

DFT STUDY OF Fe COMPLEXES
CONTAINING ELECTRONICALLY
ALTERED TERPYRIDINE DERIVATIVE

by

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Declaration

I, Evangelia Athanasopoulos, declare that the dissertation/thesis hereby handed in for the Master of Science degree in Chemistry at the University of the Free State is my own independent work and that I have not previously submitted the same work for a qualification at/in another university/faculty.

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List of Abbreviations

AD = average deviation

BIPV = building-integrated photovoltaics

BS DFT = Broken-Symmetry Density Functional Theory

bpy = 2,2'-bipyridine

bpp = 2,6-bis(pyrazol-1-yl) pyridine

CB = conduction band

CH₃CN or MeCN = acetonitrile

CVs = cyclic voltammograms

DFT = Density Functional Theory

DSSCs = Dye-Sensitized Solar Cells

EA = Electron Affinity

EPR = electron paramagnetic resonance

eeL = electronic effect of ligands

Fc⁺/Fc or FcH/FcH⁺ = ferrocene/ferrocenium

FF = fill factor

FMOs = frontier molecular orbitals

GGA = generalized gradient approximation

HF method = Hartree-Fock method

HOMO = Highest Occupied Molecular Orbital

IEFPCM = integral equation formalism variant

IET = interfacial electron transfer

IP = Ionization Potential

IPCE = incident photon-to-current efficiency

ISC = intersystem crossing

I⁻/I₃⁻ = iodide/tri-iodide

LC = ligand-centered

LDA = local density approximation

LHE = Light Harvesting Efficiency

LLCT = ligand to ligand charge transfer

LMCT = ligand-to-metal charge transfer

LUMO = Lowest Unoccupied Molecular Orbital

MAD = mean absolute deviation

MeOH = Methanol

MESP = Molecular Electrostatic Potential

MLCT = metal-to-ligand charge transfer

MM = molecular mechanics

MMCT = metal-to-metal charge transfer

MOs = molecular orbitals

NIR = near-infrared

NRF = National Research Foundation

NTOs = natural transition orbitals

NHE = normal hydrogen electrode

PCM = Polarizable Continuum Model

PET = Photoinduced Electron Transfer Rates

SAR = structure-activity relationship

SHE = standard hydrogen electrode

SOMO = Singly Occupied Molecular Orbital

TBAPF₆ = Tetrabutylammonium hexafluorophosphate

TDDFT or TD-DFT = Time-Dependent Density Functional Theory

terpy or tpy = 2,2':6',2''-Terpyridine

UV-vis = ultraviolet-visible

Abstract

Understanding the intricate interplay between structure, reactivity, and redox properties is paramount in various biological processes. Employing Density Functional Theory (DFT), this study optimized the structures of two categories of iron(II) compounds, iron(II)-terpyridine and iron(II)-tris-azinyl derivatives, in both gaseous and solvated states. The investigation encompassed an extensive analysis of various parameters. Correlations between experimentally reported iron-based oxidation, ligand-based reduction potential, and DFT-calculated reactivity parameters have been established. These relationships are emphasized for their accuracy, though the influence of the chosen reference system is also acknowledged. Notably, the study identified precise relationships for predicting the oxidation and reduction of similar iron(II) derivatives, thereby contributing to the advancement of understanding and predicting redox properties in biological contexts. Furthermore, this research contributed to the field of photovoltaic materials by conducting a comprehensive computational analysis using Time-Dependent Density Functional Theory (TD-DFT). By optimizing nineteen iron(II)-terpyridine derivatives and related compounds, the study evaluated their potential for improving the efficiency of Dye-Sensitized Solar Cells (DSSCs). The assessment encompassed various spectroscopic properties. The results underscored the pivotal role of electronic modifications in enhancing the light-harvesting capabilities and overall performance of DSSCs, consequently facilitating the development of more efficient and sustainable solar energy technologies.

Keywords: iron (II); terpyridine; tris-azinyl; DFT; TDDFT; DSSCs; redox; experimental-theoretical relationships.

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Chapter 1: Introduction

1 Chapter 1: Introduction

1.1 Motivation

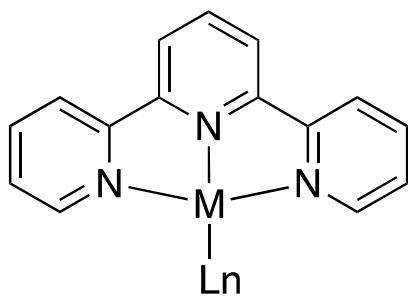
In light of the rapidly evolving global climate and diminishing fossil fuel reserves, the search for sustainable and efficient energy sources is imperative [1,2]. This thesis arises from the critical need to investigate and improve renewable energy technologies, with a particular focus on solar energy. Dye-Sensitized Solar Cells (DSSCs) represent a cost-effective and efficient solution [2,3]. At the heart of this research lies the detailed study of iron(II)-terpyridine complexes, known for their exceptional photochemical and electrochemical properties [4,5]. Employing Density Functional Theory (DFT), this work endeavors to decode the complex electronic structure, magnetic properties, and light-harvesting capabilities of these complexes [4,5]. Through computational chemistry, we aim to deepen the understanding of these complexes' roles as redox mediators and efficient dyes in DSSCs, ultimately contributing to the practical application of solar energy conversion [5,6]. The primary goal is to enrich the foundational knowledge within inorganic chemistry and photovoltaics, potentially inspiring innovative solar cell designs essential for a sustainable future [7,8].

This thesis examines the advancements in the study of iron(II)-terpyridine complexes, particularly through the lens of computational methods applied in electrochemical and photovoltaic technologies. It provides a thorough analysis of the electronic structures, redox behaviour, and their utility in DSSCs [4,5]. Terpyridine, an NNN-type Pincer ligand, offers three nitrogen coordination sites, enabling strong chelation with a variety of metal cations in an almost planar configuration. The coordination of terpyridine with metals can occur in two primary modes, either as mono-tpy Pincer complexes or as bis-tpy complexes, denoted as $[M(tpy)_2]$, as illustrated in Scheme 1.

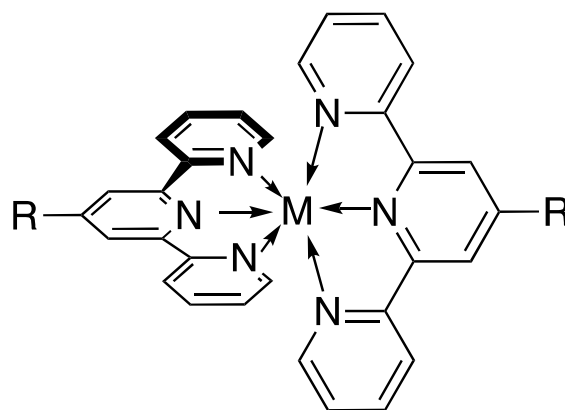
The initial segment investigates the electronic properties of various $[Fe(tpy)_2]^n$ complexes (where n ranges from 3 to 1, and tpy denotes symmetrically substituted terpyridine and tris-azinyl ligands). DFT calculations shed light on the oxidation and reduction centres, and redox behaviour of these complexes.

The subsequent section focuses on applying these iron(II)-terpyridine derivatives in renewable energy, specifically DSSCs. Time-Dependent Density Functional Theory (TD-DFT) provides a detailed computational analysis of their spectroscopic behavior, evaluating their efficacy as dyes. Insights into their absorption spectra and light-harvesting functions are compared with experimental results, highlighting the correlation between electronic alterations and the efficiency of DSSCs [5,6].

By integrating computational chemistry with photovoltaic technology, the thesis enhances the understanding of iron(II)-terpyridine complexes and underscores their potential in the development of sustainable solar energy solutions. The findings from this research may lead to the creation of novel materials and the optimization of DSSC components, contributing to more effective solar energy conversion systems [5,6].



mono tpy pincer complexes



bis-tpy complexes

Scheme 1: “Basic binding mode of terpyridine ligands” from [9]. Reprinted (adapted) with permission C. Wei, Y. He, X. Shi, Z. Song, *Terpyridine-metal complexes: Applications in catalysis and supramolecular chemistry*, *Coord. Chem. Rev.* 385 (2019) pgs. 1-19. <https://doi.org/10.1016/j.ccr.2019.01.005>. Copyright © 2019, Elsevier B.V. All rights reserved.

1.2 Objective and Overview of Thesis

This thesis investigates the electronic influence of various substituents on the terpyridine ligands on their iron(II)-terpyridine complexes, with a focus on electrochemical analysis and sophisticated computational methods such as DFT and TD-DFT. The objective is to elucidate the electronic structures, magnetic properties, and light-harvesting capabilities of these complexes. A key goal is to align theoretical calculations with experimental data, creating a predictive database for electronic behavior, redox potential, spin state transitions, and light-absorption characteristics of new iron(II) complexes. This database will assist in predicting stability, reactivity, and photophysical behavior, essential for designing complexes with specific properties for applications in advanced material science, energy conversion, catalysis, and as redox mediators and dye sensitizers in DSSCs. This research contributes significantly to the advancement of sustainable energy technologies, providing insights into more efficient and eco-friendly solar energy solutions.

This is a publication-based thesis. For a MSc two publishable articles are required. Therefore, one published and one submitted publication will form the main part of the thesis. Here is the outline of the chapters in this thesis.

Chapter one provides a motivation of this research work.

Chapter two presents the literature review on researched work.

Chapters three and four presents the published and submitted articles on the research of this thesis. *Please note that each chapter will be separate and reference numbering, schemes, tables, and figures will start from number one (1).*

Chapter three - first publication: E. Athanasopoulos, J. Conradie, Substituent effect on the oxidation and reduction of electronically altered iron(II)-terpyridine derivatives – DFT study, Inorganica Chim. Acta. 555 (2023) 121599. <https://doi.org/10.1016/j.ica.2023.121599>.
<https://www.sciencedirect.com/journal/inorganica-chimica-acta> Elsevier

Chapter four - second publication: E. Athanasopoulos, J. Conradie, DFT study of the spectroscopic behaviour of different iron(II)-terpyridine derivatives with application in DSSCs, submitted to J. Mol. Graph. Model. (submitted 31.09.2023) Manuscript ID JMGM-D-23-01121
<https://www.sciencedirect.com/journal/journal-of-molecular-graphics-and-modelling> Elsevier

Chapter five comprises the main conclusion and future perspectives of this work.

Appendixes provide the supporting information and copyright permissions of the articles of this work.

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Chapter 2: Literature study

2 Chapter 2: Literature study

This MSc thesis presents a Density Functional Theory (DFT) study on the substituent effect on the oxidation, reduction and ultraviolet–visible (UV-vis) spectroscopy of electronically altered iron(II)- 2,2':6',2''-terpyridine derivatives and other related complexes. These complexes have anti-microbial potential [1] and possible application as catalysts [2], redox mediators [3] and dye sensitizers [4] in dye sensitized solar cells (DSSCs). Therefore background on DFT methods, DSSC and the redox and UV-vis behaviour of iron(II)-2,2':6',2''-terpyridine derivatives is presented in this literature study chapter.

2.1 DSSCs

The working principle of dye-sensitized solar cells (DSSCs) revolves around converting light energy into electrical energy through a series of integrated processes, as depicted in Figure 1 [5,6]. Central to this operation are the dye sensitizers, which are light-absorbing compounds responsible for harnessing photons and initiating electron transfer within the cell [7,8]. These dyes play a pivotal role in absorbing light across a broad spectrum and generating photoexcited electrons that are subsequently injected into the semiconductor electrode, a process detailed in Figure 2 [3]. The efficient regeneration of the oxidized dye and the transport of charge carriers toward the electrodes are facilitated by redox mediators, like iodide/tri-iodide (I^-/I_3^-) and coordination complexes typically comprising metals such as cobalt, copper, or other transition metals [5,9–12]. These redox mediators act as electron shuttles, enabling the transfer of electrons between the dye molecules and the electrodes, thereby sustaining the current flow within the DSSC [10]. Figure 2 illustrates these processes, showcasing the essential role of energy levels in optimizing electron transfer and overall cell efficiency. Recent research emphasizes the importance of optimizing dyes and redox mediators improve the overall efficiency of DSSCs [5,7,9]. Recent reports on cobalt and copper polypyridine redox mediators to enhance the overall efficiency of DSSCs, highlighting the crucial roles played by both the dye sensitizers and the redox mediators in the functionality and performance of these solar cells [7,10].

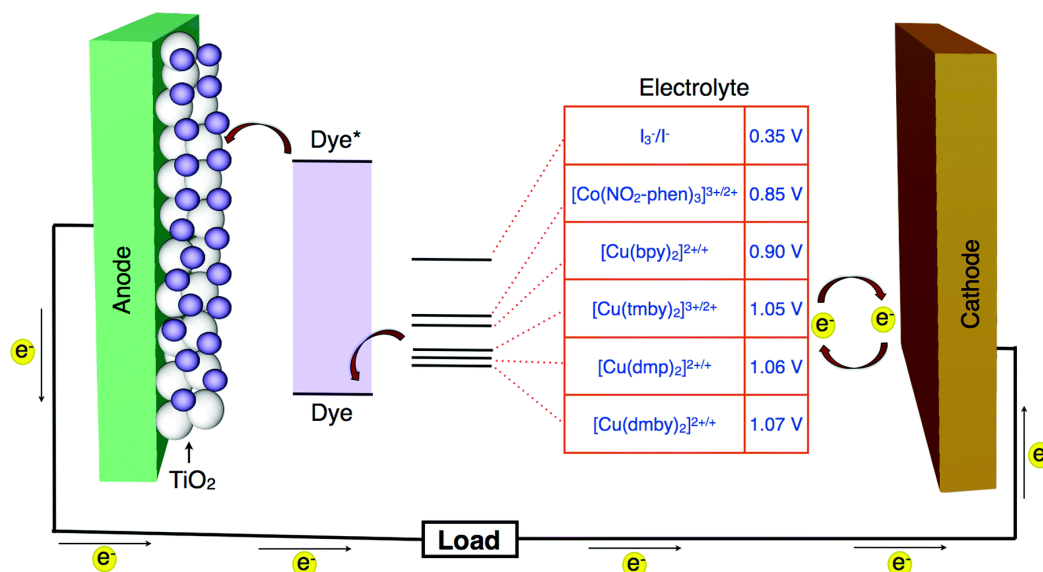


Figure 1: “Energy level diagram of a dye-sensitized solar cell (DSSC), illustrating the fundamental workings of a Grätzel cell. The dye gets excited (Dye → Dye*) as it absorbs light energy” [6]. “Reproduced from Ref. [5] (open access) under a Creative Commons Attribution-Non Commercial 3.0 Unported Licence.”

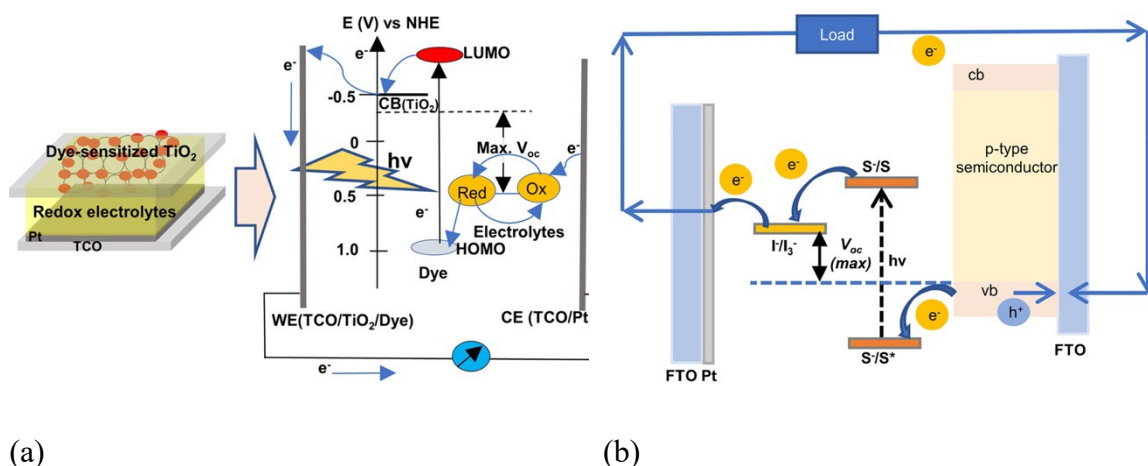


Figure 2: “(a) DSSC device structure with an n-type TiO_2 semiconductor and its working principle. (b) p-Type DSSC device structure with a p-type semiconductor and its working principle. From [3] (open access) under CC-BY-NC-ND 4.0.”

The utilization of 2,2':6',2''-terpyridine-metal complexes (also referred to as terpyridine-metal complexes or tpy-metal complexes) in various applications has gained considerable attention owing to their distinct physico-chemical properties and potential for diverse functionalities [2,13]. In the realm of solar energy conversion, iron(II) complexes incorporating terpyridine ligands have exhibited

significant promise, with extensive computational investigations shedding light on their utility as chromophores in DSSCs [4,14,15]. These studies have delved into these complexes' intricate electronic properties and redox behaviour, emphasizing their potential to facilitate efficient electron transfer processes within the solar cell framework [16,17]. Furthermore, the redox properties of various metal complexes, including cobalt and copper, have been extensively explored, highlighting their suitability as redox mediators in DSSCs [3,5,18]. These investigations underscore the significance of tailored ligand design and the precise control of electronic parameters in optimizing the performance of metal complexes for solar energy conversion applications [19–21]. The comprehensive guidance provided by recent studies has illuminated potential strategies for the development of efficient terpyridine-metal complex-based systems in the field of renewable energy technologies [22,23]. Figure 3 [19], showcases the molecular structures of benchmark Ru-polypyridine sensitizers N3, N719, and Black Dye, which are employed in DSSCs.

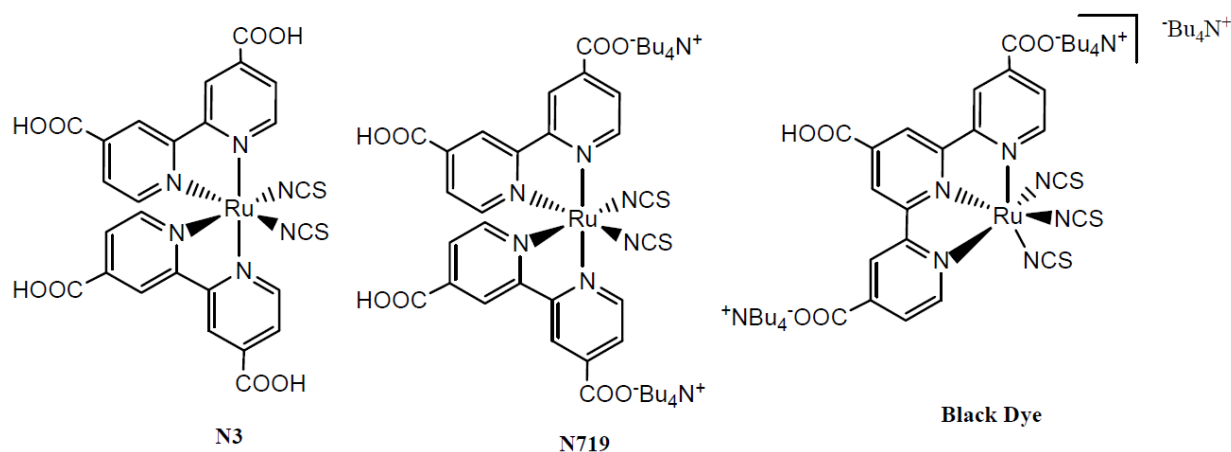


Figure 3: “Ru-polypyridine “structures for benchmark sensitizers N3, N719, and BlackDye for DSSC application.” N3 and N719 contain substituted bipyridine ligands and black dye, substituted terpyridine ligands. “From [19] (open access) under Creative Common CC BY license (<https://www.mdpi.com/openaccess>).”

As highlighted in the research conducted by Adeloye and Ajibade [19], the design of these complex structures involves strategic modifications to enhance light absorption, charge transfer, and overall efficiency of DSSCs. These complexes containing ruthenium are well-known for their capacity to absorb light efficiently over a wide range of wavelengths, aiding in the DSSC's process of transforming light energy into electrical energy.

As emphasized in the work of Masud and Kim [3], choosing appropriate redox mediators plays a crucial role in developing effective electrolytes for DSSCs. Figure 4 [3], presents a selection of important redox couples that are commonly used in the electrolytes of DSSCs as redox mediators, along with their standard redox potentials. The iodide/tri-iodide (I^-/I_3^-) redox couple is commonly

employed in DSSCs. Also shown are organic and metal containing redox couples. Many of the metal containing redox couples have polypyridine or related ligands. These redox pairs are crucial for the operation of DSSCs as they facilitate the regeneration of the photo-oxidized dye and the transport of charge carriers within the cell.

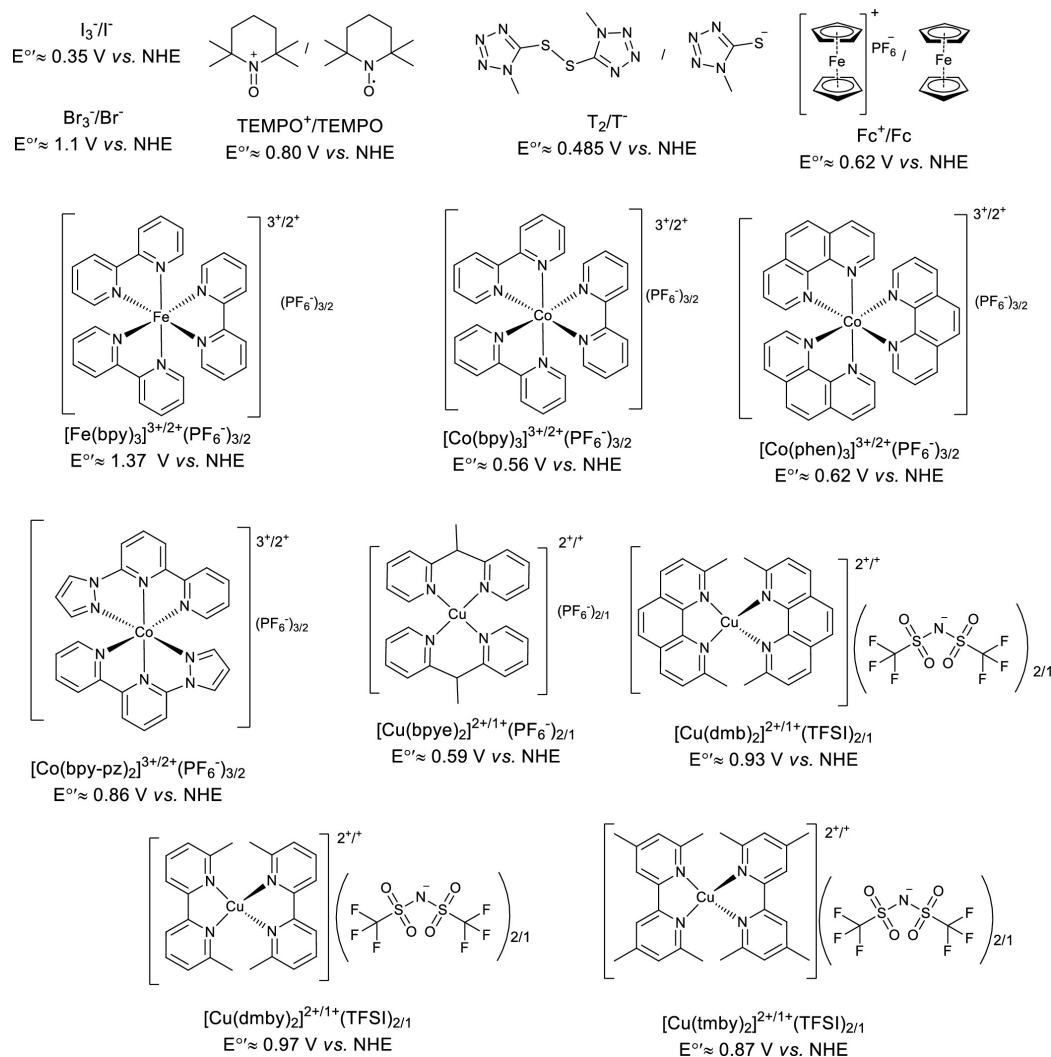


Figure 4: “Structures of some important redox couples (R^+/R) used in DSSC electrolytes as redox mediators and their standard redox potentials. From [3] (open access) under CC-BY-NC-ND 4.0.”

To conclude, Iron (Fe) has gained substantial attention in the development of DSSCs due to its cost-effectiveness in comparison to ruthenium (Ru) and cobalt (Co) complexes [18,21]. While Ru-based dyes have demonstrated high efficiency in solar energy conversion, the scarcity and high cost of Ru limit its large-scale application in solar cell technology [19]. Similarly, although Co-based redox mediators exhibit favourable performance in DSSCs, their expense and potential toxicity present practical challenges for widespread commercialization [3,24]. In contrast, Fe-based complexes offer a more economically viable alternative, given the abundant availability of iron and its low cost compared to Ru and Co, thus making Fe a promising candidate for developing cost-

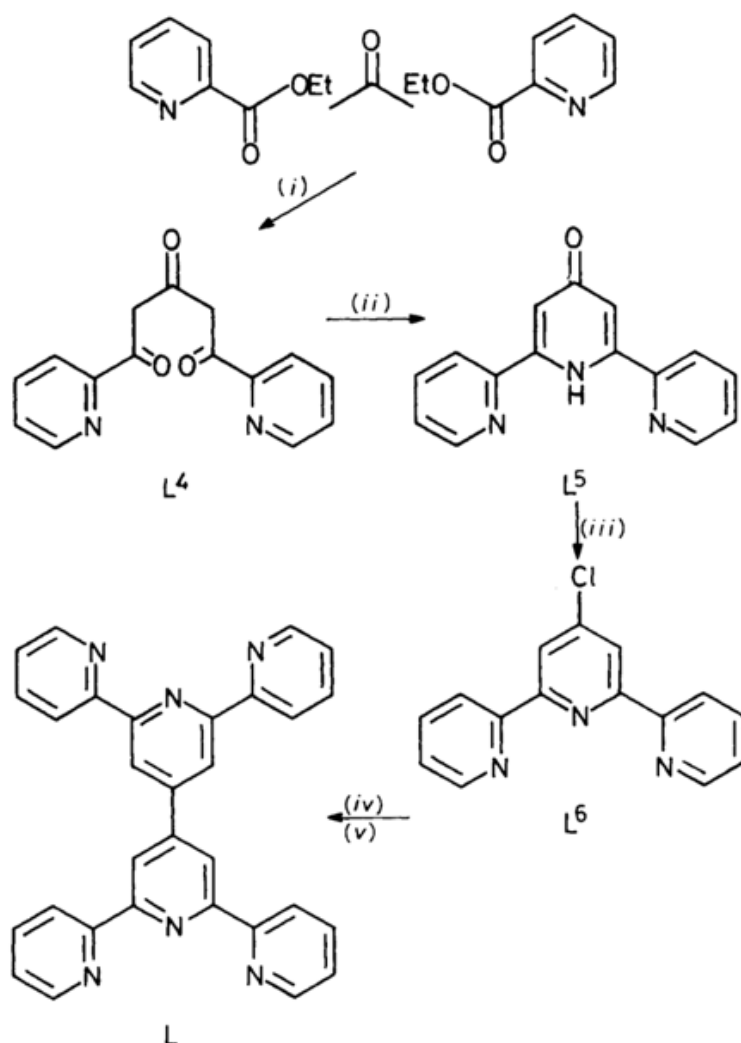
effective and sustainable solar energy conversion technologies [13,15]. Additionally, Fe's redox properties can be tuned to meet the requirements for efficient DSSCs, although its photovoltaic performance may not yet match that of Ru-based dyes. Ongoing research aims to improve the efficiency of Fe-based sensitizers and mediators to more closely compete with their Ru and Co counterparts. It is noteworthy that Fe excited states are mostly too short-lived to be used in DSSCs, except for an exceptional case to be discussed later (p.32 [16]).

2.2 *Bis(terpyridine)-iron(II) complexes*

2.2.1 Synthesis and experimental ground state

The geometry of Iron complexes with bis(terpyridine), denoted as $[\text{Fe}(\text{terpyridine})_2]^{m+}$ (where $m = 0 - 3$), exhibits a constrained octahedral structure [13]. This constrained geometry is primarily due to the structural strain imposed by the tridentate ligands. The synthesis of *bis*(2,2':6',2''-terpyridine)iron(II) perchlorate presents certain challenges owing to the complex nature of the terpyridine (tpy or terpy) ligand [25,26]. Early methods, dating back to 1932, involved the oxidative condensation of pyridine with iron(III) chloride, but the yields were extremely low and the process itself was hazardous and time-consuming [27]. Modern synthetic routes focus on constructing the tpy core through various alternative strategies, including the use of nucleophilic and electrophilic reagents like 4'-(hydroxy)-2,2':6',2''-terpyridine (OH-tpy) and 4'-(chloro)-2,2':6',2''-terpyridine (Cl-tpy) [1,28]. These intermediates allow for the introduction of diverse functional groups at the 4' position, offering greater flexibility in the synthesis of tpy derivatives. The original synthesis of Cl-tpy, aiming for the homocoupling to produce 6',6''-bis(2-pyridyl)-2,2':4,4'':2'',2'''-quaterpyridine, was reported by Constable et al. [29], as illustrated in Scheme 1 [29].

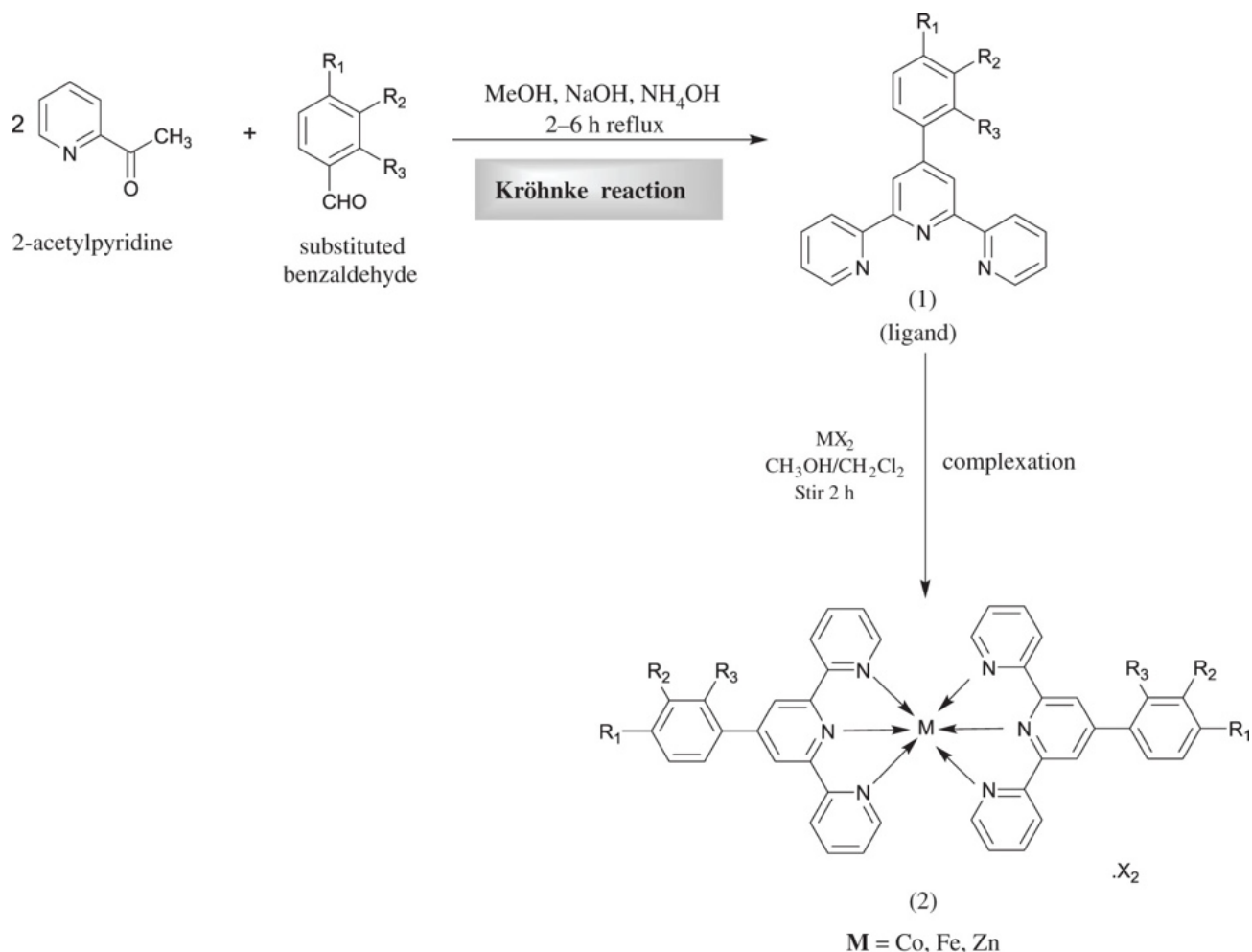
Incorporating these substituted tpy derivatives into the coordination complex of iron(II) perchlorate involves a stepwise process of ligand formation followed by the addition of perchloric acid, yielding the desired *bis*(2,2':6',2''-terpyridine)iron(II) perchlorate product [14,15,20]. This product is well-suited for further characterization and utilization in various applications, including catalysis and materials science [30].



Scheme. (i) NaH, MeOCH₂CH₂OMe; (ii) [NH₄][O₂CMe], EtOH; (iii) PCl₅, POCl₃; (iv) [Ni(PPh₃)₂Cl₂], Zn, PPh₃, dmf; (v) NaCN

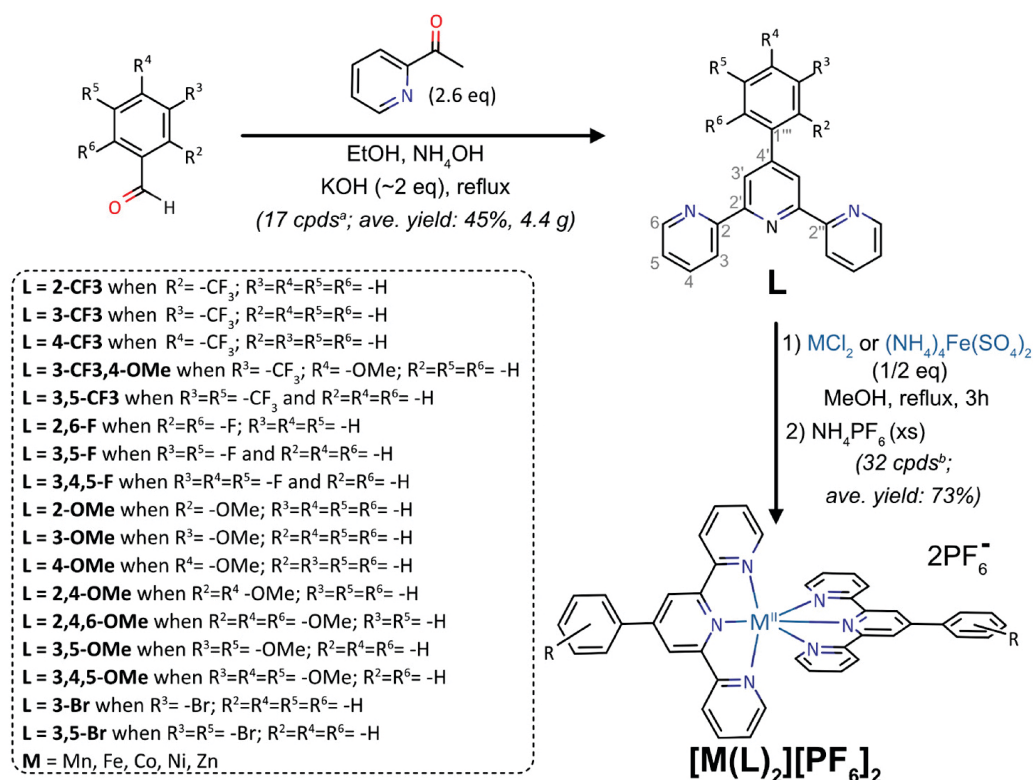
Scheme 1: “Synthesis of 4'-chloro-2,2';6',2''-terpyridine and 6',6''-bis(2-pyridyl)-2,2':4,4'':2'',2'''-quaterpyridine. Reproduced from Ref. [29] with permission from the Royal Society of Chemistry. Copyright 1990.”

In the depicted synthetic pathways, Scheme 2 and Scheme 3 outline the steps to synthesize functionalized terpyridine ligands and their subsequent metal complexes. Scheme 2, adapted from Mughal et al. [1], demonstrates the Kröhnke reaction where 2-acetylpyridine is reacted with various substituted benzaldehydes in the presence of bases and solvents to yield a range of terpyridine ligands. These ligands are first combined with metal salts in methanol and then precipitated using ammonium hexafluorophosphate, resulting in the formation of the corresponding metal complexes (where M= Co, Fe, Zn) as hexafluorophosphate salts.



Scheme 2: “Synthetic routes to substituted terpyridine ligands and their metal-complexes. Reproduced from Ref. [1] (open access) under CC BY 4.0 DEED.”

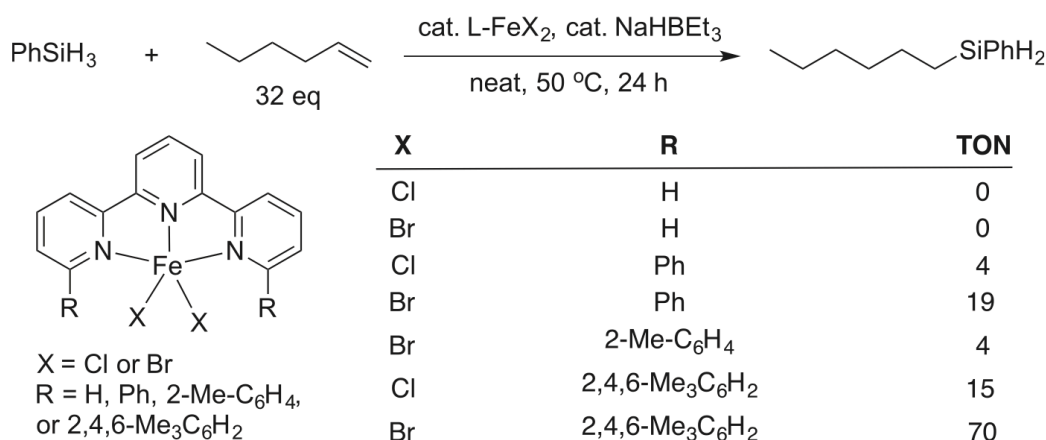
Scheme 3, from the work of Dickenson et al. [15], illustrates a similar approach with a focus on the production of 4'-aryl terpyridines. Here, the condensation of enolate species with aryl aldehydes leads to aryl-dipyridyl dione intermediates, which upon further reaction with ammonium acetate or hydroxide, close the central pyridine ring to form the terpyridine ligand. Metal complexation in this scheme may involve different metal ions (where $\text{M} = \text{Mn}, \text{Fe}, \text{Co}, \text{Ni}, \text{Zn}$) to produce a variety of metal terpyridine complexes. Both schemes emphasize the versatility and tunability of terpy ligands for forming metal complexes with varied properties.



Scheme 3: “Synthesis of different $[\text{Fe}(\text{terpyridine})_2](\text{ClO}_4)_2$ complexes, from [15]. Reprinted (adapted) with permission from J.C. Dickenson, M.E. Haley, J.T. Hyde, Z.M. Reid, T.J. Tarring, D.A. Iovan, D.P. Harrison, Fine-Tuning Metal and Ligand-Centered Redox Potentials of Homoleptic Bis-Terpyridine Complexes with 4'-Aryl Substituents, *Inorg. Chem.* **60** (2021) 9956–9969. <https://doi.org/10.1021/acs.inorgchem.1c01233>. Copyright © 2021, American Chemical Society.”

Iron(II) ions, possessing a d^6 electron configuration, are capable of forming stable octahedral complexes with as many as six ligands. Terpyridine is known for its ability to keep iron in lower oxidation states, yet the challenge in iron coordination lies in regulating the formation of mono-tpy (4 or 5 coordination) versus bis-tpy (octahedral 6 coordination) complexes, as noted in reference [31]. In their 2012 research, Nakazawa's team explored the hydrosilylation of alkenes using Fe(II) catalysts coordinated with terpyridine, as depicted in Scheme 4 [31,32]. Their observations indicated that iron complexes with plain terpyridine and either Cl or Br were ineffective, presumably forming inactive bis-tpy-Fe complexes. To address this issue, they employed ligands with large substituents at the 6,6' positions of terpyridine, achieving more favourable outcomes, particularly with iron bromide salts. Intriguingly, adding bulkiness to the 6 and/or 6'' positions of terpyridine tends to promote the high-spin state as the primary ground state configuration. This shift is linked to a decrease in ligand field strength due to alterations in the metal-ligand bond angles [30,33]. In acetonitrile solutions, these high-spin complexes were observed to transition to a low-spin state under elevated pressure, a phenomenon explained by the smaller spatial requirement of the low-spin state compared to its high-spin counterpart [30]. These catalysts consistently yielded anti-Markovnikov products, consistent

with earlier findings [31,34]. This research and its implications are further discussed and contextualized in the publication [31] which delves into the broader applications and potential of terpyridine-metal complexes in these fields.



Scheme 4: “Fe-catalyzed hydrosilylation of alkene,” from [31]. “Reprinted (adapted) with permission C. Wei, Y. He, X. Shi, Z. Song, *Terpyridine-metal complexes: Applications in catalysis and supramolecular chemistry*, *Coord. Chem. Rev.* 385 (2019) pgs. 1-19. <https://doi.org/10.1016/j.ccr.2019.01.005>. Copyright © 2019, Elsevier B.V. All rights reserved.”

Wilkins and co-workers [35] have conducted thorough investigations into the kinetics of both the formation and dissociation of terpy complexes with a range of transition metals such as Fe^{2+} , Co^{2+} , Ni^{2+} , and Cu^{2+} (Table 1). In this thesis, the primary focus is on the iron metal, which is of significant interest. Moreover, in their comprehensive study, Wilkins and colleagues established that the formation rate of the mono complex (for iron(II) terpyridine complexes) at 25°C is roughly $5.4 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ (K_1 in Scheme 5). It appears that this rate is predominantly influenced by the water exchange rate, serving as the rate-limiting step in the reaction process [13,20,30].

Iron(III) terpy complexes have also been studied, and it has been found that when terpyridine is combined with FeCl_3 , a *bis* complex does not form; instead, a mono terpyridine iron(III) complex $[\text{Fe}(\text{terpy})\text{X}_3]$ (where $\text{X} = \text{Cl}^-, \text{Br}^-, \text{SCN}^-, \text{I}^-$), is produced [30,36]. This compound forms a high-spin iron(III) complex with a $^6A_1$ ground state. Due to the prohibition of d-d transitions, it maintains a constant magnetic moment regardless of temperature changes [30,37]. Additionally, the Fe(III) bis-terpy complex can be produced by oxidizing the Fe(II) bis-terpy complex using PbO_2 in an aqueous sulfuric acid environment, followed by the introduction of sodium perchlorate [22,30,37]. The formation of the bis complex necessitates a bulky counterion; for instance, incorporating sodium chloride results in the precipitation of $[(\text{terpy})\text{FeCl}_3]$ [29,30]. The synthesized bis terpyridine complex, $[\text{Fe}^{\text{III}}(\text{tpy}^0)_2]^{3+}$, is characterized as a low-spin Fe(III) variant and intriguingly exhibits no

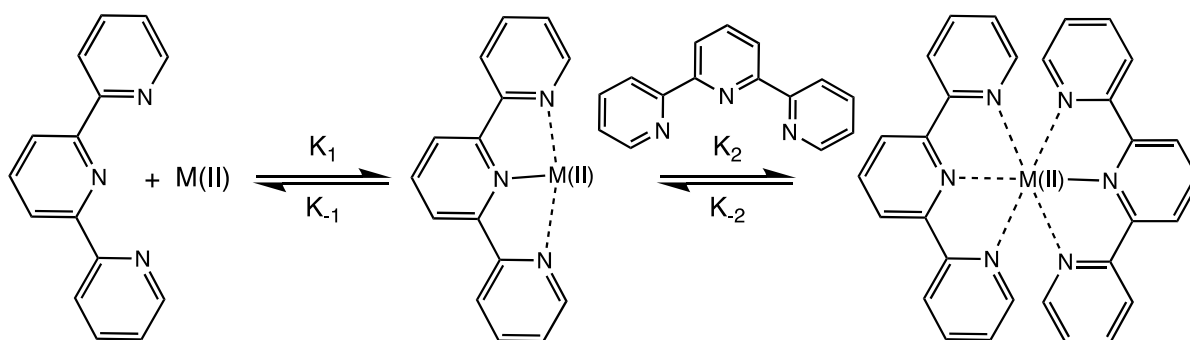
significant Jahn-Teller distortion [30,38]. Wilkins et al.'s data, which provides a thorough understanding of terpyridine-iron(II) formation kinetics (reaction in Scheme 5), is shown in Table 1 [30,35].

Table 1: “Kinetic Parameters of Terpyridine Complexation at 25 °C,” according to Scheme 5. Data from Wilkins and co-workers [35].

Ion	$\log_{K_1}(M^{-1}s^{-1})$	$\log_{K_{-1}}(s^{-1})$	$\log_{K_2}(M^{-1}s^{-1})$	$\log_{K_{-2}}(s^{-1})$
Fe	4.8	-2.2	$\sim 7.0^a$	-6.8
Co	4.4	-4	$\sim 6.7^a$	-3.2
Ni	3.1	-7.6	5.3	-5.8
Cu	$> 7.3^a$			

^a Recorded at 5 °C

The reaction rate of iron complexes for the mono complex lies between those of cobalt and nickel, while for the *bis* complex, it forms more rapidly than all others except for copper. Additionally, iron complexes exhibit a notably high kinetic stability in comparison to other bis complexes, with a dissociation constant (K_{-2}) of $1.6 \times 10^{-7} s^{-1}$. The synthesis of bis terpy complexes with transition metals involves a reversible, two-step process of ligand addition, as depicted in Scheme 5 [30]. The rate constants for formation and dissociation of the mono complex are denoted as K_1 and K_{-1} , respectively. Similarly, K_2 and K_{-2} represent the rate constants for the *bis* complex.



Scheme 5: “Reaction of terpyridine ligands with a bivalent metal salt to form a mono and subsequently a *bis* complex,” from [30].

The $[\text{Fe}(\text{tpy})_2]^{2+}$ molecule is diamagnetic [14], while the oxidized ($m = 3$) and reduced ($m = 1$) molecules are paramagnetic doublets [22]. The spin states of the $[\text{Fe}(\text{tpy})_2]^{m+}$ for $m = 1-, 0, 1+, 2+, 3+$ are summarized in Table 2 [22]. In its $2+$ oxidation state, iron is stabilized in a low-spin electronic configuration by the terpyridine ligands, which act as π -acceptors, leading to the diamagnetic nature of the $[\text{Fe}(\text{tpy})_2]^{2+}$ complex [14]. Upon oxidation to the $3+$ state, the molecule becomes a paramagnetic doublet, indicating an unpaired electron and a change in the spin state [22].

The various substituents on the terpyridine ligand has been shown to significantly affect the redox properties of the complexes. For instance, electron-donating groups can facilitate the oxidation process, whereas electron-withdrawing groups can influence the electron density on the metal center, thus decreasing the redox behaviour [15].

Table 2: Spin ground states for the electron transfer series the $[\text{Fe}(\text{terpyridine})_2]^{m+}$ for ($m = 1-, 0, 1+, 2+, \text{ and } 3+$), data from [22].

Complex	Magnetic properties	Ground State (<i>S</i>)
$[\text{Fe}^{\text{III}}(\text{tpy}^0)_2]^{3+}$	paramagnetic doublets	$\frac{1}{2}$
$[\text{Fe}^{\text{II}}(\text{tpy}^0)_2]^{2+}$	diamagnetic with neutral ligands	0
$[\text{Fe}^{\text{II}}(\text{tpy}^\bullet)(\text{tpy}^0)]^{1+}$	paramagnetic doublets (π radical monoanion and neutral ligand)	$\frac{1}{2}$
$[\text{Fe}^{\text{II}}(\text{tpy}^\bullet)_2]^0$	paramagnetic (π radical monoanions)	1
$[\text{Fe}^{\text{II}}(\text{tpy}^{\bullet\bullet})(\text{tpy}^\bullet)]^{1-}$	paramagnetic doublets (π radical dianion and monoanion)	$\frac{1}{2}$

Additionally, the study by Mughal et al. [1] investigates the structure-activity relationship of terpyridine-based ligands and their metal complexes, as depicted in Figure 5 [1]. The findings demonstrate that distinct ligand substituents play a crucial role in regulating the bioactivity of the complexes. Notably, electron-withdrawing substituents enhance antibacterial function, while the presence of bulky benzene ring substituents has the opposite effect. The potent antimicrobial activity observed in both complexes is attributed to their di-nuclear center, likely facilitated by chelation effects that modify the metal ion's polarity and improve its lipo-solubility. Consequently, the complexes exhibit strong antibacterial properties, inhibiting enzyme activity and showcasing significant potential for applications in this domain [1].

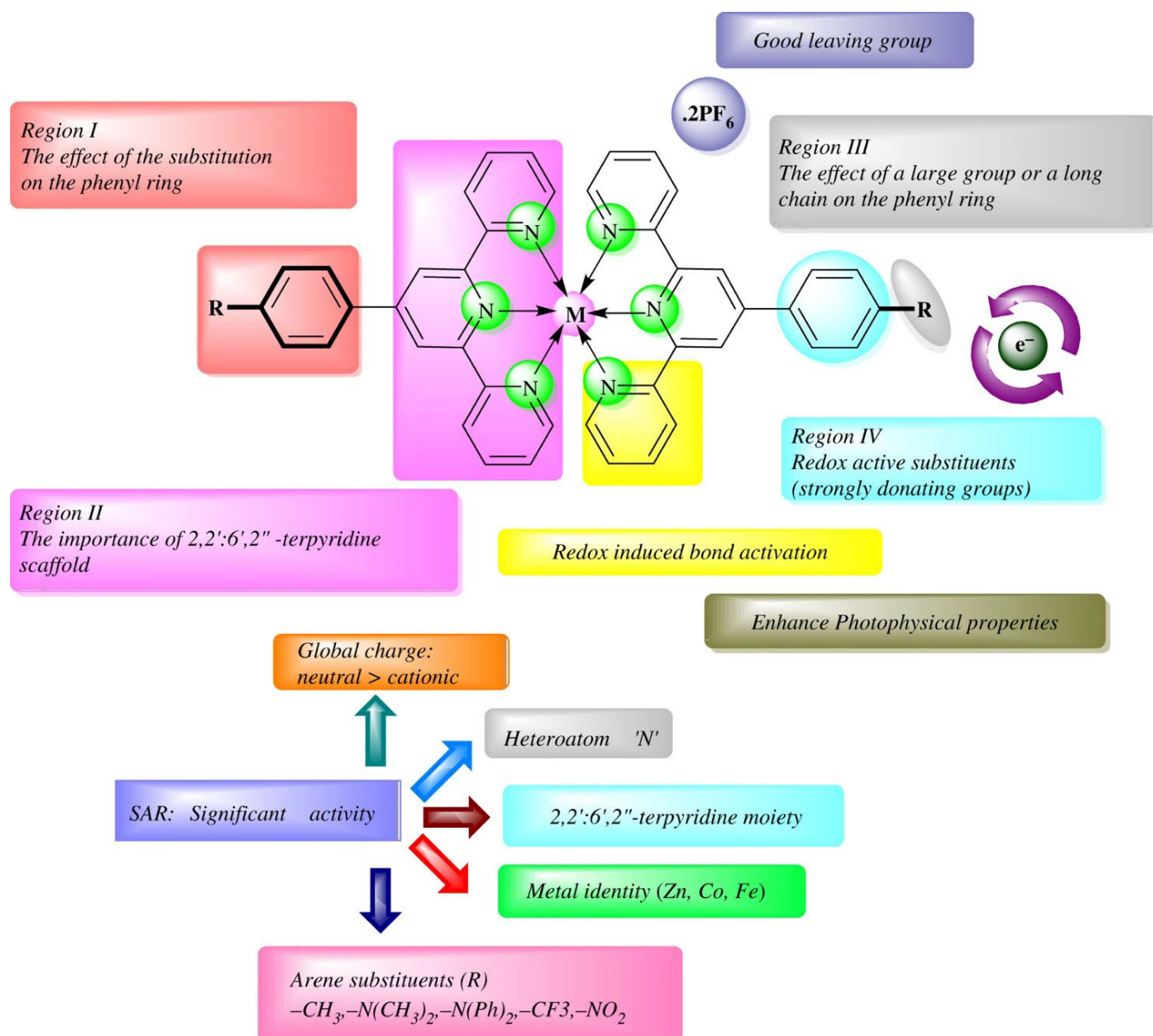


Figure 5: “Structure–activity relationship of the synthesized terpyridine-based ligands and metal complexes.”
From [1] (open access) under CC BY 4.0 DEED.

2.2.2 DFT Literature

The study by Wieghardt et al. [22] delves into the electronic structures of electron transfer complexes, specifically $[\text{Fe}(\text{tpy})_2]^n$ (where n ranges from 1- to 3+ and tpy is 2,2':6',2''-terpyridine), utilizing a combination of Mössbauer spectroscopy and DFT calculations. This research sheds light on the mechanisms of ligand-centered reductions and differentiates between low-spin and high-spin states, elucidating the ground states during one-electron reduction processes as summarized in Table

2 [22]. The diamagnetic dication $[\text{Fe}(\text{tpy})_2]^{2+}$ are characterized by the iron ion with low-spin (t_{2g})⁶ configuration paired with two neutral terpyridine ligands. The intraligand distances in these optimized structures not only align well with X-ray data but also clearly demonstrate the neutrality of the ligands. Therefore, the electronic structure of the dication is as predicted: $[\text{Fe}^{\text{II}}(\text{tpy}^0)_2]^{2+}$ with a total spin $S = 0$. Upon one-electron oxidation, the dication transitions to low-spin (t_{2g})⁵ ions, specifically $[\text{Fe}^{\text{III}}(\text{tpy}^0)_2]^{3+}$ with a spin state $S = \frac{1}{2}$. The optimized geometries and Mössbauer parameters for $[\text{Fe}^{\text{III}}(\text{tpy}^0)_2]^{3+}$ are consistent with experimental findings. Additionally, Mulliken spin population analysis alongside spin density plots substantiate that the unpaired electron is in a metal d orbital.

The monocation $[\text{Fe}(\text{tpy})_2]^{1+}$ with a spin state $S = \frac{1}{2}$ also exhibit low-spin Fe^{II} centers and are coordinated by two equivalent tpy ligands. A slight reduction in the average $C_{py} - C_{py}$ distances to approximately 1.45 Å, compared to the dication, suggests that the added electron is located in a π^* orbital of the tpy ligands. Computational models propose a delocalized electron distribution, as evidenced by the Mulliken spin population showing that each tpy ligand hosts half an electron. Although the DFT calculations yield optimized structures in which the supporting ligands are fully equivalent (i.e. the unpaired electron is delocalized), it was concluded that the electronic structure is best described by $[\text{Fe}^{\text{II}}(\text{tpy}^*)(\text{tpy}^0)]^{1+}$ [22].

The implementation of Broken-Symmetry (BS) DFT calculations has been pivotal in definitively determining the ground states for $[\text{Fe}^{\text{II}}(\text{tpy})_2]^n$ (with n being 1+, 0, 1-). These calculations reveal predominant ferromagnetic or antiferromagnetic interactions amongst ligand radicals and between ligand radicals and unpaired spins at the metal center, which underscores the interdependent nature of these ligand-centered radicals, challenging prior assumptions about their independence. For example, for the neutral complex $[\text{Fe}(\text{tpy})_2]^0$, a ground state with an $S = 1$ spin state was established using BS(4,2) formalism, which is in accordance with magnetic susceptibility measurements [22]. The calculated structure's geometry is in close agreement with that determined by X-ray studies, with terpyridine ligands showcasing intraligand bond lengths that are typical of the radical anion $(\text{tpy}^*)^{1-}$ form. Moreover, the Fe–N bond lengths in this complex are approximately 0.19 Å longer than those in the higher oxidation state complexes, suggesting a high-spin Fe^{II} configuration in the neutral complex. This proposition is further supported by spin population analysis, as indicated in Figure 6 [22], which reveals 3.69 spins at the iron center and -0.89 spins on each ligand. The exchange coupling constant calculated to be $J = -425 \text{ cm}^{-1}$ between the two $(\text{tpy}^*)^{1-}$ ligand spins and the high-spin Fe^{II} center signifies a significant antiferromagnetic metal–radical interaction [22].

The research further illustrates that the monoanionic $[\text{Fe}(\text{tpy})_2]^{1-}$ complex, with an $S = \frac{1}{2}$ ground state as per the BS(4,3) model, also exhibits a high-spin Fe^{II} center and a delocalized ligand set $[(\text{tpy}^{**})(\text{tpy}^*)]^{3-}$. This is best described as $[\text{Fe}^{\text{II}}(\text{tpy}^{**})(\text{tpy}^*)]^{1-}$, a conclusion that is verified by Mulliken

spin density analysis depicted in Figure 6 [22]. This analysis shows 3.77 unpaired spins at the iron center and -2.78 spins across the terpyridine ligands. A computed exchange coupling constant J of -251 cm^{-1} indicates that the high-spin excited state is unlikely to be significantly populated at room temperature. Nonetheless, validating these findings experimentally has been a challenge due to the $[\text{Fe}(\text{tpy})_2]^{1-}$ complex's instability in solution, which cyclic voltammetry suggests is prone to ligand dissociation [22].

This research not only enhances the comprehension of the spin states and electronic configurations of such complexes but also underscores the intricate interaction between the ligand and metal center redox processes.

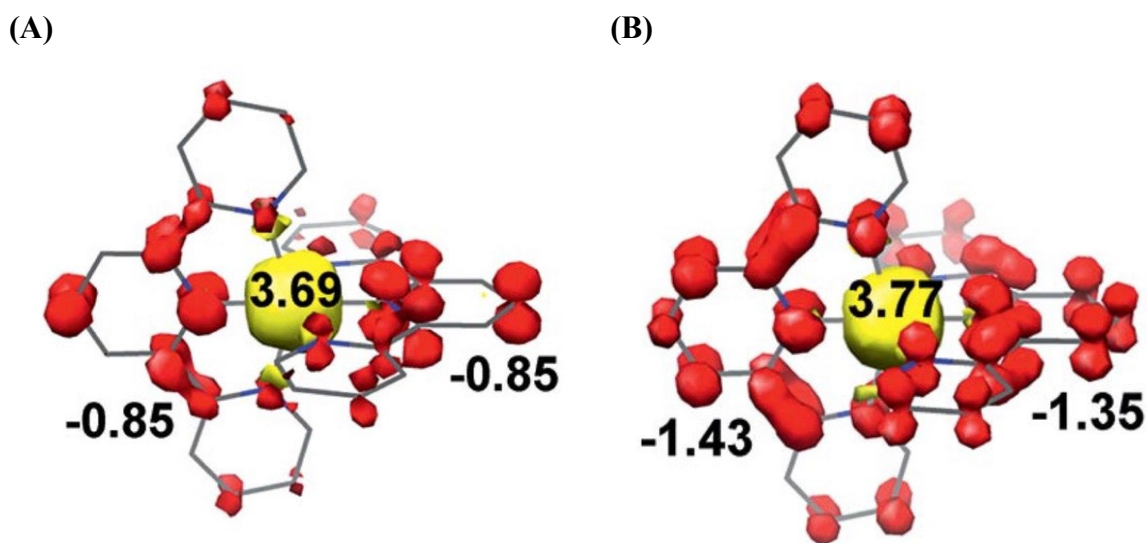
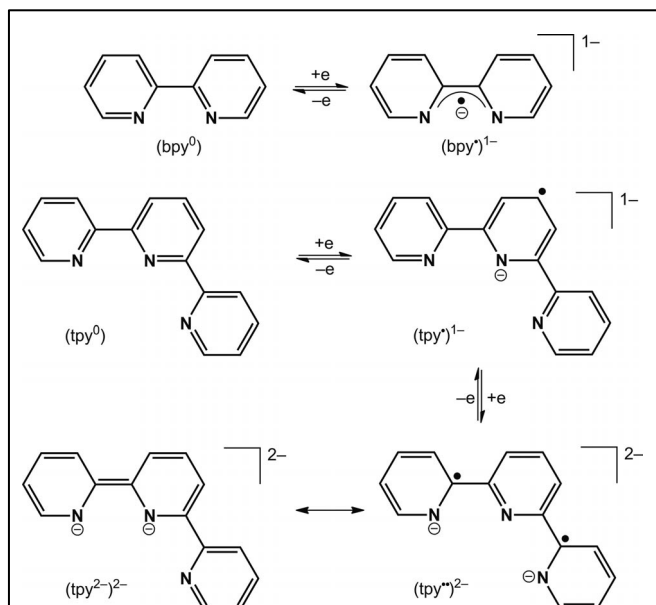


Figure 6: “Spin density plots (yellow: positive; red: negative) and Mulliken spin populations obtained from DFT calculations for the diradical complex (A) $[\text{Fe}(\text{tpy})_2]^0$ ($S = 1$) and the tpy complex (B) $[\text{Fe}^{\text{II}}(\text{tpy}^{\bullet})(\text{tpy}')]^{1-}$, ($S = 1/2$). From [22] with permission. Copyright © 2012 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.”

The research of Wieghardt et al. demonstrates that the iron center retains its divalent (d^6) state throughout the reduction processes, primarily observed as ligand-centered transitions in the diamagnetic di-cation complex $[\text{Fe}^{\text{II}}(\text{tpy}^0)_2]^{2+}$ as it transitions to its reduced forms $[\text{Fe}(\text{tpy}^0)_2]^n$ (where $n \leq 1$), as depicted in Scheme 6 [22]. This study not only advances the understanding of the spin states and electronic configurations of such complexes but also highlights the subtle interplay between ligand and metal center redox activities [22].



Scheme 6: “Ligand oxidation states. From [22] Copyright © 2012 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.”

In another DFT study, using a basic model system of substituted pyridine compounds, researchers discovered a significant relationship between the Hammett parameters and the lowest unoccupied molecular orbital (LUMO) energies of the corresponding substituted pyridine models [15], illustrated in Figure 7. This result suggests that this correlation can serve as a cost-effective predictive tool when combined with electrochemical data of the corresponding metal-tpy complexes [15].

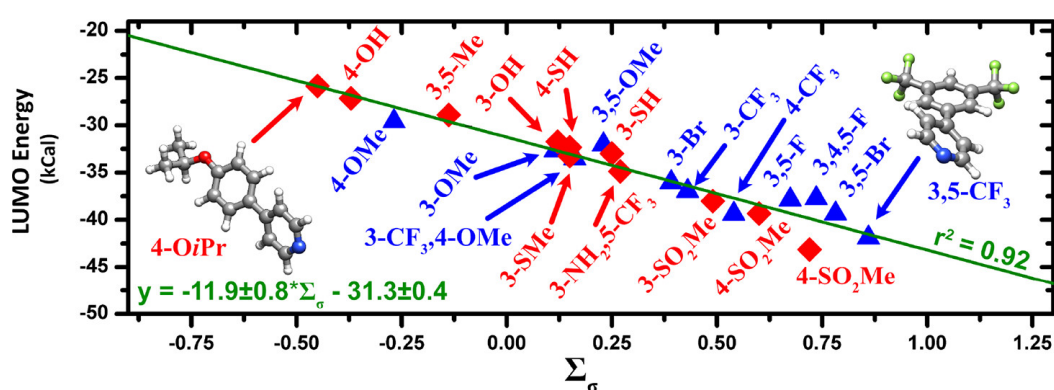


Figure 7: “Plot of LUMO energy (kcal) vs $\Sigma\sigma$ for 22 Ar-Py. Blue triangles are Ar-Py compounds with analogous $[\text{Co}(\text{L})_2]^{2+}$ complexes synthesized. Red diamonds are additional Ar-Py without analogously synthesized complexes. The green line is the regression line of all 22 Ar-Py [15]. Reprinted (adapted) with permission from J.C. Dickenson, M.E. Haley, J.T. Hyde, Z.M. Reid, T.J. Tarring, D.A. Iovan, D.P. Harrison, Fine-Tuning Metal and Ligand-Centered Redox Potentials of Homoleptic Bis-Terpyridine Complexes with 4'-Aryl Substituents, *Inorg. Chem.* 60 (2021) 9956–9969. <https://doi.org/10.1021/acs.inorgchem.1c01233>. Copyright © 2021, American Chemical Society.”

A significant contribution to the understanding of the computational aspects of Fe(II)-polypyridines as chromophores in DSSCs comes from the work by Jakubikova and Bowman [4] as shown in Figure 8. They did DFT calculations on different iron(II)-polypyridine complexes, as well as iron(II)-polypyridine-TiO₂ assemblies. Their computational perspective provides valuable insights into the electronic properties and structural dynamics of Fe(II)-polypyridine complexes, with a specific focus on their potential application in DSSCs. Through DFT calculations, the study elucidates the intricate details of the photoinduced electron transfer processes and the subsequent charge transport mechanisms within the sensitized solar cells. Additionally, the research sheds light on the factors such as the relative rates of intersystem crossing (ISC) and interfacial electron transfer (IET), the impact of linker groups anchoring Fe(II)-polypyridines onto TiO₂ surfaces, and the role of electron density on these linker groups, influencing the light-harvesting efficiency and the overall performance of the solar cells. The findings of this study are instrumental in furthering the understanding of the role of Fe(II)-polypyridines in the development of efficient and sustainable solar energy technologies. Specifically, the computational perspective offered in the study delves into the electronic properties, structural dynamics, and photoinduced electron transfer processes of Fe(II)-polypyridine complexes, which can offer valuable insights applicable to Fe(II)-terpyridine complexes [4].

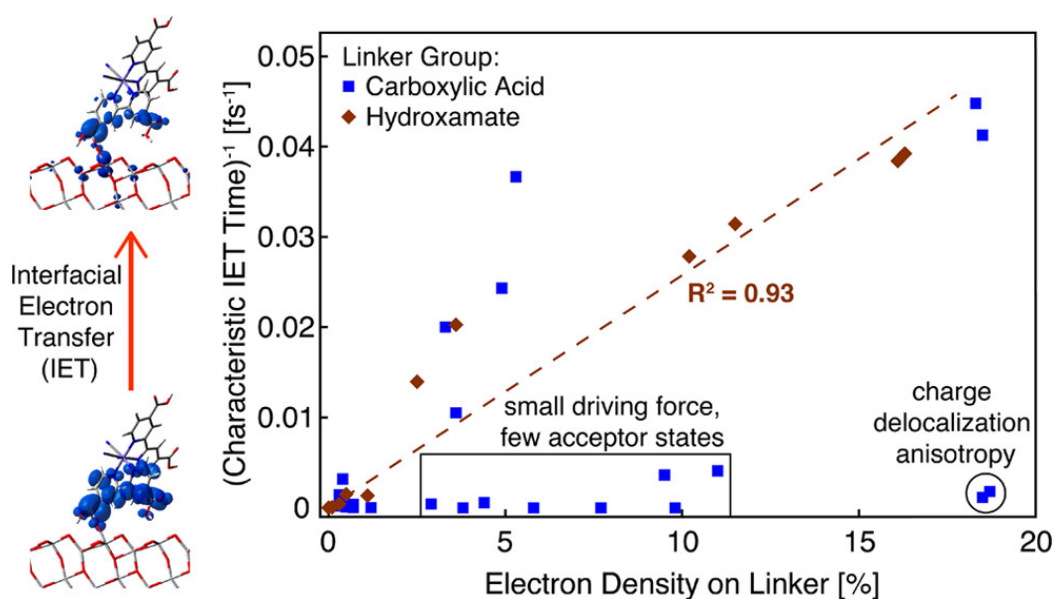
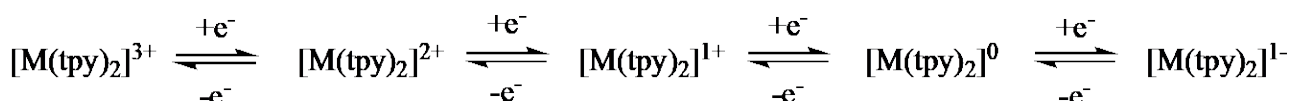


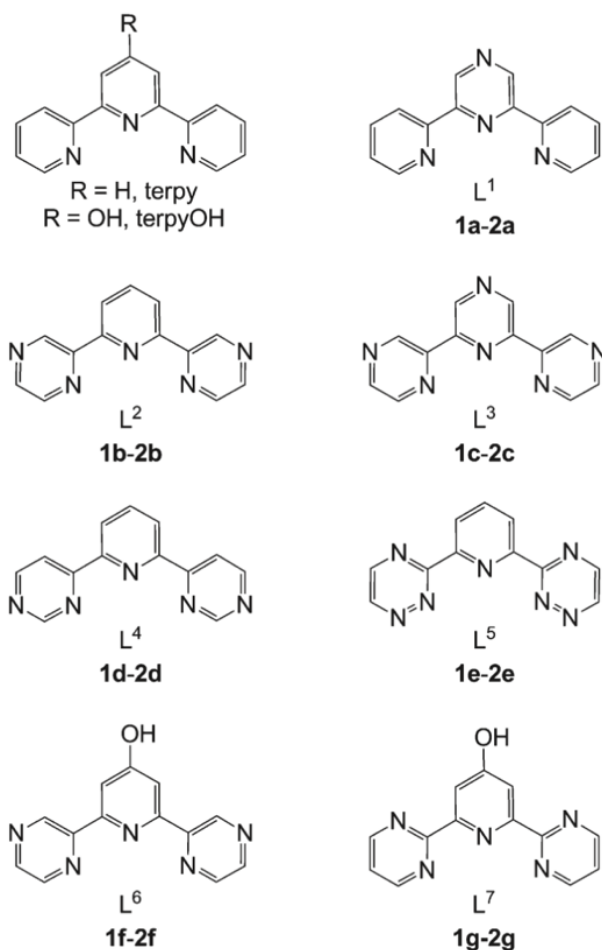
Figure 8: “Graph of characteristic interfacial electron transfer (IET) time against the percentage of electron density on the linker for various donor states in [Fe(bpy)₂(CN)₂]-TiO₂ assemblies with carboxylic acid and hydroxamate linkers, Jakubikova and Bowman [4] calculated the electron densities from Mulliken population analysis. The boxed and circled points represent IET rates involving the LUMO/LUMO+1 and LUMO+2 of [Fe(bpy-dca)₂(CN)₂], respectively. Reproduced from [4] E. Jakubikova, D.N. Bowman, Fe(II)-Polypyridines as Chromophores in DSSCs: A Computational Perspective, *Acc. Chem. Res.* 48 (2015) 1441–1449. <https://doi.org/10.1021/ar500428t>. (Open access). Copyright © 2015 American Chemical Society.”

2.2.3 CV Literature

The electrochemical behavior of iron(II)-terpyridine derivatives has been extensively documented in the literature. Table 3 summarizes the reported oxidation and reduction potentials of various iron(II) compounds, denoted as $[\text{Fe}^{\text{II}}(\text{L})_2]^{2+}$, where L is either a substituted terpyridine or a tris-azinyl derivative, as depicted in Scheme 8. Various electrochemical techniques such as cyclic voltammetry and polarography have been employed to study the electrochemical properties of $[\text{M}(\text{tpy})_2]^n$ ($\text{M} = \text{Fe}, \text{Ru}; n = 3+, 2+, 1+, 0, 1-$) complexes, revealing their patterns of oxidation and reduction, as depicted in Scheme 7 (spin states summarized in Table 2) [22].



Scheme 7: “Redox scheme for $[\text{M}(\text{tpy})_2]^n$ ($\text{M} = \text{Fe}$ or $\text{Ru}; n = 3+, 2+, 1+, 0, 1-$)” from [22].



Scheme 8: “Structure of various pyridine and pyrazine analogues (abbreviation for Fe^{II} (1a-1g) and Co^{II} (2a-2g) complexes) researched by Kershaw Cook et al [21]. Used with permission of Royal Society of Chemistry, from L.J. Kershaw Cook, F. Tuna, M.A. Halcrow, Iron(ii) and cobalt(ii) complexes of tris-azinyl analogues of 2,2':6',2''-terpyridine, *Dalt. Trans.* 42 (2013) 2254–2265. <https://doi.org/10.1039/c2dt31736b>; permission conveyed through Copyright Clearance Center, Inc. (Order license ID link: 1413863-1.)”

According to the findings of Wieghardt et al. [22], the $[\text{Fe}(\text{tpy})_2]^{2+}$ diamagnetic di-cationic complexes comprise low-spin Fe^{II} atoms at their core and are surrounded by neutral bis(terpyridine) ligands. Their tri-cationic counterparts feature Fe^{III} centers with a $(t_{2g})^5$ configuration, again with neutral ligands, marking the oxidation from di-cation to tri-cation as a metal-centered process. When the $[\text{Fe}^{\text{II}}(\text{tpy}^0)_2]^{2+}$ di-cation undergoes a one-electron reduction, they yield the mono-cation $[\text{Fe}^{\text{II}}(\text{tpy}^\bullet)(\text{tpy}^0)]^{1+}$ which have an $S=1/2$ ground state confirmed through X-band EPR spectroscopy in solution. The Mössbauer parameters for the mono-cation, similar to their di-cation counterparts, suggest they maintain a low-spin Fe^{II} ($S_{\text{Fe}} = 0$) configuration, placing the single unpaired electron in a ligand-based π^* orbital (SOMO) of $(\text{tpy}^\bullet)^1$. Consistent with prior research, the mono-cationic Fe $[\text{Fe}(\text{tpy}^\bullet)(\text{tpy}^0)]^{1+}$ ($S = 1/2$) structures suggest that the $2+/1+$ redox couples involve ligand-centered one-electron transfers, preserving the divalent low-spin $(t_{2g})^6$ (in distorted O_h symmetry) metal center configuration.

The neutral complex $[\text{Fe}^{\text{II}}(\text{tpy}^\bullet)_2]^0$, characterized by a high-spin Fe^{II} ($S_{\text{Fe}} = 2$) center exhibits a unique electronic structure where strong antiferromagnetic coupling between the iron ion and the two radical anions leads to an experimentally observed ground state with a spin of $S = 1$. This is indicative of the complex interplay between the high-spin Fe^{II} center and the radical anions, leading to a unique magnetic state. In octahedral metal complexes like $[\text{Fe}^{\text{II}}(\text{tpy}^\bullet)_2]$ with two terdentate $(\text{tpy}^\bullet)^{1-}$ radical anions and a diamagnetic central metal ion, their electronic structures are particularly intriguing due to the D_{2d} symmetry, resulting in nearly orthogonal magnetic orbitals of the two radical anions. This orientation is expected to enhance ferromagnetic couplings and reduce minor antiferromagnetic interactions. The cyclic voltammogram of $[\text{Fe}(\text{tpy})_2]^{2+}$, shown in Figure 9 [22], displays one oxidation wave and two reduction waves for the di-cationic complex, each corresponding to a one-electron process [22].

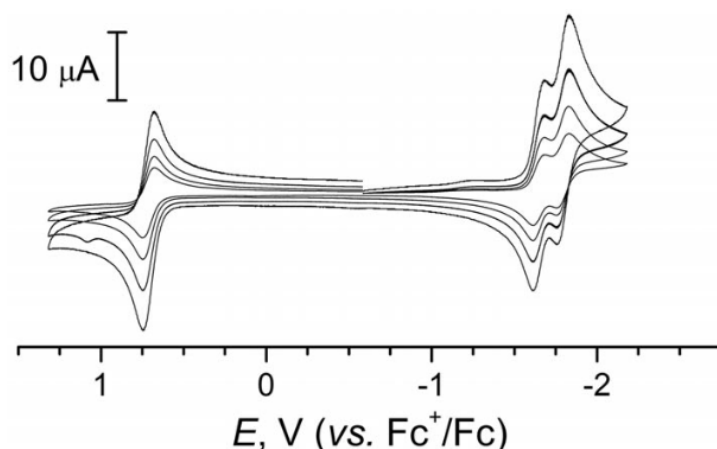


Figure 9: “CV of $[\text{Fe}(\text{tpy})_2](\text{PF}_6)_2$ was conducted at various scan rates (50, 100, 200, and 400 mV s^{-1}) at room temperature in acetonitrile (CH_3CN) solutions with a concentration of 0.2 M $[\text{N}(\text{nBu})_4](\text{PF}_6)_2$. The potential measurements were referenced against the ferrocene/ferrocenium (Fc^+/Fc) redox couple. From [22] Copyright © 2012 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.”

Only a few cyclic voltammograms (CVs), at only 0.100 V s^{-1} , are provided in the literature for a couple of $[\text{Fe}^{\text{II}}(\text{tpy})_2]^{2+}$ complexes. This includes $[\text{Fe}(4'-(\text{hydroxy})-2,2':6',2''\text{-terpyridine})_2]^{2+}$ ([21], oxidation only), $[\text{Fe}(4'-(\text{p-tolyl})-2,2':6',2''\text{-terpyridine})_2]^{2+}$ [23], $[\text{Fe}(2,2':6',2''\text{-terpyridine})_2]^{2+}$ ([14], and [24] oxidation only), $[\text{Fe}(4'-(\text{carboxylic acid})-2,2':6',2''\text{-terpyridine})_2]^{2+}$ ([16], oxidation and first reduction only), $[\text{Fe}(2,6\text{-di}(\text{pyrimidin-4-yl})\text{pyridine})_2]^{2+}$ [21], $[\text{Fe}(2,2':6',2''\text{-terpyrazine})_2]^{2+}$ [21], $[\text{Fe}(2,6\text{-di}(\text{pyrazol-1-yl})\text{pyridine})_2]^{2+}$ ([24], oxidation only) and $[\text{Fe}(4'-(4\text{-methoxyphenyl})-2,2':6',2''\text{-terpyridine})_2]^{2+}$ [15]. The only CVs shown at different scan rates for the oxidation peak are for $[\text{Fe}(2,2':6',2''\text{-terpyridine})_2]^{2+}$ [39]. The CVs depicting the redox behaviour of $[\text{Fe}(\text{tpy})_2]^{2+}$, $[\text{Fe}(\text{phen})_2]^{2+}$ and $[\text{Fe}(\text{bpy})_3]^{2+}$, are presented in Figure 10 [14].

The CVs for $[\text{Fe}(4'-(4\text{-methoxyphenyl})-2,2':6',2''\text{-terpyridine})_2]^{2+}$, $[\text{Fe}(4'-(3\text{-methoxyphenyl})-2,2':6',2''\text{-terpyridine})_2]^{2+}$, $[\text{Fe}(4'-(4\text{-(trifluoromethyl)phenyl})-2,2':6',2''\text{-terpyridine})_2]^{2+}$, and $[\text{Fe}(4'-(3,5\text{-bis(trifluoromethyl)phenyl})-2,2':6',2''\text{-terpyridine})_2]^{2+}$ are displayed in Figure 11 [15].

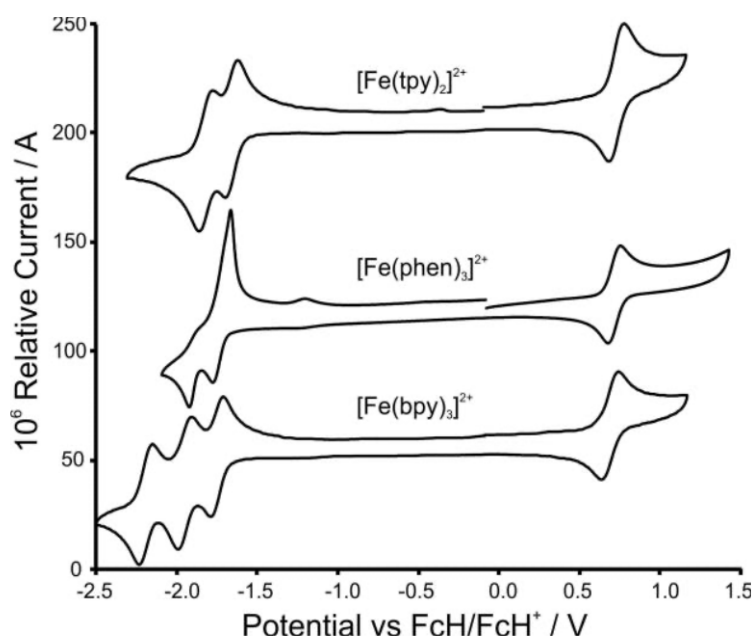


Figure 10: CVs of the oxidation of $[\text{Fe}(\text{tpy})_2]^{2+}$, $[\text{Fe}(\text{phen})_3]^{2+}$ and $[\text{Fe}(\text{bpy})_3]^{2+}$ from [14]. “Comparative wide scan cyclic voltammograms of *ca* $0.002 \text{ mol dm}^{-3}$ solutions of the indicated Fe^{II} complexes in $\text{CH}_3\text{CN} / 0.1 \text{ mol dm}^{-3}$ $[\text{n}(\text{Bu}_4)\text{N}][\text{PF}_6]$ on a glassy carbon-working electrode at a scan rate of 0.100 V s^{-1} . Scans were initiated in the positive direction from -0.01 V . Reprinted (adapted) with permission from H. Ferreira, K.G. von Eschwege, J. Conradie, Electronic properties of Fe charge transfer complexes – A combined experimental and theoretical approach, *Electrochim. Acta.* 216 (2016) 339–346. <https://doi.org/10.1016/j.electacta.2016.09.034>. © 2016 Elsevier Ltd. All rights reserved.”

The CVs presented in Figure 10 for the iron(II) complexes with terpyridine, phenanthroline, and bipyridine ligands reveal both similarities and differences in their oxidation and reduction behaviours. Although the oxidation potentials are closely grouped, indicating a similar ease of electron loss from iron(II) to iron(III), the reduction potentials display more substantial variation. This suggests that the differing ligand environments surrounding the iron(II) centers significantly influence the redox behaviour. These variations affect not only the redox potentials but also the energy and stability of the resulting oxidized and reduced species, which are crucial factors in designing these complexes for specific applications like catalysis or as redox mediators in DSSCs [14].

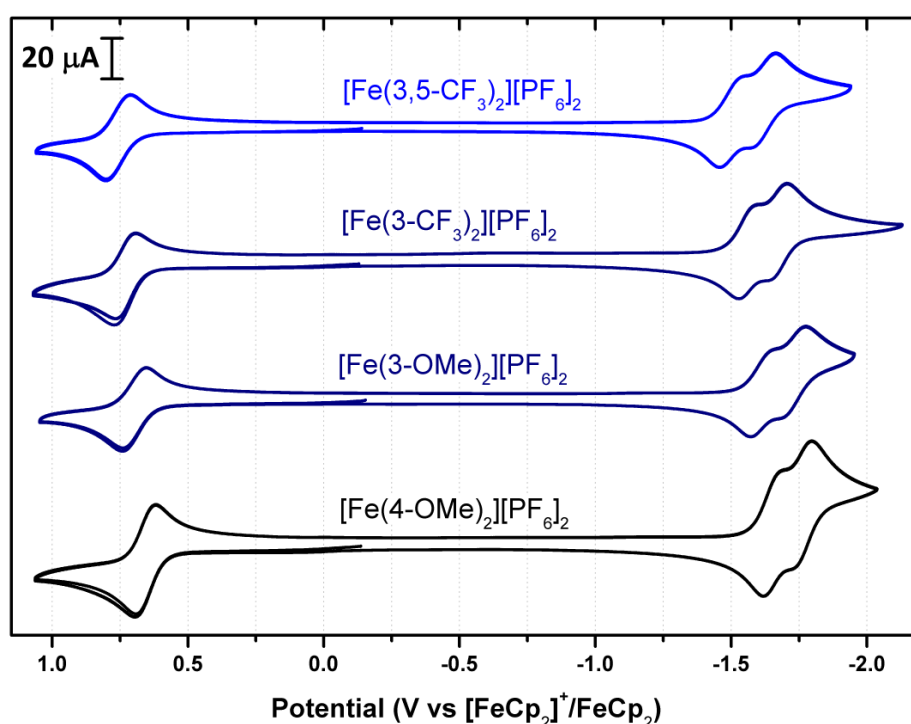


Figure 11: “CVs of $[\text{Fe}(4'-(\text{R-Ph})\text{-tpy})_2]^{2+}$ complexes (R indicated in the figure). “Collected in MeCN with 0.1M TBAPF₆ at $22 \pm 2^\circ\text{C}$. Complex concentrations listed in figure.” From [15], reprinted (adapted) with permission from J.C. Dickenson, M.E. Haley, J.T. Hyde, Z.M. Reid, T.J. Tarring, D.A. Iovan, D.P. Harrison, Fine-Tuning Metal and Ligand-Centered Redox Potentials of Homoleptic Bis-Terpyridine Complexes with 4'-Aryl Substituents, *Inorg. Chem.* 60 (2021) 9956–9969. <https://doi.org/10.1021/acs.inorgchem.1c01233>. Copyright © 2021, American Chemical Society.”

In Figure 11 [15], all $[\text{Fe}(4'-(\text{R-Ph})\text{-tpy})_2]^{2+}$ complexes demonstrate one oxidation and one reduction peak. The oxidation peak is characteristic of the one-electron transfer process typical for iron(II)/iron(III) redox couples, measured in acetonitrile with 0.1M TBAPF₆ as the supporting electrolyte. The $[\text{Fe}(4'-(3,5\text{-CF}_3)\text{-tpy})_2](\text{PF}_6)_2$ complex displays its oxidation peak at a relatively more

positive potential than that of $[\text{Fe}(4'-(4\text{-OMe})\text{-tpy})_2](\text{PF}_6)_2$, implying that the electron-withdrawing trifluoromethyl groups stabilize the oxidized state of the complex. Conversely, the oxidation peak for $[\text{Fe}(4'-(4\text{-OMe})\text{-tpy})_2](\text{PF}_6)_2$ occurs at a more negative potential, suggesting that the electron-donating methoxy groups destabilize the iron(III) state, facilitating its reduction back to iron(II). Regarding reduction, $[\text{Fe}(4'-(3\text{-CF}_3)\text{-tpy})_2](\text{PF}_6)_2$ shows its peak at a more negative potential relative to $[\text{Fe}(4'-(3\text{-OMe})\text{-tpy})_2](\text{PF}_6)_2$, once more highlighting the impact of the substituents on the ligand's capacity to stabilize the complex's reduced form. These CVs provide valuable insight into the electronic effects of substituents on the redox behavior of iron complexes, which is crucial for understanding their function in various chemical and electrochemical applications [15].

The oxidation behaviour of the molecules is observed to mainly involve iron, thus demonstrating Fe(II/III) redox activity, leading to the formation of the $[\text{Fe}^{\text{III}}(\text{tpy})_2]^{3+}$ complex [15–17,21,23,24,40], which aligns with the properties of the highest occupied molecular orbital (HOMO) as determined by DFT analysis (refer to Figure 12 [1]). In most instances, the Fe(II/III) redox pair ($E_{\text{Fe(II/III)}}$) exhibits both chemical and electrochemical reversibility [15–17,21,23,24,40]. However, the reduction process for the iron(II) complexes is attributed to the ligands that are coordinated to the metal, as indicated in the literature [15–17,21,23,24,40]. The redox potentials for the Fe(II/III) transition and the ligand-based reductions ($E_{\text{Fe(II/III)}}$ and E_{Ligand} , respectively), as reported by various research groups, show consistency when compared, as summarized in Table 3.

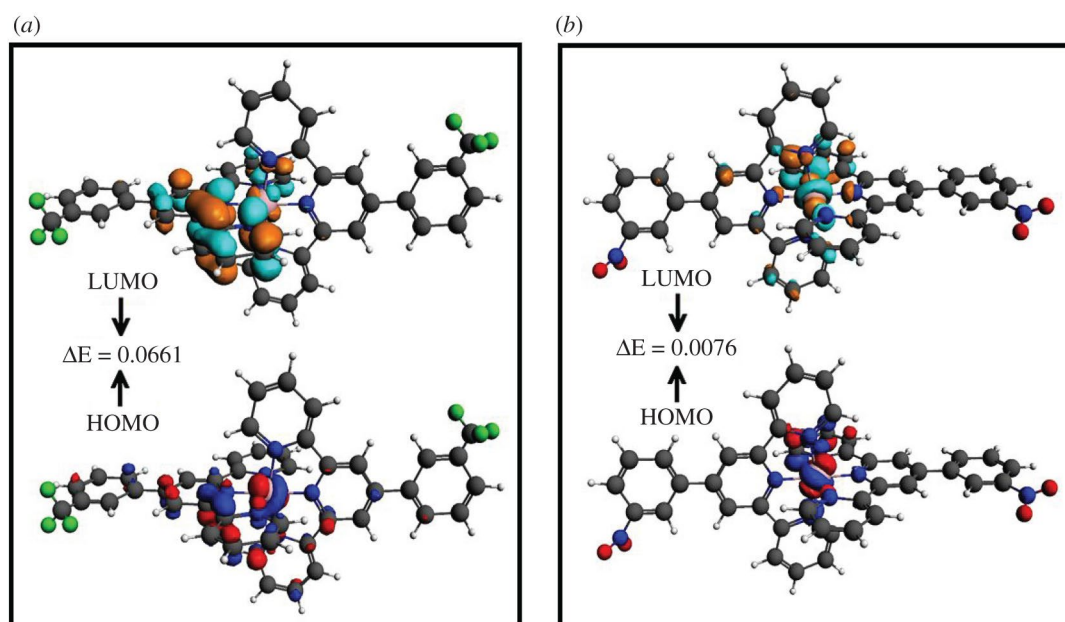


Figure 12: “DFT-B3LYP (DZ) calculated frontier molecular orbitals (FMOs) of (a) C15 and (b) C24.” From [1] (open access) under CC BY 4.0 DEED.

The electrochemical behaviours for a series of $[M^{II}(4'-(R-Ph)-tpy)_2]^{2+}$ complexes, where M represents iron or cobalt, exhibit a clear linear correlation when their M(III/II) redox potentials are plotted against the Hammett constants of substituent R, as demonstrated in Figure 13 [17]. This linear relationship signifies the impact of substituent characteristics on the metal's redox properties. Additionally, comprehensive electrochemical analyses on a suite of $[M^{II}(tpy)_2]^{2+}$ complexes with various substituents on the tpy ligand have established a robust connection between the M(III/II) oxidation and ligand-based reduction potentials with the Hammett substituent parameters, for a range of metals including manganese, iron, cobalt, nickel, and zinc [15]. These findings, showcased in Figure 14 [15], emphasize that the electronic nature of the substituents profoundly influences both the oxidation at the metal site and the reduction at the ligand in $[M^{II}(tpy)_2]^{2+}$ complexes, highlighting the substituents' roles as electron-donating or -withdrawing groups.

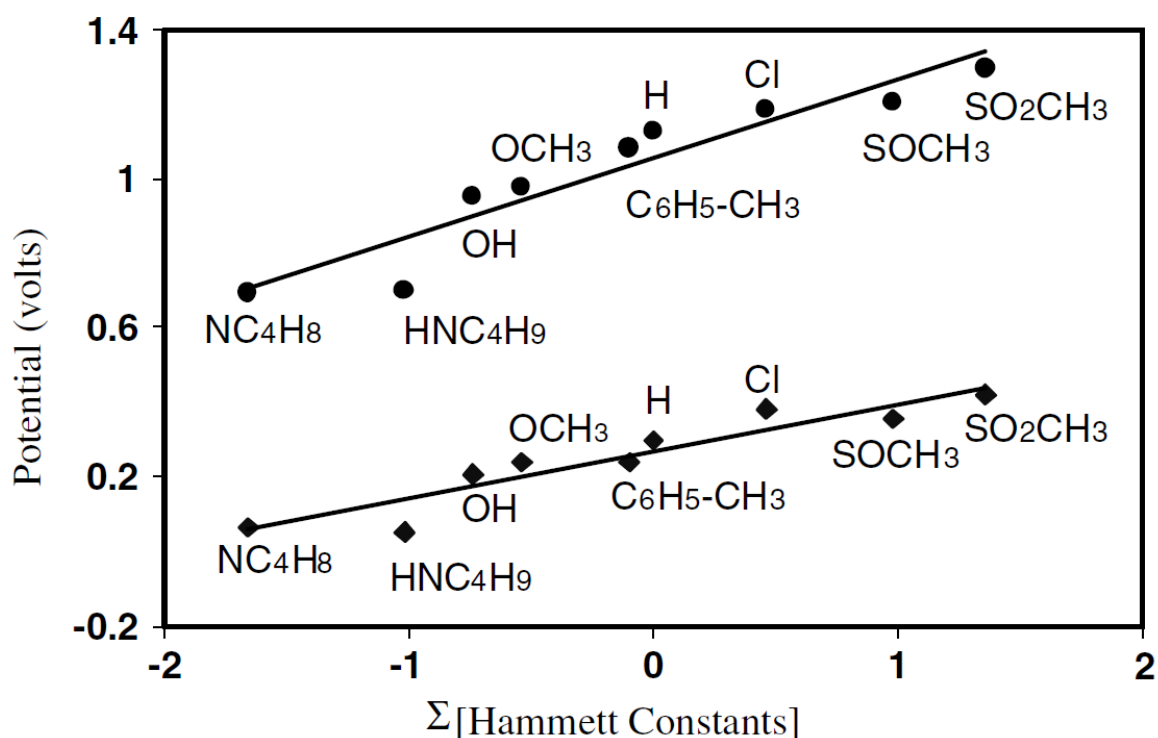


Figure 13: “A plot of Fe(III/II) couple (top line) and the Co(III/II) couple (bottom line) vs. the Hammett constants of the terpyridine substituents. The electrochemistry was measured in 0.1 M TBAH/acetonitrile using a platinum working electrode, a SSCE reference electrode, and a scan rate of 100 mV/s from [17]. Reprinted (adapted) with permission from J. Chambers, B. Eaves, D. Parker, R. Claxton, P.S. Ray, S.J. Slattery, Inductive influence of 4'-terpyridyl substituents on redox and spin state properties of iron(II) and cobalt(II) bis-terpyridyl complexes, *Inorg. Chim. Acta.* 359 (2006) 2400–2406. <https://doi.org/10.1016/j.ica.2005.12.065>. Copyright © 2006 Elsevier B.V. All rights reserved.”

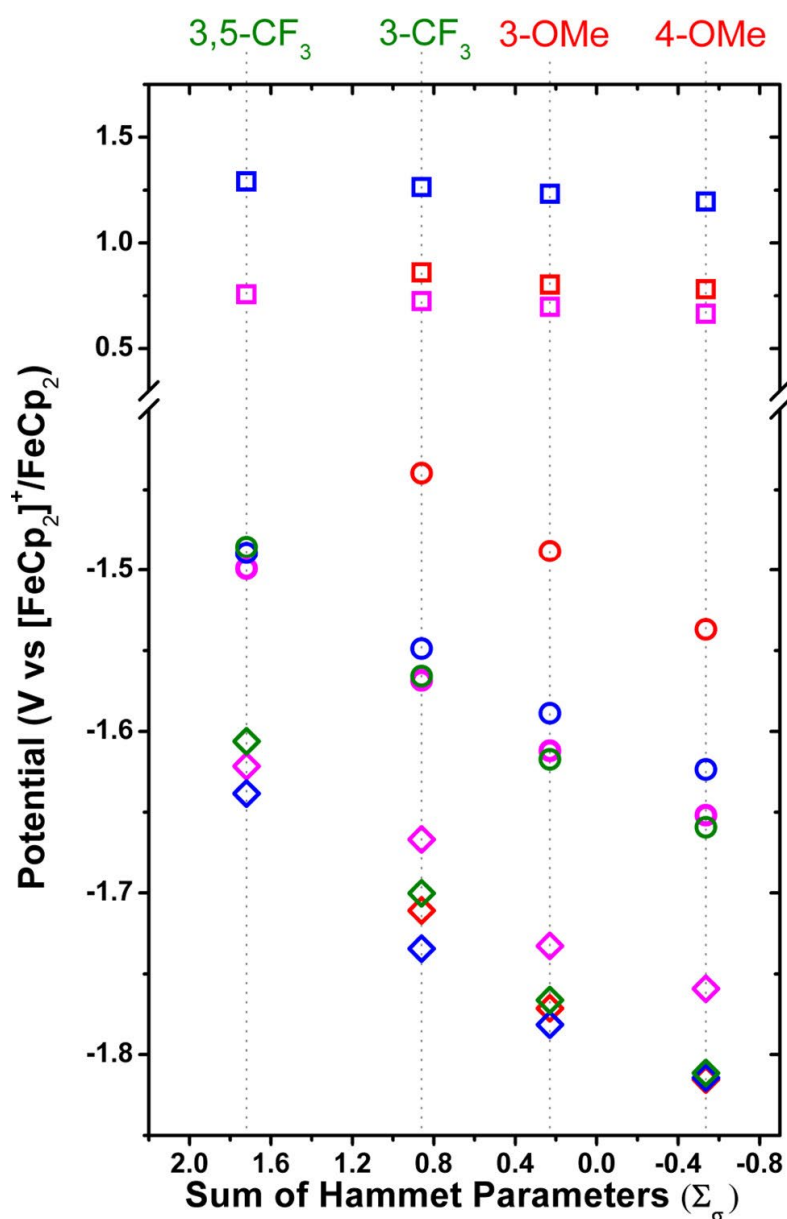


Figure 14: “Plot of reduction potentials for various $[M(L)_2]^{2+}$ complexes. Blue shapes indicate nickel complexes, red indicates manganese complexes, purple indicates iron complexes, and green indicate zinc complexes. Square symbols indicate $E_{1/2}(M^{III/II})$, circular symbols indicate $E_{1/2}(L\pi^{0/-1})$, and diamonds indicate $E_{1/2}(L\pi^{-1/-2})$.” “The coordinated ligand and their $\Sigma\sigma$ are depicted above and below the plot, respectively” from [15]. $L = 4'-(R-Ph)-tpy$, R is indicated in the plot. “Reprinted (adapted) with permission from J.C. Dickenson, M.E. Haley, J.T. Hyde, Z.M. Reid, T.J. Tarring, D.A. Iovan, D.P. Harrison, Fine-Tuning Metal and Ligand-Centered Redox Potentials of Homoleptic Bis-Terpyridine Complexes with 4'-Aryl Substituents, *Inorg. Chem.* 60 (2021) 9956–9969. <https://doi.org/10.1021/acs.inorgchem.1c01233>. Copyright © 2021, American Chemical Society.”

Table 3: “The iron-based oxidation and ligand-based first reduction potentials, $E_{\text{Fe(II/III)}}$ (expt.) (V) and E_{Ligand} vs FcH/FcH^+ (expt.)(V) of the $[\text{Fe}(\text{L})_2]^{2+}$ ($\text{L}=\text{L}^1\text{-L}^{25}$) compounds in acetonitrile as the solvent, from Ref. [15–17,21,23,24,40]. Values reported vs SSCE are converted to potentials vs FcH/FcH^+ , using a conversion constant of 0.384V reported in the literature” [41]. Data from [41] and the indicated Ref. Structures of $\text{L}1 - \text{L}7$ in Scheme 8.

Nr	Complex	$E_{\text{Fe(II/III)}}$ vs SSCE	$E_{\text{Fe(II/III)}}$ vs FcH/FcH^+	E_{Ligand} vs FcH/FcH^+	Reference
1	$[\text{Fe}(\text{tpy-NC}_4\text{H}_8)_2]^{2+}$	0.69	0.31		[17]
1	$[\text{Fe}(4'\text{-NC}_4\text{H}_8\text{-tpy})_2]^{2+}$		0.26	-1.91	[23]
2	$[\text{Fe}(\text{tpy-N}(\text{CH}_3)_2)_2]^{2+}$		0.28	-1.90	[23]
3	$[\text{Fe}(\text{tpy-NH}(\text{CH}_3(\text{CH}_2)_3)_2)]^{2+}$	0.69	0.31		[17]
4	$[\text{Fe}(\text{tpy-OH})_2]^{2+}$	0.95	0.57		[17]
4	$[\text{Fe}(4'\text{-OH-tpy})_2]^{2+}$		0.54	-1.76 ^a	[21]
4	$[\text{Fe}(\text{tpy-4-OH})_2]^{2+}$		0.55	-1.78 ^b	[23]
5	$[\text{Fe}(\text{tpy-OMe})_2]^{2+}$	0.98	0.60		[17]
6	$[\text{Fe}(\text{tpy-4-CH}_3\text{-C}_6\text{H}_4)_2]^{2+}$	1.08	0.70		[17]
6	$[\text{Fe}(4\text{-CH}_3\text{-C}_6\text{H}_4\text{-tpy})_2]^{2+}$		0.68	-1.63	[23]
7	$[\text{Fe}(\text{tpy-vinyl})_2]^{2+}$	1.08	0.69		[40]
8	$[\text{Fe}(\text{tpy})_2]^{2+}$	1.13	0.75		[17]
8	$[\text{Fe}(\text{tpy})_2]^{2+}$		0.71	-1.66	[21]
8	$[\text{Fe}(\text{tpy})_2]^{2+}$		0.72	-1.64	[23]
8	$[\text{Fe}(\text{tpy})_2]^{2+}$	1.13	0.75		[42]
8	$[\text{Fe}(\text{tpy})_2]^{2+}$	1.11	0.73		[24]
8	$[\text{Fe}(\text{tpy})_2]^{2+}$		0.72	-1.69	[14]
8	$[\text{Fe}(\text{tpy})_2]^{2+}$		0.71	-1.64	[22]
9	$[\text{Fe}(\text{tpy-L}7)_2]^{2+}$		0.75	-1.37 ^a	[21]
10	$[\text{Fe}(\text{tpy-Cl})_2]^{2+}$	1.19	0.81		[17]
10	$[\text{Fe}(\text{Cl-tpy})_2]^{2+}$		0.77	-1.54	[23]
11	$[\text{Fe}(\text{tpy-COOH})_2]^{2+}$		0.82	-1.44	[16]
12	$[\text{Fe}(\text{tpy-CH}_3\text{SO})_2]^{2+}$	1.21	0.83		[17]
13	$[\text{Fe}(\text{tpy-L}6)_2]^{2+}$		0.90	-1.09 ^a	[21]
14	$[\text{Fe}(\text{tpy-CH}_3\text{SO}_2)_2]^{2+}$	1.30	0.92		[17]
15	$[\text{Fe}(\text{tpy-L}1)_2]^{2+}$		0.95	-1.30	[21]
16	$[\text{Fe}(\text{tpy-L}4)_2]^{2+}$		0.98	-1.25	[21]
17	$[\text{Fe}(\text{tpy-L}2)_2]^{2+}$		1.07	-1.25	[21]
18	$[\text{Fe}(\text{tpy-L}5)_2]^{2+}$		1.20	-1.10 ^a	[21]
19	$[\text{Fe}(\text{tpy-L}3)_2]^{2+}$		1.36	-0.98	[21]
20	$[\text{Fe}(\text{tri-OMe-tpy})_2]^{2+}$	0.77	0.39		[42]
21	$[\text{Fe}(\text{tri-Et}_2\text{N-tpy})_2]^{2+}$	0.12	-0.26		[42]
22	$[\text{Fe}(\text{l-bpp})_2]^{2+}$	1.30 ^c	0.92		[24]
23	$[\text{Fe}(\text{tpy-methoxyphenyl})_2]^{2+}$		0.67	-1.65	[15]

a Irreversible process, E_{pc} given.

b Irreversible process, estimated value, and **c** Irreversible process, E_{pa} given.

2.2.4 UV-vis

The exploration of UV-visible (UV-vis) spectroscopy and DFT studies on various iron(II)-terpyridine derivatives within the context of DSSCs is aimed at elucidating the fundamental principles governing their optical properties and electronic transitions. UV-vis spectroscopy has emerged as a powerful technique for examining their absorption and emission characteristics. Through a comprehensive analysis of the absorption and emission spectra, researchers can develop a deeper understanding of the intricate interplay between molecular structure, electronic configurations, and optical properties of these complexes. The reported UV-visible spectra of $[\text{Fe}(\text{L}^n)_2]^{2+}$ ($\text{L} =$ a substituted terpyridine or related ligand, see Table 4), all display a peak above 500 nm (λ_{max}) in the visible region, attributed to the ligand-to-metal charge transfer band (LMCT) in the literature, along with a substantial absorbance peak at approximately 300 nm ($\lambda_{\text{A,max}}$) in the UV region, as detailed in Table 4. An example of the reported UV-visible spectra (A) and CV (B) of the unsubstituted *bis*(terpyridine)iron(II) complex, is illustrated in Figure 15 [43].

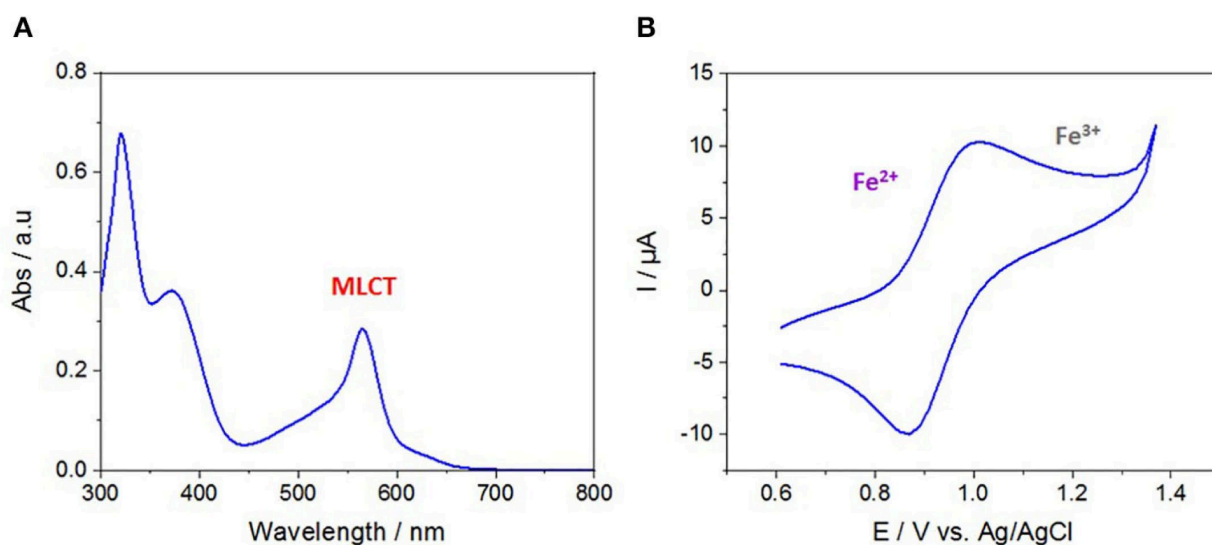


Figure 15: “(A) UV-Vis absorption spectrum of a solution containing 0.5×10^{-5} M $[\text{Fe}(\text{tpy})_2(\text{BF}_4)_2]$ in acetonitrile. (B) Cyclic voltammogram of 0.5 mM $[\text{Fe}(\text{tpy})_2(\text{BF}_4)_2]$ in 0.1 M TBABF₄ in acetonitrile at 50 mV s^{-1} . From [43] open access with Creative Commons Attribution (CC BY) license.”

Table 4: Summary of the published UV data of complexes $[\text{Fe}(\text{L}^n)_2]^{2+}$ that are relevant to the examination of iron complexes in DSSCs within this dissertation: experimental absorbance maximum wavelength ($\lambda_{\text{Abs. max}}$) and maximum wavelength (λ_{max}) in nm.

n	L	$\lambda_{\text{Abs. max}}$ (nm)	λ_{max} (nm)	Reference
1	4'-(hydroxy)-2,2':6',2''-terpyridine	243	553	[21]
2	2,6-di(pyrid-2-yl) pyrazine	278	552	[21]
3	4'-(3,5-bis(trifluoromethyl)phenyl)-2,2':6',2''-terpyridine	285	570	[12]
4	4'-(2-(trifluoromethyl) phenyl)-2,2':6',2''-terpyridine	286	572	[1]
5	4'-(4-(trifluoromethyl) phenyl)-2,2':6',2''-terpyridine	286	569	[1]
6	4'-(3-(trifluoromethyl) phenyl)-2,2':6',2''-terpyridine	286	568	[1]
7	2,6-di(pyrimidin-2-yl) pyridin-4-ol	252	545	[13]
8	2,6-di(pyrimidin-4-yl) pyridine	315	574	[13]
9	4'-(3-nitrophenyl)-2,2':6',2''-terpyridine	328	575	[1]
10	2,2':6',2''-terpyridine	319	552	[13]
11	2,6-di(pyrazinyl)pyridin-4-ol	283	586	[21]
12	2,2':6',2''-terpyrazine	282	545	[21]
13	2,6-di(pyrazinyl)pyridine	285	552	[21]
14	4'-(4-nitrophenyl)-2,2':6',2''-terpyridine	287	583	[1]
15	4-([2,2':6',2''-terpyridin]-4'-yl)-N, N-dimethylaniline	324	587	[1]
16	4'-(p-tolyl)-2,2':6',2''-terpyridine	327	571	[1]
17	4'-(4-methoxyphenyl)-2,2':6',2''-terpyridine	336	586	[1]
18	4-([2,2':6',2''-terpyridin]-4'-yl)-N, N-diphenyl aniline	437	584	[1]
19	4'-(3-methoxyphenyl)-2,2':6',2''-terpyridine	285	570	[15]

The study by Gros and co-workers [16] focuses on investigating the photophysical and photovoltaic properties of specific iron complexes, namely *bis*(2,2':6',2''-terpyridine carboxylic acid) iron(II) and two related homoleptic iron complexes with tridentate bis-carbene ligands, see Figure 16 [16]. These complexes were studied for their potential application as dye sensitizers in DSSCs. In addition to the experimental investigation, the researchers also conducted a comprehensive time-dependent DFT study to complement their experimental findings [16].

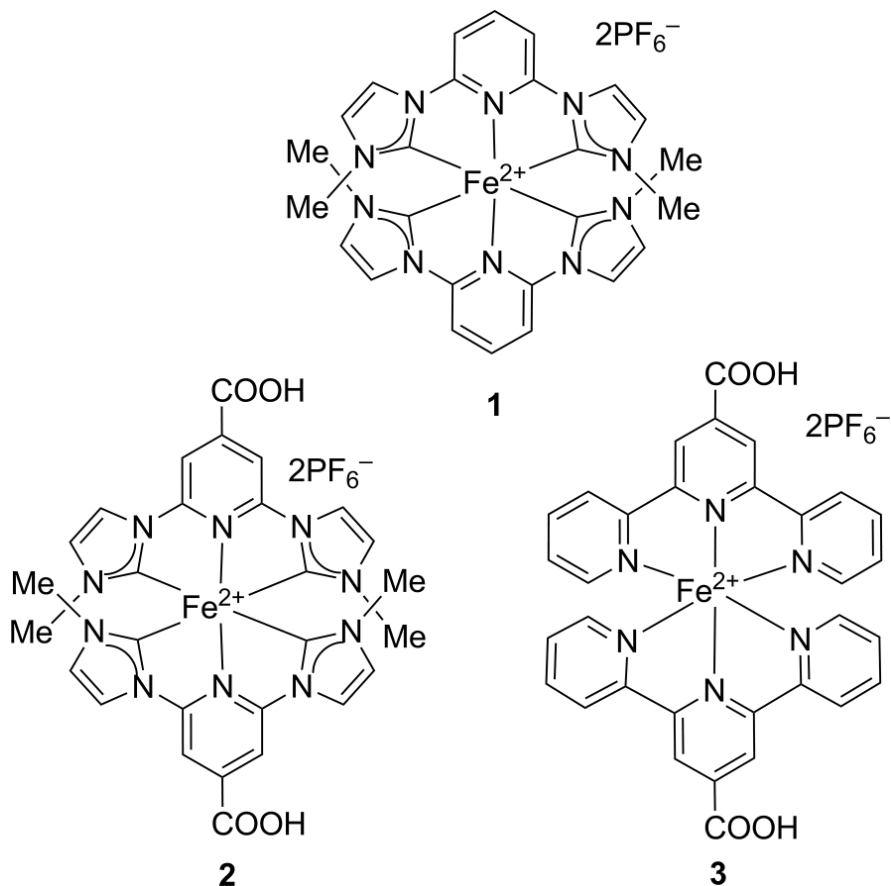


Figure 16: “Bis(2,2':6',2''-terpyridine carboxylic acid) iron(II) and two homoleptic iron complexes with tridentate bis-carbene ligands. From [16] T. Duchanois, T. Etienne, C. Cebrián, L. Liu, A. Monari, M. Beley, X. Assfeld, S. Haacke, P.C. Gros, An iron-based photosensitizer with extended excited-state lifetime: Photophysical and photovoltaic properties, *Eur. J. Inorg. Chem.* 2015 (2015) 2469–2477. <https://doi.org/10.1002/ejic.201500142>. Copyright © 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.”

The study by Gros and co-workers [16] highlights key findings on the absorption behaviour of three complexes, revealing distinct bands associated with various electronic transitions, notably π – π^* transitions at 300–320 nm and a less influenced band at 360–380 nm, as depict in Figure 17 (left) [16]. The iron center demonstrates two metal-to-ligand charge transfer (MLCT) transitions, with complexes containing carbenes (complexes 1 and 2 in Figure 16) displaying blue-shifted MLCT transitions compared to bis(2,2':6',2''-terpyridine carboxylic acid) iron(II), complex 3, in Figure 16. Complex 2 (Figure 16) exhibits substantial light absorption potential ($\epsilon > 5 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$) in the 380–500 nm range, indicating its suitability for effective light harvesting in DSSCs. Moreover, the DSSC assembled with complex 2 demonstrates high incident photon-to-current efficiency (IPCE) across a wide spectral range (400–600 nm), suggesting its promise as a sensitizer in DSSCs.

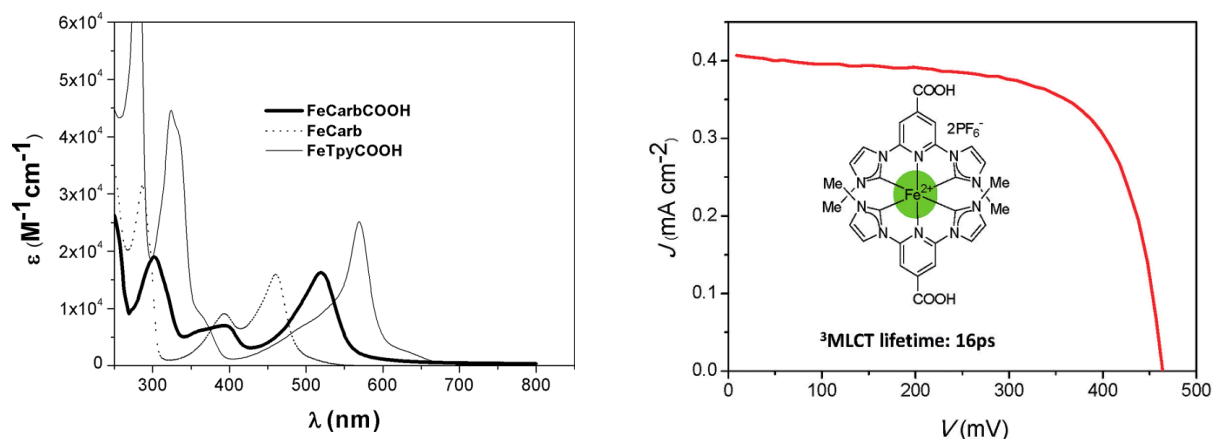


Figure 17: “Absorption spectra of three Fe complexes (left) in acetonitrile, and novel iron(II) complex with $^3\text{MLCT}$ lifetime: 16ps (right). From [16] with Copyright © 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.”

In conclusion, the research introduces a novel iron(II) complex boasting an unprecedented 16ps lifetime for the triplet MLCT ($^3\text{MLCT}$) state, see Figure 17 (right) [16]. This complex was assessed as a photosensitizer in a laboratory DSSC, resulting in observable photocurrent and enhanced power-conversion efficiency. The significant enhancement of the photophysical characteristics of iron-based complexes indicates potential applications extending well beyond energy generation [16].

The study conducted by Kershaw Cook et al. [21] details the syntheses of various pyridine and pyrazine analogues (Scheme 8). The study revealed that the UV/vis spectra of the analysed complexes in MeCN closely resemble those of $[\text{Fe}(\text{tpy})_2]^{2+}$ and $[\text{Co}(\text{tpy})_2]^{2+}$ derivatives. The spectra exhibits the anticipated MLCT absorptions falling within the range of 450–590 nm, see Figure 18 [21]. Notably, the hydroxylated complexes demonstrate significantly broader MLCT maxima, potentially due to hydrogen bonding interactions with the solvent. While the extinction coefficients vary, the MLCT λ_{max} values for $[\text{Fe}(\text{tpy})_2][\text{BF}_4]_2$, $[\text{Fe}(4'\text{-OH-tpy})_2][\text{BF}_4]_2$, and 1a–1c ($\text{L}^1\text{-L}^3$ in Scheme 8) are nearly indistinguishable within experimental margins, whereas other iron complexes exhibit more pronounced differences [21].

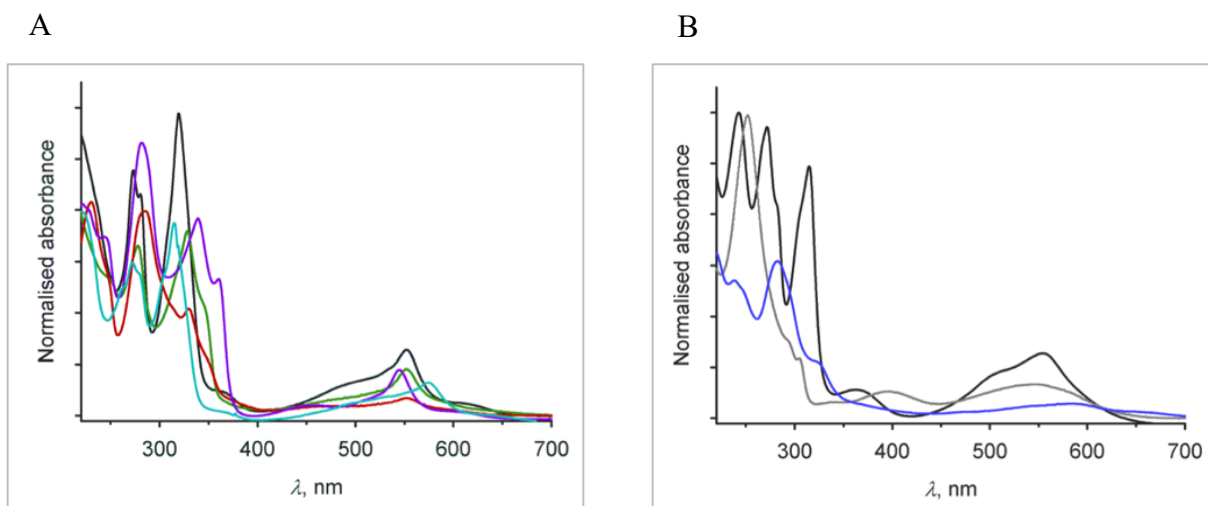
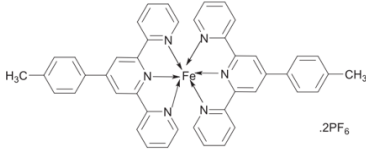
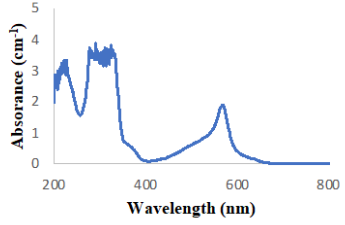
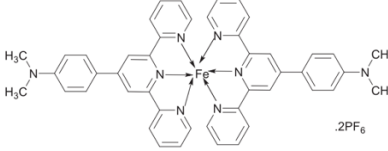
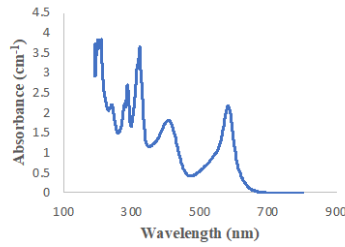
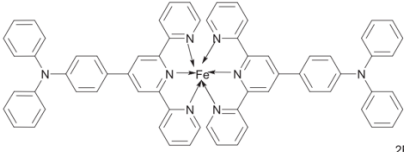
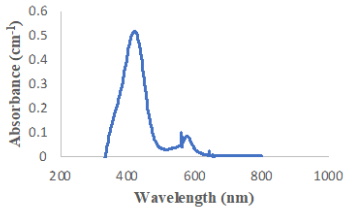
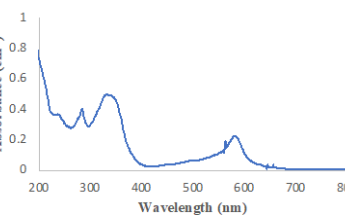
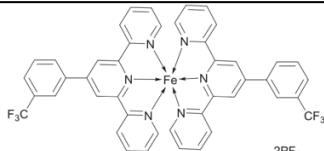
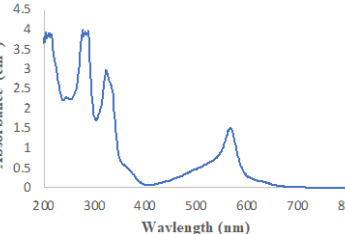
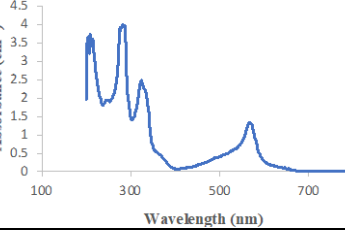
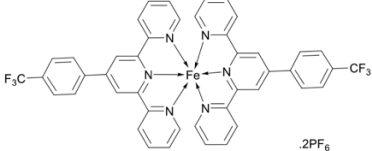
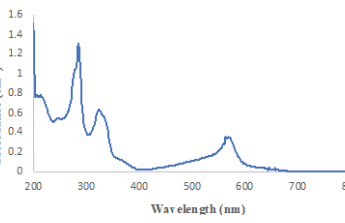
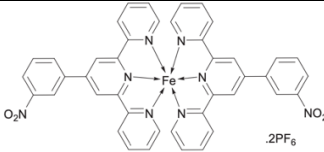
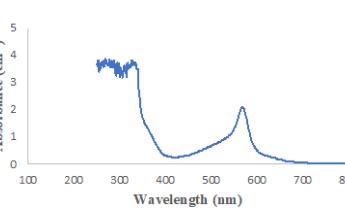


Figure 18: “(A) UV/vis spectra (MeCN, 298 K) of $[\text{Fe}(\text{terpy})_2][\text{BF}_4]_2$ (black), 1a (green), 1b (red), 1c (purple) and 1d (cyan). (B) UV/vis spectra (MeCN, 298 K) of $[\text{Fe}(\text{terpyOH})_2][\text{BF}_4]_2$ (black), 1f (blue) and 1g (grey). Terpy-OH = 4'-OH-tpy. From [21], UV/vis spectra of the indicated complexes (Ligand structures in Scheme 8). Used with permission of Royal Society of Chemistry, from L.J. Kershaw Cook, F. Tuna, M.A. Halcrow, Iron(II) and cobalt(II) complexes of tris-aziny analogues of 2,2':6',2''-terpyridine, *Dalt. Trans.* 42 (2013) 2254–2265. <https://doi.org/10.1039/c2dt31736b>; permission conveyed through Copyright Clearance Center, Inc. (Order license ID link: 1413863-1.)”

Mughal and colleagues [1] explored how various substituents impact the physical, chemical, and anti-microbial characteristics of a range of tpy-metal (II) complexes, which encompassed several iron (II) variants. Their experimental observations were further supported by a DFT and Time-Dependent Density Functional Theory (TDDFT) analysis of two iron complexes with asymmetrically substituted tpy ligands [1]. The combined experimental and theoretical approach sheds light on the intricate interplay between structural modifications and the ensuing alterations in the physicochemical properties of the tpy-metal (II) complexes, thereby providing a deeper understanding of the relationship between structure and function.

In summary, Mughal et al. [1] reported that differences in absorption wavelengths and intensities are attributed to the varying substituents at the 4' position of the terpyridine. The UV-Vis spectra of terpyridine-based metal complexes exhibit the characteristic MLCT shift associated with the Fe(II)-terpyridine system in complexes C₃, C₆, C₉, C₁₂, C₁₅, C₁₈, C₂₁, C₂₄, and C₂₇ (see Figure 19:, left), with a $\lambda_{\text{max}} = 587$ nm. These spectra are also accompanied by bands at 284 nm and 426 nm, arising from ligand-centered (LC) transitions. A minor redshift, in comparison to the reference Fe(II)-terpyridine complex, is observed. Notably, the spin-allowed MLCT band in the visible region exhibits an increase in intensity and a redshift, regardless of the substituents' electron-donating or -accepting nature (see Figure 19:, right) [1], as reported in Table 4.

C₃	 .2PF₆	
C₆	 .2PF₆	
C₉	 .2PF₆	
C₁₂	 .2PF₆	
C₁₅	 .2PF₆	
C₁₈	 .2PF₆	
C₂₁	 .2PF₆	
C₂₄	 .2PF₆	

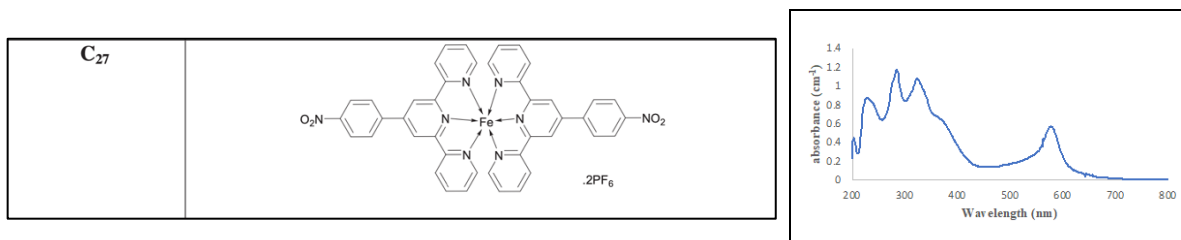


Figure 19: “The UV-Vis spectra and structure of Fe (II)-terpyridine-based complexes (C₃, C₆, C₉, C₁₂, C₁₅, C₁₈, C₂₁, C₂₄, C₂₇), MLCT shift at $\lambda_{\text{max}} = 587$ nm. From [1] (open access) under CC BY 4.0 DEED.”

The DFT and TDDFT study carried out on the iron complexes with unsymmetrically substituted tpy ligands, namely C₁₅ and C₂₄ (structures in Figure 19), serves to complement and validate the experimental findings, see Figure 20 [1]. The theoretical investigation aids in elucidating the electronic structure, optical properties, and charge transfer dynamics within the complexes, enabling a comprehensive understanding of their reactivity and stability. By integrating theoretical insights with experimental results, the researchers can effectively rationalize the observed trends and phenomena, facilitating the prediction and design of novel tpy-metal (II) complexes with tailored functionalities.

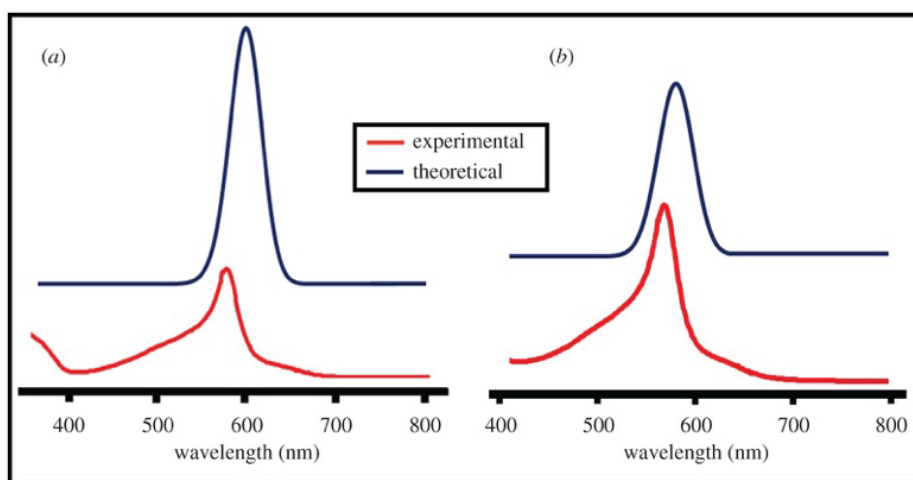


Figure 20: “Experimental and DFT-B3LYP* (DZ) calculated UV-Vis spectra of representative metal complexes of ligands L5 and L8: (a) C₁₅ and (b) C₂₄, respectively. From [1] (open access) under CC BY 4.0 DEED.”

Furthermore, the exploration of the anti-microbial potential of the complexes (C₃, C₆, C₉, C₁₂, C₁₅, C₁₈, C₂₁, C₂₄, C₂₇ in Figure 19:) highlights their potential applicability in medicinal and therapeutic contexts. The findings suggest the promise of these complexes as potential candidates for antimicrobial agents, thereby emphasizing the significance of the study in the broader context of pharmaceutical research and development. This work sets the stage for further investigations into the

design and synthesis of tpy-metal (II) complexes with optimized properties, laying the groundwork for their potential utilization in various technological and biomedical applications [1].

Additionally, in the study by Dickenson et al. [15], the authors focused on fine-tuning the metal and ligand-centered redox potentials of homoleptic *bis*-terpyridine complexes with 4'-aryl substituents. The research outlined a detailed investigation of the UV-visible spectra, providing insights into the precise tuning of electronic properties for the enhancement of various functional applications, see Figure 21 [15].

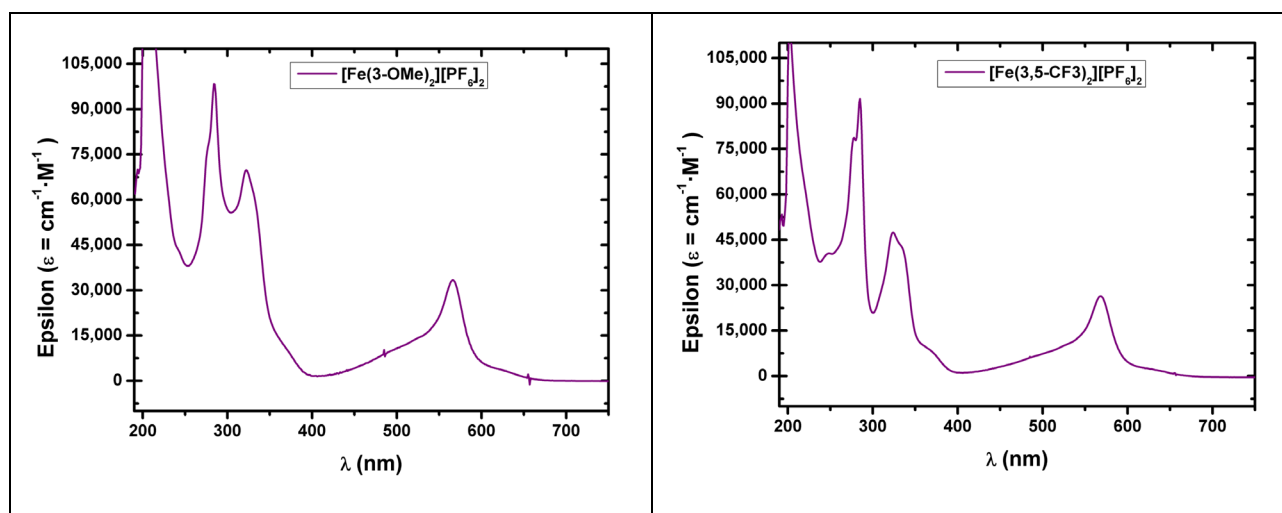


Figure 21: “UV-Vis Spectra of the indicated Fe complexes in MeCN from [15]. Reprinted (adapted) with permission from J.C. Dickenson, M.E. Haley, J.T. Hyde, Z.M. Reid, T.J. Tarring, D.A. Iovan, D.P. Harrison, Fine-Tuning Metal and Ligand-Centered Redox Potentials of Homoleptic Bis-Terpyridine Complexes with 4'-Aryl Substituents, *Inorg. Chem.* 60 (2021) 9956–9969. <https://doi.org/10.1021/acs.inorgchem.1c01233>. Copyright © 2021, American Chemical Society.”

2.3 Computational Chemistry

2.3.1 Computational methods

When discussing computational chemistry methods, it's important to differentiate between various approaches based on their principles, applications, and limitations. Below is an overview of different methods, including ab initio [44], molecular mechanics (MM) [45], DFT [6,46–48], empirical, and semi-empirical methods [48].

2.3.1.1 *Ab initio methods:*

These methods are grounded in quantum mechanics and aim to solve the Schrödinger equation without incorporating empirical data. Ab initio calculations can be very accurate but are computationally demanding. They are typically applied to small molecular systems. One of the most common ab initio methods is the Hartree-Fock (HF) method, which approximates the many-electron wave function with a single determinant of one-electron wave functions [44].

2.3.1.2 *Molecular mechanics (MM):*

MM methods use parameterized force fields to predict molecular geometry, energy, and other properties. They are particularly useful for simulating large systems like proteins or polymers where quantum mechanical treatments are impractical. MM treats atoms as spheres and bonds as springs, ignoring the electronic structure [45].

2.3.1.3 *Density Functional Theory (DFT):*

DFT is a quantum mechanical method that calculates the electronic structure based on electron density rather than wave functions. It is less computationally intensive than ab initio methods and is widely used for a variety of systems. DFT has several functionals, like the local density approximation (LDA), generalized gradient approximation (GGA), and hybrid functionals like B3LYP [6,46,47,49].

2.3.1.4 *Empirical methods:*

These methods rely on experimental data to create models and predict outcomes. They are generally less accurate than quantum mechanical methods but are faster and can be useful for screening large numbers of compounds or materials. The accuracy of empirical methods depends heavily on the quality and relevance of the experimental data used to create them.

2.3.1.5 *Semi-empirical methods:*

Semi-empirical methods use a combination of theoretical calculations and empirical adjustments. They are faster than fully ab initio methods and can sometimes offer better accuracy than MM [45],

especially for electronic properties. These methods, such as the MNDO [50], AM1 [51], and PM3 [52], parameterize certain parts of the Hamiltonian using empirical data [48].

The actual implementation of these methods in computational chemistry software packages allows researchers to tackle a wide range of chemical problems, from the prediction of molecular properties to the simulation of complex reactions [44].

2.3.2 Basis sets and functionals

Functionals are at the heart of DFT calculations and they determine how the electron density is used to calculate the energy of the system. The B3LYP [46,47] functional, a hybrid functional that includes both Becke's three-parameter exchange functional and the Lee-Yang-Parr correlation functional, is widely used due to its effective balance of computational efficiency and accuracy across a wide range of systems. This functional is widely used because it incorporates a portion of exact exchange energy, which often improves the accuracy of the calculations, especially for systems involving transition metals like iron. It has been particularly successful for main group elements but can sometimes struggle with transition metals due to the more complex d-orbital interactions [6,49].

For spin unrestricted calculations, the unrestricted form of B3LYP (UB3LYP) is used. UB3LYP [6,49] variant allows for different spatial orbitals for different spins, which is important for systems with unpaired electrons such as the Fe(III) complexes. This allows the spatial part of the spin-up and spin-down orbitals to be different, which is important for correctly describing systems with unpaired electrons. Other functionals like M06 [48], PBEh1PBE [53], and BP86 [46,54,55] offer different balances between accuracy and computational cost. M06 is a meta-GGA functional designed to improve the description of non-covalent interactions and transition states. PBEh1PBE is a hybrid version of the Perdew-Burke-Ernzerhof functional, aiming to improve performance on thermochemistry and kinetics. BP86 is a GGA functional combining Becke's exchange functional with Perdew's correlation functional, known for its robustness in predicting geometries [49].

Each functional offers a trade-off between computational demand and the type of chemical accuracy required for a particular study. The choice of functional can significantly affect the predicted properties of molecules, and the best choice often depends on the specific characteristics of the system under study.

Basis sets are a collection of functions used to describe the electron orbitals in a system. The 6-311G(d,p) [14] basis set is a triple- ζ basis set that includes polarization functions, helping to better describe the electron distribution within a molecule. It includes d-type orbitals on non-hydrogen atoms and p-type orbitals on hydrogen, allowing for more accurate modeling of the electronic

structure, especially in transition metal complexes where d-orbitals play a crucial role. This set is a good choice as it provides a good balance between accuracy in electronic distribution and computational cost [53]. When optimizing a molecule, it is good to test a variety of basis sets alongside different functionals to find the most suitable combination for the complexes in question. CEP-121G [56–58], aug-cc-pVDZ [59,60], cc-pVTZ [59–64], def2tzvpp [65], and SDD [66] are among the tested basis sets, each with different characteristics. For example, CEP-121G is a split-valence basis set that is computationally less demanding and can be used effectively for larger systems. Aug-cc-pVDZ and cc-pVTZ are part of the correlation-consistent polarized valence basis sets, which systematically improve accuracy by including more functions, particularly suited for correlated methods like DFT. Def2tzvpp is a triple- ζ valence basis set with polarization functions [65], and SDD is a Stuttgart/Dresden ECP basis set, which includes effective core potentials for heavier elements to reduce computational time [66].

The optimization of a molecule using various functionals (B3LYP, M06, PBEh1PBE, and BP86) and basis sets (CEP-121G, aug-cc-pVDZ, cc-pVTZ, def2tzvpp, and SDD) can yield different results with each combination of functional and basis set. The choice depends on the balance between computational demand and the level of accuracy required for the properties of interest [53].

2.3.3 Solvent models

The Polarizable Continuum Model (PCM) [67] is a widely used implicit solvent model in computational chemistry. It treats the solvent as a continuous medium with a uniform dielectric constant rather than simulating each solvent molecule explicitly. This approach significantly reduces computational effort while still accounting for the overall effect of the solvent on the solute. The integral equation formalism variant (IEFPCM) [49,68] is a sophisticated version of PCM that uses an integral equation to determine the polarization of the solvent. By using the dielectric constant of a solvent, IEFPCM captures the polarizing effect of this solvent on the solute, which is essential for systems where solvent-solute interactions play a significant role, such as in iron complexes. The inclusion of solvent effects through IEFPCM is crucial for a realistic description of the molecules in environments similar to experimental conditions. For instance, in DSSCs, the solvent can influence the charge transfer processes, which are critical for the device's performance [6,49].

Standard DFT functionals often lack the ability to accurately describe dispersion forces. Grimme's D3 dispersion correction [6,49,69] is an empirical addition to DFT calculations that improves the treatment of these forces. Inclusion of the D3 correction is particularly significant when modeling larger molecular systems or when dealing with interactions that involve non-covalent

contact, such as π - π stacking, hydrogen bonding, or van der Waals interactions. For systems with extensive non-covalent interactions, such as molecular assemblies or complexes used in DSSCs, neglecting dispersion forces can lead to inaccuracies in predicted geometries and energies.

Therefore, using both the IEFPCM [68] solvent model and Grimme's D3 correction in Gaussian 16 provides [70] a more comprehensive and accurate representation of the molecular system in question, especially when modeling the solvent effects of a solvent and the dispersion forces in large or complex molecular systems

2.3.4 DFT Electronic Descriptors

DFT calculations are widely used to predict various electronic properties of molecules. Some of these properties ionization potential, electron affinity [71,72], Mulliken electronegativity [73,74] global electrophilicity index [75], electronic chemical potential [76], chemical hardness [77,78], molecular electrostatic potential and charges [79,80] and absolute redox potentials [81]. Here, we will discuss these properties and provide the relevant formulas.

Ionization Potential (IP): is the energy required to remove an electron from a neutral isolated atom or molecule, resulting in a cation.

Electron Affinity (EA): is the energy change accompanying the addition of an electron to a neutral isolated atom or molecule, resulting in an anion. According to Koopman's theorem, the EA and IP of a system can be approximated by the frontier orbital energies [71,72]:

$$\text{IP} = -E_{\text{HOMO}} \text{ and } \text{EA} = -E_{\text{LUMO}}$$

where E_{HOMO} represents the energy of the highest occupied molecular orbital and E_{LUMO} represents the energy of the lowest unoccupied molecular orbital.

Mulliken Electronegativity (χ): is a measure of the tendency of an atom to attract electrons. It can be calculated using the formula [73] [74]:

$$\chi = \frac{(\text{IP} + \text{EA})}{2}$$

Global Electrophilicity Index (ω): is a descriptor of the reactivity of a molecule, indicating its ability to accept electrons. Defined by Parr and co-workers as the electrophilic power of atoms and molecules [75], it can be calculated using the formula:

$$\omega = \frac{\mu^2}{(2\eta)}$$

where $\mu = -(\text{IP} + \text{EA})/2$ is the electronic chemical potential (the same as $-\chi$) [76]. The electronic chemical potential (μ) is a measure of the reactivity and stability of a molecule. Furthermore, $\eta = (\text{IP} - \text{EA})$ [77,78] represents the chemical hardness (η) of the ground state of atoms and molecules. The chemical hardness is a measure of the resistance of a molecule to alterations in its electron density caused by an external disturbance.

Molecular Electrostatic Potential (MESP): is a map of the electrostatic potential in the vicinity of a molecule, providing insights into its reactivity. MESP analysis are performed on optimized geometries, using the chelp (charges from electrostatic potential) keyword in Gaussian. The MESP, $V(r)$ at a point r is calculated using the standard equation,

$$V(r) = \sum_A^{N_A} \frac{Z_A}{|r - R_A|} - \int \frac{\rho(r') d^3r'}{|r - r'|}$$

where the summation runs over all the nuclei A in the compound. Z_A is the charge on the nucleus A at position R_A , $\rho(r')$ is the electron density and N_A is the total number of nuclei [79,80].

Absolute Redox Potentials: represent the tendency of a molecule to undergo reduction or oxidation. They can be calculated using specialized computational methods, often derived from thermodynamic cycles or experimental data. The absolute redox potential was calculated by application of the following formula:

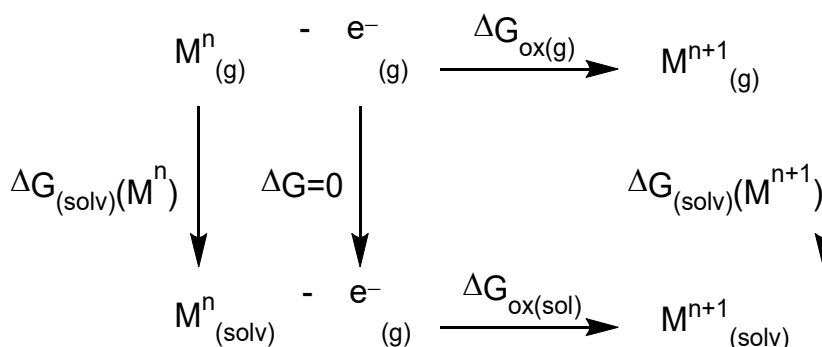
$$E_{\text{calc,abs.}} = \frac{-\Delta G_{\text{ox(sol)}}}{nF}$$

where F = Faraday constant and n = number of transferred electrons. The thermodynamic cycle shown in Scheme 9, similar to the thermodynamic cycle used to determine the absolute potential of the SHE [81] was used to acquire Gibbs free energy change in solution ($\Delta G_{\text{ox(sol)}}$) of a molecule M .

By subtracting the absolute reduction potential of ferrocene/ferrocenium (FcH/FcH^+) in the solvent from the absolute redox potential calculation ($E_{\text{calc,abs.}}$), the absolute redox potential can be converted to a relative redox potential versus (FcH/FcH^+), $E_{\text{calc. vs FcH/FcH}^+}$ as follows:

$$E_{\text{calc. vs FcH/FcH}^+} = \frac{-\Delta G_{\text{ox(sol)}}}{nF} - E_{\text{FcH/FcH}^+}$$

These properties, obtained through DFT calculations, offer valuable insights into the reactivity and stability of molecules, guiding their applications in various fields, including materials science, catalysis, and drug design.



Scheme 9: “Thermodynamic cycle to calculate absolute redox potential of a molecule M , using Gibbs free energy, $\Delta G_{\text{ox(sol)}} =$ change of free energy in solution, $\Delta G_{\text{ox(g)}} =$ free energy change in gas phase and $\Delta G_{\text{(solv)}} =$ solvation energy of gas phase species.”

2.3.5 Time-Dependent Density Functional Theory

Time-Dependent DFT is an extension of the ground-state DFT that enables the calculation of excited-state properties of molecules and materials. TDDFT has become a widely used theoretical framework in the study of various properties and processes, including those relevant to the application of DSSCs. In the context of the application to DSSCs, TDDFT calculations are crucial for understanding the optical properties and electronic transitions involved in the operation of DSSCs. From TDDFT calculations, several key properties are derived to assess the performance and efficiency of the dyes within DSSCs [1,4,6,7,46–48]:

Absorption Spectra: TDDFT can predict the absorption spectra of dye molecules used in DSSCs, providing insights into the wavelengths (λ) at which these dyes can efficiently harvest solar energy. Understanding the absorption spectra is essential for optimizing the design and performance of DSSCs [4].

Excited-State Energies: TDDFT allows for the determination of excited-state energies, which are crucial for understanding the electron transfer processes that occur upon absorption of light in DSSCs. This information is valuable for the development of efficient light-harvesting materials [16,82].

Excited State Lifetime (τ) of dyes: reflects the stability of the excited state and can be evaluated as [82]:

$$\tau \text{ (in secs)} = 1.499 / (fE_{\lambda}^2),$$

The equation takes into account the calculated transition energy (E_{λ} , in cm^{-1}) and the oscillator strength (f) of the excited state corresponding to the specific wavelength (λ). The longer the excited state lifetime, the greater the probability of charge injection and reduced recombination, leading to improved DSSC efficiency.

Light Harvesting Efficiency (LHE): The light harvesting efficiency, as expressed [82,83]:

$$\text{LHE} = 1 - 10^{-f}$$

LHE is determined from the oscillator strength (f) of the absorption bands. It provides an understanding of the dye's ability to efficiently capture incident photons for the generation of charge carriers. A higher LHE value suggests a more effective light-harvesting capability of the dye in the DSSC system.

Charge Transfer Dynamics: TDDFT can provide information about the dynamics of charge transfer processes, such as electron injection and regeneration, which are central to the functioning of DSSCs. Understanding these processes is essential for improving the overall efficiency and stability of DSSCs [4].

Injection and Regeneration Driving Forces (ΔG_{inject} and $\Delta G_{\text{regenerate}}$): The injection driving force (ΔG_{inject}) and the regeneration driving force ($\Delta G_{\text{regenerate}}$) of a dye are calculated based on its oxidation potential, as described [6,14]:

$$\Delta G_{\text{inject}} = E_{\text{dye}}^* - E_{\text{CB}} = E_{\text{dye}} - E_{\lambda} - E_{\text{CB}}$$

$$\Delta G_{\text{regenerate}} = (E_{\text{I}^-/\text{I}_3^-}) - (E_{\text{dye}})$$

ΔG_{inject} is determined by the disparity in energy between the dye's oxidation potential (E_{dye} , approximated by the energy of the highest occupied molecular orbital) and the reduction potential

(E_{CB}) of the conduction band edge of TiO_2 (-4.0 eV vs. vacuum or -0.5 eV vs. NHE [8,84]). E_λ represents the vertical transition energy associated with the wavelength λ .

On the other hand, $\Delta G_{regenerate}$ accounts for the redox potential difference between the dye (E_{dye}) and the redox potential (E_{I^-/I_3^-}) of the electrolyte I^-/I_3^- redox couple (-4.8 eV vs vacuum or 0.3 eV vs NHE) [85]. These parameters are essential for assessing the efficiency of charge injection and regeneration processes, which are critical steps in the operation of DSSCs.

Electron-Hole Binding Energies (E_h): TDDFT enables the calculation of electron-hole binding energies, which are important for evaluating the stability and recombination properties of photoexcited states in DSSCs. Optimizing the electron-hole binding energies is crucial for enhancing the charge separation and collection efficiency in DSSCs. The electron-hole binding energy (E_h) in the context of TDDFT can be computed using the equation [46–48]:

$$E_h = E_{excited} - (E_{HOMO} + E_{LUMO})$$

Where E_h is the electron-hole binding energy, $E_{excited}$ is the energy of the excited state.

Photoinduced Electron Transfer Rates (PET): TDDFT calculations can predict the rates of photoinduced electron transfer between the dye and semiconductor components in DSSCs. Understanding these rates helps in the design of efficient DSSC architectures and materials with improved charge transport properties [16,86]. Marcus Theory is often used in combination with TDDFT to predict electron transfer rates. The theory provides a widely accepted formula for calculating PET rates, which is often referenced in the context of DSSCs and other photochemical processes. Here's the Marcus formula for the rate of electron transfer (k_{ET}):

$$k_{ET} = \frac{2\pi}{\hbar} |V_{DA}|^2 \frac{1}{\sqrt{4\pi\lambda k_B T}} \exp\left(-\frac{(\Delta G^0 + \lambda)^2}{4\lambda k_B T}\right)$$

Here, k_{ET} is the rate of electron transfer, $\hbar$ is the reduced Planck constant, V_{DA} is the electronic coupling between donor and acceptor, λ is the reorganization energy, k_B is the Boltzmann constant, T is the temperature, and ΔG^0 is the free energy change for the reaction.

By providing insights into these properties, TDDFT plays a crucial role in the rational design and optimization of dye molecules, sensitizers, and semiconductor materials for enhancing the efficiency and performance of DSSCs. It enables researchers to make informed decisions in the development of sustainable and cost-effective solar energy conversion technologies.

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Chapter 3: Results and Discussion

Chapter 3: published article 1:

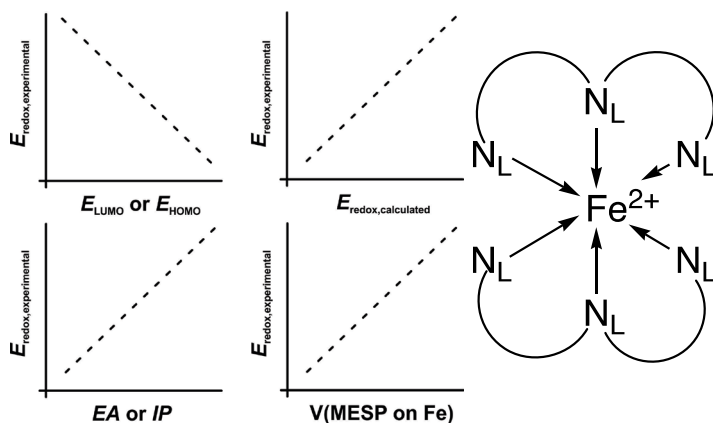
E. Athanasopoulos, J. Conradie, Substituent effect on the oxidation and reduction of electronically altered iron(II)-terpyridine derivatives – DFT study, *Inorganica Chim. Acta*. 555 (2023) 121599.
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Appendix A:

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Supporting information associated with article *Inorganica Chimica Acta*, 555, 121599: Figures S1-S2 and Tables S1 – S10. Optimized coordinates of the DFT calculations as xyz files (also available online at: <https://doi.org/10.1016/J.ICA.2023.121599>).

TOC



Keywords

iron (II); terpyridine; DFT; redox; experimental-theoretical relationships

Research highlights

- DFT study of electronically altered iron(II)-terpyridine derivatives
- Correlations between experimental redox and theoretically computed energies
- Visualization of the oxidation and reduction center of the iron(II)-terpyridine derivative
- Similar behavior of iron(II)-terpyridine and iron(II)-tris-azinyl derivatives

- Iron (II)-terpyridine and iron (II)-tris-azinyl follow same “redox-DFT reaction descriptor” relationships

Abstract

Structure, reactivity, and redox properties play an important role in many biological processes. The structures of two types of series of related iron(II) compounds, namely iron(II)-terpyridine and iron(II)-tris-azinyl derivatives, were optimized in the gaseous as well as solvated states by means of density functional theory (DFT). From the optimized geometries of the molecules, their frontier orbital energies ($E_{\text{LUMO}}/E_{\text{HOMO}}$), electronic chemical potential (μ), electrophilicity index, (ω), Merz-Kollman electric potential, Gibbs Free energy, Mulliken and Natural Bond Orbital charges were determined. The DFT calculated reactivity parameters were related to the experimentally reported iron-based oxidation and ligand-based reduction potential of the series of iron(II)-terpyridine and tris-azinyl derivatives. Results obtained show that the relationship between the experimental and DFT calculated Fe(II/III) redox potential gave the most accurate relationship ($R^2 = 0.97$), though a systematic error, depending on the choice of the reference system, was obtained. Relationships between the experimental iron-based oxidation ($E_{\text{Fe(II/III)}}$) or ligand-based reduction (E_{Ligand}) of the iron(II) complexes, and solvent phase calculated HOMO and LUMO energies respectively ($R^2 = 0.96$ and 0.95 respectively), lead to more accurate relationships with higher R^2 values than the relationships involving the gas phase calculations ($R^2 = 0.87$ and 0.88 respectively). More relationships, that can be used to predict the oxidation and reduction of related iron(II) derivatives containing two substituted terpyridine or tris-azinyl analogues of the terpyridine ligand, were obtained to a high accuracy.

1 Introduction

2,2':6',2''-Terpyridine (tpy) is a tridentate ligand that comprises three N-heteroaromatic ring coordination sites, making it an important family of aromatic heterocyclic compounds [1]. The ligand was first isolated by Morgan and Burstall in 1937 [2]. The general structure, including the conventional ligand numbering, may be viewed in Figure 1 (a). The electrochemical and optical characteristics exhibited by tpy ligands and their derivatives have captivated scientists, especially in the field of coordination chemistry. Spin-crossover [2] and fluorescence [3–5] are particularly important applications acquired by the terpyridine complexes. The variety of substituents that tpy derivatives can bear, and the ease at which they are synthesized [6,7], allows for its binding sites to be incorporated into various types of nano-chemical and molecular devices [4,5,8–12], redox catalysis [13–16], dendrimers [9,17] and metal-containing polymers [8,9]. Also, complexes containing tris-azine terpyridine analogs have shown significance in photochemical devices and supramolecular chemistry [6,7]. All of which inspires continuous research in the photophysical [11,12,18,19] spin

state [13,20], reversible reduction and oxidation [13–20], as well as metal-to-ligand charge transfer properties of various types of tpy derivatives [6,7].

The group of Wieghardt [21] did a thorough study on the electronic structures of electron transfer complex $[\text{Fe}(\text{tpy})_2]^n$ for $n = 1-, 0, 1+, 2+, 3+$, using the field of computational chemistry, using density functional theory (DFT) calculations. Gros and co-workers [22] reported on the experimental photophysical and photovoltaic properties of bis(2,2':6',2''-terpyridine carboxylic acid) iron(II) (complex $[\text{Fe}(\text{L}^{11})_2]^{2+}$ in Table 1) and two related homoleptic iron complexes bearing tridentate bis-carbene ligands for application as dye sensitizers in dye-sensitized solar cells (DSSCs). A time-dependent DFT study complemented the experimental work [22]. Mughal et al. [1] reported on the effect of different substituents on the physicochemical properties and anti-microbial potential of a series of tpy-metal(II) complexes, including some iron(II) complexes. A DFT and TDDFT study on two iron complexes containing unsymmetrically substituted tpy ligands complemented the experimental findings [1]. Recently, an experimental electrochemical study on a series of bis(tpy)metal(II) complexes containing substituted derivatives of tpy revealed a strong correlation between the redox potential of the complexes and the Hammett parameter of the tpy substituents for metal = Mn, Fe, Co, Ni, and Zn [23]. In addition, a DFT study on a simple model system of substituted pyridine models revealed a strong correlation between the Hammett parameters and the lowest unoccupied molecular orbital (LUMO) energies of the corresponding substituted pyridine models [23], suggesting an inexpensive predictive tool when coupled with the electrochemical data.

In this study, for the first time, DFT calculated energies will be compared to the experimental redox potentials for a series of 25 $[\text{Fe}(\text{tpy})_2]^n$ complexes ($n = 3 - 1$ and tpy = a series of differently symmetrically substituted terpyridine and tris-azinyl ligands as given in Table 1). The DFT calculated energies include Ionization Potential, Electron Affinity, Mulliken Electronegativity [24,25], Global Electrophilicity Index [26], Electronic Chemical Potential [27], Chemical Hardness [28,29], Molecular Electrostatic Potential and Charges [30] and Absolute Redox Potentials.

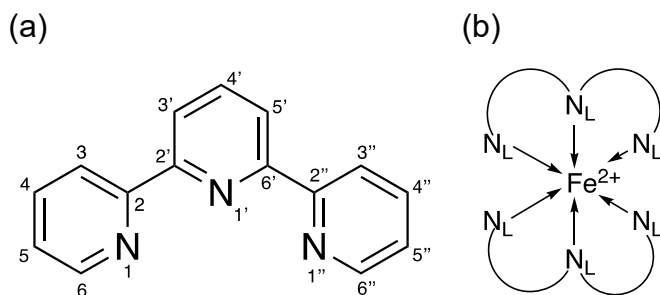


Figure 1: (a) General structure of 2,2':6',2''-Terpyridine framework. (b) $[\text{Fe}(\text{L})_2]^{2+}$ complex where L = various 4,4',4''-substituted substituted (R-groups) terpyridine and tris-azinyl derivates of terpyridine as ligands, see Table 1.

Due to the ligands' strong chelating tendency, it is commonly comprehended for two terpyridine ligands (bis-terpyridine) to coordinate with transition metals, e.g. $[\text{Fe}(\text{R-tpy})_2]^{2+}$ [6,7], $[\text{Co}(\text{R-tpy})_2]^{2+}$ [23,31–33] and $[\text{Cu}(\text{R-tpy})_2]^{2+}$ [34], forming $[\text{M}(\text{R-tpy})_2]^{n+}$ type complexes. The metal center associates with bis-terpyridine at three meridional sites and the achiral Fe(II) complex will serve as the base structure for the various 4'-substituted (R-groups) terpyridine ($\text{L}^1 - \text{L}^8$, $\text{L}^{10} - \text{L}^{12}$, L^{14} , L^{21} , L^{25}), 4,4',4''-substituted (R-groups) terpyridine (L^{20} , L^{22} , L^{23}), tris-azinyl derivatives of terpyridine (L^9 , L^{13} , L^{15} - L^{19}) and related (L^{24}) complexes, illustrated in Figure 1 (b) and Table 1.

In literature [7], the influence of a single electron donating or withdrawing substituent in the 4'-position of terpyridine on the Fe(III/II) redox couple was investigated by means of cyclic voltammetry. Substitution at the 4'-position of terpyridine allows for a wide range of substituents having different electron donating or withdrawing properties and hence various inductive influences. The voltametric behaviour of a series of Fe(II) complexes containing tris-azine terpyridine analogs showed that the Fe(III/II) redox couple becomes more positive as the nitrogen content of the ligands increases [6].

Mughal et al. [1] used docking analyses to analyze the binding affinity of terpyridine-based ligands with shikimate dehydrogenase and penicillin-binding sites to assess the anti-microbial potential of ligands and complexes, which showed moderate to good binding affinity overall. Their established study on a structure-activity relationship (SAR) between biological and spectrophotometric properties of terpyridine-transition metal complexes showed that the antibacterial activity of the initial metal complex was enhanced due to electron-withdrawing substituents on the ligand, whereas the opposite is true for electron-donating substituents. The strong anti-microbial activity exhibited by the terpyridine moiety serves as a useful benchmark for developing more powerful anti-microbial drugs.

Table 1: The twenty-five [Fe(L)₂]²⁺ complexes (L = L¹-L²⁵, general structure in Figure 1 (b)) of this study. Ligand name and structure are indicated.

4'-(pyrrolidin-1-yl)-2,2':6',2''-terpyridine L¹	N,N-dimethyl-[2,2':6',2''-terpyridin]-4'-amine L²	4'-(n-butylamine)-2,2':6',2''-terpyridine L³
4'-(hydroxy)-2,2':6',2''-terpyridine L⁴	4'-(methoxy)-2,2':6',2''-terpyridine L⁵	4'-(p-tolyl)-2,2':6',2''-terpyridine L⁶
4'-vinyl-2,2':6',2''-terpyridine L⁷	2,2':6',2''-terpyridine L⁸	2,6-di(pyrimidin-2-yl) pyridin-4-ol L⁹
4'-(chloro)-2,2':6',2''-terpyridine L¹⁰	2,2':6',2''-terpyridine-4'-carboxylic acid L¹¹	4'-(methylsulfinyl)-2,2':6',2''-terpyridine L¹²
2,6-di(pyrazinyl)pyridin-4-ol L¹³	4'-(methylsulfonyl)-2,2':6',2''-terpyridine L¹⁴	2,6-di(pyrid-2-yl) pyrazine L¹⁵
2,6-di(pyrimidin-4-yl) pyridine L¹⁶	2,6-di(pyrazinyl) pyridine L¹⁷	2,6-di(1,2,4-triazin-3-yl) pyridine L¹⁸
2,2':6',2''-terpyrazine L¹⁹	4,4',4''-tri-tert-butyl-2,2':6',2''-terpyridine L²⁰	4'-(4-chlorophenyl)-2,2':6',2''-terpyridine L²¹
4,4',4''-trimethoxy-2,2':6',2''-terpyridine L²²	N4, N4',N4''-tris(diethylamino)-2,2':6',2''-terpyridine L²³	2,6-di(pyrazol-1-yl) pyridine L²⁴
	4'-(4-methoxyphenyl)-2,2':6',2''-terpyridine L²⁵	

The focus of this work is to determine the electronic influence of mainly two types of series of related iron(II) compounds, containing different symmetrically substituted terpyridine and tris-azanyl ligands (L), on the iron metal it is coordinated to, in order to obtain relationships between theoretical calculations and experimental values. The data obtained can be used to build up a database utilizing quantum computational data that can be used to forecast the electronic behaviour of new octahedral Fe(II)(L)₂ complexes. The Fe(II) complexes investigated here are all diamagnetic, low spin (S=0). The tpy ligand stabilizes metals in lower oxidation states as these ligands are pi-acceptors, giving rise to the low-spin electronic configuration of the metallic compound [6,7].

2 Experimental

2.1 Synthesis and electrochemistry

Bis(2,2':6',2''-terpyridine)iron(II) perchlorate, [Fe(L⁸)₂](ClO₄)₂, was synthesized and characterized as described in the literature [35,36]. The cyclic voltammograms were conducted in acetonitrile on a BAS 100B/W electrochemical analyzer under conditions as previously described [36] and reported versus the redox couple of iron(II) in ferrocene (FcH/FcH⁺).

2.2 Computational methods

Density functional theory (DFT) calculations were performed on the Fe(II) (Q = 2) and the oxidized Fe(III) (Q = 3), and the reduced (Q = 1) molecules. The B3LYP functional (and UB3LYP for spin unrestricted calculations) as implemented in the Gaussian 16 package [37], with the triple- ζ basis set 6-311G(d, p) was used. Spin S = 0 for Fe(II) and spin S = ½ for Fe(III) and the reduced molecules. All calculations were successfully executed in both the gas phase as well as in the solvent acetonitrile (CH₃CN). The default solvent model IEFPCM in Gaussian was used to perform calculations in CH₃CN (dielectric constant = 36.64). A frequency analysis was done on all compounds to confirm that the optimized structures did not exhibit any imaginary frequencies, thus, are real minimum energy structures.

The adiabatic ionization potential (IP) and adiabatic electron affinity (EA) of a molecule Mⁿ of charge n, [Fe(L)₂]²⁺ with n = 2 here, is defined as:

$$\text{IP}(\text{M}^n) = E(\text{M}^n) - E(\text{M}^{n+1}) \quad \text{Equation 1}$$

$$\text{EA}(\text{M}^n) = E(\text{M}^{n-1}) - E(\text{M}^n) \quad \text{Equation 2}$$

According to Koopman's theorem, the EA and IP of a system can be approximated by the frontier orbital energies [38,39]:

$$\text{IP} = -E_{\text{HOMO}} \text{ and } \text{EA} = -E_{\text{LUMO}} \quad \text{Equation 3}$$

The Mulliken electronegativity (χ) was calculated by application of the following formula [24,25]:

$$\chi = (\text{IP} + \text{EA})/2 \quad \text{Equation 4}$$

The global electrophilicity index (ω), defined by Parr and co-workers as the electrophilic power of atoms and molecules [26], was calculated by application of the following formula:

$$\omega = \mu^2 / (2 \eta) \quad \text{Equation 5}$$

where $\mu = -(\text{IP} + \text{EA})/2$ is the electronic chemical potential (the same as $-\chi$) [27], and $\eta = (\text{IP} - \text{EA})$ [28,29] is the chemical hardness of the ground state of atoms and molecules.

The Molecular Electrostatic Potential, MESP, analysis were performed on the optimized B3LYP geometries, using the chelp (charges from electrostatic potential) keyword in Gaussian. The MESP, $V(r)$ at a point r is calculated using the standard equation,

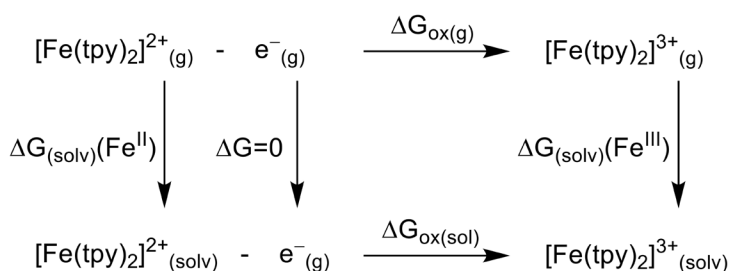
$$V(r) = \sum_A^{N_A} \frac{Z_A}{|r-R_A|} - \int \frac{\rho(r') d^3 r'}{|r-r'|} \quad \text{Equation 6}$$

where the summation runs over all the nuclei A in the compound. Z_A is the charge on the nucleus A at position R_A , $\rho(r')$ is the electron density and N_A is the total number of nuclei [30,40].

The absolute redox potential was calculated by application of the following formula:

$$E_{\text{calc,abs.}} = \frac{-\Delta G_{\text{ox(sol)}}}{nF} \quad \text{Equation 7}$$

where F = Faraday constant and n = number of transferred electrons. The thermodynamic cycle shown in Scheme 1, similar to the thermodynamic cycle used to determine the absolute potential of the SHE [41], was used to acquire Gibbs free energy change in solution ($\Delta G_{\text{ox(sol)}}$).



Scheme 1: Thermodynamic cycle used in this study to calculate absolute redox potential, using Gibbs free energy, $\Delta G_{\text{ox(sol)}}$ = change of free energy in solution, $\Delta G_{\text{ox(g)}}$ = free energy change in gas phase and $\Delta G_{\text{(solv)}}$ = solvation energy of gas phase species.

By subtracting the absolute reduction potential of ferrocene/ferrocenium (FcH/FcH^+) in CH_3CN from the application of Equation 7 for absolute redox potential ($E_{\text{calc,abs.}}$), the absolute redox potential was converted to a relative redox potential versus (FcH/FcH^+), $E_{\text{calc. vs FcH/FcH}^+}$ as follows:

$$E_{\text{calc. vs FcH/FcH}^+} = \frac{-\Delta G_{\text{ox(sol)}}}{nF} - E_{\text{FcH/FcH}^+} \quad \text{Equation 8}$$

3 Results and Discussion

3.1 Geometry and electronic structure

The geometry of the $[\text{Fe}(\text{L}^n)_2]^{m+}$ ($m = 1 - 3$, $n = 1 - 25$, L^n shown in Table 1) complexes is constrained octahedral [42] due to the strain of the tridentate ligands L^n . The $[\text{Fe}(\text{L}^n)_2]^{2+}$ molecule is diamagnetic [36], while the oxidized ($m = 3$) and reduced ($m = 1$) molecules are paramagnetic doublets [21]. The highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO, respectively) of a molecule, are the MOs of favourable energy where an electron is removed or added upon oxidation or reduction. The HOMO and LUMO of $[\text{Fe}(\text{L}^8)_2]^{m+}$ ($m = 2$), Figure S2 in the supporting information, shows the locus of the oxidation (on iron) and reduction (on the terpyridine ligand). The locus of the unpaired electron on the molecule because of oxidation or reduction is visualized by the spin density plots of the oxidized ($m = 3$) and reduced ($m = 1$) molecules in Figure 2, confirming iron-based oxidation and ligand-based reduction. Although the LUMO of $[\text{Fe}(\text{L}^8)_2]^{2+}$ is on both ligands, the first reduction occurs on one ligand, as can be seen by the spin plot of the reduced $[\text{Fe}(\text{L}^8)_2]^{1+}$ in Figure 2. The reduced ($m = 1$) molecule thus has a d^6 iron(II) centre, one neutral ligand, and one radical ligand. Thus upon reduction of $[\text{Fe}(\text{L}^8)_2]^{2+}$, an electron is first added to the one ligand (first reduction, α electron in LUMO of $m = 2$), and then another electron is added to the other ligand (second reduction, addition of another α electron to obtain the paramagnetic doubly reduced molecule), see Figure S2 in the supporting information. The spin density plot of the doubly reduced molecule ($m = 0$) shows the locus of the two added electrons on the two ligands, Figure 2.

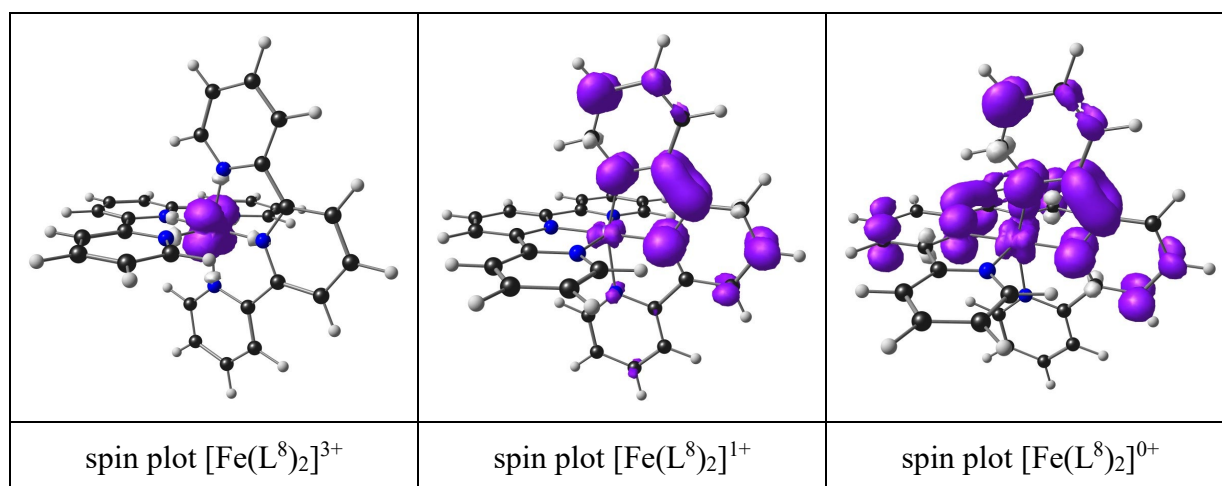


Figure 2: Selected spin plots of $[\text{Fe}(\text{L}^8)_2]^{m+}$ ($\text{L}^8 = \text{tpy}$, $m = 0, 1, 3$).

3.2 Cyclic voltammetry

The electrochemical behaviour of iron(II)-terpyridine derivatives are well reported in the literature. Reported oxidation and reduction potentials from the literature of the series of related iron(II) compounds of the type $[\text{Fe}^{\text{II}}(\text{L})_2]^{2+}$, with L, a substituted terpyridine or tris-azinyl derivative as shown in Table 1, are summarized in Table 2. However, only a few cyclic voltammograms (CVs), at only 0.100 V s^{-1} , are provided in the literature for a couple of $[\text{Fe}^{\text{II}}(\text{L})_2]^{2+}$ complexes. This include $[\text{Fe}^{\text{II}}(\text{L}^4)_2]^{2+}$ ([6], oxidation only), $[\text{Fe}^{\text{II}}(\text{L}^6)_2]^{2+}$ [43], $[\text{Fe}^{\text{II}}(\text{L}^8)_2]^{2+}$ ([36], and [44] oxidation only), $[\text{Fe}^{\text{II}}(\text{L}^{11})_2]^{2+}$ ([22], oxidation and first reduction only), $[\text{Fe}^{\text{II}}(\text{L}^{16})_2]^{2+}$ [6], $[\text{Fe}^{\text{II}}(\text{L}^{19})_2]^{2+}$ [6], $[\text{Fe}^{\text{II}}(\text{L}^{24})_2]^{2+}$ ([44], oxidation only) and $[\text{Fe}^{\text{II}}(\text{L}^{25})_2]^{2+}$ [23]. The only CVs shown at different scan rates for the oxidation peak are for $[\text{Fe}^{\text{II}}(\text{L}^8)_2]^{2+}$ [45]. No CV or redox data could be found in the literature for the reduction of any $[\text{Fe}^{\text{II}}(\text{L})_2]^{2+}$ complex at a scan rate different from 0.100 V s^{-1} . It is important to evaluate CVs at scan rates over at least one order of magnitude to ensure the observed redox behaviour does not change at higher scan rates. Therefore, as an example of the typical electrochemical behaviour of the iron(II)-terpyridine derivatives at different scan rates and scan directions, the cyclic voltammogram of $[\text{Fe}(\text{L}^8)_2]^{2+}$ ($\text{L}^8 = \text{tpy}$) is shown in Figure 3, showing one oxidation and two reduction peaks at scan rates 0.100 and 1.024 V s^{-1} . The oxidation of the molecules is reported to be iron-based; thus, Fe(II/III) oxidation, giving $[\text{Fe}^{\text{III}}(\text{L})_2]^{3+}$ ([6,7,22,23,43,44,46]), in agreement with the character of the DFT calculated HOMO (Figure S2 in the supporting information). The Fe(II/III) redox couple, $E_{\text{Fe(II/III)}}$, is in most cases chemically and electrochemically reversible ([6,7,22,23,43,44,46]). The reduction of the iron(II) complexes, however, is reported to occur on the coordinated ligands ([6,7,22,23,43,44,46]). Thus, as predicted by DFT, the first one electron reduction leads to a complex containing an iron(II) centre, one neutral ligand, and one ligand radical: $[\text{Fe}^{\text{II}}(\text{L})(\text{L}^{\cdot})]^{1+}$. The notation $E_{\text{Fe(II/III)}}$ and E_{Ligand} will be used to indicate the iron-based oxidation and the ligand-based reduction potentials, respectively. Reported $E_{\text{Fe(II/III)}}$ and E_{Ligand} values from different laboratories are generally in good agreement, see Table 2.

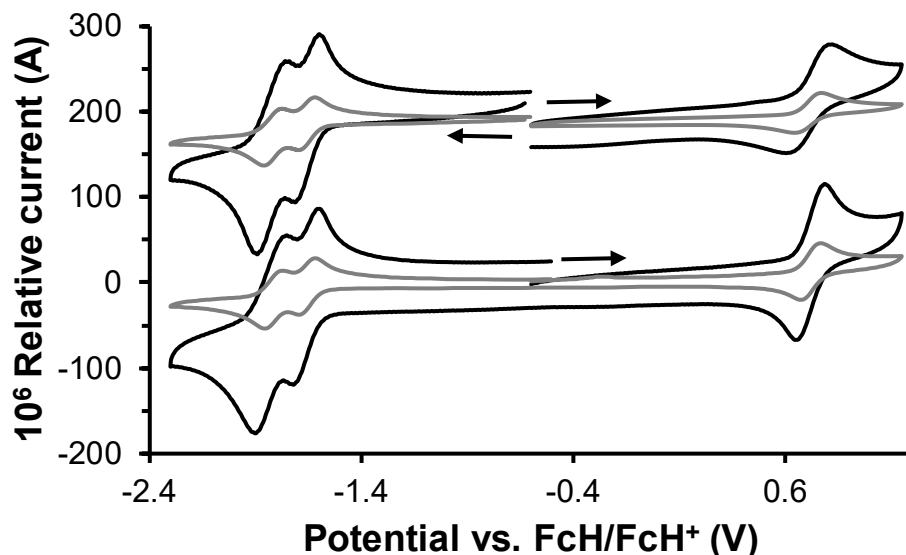


Figure 3: CV of a 0.002 mol dm⁻³ solution of [Fe(L⁸)₂](ClO₄)₂ in acetonitrile with 0.1 mol dm⁻³ with tetra-*n*-butylammonium hexafluorophosphate as supporting electrolyte, a glassy carbon-working electrode at a scan rate of 0.100 (grey) and 1.024 (black) V s⁻¹ at 25°C. The arrows indicate the initial scan direction.

Table 2: The iron-based oxidation and ligand-based first reduction potentials, E_{Fe(II/III)} (expt.) (V) and E_{Ligand} vs FcH/FcH⁺ (expt.) (V) of the [Fe(L)₂]²⁺ (L = L¹-L²⁵) compounds in acetonitrile as solvent, from ref [6,7,22,23,43,44,46]. Values reported vs SSCE are converted to potentials vs FcH/FcH⁺, using a conversion constant of 0.384 V reported in the literature [47]. The potential values in bold were used in this study.

Nr	Complex	E _{Fe(II/III)} vs SSCE	E _{Fe(II/III)} vs FcH/FcH ⁺	E _{Ligand} vs FcH/FcH ⁺	Reference
1	[Fe(tpy-NC ₄ H ₈) ₂] ²⁺	0.69	0.31		[7]
1	[Fe(tpy-NC ₄ H ₈) ₂] ²⁺		0.26	-1.91	[43]
2	[Fe(tpy-N(CH ₃) ₂) ₂] ²⁺		0.28	-1.90	[43]
3	[Fe(tpy-NH(CH ₃ (CH ₂) ₃) ₂)] ²⁺	0.69	0.31		[7]
4	[Fe(tpy-OH) ₂] ²⁺	0.95	0.57		[7]
4	[Fe(tpy-OH) ₂] ²⁺		0.54	-1.76 ^a	[6]
4	[Fe(tpy-OH) ₂] ²⁺		0.55	-1.78 ^b	[43]
5	[Fe(tpy-OMe) ₂] ²⁺	0.98	0.60		[7]
6	[Fe(tpy-4-CH ₃ -C ₆ H ₄) ₂] ²⁺	1.08	0.70		[7]
6	[Fe(tpy-4-CH ₃ -C ₆ H ₄) ₂] ²⁺		0.68	-1.63	[43]
7	[Fe(tpy-vinyl) ₂] ²⁺	1.08	0.70		[46]
8	[Fe(tpy) ₂] ²⁺	1.13	0.75		[7]
8	[Fe(tpy) ₂] ²⁺		0.71	-1.66	[6]
8	[Fe(tpy) ₂] ²⁺		0.72	-1.64	[43]
8	[Fe(tpy) ₂] ²⁺	1.13	0.75		[13]
8	[Fe(tpy) ₂] ²⁺	1.11	0.73		[44]
8	[Fe(tpy) ₂] ²⁺		0.72	-1.69	[36]
8	[Fe(tpy) ₂] ²⁺		0.71	-1.64	[21]
8	[Fe(tpy) ₂] ²⁺		0.72	-1.69	this study
9	[Fe(tpy-L7) ₂] ²⁺		0.75	-1.37 ^a	[6]
10	[Fe(tpy-Cl) ₂] ²⁺	1.19	0.81		[7]

10	[Fe(tpy-Cl) ₂] ²⁺		0.77	-1.54	[43]
11	[Fe(tpy-COOH) ₂] ²⁺		0.82	-1.44	[22]
12	[Fe(tpy-CH ₃ SO) ₂] ²⁺	1.21	0.83		[7]
13	[Fe(tpy-L6) ₂] ²⁺		0.90	-1.09 ^a	[6]
14	[Fe(tpy-CH ₃ SO ₂) ₂] ²⁺	1.30	0.92		[7]
15	[Fe(tpy-L1) ₂] ²⁺		0.95	-1.30	[6]
16	[Fe(tpy-L4) ₂] ²⁺		0.98	-1.25	[6]
17	[Fe(tpy-L2) ₂] ²⁺		1.07	-1.25	[6]
18	[Fe(tpy-L5) ₂] ²⁺		1.20	-1.10 ^a	[6]
19	[Fe(tpy-L3) ₂] ²⁺		1.36	-0.98	[6]
20	[Fe(tpy-tri-tert-Butyl) ₂] ²⁺				
21	[Fe(tpy-chlorophenyl) ₂] ²⁺				
22	[Fe(tri-OMe-tpy) ₂] ²⁺	0.77	0.39		[13]
23	[Fe(tri-Et ₂ N-tpy) ₂] ²⁺	0.12	-0.26		[13]
24	[Fe(1-bpp) ₂] ²⁺	1.30 ^c	0.92		[44]
25	[Fe(tpy-methoxyphenyl) ₂] ²⁺		0.67	-1.65	[23]

a Irreversible process, E_{pc} given.

b Irreversible process, estimated value.

c Irreversible process, E_{pa} given.

3.3 Redox potential relationships

DFT calculations were carried out on the [Fe(L)₂]¹⁺, [Fe(L)₂]²⁺, and [Fe(L)₂]³⁺ complexes containing ligands L¹-L²⁵, with the structures shown in Table 1. The obtained optimized geometry provided electronic and other energies, which were used in correlations with experimentally obtained redox potentials from the literature [6,7,22,23,43,44,46], given in Table 2.

The coordination of substituted ligands (L¹-L²⁵) on the 4'-position of terpyridine and triz-azine analogues of terpyridine to Fe(II) produces various electronic influences. The electron-withdrawing and/or donating properties of the R-groups on the L¹-L²⁵ will influence the electron density of the metal via conjugations. Electron-donating groups will subsequently allow more effortless oxidation and/or reduction of the molecule. The order of electronegativity of the substituent groups on L¹-L⁸, L¹⁰-L¹², L¹⁴, and L²⁰-L²⁵ from least to most electron-withdrawing are as follows, according to reported Hammett para substituents constants (σ_p) [7,48]:

(most electron donation): -tri-NEt₂ (-2.16) < -NC₄H₈ and -N(CH₃)₂ (-0.83) < -tri-OMe (-0.81) < -tri-tert-Butyl (-0.60) < -NHC₄H₉ (-0.51) < -OH (-0.37) < -OCH₃ (-0.27) < -4-CH₃-C₆H₄ (-0.05) < -Vinyl (-0.04) < -H (0) < -4-Cl-C₆H₄ (0.12) < -Cl (0.23) < -COOH (0.45) < -SOCH₃ (0.49) < -SO₂CH₃ (0.68) (least electron donation).

Thus, the order of ease of oxidation of the ligand containing iron(II) complexes, from complexes containing most to least electron-donating ligands, should follow the same order as above. The sum of the *para* Hammett parameter on one *tpy* ligand on the iron(II) complexes (containing ligands $L = L^1 - L^8, L^{10} - L^{12}, L^{14}, L^{22}, L^{23}, L^{25}$) displays a good correlation between the redox potentials $E_{Fe(II/III)}$ oxidation (Figure 4a), as well as with the reduction potential E_{Ligand} (Figure 4b). The sum of the *para* Hammett parameter on the free uncoordinated *tpy*-ligands also gave a good relationship with the experimental irreversible reduction potential of the free uncoordinated *tpy*-ligand [49].

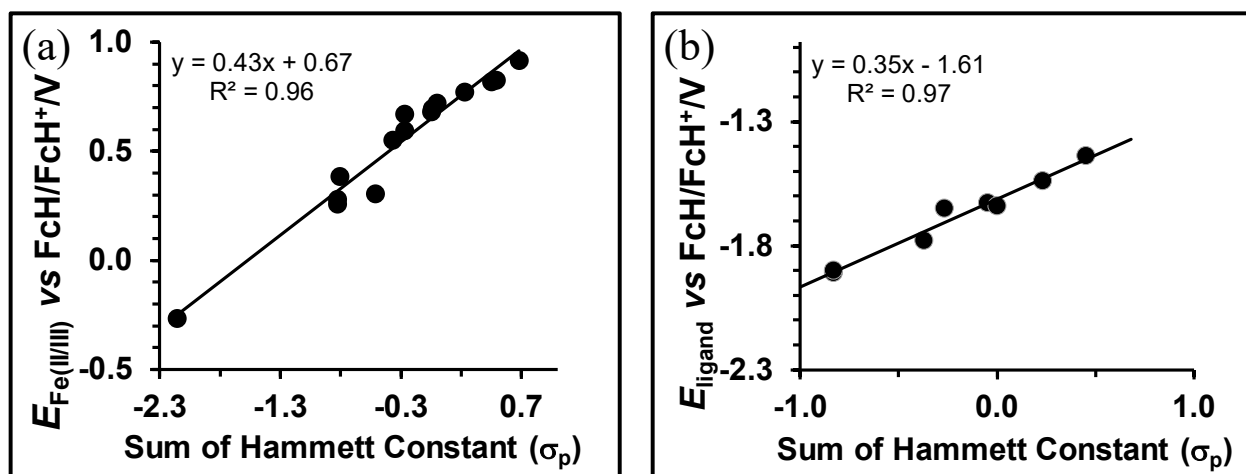


Figure 4: Linear correlation graph between the sum of the Hammett constants and (a) the iron-based oxidation $E_{Fe(II/III)}$ vs FcH/FcH^+ (expt.) (V) and (b) the ligand based reduction of the iron(II) complexes containing ligands $L^1 - L^8, L^{10} - L^{12}, L^{14}, L^{22}, L^{23}$ and L^{25} , for which experimental data were available. Redox data from Table 2. No Hammett values available for $L^9, L^{13}, L^{15} - L^{19}, L^{24}$.

The optimization of a $[Fe(L)_2]^{2+}$ complex allows for the energy of the frontier orbital (HOMO for oxidation and LUMO for reduction) of the $[Fe(L)_2]^{2+}$ complex to be determined [39]. The DFT calculated gas phase data for different $[Fe(L)_2]^{2+}$ structures are summarized in Table S1 in the supporting information. The good relationships obtained between the oxidation $E_{Fe(II/III)}$ (respective reduction E_{Ligand}) potential and the gas phase calculated energy of the HOMO (respective LUMO) of the $[Fe(L)_2]^{2+}$ complexes are shown in Figure 5 (a) and (b). The good relationships obtained with R^2 up to 0.88 are thereby achieved through a large HOMO/LUMO energy and oxidation/reduction potential range (1.6 V for oxidation and 0.9 V for reduction).

The correlation between the iron-based oxidation $E_{Fe(II/III)}$ vs FcH/FcH^+ (expt.) (V) and calculated E_{HOMO} (DFT) (eV) for the oxidation of the $[Fe(L)_2]^{2+}$ complexes containing substituted ligands $L^1-L^{19}, L^{22}-L^{25}$, is $R^2 = 0.87$, see Figure 5 (a). The obtained linear equation ($y = -0.36x - 3.39$), was used to calculate $E_{Fe(II/III)}$ of $[Fe(L^{20})_2]^{2+}$ ($y = 0.43$) and $[Fe(L^{21})_2]^{2+}$ ($y = 0.53$) that could not be found in literature in acetonitrile as the solvent, see Table 3. During oxidation, the electron in the

HOMO is removed; therefore, linear trends are followed correlating to experimental oxidation potentials with the HOMO energies. The data point of $[\text{Fe}(\text{L}^{25})_2]^{2+}$, with the methoxyphenyl-containing ligand L^{25} , lies above the line. It is not uncommon for data of molecules containing ligands with alkoxy groups on the *ortho* and *para* positions of phenyl rings to deviate from “experimental redox – DFT calculated energies” relationships. This is because alkoxy groups on the *ortho* and *para* positions donate electron density to the phenyl ring through both induction and resonance (lone pair on oxygen) [50,51].

Due to the function of the LUMO in the reduction of the $[\text{Fe}(\text{L})_2]^{2+}$ complex, it is predicted that the energy of the LUMO (E_{LUMO}) (calc.) (eV) will correlate with the experimentally measured reduction potential, E_{Ligand} vs FcH/FcH^+ (expt.) (V), see Figure 5 (b). This is expected, as, during reduction, a lower LUMO energy can accept the addition of an electron with more ease, thereby leading to a more positive reduction potential. As expected, the correlations show an inversely proportional linear relationship, with $R^2 = 0.88$. The obtained linear equation ($y = -0.41x - 4.73$), was utilized to predict the values of $[\text{Fe}(\text{R-tpy})_2]^{2+}$ complex with ligands L^3 , L^5 , L^7 , L^{12} , L^{14} , and L^{20} - L^{24} (in acetonitrile as solvent), see Table 4. These experimentally measured values could not be found in the literature [6,7,22,23,43,44,46].

DFT calculations can also be used to analyze significant properties of a chemical structure such as an atom, ion, molecule, or radical [35]. These DFT properties are electronic chemical potential, μ , and electrophilicity index, ω . The electrophilicity index is the electrophilic power of a chemical class that is measured [35]. Good linear correlations are achieved between $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (expt.) (V) and the DFT calculated parameters such as electrophilicity index, ω , and electronic chemical potential, μ , see Figure 5 (c) and (d), respectively.

A MESP analysis of molecules can be used as a descriptor of chemical reactivity and stability [52,53] and to describe the total electronic effect of ligands (eeL) on the metal it is coordinated to. The calculated MESP potential of a metal is reported to be related to the metal-based redox potential of molecules [52,54–57]. The calculated Merz-Kollman electric potential on Fe, obtained from the MESP analysis of the gas phase $[\text{Fe}(\text{L})_2]^{2+}$ molecules, relates to the $E_{\text{Fe(II/III)}}$ with $R^2 = 0.93$, see Figure 5 (e). The calculated Merz-Kollman electric potential on Fe thus increases as the electron-withdrawing tendency of the substituents on the ligands increases, leading to a higher $E_{\text{Fe(II/III)}}$. Molecule $[\text{Fe}(\text{L}^{19})_2]^{2+}$ with the highest $E_{\text{Fe(II/III)}}$ also has the highest calculated Merz-Kollman electric potential on Fe.

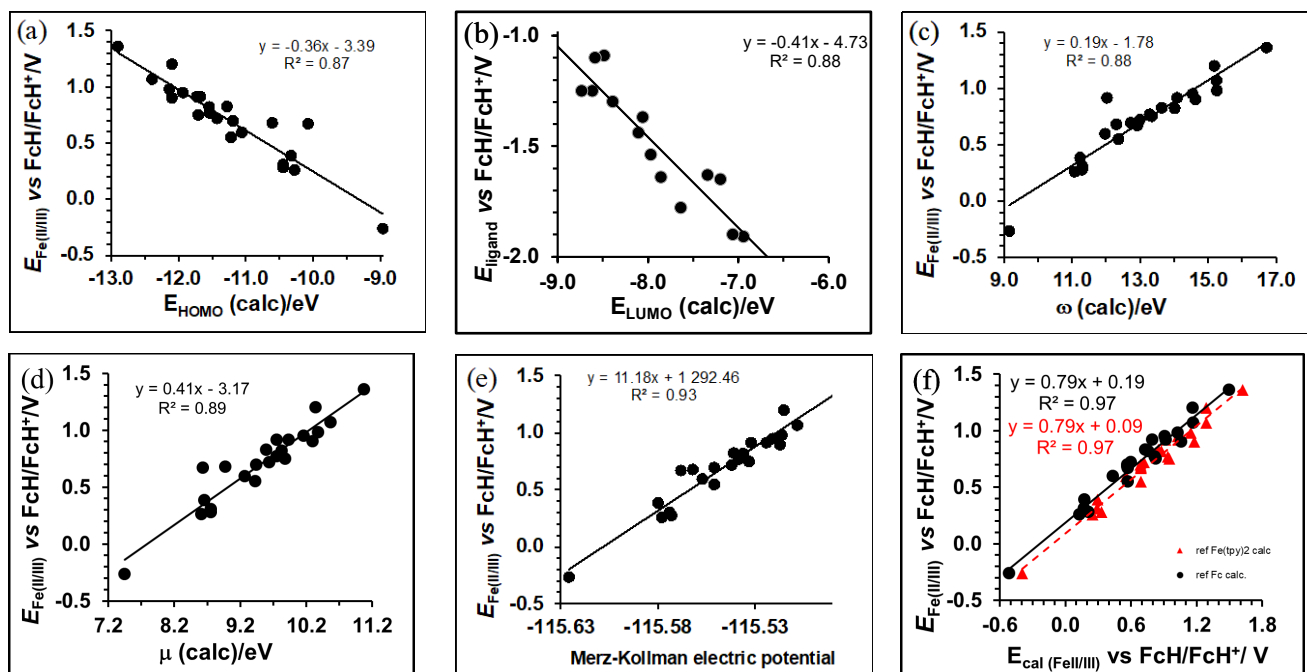


Figure 5: Linear correlation graph between iron-based oxidation $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (expt.) (V) and DFT calculated E_{HOMO} (eV) graph (a), electrophilicity index, ω (eV) graph (c), electronic chemical potential, μ (eV) graph (d) and Merz-Kollman electric potential (au), graph (e). Inversely proportional linear relationship between ligand-based reduction E_{Ligand} vs FcH/FcH^+ (expt.) (V) and DFT calculated E_{LUMO} (eV), graph (b). Linear correlation between $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (expt.) (V) and $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (calc.) (V), see graph (f). Only known experimental data were used in the linear fit. For unknown predictions, see Table 3 and Table 4. Redox data from Table 2 and DFT data for (a) – (e) obtained from the **optimized gas phase** $[\text{Fe}(\text{L})_2]^{2+}$ structures ($\text{L} = \text{L}^1$ – L^{25}), see data in Table S1 in the supporting information. μ and ω are calculated using $\text{IP} = -E_{\text{HOMO}}$ and $\text{EA} = -E_{\text{LUMO}}$. $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (calc.) data for (f) in Table S3 in the supporting information.

Furthermore, to evaluate the relationship between the experimental iron-based oxidation $E_{\text{Fe(II/III)}}$ (expt.) and calculated redox potential, $E_{\text{Fe(II/III)}}$ (calc.), a linear correlation graph is presented, see Figure 5 (f). The theoretical redox potentials were computed from the optimized geometries of the $[\text{Fe}(\text{L})_2]^{2+}$ and $[\text{Fe}(\text{L})_2]^{3+}$ molecules using Scheme 1; see data summarized in Table S3 in the supporting information. When using a reported high-level *ab initio* molecular orbital theory determined absolute reduction potential of FcH/FcH^+ in CH_3CN , $E_{\text{FcH/FcH}^+} = 4.980 \text{ V}$ [58], in Equation 8, a systematic error of 0.19 V is obtained (top graph in Figure 5 (f)). When using the experimental potential vs. FcH/FcH^+ of $[\text{Fe}(\text{tpy})_2]^{2+}$ to convert the calculated absolute redox potential to potentials vs. FcH/FcH^+ [59] (bottom graph in Figure 5 (f)), the systematic error decreases to 0.09 V. The results in Figure 5 (f) thus show that although $E_{\text{Fe(II/III)}}$ (exp.) versus $E_{\text{Fe(II/III)}}$ (calc.) gives a linear relationship, the values do not coincide with each other, giving a systematic error. Systematic errors when calculating redox potentials are often obtained [60–63] and depend *inter alia* on the DFT level of theory, and the reference used [59]. The DFT calculated redox potentials (and energies) could be improved, for example, by changing the level of theory [58,63], by using another free energy cycle

for the redox calculation [60,64], the choice of the reference used [59], by adding correction factors [60,64], using explicit solvation [65], by adding the counterions during the optimization [31,66], or by using solution phase optimized geometries and frequencies [61,67].

Thus to eliminate the systematic error, predicted redox potentials $E_{\text{Fe(II/III)}}^{\text{(predicted)}}$, obtained from the linear relationship between $E_{\text{Fe(II/III)}}^{\text{(expt.)}}$ and $E_{\text{Fe(II/III)}}^{\text{(calc.)}}$ in Figure 5 (f) is used, see values in the 4th column of Table S3 in the supporting information. Irrespective of the systematic error, the DFT calculated redox potential, $E_{\text{Fe(II/III)}}^{\text{(calc.)}}$, in Figure 5 (f) gave a more accurate linear relationship with $E_{\text{Fe(II/III)}}^{\text{(expt.)}}$ ($R^2 = 0.97$) than the DFT calculated energies in Figure 5 (a), (c), (d) and (e). The degree of accuracy in reproducing the experimental redox potential, $E_{\text{Fe(II/III)}}^{\text{(expt.)}}$, from the linear relationship obtained in Figure 5 (f) can also be evaluated from the mean absolute deviation (MAD) of $E_{\text{Fe(II/III)}}^{\text{(predicted)}}$ from $E_{\text{Fe(II/III)}}^{\text{(expt.)}}$ of 0.05 V. It should be noted that the reported experimental values of $[\text{Fe}(\text{L}^1)_2]^{2+}$ differ with 0.05 V, and that of $[\text{Fe}(\text{L}^8)_2]^{2+}$ and $[\text{Fe}(\text{L}^{10})_2]^{2+}$ up to 0.04 V (Table 2). Thus the DFT method used here to obtain a linear relationship between the experimental $E_{\text{Fe(II/III)}}^{\text{(expt.)}}$ and the calculated $E_{\text{Fe(II/III)}}^{\text{(calc.)}}$ redox potential to predict redox potentials $E_{\text{Fe(II/III)}}^{\text{(predicted)}}$, could be considered as highly efficient to reproduce experimental redox potential of $[\text{Fe}(\text{L})_2]^{2+}$ type of molecules (Table 3).

By optimizing $[\text{FeL}_2]^n$ ($n = 1, 2, 3$) in the gas phase, the adiabatic EA_a and IP_a can be calculated. Using EA_a and IP_a , μ and ω can be calculated. Relationships obtained between the oxidation $E_{\text{Fe(II/III)}}$ (respective reduction E_{Ligand}) potential and the gas phase calculated IP_a (respective EA_a), Figure 6 (a) and (b), gave slightly higher R^2 values as the relationships involving the gas phase calculated energy of the HOMO (respective LUMO) of the $[\text{Fe}(\text{L})_2]^{2+}$ complexes, Figure 5 (a) and (b). Similarly, the relationships involving μ and ω in Figure 6 (c) and (d) and in Figure 5 (c) and (d) gave slightly higher or similar R^2 values. The relationships in Figure 5 (a) – (e) were obtained from the gas phase optimized $[\text{FeL}_2]^{2+}$ molecules, while the relationships in Figure 6 were obtained from the gas phase optimized $[\text{FeL}_2]^n$ ($n = 1, 2, 3$) molecules. It is expected that relaxation of the molecules upon oxidation ($m = 3$) and reduction ($m = 1$) gives better results. Optimizing $[\text{FeL}_2]^n$ ($n = 1, 2, 3$) needs more than three times the computational resources (CPU hours) than optimizing the closed shell $[\text{FeL}_2]^{2+}$ molecules (restricted calculations) only. In light of the slight increase in R^2 values of ca 2%, only the $[\text{FeL}_2]^{2+}$ molecules were optimized in the solvent phase (using the experimental solvent CH_3CN as implicit solvent model) to evaluate if solvent phase calculated energies will lead to more accurate relationships with $E_{\text{Fe(II/III)}}$ and E_{Ligand} .

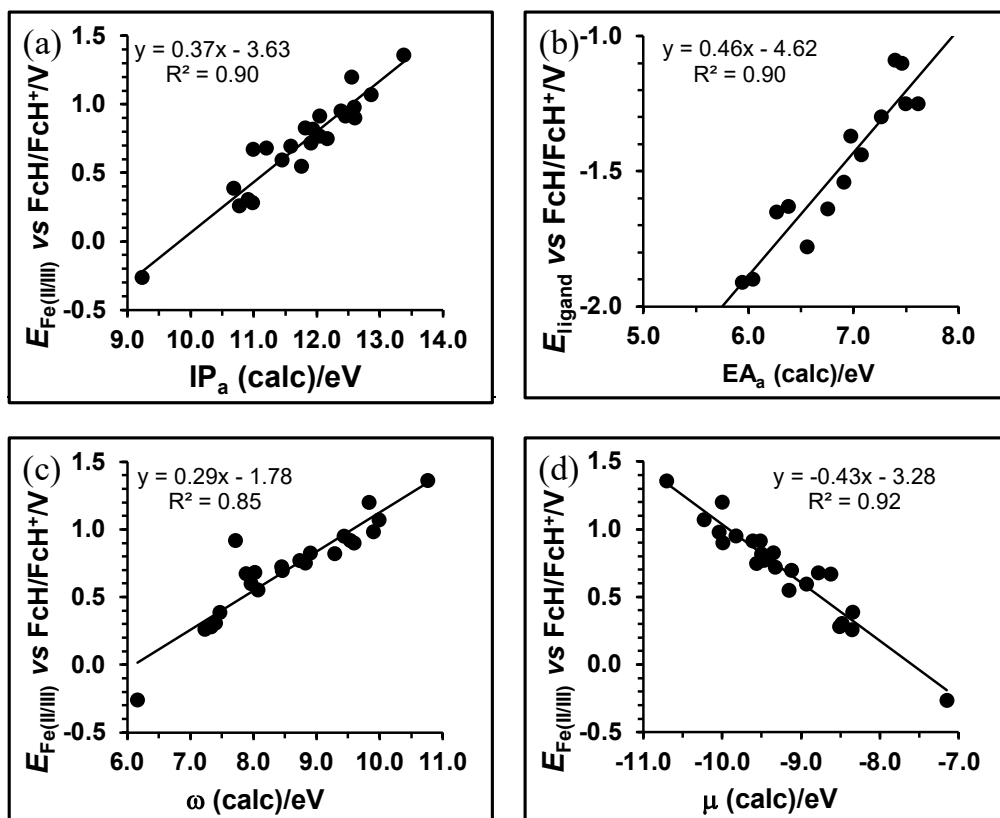


Figure 6: Linear correlation graph between iron-based oxidation $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (expt.) (V) and (a) the adiabatic IP_a , (b) adiabatic EA_a , (c) global electrophilicity index (ω) (eV) and (d) electronic chemical potential (μ) (eV) in gas phase. Data of graph (a) – (d) obtained from the optimized $[\text{FeL}_2]^n$ ($n = 1, 2, 3$) gas phase calculations. Redox data from Table 2 and DFT data in Table S2 in the supporting information. μ and ω are calculated using EA_a and IP_a .

DFT calculated data for optimized $[\text{Fe}(\text{L})_2]^{2+}$ structures in the solvent (CH_3CN) phase can be viewed in Table S4 in the supporting information. Relationships obtained between the experimental iron-based oxidation $E_{\text{Fe(II/III)}}$ (expt.) or ligand-based reduction E_{Ligand} (expt.) and solvent phase calculated HOMO and LUMO energies (Figure 7 (a) and (b) with $R^2 = 0.96$ and 0.95), lead to more accurate relationships with higher R^2 values than the relationships involving the gas phase calculations (Figure 5 (a) and (b) with $R^2 = 0.87$ and 0.88). The solvent used to obtain the experimental redox potentials, CH_3CN , was used for the solvent phase DFT calculations. The linear equations in Figure 7 were utilized to predict the oxidation and ligand-based reduction values of $[\text{Fe}(\text{R-tpy})_2]^{2+}$ complexes with ligands L^{20} and L^{21} (Table 3) and L^3 , L^5 , L^7 , L^{12} , L^{14} and L^{20} - L^{24} (Table 4), respectively. These experimentally measured values could not be found in the literature (Table 2) [6,7,22,23,43,44,46].

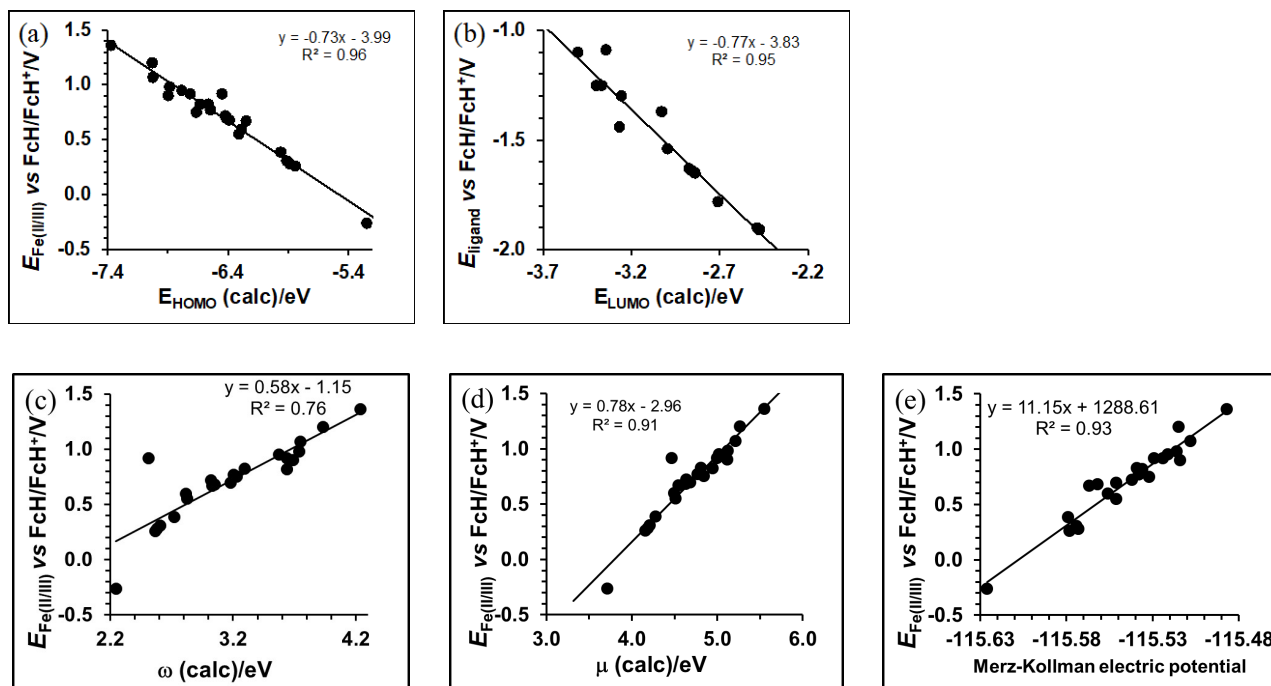


Figure 7: Linear correlation graph between iron-based oxidation $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (expt.) (V) and DFT calculated E_{HOMO} (eV) graph (a), calculated E_{LUMO} (eV), graph (b), electrophilicity index, ω (eV) graph (c), electronic chemical potential, μ (eV) graph (d) and Merz-Kollman electric potential (au), graph (e). Only known experimental data were used in the linear fit. For unknown predictions, see Table 3 and Table 4. DFT data obtained from optimized $[\text{Fe}(\text{L})_2]^{2+}$ structures ($\text{L} = \text{L}^1\text{-L}^{25}$) in solvent (CH_3CN) phase, see data in Table S4 in the supporting information. $E_{\text{Fe(II/III)}}$ vs FcH/FcH^+ (expt.) (V) and E_{Ligand} vs FcH/FcH^+ (expt.) (V) from Table 2.

DFT calculated data Natural Bond Orbital (NBO) charges on Fe, and the coordinating N's for optimized $[\text{Fe}(\text{L})_2]^{n+}$ ($n = 2$ and 3) structures in the indicated phase can be viewed in Table S5-S7 in the supporting information. NBO analysis is a helpful tool for determining the delocalization of the electron density onto the different atoms in a molecule. Relationships obtained between the experimental iron-based oxidation $E_{\text{Fe(II/III)}}$ (expt.) or ligand-based reduction E_{Ligand} (expt.) and the sum of the calculated NBO charges on Fe and the coordinated N's, are shown in Figure 8. Data of complexes containing tris-azinyl ligands L^9 , L^{16} , L^{18} , and L^{24} were omitted from the relationships. These tris-azinyl analogues of terpyridine have nitrogen in an *ortho* or *meta* position of the “pyridine” rings. The complexes containing the tris-azinyl analogues of terpyridine, having nitrogen in a *para* position of the “pyridine” rings (L^{13} , L^{15} , L^{17} , L^{19}), did fit the relationship shown in Figure 8. $[\text{Fe}(\text{L}^{24})_2]^{2+}$, contains L^{24} (2,6-di(pyrazol-1-yl) pyridine) with one six-membered pyridine and two five-membered pyrazole rings, contrary to the terpyridine complexes (e.g. $[\text{Fe}(\text{L}^8)_2]^{2+}$) all containing terpyridine with three six-membered pyridine rings. The ring size as well as the extra N's in pyrazole decrease the NBO charges on the coordinating N's in $[\text{Fe}(\text{L}^{24})_2]^{2+}$ compared to $[\text{Fe}(\text{L}^8)_2]^{2+}$.

The relationship between $E_{\text{Fe(II/III)}}$ and the sum of the calculated NBO charges on Fe and the coordinated N's (both gas and solvent phase calculations, Figure 8 (a) and (c)) gave a very high R^2 value of 0.95. This suggests that $E_{\text{Fe(II/III)}}$ is dependent of the charge on the iron(II) atom and it's

environment (the N-atoms it is coordinated to), and not only the charge on iron only, before oxidation. The data point of $[\text{Fe}(\text{L}^{22})_2]^{2+}$, with the tri-OMe-tpy ligand L^{22} , generally lay slightly above the lines in Figure 8 (a) - (e).

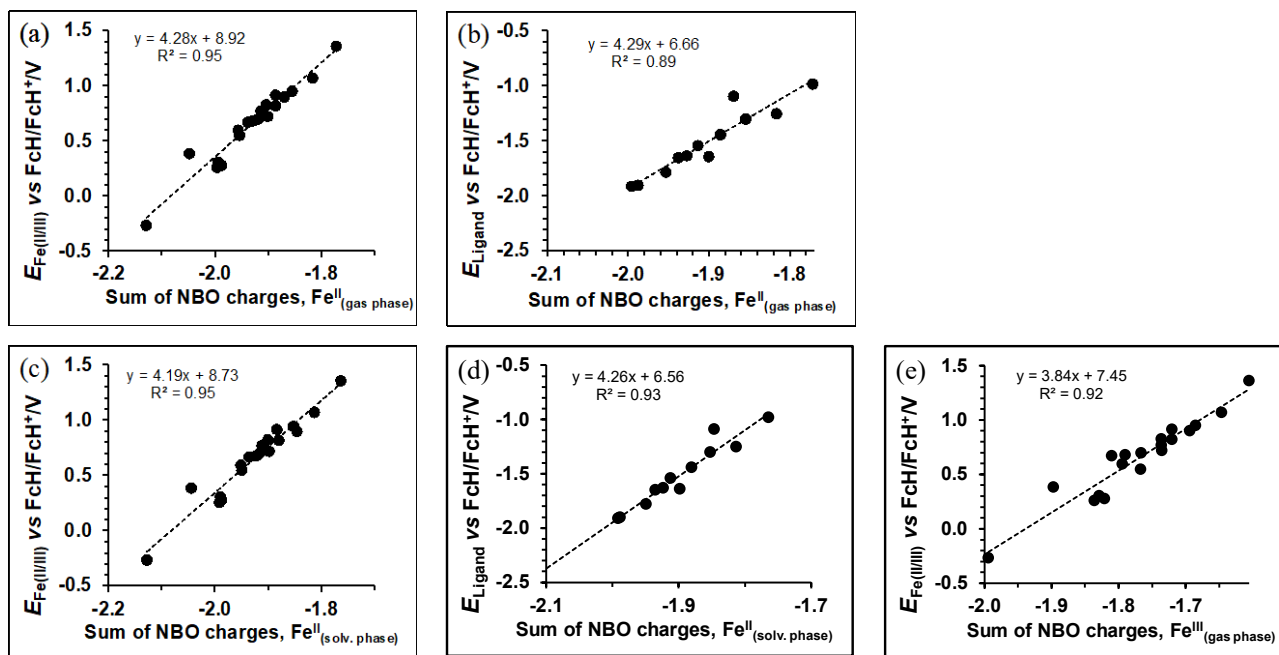


Figure 8: Relationships obtained between (a) $E_{\text{Fe(II/III)}}$ and the sum of the calculated NBO charges on Fe and the coordinated N's, obtained from the optimized Fe^{II} gas phase calculations, (b) the ligand based reduction of the Fe(II) complexes and the sum of the calculated NBO charges on Fe and the coordinated N's, obtained from the optimized Fe^{II} gas phase calculations, (c) $E_{\text{Fe(II/III)}}$ and the sum of the calculated NBO charges on Fe and the coordinated N's, obtained from the optimized Fe^{II} solvent phase calculations, (d) the ligand based reduction of the Fe(II) complexes and the sum of the calculated NBO charges on Fe and the coordinated N's, obtained from the optimized Fe^{II} solvent phase calculations, and (e) $E_{\text{Fe(II/III)}}$ and the sum of the calculated NBO charges on Fe and the coordinated N's, obtained from the optimized $[\text{Fe}(\text{L})_2]^{3+}$ ($\text{L} = \text{L}^1\text{-L}^{25}$) gas phase calculations. Data of complexes containing tris-azinyl ligands L^9 , L^{16} , L^{18} and L^{24} omitted. Redox data from Table 2 and DFT data in Tables S5 – S7 in the supporting information. Note (i) no $E_{\text{Fe(II/III)}}$ experimental values for L^{20} and L^{21} and (ii) no ligand based reduction of the Fe(II) complexes values for L^3 , L^5 , L^7 , L^{12} , L^{14} and $\text{L}^{20}\text{-L}^{24}$.

The same conclusion is obtained from the good relationship between $E_{\text{Fe(II/III)}}$ (and the ligand-based reduction) and the sum of the calculated Mulliken charges on Fe and the coordinated N's (gas phase calculations, Figure 9 (a) and (b) with data in Table S8-S10 in the supporting information). In Figure 9, only the data of the 4'-substituted (R-groups) terpyridine complexes ($\text{L}^1 - \text{L}^8$, $\text{L}^{10} - \text{L}^{12}$, L^{14} , L^{25}) were considered. Data of related complexes, containing 4,4',4''-substituted (R-groups) terpyridine (L^{22} , L^{23}), tris-azinyl derivatives of terpyridine (L^9 , L^{13} , $\text{L}^{15}\text{-L}^{19}$) and (L^{24}) did not fit the trend.

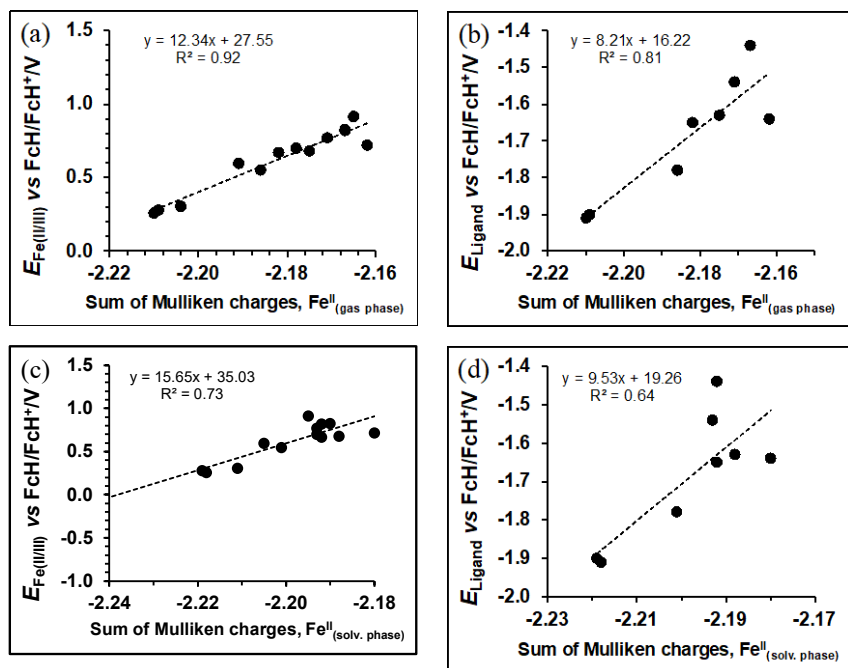


Figure 9: Relationships obtained between the (a) $E_{\text{Fe(II/III)}}$ and the sum of the calculated Mulliken charges on Fe and the coordinated N's, obtained from the optimized Fe^{II} gas phase calculations, (b) the ligand based reduction of the Fe(II) complexes and the sum of the calculated Mulliken charges on Fe and the coordinated N's, obtained from the optimized [Fe(L)₂]²⁺ gas phase calculations, (c) $E_{\text{Fe(II/III)}}$ and the sum of the calculated Mulliken charges on Fe and the coordinated N's, obtained from the optimized Fe^{II} solvent phase calculations and (d) the ligand based reduction of the Fe(II) complexes and the sum of the calculated Mulliken charges on Fe and the coordinated N's, obtained from the optimized [Fe(L)₂]²⁺ solvent phase calculations. Data of 4'-substituted (R-groups) terpyridine complexes (L¹ – L⁸, L¹⁰ - L¹², L¹⁴, L²⁵) used. Data of 4,4',4''-substituted (R-groups) terpyridine (L²², L²³), tris-azinyl derivatives of terpyridine (L⁹, L¹³, L¹⁵-L¹⁹) and related (L²⁴) complexes not included. Redox data from Table 2 and DFT data in Table S8-S10 in the supporting information.

In conclusion, the different relationships between the experimental redox potentials and DFT calculated energies, including the R^2 value of the relationship and the MAD of the specific relationship (method), presented in this study in Figure 4 - Figure 9, are summarized in Table 3 and Table 4. From these equations, the iron-based oxidation and the ligand-based reduction potential of some complexes, of which the experimental data could not be found, are predicted from the linear relationships; see Table 3 and Table 4. The predicted redox potential of 0.67 vs FcH/FcH⁺ (0.69 V vs FcH/FcH⁺ experimentally) of the iron-based oxidation of [Fe(L⁷)₂]²⁺, for example, is predicted with a MAD of 0.02, a value less than the difference between reported oxidation potentials from different laboratories, 0.04 V, in Table 2. The ligand-based reduction potential of [Fe(L⁷)₂]²⁺ ([Fe(tpy-vinyl)₂]²⁺) is predicted to be -1.60 V vs FcH/FcH⁺ (MAD of 0.03 V). The predicted value of [Fe(L⁷)₂]²⁺ is very near to the reported value of -1.57 V vs FcH/FcH⁺ (-1.19 V vs SSCE), from literature [46]. The prediction of reduction potentials gave a higher MAD in some cases (Table 4). It is important to note that the predicted redox value and the MAD of prediction depend on the amount

of methods used and the accuracy of the methods included (R^2 and MAD values of the specific method). Here, all methods presented in this work, were included in the predictions in Table 3 and Table 4.

Predicting the redox potential of molecules has important practical applications. For example, for a complex to be considered to be used as a redox mediator in a DSSC, the redox mediators may have redox potentials up to 0.5 V more positive than that of the commonly used iodide/triiodide (I_3^-/I^-) redox mediator [68] (-0.34 ± 0.02 V vs. FcH/FcH^+ in acetonitrile [69]). Thus, using available redox potential-DFT relationships to design complexes with redox potentials in the range $(-0.34) - (+0.24)$ vs. Fc/Fc^+ , a suitable redox mediator may be identified, depending on the electronic properties of the specific dye in the DSSC [70,71].

The results (Table 3 and Table 4) further show that the relationship between the experimental and DFT calculated $Fe(II/III)$ redox potential in Figure 5 (f) gave the most accurate relationship with $E_{Fe(II/III)}$ (expt.) ($R^2 = 0.97$ with MAD 0.05). It is also observed that the relationships between the experimental iron-based oxidation $E_{Fe(II/III)}$ (expt.) or ligand-based reduction E_{Ligand} (expt.), and solvent phase calculated HOMO and LUMO energies respectively (Figure 7 (a) and (b) with $R^2 = 0.96$ and 0.95 and MAD 0.05 and 0.04 respectively), lead to more accurate relationships with higher R^2 values than the relationships involving the gas phase calculations (Figure 5 (a) and (b) with $R^2 = 0.87$ and 0.88 and MAD 0.09 and 0.08 respectively).

Table 3: Table of linear equations, R^2 , MAD and predicted unknown values (predicted $E_{Fe(II/III)}$ vs FcH/FcH^+), for $[Fe(L^n)_2]^{2+}$ complexes containing L^{20} and L^{21} , obtained by using the linear equation of the graphs between the experimental iron-based oxidation $E_{Fe(II/III)}$ vs FcH/FcH^+ (expt.) (V) and the indicated DFT calculated value.

Relationship $E_{Fe(II/III)}$ vs x	Equation	R^2 of method	MAD ^a of method	Figure	L^{20}	L^{21}
Hammett	$y = 0.43x + 0.67$	0.96	0.05	Figure 4 a	0.58	0.72
$E_{HOMO,Fe(II),gas}$	$y = -0.36x - 3.39$	0.87	0.09	Figure 5 a	0.43	0.53
$\omega_{Fe(II),gas}$	$y = 0.19x - 1.78$	0.88	0.08	Figure 5 c	0.26	0.69
$\mu_{Fe(II),gas}$	$y = 0.41x - 3.17$	0.89	0.09	Figure 5 d	0.39	0.57
$V_{Mers-Kollman,Fe(II),gas}$	$y = 11.18x + 1292.46$	0.93	0.07	Figure 5 e	0.38	0.60
$E_{Fe(II/III),calc}$	$y = 0.79x + 0.09$	0.97	0.05	Figure 5 f	0.50	0.69
IP_{gas}	$y = 0.37x - 3.63$	0.90	0.09	Figure 6 a	0.37	0.59
$\omega_{adiabatic,gas}$	$y = 0.29x - 1.78$	0.85	0.09	Figure 6 c	0.37	0.63
$\mu_{adiabatic,gas}$	$y = -0.43x - 3.28$	0.92	0.08	Figure 6 d	0.34	0.58
$E_{HOMO,Fe(II),solvent}$	$y = -0.73x - 3.99$	0.96	0.05	Figure 7 a	0.54	0.71
$\omega_{Fe(II),solvent}$	$y = 0.58x - 1.15$	0.76	0.10	Figure 7 c	0.47	0.68
$\mu_{Fe(II),solvent}$	$y = 0.78x - 2.96$	0.91	0.06	Figure 7 d	0.50	0.70
$V_{Mers-Kollman,Fe(II),solvent}$	$y = 11.15x + 1288.61$	0.93	0.07	Figure 7 e	0.38	0.61

NBO charges _{(FeII),gas}	$y = 4.28x + 8.92$	0.95	0.06	Figure 8 a	0.67	0.69
NBO charges _{(FeII),solv.}	$y = 4.19x + 8.73$	0.95	0.06	Figure 8 c	0.66	0.69
NBO charges _{(FeIII),gas.}	$y = 3.84x + 7.45$	0.92	0.08	Figure 8 e	0.73	0.59
Mulliken charges _{(FeII),gas.}	$y = 12.34x + 27.55$	0.92	0.04	Figure 9 a	0.46	0.69
Mulliken charges _{(FeII),solv.}	$y = 15.65x + 35.03$	0.73	0.09	Figure 9 c	0.37	0.76
Average predicted^b					0.47	0.65
MAD^a of prediction^b					0.10	0.06

a MAD = mean absolute deviation.

b Average and MAD of prediction (MAD across all the methods) depend on the amount of methods used and the accuracy of the methods (R^2 and MAD of method).

Table 4: Table of linear equations, R^2 , MAD and predicted unknown values (predicted E_{Ligand} vs $F_{\text{CH}}/F_{\text{CH}^+}$), for $[\text{Fe}(\text{L}^n)_2]^{2+}$ complexes containing L^3 , L^5 , L^7 , L^{12} , L^{14} and L^{20} - L^{24} , obtained by using linear equation of the graphs for between the experimental ligand-based reduction E_{Ligand} vs $F_{\text{CH}}/F_{\text{CH}^+}$ (expt.) (V) and the indicated DFT calculated value.

Relationship E_{Ligand} vs	Equation	R^2 of method	MAD ^a of method	Figure	L^3	L^5	L^7	L^{12}	L^{14}	L^{20}	L^{21}	L^{22}	L^{23}	L^{24}
Hammett	$y = 0.35x - 1.61$	0.97	0.02	Figure 4 b	-1.79	-1.70	-1.62	-1.44	-1.37	-1.68	-1.57	-1.89	-2.37	
$E_{\text{LUMO,Fe(II),gas}}$	$y = -0.41x - 4.73$	0.88	0.08	Figure 5 b	-1.84	-1.67	-1.58	-1.49	-1.38	-1.88	-1.64	-1.86	-2.30	-1.54
$E_{\text{A}_{\text{gas}}}$	$y = 0.46x - 4.62$	0.90	0.07	Figure 6 b	-1.86	-1.69	-1.58	-1.48	-1.34	-1.88	-1.64	-1.88	-2.30	-1.62
$E_{\text{LUMO,Fe(II),solvent}}$	$y = -0.77x - 3.83$	0.95	0.04	Figure 7 b	-1.90	-1.75	-1.55	-1.48	-1.30	-1.77	-1.56	-1.83	-2.15	-1.92
NBO charges _{(FeII),gas}	$y = 4.29x + 6.66$	0.89	0.06	Figure 8 b	-1.89	-1.74	-1.57	-1.51	-1.43	-1.61	-1.59	-2.13	-2.47	c
NBO charges _{(FeII),solv}	$y = 4.26x + 6.56$	0.93	0.05	Figure 8 d	-1.92	-1.76	-1.61	-1.54	-1.47	-1.60	-1.58	-2.11	-2.47	c
Mulliken charges _{(FeII),gas}	$y = 8.21x + 16.22$	0.81	0.05	Figure 9 b	-1.86	-1.76	-1.65	-1.56	-1.54	d	-1.64	d	d	d
Mulliken charges _{(FeII),solv}	$y = 9.53x + 19.26$	0.64	0.07	Figure 9 d	-1.81	-1.75	-1.64	-1.61	-1.66	d	-1.61	d	d	d
Average predicted^b					-1.86	-1.73	-1.60	-1.51	-1.44	-1.74	-1.60	-1.95	-2.34	-1.69
MAD^a of prediction^b					0.04	0.03	0.03	0.04	0.09	0.11	0.03	0.11	0.09	0.15

a MAD = mean absolute deviation.

b Average and MAD of prediction (MAD across all the methods), depend on the amount of methods used and the accuracy of the methods (R^2 and MAD of method).

c Data of complexes containing tris-azinyl ligands L^9 , L^{16} , L^{18} , and L^{24} with *ortho* or *meta* N were omitted from the relationships.

d Data of complexes, containing 4,4',4''-substituted (R-groups) terpyridine (L^{20} , L^{22} , L^{23}), tris-azinyl derivatives of terpyridine (L^9 , L^{13} , L^{15} - L^{19}) and (L^{24}) did not fit the trend.

4 Conclusions

Different DFT computational calculated energies, potentials and charges revealed a good linear relationship to the combination of different experimental studies. The linear relationships obtained involve the experimental oxidation and reduction potentials obtained from the reported cyclic voltammetry studies, and the DFT calculated energies, potentials and charges in this study, namely molecular orbitals energies ($E_{\text{LUMO}}/E_{\text{HOMO}}$), electronic chemical potential (μ), electrophilicity index, (ω), Merz-Kollman electric potential and Mulliken and NBO charges. These relationships can be utilized to predict the oxidation and reduction potential of a complex by optimizing its structure with the DFT methods used in this study.

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Credit author statement

Evangelia Athanasopoulos: Methodology, Visualization, Data curation, Formal analysis, Investigation, Writing - original draft, Writing - review & editing.

Jeanet Conradie: Supervision, Validation, Methodology, Conceptualization, Funding acquisition, Project administration, Writing - review & editing.

Supporting Information

Figures S1-S2 and Tables S1 – S10. Optimized coordinates of the DFT calculations as xyz files.

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<https://doi.org/10.1016/j.elecom.2022.107225>.

Chapter 4: Results and Discussions

Chapter 4: submitted article 2.

E. Athanasopoulos, J. Conradie, DFT study of the spectroscopic behaviour of different iron(II)-terpyridine derivatives with application in DSSCs, submitted to J. Mol. Graph. Model. (submitted 31.09.2023) Manuscript ID JMGM-D-23-01121 <https://www.sciencedirect.com/journal/journal-of-molecular-graphics-and-modelling> Elsevier

Appendix B:

Supplementary material associated with article J. Mol. Graph. Model. (submitted 31.09.2023) Manuscript ID JMGM-D-23-01121: Optimized coordinates of the DFT calculations, Table S1, Figures S1 – S9.

Highlights

- TDDFT study of electronically altered iron(II)-terpyridine derivatives
- MMCT (lowest energy), CLCT and LLCT (highest energy) bands identified
- Properties needed to qualify as dyes in DSSCs evaluated

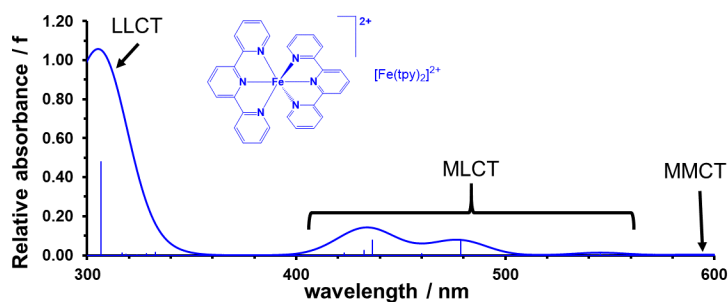
Abstract

Through a comprehensive computational analysis utilizing Density Functional Theory (DFT), we clarify the electronic structure and spectroscopic properties of modified iron(II)-terpyridine derivatives, with the aim of enhancing the efficiency of Dye-Sensitized Solar Cells (DSSCs). We optimized a series of nineteen iron(II)-terpyridine derivatives and related compounds in acetonitrile (MeCN) as the solvent using time-dependent Density Functional Theory (TDDFT), evaluating their potential as dyes for DSSCs. From the conducted computations on the optimized geometries of the nineteen $[\text{Fe}(\text{L}^n)_2]^{2+}$ complexes, containing substituted terpyridine and related ligands $\text{L}^1\text{-L}^{19}$, we determined the maximum wavelengths ($\lambda_{\text{max}}/\text{nm}$), transition energy (E in eV), oscillator strength (f), type of transitions, excited state lifetime (τ), light harvesting efficiency (LHE), frontier orbital energies and their energies ($E_{\text{LUMO}}/E_{\text{HOMO}}$), natural transition orbitals (NTOs), injection driving force of a dye (ΔG_{inject}), and regeneration driving force of a dye ($\Delta G_{\text{regenerate}}$). Results show that the theoretically calculated values for assessing dye efficiency in a DSSC correlate with available experimental values. The UV-visible spectra of $[\text{Fe}(\text{L}^n)_2]^{2+}$ exhibited a peak above 500 nm (λ_{max}) in the visible region, attributed to the ligand-to-metal charge transfer band (LMCT) in literature, and a significant absorbance peak at approximately 300 nm ($\lambda_{\text{A,max}}$) in the UV region. The M06-D3/CEP-121G method replicated all reported λ_{max} and $\lambda_{\text{A,max}}$ values with a mean absolute deviation (MAD) of 21 and 18 nm, respectively. Our findings underscore the connections between electronic modifications and absorption spectra, emphasizing their impact on the light-harvesting capabilities and overall performance of DSSCs. This research contributes to the advancement of fundamental principles governing the design and optimization of novel photovoltaic materials, facilitating the development of more efficient and sustainable solar energy technologies.

Keywords

Iron(II); terpyridine; tris-azinyl; DFT; TDDFT; DSSCs

SYNOPSIS TOC



SYNOPSIS TEXT

Simulated UV-vis spectra and properties related to dyes to be used in Dye-Sensitized Solar Cells for nineteen $[\text{Fe}(\text{L}^n)_2]^{2+}$ complexes with L = terpyridine and related ligands.

1 Introduction

Dye-sensitized solar cells (DSSCs), also known as Grätzel cells or simply "sensitized solar cells," are a type of solar-powered device (photovoltaic device) used to convert sunlight into electricity [1]. DSSCs operate on a different principle compared to traditional solar cells [2]. They use a photoelectrochemical system where a photosensitive dye (e.g., organic molecules, Ru, Zn, Cu, or Cu-based complexes) absorbs photons from sunlight and generates electron-hole pairs. They consist of the following components: an electrolyte, a photoanode, and a counter electrode. The photoanode consists of a mesoporous layer of titanium dioxide (TiO_2) nanoparticles coated with the light-absorbing dye where the photogenerated electrons are collected. The excited electrons in the dye are injected into the TiO_2 , creating an electrical current. DSSCs are known for their cost-effectiveness, flexibility, transparency, and suitability for low-light conditions [3]. However, research is ongoing to improve the production of toxic electrolytes, which is unsafe for the environment, and improve efficiency and stability for broader applications [4]. Moreover, due to its flexibility and transparency, DSSCs are helpful in applications such as portable electronic devices, solar chargers, and building-integrated photovoltaics (BIPV).

In summary, dye-sensitized solar cells are an innovative and promising technology for harnessing solar energy. It offers unique cost, flexibility, and low-light performance advantages. However, to explore their potential for broader applications, including large-scale energy generation, their efficiency and stability still require further development to compete with traditional silicon-based solar cells in mainstream energy generation.

Ruthenium-based dyes, e.g., N3, N719, and Black Dye, have historically demonstrated very high efficiency and performance as dyes for DSSCs [5,6], while iron-based sensitizers are not that well

known [7,8]. Iron is a much more abundant and less expensive element than ruthenium. Iron-based dyes can reduce the overall cost of manufacturing DSSCs, making them more accessible for large-scale deployment. Ruthenium is a rare and precious metal, and its extraction and use can have a more significant environmental impact than iron. By using iron compounds, DSSCs can be considered more environmentally friendly and sustainable. Many iron compounds are less toxic than ruthenium compounds, which is important for the environmental and health aspects of DSSC production and disposal.

Research into iron-based DSSCs has increased over the years, and scientists have been working to improve their performance, stability, and efficiency. This growing interest in iron-based DSSCs may lead to significant technological advancements [5,6]. In order to explore and seek to develop new, more efficient, and cost-effective dyes, this theoretical study, using density functional theory calculations, presents and discusses various properties of a series of nineteen iron(II)-terpyridine (Figure 1) and derivatives and related compounds (Scheme 1), to evaluate them as possible dyes for DSSCs. The results can be used to design related iron-based dyes to be tested experimentally for application as dyes in DSSCs.

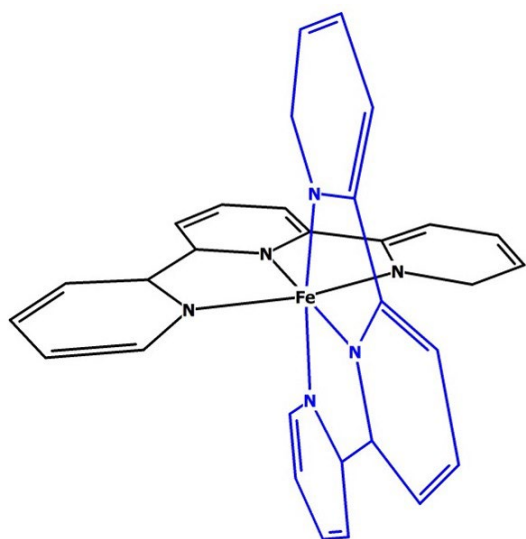
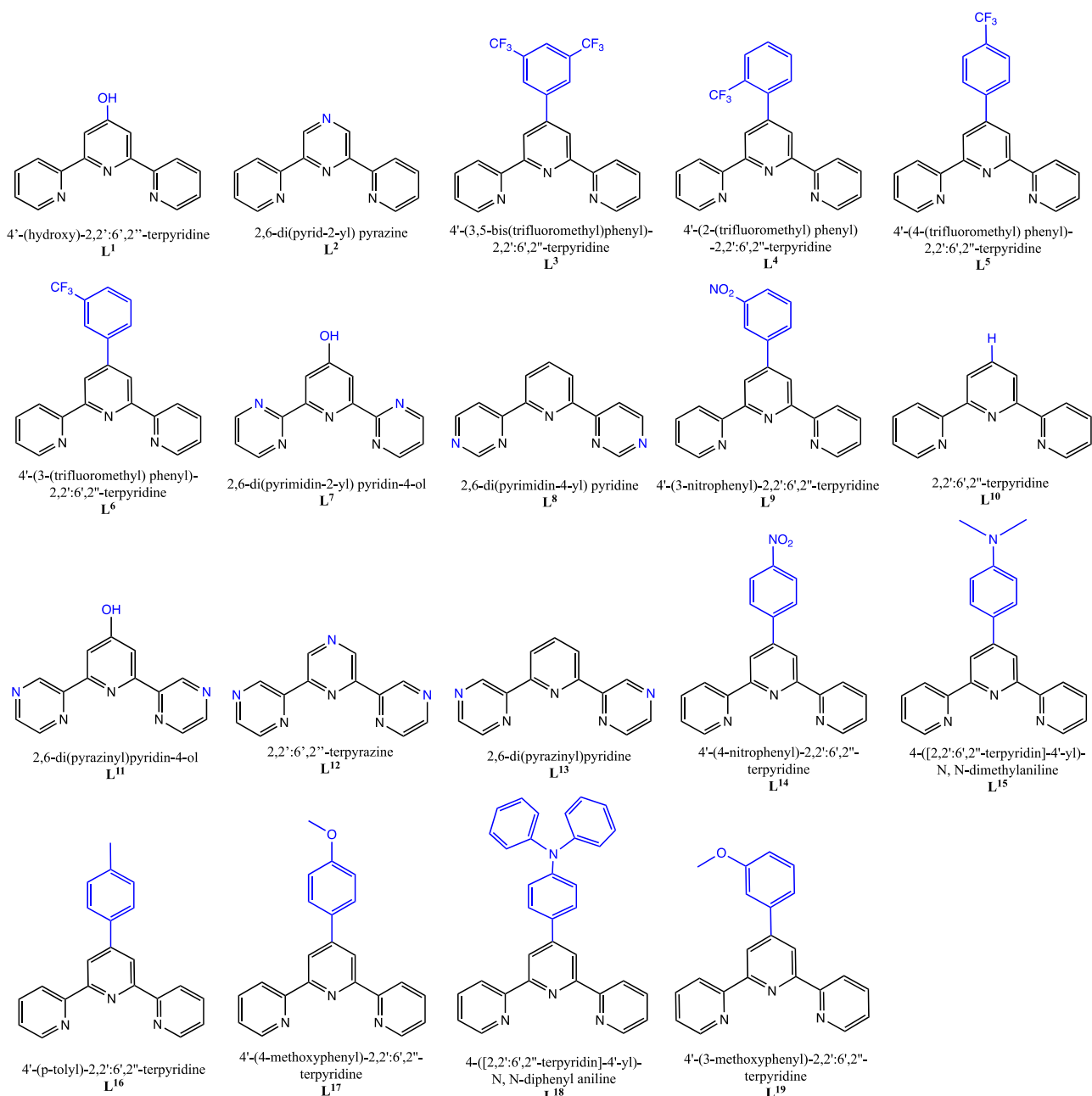


Figure 1: General structure of $[\text{Fe}(\text{L}^n)_2]^{2+}$ complexes, here with $\text{L} = 2,2':6',2''$ -terpyridine (created using Chemcraft [9]).



Scheme 1. The nineteen $[\text{Fe}(\text{L}^n)_2]^{2+}$ complexes **1 – 19**, containing ligands **L¹-L¹⁹**. Ligands name and structures are noted.

2 Computational methods

Density functional theory (DFT) computations were conducted on the Fe(II) ($Q = 2$) molecules with spin $S = 0$ using the Gaussian 16 software package [10]. To determine the most suitable DFT method for all complexes, optimization of iron(II)-terpyridine, complex 10, was carried out using various functionals: (i) B3LYP [11,12], (ii) M06 [13], (iii) PBEh1PBE [14], and (iv) BP86 [11,15,16], in conjunction with CEP-121G [17–19], aug-cc-pVDZ [20,21], cc-pVTZ [20–25], def2tzvpp [26], and SDD [27] basis sets. The Grimme's D3 empirical dispersion correction was applied as specified [28].

Optimizations were performed in acetonitrile (MeCN) as the solvent. The implicit solvent Polarizable Continuum Model (PCM) [29] employing the integral equation formalism variant (IEFPCM) [30] was utilized for solvent calculations in Gaussian. The input coordinates for the compounds were generated using Chemcraft [9]. Time-dependent density functional theory (TDDFT) computations were conducted on the M06 optimized geometries for all complexes (1 - 19) using the M06 functional [13] and the CEP-121G basis set [17–19]. The Grimme's D3 empirical dispersion correction was employed for all complexes.

The nature and energy of the (Kohn–Sham) molecular orbitals (MOs) were obtained from the DFT output files and visualized using Chemcraft.

From the time-dependent density functional theory (TD-DFT) findings, the following were obtained:

- a) λ with the corresponding calculated transition energy E (cm^{-1}) and the calculated oscillator strength (f) of the excited state.

- b) The excited state lifetime (τ) of dyes (in seconds) can be evaluated by equation (1) [31]:

$$\tau \text{ (in s)} = 1.499 / (fE_{\lambda}^2), \quad (1)$$

Where E_{λ} is the calculated transition energy (cm^{-1}), and f is the calculated oscillator strength of the excited state corresponding to the specified wavelength λ .

- c) The light harvesting efficiency (LHE), calculated from the oscillator strength (f) of the absorption bands, can be expressed as equation (2) [32,33]:

$$\text{LHE} = 1 - 10^{-f} \quad (2)$$

- d) Additionally, the injection driving force of a dye (ΔG_{inject}) and the regeneration driving force of a dye ($\Delta G_{\text{regenerate}}$) are calculated from oxidation potentials by equations (3) and (4), respectively [31,34]:

$$\Delta G_{\text{inject}} = E_{\text{dye}}^* - E_{\text{CB}} = E_{\text{dye}} - E_{\lambda} - E_{\text{CB}}, \quad (3)$$

$$\Delta G_{\text{regenerate}} = (E_{\text{I}^-/\text{I}_3^-}) - (E_{\text{dye}}) \quad (4)$$

Where E_{dye} represents the dye's oxidation potential that is approximated by the energy of the highest occupied molecular orbital. E_{CB} signifies the reduction potential of the conduction band edge of TiO_2 (-4.0 eV vs. vacuum or -0.5 eV vs. NHE [35,36]). E_{λ} denotes the electronic vertical transition energy corresponding to the wavelength λ_{max} , and $E_{\text{I}^-/\text{I}_3^-}$ indicates the redox potential of the electrolyte I^-/I_3^- redox couple (-4.8 eV vs vacuum or 0.3 eV vs NHE) [37].

3 Results and Discussion

3.1 Motivation of DFT method

The reported UV-visible spectra of $[\text{Fe}(\text{L}^n)_2]^{2+}$ all show a peak above 500 nm (λ_{max}) in the visible region, ascribe to the ligand-to-metal charge transfer band (LMCT) in literature, and a large absorbance maximum peak at ca 300 nm ($\lambda_{\text{A,max}}$) in the UV region, see data in Table 1. An example of reported UV-visible spectra of the unsubstituted bis(terpyridine)iron(II) complex, $[\text{Fe}(\text{L}^{10})_2]^{2+}$ [38], is shown in Figure 2. In order to explore the best DFT method to reproduce the experimental UV-vis nm λ_{max} and $\lambda_{\text{A,max}}$ values, the TDDFT simulated spectrum of complex 10, $[\text{Fe}(\text{L}^{10})_2]$, is determined using a selection of DFT functionals that previously proved to give simulated spectra in agreement with experiment for related metal-polypyridine and 6-coordinated iron(II) complexes, namely B3LYP [39–41], BP86 [42], M06 [43] and PBEh1PBE [44]. The results are shown in Figure 3. Both the B3LYP and M06 calculated spectra gave reasonable agreement with the reported values of 319 and 552 nm for $\lambda_{\text{A, max}}$, and λ_{max} for complex 10. The M06-D3/CEP-121G method reproduced the experimental λ_{max} and $\lambda_{\text{A,max}}$ values within 7 and 12 nm, respectively. The M06-D3/CEP-121G method was chosen to calculate the spectra of complexes $[\text{Fe}(\text{L}^n)_2]^{2+}$, where $n = 1 - 19$. Results of the TDDFT calculated λ_{max} and $\lambda_{\text{A,max}}$ values, together with the reported values, are presented in Table 2. The M06-D3/CEP-121G method reproduced all reported λ_{max} and $\lambda_{\text{A,max}}$ values with a mean absolute deviation (MAD) of 21 and 18 nm, respectively.

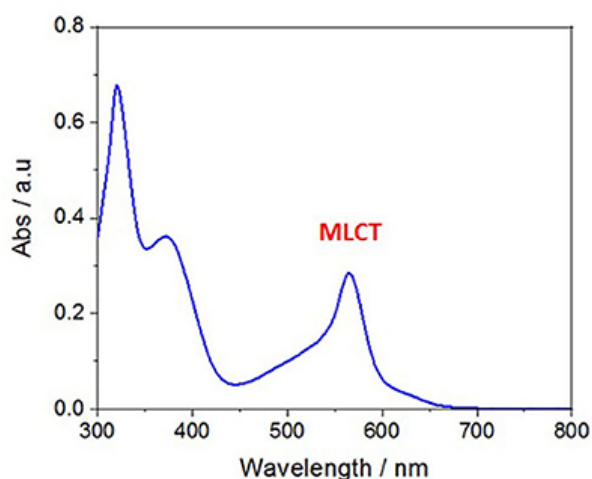


Figure 2: “UV-Vis absorption spectrum of a solution containing 0.5×10^{-5} M $[\text{Fe}(\text{tpy})_2(\text{BF}_4)_2]$ in acetonitrile” from [38] open access with Creative Commons Attribution (CC BY) license.

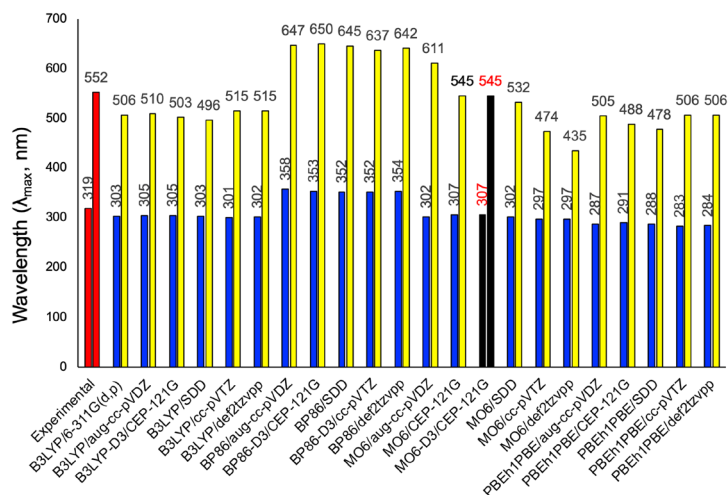


Figure 3: Calculated wavelength of the absorbance maximum peak ($\lambda_{A,max}$) and the maximum wavelength peak (λ_{max} , nm on y-axis) in the region 200–700 nm using the indicated DFT methods (x-axis), compared to the experimental absorption value, $\lambda_{Abs,max} = 319$ nm and $\lambda_{max} = 552$ nm of complex 10, $[\text{Fe}(\text{Terpy})_2]^{2+}$, indicated in red. The DFT method in best agreement with experimental absorption is written in red, $\lambda_{Abs,max} = 307$ nm and $\lambda_{max} = 545$ nm. MO6-D3/CEP-121G, was used to run all complexes of $[\text{Fe}(\text{L}^n)_2]^{2+}$ type.

Table 1: DFT calculated absorbance maximum wavelength ($\lambda_{Abs,max}$) and maximum wavelength (λ_{max}) compared to experimental absorbance maximum wavelength ($\lambda_{Abs,max}$) and maximum wavelength (λ_{max}) in nm.

Complex Nr.	DFT calculated		Experimental Data		Reference
	$\lambda_{Abs,max}$ (nm)	λ_{max} (nm)	$\lambda_{Abs,max}$ (nm)	λ_{max} (nm)	
1	247.87	530.63	243	553	[45]
2	277.84	553.21	278	552	[45]
3	279.71	560.47	285	570	[46]
4	281.69	551.92	286	572	[47]
5	282.64	557.91	286	569	[47]
6	285.07	555.18	286	568	[47]
7	287.70	519.81	252	545	[45]
8	300.75	557.21	315	574	[45]
9	300.85	556.31	328	575	[47]
10	306.64	545.47	319	552	[45]
11	309.46	524.32	283	586	[45]
12	314.29	538.15	282	545	[45]
13	317.43	529.33	285	552	[45]
14	320.15	573.09	287	583	[47]
15	320.44	545.32	324	587	[47]
16	327.95	549.15	327	571	[47]
17	353.19	548.24	336	586	[47]
18	358.28	549.70	437	584	[47]
19	298.23	551.35	285	570	[46]

3.2 Type of excitation (MOs and NTOs)

To get more insight into the type of excitation involved in the $\lambda_{\max}$ and $\lambda_{A,\max}$ peaks, the molecular orbitals contributing to the peaks are listed in Table 2 and visualized in Figure 5 for bis(terpyridine)iron(II), complex 10. For $[\text{Fe}(\text{L}^{10})_2]^{2+}$, TDDFT predicts two near-degenerate, very weak peaks at 592.2 nm. This peak is too small to be experimentally observed and involves mainly excitation from HOMO-1/HOMO-2 to LUMO+10/LUMO+11 (details of the % contribution are in Table 2). The MOs involved in this excitation are shown in Figure 5. The four MOs that contribute to more than 90 % of the excitation are iron-based; thus, the experimentally unobserved near degenerate excitations at 592.2 nm are of metal-to-metal charge transfer (MMCT) character. At 545.5 nm, the two near degenerate calculated peaks, which corresponds to the experimental peak $\lambda_{\max}$ at 552 nm, involve excitation mainly from the metal-based HOMO to the ligand-based LUMO and LUMO+1, see Figure 5. Thus, these peaks are of metal to ligand charge transfer (MLCT), or more specifically, Fe- $d\pi$ to ligand- π^* character, in agreement with experimental ([45,47]) assignments. In addition, two more strong peaks at 478.6 and 436.5 nm (Figure 4), also of MLCT character, are observed in the visible region between 400-500 nm (Table 2 and Figure 5). The strongest absorption bands appear at 319 nm experimentally and are reproduced by the two near-degenerate calculated peaks at 306.6 nm (Figure 4). The MOs involved in this transition (Table 2) are HOMO-3/HOMO-4 to LUMO/LUMO+1, all with ligand character (see Figure 5), thus exhibiting ligand to ligand charge transfer (LLCT) characteristics. The LLCT can be described as π to π^* electronic transitions within the aromatic system of the terpyridines.

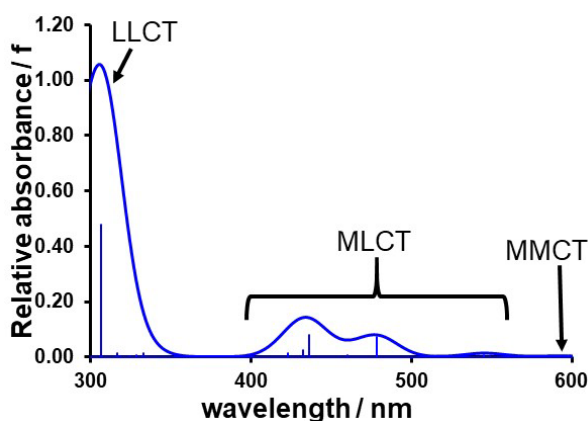


Figure 4: Experimental absorption spectra of the Fe(II) terpyridine complex 10 in MeCN (smooth curves) overlaid with the M06-D3/CEP-121G calculated oscillators (bar graphs of wavenumber versus the oscillator strengths).

Table 2: Computed wavelengths (λ in nm), transition energy (E in eV), oscillator strength (f), percentage (%) contribution, and type of transitions involved in the excitation of complex 10. N = no of excited state.

N	E/eV	λ_{max}/nm	f	From	To	% Contribution	Transition Type
2	2.09	592.21	0.0016	HOMO-2	LUMO + 10	48.1	MMCT
				HOMO-1	LUMO + 11	38.8	MMCT
				HOMO	LUMO + 1	9.5	MLCT
3	2.09	592.20	0.0016	HOMO-2	LUMO + 11	38.8	MMCT
				HOMO-1	LUMO + 10	48.1	MMCT
				HOMO	LUMO	9.5	MLCT
4	2.27	545.47	0.0066	HOMO-2	LUMO + 10	3.2	MMCT
				HOMO-1	LUMO + 3	2.8	MLCT
				HOMO-1	LUMO + 11	7.0	MMCT
				HOMO	LUMO + 1	85.2	MLCT
5	2.27	545.47	0.0066	HOMO-2	LUMO + 3	2.8	MLCT
				HOMO-2	LUMO + 11	7.0	MMCT
				HOMO-1	LUMO + 10	3.2	MMCT
				HOMO	LUMO	85.3	MLCT
8	2.59	478.55	0.0731	HOMO-2	LUMO + 1	47.4	MLCT
				HOMO-1	LUMO	47.4	MLCT
				HOMO	LUMO+2	4.0	MLCT
12	2.84	436.50	0.0787	HOMO	LUMO + 2	94.9	MLCT
30	4.04	306.64	0.4794	HOMO-4	LUMO + 1	22.7	LLCT
				HOMO-3	LUMO	59.6	LLCT
				HOMO	LUMO + 5	13.4	MLCT
31	4.04	306.64	0.4793	HOMO-4	LUMO	22.7	LLCT
				HOMO-3	LUMO + 1	59.6	LLCT
				HOMO	LUMO + 6	13.4	MLCT

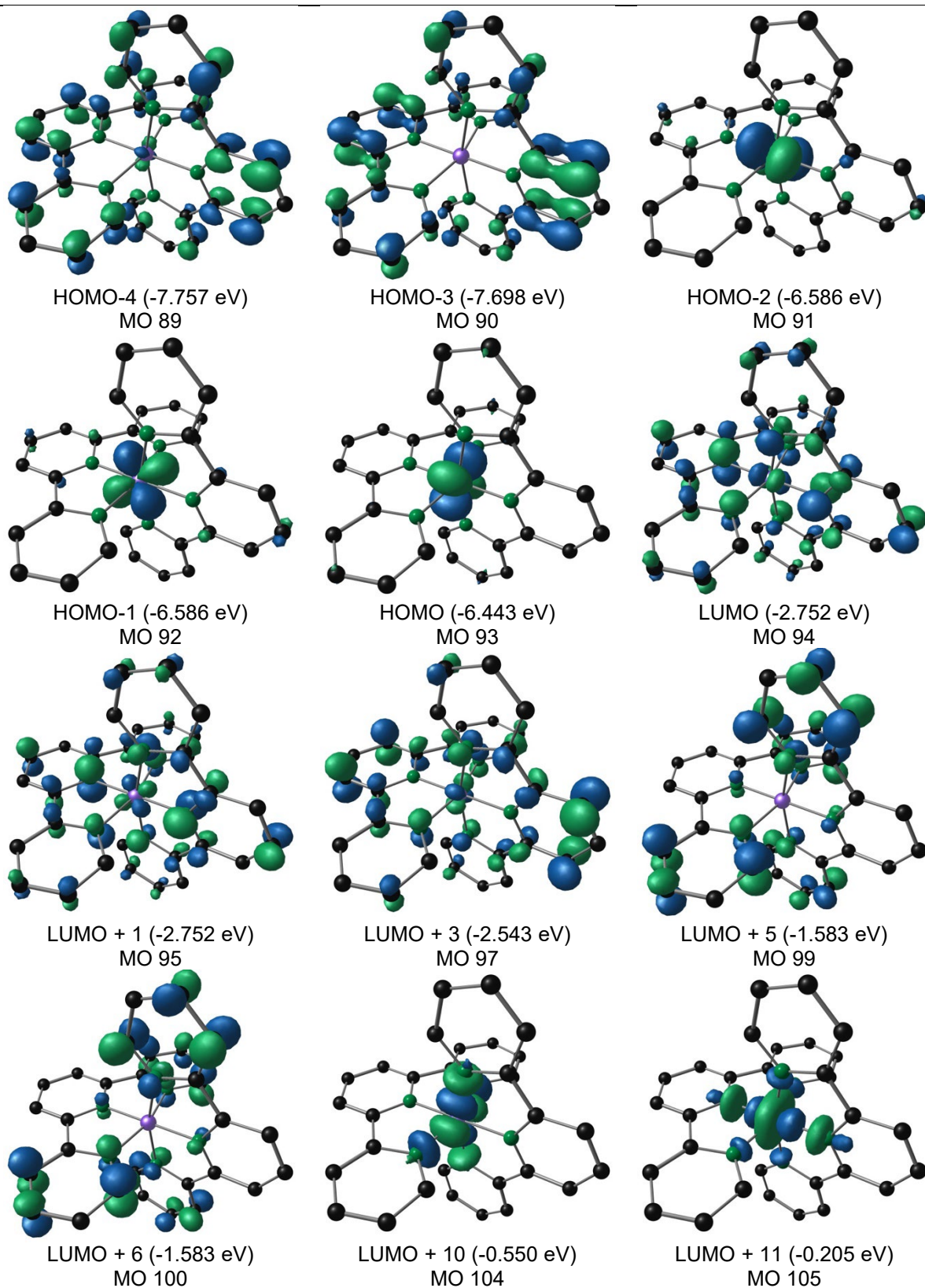


Figure 5: Selected MOs of complex 10, energy given in eV in brackets, calculated at the M06-D3/CEP-121G level in MeCN solution.

Similarly, the TDDFT calculated spectra of 1 – 19 can be divided into four regions (Figure 6), namely:

- (i) small experimentally unobserved MMCT peak above 580 nm (Figure 7)
- (ii) the experimentally observed MLCT λ_{max} , peak at ca 520-570 nm
- (iii) more MLCT peaks in the visible region between 400-500 nm (stronger peaks at ca 530 nm for 14, 15, and 18 are discussed below)
- (iv) the LLCT absorbance maximum peak in the UV region at below 360 nm

The MOs contributing to the different peaks of complexes 1 – 19, confirming the assigned character of the peaks, are summarized in Table S1 of the supporting information.

Comparing complexes 9 and 14, both containing a nitro group, with complex 10, it is observed that the peaks are more red-shifted to longer wavelengths in going from 10 (containing the unsubstituted terpyridine ligand) to 9 (containing a 4' *m*-NO₂-phenyl group) to 14 (containing a 4' *p*-NO₂-phenyl group), see Figure 6 bottom left graph. The shift in wavelength is more pronounced for 14, especially for the peak at 526 nm. The latter peak is also an MLCT, from metal-based HOMO-1/HOMO-2 to ligand-based LUMO/LUMO+1. However, the near degenerate LUMO and LUMO+1 are located on the nitro group (Figure 8 for 14), lowering the energy of the LUMO, thereby lowering the LUMO energy (-3.60 eV) compared to the terpyridine-based LUMO+2 (-2.813 eV). The energy of the terpyridine-based LUMO+2 of 14 is similar to that of the terpyridine-based LUMO of 10 (-2.75 eV). It is well known that a para substituent has a larger electronic influence as a meta substituent on the ligand or complexes to which it is attached [48–50].

When comparing complex 10 with complex 15 and 18, both containing an amide group, it is observed that both 15 and 18 have a strong peak at approximately 530 nm (Figure 6, bottom right graph). These peaks are mainly excitation from HOMO/HOMO-1 to LUMO/LUMO+1 (details of the % contribution are in Table S1 in the supporting information), where the HOMO and HOMO-1 are on the amide group and are not metal-based, see Figure 9 for 15 as an example (Figure S1 for 18). Therefore, these two strong peaks of 15 and 18 at ca 530 nm are of LLCT character, involving the amide group. The MLCT peaks of 15 (421 and 447 nm) and 18 (452 nm) are below 500 nm in the 400-500 nm region.

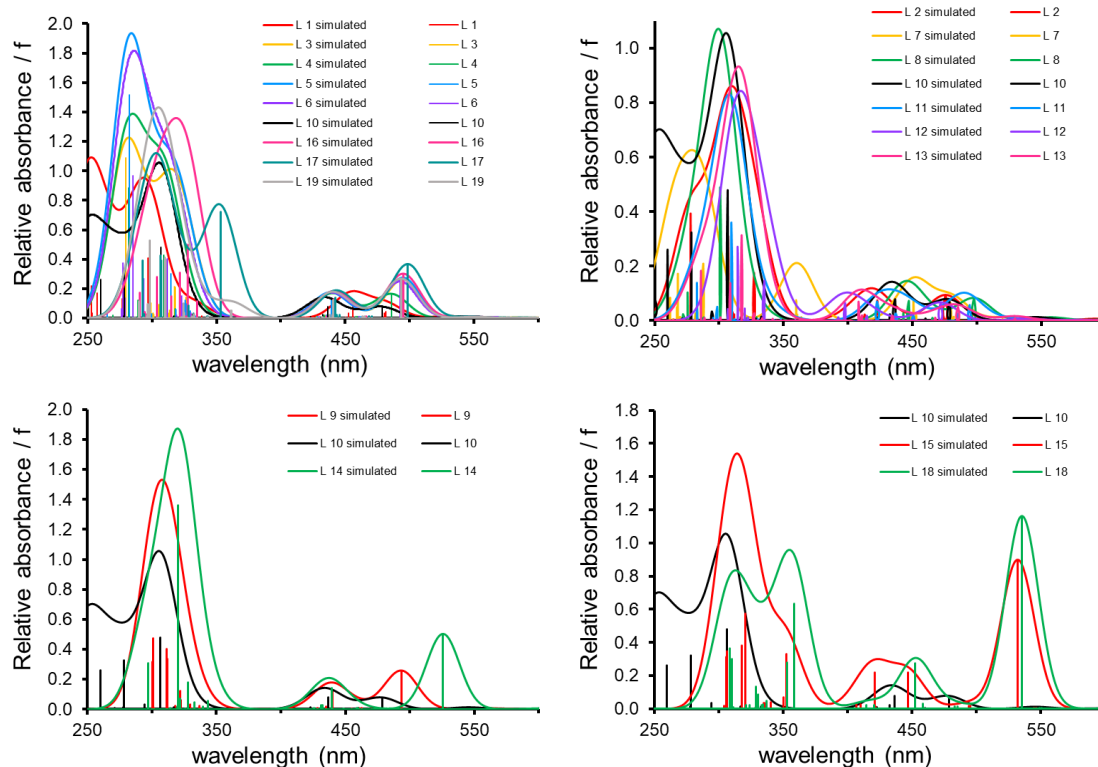


Figure 6: Experimental absorption spectra of the $[\text{FeL}'_n]^{2+}$ in MeCN (smooth curves) overlaid with the M06-D3/CEP-121G calculated oscillators (bar graphs of wavenumber versus the oscillator strengths) in the region 250-600 nm. $n = 1 - 19$. Top left, graph of complexes 1, 3, 4, 5, 6, 10, 16, 17, 1, all containing substituted terpyridine ligands. Top right, graph of complexes 2, 7, 8, 11, 12, 13, all containing tris-azinyl analogues of the terpyridine ligand, including 10 for comparative reasons. Left bottom, graph of complexes 9 and 14, containing a nitro group, including 10 for comparative reasons. Right bottom, graph of complexes 15 and 18, containing an amide group, including 10 for comparative reasons.

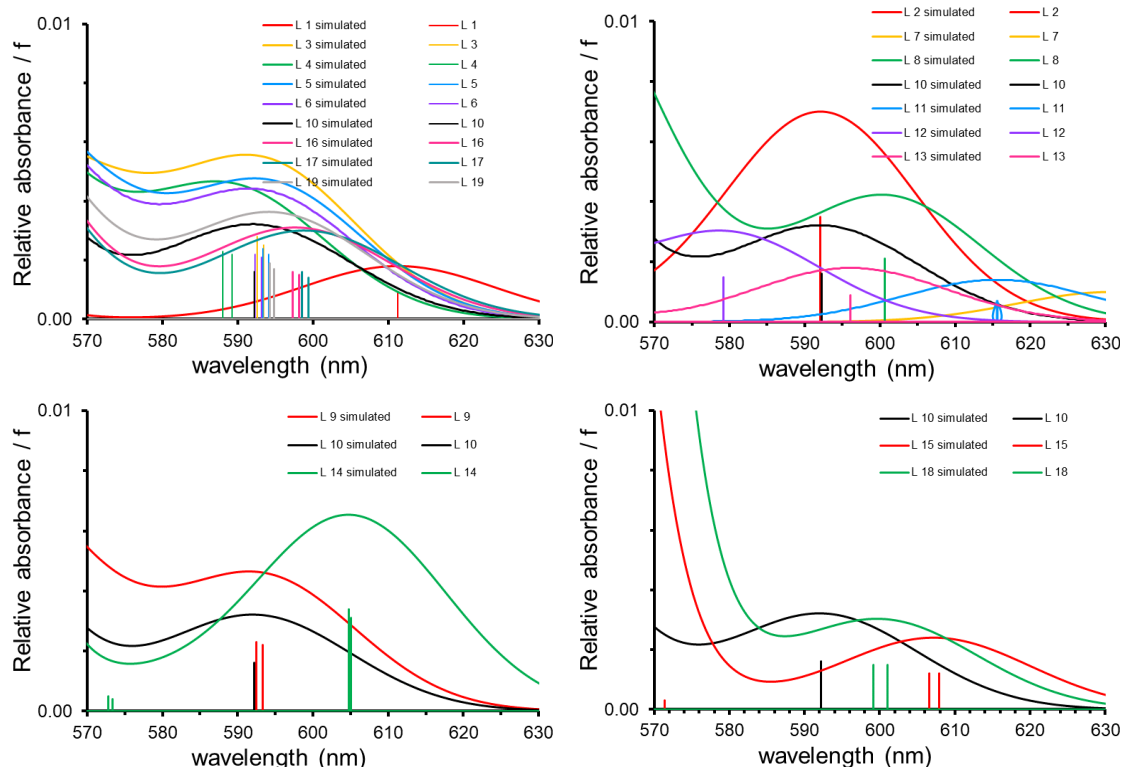


Figure 7: Experimental absorption spectra of complexes 1 – 19, $[\text{FeL}_n]^{2+}$, $n = 1 - 19$, in MeCN (smooth curves) overlaid with the M06-D3/CEP-121G calculated oscillators (bar graphs of wavenumber versus the oscillator strengths) showing the MMCT bands in the region 570-630 nm. Top left, graph of complexes 1, 3, 4, 5, 6, 10, 16, 17, 19, all containing substituted terpyridine ligands. Top right, graph of complexes 2, 7, 8, 11, 12, 13, all containing tris-azanyl analogues of the terpyridine ligand, including 10 for comparative reasons. Left bottom, graph of complexes 9 and 14, containing a nitro group, including 10 for comparative reasons. Right bottom, graph of complexes 15 and 18, containing an amide group, including 10 for comparative reasons.

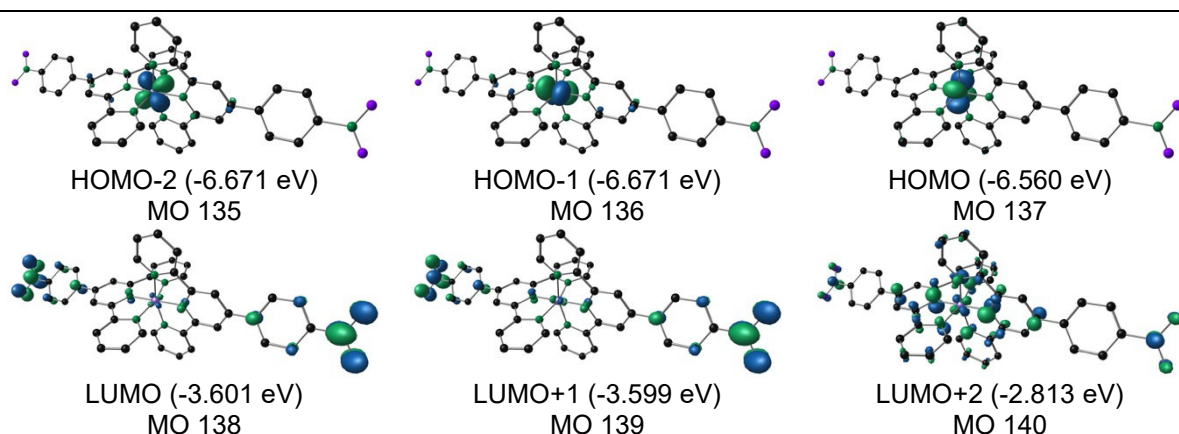


Figure 8: Selected MOs of complex 14, containing a nitro group, energy given in eV in brackets, calculated at the M06-D3/CEP-121G level in MeCN solution.

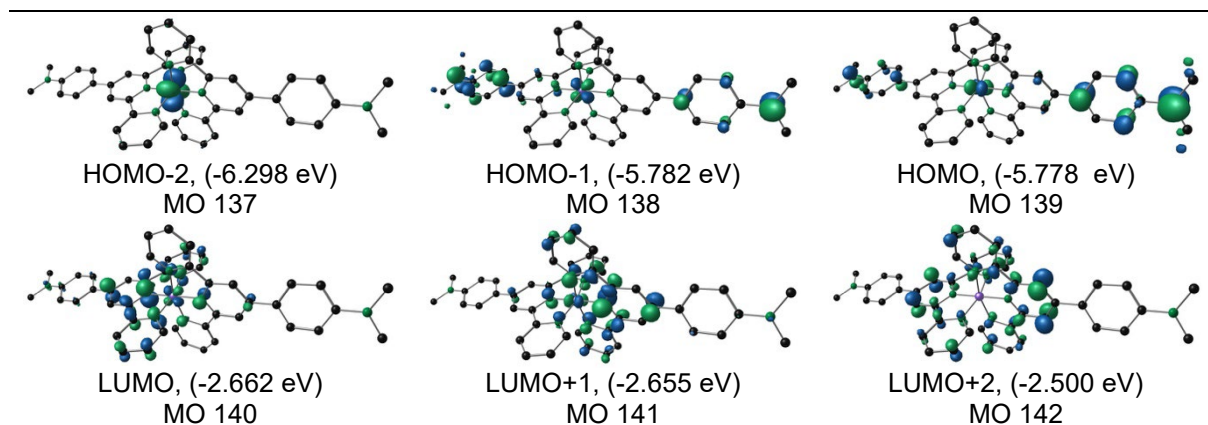


Figure 9: Selected MOs of complex 15, containing an amide group, energy given in eV in brackets, calculated at the M06-D3/CEP-121G level in MeCN solution.

Another way of identifying the type of excitation is to determine the natural transition orbitals (NTOs) involved in each citation. NTOs provide a clear picture of the molecular orbitals involved in the electronic transitions responsible for UV-Vis absorption bands. They enable the identification of the nature of the transitions. NTOs are represented as a linear combination of the occupied (particle) and unoccupied (hole) molecular orbitals [51]. They provide a visual and quantitative description of the orbitals involved in these transitions [52]. The NTOs involved in the transitions at 592.2 nm (excited state S2 and S3), 545.5 nm (excited state S4 and S5), 478 and 436 nm (excited state S8 and S12) and 306.6 nm (excited state S30 and S31) for $[\text{Fe}(\text{L}^{10})_2]^{2+}$ are graphically visualized, as a pair of orbitals that describe the initial and final states of the electronic transition, in Figure 10, Figure 11, Figure 12 and Figure 13, respectively. The character of the NTOs shown that:

- (i) peaks at 592.2 nm (excited state S2 and S3) are MMCT of character (Figure 10).
- (ii) peaks at 545.5 nm (excited state S4 and S5) are MLCT of character (Figure 11), and
- (iii) peaks at 478 and 436 nm (excited state S8 and S12) are MLCT of character (Figure 12).
- (iv) peaks at 306.6 nm (excited state S30 and S31) are LLCT of character (Figure 13). Thus, the information obtained from the NTO analysis regarding the spatial distribution of electron density changes during electronic transitions agrees with the information obtained from the MOs involved in the electronic transitions from Table 2. The NTOs, however, are a more compact tool to provide a visual and quantitative description of the orbitals involved in specific transitions [52].

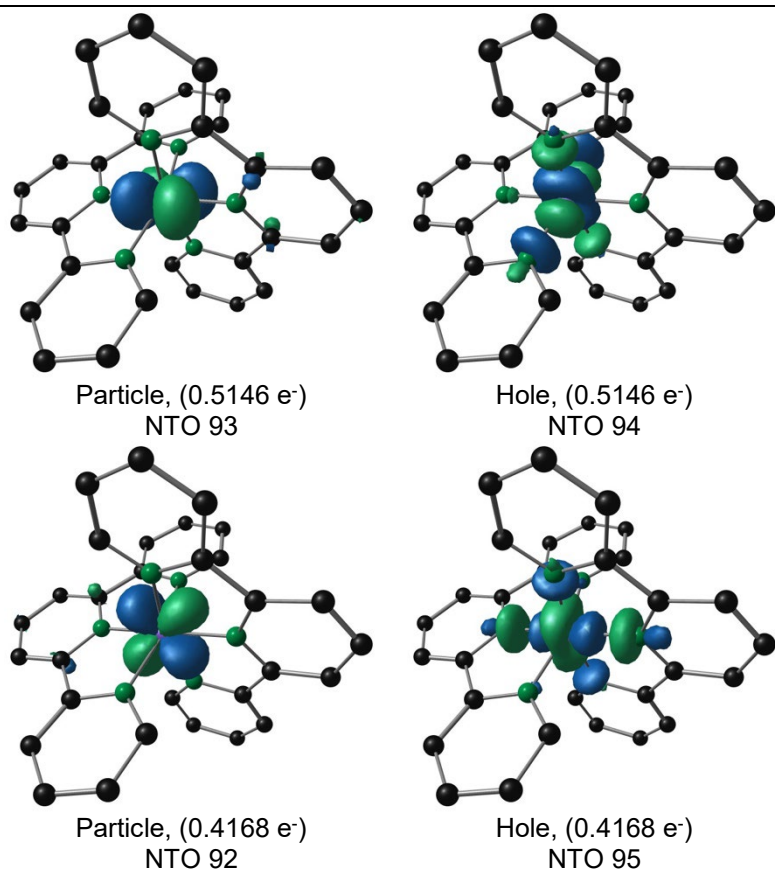


Figure 10: NTOs of excited state 2 (contr. value 0.05), peak at 592.2 nm of 10. The electron occupation of the occupied (particle) and unoccupied (hole) NTO pairs are indicated. NTOs of 0.0969 e^- in Figure S2 of supporting information. Excited state 3 is similar, see supporting information Figure S3. A contour of 0.05 $e/\text{\AA}^3$ was used for the orbital plot. Atoms are colour coded (online version) as follows: Fe (purple), C (black), N (green).

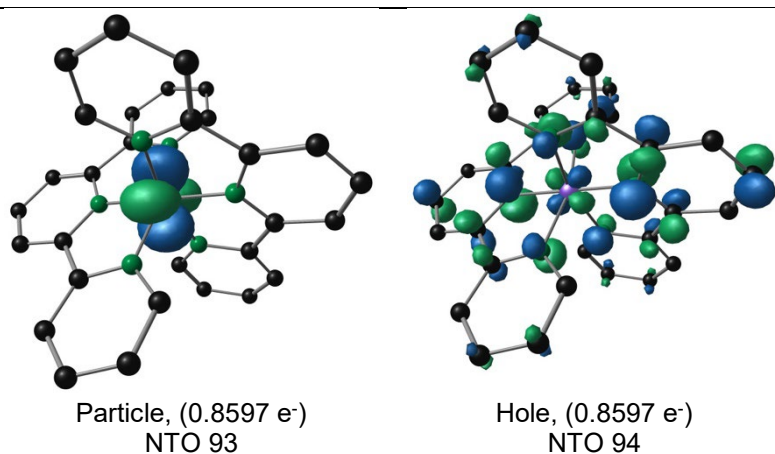


Figure 11: NTOs of excited state 4 (contr. value 0.05), peak at 545.5 nm of 10. NTOs of 0.0441 e^- and 0.0339 e^- in supporting information Figure S4. Excited state 5 is similar, see supporting information Figure S5. See caption of Figure 10 for more info.

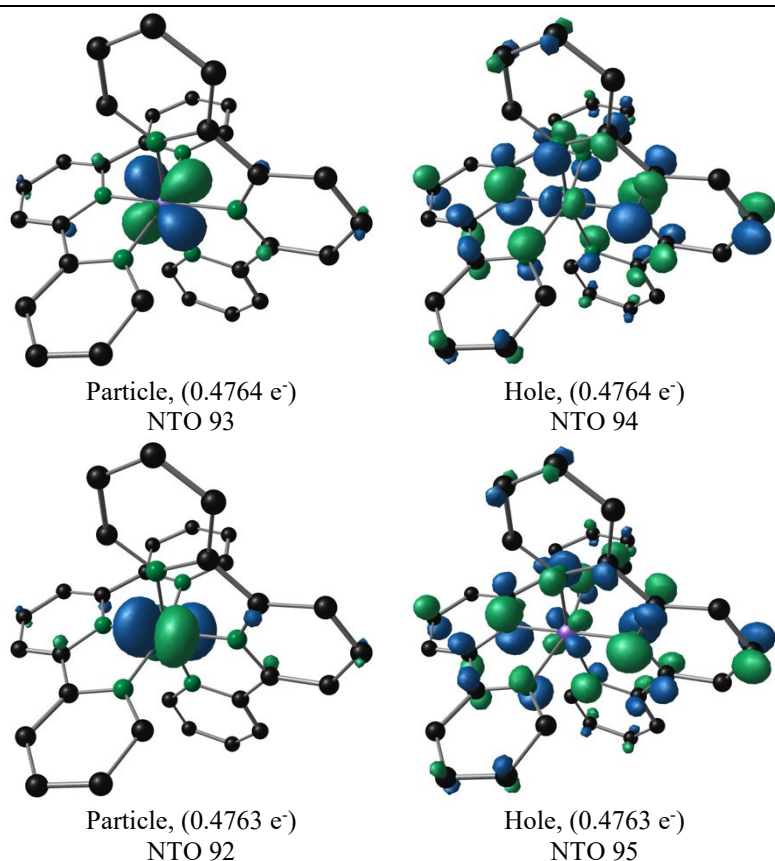


Figure 12: NTOs of excited state S8 (contr. value 0.05), peak at 478 NTOs of 0.0441 e^- in supporting information Figure S6. Excited state 12, peak at 436 nm of 10, is similar, see supporting information Figure S7. See caption of Figure 10 for more info.

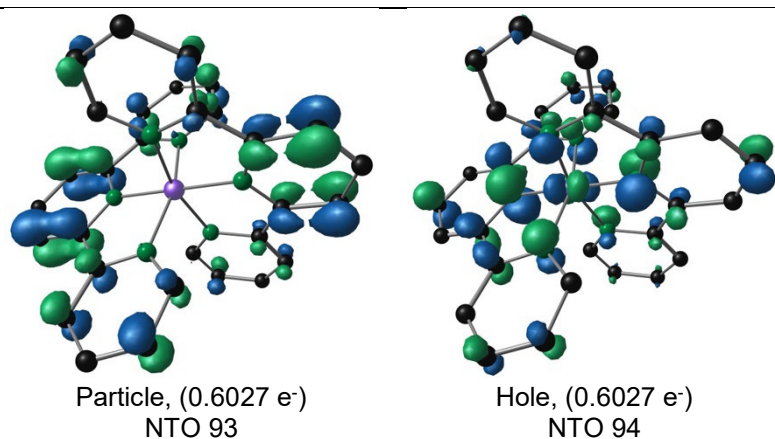


Figure 13: NTOs of excited state 30 (contr. value 0.05), peak at 306.6 nm of 10. NTOs of 0.2280 e^- and 0.1339 e^- in supporting information Figure S8. Excited state 31 is similar, see supporting information Figure S9. See caption of Figure 10 for more info.

3.3 Theoretical Criteria for Evaluating DSSC Efficiency

This section discusses the relationship between specific theoretically calculated values used to assess the efficiency of a dye in a DSSC and experimental values for the same purpose.

Experimentally, critical parameters used to assess the effectiveness of DSSCs include (a) the short-circuit current density (J_{sc}), (b) the open-circuit photovoltage (V_{oc}), (c) the fill factor (FF), and (d) the energy conversion efficiency (η) [53–55]. η reflects how well the DSSC can harness and convert the energy from incident sunlight into electrical power and is the maximum output power divided by the incident solar power on the cell (P_{inc}) [53–59]:

$$\eta = \frac{I_{mp}V_{mp}}{P_{inc}}$$

With I_{mp} , the maximum power point current, and V_{mp} , the maximum power point voltage. FF is a measure of how effectively the solar cell converts light into electrical energy, defined as the maximum output power divided by the product of J_{sc} and V_{oc} [53–56]:

$$FF = \frac{I_{mp}V_{mp}}{J_{sc}V_{oc}}$$

From the above equations, it follows that η is determined by both J_{sc} and V_{oc} [53–59]:

$$\eta = \frac{I_{mp}V_{mp}}{P_{inc}} = \frac{J_{sc}V_{oc}FF}{P_{inc}}$$

J_{sc} represents the maximum current that the cell can generate when the terminals are short-circuited, i.e., when there is no external load connected to the cell, and it is exposed to maximum illumination (sunlight) and is thus primarily determined by the amount of light absorbed by the dye molecules or other sensitizing materials in the DSSC. The J_{sc} in DSSCs can be written as the following integral equation [53,55,57,59]:

$$J_{sc} = \int_{\lambda} LHE(\lambda)\phi_{inject}\eta_{collect}d\lambda$$

$\eta_{collect}$ is the charge collection efficiency, assumed to be a constant for a specific DSSC independent of the type of sensitizer. ϕ_{inject} is the electron injection efficiency, and $LHE(\lambda)$ is the light harvesting efficiency at a given wavelength.

From the discussion above, it follows that high J_{sc} (and thus better η) can be obtained by high $LHE(\lambda)$ and ϕ_{inject} . $LHE(\lambda)$ is determined by the oscillator strength (f) of the absorption peaks, obtained by TDDFT calculations, using equation (2) [32,33,53,57,59,60]. ϕ_{inject} is closely related to ΔG_{inject} , that is, the injection driving force calculated by equation (3) [31,34,53,57,59–61].

Furthermore, assessing the performance of DSSCs includes considering the efficiency of dye regeneration while in the excited state, which is estimated through the regeneration driving force $\Delta G_{regenerate}$. $\Delta G_{regenerate}$ is determined from the difference between the ground state oxidation potential of the dye and the redox potential of the iodide/tri-iodide redox couple, as shown in equation (4) [31,34,53,60,61]. The DFT calculated values of ΔG_{inject} and $\Delta G_{regenerate}$ for 1 – 19 are provided in Table 3 and discussed in section 3.4.4 below.

3.4 Suitability of 1 – 19 as dyes in DSSCs

DSSCs are a type of solar cell that relies on various materials and interfaces for their functionality. DFT calculations can provide valuable insights into the electronic structure and properties of these materials, helping researchers optimize DSSCs. To further systematically explore the properties of complexes 1 – 19, properties essential to characterize a dye to be used in DSSCs containing a TiO₂ semiconductor as photo anode, and the I⁻/I₃⁻ redox mediator are determined and tabulated in Table 3.

3.4.1 UV regions

Choosing a dye that can harness the complete solar spectrum, spanning ultraviolet (UV) to visible (VIS) and near-infrared (NIR) wavelengths, is crucial for optimizing DSSC efficiency. Typically, dyes used in DSSCs are designed to absorb within the visible range, covering wavelengths from approximately 400 nm to 700 nm, considering the significant portion of solar radiation falling within this spectrum. DFT calculations play a vital role in predicting the adsorption energies of dyes on semiconductor surfaces, with strong adsorption being essential for anchoring dye molecules and facilitating efficient charge transfer. Notably, the MLCT peak of 1-19 falls within the range of 545-587 nm experimentally and 400-600 nm calculated. Additionally, the $\lambda_{A,max}$ peaks lie in the UV region, specifically 243-328 nm experimentally (248-358 nm calculated). Any experimentally unobserved peaks (calculated above 580 nm) are too weak to be considered effective dyes for DSSCs.

3.4.2 HOMO-LUMO

DFT calculations are necessary for determining the alignment of energy levels at interfaces within the DSSC, a critical factor for effective charge injection and collection. To ensure the effectiveness of compounds 1 - 19 as dye sensitizers for DSSCs, it is crucial that their excited state energy levels (LUMOs involved in the excitations) are positioned higher than the CB of the semiconductor (TiO₂). Simultaneously, their redox potentials must be sufficiently positive (relative to the Normal Hydrogen Electrode, NHE) to facilitate regeneration via electron donation from the I⁻/I₃⁻ redox electrolyte [60]. Consequently, the HOMO levels of the dye sensitizers must be positioned below the electrolyte's redox potential concerning the vacuum [4].

The HOMOs and LUMOs of bis(terpyridine)iron(II), [Fe(L¹⁰)₂]²⁺, illustrated in Figure 14, together with the potential (E_{CB}) of the TiO₂ and the redox potential of the I⁻/I₃⁻ electrolyte, adhere to these requirements. Similarly, the LUMO and HOMO energies of 1 - 19 are suitably higher than the CB of the TiO₂ (-4.0 eV) and lower than the redox potential of the I⁻/I₃⁻ electrolyte (-4.8 eV); see LUMO (-2.7 – -3.8 eV) and HOMO (-5.8 – -7.6 eV) energies in Table 3. The HOMO energy levels

of CYC-B11, an exceptionally efficient light-absorbing ruthenium dye sensitizer [62] (-5.26 eV as reported [63]), are marginally greater than the HOMO energies of 1 - 19.

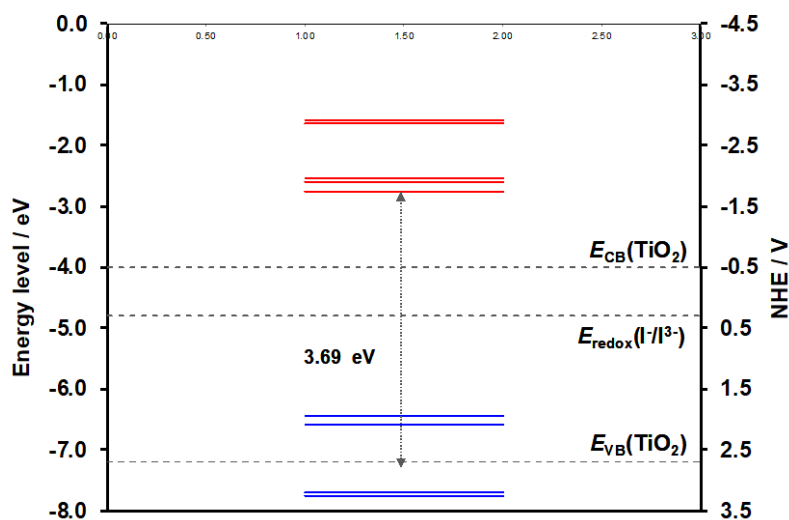


Figure 14: MO energy level and HOMO-LUMO gap of Fe^{II} terpyridine complex 10, calculated at the M06-D3/CEP-121G level in MeCN solution.

3.4.3 Oscillator strength f , LHE and τ

The DFT calculated oscillator strength quantifies the likelihood of an electronic transition occurring between two states within a molecule or atom, such as from the ground state to an excited state. It is connected to the experimental absorption intensity of the molecule in the UV-visible range.

While a greater oscillator strength signifies an increased chance of electronic transition and, consequently, stronger light absorption in the UV-visible region, it does not directly measure the charge transfer rate [64–66]. The oscillator strength further determines the LHE through equation 2. The concept of LHE is central to the operation of DSSCs because it is the initial step in which light energy is captured and converted into electrical energy. The LHE for 1 – 19 for the LMCT bands in the 400-570 nm range up to 0.69 (for complex 14) and the LLCT bands below 360 nm up to 0.97 (complex 14), see Table 3. The LHE of the well-known ruthenium-based dyes CYC-B11 [62] and N3 are 0.34 (calculated from $f = 0.179$ [63]) and 0.23 (calculated from $f = 0.11$ [63]), respectively. On the grounds of LHE, complex 14 (containing a 4' *p*-NO₂-phenyl group) thus shows promising results and could be, with modification, considered to be tested as a dye.

The excited state lifetime (τ) of a dye provides insight into the time a dye molecule remains in an excited state after absorbing a photon. This information is crucial for optimizing the efficiency of DSSCs. Longer excited state lifetimes can lead to increased electron injection into the semiconductor, which is a key factor in enhancing the overall efficiency of the solar cell. The τ for 1

– 19 for the LMCT band at 479 nm of 10 is 47 ns (Table 3), which is similar to the calculated excited state lifetime of CYC-B11 [62] of 27 ns (calculated from $f = 0.179$ and $E_{\lambda} = 2.17$ eV from [63]).

3.4.4 $\Delta G_{\text{regenerate}}$ and ΔG_{inject}

The driving force for dye regeneration, referred to as $\Delta G_{\text{regenerate}}$, is defined as the energy gap between the HOMO of the dye and the reduction potential (E_{redox}) of the electrolyte. To ensure the effectiveness of a DSSC, ΔG_{reg} should be at least 0.2 – 0.3 eV [67]. The energies of the HOMOs of 1-19 are below the potential of the I^-/I_3^- electrolyte, ensuring a large enough driving force for dye regeneration with $\Delta G_{\text{regenerate}}$ values for 1 – 19 between 0.9 - 2.8 eV, see Table 3.

Meanwhile, the driving force for electron injection, known as ΔG_{inject} , is defined by the variance in energy between the excited state of the dye (approximated via the energy of the unoccupied molecular orbitals engaged in the excitation) and the conduction band (CB) of the semiconductor. For efficient injection of the excited electrons, the energy level of the dye's excited state must be at a higher potential (relative to the vacuum level) than the energy level of the conduction band (E_{CB}) of titanium dioxide (TiO_2) [68]. To ensure the effectiveness of a DSSC, it is crucial that ΔG_{inject} exceeds 0.2 eV [67,69]. ΔG_{inject} values depend on the energy of the excited state of the dye (equation 3) and are thus different for each peak of 1 – 19. From Table 3, it is clear that the ΔG_{inject} values of most of the MLCT and LLCT peaks are favourable for electron injection from the dye into the CB of a TiO_2 semiconductor. Greater values for both ΔG_{inject} and $\Delta G_{\text{regenerate}}$ facilitate the process of charge transfer between the conduction band of the semiconductor and the electrolyte [70].

3.4.5 Reorganization E

Reorganization energy for electron λ_e and reorganization energy for hole λ_h are calculated from the electronic energies by [71–74]:

$$\lambda_e = [E_a(Q_n) - E_a(Q_a)] + [(E_n(Q_a) - E_n(Q_n))]$$

$$\lambda_h = [E_c(Q_n) - E_c(Q_c)] + [(E_n(Q_c) - E_n(Q_n))]$$

“ $E_n(Q_n)$, $E_a(Q_a)$, and $E_c(Q_c)$ are the electronic energies of the optimized neutral, anion and cation molecules, respectively. $E_n(Q_a)$ and $E_n(Q_c)$ are the electronic energies of the neutral molecule, calculated from the optimized anion and cation molecules, respectively. $E_a(Q_n)$ and $E_c(Q_n)$ are the electronic energies of the anion and cation, respectively, calculated from the optimized neutral molecule,” [43] where bis(terpyridine)iron(II) is considered the “neutral” molecules.

The reorganization energy is another element that plays a role in determining the effectiveness of DSSCs [75]. Reorganization energy regarding DSSCs refers to the energy required to reorganize

the surrounding environment (including the solvent and other molecules) when an electron is transferred from the dye molecule to the semiconductor (TiO₂) upon photon absorption. Lower reorganization energy leads to more efficient charge separation and a higher J_{sc}, as it allows a greater fraction of the photogenerated electrons to contribute to the photocurrent, ultimately enhancing the overall performance of the DSSC as a solar energy conversion device [76,77]. Reduced total reorganization energy (λ_{total}), comprised of hole (λ_{h}) and electron (λ_{e}) reorganization energies [78], could elevate J_{sc} [77]. Essentially, achieving a lower λ_{total} value leads to swifter charge-carrier transport rates [79]. The computed λ_{h} and λ_{e} for complex 10 is 0.39 and 0.05 respectively. A smaller λ indicates a faster charge transport rate [79], indicating that the electron transport is faster than the hole transport for 10. The small value of $\lambda_{\text{total}} = 0.44$ is advantageous for J_{sc} [77].

3.4.6 V_{oc} and E_{LUMO}

Based on the sensitized mechanism (where electrons are injected from the excited dyes to the semiconductor conduction band) and employing the single electron and single state approximation, a mathematical correlation between V_{oc} and E_{LUMO} [80] can be defined as follows:

$$V_{\text{oc}} = (E_{\text{LUMO}} - E_{\text{CB}})/e$$

It should be noted that this represents an analytical relationship that requires additional validation through experimental testing and theoretical calculations. Nevertheless, the relationship suggests that higher E_{LUMO} values correspond to larger V_{oc}, thus indicating improved energy conversion efficiency (η). Calculated V_{oc} for 1 – 19 are provided in Table 3, with complex 1 having the highest V_{oc}.

Table 3: Computed wavelengths (λ in nm), transition energy (E in eV), oscillator strength (f), LHE, excited lifetime (τ in ns), HOMO and LUMO energy (in eV), ΔG_{inject} (eV), $\Delta G_{\text{regenerate}}$ (eV) and V_{oc} (V) of complexes 1-19, for selected wavelengths. N = excited state

complex	N	λ	f	E	LHE	τ	LUMO	HOMO	ΔG_{inject}	$\Delta G_{\text{regenerate}}$	V _{oc} ^a
1	2	611.31	0.0009	2.03	0.00	6224.18	-2.660	-6.376	-0.35	1.58	1.34
	5	530.78	0.0074	2.34	0.02	570.69	-2.660	-6.376	-0.04	1.58	1.34
	8	481.71	0.0432	2.57	0.09	80.52	-2.660	-6.376	0.20	1.58	1.34
	12	455.84	0.0991	2.72	0.20	31.43	-2.660	-6.376	0.34	1.58	1.34
	48	247.87	0.4707	5.00	0.66	1.96	-2.660	-6.376	2.63	1.58	1.34
2	2	592.10	0.0035	2.09	0.01	1501.49	-3.230	-6.855	-0.76	2.05	0.77
	5	553.21	0.0002	2.24	0.00	22937.80	-3.230	-6.855	-0.61	2.05	0.77
	8	475.58	0.0941	2.61	0.19	36.03	-3.230	-6.855	-0.25	2.05	0.77
	13	422.65	0.0745	2.93	0.16	35.94	-3.230	-6.855	0.08	2.05	0.77
	44	277.84	0.3934	4.46	0.60	2.94	-3.230	-6.855	1.61	2.05	0.77

3	2	593.38	0.0025	2.09	0.01	2111.19	-3.026	-6.572	-0.48	1.77	0.97
	5	561.03	0.003	2.21	0.01	1572.72	-3.026	-6.572	-0.36	1.77	0.97
	8	494.98	0.2660	2.50	0.46	13.81	-3.026	-6.572	-0.07	1.77	0.97
	12	440.67	0.1230	2.81	0.25	23.67	-3.026	-6.572	0.24	1.77	0.97
	48	279.71	1.0870	4.43	0.92	1.08	-3.026	-6.572	1.86	1.77	0.97
4	2	589.18	0.0022	2.10	0.01	2365.24	-2.871	-6.509	-0.40	1.71	1.13
	4	552.17	0.0045	2.25	0.01	1015.63	-2.871	-6.509	-0.26	1.71	1.13
	8	485.77	0.1636	2.55	0.31	21.62	-2.871	-6.509	0.04	1.71	1.13
	12	441.98	0.1171	2.81	0.24	25.01	-2.871	-6.509	0.30	1.71	1.13
	42	281.69	0.8823	4.40	0.87	1.35	-2.871	-6.509	1.89	1.71	1.13
5	2	594.07	0.0022	2.09	0.01	2404.66	-2.953	-6.520	-0.43	1.72	1.05
	5	558.43	0.0038	2.22	0.01	1230.14	-2.953	-6.520	-0.30	1.72	1.05
	8	494.77	0.2752	2.51	0.47	13.33	-2.953	-6.520	-0.01	1.72	1.05
	12	439.45	0.1233	2.82	0.25	23.48	-2.953	-6.520	0.30	1.72	1.05
	41	282.64	1.514	4.39	0.97	0.79	-2.953	-6.520	1.87	1.72	1.05
6	2	593.15	0.0021	2.09	0.00	2511.37	-2.908	-6.504	-0.41	1.70	1.09
	5	555.62	0.0042	2.23	0.01	1101.81	-2.908	-6.504	-0.27	1.70	1.09
	8	492.84	0.2497	2.52	0.44	14.58	-2.908	-6.504	0.01	1.70	1.09
	12	440.88	0.1216	2.81	0.24	23.96	-2.908	-6.504	0.31	1.70	1.09
	41	285.07	0.9685	4.35	0.89	1.26	-2.908	-6.504	1.84	1.70	1.09
7	2	630.82	0.0005	1.97	0.00	11930.06	-3.074	-6.820	-0.85	2.02	0.93
	5	519.84	0.0061	2.39	0.01	664.07	-3.074	-6.820	-0.43	2.02	0.93
	10	479.35	0.0660	2.59	0.14	52.19	-3.074	-6.820	-0.23	2.02	0.93
	14	450.73	0.0768	2.75	0.16	39.65	-3.074	-6.820	-0.07	2.02	0.93
	35	287.70	0.2093	4.31	0.38	5.93	-3.074	-6.820	1.49	2.02	0.93
8	2	600.63	0.0021	2.06	0.00	2575.11	-3.360	-6.986	-0.92	2.19	0.64
	5	557.21	0.0061	2.23	0.01	762.97	-3.360	-6.986	-0.76	2.19	0.64
	8	497.62	0.0828	2.49	0.17	44.83	-3.360	-6.986	-0.49	2.19	0.64
	12	447.13	0.0729	2.77	0.15	41.11	-3.360	-6.986	-0.21	2.19	0.64
	35	300.75	0.4894	4.12	0.68	2.77	-3.360	-6.986	1.14	2.19	0.64
9	2	593.33	0.0022	2.09	0.01	2398.68	-3.507	-6.523	-0.43	1.72	0.49
	5	556.82	0.0029	2.23	0.01	1602.63	-3.507	-6.523	-0.30	1.72	0.49
	8	493.45	0.2544	2.51	0.44	14.35	-3.507	-6.523	-0.01	1.72	0.49
	18	440.25	0.1232	2.82	0.25	23.58	-3.507	-6.523	0.29	1.72	0.49
	49	300.85	0.4752	4.12	0.67	3.06	-3.507	-6.523	1.60	1.72	0.49
10	2	592.21	0.0016	2.09	0.00	3285.74	-2.752	-6.443	-0.35	1.64	1.25
	4	545.47	0.0066	2.27	0.02	675.77	-2.752	-6.443	-0.17	1.64	1.25
	8	478.55	0.0731	2.59	0.15	46.96	-2.752	-6.443	0.15	1.64	1.25
	12	436.50	0.0787	2.84	0.17	36.29	-2.752	-6.443	0.40	1.64	1.25
	30	306.64	0.4794	4.04	0.67	2.94	-2.752	-6.443	1.60	1.64	1.25
11	2	615.61	0.0007	2.01	0.00	8115.49	-3.315	-7.027	-1.01	2.23	0.69
	5	524.43	0.0047	2.36	0.01	877.16	-3.315	-7.027	-0.66	2.23	0.69
	8	494.31	0.0574	2.51	0.12	63.81	-3.315	-7.027	-0.52	2.23	0.69

	16	422.39	0.0704	2.94	0.15	37.99	-3.315	-7.027	-0.09	2.23	0.69
	35	309.48	0.3602	4.01	0.56	3.99	-3.315	-7.027	0.98	2.23	0.69
12	2	579.22	0.0015	2.14	0.00	3352.72	-3.778	-7.547	-1.41	2.75	0.22
	5	538.15	0.0037	2.30	0.01	1173.29	-3.778	-7.547	-1.24	2.75	0.22
	8	471.89	0.0655	2.63	0.14	50.96	-3.778	-7.547	-0.92	2.75	0.22
	15	397.69	0.0651	3.12	0.14	36.42	-3.778	-7.547	-0.43	2.75	0.22
	40	314.29	0.2714	3.94	0.46	5.46	-3.778	-7.547	0.40	2.75	0.22
13	2	596.09	0.0009	2.08	0.00	5918.11	-3.394	-7.152	-1.07	2.35	0.61
	5	529.33	0.0083	2.34	0.02	506.03	-3.394	-7.152	-0.81	2.35	0.61
	8	485.23	0.0502	2.56	0.11	70.31	-3.394	-7.152	-0.60	2.35	0.61
	16	408.11	0.0697	3.04	0.15	35.82	-3.394	-7.152	-0.11	2.35	0.61
	34	317.43	0.3136	3.91	0.51	4.82	-3.394	-7.152	0.75	2.35	0.61
14	2	605.05	0.0031	2.05	0.01	1770.20	-3.601	-6.560	-0.51	1.76	0.40
	5	573.36	0.0004	2.16	0.00	12319.59	-3.601	-6.560	-0.40	1.76	0.40
	8	525.73	0.5029	2.36	0.69	8.24	-3.601	-6.560	-0.20	1.76	0.40
	14	439.58	0.1427	2.82	0.28	20.30	-3.601	-6.560	0.26	1.76	0.40
	38	320.15	1.3631	3.87	0.96	1.13	-3.601	-6.560	1.31	1.76	0.40
15	2	607.93	0.0012	2.04	0.00	4616.66	-2.662	-5.778	0.26	0.98	1.34
	5	545.97	0.0058	2.27	0.01	770.39	-2.662	-5.778	0.49	0.98	1.34
	8	531.81	0.8920	2.33	0.87	4.75	-2.662	-5.778	0.55	0.98	1.34
	16	446.82	0.2207	2.77	0.40	13.56	-2.662	-5.778	1.00	0.98	1.34
	19	421.07	0.2198	2.94	0.40	12.09	-2.662	-5.778	1.17	0.98	1.34
	38	320.44	0.5754	3.87	0.73	2.68	-2.662	-5.778	2.09	0.98	1.34
16	2	598.13	0.0015	2.07	0.00	3575.21	-2.785	-6.416	-0.34	1.62	1.22
	5	549.6	0.0058	2.26	0.01	780.67	-2.785	-6.416	-0.16	1.62	1.22
	8	495.11	0.3005	2.50	0.50	12.23	-2.785	-6.416	0.09	1.62	1.22
	13	441.07	0.1294	2.81	0.26	22.54	-2.785	-6.416	0.39	1.62	1.22
	24	327.95	0.4970	3.78	0.68	3.24	-2.785	-6.416	1.36	1.62	1.22
17	2	599.39	0.0014	2.07	0.00	3846.74	-2.768	-6.379	-0.31	1.58	1.23
	5	548.7	0.0060	2.26	0.01	775.51	-2.768	-6.379	-0.12	1.58	1.23
	8	498.64	0.3660	2.49	0.57	10.18	-2.768	-6.379	0.11	1.58	1.23
	14	442.27	0.1400	2.80	0.28	20.94	-2.768	-6.379	0.42	1.58	1.23
	19	353.19	0.7222	3.51	0.81	2.59	-2.768	-6.379	1.13	1.58	1.23
18	2	601.09	0.0015	2.06	0.00	3610.68	-2.760	-5.770	0.29	0.97	1.24
	5	550.34	0.0055	2.25	0.01	825.47	-2.760	-5.770	0.48	0.97	1.24
	7	535.15	1.1572	2.32	0.93	3.71	-2.760	-5.770	0.55	0.97	1.24
	15	452.26	0.2745	2.74	0.47	11.17	-2.760	-5.770	0.97	0.97	1.24
	27	358.28	0.6322	3.46	0.77	3.04	-2.760	-5.770	1.69	0.97	1.24
19	2	594.83	0.0017	2.08	0.00	3119.88	-2.822	-6.444	-0.36	1.64	1.18
	5	551.86	0.0053	2.25	0.01	861.36	-2.822	-6.444	-0.20	1.64	1.18
	8	493.53	0.2674	2.51	0.46	13.65	-2.822	-6.444	0.07	1.64	1.18
	12	440.58	0.1242	2.81	0.25	23.43	-2.822	-6.444	0.37	1.64	1.18
	41	298.23	0.5274	4.16	0.70	2.53	-2.822	-6.444	1.71	1.64	1.18

4 Conclusions

In summary, selecting an appropriate dye is crucial for maximizing the efficiency of a Dye-sensitized solar cell (DSSC) by ensuring optimal solar spectrum utilization. The strategic alignment of the dye's absorption properties with the solar spectrum is integral to enhancing the overall performance of DSSCs. This comprehensive study utilizing the Density Functional Theory (DFT) method to analyze the spectroscopic behavior of electronically altered iron(II)-terpyridine derivatives has shed substantial light on their potential applications in Dye-Sensitized Solar Cells (DSSCs). The exploration utilizing DFT calculations has made significant strides in comprehending the intricate interplay between the structural features, electronic properties, and absorption spectra of DSSCs. This deeper understanding has led to evaluating dye suitability for optimal solar energy conversion. Notably, the alignment of complexes 1-19's absorption properties with the visible range of the solar spectrum underscores their potential as efficient dyes for DSSCs. Their strong light absorption and charge transfer capabilities further emphasize the significance of these compounds in facilitating effective solar energy conversion.

Moreover, the DFT calculations have successfully elucidated the effects of electronic alterations on the absorption spectra, elucidating the relationship between the molecular structure and the absorption characteristics of the iron(II)-terpyridine derivatives. Notably, utilizing natural transition orbitals (NTOs) has enhanced the understanding of the excitations in the UV-Vis absorption bands, offering a valuable analytical tool for further investigations. DFT calculations have proven instrumental in predicting the adsorption energies of dyes on semiconductor surfaces, a critical factor for securing strong adsorption and efficient charge transfer within the DSSC. In this context, the peak absorption wavelength in the 545 to 587 nm range for the MLCT peak of complexes 1-19 aligns well with the visible spectrum, affirming their potential suitability for effective light absorption and conversion. Conversely, the observation that the experimentally unobserved peaks fall beyond 580 nm indicates weak absorbance, highlighting their limited viability as efficient dyes for DSSCs. In conclusion, the DFT study has not only contributed to the fundamental understanding of the spectroscopic behavior of electronically modified iron(II)-terpyridine derivatives but has also opened up new avenues for the development of high-performance DSSCs, thereby positioning these derivatives as promising candidates for the advancement of renewable energy technologies. Further experimental validation and refinement are imperative to accelerate the practical application of these compounds in real-world solar energy conversion devices.

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Credit author statement

Evangelia Athanasopoulos: “Methodology, Visualization, Data curation, Formal analysis, Investigation, Writing - original draft, Writing - review & editing.”

Jeanet Conradie: “Supervision, Validation, Methodology, Conceptualization, Funding acquisition, Project administration, Writing - review & editing.”

Supporting Information

Optimized coordinates of the DFT calculations, Table S1, Figures S1 – S9.

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Chapter 5: Conclusion & Future Perspectives

Chapter 5: Conclusion and Future Perspectives

5.1 Conclusion

The success of Dye-Sensitized Solar Cells (DSSCs) pivots on the strategic selection and optimization of the photoactive dye, which directly influences solar energy conversion efficacy. This thesis has utilized Density Functional Theory (DFT) to thoroughly analyze the electronic and spectroscopic attributes of Fe(II)-terpyridine derivatives, revealing their potential utility in DSSCs. The DFT-based exploration has greatly enhanced our understanding of the correlation between structural intricacies, electronic attributes, and absorption spectra, which are pivotal for evaluating dye suitability. Crucially, the study has highlighted how the absorption characteristics of complexes 1-19 (Scheme 1, Chapter 4) are harmoniously attuned with the visible solar spectrum, signifying their potential as potent dyes for DSSCs. Their pronounced light absorption and charge transfer proficiency underscore their importance in solar energy conversion.

The DFT computations have not only clarified the impact of electronic modifications on the absorption spectra but have also elucidated the connection between molecular architecture and absorptive behavior, with natural transition orbitals (NTOs) offering a more profound understanding of UV-vis absorption bands. The calculated molecular orbital energies (HOMO/LUMO), electronic chemical potential (μ), electrophilicity index (ω), and electric potentials (Merz-Kollman) underscore the feasibility of using these theoretical insights to predict and enhance the redox potential of novel complexes. The observance of a linear relationship between these calculated properties and experimental electrochemical data underscores the potential of DFT methods in predicting and tailoring redox mediator's characteristics for superior solar harvesting.

In conclusion, this study's DFT analyses have not only enriched the fundamental comprehension of the spectroscopic and electronic behaviour of electronically tailored iron(II)-terpyridine derivatives but have also charted new pathways for the engineering of high-efficiency DSSCs. These derivatives emerge as compelling candidates for propelling renewable energy technologies forward. To transition from theoretical models to tangible solar energy harvesting innovations, further experimental validation and optimization are vital, promising to expedite the deployment of these compounds in practical solar energy devices.

5.2 *Future Perspectives*

- ◆ ***Enhance Computational Models:*** Streamline models for better redox property predictions of iron(II)-terpyridine derivatives.
- ◆ ***Synthesize New Derivatives:*** Use models to create derivatives with desired electronic characteristics.
- ◆ ***DSSCs and Electronics Use:*** Apply these derivatives in solar cells and electronics for improved performance.
- ◆ ***Biomedical Exploration:*** Examine the potential of these compounds in medicine and biology.
- ◆ ***Environmental Assessment:*** Study the ecological effects and degradation patterns of these compounds.
- ◆ ***Photo-catalysis:*** Explore the application of iron(II)-terpyridine derivatives in photo-catalytic processes for environmental and industrial purposes.

5.3 *Publications from this study*

5.3.1 Publications

1. E. Athanasopoulos, J. Conradie, Substituent effect on the oxidation and reduction of electronically altered iron(II)-terpyridine derivatives – DFT study, *Inorganica Chim. Acta*. 555 (2023) 121599. <https://doi.org/10.1016/j.ica.2023.121599>.
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2. E. Athanasopoulos, J. Conradie, DFT study of the spectroscopic behaviour of different iron(II)-terpyridine derivatives with application in DSSCs, submitted to *J. Mol. Graph. Model.* (31.09.2023) Manuscript ID JMGM-D-23-01121
<https://www.sciencedirect.com/journal/journal-of-molecular-graphics-and-modelling> Elsevier.

Appendix A

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- Supporting information associated with article *Inorganica Chimica Acta*, 555, 121599: Figures S1-S2 and Tables S1 – S10. Optimized coordinates of the DFT calculations as xyz files (also available online at: <https://doi.org/10.1016/J.ICA.2023.121599>).

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Substituent effect on the oxidation and reduction of electronically altered iron(II)-terpyridine derivatives – DFT study
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Supplementary material to article *Inorganica Chimica Acta*, 555, 121599:

Supporting information

1 Figures

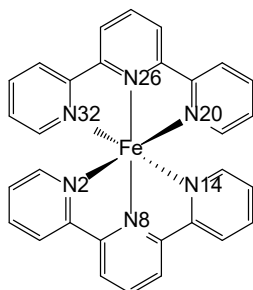


Figure S 1: Atom numbering used in Table S 5 – Table S 10 for coordinating N's.

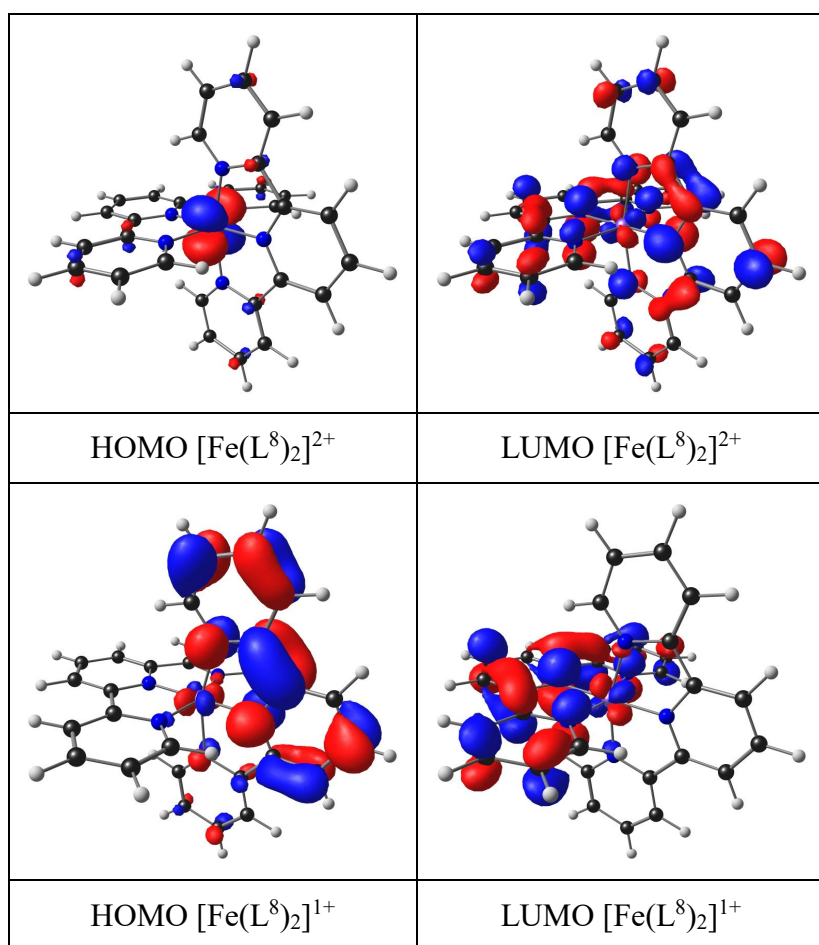


Figure S 2: Selected MOs of $[\text{Fe}(\text{L}^8)_2]^{m+}$ ($\text{L}^8 = \text{tpy}$, $m = 1 - 2$).

2 Tables

Table S 1: DFT calculated data obtained from the gas phase optimized $[\text{Fe}(\text{L})_2]^{2+}$ structures ($\text{L} = \text{L}^1\text{-L}^{25}$). DFT computed HOMO ($E_{\text{HOMO}} = -\text{IP}$) and LUMO ($E_{\text{LUMO}} = -\text{EA}$) energies, electronic chemical potential (μ) (eV), chemical hardness (η) (eV), global electrophilicity index (ω) (eV) and DFT calculated Merz-Kollman atomic charge and electric potential.

L	Electronic energy of calculated $[\text{Fe}(\text{L})_2]^{2+}$ in gas phase, DFT analysis.						
	E_{HOMO} (eV)	E_{LUMO} (eV)	μ (eV)	η (eV)	ω (eV)	Merz-Kollman	
						Atomic charge	Electric potential
L^1	-10.282	-6.937	-8.609	3.345	11.079	-0.500	-115.578
L^2	-10.449	-7.057	-8.753	3.392	11.294	-0.522	-115.573
L^3	-10.447	-7.058	-8.753	3.389	11.302	-0.463	-115.574
L^4	-11.229	-7.630	-9.429	3.598	12.356	-0.430	-115.551
L^5	-10.065	-7.473	-9.269	3.591	11.962	-0.396	-115.557
L^6	-10.612	-7.338	-8.975	3.274	12.302	-0.492	-115.562
L^7	-11.192	-7.691	-9.442	3.502	12.729	-0.413	-115.551
L^8	-11.432	-7.854	-9.643	3.578	12.994	-0.671	-115.542
L^9	-11.712	-8.053	-9.883	3.660	13.343	-0.434	-115.533
L^{10}	-10.544	-7.963	-9.753	3.580	13.286	-0.507	-115.538
L^{11}	-11.550	-8.104	-9.827	3.446	14.014	-0.498	-115.536
L^{12}	-11.287	-7.908	-9.597	3.378	13.632	-0.449	-115.541
L^{13}	-12.106	-8.482	-10.294	3.623	14.625	-0.707	-115.517
L^{14}	-11.684	-8.183	-9.933	3.501	14.091	-0.572	-115.532
L^{15}	-11.941	-8.387	-10.164	3.554	14.533	-0.822	-115.521
L^{16}	-12.143	-8.612	-10.378	3.531	15.251	-0.737	-115.516
L^{17}	-12.399	-8.734	-10.567	3.665	15.232	-0.919	-115.508
L^{18}	-12.102	-8.580	-10.341	3.523	15.179	-1.633	-115.515
L^{19}	-12.908	-9.241	-11.074	3.667	16.722	-1.175	-115.487
L^{20}	-10.494	-6.953	-8.724	3.541	10.746	-0.377	-115.575
L^{21}	-10.770	-7.544	-9.157	3.226	12.994	-0.587	-115.555
L^{22}	-10.329	-6.991	-8.660	3.338	11.235	0.226	-115.580
L^{23}	-8.964	-5.935	-7.450	3.029	9.162	-0.212	-115.626
L^{24}	-11.734	-7.775	-9.755	3.959	12.019	0.138	-115.524
L^{25}	-10.080	-7.193	-8.637	2.887	12.919	-0.516	-115.568

Table S 2: DFT calculated energies. The DFT optimized [FeL₂]ⁿ (n = 1, 2, 3) electronic energy was used to calculate adiabatic ionization potentials (IP_a) (eV), the adiabatic electron affinity (EA_a) (eV), electronic chemical potential (μ) (eV), chemical hardness (η) (eV) and global electrophilicity index (ω) (eV) in gas phase.

L	Adiabatic IP (eV) calc.	Adiabatic EA (eV) calc.	μ (eV)	η (eV)	ω (eV)
L ¹	10.77	5.94	-8.357	4.827	7.234
L ²	10.98	6.04	-8.512	4.940	7.333
L ³	10.91	6.05	-8.481	4.861	7.398
L ⁴	11.75	6.56	-9.154	5.194	8.067
L ⁵	11.44	6.43	-8.935	5.011	7.966
L ⁶	11.19	6.38	-8.786	4.810	8.025
L ⁷	11.58	6.66	-9.121	4.918	8.459
L ⁸	11.91	6.75	-9.329	5.154	8.443
L ⁹	12.16	6.97	-9.568	5.185	8.827
L ¹⁰	12.04	6.91	-9.475	5.139	8.735
L ¹¹	11.93	7.07	-9.501	4.859	9.29
L ¹²	11.81	6.90	-9.353	4.912	8.904
L ¹³	12.60	7.39	-9.995	5.205	9.596
L ¹⁴	12.04	7.19	-9.614	4.848	9.533
L ¹⁵	12.38	7.27	-9.825	5.117	9.432
L ¹⁶	12.59	7.50	-10.043	5.091	9.904
L ¹⁷	12.86	7.61	-10.234	5.244	9.987
L ¹⁸	12.55	7.46	-10.004	5.088	9.835
L ¹⁹	13.37	8.04	-10.706	5.327	10.759
L ²⁰	10.79	-	-	-	-
L ²¹	11.38	6.53	-8.956	4.845	8.278
L ²²	10.67	6.01	-8.345	4.660	7.471
L ²³	9.23	5.08	-7.156	4.151	6.167
L ²⁴	12.45	6.58	-9.517	5.872	7.713
L ²⁵	10.99	6.27	-8.629	4.720	7.889

Table S 3: DFT calculated $\text{Fe}^{\text{II/III}}$ redox potential ($E_{\text{calc. vs FcH/FcH}^+}$) in V.

L	$E_{\text{cal}}(\text{Fe}^{\text{II/III}})$ vs FcH/FcH^+ (V) from Eq 8, using $E_{\text{FcH/FcH}^+} = 4.980$ V [1]	$E_{\text{cal}}(\text{Fe}^{\text{II/III}})$ vs FcH/FcH^+ (V) using the experimental potential vs FcH/FcH^+ of $[\text{Fe}(\text{tpy})_2]^{2+}$ [2]	$E_{\text{predicted}}(\text{Fe}^{\text{II/III}})$ vs FcH/FcH^+ (V) using the linear equation Figure 5(f)	% error predicted using the linear eq Figure 5 (f) from exp. ^a
L ¹	0.129	0.249	0.29	12%
L ²	0.210	0.330	0.36	27%
L ³	0.171	0.291	0.32	6%
L ⁴	0.570	0.690	0.64	17%
L ⁵	0.433	0.553	0.53	11%
L ⁶	0.569	0.689	0.64	6%
L ⁷	0.566	0.686	0.64	8%
L ⁸	0.600	0.720	0.66	8%
L ⁹	0.828	0.948	0.85	13%
L ¹⁰	0.818	0.938	0.84	9%
L ¹¹	0.758	0.878	0.79	4%
L ¹²	0.731	0.851	0.77	7%
L ¹³	1.059	1.179	1.03	14%
L ¹⁴	0.920	1.040	0.92	0%
L ¹⁵	0.909	1.029	0.91	4%
L ¹⁶	1.025	1.145	1.00	2%
L ¹⁷	1.167	1.287	1.12	4%
L ¹⁸	1.165	1.285	1.11	7%
L ¹⁹	1.499	1.619	1.38	1%
L ²⁰	0.397	0.517	0.50	
L ²¹	0.636	0.756	0.69	
L ²²	0.176	0.296	0.33	15%
L ²³	-0.515	-0.395	-0.22	16%
L ²⁴	0.795	0.915	0.82	11%
L ²⁵	0.570	0.690	0.64	4%
MAD		0.05	0.05	average: 9%

^a % depends on the value used to convert absolute redox potential to potential vs FcH/FcH^+ .

Table S 4: DFT calculated data obtained from the solvent (CH₃CN) phase optimized [Fe(L)₂]²⁺ structures (L = L¹-L²⁵). DFT calculated HOMO (E_{HOMO}) and LUMO (E_{LUMO}) energies, electronic chemical potential (μ) (eV), chemical hardness (η) (eV), global electrophilicity index (ω) (eV), Merz-Kollman atomic charge and electric potential.

L	Electronic energy of calculated [Fe(L) ₂] ²⁺ in solvent (CH ₃ CN) phase. DFT analysis						
	E _{HOMO} (eV)	E _{LUMO} (eV)	μ (eV)	η (eV)	ω (eV)	Merz-Kollman	
						Atomic charge	Electric potential
L ¹	-5.843	-2.476	-4.159	3.367	2.569	-0.558	-115.578
L ²	-5.891	-2.491	-4.191	3.400	2.583	-0.580	-115.573
L ³	-5.918	-2.511	-4.214	3.407	2.606	-0.445	-115.574
L ⁴	-6.311	-2.712	-4.512	3.598	2.828	-0.298	-115.551
L ⁵	-6.290	-2.701	-4.495	3.589	2.816	-0.362	-115.556
L ⁶	-6.390	-2.875	-4.632	3.515	3.052	-0.534	-115.562
L ⁷	-6.415	-2.960	-4.688	3.456	3.179	-0.426	-115.551
L ⁸	-6.424	-2.860	-4.642	3.565	3.022	-0.679	-115.542
L ⁹	-6.665	-3.028	-4.847	3.637	3.230	-0.447	-115.532
L ¹⁰	-6.549	-2.998	-4.773	3.552	3.208	-0.540	-115.538
L ¹¹	-6.630	-3.268	-4.949	3.363	3.642	-0.600	-115.536
L ¹²	-6.564	-3.053	-4.809	3.511	3.293	-0.330	-115.539
L ¹³	-6.897	-3.345	-5.121	3.552	3.691	-0.481	-115.514
L ¹⁴	-6.718	-3.282	-5.000	3.437	3.637	-0.579	-115.529
L ¹⁵	-6.784	-3.258	-5.021	3.527	3.574	-0.838	-115.521
L ¹⁶	-6.885	-3.369	-5.127	3.515	3.739	-0.577	-115.516
L ¹⁷	-7.028	-3.401	-5.215	3.627	3.749	-0.825	-115.508
L ¹⁸	-7.029	-3.503	-5.266	3.526	3.933	-1.456	-115.515
L ¹⁹	-7.374	-3.734	-5.554	3.640	4.237	-1.024	-115.487
L ²⁰	-6.208	-2.675	-4.441	3.534	2.791	-0.350	-115.575
L ²¹	-6.441	-2.944	-4.692	3.497	3.148	-0.537	-115.554
L ²²	-5.965	-2.596	-4.280	3.368	2.720	0.079	-115.579
L ²³	-5.249	-2.179	-3.714	3.069	2.247	-0.285	-115.626
L ²⁴	-6.453	-2.480	-4.466	3.973	2.510	0.020	-115.524
L ²⁵	-6.252	-2.840	-4.546	3.411	3.029	-0.539	-115.567

Table S 5: NBO charges on Fe and the coordinated N's of the DFT gas phase optimized [Fe(L)₂]²⁺ complexes (L = L¹-L²⁵). Atom numbering as in Error! Reference source not found. (c).

Atom No.	L ¹	L ²	L ³	L ⁴	L ⁵	L ⁶	L ⁷	L ⁸	L ⁹	L ¹⁰	L ¹¹	L ¹²	L ¹³
Fe (1)	1.140	1.140	1.140	1.140	1.139	1.138	1.139	1.137	1.148	1.140	1.140	1.140	1.138
N (2)	-0.505	-0.505	-0.505	-0.506	-0.506	-0.505	-0.505	-0.505	-0.538	-0.505	-0.506	-0.506	-0.482
N (8)	-0.558	-0.554	-0.557	-0.536	-0.537	-0.523	-0.519	-0.509	-0.535	-0.517	-0.502	-0.511	-0.540
N (14)	-0.505	-0.505	-0.505	-0.505	-0.505	-0.505	-0.505	-0.505	-0.537	-0.505	-0.505	-0.505	-0.482
N (20)	-0.505	-0.505	-0.505	-0.505	-0.505	-0.505	-0.505	-0.505	-0.538	-0.505	-0.505	-0.505	-0.482
N (26)	-0.558	-0.554	-0.557	-0.536	-0.537	-0.523	-0.519	-0.509	-0.535	-0.517	-0.502	-0.511	-0.540
N (32)	-0.505	-0.505	-0.505	-0.506	-0.506	-0.505	-0.505	-0.505	-0.537	-0.505	-0.506	-0.506	-0.482
	L ¹⁴	L ¹⁵	L ¹⁶	L ¹⁷	L ¹⁸	L ¹⁹	L ²⁰	L ²¹	L ²²	L ²³	L ²⁴	L ²⁵	
Fe (1)	1.140	1.143	1.138	1.135	1.097	1.141	1.134	1.138	1.142	1.139	1.129	1.138	
N (2)	-0.506	-0.508	-0.538	-0.482	-0.308	-0.485	-0.509	-0.505	-0.532	-0.544	-0.353	-0.482	
N (8)	-0.502	-0.483	-0.502	-0.512	-0.463	-0.486	-0.512	-0.521	-0.532	-0.545	-0.353	-0.540	
N (14)	-0.505	-0.508	-0.538	-0.482	-0.308	-0.485	-0.510	-0.505	-0.532	-0.545	-0.353	-0.482	
N (20)	-0.505	-0.508	-0.538	-0.482	-0.308	-0.485	-0.509	-0.505	-0.532	-0.545	-0.54	-0.482	
N (26)	-0.502	-0.483	-0.502	-0.512	-0.463	-0.487	-0.512	-0.521	-0.532	-0.544	-0.353	-0.540	
N (32)	-0.506	-0.508	-0.538	-0.482	-0.308	-0.485	-0.510	-0.505	-0.532	-0.545	-0.54	-0.482	

Table S 6: NBO charges on Fe and the coordinated N's of the DFT gas phase optimized [Fe(L)₂]³⁺ complexes (L = L¹-L²⁵). Atom numbering as in Error! Reference source not found. (c).

Atom No.	L ¹	L ²	L ³	L ⁴	L ⁵	L ⁶	L ⁷	L ⁸	L ⁹	L ¹⁰	L ¹¹	L ¹²	L ¹³
Fe (1)	1.394	1.377	1.398	1.396	1.380	1.376	1.376	1.373	1.388	1.414	1.390	1.394	1.406
N (2)	-0.522	-0.510	-0.523	-0.513	-0.517	-0.518	-0.517	-0.518	-0.550	-0.514	-0.527	-0.528	-0.490
N (8)	-0.587	-0.582	-0.585	-0.566	-0.553	-0.547	-0.536	-0.518	-0.548	-0.547	-0.518	-0.529	-0.570
N (14)	-0.506	-0.510	-0.505	-0.512	-0.517	-0.518	-0.518	-0.518	-0.550	-0.514	-0.510	-0.508	-0.490
N (20)	-0.522	-0.508	-0.522	-0.508	-0.517	-0.518	-0.518	-0.518	-0.550	-0.514	-0.510	-0.508	-0.490
N (26)	-0.587	-0.580	-0.585	-0.555	-0.553	-0.547	-0.536	-0.518	-0.548	-0.547	-0.518	-0.529	-0.570
N (32)	-0.506	-0.508	-0.507	-0.509	-0.517	-0.518	-0.517	-0.518	-0.550	-0.514	-0.527	-0.528	-0.490
	L ¹⁴	L ¹⁵	L ¹⁶	L ¹⁷	L ¹⁸	L ¹⁹	L ²⁰	L ²¹	L ²²	L ²³	L ²⁴	L ²⁵	
Fe (1)	1.388	1.385	1.391	1.402	1.357	1.400	1.364	1.376	1.382	1.366	1.343	1.378	
N (2)	-0.511	-0.510	-0.560	-0.487	-0.339	-0.490	-0.522	-0.518	-0.553	-0.57	-0.368	-0.518	
N (8)	-0.518	-0.496	-0.517	-0.531	-0.482	-0.504	-0.523	-0.545	-0.548	-0.563	-0.368	-0.558	
N (14)	-0.525	-0.530	-0.543	-0.506	-0.314	-0.509	-0.502	-0.518	-0.539	-0.549	-0.368	-0.518	
N (20)	-0.526	-0.523	-0.542	-0.488	-0.315	-0.508	-0.522	-0.518	-0.553	-0.559	-0.544	-0.518	
N (26)	-0.518	-0.494	-0.517	-0.530	-0.482	-0.503	-0.522	-0.545	-0.548	-0.559	-0.368	-0.558	
N (32)	-0.51	-0.517	-0.561	-0.506	-0.338	-0.491	-0.522	-0.518	-0.538	-0.56	-0.544	-0.518	

Table S 7: NBO charges on Fe and the coordinated N's of the DFT solvent (CH₃CN) phase optimized [Fe(L)₂]²⁺ complexes (L = L¹-L²⁵). Atom numbering as in Error! Reference source not found. (c).

Atom No.	L ¹	L ²	L ³	L ⁴	L ⁵	L ⁶	L ⁷	L ⁸	L ⁹	L ¹⁰	L ¹¹	L ¹²	L ¹³
Fe (1)	1.132	1.131	1.132	1.130	1.130	1.128	1.130	1.127	1.136	1.129	1.129	1.128	1.126
N (2)	-0.503	-0.504	-0.504	-0.504	-0.504	-0.503	-0.503	-0.503	-0.536	-0.503	-0.503	-0.503	-0.479
N (8)	-0.556	-0.552	-0.554	-0.533	-0.534	-0.520	-0.517	-0.507	-0.532	-0.515	-0.499	-0.509	-0.537
N (14)	-0.503	-0.504	-0.503	-0.503	-0.503	-0.503	-0.504	-0.503	-0.535	-0.503	-0.503	-0.503	-0.478
N (20)	-0.503	-0.504	-0.503	-0.503	-0.503	-0.503	-0.503	-0.503	-0.536	-0.503	-0.503	-0.503	-0.479
N (26)	-0.556	-0.552	-0.554	-0.533	-0.534	-0.520	-0.517	-0.507	-0.532	-0.515	-0.499	-0.509	-0.521
N (32)	-0.503	-0.504	-0.504	-0.504	-0.504	-0.503	-0.503	-0.503	-0.535	-0.503	-0.503	-0.503	-0.479
	L ¹⁴	L ¹⁵	L ¹⁶	L ¹⁷	L ¹⁸	L ¹⁹	L ²⁰	L ²¹	L ²²	L ²³	L ²⁴	L ²⁵	
Fe (1)	1.128	1.133	1.131	1.122	1.084	1.129	1.126	1.128	1.133	1.135	1.115	1.128	
N (2)	-0.503	-0.506	-0.537	-0.479	-0.306	-0.482	-0.508	-0.503	-0.529	-0.544	-0.351	-0.504	
N (8)	-0.500	-0.481	-0.500	-0.510	-0.460	-0.483	-0.510	-0.518	-0.53	-0.544	-0.351	-0.525	
N (14)	-0.503	-0.506	-0.537	-0.479	-0.306	-0.482	-0.508	-0.503	-0.53	-0.544	-0.351	-0.503	
N (20)	-0.503	-0.506	-0.537	-0.479	-0.306	-0.482	-0.508	-0.503	-0.529	-0.544	-0.537	-0.503	
N (26)	-0.500	-0.481	-0.500	-0.510	-0.46	-0.483	-0.510	-0.518	-0.53	-0.543	-0.351	-0.525	
N (32)	-0.503	-0.506	-0.537	-0.479	-0.306	-0.482	-0.508	-0.503	-0.53	-0.544	-0.537	-0.504	

Table S 8: Mulliken charges on Fe and the coordinated N's of the DFT gas phase optimized [Fe(L)₂]²⁺ complexes (L = L¹-L²⁵). Atom numbering as in Error! Reference source not found.

(c).

Analysis of Sum of Mulliken Charges with summed hydrogen in the DFT-optimized geometries of Fe ^{II} L ₁ -L ₂₅ in gas phase.													
Atom No.	L ₁	L ₂	L ₃	L ₄	L ₅	L ₆	L ₇	L ₈	L ₉	L ₁₀	L ₁₁	L ₁₂	L ₁₃
Fe (1)	1.312	1.311	1.310	1.308	1.309	1.307	1.308	1.304	1.324	1.307	1.307	1.307	1.308
N (2)	-0.545	-0.546	-0.546	-0.549	-0.549	-0.548	-0.550	-0.550	-0.527	-0.550	-0.552	-0.550	-0.504
N (8)	-0.671	-0.668	-0.666	-0.651	-0.654	-0.645	-0.644	-0.633	-0.654	-0.639	-0.634	-0.636	-0.659
N (14)	-0.545	-0.546	-0.545	-0.547	-0.547	-0.548	-0.549	-0.550	-0.525	-0.550	-0.551	-0.551	-0.502
N (20)	-0.545	-0.546	-0.545	-0.547	-0.547	-0.548	-0.549	-0.550	-0.527	-0.550	-0.551	-0.551	-0.502
N (26)	-0.671	-0.668	-0.666	-0.651	-0.654	-0.645	-0.644	-0.633	-0.654	-0.639	-0.634	-0.636	-0.659
N (32)	-0.545	-0.546	-0.546	-0.549	-0.549	-0.548	-0.550	-0.550	-0.525	-0.550	-0.552	-0.550	-0.504
Atom No.	L ₁₄	L ₁₅	L ₁₆	L ₁₇	L ₁₈	L ₁₉	L ₂₀	L ₂₁	L ₂₂	L ₂₃	L ₂₄	L ₂₅	
Fe (1)	1.306	1.311	1.306	1.304	1.264	1.311	1.310	1.307	1.313	1.314	1.314	1.308	
N (2)	-0.552	-0.553	-0.541	-0.505	-0.436	-0.507	-0.558	-0.549	-0.567	-0.570	-0.346	-0.548	
N (8)	-0.632	-0.586	-0.633	-0.640	-0.640	-0.590	-0.640	-0.644	-0.649	-0.656	-0.665	-0.649	
N (14)	-0.5521	-0.553	-0.541	-0.505	-0.436	-0.507	-0.553	-0.549	-0.561	-0.570	-0.346	-0.548	
N (20)	-0.551	-0.553	-0.541	-0.505	-0.436	-0.507	-0.557	-0.549	-0.567	-0.570	-0.346	-0.548	
N (26)	-0.632	-0.586	-0.633	-0.640	-0.640	-0.590	-0.639	-0.644	-0.649	-0.655	-0.665	-0.649	
N (32)	-0.552	-0.553	-0.541	-0.505	-0.436	-0.507	-0.558	-0.549	-0.561	-0.570	-0.346	-0.548	

Table S 9: Mulliken charges on Fe and the coordinated N's of the DFT gas phase optimized [Fe(L)₂]³⁺ complexes (L = L¹-L²⁵). Atom numbering as in Error! Reference source not found. (c).

Analysis of Sum of Mulliken Charges with summed hydrogen in the DFT-optimized geometries of Fe ^{III} L ₁ -L ₂₅ in gas phase													
Atom Nr.	L ₁	L ₂	L ₃	L ₄	L ₅	L ₆	L ₇	L ₈	L ₉	L ₁₀	L ₁₁	L ₁₂	L ₁₃
Fe (1)	1.431	1.421	1.431	1.425	1.417	1.414	1.413	1.408	1.437	1.431	1.420	1.423	1.432
N (2)	-0.585	-0.566	-0.587	-0.572	-0.593	-0.592	-0.594	-0.595	-0.569	-0.583	-0.601	-0.599	-0.530
N (8)	-0.726	-0.741	-0.721	-0.722	-0.682	-0.678	-0.669	-0.653	-0.681	-0.696	-0.662	-0.668	-0.719
N (14)	-0.573	-0.566	-0.572	-0.570	-0.591	-0.592	-0.593	-0.595	-0.567	-0.583	-0.587	-0.585	-0.532
N (20)	-0.585	-0.580	-0.587	-0.584	-0.591	-0.592	-0.593	-0.595	-0.569	-0.583	-0.587	-0.585	-0.530
N (26)	-0.726	-0.741	-0.718	-0.692	-0.682	-0.678	-0.669	-0.653	-0.681	-0.696	-0.662	-0.668	-0.719
N (32)	-0.573	-0.580	-0.576	-0.587	-0.593	-0.592	-0.594	-0.595	-0.567	-0.583	-0.601	-0.599	-0.532
Atom Nr.	L ₁₄	L ₁₅	L ₁₆	L ₁₇	L ₁₈	L ₁₉	L ₂₀	L ₂₁	L ²²	L ²³	L ²⁴	L ²⁵	
Fe (1)	1.417	1.419	1.422	1.428	1.383	1.432	1.410	1.414	1.424	1.418	1.417	1.416	
N (2)	-0.600	-0.586	-0.588	-0.535	-0.473	-0.537	-0.605	-0.593	-0.621	-0.626	-0.373	-0.519	
N (8)	-0.659	-0.609	-0.662	-0.678	-0.672	-0.620	-0.660	-0.676	-0.679	-0.689	-0.691	-0.686	
N (14)	-0.588	-0.603	-0.575	-0.549	-0.458	-0.552	-0.600	-0.593	-0.600	-0.606	-0.373	-0.592	
N (20)	-0.600	-0.599	-0.573	-0.536	-0.459	-0.552	-0.600	-0.593	-0.621	-0.619	-0.373	-0.592	
N (26)	-0.660	-0.604	-0.663	-0.677	-0.671	-0.619	-0.660	-0.676	-0.679	-0.681	-0.691	-0.686	
N (32)	-0.587	-0.595	-0.588	-0.549	-0.473	-0.538	-0.605	-0.593	-0.600	-0.621	-0.373	-0.591	

Table S 10: Mulliken charges on Fe and the coordinated N's of the DFT solvent (CH₃CN) phase optimized [Fe(L)₂]²⁺ complexes (L = L¹-L²⁵). Atom numbering as in Error! Reference source not found. (c).

Analysis of Sum of Mulliken Charges with summed hydrogen in the DFT-optimized geometries of Fe^{II} L¹-L²⁵ in solvent (CH₃CN) phase													
Atom Nr.	L ₁	L ₂	L ₃	L ₄	L ₅	L ₆	L ₇	L ₈	L ₉	L ₁₀	L ₁₁	L ₁₂	L ₁₃
Fe (1)	1.308	1.307	1.307	1.304	1.305	1.304	1.305	1.300	1.323	1.303	1.304	1.302	1.305
N (2)	-0.545	-0.546	-0.546	-0.549	-0.549	-0.550	-0.551	-0.551	-0.529	-0.552	-0.554	-0.552	-0.507
N (8)	-0.673	-0.671	-0.668	-0.655	-0.658	-0.646	-0.647	-0.638	-0.660	-0.644	-0.640	-0.642	-0.668
N (14)	-0.545	-0.546	-0.545	-0.548	-0.548	-0.550	-0.551	-0.551	-0.529	-0.552	-0.554	-0.552	-0.506
N (20)	-0.545	-0.546	-0.545	-0.549	-0.548	-0.550	-0.551	-0.551	-0.529	-0.552	-0.554	-0.552	-0.507
N (26)	-0.673	-0.671	-0.668	-0.655	-0.658	-0.646	-0.647	-0.638	-0.660	-0.644	-0.640	-0.642	-0.659
N (32)	-0.545	-0.546	-0.546	-0.549	-0.549	-0.550	-0.551	-0.551	-0.529	-0.552	-0.554	-0.552	-0.507
Atom Nr.	L ₁₄	L ₁₅	L ₁₆	L ₁₇	L ₁₈	L ₁₉	L ₂₀	L ₂₁	L ²²	L ²³	L ²⁴	L ²⁵	
Fe (1)	1.303	1.308	1.305	1.300	1.260	1.309	1.306	1.304	1.309	1.310	1.310	1.304	
N (2)	-0.554	-0.555	-0.544	-0.508	-0.433	-0.510	-0.559	-0.551	-0.566	-0.568	-0.340	-0.550	
N (8)	-0.641	-0.593	-0.643	-0.649	-0.640	-0.600	-0.646	-0.645	-0.654	-0.658	-0.669	-0.648	
N (14)	-0.554	-0.555	-0.544	-0.508	-0.433	-0.510	-0.554	-0.551	-0.561	-0.568	-0.340	-0.550	
N (20)	-0.554	-0.555	-0.544	-0.508	-0.432	-0.510	-0.558	-0.551	-0.566	-0.568	-0.340	-0.550	
N (26)	-0.641	-0.593	-0.643	-0.649	-0.640	-0.600	-0.645	-0.645	-0.654	-0.657	-0.669	-0.648	
N (32)	-0.554	-0.555	-0.544	-0.508	-0.433	-0.510	-0.559	-0.551	-0.561	-0.568	-0.340	-0.550	

3 References

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- [2] L.E. Roy, E. Jakubikova, M. Graham Guthrie, E.R. Batista, Calculation of one-electron redox potentials revisited. Is it possible to calculate accurate potentials with density functional methods?, *J. Phys. Chem. A.* 113 (2009) 6745–6750. <https://doi.org/10.1021/jp811388w>.

Optimized Cartesian coordinates (Å) of the DFT calculations in gas phase:

i) [Fe(L1)2]1+

26	0.000002000	-0.000019000	-0.000228000
7	0.325952000	1.402695000	1.402323000
6	1.656056000	1.640190000	1.636603000
6	2.058802000	2.591286000	2.583410000
6	1.102288000	3.299832000	3.292983000
6	-0.248361000	3.051149000	3.048972000
6	-0.584172000	2.095347000	2.095713000
7	1.910701000	0.000101000	-0.000222000
6	2.572288000	0.832020000	0.828814000
6	3.970722000	0.860761000	0.860048000
6	4.700345000	-0.000006000	0.000064000
6	3.970858000	-0.860718000	-0.860043000
6	2.572395000	-0.831910000	-0.829116000
7	0.326131000	-1.402597000	-1.402820000
6	1.656279000	-1.640028000	-1.637022000
6	2.059114000	-2.591029000	-2.583915000
6	1.102678000	-3.299535000	-3.293601000
6	-0.248019000	-3.050926000	-3.049651000
6	-0.583919000	-2.095216000	-2.096343000
7	-0.326209000	1.402702000	-1.402674000
6	-1.656363000	1.640104000	-1.636837000
6	-2.059256000	2.591301000	-2.583483000
6	-1.102864000	3.300071000	-3.292985000
6	0.247831000	3.051505000	-3.049077000
6	0.583794000	2.095581000	-2.096003000
7	-1.910694000	-0.000113000	-0.000126000
6	-2.572447000	0.831782000	-0.829047000
6	-3.970898000	0.860445000	-0.860107000
6	-4.700349000	-0.000335000	0.000017000
6	-3.970702000	-0.860946000	0.860076000
6	-2.572220000	-0.832097000	0.828949000
7	-0.325830000	-1.402664000	1.402338000
6	-1.655977000	-1.640069000	1.636791000
6	-2.058638000	-2.590936000	2.583911000
6	-1.102104000	-3.299303000	3.293576000
6	0.248566000	-3.050721000	3.049381000
6	0.584304000	-2.095177000	2.095857000
1	3.111871000	2.768799000	2.755907000
1	1.403052000	4.037394000	4.027562000
1	-1.027561000	3.581263000	3.580253000
1	-1.619951000	1.870714000	1.873711000
1	4.485687000	1.518561000	1.542209000
1	4.485925000	-1.518595000	-1.542056000
1	3.112203000	-2.768466000	-2.756383000

1	1.403512000	-4.037017000	-4.028233000
1	-1.027161000	-3.581042000	-3.581013000
1	-1.619721000	-1.870643000	-1.874378000
1	-3.112359000	2.768712000	-2.755886000
1	-1.403744000	4.037720000	-4.027429000
1	1.026940000	3.581807000	-3.580304000
1	1.619611000	1.871007000	-1.874109000
1	-4.485983000	1.518154000	-1.542265000
1	-4.485637000	-1.518827000	1.542185000
1	-3.111702000	-2.768351000	2.756556000
1	-1.402819000	-4.036660000	4.028382000
1	1.027794000	-3.580727000	3.580725000
1	1.620078000	-1.870668000	1.873692000
7	-6.058342000	-0.000473000	0.000022000
6	-6.878371000	-0.924106000	0.795738000
1	-6.830916000	-0.664806000	1.861704000
1	-6.525321000	-1.952979000	0.683415000
1	-9.063868000	-0.946724000	0.973994000
6	-8.292228000	-0.731531000	0.234063000
1	-8.448318000	-1.399768000	-0.617486000
6	-8.292184000	0.731067000	-0.232785000
1	-8.447561000	1.399347000	0.618861000
1	-9.064226000	0.946460000	-0.972238000
6	-6.878622000	0.923258000	-0.795326000
1	-6.525265000	1.952057000	-0.683343000
1	-6.831882000	0.663808000	-1.861286000
7	6.058317000	-0.000031000	0.000189000
6	6.878449000	0.923697000	0.795724000
1	6.831211000	0.664422000	1.861702000
1	6.525304000	1.952534000	0.683414000
1	9.063996000	0.946537000	0.973497000
6	8.292203000	0.731165000	0.233779000
1	8.448038000	1.399284000	-0.617912000
6	8.292173000	-0.731489000	-0.232853000
1	8.447731000	-1.399624000	0.618877000
1	9.064119000	-0.946950000	-0.972385000
6	6.878531000	-0.923865000	-0.795136000
1	6.525230000	-1.952657000	-0.682896000
1	6.831569000	-0.664598000	-1.861127000

ii) [Fe(L2)2]1+

26	0.000001000	-0.000329000	-0.000003000
7	0.326941000	-1.404359000	1.401267000
6	1.657241000	-1.639913000	1.636494000
6	2.060820000	-2.589569000	2.584215000
6	1.104862000	-3.299947000	3.292861000
6	-0.245888000	-3.054055000	3.047192000
6	-0.582546000	-2.098660000	2.093842000
7	1.909988000	-0.000159000	-0.000481000
6	2.572206000	-0.830414000	0.828567000
6	3.971213000	-0.859650000	0.858105000
6	4.702425000	0.000723000	-0.000708000
6	3.970616000	0.860620000	-0.859279000
6	2.571524000	0.830591000	-0.829656000
7	0.325822000	1.403469000	-1.401714000
6	1.656056000	1.639479000	-1.637386000
6	2.058945000	2.589001000	-2.585621000
6	1.102533000	3.298658000	-3.294281000
6	-0.248109000	3.052256000	-3.048196000
6	-0.584090000	2.097100000	-2.094392000
7	-0.325837000	1.401110000	1.404062000

6	-1.656073000	1.636805000	1.640034000
6	-2.058973000	2.584801000	2.589790000
6	-1.102568000	3.293232000	3.299687000
6	0.248076000	3.047136000	3.053310000
6	0.584068000	2.093533000	2.097956000
7	-1.909987000	-0.000182000	0.000475000
6	-2.571532000	0.829248000	0.830963000
6	-3.970624000	0.859234000	0.860615000
6	-4.702426000	0.000668000	0.000710000
6	-3.971203000	-0.858356000	-0.859449000
6	-2.572197000	-0.829131000	-0.829885000
7	-0.326925000	-1.402005000	-1.403631000
6	-1.657221000	-1.637273000	-1.639159000
6	-2.060790000	-2.585404000	-2.588410000
6	-1.104824000	-3.294528000	-3.298300000
6	0.245923000	-3.048915000	-3.052337000
6	0.582571000	-2.095073000	-2.097430000
1	3.113935000	-2.764510000	2.759014000
1	1.406270000	-4.036622000	4.028029000
1	-1.024633000	-3.585739000	3.577551000
1	-1.618598000	-1.875798000	1.871377000
1	4.479733000	-1.531997000	1.529501000
1	4.478603000	1.533375000	-1.530674000
1	3.111937000	2.764331000	-2.760786000
1	1.403437000	4.035189000	-4.029801000
1	-1.027218000	3.583408000	-3.578548000
1	-1.620004000	1.873965000	-1.871545000
1	-3.111966000	2.759914000	2.765160000
1	-1.403481000	4.028577000	4.036388000
1	1.027180000	3.577357000	3.584601000
1	1.619984000	1.870699000	1.874821000
1	-4.478625000	1.530931000	1.533061000
1	-4.479708000	-1.529654000	-1.531901000
1	-3.113903000	-2.760149000	-2.763416000
1	-1.406223000	-4.030019000	-4.034656000
1	1.024675000	-3.579648000	-3.583639000
1	1.618620000	-1.872491000	-1.874673000
7	-6.067793000	0.001077000	0.000787000
7	6.067787000	0.001112000	-0.000743000
6	-6.806413000	-0.886922000	-0.889405000
1	-7.872698000	-0.735845000	-0.737884000
1	-6.582944000	-0.681139000	-1.941987000
1	-6.582892000	-1.939962000	-0.686130000
6	-6.805612000	0.890378000	0.890301000
1	-6.581654000	0.685628000	1.942973000
1	-6.581725000	1.943139000	0.685840000
1	-7.872042000	0.739583000	0.739532000
6	6.806328000	-0.888193000	0.888208000
1	7.872627000	-0.736889000	0.737017000
1	6.582753000	-0.683949000	1.941066000
1	6.582825000	-1.940937000	0.683375000
6	6.805685000	0.891606000	-0.889003000
1	6.581751000	0.688327000	-1.941964000
1	6.581861000	1.944097000	-0.683092000
1	7.872101000	0.740537000	-0.738412000

iii) [Fe(L3)2]1+

26	-0.000005000	-0.514348000	0.000012000
7	0.259625000	-1.921679000	1.416791000
6	1.571059000	-2.154593000	1.725075000
6	1.927540000	-3.103059000	2.687942000

6	0.935103000	-3.817747000	3.344905000
6	-0.398064000	-3.573064000	3.027927000
6	-0.686379000	-2.618102000	2.057844000
7	1.908693000	-0.514637000	0.100106000
6	2.529716000	-1.336008000	0.967447000
6	3.917674000	-1.352513000	1.079512000
6	4.687010000	-0.482734000	0.260531000
6	4.010575000	0.373158000	-0.630433000
6	2.607872000	0.327680000	-0.691984000
7	0.393017000	0.883151000	-1.385978000
6	1.737670000	1.122721000	-1.550023000
6	2.186830000	2.066259000	-2.487471000
6	1.269557000	2.766355000	-3.250705000
6	-0.094877000	2.518547000	-3.074335000
6	-0.477980000	1.569283000	-2.134094000
7	-0.393243000	0.882203000	1.386940000
6	-1.737902000	1.121605000	1.551009000
6	-2.187208000	2.064467000	2.489047000
6	-1.270034000	2.764087000	3.252858000
6	0.094415000	2.516457000	3.076461000
6	0.477657000	1.567846000	2.135609000
7	-1.908699000	-0.514763000	-0.100119000
6	-2.607996000	0.327062000	0.692349000
6	-4.010679000	0.372597000	0.630645000
6	-4.686989000	-0.482807000	-0.260906000
6	-3.917549000	-1.352068000	-1.080298000
6	-2.529584000	-1.335640000	-0.968050000
7	-0.259414000	-1.920911000	-1.417539000
6	-1.570838000	-2.153763000	-1.726002000
6	-1.927194000	-3.101833000	-2.689326000
6	-0.934684000	-3.816153000	-3.346553000
6	0.398463000	-3.571528000	-3.029392000
6	0.686656000	-2.616991000	-2.058857000
1	2.970489000	-3.276087000	2.916797000
1	1.198086000	-4.554844000	4.094183000
1	-1.203316000	-4.105080000	3.517134000
1	-1.708988000	-2.395753000	1.780335000
1	4.414733000	-2.017163000	1.773584000
1	4.558570000	1.060795000	-1.255705000
1	3.247462000	2.240993000	-2.610379000
1	1.607463000	3.497131000	-3.975818000
1	-0.845865000	3.045420000	-3.647572000
1	-1.524286000	1.345912000	-1.965994000
1	-3.247860000	2.239059000	2.611974000
1	-1.608046000	3.494353000	3.978435000
1	0.845322000	3.042977000	3.650128000
1	1.523988000	1.344635000	1.967449000
1	-4.558759000	1.059905000	1.256204000
1	-4.414521000	-2.016300000	-1.774832000
1	-2.970121000	-3.274845000	-2.918299000
1	-1.197579000	-4.552932000	-4.096174000
1	1.203777000	-4.103258000	-3.518805000
1	1.709239000	-2.394697000	-1.781207000
7	-6.045640000	-0.520388000	-0.351565000
1	-6.431341000	-1.105680000	-1.075029000
7	6.045660000	-0.520326000	0.351017000
1	6.431505000	-1.106388000	1.073765000
6	-7.185457000	1.724323000	-0.288714000
1	-7.537791000	1.583532000	-1.317211000
1	-6.220900000	2.239335000	-0.361344000
6	-8.182308000	2.594524000	0.485288000
1	-9.141090000	2.067932000	0.560652000

1	-7.827160000	2.726278000	1.514725000
6	-8.404358000	3.966671000	-0.156727000
1	-7.470324000	4.533697000	-0.214331000
1	-8.796340000	3.868871000	-1.173294000
1	-9.118500000	4.561098000	0.417902000
6	-6.980683000	0.345807000	0.356489000
1	-6.645428000	0.453940000	1.392624000
1	-7.935405000	-0.184970000	0.403901000
6	6.980655000	0.346008000	-0.356945000
1	6.645297000	0.454402000	-1.393028000
1	7.935351000	-0.184791000	-0.404549000
6	7.185550000	1.724342000	0.288598000
1	7.538126000	1.583264000	1.316970000
6	8.182203000	2.594777000	-0.485400000
1	9.140934000	2.068159000	-0.561261000
1	7.826742000	2.726928000	-1.514677000
1	6.221013000	2.239333000	0.361605000
1	7.470520000	4.533680000	0.215269000
6	8.404526000	3.966669000	0.157053000
1	9.118426000	4.561316000	-0.417651000
1	8.796936000	3.868479000	1.173417000

iv) [Fe(L4)2]1+

26	-0.000009000	0.000053000	-0.007951000
7	-0.376791000	-1.392128000	-1.420341000
6	-1.704310000	-1.599576000	-1.651882000
6	-2.142108000	-2.527341000	-2.594834000
6	-1.206261000	-3.263657000	-3.313092000
6	0.146094000	-3.052669000	-3.069870000
6	0.515153000	-2.108211000	-2.118224000
7	-1.910947000	0.045478000	-0.005040000
6	-2.599753000	-0.769248000	-0.822622000
6	-3.989217000	-0.789454000	-0.827506000
6	-4.661192000	0.075425000	0.060870000
6	-3.945013000	0.913795000	0.907502000
6	-2.535307000	0.886844000	0.858832000
7	-0.274652000	1.417709000	1.382880000
6	-1.605227000	1.680010000	1.636466000
6	-1.976117000	2.659368000	2.574695000
6	-1.001636000	3.363088000	3.254876000
6	0.347058000	3.088227000	2.992650000
6	0.652411000	2.115390000	2.051225000
7	0.376446000	1.392207000	-1.420457000
6	1.703934000	1.599673000	-1.652164000
6	2.141562000	2.527307000	-2.595349000
6	1.205595000	3.263465000	-3.313589000
6	-0.146721000	3.052478000	-3.070158000
6	-0.515606000	2.108128000	-2.118327000
7	1.910964000	-0.045313000	-0.005331000
6	2.599531000	0.769532000	-0.822946000
6	3.989030000	0.789975000	-0.827920000
6	4.661185000	-0.074782000	0.060411000
6	3.945206000	-0.913325000	0.907051000
6	2.535471000	-0.886627000	0.858408000
7	0.274941000	-1.417948000	1.382587000
6	1.605559000	-1.680115000	1.635951000
6	1.976703000	-2.659725000	2.573806000
6	1.002378000	-3.363875000	3.253795000
6	-0.346369000	-3.089187000	2.991742000
6	-0.651956000	-2.116041000	2.050696000
1	-3.200955000	-2.670919000	-2.763035000

1	-1.529667000	-3.990299000	-4.048433000
1	0.908676000	-3.605796000	-3.602582000
1	1.557257000	-1.914084000	-1.899214000
1	-4.566277000	-1.438524000	-1.469468000
1	-4.463961000	1.571142000	1.594247000
1	-3.023514000	2.860117000	2.759157000
1	-1.278882000	4.117783000	3.980911000
1	1.142233000	3.611186000	3.506602000
1	1.682953000	1.874092000	1.821625000
1	3.200380000	2.670862000	-2.763746000
1	1.528871000	3.989993000	-4.049101000
1	-0.909389000	3.605511000	-3.602841000
1	-1.557675000	1.913960000	-1.899173000
1	4.565907000	1.439168000	-1.469915000
1	4.464310000	-1.570530000	1.593808000
1	3.024143000	-2.860372000	2.758120000
1	1.279819000	-4.118783000	3.979535000
1	-1.141420000	-3.612462000	3.505564000
1	-1.682557000	-1.874800000	1.821290000
8	-6.010358000	0.026335000	0.030929000
1	-6.387165000	0.642176000	0.669839000
8	6.010323000	-0.025434000	0.030467000
1	6.387264000	-0.641256000	0.669315000

v) [Fe(L5)2]1+

26	0.000000000	0.000003000	-0.058573000
7	-0.289153000	1.415593000	-1.470099000
6	-1.599683000	1.709338000	-1.702989000
6	-1.975603000	2.667275000	-2.641354000
6	-0.993788000	3.346184000	-3.355017000
6	0.342016000	3.048001000	-3.109956000
6	0.648519000	2.078001000	-2.163022000
7	-1.909287000	0.077755000	-0.056037000
6	-2.547268000	0.935212000	-0.875150000
6	-3.927051000	1.043635000	-0.877204000
6	-4.663076000	0.226019000	0.014713000
6	-3.999013000	-0.654858000	0.862410000
6	-2.590158000	-0.717913000	0.808896000
7	-0.369431000	-1.398140000	1.329701000
6	-1.715333000	-1.573420000	1.583762000
6	-2.148357000	-2.532955000	2.516285000
6	-1.222666000	-3.303698000	3.190766000
6	0.142015000	-3.116805000	2.927958000
6	0.509836000	-2.161478000	1.992391000
7	0.369437000	1.398114000	1.329730000
6	1.715341000	1.573386000	1.583791000
6	2.148370000	2.532900000	2.516333000
6	1.222683000	3.303632000	3.190833000
6	-0.141999000	3.116748000	2.928024000
6	-0.509826000	2.161442000	1.992438000
7	1.909287000	-0.077751000	-0.056047000
6	2.590162000	0.717894000	0.808903000
6	3.999017000	0.654833000	0.862413000
6	4.663076000	-0.226027000	0.014695000
6	3.927046000	-1.043620000	-0.877240000
6	2.547264000	-0.935192000	-0.875181000
7	0.289146000	-1.415556000	-1.470134000
6	1.599674000	-1.709296000	-1.703035000
6	1.975589000	-2.667211000	-2.641425000
6	0.993771000	-3.346101000	-3.355102000
6	-0.342031000	-3.047922000	-3.110029000

6	-0.648529000	-2.077944000	-2.163070000
1	-3.023081000	2.878786000	-2.809502000
1	-1.268775000	4.095492000	-4.087250000
1	1.139315000	3.553897000	-3.638933000
1	1.675570000	1.816672000	-1.942786000
1	-4.463220000	1.727501000	-1.518845000
1	-4.542482000	-1.279463000	1.554904000
1	-3.206642000	-2.666219000	2.700023000
1	-1.548536000	-4.043144000	3.912269000
1	0.901362000	-3.693749000	3.438408000
1	1.553840000	-1.987222000	1.762760000
1	3.206656000	2.666158000	2.700070000
1	1.548557000	4.043062000	3.912349000
1	-0.901343000	3.693684000	3.438488000
1	-1.553831000	1.987193000	1.762807000
1	4.542489000	1.279419000	1.554923000
1	4.463211000	-1.727474000	-1.518896000
1	3.023066000	-2.878720000	-2.809581000
1	1.268754000	-4.095392000	-4.087353000
1	-1.139333000	-3.553803000	-3.639016000
1	-1.675579000	-1.816619000	-1.942825000
8	5.998354000	-0.388252000	-0.040405000
6	6.831473000	0.385978000	0.825361000
1	6.716421000	1.456044000	0.628029000
1	6.612154000	0.172913000	1.875893000
1	7.850414000	0.082195000	0.598135000
8	-5.998355000	0.388237000	-0.040383000
6	-6.831470000	-0.386028000	0.825355000
1	-6.716415000	-1.456087000	0.627984000
1	-6.612149000	-0.173001000	1.875894000
1	-7.850412000	-0.082240000	0.598142000

vi) [Fe(L6)2]1+

26	0.000000000	0.000121000	-0.000155000
7	0.338835000	-1.396653000	-1.412684000
6	1.667382000	-1.644415000	-1.647786000
6	2.069603000	-2.563225000	-2.621748000
6	1.115701000	-3.239526000	-3.364018000
6	-0.236623000	-2.980192000	-3.122100000
6	-0.572891000	-2.055709000	-2.146846000
7	1.904593000	0.001186000	-0.000149000
6	2.575917000	-0.852486000	-0.817571000
6	3.963742000	-0.870142000	-0.831481000
6	4.692983000	0.002052000	0.000538000
6	3.962713000	0.873620000	0.832463000
6	2.575000000	0.855128000	0.817681000
7	0.337289000	1.397521000	1.412179000
6	1.665505000	1.646447000	1.647596000
6	2.066740000	2.565883000	2.621320000
6	1.112069000	3.241685000	3.363105000
6	-0.239937000	2.981220000	3.120844000
6	-0.575192000	2.056145000	2.145784000
7	-0.337100000	-1.396938000	1.412558000
6	-1.665285000	-1.645920000	1.648095000
6	-2.066402000	-2.565123000	2.622086000
6	-1.111644000	-3.240624000	3.364035000
6	0.240328000	-2.980087000	3.121668000
6	0.575465000	-2.055259000	2.146333000
7	-1.904593000	-0.001004000	0.000039000
6	-2.574886000	-0.854876000	0.818034000
6	-3.962596000	-0.873544000	0.832825000

6	-4.692983000	-0.002238000	0.000728000
6	-3.963859000	0.869877000	-0.831476000
6	-2.576031000	0.852403000	-0.817569000
7	-0.339024000	1.396652000	-1.412881000
6	-1.667602000	1.644265000	-1.647963000
6	-2.069940000	2.562910000	-2.622033000
6	-1.116126000	3.239205000	-3.364419000
6	0.236232000	2.980039000	-3.122504000
6	0.572617000	2.055707000	-2.147146000
1	3.123251000	-2.739860000	-2.794391000
1	1.415218000	-3.954419000	-4.120488000
1	-1.016244000	-3.486618000	-3.675942000
1	-1.608861000	-1.827757000	-1.930138000
1	4.492594000	-1.531762000	-1.504303000
1	4.490951000	1.535222000	1.505776000
1	3.120197000	2.743475000	2.794125000
1	1.410799000	3.957080000	4.119409000
1	-1.020129000	3.487223000	3.674272000
1	-1.610913000	1.827309000	1.928829000
1	-3.119837000	-2.742761000	2.794978000
1	-1.410283000	-3.955836000	4.120549000
1	1.020586000	-3.485849000	3.675223000
1	1.611159000	-1.826393000	1.929281000
1	-4.490746000	-1.535087000	1.506266000
1	-4.492799000	1.531279000	-1.504442000
1	-3.123610000	2.739431000	-2.794659000
1	-1.415733000	3.953973000	-4.120971000
1	1.015786000	3.486477000	-3.676429000
1	1.608614000	1.827871000	-1.930444000
6	6.170228000	0.002983000	0.000616000
6	6.895415000	1.189712000	0.178629000
6	6.897111000	-1.185866000	-0.177794000
6	8.286006000	1.186479000	0.176054000
6	8.284778000	-1.182493000	-0.175062000
6	9.009351000	0.003512000	0.000597000
1	6.371122000	2.132683000	0.286598000
1	6.372057000	-2.128452000	-0.285653000
1	8.818661000	2.122762000	0.303712000
1	8.817772000	-2.119178000	-0.302145000
6	-6.170227000	-0.003359000	0.000811000
6	-6.895263000	-1.190145000	0.179063000
6	-6.897262000	1.185361000	-0.177836000
6	-8.285854000	-1.187089000	0.176490000
6	-8.284929000	1.181813000	-0.175100000
6	-9.009351000	-0.004250000	0.000798000
1	-6.370850000	-2.133028000	0.287219000
1	-6.372327000	2.127992000	-0.285885000
1	-8.818391000	-2.123415000	0.304337000
1	-8.818042000	2.118404000	-0.302369000
6	10.517026000	-0.005759000	-0.001106000
1	10.923076000	0.994778000	0.155235000
1	10.907731000	-0.654473000	0.788532000
1	10.907824000	-0.382502000	-0.951093000
6	-10.517026000	0.004828000	-0.000909000
1	-10.922949000	-0.995721000	0.155686000
1	-10.907816000	0.653695000	0.788562000
1	-10.907871000	0.381278000	-0.950994000

vii) [Fe(L7)2]1+

26	0.000000000	0.000001000	-0.031633000
7	-0.252404000	1.426334000	-1.430724000

6	-1.566896000	1.729224000	-1.686639000
6	-1.911039000	2.718069000	-2.615932000
6	-0.915615000	3.401315000	-3.292238000
6	0.421411000	3.089561000	-3.024760000
6	0.699917000	2.105451000	-2.090373000
7	-1.901143000	0.106007000	-0.032320000
6	-2.520345000	0.957725000	-0.895669000
6	-3.908608000	1.036423000	-0.922116000
6	-4.686417000	0.247529000	-0.057825000
6	-4.004454000	-0.625608000	0.824131000
6	-2.622815000	-0.674731000	0.811632000
7	-0.422037000	-1.385686000	1.373969000
6	-1.757644000	-1.546527000	1.620276000
6	-2.214750000	-2.481774000	2.549585000
6	-1.302117000	-3.266431000	3.239263000
6	0.058768000	-3.101633000	2.980348000
6	0.449660000	-2.156934000	2.044120000
7	0.422040000	1.385683000	1.373973000
6	1.757648000	1.546522000	1.620280000
6	2.214756000	2.481766000	2.549591000
6	1.302124000	3.266421000	3.239271000
6	-0.058762000	3.101626000	2.980357000
6	-0.449656000	2.156930000	2.044127000
7	1.901143000	-0.106006000	-0.032324000
6	2.622817000	0.674728000	0.811632000
6	4.004456000	0.625601000	0.824131000
6	4.686416000	-0.247534000	-0.057829000
6	3.908606000	-1.036424000	-0.922122000
6	2.520343000	-0.957723000	-0.895675000
7	0.252401000	-1.426327000	-1.430729000
6	1.566892000	-1.729217000	-1.686647000
6	1.911034000	-2.718059000	-2.615944000
6	0.915608000	-3.401301000	-3.292252000
6	-0.421417000	-3.089547000	-3.024772000
6	-0.699921000	-2.105440000	-2.090381000
1	-2.952819000	2.946212000	-2.799861000
1	-1.170584000	4.166496000	-4.015169000
1	1.231815000	3.595432000	-3.532806000
1	1.721919000	1.834957000	-1.856660000
1	-4.403660000	1.711505000	-1.609240000
1	-4.563553000	-1.259100000	1.498579000
1	-3.276184000	-2.593370000	2.727391000
1	-1.643463000	-3.995415000	3.963896000
1	0.806420000	-3.691317000	3.494634000
1	1.495730000	-1.998926000	1.814836000
1	3.276190000	2.593360000	2.727395000
1	1.643471000	3.995403000	3.963907000
1	-0.806413000	3.691310000	3.494645000
1	-1.495726000	1.998924000	1.814843000
1	4.563556000	1.259089000	1.498582000
1	4.403657000	-1.711505000	-1.609248000
1	2.952813000	-2.946203000	-2.799875000
1	1.170576000	-4.166480000	-4.015186000
1	-1.231822000	-3.595415000	-3.532820000
1	-1.721922000	-1.834946000	-1.856666000
6	6.144190000	-0.356139000	-0.105750000
1	6.524631000	-1.047814000	-0.852894000
6	7.028501000	0.292945000	0.660897000
1	6.739114000	0.996788000	1.432966000
1	8.091708000	0.132645000	0.535479000
6	-6.144190000	0.356131000	-0.105746000
1	-6.524633000	1.047802000	-0.852892000

6	-7.028499000	-0.292952000	0.660904000
1	-6.739111000	-0.996790000	1.432976000
1	-8.091707000	-0.132654000	0.535486000
viii) [Fe(L8)2]1+			
26	0.000000000	0.000023000	0.000007000
7	-0.334342000	1.410578000	1.398032000
6	-1.662323000	1.644680000	1.649090000
6	-2.063750000	2.615448000	2.572202000
6	-1.108915000	3.355048000	3.249630000
6	0.243052000	3.114602000	2.986643000
6	0.578177000	2.143050000	2.057854000
7	-1.905892000	-0.001508000	-0.000908000
6	-2.571727000	0.820735000	0.855377000
6	-3.963100000	0.832232000	0.873682000
6	-4.659968000	-0.003653000	-0.002308000
6	-3.960895000	-0.838453000	-0.877595000
6	-2.569569000	-0.824769000	-0.857864000
7	-0.330705000	-1.411150000	-1.398251000
6	-1.658066000	-1.647310000	-1.650652000
6	-2.057077000	-2.618741000	-2.574101000
6	-1.100431000	-3.356959000	-3.250490000
6	0.250890000	-3.114458000	-2.986112000
6	0.583593000	-2.142313000	-2.057071000
7	0.333039000	-1.410434000	1.398449000
6	1.660785000	-1.644748000	1.650522000
6	2.061360000	-2.615429000	2.574084000
6	1.105893000	-3.354727000	3.250960000
6	-0.245830000	-3.114045000	2.986974000
6	-0.580096000	-2.142592000	2.057767000
7	1.905893000	0.001413000	0.000725000
6	2.570942000	-0.821038000	0.857401000
6	3.962291000	-0.832957000	0.876599000
6	4.659969000	0.002736000	0.001051000
6	3.961706000	0.837728000	-0.874679000
6	2.570354000	0.824466000	-0.855841000
7	0.332007000	1.411297000	-1.397832000
6	1.659603000	1.647243000	-1.649223000
6	2.059466000	2.618760000	-2.572222000
6	1.103452000	3.357284000	-3.249162000
6	-0.248114000	3.115022000	-2.985779000
6	-0.581675000	2.142777000	-2.057154000
1	-3.117065000	2.787134000	2.751830000
1	-1.407216000	4.108214000	3.968438000
1	1.023305000	3.666500000	3.494144000
1	1.613987000	1.927990000	1.827935000
1	-4.502618000	1.480699000	1.551392000
1	-5.742465000	-0.004501000	-0.002860000
1	-4.498708000	-1.487757000	-1.555856000
1	-3.109947000	-2.792023000	-2.754800000
1	-1.396855000	-4.110625000	-3.969551000
1	1.032503000	-3.665229000	-3.492745000
1	1.618846000	-1.925666000	-1.826146000
1	3.114513000	-2.787269000	2.754517000
1	1.403531000	-4.107822000	3.970117000
1	-1.026559000	-3.665686000	3.494021000
1	-1.615700000	-1.927378000	1.827072000
1	4.501186000	-1.481608000	1.554628000
1	5.742467000	0.003255000	0.001182000
1	4.500142000	1.486847000	-1.552625000
1	3.112500000	2.791886000	-2.752119000

1	1.400539000	4.111020000	-3.967875000
1	-1.029251000	3.666052000	-3.492864000
1	-1.617134000	1.926286000	-1.827003000
ix) [Fe(L9)2]1+			
26	0.000003000	-0.000074000	0.011927000
7	-0.374434000	1.400745000	1.422775000
6	-1.703159000	1.612756000	1.650397000
7	-2.204570000	2.479694000	2.518922000
6	-1.333182000	3.210567000	3.222782000
6	0.041029000	3.078466000	3.062387000
6	0.485384000	2.142061000	2.136076000
7	-1.912209000	-0.029931000	0.010410000
6	-2.601667000	0.782460000	0.826697000
6	-3.987575000	0.810395000	0.843754000
6	-4.666645000	-0.056530000	-0.041214000
6	-3.952289000	-0.897064000	-0.892443000
6	-2.547844000	-0.862171000	-0.844164000
7	-0.292859000	-1.414050000	-1.386333000
6	-1.628569000	-1.657247000	-1.632898000
7	-2.090486000	-2.555728000	-2.514193000
6	-1.191857000	-3.251284000	-3.198628000
6	0.186344000	-3.078712000	-3.024135000
6	0.587890000	-2.133908000	-2.087118000
7	0.374449000	-1.401524000	1.422161000
6	1.703176000	-1.613633000	1.649658000
7	2.204615000	-2.480867000	2.517864000
6	1.333234000	-3.211919000	3.221565000
6	-0.040972000	-3.079757000	3.061253000
6	-0.485354000	-2.143042000	2.135262000
7	1.912198000	0.029766000	0.010364000
6	2.601679000	-0.783000000	0.826263000
6	3.987574000	-0.810957000	0.843286000
6	4.666638000	0.056401000	-0.041292000
6	3.952272000	0.897363000	-0.892069000
6	2.547816000	0.862456000	-0.843782000
7	0.292829000	1.414725000	-1.385548000
6	1.628547000	1.658017000	-1.632018000
7	2.090460000	2.557036000	-2.512771000
6	1.191824000	3.253096000	-3.196687000
6	-0.186373000	3.080535000	-3.022179000
6	-0.587916000	2.135117000	-2.085770000
1	0.740173000	3.675739000	3.631954000
1	1.539464000	1.974748000	1.952315000
1	-4.528986000	1.472753000	1.503228000
1	-4.441291000	-1.570441000	-1.585604000
1	0.909103000	-3.648481000	-3.590994000
1	1.636136000	-1.940115000	-1.892048000
1	-0.740109000	-3.677217000	3.630634000
1	-1.539439000	-1.975667000	1.951589000
1	4.529000000	-1.473610000	1.502451000
1	4.441252000	1.571111000	-1.584885000
1	-0.909140000	3.650743000	-3.588585000
1	-1.636165000	1.941257000	-1.890774000
8	6.012458000	0.010700000	-0.006112000
1	6.390445000	0.629553000	-0.642140000
8	-6.012469000	-0.010887000	-0.005980000
1	-6.390460000	-0.629422000	-0.642314000
1	1.579036000	3.975058000	-3.909346000
1	1.755759000	-3.918873000	3.927959000
1	-1.579067000	-3.972802000	-3.911738000

1	-1.755678000	3.917228000	3.929488000
x)	[Fe(L10)2]1+		
26	0.000000000	-0.000028000	0.000052000
7	0.336241000	1.411447000	1.399514000
6	1.663828000	1.646767000	1.650399000
6	2.066827000	2.616319000	2.573395000
6	1.112085000	3.354964000	3.252494000
6	-0.239583000	3.113834000	2.990646000
6	-0.575649000	2.142844000	2.061217000
7	1.905927000	-0.000131000	0.000015000
6	2.572075000	0.822118000	0.854983000
6	3.961738000	0.839716000	0.878649000
6	4.649949000	-0.000131000	-0.000197000
6	3.961600000	-0.839968000	-0.878945000
6	2.571944000	-0.822365000	-0.855071000
7	0.336019000	-1.411535000	-1.399426000
6	1.663573000	-1.646988000	-1.650377000
6	2.066440000	-2.616671000	-2.573289000
6	1.111600000	-3.355344000	-3.252222000
6	-0.240031000	-3.114110000	-2.990278000
6	-0.575967000	-2.142981000	-2.060952000
7	-0.336020000	1.411567000	-1.399395000
6	-1.663557000	1.647003000	-1.650362000
6	-2.066434000	2.616692000	-2.573251000
6	-1.111590000	3.355411000	-3.252144000
6	0.240031000	3.114209000	-2.990168000
6	0.575970000	2.143045000	-2.060873000
7	-1.905930000	0.000089000	-0.000033000
6	-2.571946000	0.822340000	-0.855067000
6	-3.961590000	0.839987000	-0.878943000
6	-4.649946000	0.000122000	-0.000193000
6	-3.961749000	-0.839736000	0.878617000
6	-2.572070000	-0.822179000	0.854951000
7	-0.336236000	-1.411464000	1.399505000
6	-1.663842000	-1.646815000	1.650351000
6	-2.066836000	-2.616398000	2.573330000
6	-1.112099000	-3.355014000	3.252453000
6	0.239580000	-3.113834000	2.990662000
6	0.575646000	-2.142842000	2.061239000
1	3.120117000	2.788707000	2.752613000
1	1.410733000	4.107586000	3.971628000
1	-1.019585000	3.664886000	3.499430000
1	-1.611787000	1.928134000	1.832751000
1	4.509345000	1.485272000	1.550567000
1	4.509105000	-1.485507000	-1.550964000
1	3.119706000	-2.789154000	-2.752555000
1	1.410144000	-4.108077000	-3.971283000
1	-1.020107000	-3.665197000	-3.498912000
1	-1.612074000	-1.928184000	-1.832433000
1	-3.119699000	2.789152000	-2.752541000
1	-1.410136000	4.108158000	-3.971189000
1	1.020107000	3.665338000	-3.498758000
1	1.612076000	1.928253000	-1.832343000
1	-4.509090000	1.485561000	-1.550928000
1	-4.509361000	-1.485286000	1.550539000
1	-3.120127000	-2.788825000	2.752508000
1	-1.410748000	-4.107651000	3.971572000
1	1.019579000	-3.664855000	3.499481000
1	1.611787000	-1.928112000	1.832802000
17	-6.393719000	0.000179000	-0.000312000

17	6.393720000	-0.000135000	-0.000329000
xi) [Fe(L11)2]1+			
26	0.000001000	0.000005000	0.005960000
7	0.328069000	1.406911000	1.415129000
6	1.651430000	1.640541000	1.671085000
6	2.051567000	2.595641000	2.608716000
6	1.092159000	3.322898000	3.295552000
6	-0.256696000	3.084188000	3.027288000
6	-0.589038000	2.125099000	2.083264000
7	1.900968000	0.008203000	0.004994000
6	2.566579000	0.827327000	0.866717000
6	3.950543000	0.851761000	0.885705000
6	4.662258000	0.023810000	0.001377000
6	3.960710000	-0.812654000	-0.881504000
6	2.573411000	-0.803064000	-0.857796000
7	0.339686000	-1.405388000	-1.400865000
6	1.665594000	-1.626827000	-1.658454000
6	2.071816000	-2.582335000	-2.593785000
6	1.118337000	-3.321651000	-3.275311000
6	-0.232529000	-3.095408000	-3.004637000
6	-0.571568000	-2.135879000	-2.063710000
7	-0.339696000	1.405365000	-1.400894000
6	-1.665607000	1.626797000	-1.658478000
6	-2.071837000	2.582284000	-2.593827000
6	-1.118364000	3.321586000	-3.275377000
6	0.232505000	3.095350000	-3.004709000
6	0.571552000	2.135842000	-2.063762000
7	-1.900967000	-0.008194000	0.005010000
6	-2.573417000	0.803051000	-0.857794000
6	-3.960717000	0.812640000	-0.881493000
6	-4.662258000	-0.023804000	0.001413000
6	-3.950535000	-0.851734000	0.885755000
6	-2.566570000	-0.827299000	0.866756000
7	-0.328056000	-1.406869000	1.415165000
6	-1.651415000	-1.640493000	1.671136000
6	-2.051544000	-2.595571000	2.608793000
6	-1.092130000	-3.322811000	3.295640000
6	0.256722000	-3.084107000	3.027359000
6	0.589057000	-2.125040000	2.083310000
1	3.104575000	2.764165000	2.792252000
1	1.387679000	4.065270000	4.026702000
1	-1.038954000	3.627247000	3.541244000
1	-1.623763000	1.910635000	1.848525000
1	4.508603000	1.492133000	1.555534000
1	4.508611000	-1.452017000	-1.558917000
1	3.125721000	-2.742679000	-2.779469000
1	1.419375000	-4.064310000	-4.003929000
1	-1.010632000	-3.648613000	-3.513997000
1	-1.607781000	-1.931133000	-1.826846000
1	-3.125743000	2.742623000	-2.779506000
1	-1.419408000	4.064227000	-4.004009000
1	1.010603000	3.648543000	-3.514087000
1	1.607766000	1.931101000	-1.826902000
1	-4.508623000	1.451986000	-1.558915000
1	-4.508588000	-1.492091000	1.555603000
1	-3.104550000	-2.764092000	2.792341000
1	-1.387644000	-4.065166000	4.026810000
1	1.038985000	-3.627152000	3.541323000
1	1.623780000	-1.910581000	1.848558000
6	6.144113000	0.076229000	0.045636000

8	6.775645000	0.781986000	0.795078000
8	6.720564000	-0.757408000	-0.850414000
1	7.679368000	-0.658910000	-0.752346000
6	-6.144116000	-0.076221000	0.045689000
8	-6.775641000	-0.782026000	0.795091000
8	-6.720582000	0.757308000	-0.850452000
1	-7.679385000	0.658756000	-0.752426000

xii) [Fe(L12)2]1+

26	0.000001000	0.000005000	-0.068546000
7	-0.310965000	1.414947000	-1.471466000
6	-1.633121000	1.657163000	-1.738189000
6	-2.018553000	2.625858000	-2.669017000
6	-1.051155000	3.357843000	-3.338084000
6	0.295109000	3.111641000	-3.057281000
6	0.613832000	2.140537000	-2.121672000
7	-1.904765000	0.027008000	-0.075189000
6	-2.557189000	0.841697000	-0.949368000
6	-3.947042000	0.849811000	-1.000591000
6	-4.645097000	0.017746000	-0.120669000
6	-3.972141000	-0.823236000	0.764260000
6	-2.583390000	-0.801798000	0.768245000
7	-0.355872000	-1.405199000	1.331707000
6	-1.686577000	-1.630614000	1.569717000
6	-2.107364000	-2.596120000	2.489516000
6	-1.164134000	-3.339307000	3.179374000
6	0.191829000	-3.106311000	2.932882000
6	0.544673000	-2.139748000	2.004863000
7	0.355891000	1.405161000	1.331750000
6	1.686599000	1.630560000	1.569761000
6	2.107396000	2.596034000	2.489588000
6	1.164175000	3.339207000	3.179473000
6	-0.191792000	3.106229000	2.932979000
6	-0.544646000	2.139697000	2.004932000
7	1.904766000	-0.027002000	-0.075209000
6	2.583401000	0.801765000	0.768256000
6	3.972153000	0.823186000	0.764271000
6	4.645098000	-0.017770000	-0.120690000
6	3.947033000	-0.849796000	-1.000641000
6	2.557180000	-0.841667000	-0.949416000
7	0.310950000	-1.414883000	-1.471524000
6	1.633102000	-1.657097000	-1.738264000
6	2.018524000	-2.625755000	-2.669135000
6	1.051117000	-3.357706000	-3.338227000
6	-0.295143000	-3.111507000	-3.057407000
6	-0.613855000	-2.140440000	-2.121756000
1	-3.068476000	2.803821000	-2.862074000
1	-1.336509000	4.109950000	-4.063193000
1	1.084619000	3.659062000	-3.555188000
1	1.645712000	1.921955000	-1.878463000
1	-4.474057000	1.478520000	-1.708162000
1	-4.560324000	-1.481976000	1.393709000
1	-3.164442000	-2.758981000	2.654700000
1	-1.475223000	-4.089263000	3.896090000
1	0.962344000	-3.660500000	3.452678000
1	1.584277000	-1.930814000	1.786735000
1	3.164476000	2.758884000	2.654772000
1	1.475273000	4.089138000	3.896210000
1	-0.962300000	3.660407000	3.452796000
1	-1.584253000	1.930776000	1.786802000
1	4.560344000	1.481894000	1.393747000

1	4.474040000	-1.478487000	-1.708234000
1	3.068444000	-2.803717000	-2.862205000
1	1.336463000	-4.109785000	-4.063368000
1	-1.084659000	-3.658902000	-3.555333000
1	-1.645733000	-1.921862000	-1.878533000
16	6.469346000	0.142032000	-0.162322000
8	6.784442000	1.299881000	0.751516000
6	6.853220000	-1.387910000	0.783208000
1	6.486280000	-2.261922000	0.243067000
1	6.401850000	-1.308286000	1.771983000
1	7.939390000	-1.427675000	0.866498000
16	-6.469345000	-0.142072000	-0.162303000
8	-6.784444000	-1.299913000	0.751544000
6	-6.853242000	1.387886000	0.783196000
1	-6.486327000	2.261894000	0.243032000
1	-7.939412000	1.427630000	0.866503000
1	-6.401854000	1.308291000	1.771966000

xiii) [Fe(L13)2]1+

26	-0.000013000	0.000338000	-0.002006000
7	-0.352963000	1.413902000	-1.379191000
6	-1.681695000	1.661324000	-1.601947000
6	-2.066969000	2.661423000	-2.497740000
7	-1.195153000	3.405836000	-3.169664000
6	0.102028000	3.154325000	-2.941702000
6	0.524482000	2.173287000	-2.055899000
7	-1.916604000	-0.017441000	0.001764000
6	-2.592628000	0.822448000	-0.818775000
6	-3.977056000	0.842789000	-0.834491000
6	-4.670293000	-0.025365000	0.026676000
6	-3.961586000	-0.885504000	0.872132000
6	-2.567871000	-0.863521000	0.836764000
7	-0.313447000	-1.424548000	1.364937000
6	-1.642623000	-1.691743000	1.599090000
6	-2.002302000	-2.712535000	2.486908000
7	-1.118510000	-3.452996000	3.139869000
6	0.178030000	-3.180540000	2.901469000
6	0.577327000	-2.185668000	2.023996000
7	0.314680000	1.425279000	1.364478000
6	1.644073000	1.692031000	1.597847000
6	2.004600000	2.712857000	2.485308000
7	1.121423000	3.453730000	3.138621000
6	-0.175355000	3.181695000	2.900967000
6	-0.575487000	2.186848000	2.023860000
7	1.916561000	0.017805000	0.000180000
6	2.568604000	0.863400000	0.835154000
6	3.962350000	0.884413000	0.870199000
6	4.670297000	0.023807000	0.024623000
6	3.976268000	-0.844089000	-0.836222000
6	2.591891000	-0.822773000	-0.820185000
7	0.351736000	-1.413606000	-1.379394000
6	1.680205000	-1.661432000	-1.602846000
6	2.064726000	-2.661606000	-2.498849000
7	1.192277000	-3.405747000	-3.170324000
6	-0.104655000	-3.153805000	-2.941723000
6	-0.526341000	-2.172603000	-2.055693000
1	-3.118012000	2.864889000	-2.675309000
1	0.824677000	3.752109000	-3.485901000
1	1.576109000	1.983108000	-1.884915000
1	-4.542204000	1.502112000	-1.478604000
1	-4.490362000	-1.554886000	1.539936000

1	-3.049277000	-2.934494000	2.670172000
1	0.913040000	-3.774258000	3.432675000
1	1.625490000	-1.981846000	1.846371000
1	3.051746000	2.934574000	2.667879000
1	-0.909863000	3.775737000	3.432505000
1	-1.623805000	1.983360000	1.846766000
1	4.491739000	1.553359000	1.537959000
1	4.540851000	-1.503994000	-1.480230000
1	3.115588000	-2.865423000	-2.677025000
1	-0.827804000	-3.751310000	-3.485571000
1	-1.577809000	-1.982035000	-1.884182000
8	6.015403000	-0.033539000	-0.021267000
1	6.413457000	0.589564000	0.597785000
8	-6.015457000	0.031100000	-0.018865000
1	-6.412926000	-0.592118000	0.600443000

xiv) [Fe(L14)2]1+

26	0.000000000	0.000006000	-0.052667000
7	0.299647000	1.409897000	1.360486000
6	1.618411000	1.644257000	1.641453000
6	2.000930000	2.593700000	2.592344000
6	1.028920000	3.316261000	3.266137000
6	-0.314601000	3.079822000	2.970121000
6	-0.629317000	2.125565000	2.015081000
7	1.901821000	0.034731000	-0.042978000
6	2.547711000	0.838437000	0.848300000
6	3.933962000	0.840472000	0.918702000
6	4.640186000	0.004306000	0.047447000
6	3.975233000	-0.827459000	-0.857445000
6	2.586965000	-0.794561000	-0.881214000
7	0.364360000	-1.403003000	-1.453477000
6	1.694995000	-1.625179000	-1.688574000
6	2.118769000	-2.589543000	-2.607654000
6	1.177925000	-3.335488000	-3.298469000
6	-0.178154000	-3.106097000	-3.053969000
6	-0.534159000	-2.139767000	-2.126732000
7	-0.364369000	1.403020000	-1.453469000
6	-1.695005000	1.625191000	-1.688561000
6	-2.118786000	2.589558000	-2.607636000
6	-1.177947000	3.335511000	-3.298448000
6	0.178135000	3.106125000	-3.053952000
6	0.534145000	2.139791000	-2.126721000
7	-1.901820000	-0.034723000	-0.042968000
6	-2.586970000	0.794566000	-0.881203000
6	-3.975239000	0.827452000	-0.857436000
6	-4.640186000	-0.004319000	0.047454000
6	-3.933956000	-0.840482000	0.918707000
6	-2.547705000	-0.838437000	0.848306000
7	-0.299637000	-1.409889000	1.360486000
6	-1.618400000	-1.644254000	1.641456000
6	-2.000913000	-2.593698000	2.592348000
6	-1.028898000	-3.316255000	3.266139000
6	0.314621000	-3.079810000	2.970120000
6	0.629331000	-2.125553000	2.015080000
1	3.049891000	2.761811000	2.798435000
1	1.310422000	4.053031000	4.008311000
1	-1.106855000	3.619762000	3.471823000
1	-1.660219000	1.913510000	1.762580000
1	4.471398000	1.436693000	1.644064000
1	4.544112000	-1.505570000	-1.479659000
1	3.175751000	-2.752908000	-2.772576000

1	1.491864000	-4.085651000	-4.013713000
1	-0.946495000	-3.663622000	-3.573350000
1	-1.574250000	-1.934107000	-1.908241000
1	-3.175768000	2.752920000	-2.772554000
1	-1.491890000	4.085677000	-4.013687000
1	0.946472000	3.663658000	-3.573330000
1	1.574237000	1.934135000	-1.908232000
1	-4.544122000	1.505560000	-1.479649000
1	-4.471388000	-1.436710000	1.644066000
1	-3.049873000	-2.761813000	2.798441000
1	-1.310396000	-4.053026000	4.008314000
1	1.106879000	-3.619747000	3.471820000
1	1.660232000	-1.913494000	1.762576000
16	-6.439951000	0.092693000	0.178217000
8	-6.826940000	1.404376000	-0.342474000
6	-7.050284000	-1.158802000	-0.973062000
1	-6.692924000	-2.139143000	-0.661801000
1	-6.723456000	-0.909994000	-1.981480000
1	-8.137867000	-1.113781000	-0.905838000
16	6.439950000	-0.092719000	0.178210000
8	6.826928000	-1.404405000	-0.342481000
6	7.050293000	1.158772000	-0.973068000
1	6.692941000	2.139116000	-0.661806000
1	8.137876000	1.113742000	-0.905844000
1	6.723463000	0.909968000	-1.981486000
8	6.784576000	0.340598000	1.532629000
8	-6.784577000	-0.340628000	1.532634000

xv) [Fe(L15)2]1+

26	0.000000000	0.000019000	0.000012000
7	0.347260000	1.409089000	1.411066000
6	1.676187000	1.631583000	1.663564000
6	2.088403000	2.588174000	2.595400000
6	1.138124000	3.327983000	3.280484000
6	-0.214556000	3.101528000	3.016249000
6	-0.559400000	2.141444000	2.077914000
7	1.890825000	-0.000710000	-0.000378000
6	2.570570000	0.806425000	0.857509000
6	3.962277000	0.782305000	0.836678000
7	4.655469000	-0.001730000	-0.001013000
6	3.961314000	-0.785245000	-0.838390000
6	2.569578000	-0.808345000	-0.858579000
7	0.345567000	-1.409373000	-1.411123000
6	1.674221000	-1.632852000	-1.664213000
6	2.085317000	-2.589791000	-2.596186000
6	1.134194000	-3.328956000	-3.280792000
6	-0.218200000	-3.101517000	-3.015940000
6	-0.561922000	-2.141125000	-2.077508000
7	-0.346112000	1.409435000	-1.410959000
6	-1.674862000	1.632847000	-1.663604000
6	-2.086317000	2.589810000	-2.595397000
6	-1.135459000	3.329067000	-3.280270000
6	0.217036000	3.101700000	-3.015863000
6	0.561119000	2.141281000	-2.077592000
7	-1.890825000	0.000703000	0.000312000
6	-2.569904000	0.808264000	-0.857705000
6	-3.961634000	0.785013000	-0.837122000
7	-4.655469000	0.001418000	0.000439000
6	-3.961957000	-0.782555000	0.837928000
6	-2.570243000	-0.806525000	0.858367000
7	-0.346715000	-1.409041000	1.411219000

6	-1.675546000	-1.631615000	1.664146000
6	-2.087404000	-2.588200000	2.596145000
6	-1.136859000	-3.327919000	3.280960000
6	0.215721000	-3.101375000	3.016297000
6	0.560204000	-2.141302000	2.077816000
1	3.143667000	2.747946000	2.774789000
1	1.442333000	4.071324000	4.007020000
1	-0.989811000	3.655121000	3.529462000
1	-1.597474000	1.938062000	1.847660000
1	4.546673000	1.406896000	1.503724000
1	4.544943000	-1.410268000	-1.505703000
1	3.140384000	-2.750334000	-2.776048000
1	1.437534000	-4.072555000	-4.007427000
1	-0.994090000	-3.654587000	-3.528755000
1	-1.599746000	-1.936982000	-1.846806000
1	-3.141451000	2.750305000	-2.774905000
1	-1.439077000	4.072686000	-4.006768000
1	0.992727000	3.654846000	-3.528898000
1	1.599028000	1.937185000	-1.847233000
1	-4.545517000	1.409973000	-1.504274000
1	-4.546100000	-1.407228000	1.505119000
1	-3.142600000	-2.748032000	2.775876000
1	-1.440789000	-4.071253000	4.007619000
1	0.991176000	-3.654892000	3.529289000
1	1.598192000	-1.937860000	1.847232000

xvi) [Fe(L16)2]1+

26	0.000015000	-0.000004000	-0.000066000
7	-0.341839000	-1.404133000	1.403368000
6	-1.670771000	-1.623628000	1.664366000
6	-2.041631000	-2.585104000	2.606374000
6	-1.032074000	-3.280495000	3.250014000
6	0.546027000	-2.148882000	2.081214000
7	-1.908532000	0.002114000	-0.000564000
6	-2.577230000	-0.806820000	0.865274000
6	-3.968802000	-0.818120000	0.885001000
6	-3.966419000	0.826218000	-0.888080000
6	-2.574887000	0.812352000	-0.867028000
7	-0.337828000	1.405252000	-1.403302000
6	-1.666183000	1.627520000	-1.665187000
6	-2.034386000	2.590259000	-2.606943000
6	-1.022977000	3.284085000	-3.249329000
6	0.551999000	2.148719000	-2.079958000
7	0.338317000	-1.404657000	-1.403760000
6	1.666743000	-1.626735000	-1.665362000
6	2.035297000	-2.589109000	-2.607336000
6	1.024096000	-3.282792000	-3.250244000
6	-0.551277000	-2.147958000	-2.080895000
7	1.908538000	-0.002043000	0.000057000
6	2.575182000	-0.811799000	-0.866627000
6	3.966728000	-0.825475000	-0.887369000
6	3.968491000	0.818032000	0.886468000
6	2.576931000	0.806542000	0.866385000
7	0.341334000	1.403460000	1.404201000
6	1.670168000	1.622914000	1.665674000
6	2.040737000	2.583876000	2.608265000
6	1.030928000	3.278858000	3.252016000
6	-0.546776000	2.147727000	2.082232000
1	-3.081167000	-2.784700000	2.829768000
1	-1.258933000	-4.034107000	3.996452000
1	1.591402000	-1.968983000	1.857931000

1	-4.506568000	-1.457884000	1.572476000
1	-4.502302000	1.466953000	-1.576117000
1	-3.073344000	2.792073000	-2.831050000
1	-1.247775000	4.038594000	-3.995485000
1	3.074326000	-2.790793000	-2.831220000
1	1.249172000	-4.037024000	-3.996600000
1	4.502842000	-1.465809000	-1.575599000
1	4.506004000	1.457560000	1.574356000
1	3.080191000	2.783441000	2.832060000
1	1.257561000	4.032080000	3.998922000
6	-4.666106000	0.004703000	-0.001869000
6	4.666104000	-0.004295000	-0.000629000
1	-5.748401000	0.005721000	-0.002395000
1	5.748400000	-0.005174000	-0.000912000
7	0.278568000	3.068391000	-2.989009000
7	0.270065000	-3.067475000	2.990612000
7	-0.277509000	-3.067294000	-2.990197000
7	-0.271094000	3.065836000	2.992205000
1	-1.596200000	-1.965961000	-1.857217000
1	1.596852000	1.966568000	-1.856065000
1	-1.592074000	1.967868000	1.858586000

xvii) [Fe(L17)2]1+

26	0.000001000	-0.000068000	-0.000013000
7	-0.326699000	-1.415702000	-1.379061000
6	-1.653490000	-1.667018000	-1.615467000
6	-2.022624000	-2.669707000	-2.519775000
6	0.154702000	-3.150808000	-2.939149000
6	0.561630000	-2.171231000	-2.045956000
7	-1.912496000	-0.003124000	0.000271000
6	-2.572853000	-0.841020000	-0.839475000
6	-3.965476000	-0.858103000	-0.860027000
6	-3.967980000	0.846716000	0.859639000
6	-2.575359000	0.833203000	0.839640000
7	-0.330902000	1.414052000	1.379713000
6	-1.658392000	1.661628000	1.615945000
6	-2.030454000	2.662859000	2.520657000
6	0.145475000	3.149394000	2.941053000
6	0.555248000	2.171438000	2.047366000
7	0.325947000	1.415589000	-1.379296000
6	1.652607000	1.667020000	-1.616272000
6	2.021282000	2.669685000	-2.520769000
6	-0.156253000	3.150522000	-2.939298000
6	-0.562734000	2.170957000	-2.045867000
7	1.912481000	0.003089000	-0.000704000
6	2.572391000	0.841124000	-0.840638000
6	3.965003000	0.858493000	-0.861654000
6	3.968424000	-0.846266000	0.858053000
6	2.575792000	-0.833037000	0.838505000
7	0.331629000	-1.414152000	1.379545000
6	1.659247000	-1.661594000	1.615192000
6	2.031828000	-2.662823000	2.519670000
6	-0.143863000	-3.149592000	2.941015000
6	-0.554155000	-2.171648000	2.047530000
1	-3.070600000	-2.879210000	-2.708963000
1	0.885378000	-3.743743000	-3.477446000
1	1.610558000	-1.977578000	-1.862347000
1	-4.502736000	-1.519783000	-1.526425000
1	-4.507237000	1.507072000	1.525739000
1	-3.079029000	2.869520000	2.709641000
1	0.874415000	3.743879000	3.479994000

1	1.604730000	1.980708000	1.863851000
1	3.069150000	2.879256000	-2.710455000
1	-0.887203000	3.743357000	-3.477336000
1	-1.611565000	1.977205000	-1.861808000
1	4.501904000	1.520292000	-1.528223000
1	4.508030000	-1.506475000	1.524017000
1	3.080501000	-2.869383000	2.708204000
1	-0.872504000	-3.744159000	3.480272000
1	-1.603731000	-1.981008000	1.864467000
6	-4.661694000	-0.006612000	-0.000337000
6	4.661680000	0.007163000	-0.002178000
1	5.744252000	0.008766000	-0.002732000
1	-5.744267000	-0.007978000	-0.000551000
7	-1.140914000	-3.406406000	-3.182092000
7	-1.150872000	3.401499000	3.183658000
7	1.139222000	3.406249000	-3.182761000
7	1.152611000	-3.401582000	3.183015000

xviii) [Fe(L18)2]1+

26	0.000053000	0.000477000	0.000270000
7	-0.335762000	1.409356000	1.345272000
6	-1.662493000	1.673482000	1.576642000
7	-2.109297000	2.612023000	2.402164000
6	-1.182867000	3.333761000	3.021197000
7	0.592330000	2.149375000	1.952542000
7	-1.907810000	-0.011216000	-0.002995000
6	-2.574284000	0.829748000	0.807862000
6	-3.965122000	0.849063000	0.832489000
6	-3.951576000	-0.895682000	-0.846485000
6	-2.561240000	-0.859842000	-0.816320000
7	-0.313998000	-1.413245000	-1.344682000
6	-1.636465000	-1.693100000	-1.581364000
7	-2.068897000	-2.637279000	-2.407920000
6	-1.131485000	-3.348850000	-3.022452000
7	0.625380000	-2.143408000	-1.947031000
7	0.331817000	-1.408317000	1.346346000
6	1.657813000	-1.673020000	1.581150000
7	2.102042000	-2.611543000	2.408005000
6	1.173719000	-3.332688000	3.024973000
7	1.907897000	0.011361000	0.001965000
6	2.572025000	-0.829996000	0.814256000
6	3.962760000	-0.850782000	0.841633000
6	3.954114000	0.893055000	-0.838339000
6	2.563671000	0.858772000	-0.810845000
7	0.317889000	1.413691000	-1.343924000
6	1.641103000	1.692369000	-1.578115000
6	1.140497000	3.348176000	-3.020584000
1	-1.515715000	4.103457000	3.708540000
1	-4.479416000	1.535803000	1.491496000
1	-4.455006000	-1.588515000	-1.507475000
1	-1.452576000	-4.122575000	-3.710841000
1	1.504585000	-4.102359000	3.713295000
1	4.474909000	-1.537889000	1.501913000
1	4.459630000	1.584878000	-1.498821000
1	1.463519000	4.121094000	-3.708960000
6	-4.653912000	-0.027391000	-0.008351000
6	4.654001000	0.024524000	0.001707000
6	0.229078000	-3.098423000	-2.772405000
6	0.181656000	3.099025000	2.777158000
6	-0.190074000	-3.097233000	2.777509000
7	-0.619640000	2.144853000	-1.947924000

6	-0.220855000	3.099479000	-2.772546000
7	2.076039000	2.635818000	-2.404173000
1	-1.007170000	3.673971000	-3.248001000
7	-0.598221000	-2.147653000	1.951677000
1	-0.970613000	-3.678701000	3.253970000
1	1.016855000	-3.672012000	-3.246512000
1	0.960747000	3.681020000	3.255320000
1	5.736750000	0.029816000	0.001654000
1	-5.736651000	-0.033763000	-0.010459000

xix) [Fe (L19) 2] 1+

26	0.014535000	-0.000511000	-0.000100000
7	0.345400000	0.055031000	-1.984884000
6	1.665988000	0.063915000	-2.320749000
6	2.050349000	0.101996000	-3.661828000
6	-0.123784000	0.121986000	-4.314143000
6	-0.541629000	0.084160000	-2.984148000
7	1.901784000	-0.001344000	0.001748000
6	2.573291000	0.030880000	-1.167759000
6	3.970487000	0.029280000	-1.141994000
6	3.968142000	-0.034627000	1.149632000
6	2.570911000	-0.034197000	1.172588000
7	0.341350000	-0.055027000	1.985283000
6	1.661265000	-0.064980000	2.323809000
6	2.042892000	-0.101115000	3.665723000
6	-0.132554000	-0.116859000	4.313737000
6	-0.547697000	-0.080963000	2.982856000
7	-0.341708000	-1.980600000	-0.055357000
6	-1.677817000	-2.317071000	-0.065569000
6	-2.051695000	-3.671515000	-0.103174000
6	0.125005000	-4.319233000	-0.119633000
6	0.538581000	-3.001256000	-0.082945000
7	-1.890146000	0.000190000	-0.001919000
6	-2.573415000	-1.183768000	-0.034870000
6	-3.964149000	-1.148183000	-0.034609000
6	-3.963321000	1.150371000	0.029138000
6	-2.572126000	1.185152000	0.030687000
7	-0.339743000	1.979606000	0.054303000
6	-1.675820000	2.317234000	0.062605000
6	-2.048435000	3.672256000	0.099443000
6	0.128893000	4.317920000	0.118736000
6	0.541298000	2.999706000	0.082867000
1	3.098445000	0.109359000	-3.942219000
1	-0.850813000	0.145543000	-5.118453000
1	-1.589796000	0.076973000	-2.715487000
1	4.555638000	0.054290000	-2.054635000
1	4.551388000	-0.060493000	2.063462000
1	3.090420000	-0.109356000	3.948215000
1	-0.861212000	-0.137740000	5.116644000
1	-1.595320000	-0.072908000	2.712115000
1	-3.102960000	-3.942775000	-0.111314000
1	0.849027000	-5.125318000	-0.141402000
1	1.591846000	-2.749468000	-0.075196000
1	-4.550392000	-2.060632000	-0.060123000
1	-4.548617000	2.063510000	0.054269000
1	-3.099529000	3.944327000	0.106061000
1	0.853493000	5.123432000	0.141317000
1	1.594388000	2.747092000	0.076623000
7	1.164958000	0.130936000	-4.654992000
7	1.155503000	-0.127013000	4.657170000
7	-1.179498000	-4.663104000	-0.129967000

7	-1.175621000	4.662987000	0.127248000
7	4.652267000	-0.003246000	0.004494000
7	-4.656244000	0.001717000	-0.003077000

xx) [Fe(L20)2]1+

26	-0.006620000	-0.007183000	-0.001427000
7	0.385211000	1.341327000	1.443818000
6	1.712417000	1.503275000	1.720963000
6	2.154425000	2.423049000	2.675617000
6	1.253711000	3.212738000	3.385478000
6	-0.107049000	3.028382000	3.076019000
6	-0.487827000	2.106709000	2.119201000
7	1.894428000	-0.105962000	0.029645000
6	2.593739000	0.653342000	0.910825000
6	3.979155000	0.597150000	0.944369000
6	4.684179000	-0.242431000	0.058301000
6	3.927519000	-1.005185000	-0.839824000
6	2.535159000	-0.928375000	-0.839380000
7	0.281354000	-1.389060000	-1.434254000
6	1.600120000	-1.681455000	-1.675236000
6	1.968574000	-2.635871000	-2.624330000
6	1.012678000	-3.326344000	-3.369587000
6	-0.328403000	-3.008389000	-3.100196000
6	-0.639171000	-2.056168000	-2.141437000
7	-0.245168000	1.458375000	-1.356463000
6	-1.557189000	1.762959000	-1.629451000
6	-1.892829000	2.785293000	-2.531907000
6	-0.915182000	3.522195000	-3.184075000
6	0.424463000	3.188998000	-2.879761000
6	0.701302000	2.179716000	-1.979564000
7	-1.909760000	0.088183000	-0.035472000
6	-2.516415000	0.963168000	-0.886791000
6	-3.912583000	1.030198000	-0.937672000
6	-4.699178000	0.216510000	-0.119863000
6	-4.026119000	-0.674113000	0.749718000
6	-2.642640000	-0.719786000	0.769461000
7	-0.453578000	-1.431701000	1.355571000
6	-1.789816000	-1.608513000	1.571682000
6	-2.265918000	-2.570163000	2.466156000
6	-1.392013000	-3.389258000	3.176568000
6	-0.020824000	-3.188494000	2.931378000
6	0.394272000	-2.223960000	2.033261000
1	3.216206000	2.513728000	2.852728000
1	-0.877039000	3.598772000	3.578611000
1	-1.532513000	1.960436000	1.874674000
1	4.519535000	1.209507000	1.653391000
1	4.418641000	-1.663545000	-1.541167000
1	3.021058000	-2.836490000	-2.775379000
1	-1.138921000	-3.487885000	-3.629549000
1	-1.671386000	-1.804951000	-1.930352000
1	-2.938865000	2.991009000	-2.707775000
1	1.251071000	3.709316000	-3.344755000
1	1.725956000	1.919582000	-1.742908000
1	-4.378917000	1.725301000	-1.620608000
1	-4.592341000	-1.328663000	1.397954000
1	-3.333653000	-2.668314000	2.596852000
1	0.730606000	-3.778736000	3.439214000
1	1.447923000	-2.064360000	1.840713000
6	1.680678000	4.235149000	4.445630000
6	1.035982000	3.856513000	5.800206000
6	1.194988000	5.640320000	4.017653000

1	1.634285000	5.933857000	3.060616000
1	0.108276000	5.684399000	3.917247000
1	1.488959000	6.380430000	4.766506000
1	-0.054938000	3.851249000	5.746617000
1	1.326673000	4.579837000	6.566535000
1	1.362459000	2.866087000	6.128218000
6	6.219133000	-0.287255000	0.105370000
6	6.674426000	-0.745025000	1.511352000
6	6.780426000	1.125509000	-0.182950000
1	6.476540000	1.474211000	-1.173489000
1	6.440035000	1.859550000	0.551200000
1	7.873081000	1.108904000	-0.150608000
1	6.329912000	-0.066327000	2.295133000
1	7.766104000	-0.777783000	1.559882000
1	6.295539000	-1.744505000	1.740900000
6	-1.858119000	-4.457470000	4.173171000
6	-3.391418000	-4.515623000	4.290881000
6	-1.271316000	-4.136090000	5.568271000
1	-0.179116000	-4.126180000	5.560229000
1	-1.614953000	-3.161409000	5.924631000
1	-1.590596000	-4.892292000	6.290206000
1	-3.810329000	-3.570310000	4.646957000
1	-3.672658000	-5.287711000	5.010382000
1	-3.865250000	-4.769606000	3.338579000
6	-6.234784000	0.251769000	-0.133240000
6	-6.785670000	1.279646000	-1.137706000
6	-6.750053000	0.627459000	1.276446000
1	-6.431782000	-0.092008000	2.034596000
1	-6.387795000	1.614437000	1.576202000
1	-7.843099000	0.651785000	1.282911000
1	-6.464215000	2.297195000	-0.898857000
1	-7.877553000	1.267922000	-1.109972000
1	-6.483087000	1.051591000	-2.163464000
6	1.438487000	-4.367359000	-4.414458000
6	2.245573000	-5.488028000	-3.717768000
6	2.322319000	-3.682337000	-5.483371000
1	1.777269000	-2.881651000	-5.990034000
1	3.228258000	-3.251502000	-5.050585000
1	2.630205000	-4.411953000	-6.237062000
1	3.149455000	-5.104361000	-3.238755000
1	2.552809000	-6.238189000	-4.451280000
1	1.645136000	-5.988206000	-2.953366000
6	-1.227006000	4.642903000	-4.183110000
6	-0.608817000	5.965549000	-3.671468000
6	-2.739636000	4.853895000	-4.371348000
1	-3.231192000	3.958341000	-4.761473000
1	-3.231120000	5.141185000	-3.437625000
1	-2.909501000	5.658531000	-5.090330000
1	-1.028841000	6.245785000	-2.701784000
1	-0.817476000	6.773803000	-4.377520000
1	0.475416000	5.893824000	-3.560632000
6	0.228704000	-5.006010000	-5.120212000
1	-0.422928000	-5.532561000	-4.417734000
1	-0.368798000	-4.264702000	-5.657554000
1	0.578237000	-5.737102000	-5.852613000
6	-1.349542000	-5.841814000	3.705810000
1	-0.259433000	-5.879031000	3.648277000
1	-1.670813000	-6.614031000	4.409672000
1	-1.748371000	-6.095202000	2.719993000
6	-6.775597000	-1.144545000	-0.522950000
1	-6.458313000	-1.918082000	0.180410000
1	-7.868862000	-1.135145000	-0.531856000

1	-6.431550000	-1.434148000	-1.519427000
6	-0.609248000	4.282595000	-5.555147000
1	-1.030819000	3.351449000	-5.942974000
1	-0.816446000	5.075726000	-6.278585000
1	0.474754000	4.162332000	-5.496174000
6	3.207932000	4.282050000	4.628839000
1	3.721244000	4.575362000	3.708813000
1	3.460888000	5.021097000	5.392188000
1	3.609696000	3.320514000	4.960560000
6	6.805539000	-1.260731000	-0.932760000
1	6.547015000	-0.972786000	-1.955538000
1	7.895315000	-1.258122000	-0.859886000
1	6.470381000	-2.288089000	-0.765112000

xxi) [Fe(L21)2]1+

26	0.011236000	-0.023782000	0.018594000
7	0.337339000	1.263758000	1.531216000
6	1.656652000	1.485542000	1.794134000
6	2.061795000	2.333552000	2.823431000
6	1.100626000	2.971989000	3.597435000
6	-0.244401000	2.743843000	3.323219000
6	-0.580326000	1.882632000	2.285750000
7	1.909951000	-0.032616000	0.028292000
6	2.574025000	0.747947000	0.906944000
6	3.965662000	0.784384000	0.914437000
6	4.690608000	0.003425000	-0.000693000
6	3.967637000	-0.796928000	-0.899720000
6	2.575653000	-0.799424000	-0.861852000
7	0.340044000	-1.339311000	-1.469031000
6	1.660238000	-1.568560000	-1.722799000
6	2.067054000	-2.465599000	-2.709322000
6	1.107420000	-3.137918000	-3.455704000
6	-0.238380000	-2.898460000	-3.193861000
6	-0.576096000	-1.996269000	-2.192506000
7	-0.305919000	1.477245000	-1.287219000
6	-1.637890000	1.748517000	-1.523464000
6	-2.014555000	2.767347000	-2.412186000
6	-1.049929000	3.510675000	-3.061946000
6	0.303462000	3.229475000	-2.816454000
6	0.617145000	2.215756000	-1.931462000
7	-1.897668000	-0.006592000	0.002257000
6	-2.555821000	0.903398000	-0.781325000
6	-3.941695000	0.932249000	-0.804213000
6	-4.689912000	0.026173000	-0.022636000
6	-3.976177000	-0.898052000	0.773036000
6	-2.591083000	-0.899416000	0.773336000
7	-0.363950000	-1.519201000	1.318501000
6	-1.703933000	-1.764922000	1.532130000
6	-2.115602000	-2.775537000	2.411985000
6	-1.176078000	-3.538873000	3.077666000
6	0.185932000	-3.283724000	2.854881000
6	0.535149000	-2.275892000	1.976761000
1	3.114299000	2.490626000	3.019134000
1	1.397131000	3.634907000	4.401023000
1	-1.026008000	3.221763000	3.899372000
1	-1.613199000	1.674334000	2.038551000
1	4.492557000	1.393378000	1.636175000
1	4.494942000	-1.385003000	-1.638382000
1	3.119892000	-2.636764000	-2.891013000
1	1.405381000	-3.836602000	-4.227834000
1	-1.018906000	-3.397723000	-3.753105000

1	-1.609440000	-1.780391000	-1.953868000
1	-3.064746000	2.964266000	-2.584765000
1	-1.334463000	4.297272000	-3.749968000
1	1.093700000	3.785547000	-3.303220000
1	1.651379000	1.972703000	-1.720152000
1	-4.457140000	1.633788000	-1.446844000
1	-4.518403000	-1.587276000	1.406812000
1	-3.172284000	-2.952092000	2.566251000
1	-1.487301000	-4.320391000	3.759786000
1	0.956610000	-3.856048000	3.354226000
1	1.577066000	-2.052277000	1.782305000
6	6.170221000	0.025379000	-0.018514000
6	6.903954000	-1.145758000	-0.257815000
6	6.875071000	1.217470000	0.203612000
6	8.292942000	-1.132749000	-0.271882000
6	8.263778000	1.244879000	0.184180000
6	8.966172000	0.066083000	-0.052145000
1	6.389465000	-2.088650000	-0.402442000
1	6.337104000	2.145076000	0.361121000
1	8.851430000	-2.043733000	-0.442680000
1	8.799460000	2.171785000	0.341867000
6	-6.166042000	0.042836000	-0.035611000
6	-6.878725000	1.244360000	-0.184735000
6	-6.907825000	-1.142460000	0.100874000
6	-8.267676000	1.266816000	-0.198184000
6	-8.296975000	-1.134058000	0.089481000
6	-8.971319000	0.074030000	-0.060516000
1	-6.344276000	2.184231000	-0.259575000
1	-6.395854000	-2.093968000	0.185266000
1	-8.802664000	2.201902000	-0.302207000
1	-8.854403000	-2.056977000	0.183918000
17	10.713723000	0.091545000	-0.073093000
17	-10.724109000	0.093556000	-0.075953000

xxii) [Fe (L22) 2]1+

26	0.000000000	-0.055230000	0.000000000
7	0.557066000	-1.462297000	-1.329334000
6	1.899171000	-1.701721000	-1.343814000
6	2.475662000	-2.648807000	-2.195634000
6	1.654339000	-3.372907000	-3.061652000
6	0.273847000	-3.119390000	-3.043166000
6	-0.216417000	-2.168035000	-2.169541000
7	1.884566000	-0.055779000	0.315488000
6	2.671185000	-0.887583000	-0.396596000
6	4.053699000	-0.910527000	-0.195656000
6	4.604364000	-0.045521000	0.768633000
6	3.779735000	0.812205000	1.499858000
6	2.392158000	0.780255000	1.242015000
7	0.085609000	1.348022000	1.438741000
6	1.362509000	1.586033000	1.891021000
6	1.614730000	2.524662000	2.889637000
6	0.556838000	3.245201000	3.448552000
6	-0.742693000	2.999680000	2.982997000
6	-0.911364000	2.045322000	1.984583000
7	-0.557059000	-1.462315000	1.329316000
6	-1.899164000	-1.701743000	1.343796000
6	-2.475651000	-2.648841000	2.195605000
6	-1.654325000	-3.372949000	3.061613000
6	-0.273834000	-3.119427000	3.043128000
6	0.216427000	-2.168060000	2.169515000
7	-1.884566000	-0.055782000	-0.315488000

6	-2.671182000	-0.887597000	0.396587000
6	-4.053696000	-0.910543000	0.195649000
6	-4.604364000	-0.045528000	-0.768629000
6	-3.779739000	0.812209000	-1.499847000
6	-2.392161000	0.780260000	-1.242005000
7	-0.085615000	1.348038000	-1.438726000
6	-1.362515000	1.586049000	-1.891004000
6	-1.614741000	2.524687000	-2.889609000
6	-0.556851000	3.245235000	-3.448518000
6	0.742681000	2.999714000	-2.982967000
6	0.911355000	2.045346000	-1.984561000
1	3.543222000	-2.806245000	-2.170217000
1	-0.382134000	-3.666738000	-3.705973000
1	-1.276847000	-1.952787000	-2.133287000
1	4.715184000	-1.561851000	-0.747501000
1	4.180624000	1.483846000	2.242479000
1	2.616264000	2.713577000	3.250056000
1	-1.605695000	3.521006000	3.369255000
1	-1.903235000	1.833049000	1.604427000
1	-3.543211000	-2.806283000	2.170187000
1	0.382149000	-3.666782000	3.705928000
1	1.276856000	-1.952809000	2.133262000
1	-4.715178000	-1.561875000	0.747487000
1	-4.180631000	1.483858000	-2.242459000
1	-2.616275000	2.713601000	-3.250027000
1	1.605681000	3.521047000	-3.369220000
1	1.903228000	1.833073000	-1.604409000
8	-5.942068000	-0.122558000	-0.908996000
6	-6.592981000	0.713682000	-1.867602000
1	-6.445571000	1.771898000	-1.632078000
1	-6.236893000	0.503019000	-2.880388000
1	-7.650415000	0.470085000	-1.796707000
8	5.942068000	-0.122549000	0.908999000
6	6.592977000	0.713682000	1.867616000
1	6.445564000	1.771901000	1.632104000
1	6.236889000	0.503006000	2.880399000
1	7.650412000	0.470089000	1.796719000
8	2.077784000	-4.308052000	-3.926996000
6	3.472551000	-4.618166000	-3.994733000
1	4.055783000	-3.742640000	-4.294673000
1	3.836627000	-5.002378000	-3.037433000
1	3.561906000	-5.391324000	-4.753884000
8	0.882029000	4.131741000	4.405773000
6	-0.154688000	4.901025000	5.022201000
1	-0.669298000	5.527311000	4.287874000
1	-0.873811000	4.254064000	5.532654000
1	0.346492000	5.533226000	5.751221000
8	-0.882046000	4.131783000	-4.405730000
6	0.154668000	4.901077000	-5.022150000
1	0.669277000	5.527358000	-4.287818000
1	0.873793000	4.254123000	-5.532611000
1	-0.346514000	5.533283000	-5.751164000
8	-2.077766000	-4.308106000	3.926946000
6	-3.472532000	-4.618225000	3.994681000
1	-4.055767000	-3.742705000	4.294632000
1	-3.836608000	-5.002427000	3.037377000
1	-3.561883000	-5.391393000	4.753823000

xxiii) [Fe(L23)2]1+

26	-0.004231000	0.030448000	-0.037619000
7	-0.681443000	1.188349000	-1.535864000

6	-2.046517000	1.232552000	-1.629544000
6	-2.697245000	1.970530000	-2.615662000
6	-1.965047000	2.719675000	-3.562851000
6	-0.554258000	2.658275000	-3.437732000
6	0.013965000	1.894176000	-2.434336000
7	-1.885098000	-0.194311000	0.212148000
6	-2.743752000	0.433685000	-0.614202000
6	-4.129662000	0.300821000	-0.455006000
6	-4.641121000	-0.520746000	0.580591000
6	-3.704650000	-1.170789000	1.422312000
6	-2.332270000	-0.977343000	1.213252000
7	0.014447000	-1.206533000	1.547949000
6	-1.232165000	-1.563302000	1.987904000
6	-1.417711000	-2.404034000	3.083380000
6	-0.313587000	-2.935194000	3.785317000
6	0.963670000	-2.550969000	3.304598000
6	1.061381000	-1.705200000	2.214280000
7	0.300877000	1.630975000	1.140848000
6	1.603434000	2.050637000	1.180909000
6	2.006809000	3.139674000	1.950349000
6	1.074785000	3.866861000	2.723000000
6	-0.265961000	3.410556000	2.659243000
6	-0.582823000	2.316322000	1.874565000
7	1.875983000	0.255273000	-0.287421000
6	2.516259000	1.251989000	0.353772000
6	3.896425000	1.441646000	0.201063000
6	4.634414000	0.581053000	-0.649654000
6	3.925205000	-0.463960000	-1.293018000
6	2.544076000	-0.592313000	-1.093371000
7	0.349409000	-1.492858000	-1.301833000
6	1.659472000	-1.604581000	-1.683174000
6	2.092836000	-2.595061000	-2.561702000
6	1.187657000	-3.539928000	-3.092964000
6	-0.160598000	-3.401251000	-2.677216000
6	-0.510153000	-2.384655000	-1.806671000
1	-3.774723000	1.941381000	-2.652761000
1	0.100518000	3.206523000	-4.097620000
1	1.092275000	1.847805000	-2.338767000
1	-4.792391000	0.845469000	-1.107050000
1	-4.032748000	-1.831404000	2.207749000
1	-2.425671000	-2.625347000	3.396785000
1	1.874730000	-2.912780000	3.756057000
1	2.037755000	-1.412552000	1.846632000
1	3.051633000	3.407112000	1.955537000
1	-1.061716000	3.904041000	3.195900000
1	-1.607987000	1.969115000	1.824401000
1	4.381509000	2.240189000	0.736991000
1	4.433736000	-1.168958000	-1.929039000
1	3.133749000	-2.613352000	-2.843366000
1	-0.931375000	-4.080299000	-3.008231000
1	-1.540431000	-2.279831000	-1.487925000
7	5.983746000	0.759283000	-0.851489000
7	-5.993564000	-0.680493000	0.761540000
6	6.743696000	-0.131496000	-1.731627000
1	7.620294000	0.424089000	-2.071241000
1	6.152550000	-0.332442000	-2.629565000
6	6.717154000	1.832596000	-0.176353000
1	6.114537000	2.745024000	-0.200515000
1	7.602167000	2.045125000	-0.779593000
6	-6.971737000	-0.112126000	-0.167134000
1	-7.848769000	-0.764562000	-0.155065000
1	-6.576275000	-0.167411000	-1.183894000

6	-6.540224000	-1.428030000	1.894962000
1	-5.918461000	-1.251083000	2.775533000
1	-7.515928000	-0.994695000	2.129914000
6	7.193956000	-1.449025000	-1.087630000
1	7.726450000	-2.061880000	-1.820765000
1	7.868993000	-1.268001000	-0.248604000
1	6.343022000	-2.023821000	-0.716017000
6	-6.694760000	-2.930746000	1.634256000
1	-7.124736000	-3.426486000	2.509218000
1	-7.358287000	-3.114470000	0.785389000
1	-5.732299000	-3.397050000	1.413025000
6	-7.393446000	1.322019000	0.172588000
1	-8.136711000	1.680309000	-0.545312000
1	-7.838721000	1.373344000	1.169436000
1	-6.539680000	2.002759000	0.152601000
6	7.145275000	1.518107000	1.262754000
1	7.658242000	2.380498000	1.698337000
1	6.285666000	1.278729000	1.892270000
1	7.831203000	0.669028000	1.293903000
7	-0.465553000	-3.767373000	4.862012000
6	-1.781648000	-4.243863000	5.291392000
6	-2.491468000	-3.305863000	6.273968000
6	0.681965000	-4.233170000	5.644925000
6	1.323985000	-5.514407000	5.102376000
1	1.420084000	-3.431177000	5.712847000
1	2.158246000	-5.820034000	5.739822000
1	0.330763000	-4.400539000	6.666321000
1	0.601881000	-6.334514000	5.077830000
1	-1.636668000	-5.222219000	5.756422000
1	-2.403823000	-4.423807000	4.411472000
1	-1.895421000	-3.163764000	7.178898000
1	-3.456756000	-3.725857000	6.570293000
1	-2.665905000	-2.322829000	5.831195000
1	1.702705000	-5.370618000	4.088235000
7	1.441312000	4.943735000	3.485055000
6	2.806229000	5.473312000	3.470055000
6	3.744764000	4.798138000	4.476185000
6	0.486341000	5.632190000	4.357382000
6	-0.297701000	6.748492000	3.659397000
1	-0.194234000	4.898803000	4.795049000
1	-0.975605000	7.235036000	4.366111000
1	1.053388000	6.047412000	5.194405000
1	0.376589000	7.511007000	3.261273000
1	2.741839000	6.542484000	3.687149000
1	3.209435000	5.401003000	2.457179000
1	3.371825000	4.913267000	5.496980000
1	4.739974000	5.249054000	4.429451000
1	3.842197000	3.729145000	4.274751000
7	1.585511000	-4.526481000	-3.954986000
6	0.624331000	-5.439861000	-4.578481000
6	0.319241000	-6.685788000	-3.740263000
6	2.993435000	-4.728788000	-4.302049000
6	3.466436000	-3.887074000	-5.492386000
1	3.612208000	-4.535824000	-3.422494000
1	4.516821000	-4.097038000	-5.712792000
1	3.122675000	-5.790311000	-4.527661000
1	2.883644000	-4.114719000	-6.388425000
1	1.040258000	-5.737787000	-5.544314000
1	-0.293904000	-4.894503000	-4.806590000
1	1.228218000	-7.261956000	-3.549499000
1	-0.385551000	-7.334541000	-4.267623000
1	-0.117209000	-6.418806000	-2.775479000

7	-2.577565000	3.457326000	-4.540243000
6	-1.810327000	4.152034000	-5.577369000
6	-1.369610000	5.564963000	-5.180634000
6	-4.033468000	3.598174000	-4.604814000
6	-4.730030000	2.486781000	-5.397744000
1	-4.434656000	3.658239000	-3.590325000
1	-5.809622000	2.659108000	-5.425387000
1	-4.245667000	4.566587000	-5.064752000
1	-4.368603000	2.456534000	-6.428671000
1	-2.440020000	4.198780000	-6.469491000
1	-0.947491000	3.542914000	-5.855006000
1	-2.232795000	6.193955000	-4.948496000
1	-0.821448000	6.035874000	-6.001291000
1	-0.721620000	5.547173000	-4.301790000
1	-4.549985000	1.506178000	-4.951811000
1	-0.890572000	6.358708000	2.829253000
1	3.364727000	-2.818571000	-5.290421000

xxiv) [Fe(L24)2]1+

26	0.000000000	0.000090000	-0.000011000
7	-0.369069000	1.393721000	-1.402028000
7	-1.715260000	1.588679000	-1.608077000
6	-1.923745000	2.563572000	-2.542381000
7	-1.915393000	-0.000009000	0.000450000
6	-2.597662000	0.813856000	-0.839937000
6	-3.977565000	0.845583000	-0.877402000
6	-4.673990000	-0.000578000	0.000693000
6	-3.977055000	-0.846499000	0.878626000
6	-2.597176000	-0.814217000	0.840891000
7	-0.368245000	-1.393574000	1.402181000
7	-1.714315000	-1.588790000	1.608763000
6	-1.922241000	-2.563644000	2.543231000
7	0.368943000	1.393760000	1.402014000
7	1.715118000	1.588797000	1.608099000
6	-0.246538000	2.253753000	2.210752000
7	1.915393000	0.000132000	-0.000436000
6	2.597587000	0.814001000	0.840012000
6	3.977487000	0.845748000	0.877577000
6	4.673989000	-0.000390000	-0.000476000
6	3.977132000	-0.846325000	-0.878461000
6	2.597251000	-0.814067000	-0.840821000
7	0.368370000	-1.393532000	-1.402197000
1	-2.915996000	2.861942000	-2.835178000
1	-4.508933000	1.500535000	-1.554126000
1	-5.755407000	-0.000795000	0.000798000
1	-4.508031000	-1.501709000	1.555408000
1	-2.914319000	-2.862173000	2.836454000
1	-0.478444000	-3.772271000	3.678365000
1	-1.323725000	2.293798000	2.233922000
1	4.508796000	1.500695000	1.554353000
1	5.755406000	-0.000588000	-0.000502000
1	4.508168000	-1.501530000	-1.555200000
7	1.714457000	-1.588664000	-1.608750000
6	1.922465000	-2.563431000	-2.543288000
6	-0.247456000	-2.253242000	-2.210969000
6	0.684458000	-3.007787000	-2.948347000
1	-1.324654000	-2.293177000	-2.233806000
1	0.478767000	-3.771977000	-3.678636000
1	2.914568000	-2.861884000	-2.836504000
6	0.685687000	3.008440000	2.947587000
6	1.923522000	2.563779000	2.542330000

1	2.915748000	2.862221000	2.835139000
1	0.480307000	3.772885000	3.677695000
6	-0.684198000	-3.008006000	2.948173000
6	0.247653000	-2.253312000	2.210869000
1	1.324853000	-2.293182000	2.233679000
6	-0.685947000	3.008244000	-2.947737000
1	-0.480630000	3.772634000	-3.677921000
6	0.246343000	2.253664000	-2.210872000
1	1.323526000	2.293760000	-2.234083000

xxv) [Fe (L25) 2] 1+

26	0.000000000	0.000003000	0.009979000
7	-0.306468000	-1.403276000	1.422997000
6	-1.629115000	-1.681920000	1.658216000
6	-2.009661000	-2.608891000	2.633183000
6	-1.040397000	-3.261755000	3.376455000
6	0.305668000	-2.970896000	3.134435000
6	0.620279000	-2.039971000	2.158186000
7	-1.904462000	-0.043654000	0.009654000
6	-2.555907000	-0.912346000	0.827015000
6	-3.942687000	-0.962967000	0.840800000
6	-4.694308000	-0.110862000	0.006387000
6	-3.982717000	0.776013000	-0.826802000
6	-2.595106000	0.792389000	-0.809597000
7	-0.370389000	1.387926000	-1.403246000
6	-1.704378000	1.604358000	-1.639946000
6	-2.126684000	2.512568000	-2.615364000
6	-1.188230000	3.210340000	-3.357380000
6	0.169702000	2.983061000	-3.113602000
6	0.526348000	2.067709000	-2.137087000
7	0.370382000	-1.387901000	-1.403266000
6	1.704369000	-1.604332000	-1.639974000
6	2.126670000	-2.512529000	-2.615406000
6	1.188213000	-3.210289000	-3.357429000
6	-0.169718000	-2.983011000	-3.113644000
6	-0.526359000	-2.067671000	-2.137114000
7	1.904462000	0.043660000	0.009647000
6	2.595102000	-0.792376000	-0.809617000
6	3.982713000	-0.776003000	-0.826826000
6	4.694308000	0.110860000	0.006373000
6	3.942692000	0.962956000	0.840799000
6	2.555912000	0.912338000	0.827017000
7	0.306475000	1.403265000	1.423013000
6	1.629124000	1.681904000	1.658231000
6	2.009674000	2.608863000	2.633207000
6	1.040414000	3.261721000	3.376489000
6	-0.305653000	2.970867000	3.134471000
6	-0.620268000	2.039953000	2.158212000
1	-3.058915000	-2.810105000	2.805755000
1	-1.323259000	-3.982608000	4.133684000
1	1.096882000	-3.458170000	3.689042000
1	1.650628000	-1.787870000	1.941273000
1	-4.454236000	-1.635505000	1.516103000
1	-4.524674000	1.421715000	-1.504624000
1	-3.184024000	2.664332000	-2.789182000
1	-1.503587000	3.917234000	-4.114941000
1	0.937924000	3.507187000	-3.666919000
1	1.567122000	1.864378000	-1.918850000
1	3.184010000	-2.664292000	-2.789230000
1	1.503566000	-3.917172000	-4.115001000
1	-0.937942000	-3.507127000	-3.666966000

1	-1.567132000	-1.864342000	-1.918871000
1	4.524667000	-1.421699000	-1.504656000
1	4.454244000	1.635484000	1.516109000
1	3.058930000	2.810074000	2.805777000
1	1.323280000	3.982564000	4.133726000
1	-1.096863000	3.458136000	3.689085000
1	-1.650618000	1.787856000	1.941299000
6	-6.168766000	-0.147514000	0.005825000
6	-6.927419000	1.012118000	-0.199243000
6	-6.868839000	-1.351901000	0.213811000
6	-8.318824000	0.988968000	-0.197354000
6	-8.250066000	-1.391590000	0.213605000
6	-8.993567000	-0.219413000	0.009048000
1	-6.429080000	1.966154000	-0.329534000
1	-6.321784000	-2.278726000	0.343970000
1	-8.862847000	1.911834000	-0.344558000
1	-8.786343000	-2.321248000	0.358168000
6	6.168766000	0.147507000	0.005809000
6	6.927415000	-1.012125000	-0.199276000
6	6.868844000	1.351890000	0.213808000
6	8.318821000	-0.988978000	-0.197390000
6	8.250070000	1.391574000	0.213599000
6	8.993568000	0.219398000	0.009026000
1	6.429074000	-1.966157000	-0.329578000
1	6.321791000	2.278714000	0.343979000
1	8.862840000	-1.911844000	-0.344606000
1	8.786350000	2.321230000	0.358172000
8	10.338731000	0.363273000	0.029689000
6	11.159389000	-0.783459000	-0.180200000
1	10.997048000	-1.536423000	0.597785000
1	10.980335000	-1.225396000	-1.165706000
1	12.184883000	-0.424545000	-0.126377000
8	-10.338730000	-0.363293000	0.029713000
6	-11.159391000	0.783440000	-0.180160000
1	-10.997051000	1.536395000	0.597834000
1	-10.980342000	1.225390000	-1.165661000
1	-12.184884000	0.424522000	-0.126339000

i) [Fe(L1)2]2+

26	0.000001000	0.000042000	0.000125000
7	0.347703000	1.409560000	1.409251000
6	1.669846000	1.648399000	1.646602000
6	2.080378000	2.589742000	2.587037000
6	1.127101000	3.304465000	3.303195000
6	-0.219339000	3.057929000	3.058503000
6	-0.561782000	2.105882000	2.106685000
7	1.917576000	-0.000088000	0.000048000
6	2.589830000	0.829001000	0.826020000
6	3.971477000	0.859639000	0.857342000
6	4.717385000	-0.000144000	-0.000197000
6	3.971291000	-0.859886000	-0.857614000
6	2.589651000	-0.829194000	-0.826050000
7	0.347395000	-1.409567000	-1.408992000
6	1.669491000	-1.648541000	-1.646484000
6	2.079829000	-2.589985000	-2.586901000
6	1.126409000	-3.304679000	-3.302896000
6	-0.219981000	-3.058013000	-3.058057000
6	-0.562228000	-2.105869000	-2.106267000
7	-0.347472000	1.408974000	-1.409649000
6	-1.669580000	1.647780000	-1.647239000
6	-2.079967000	2.588761000	-2.588099000

6	-1.126583000	3.303155000	-3.304441000
6	0.219820000	3.056665000	-3.059496000
6	0.562117000	2.104986000	-2.107258000
7	-1.917574000	0.000146000	0.000126000
6	-2.589695000	0.828792000	-0.826397000
6	-3.971336000	0.859386000	-0.857984000
6	-4.717386000	0.000033000	-0.000136000
6	-3.971428000	-0.859278000	0.857834000
6	-2.589784000	-0.828572000	0.826506000
7	-0.347624000	-1.408766000	1.409981000
6	-1.669756000	-1.647510000	1.647497000
6	-2.080238000	-2.588348000	2.588458000
6	-1.126926000	-3.302653000	3.304984000
6	0.219502000	-3.056214000	3.060125000
6	0.561896000	-2.104680000	2.107777000
1	3.133898000	2.764257000	2.759674000
1	1.431312000	4.039649000	4.038012000
1	-0.996014000	3.590263000	3.592004000
1	-1.599205000	1.887027000	1.889014000
1	4.485308000	1.523211000	1.535795000
1	4.484977000	-1.523464000	-1.536172000
1	3.133314000	-2.764609000	-2.759642000
1	1.430470000	-4.039943000	-4.037695000
1	-0.996766000	-3.590321000	-3.591424000
1	-1.599609000	-1.886912000	-1.888497000
1	-3.133460000	2.763261000	-2.760910000
1	-1.430682000	4.038056000	-4.039588000
1	0.996577000	3.588754000	-3.593122000
1	1.599508000	1.886172000	-1.889396000
1	-4.485056000	1.522586000	-1.536885000
1	-4.485221000	-1.522548000	1.536611000
1	-3.133749000	-2.762792000	2.761220000
1	-1.431099000	-4.037441000	4.040214000
1	0.996205000	-3.588231000	3.593902000
1	1.599308000	-1.885919000	1.889961000
7	-6.062466000	-0.000017000	-0.000256000
6	-6.890653000	-0.922873000	0.801733000
1	-6.841356000	-0.649407000	1.862672000
1	-6.536324000	-1.951108000	0.694128000
1	-9.072951000	-0.941564000	0.975927000
6	-8.302019000	-0.730556000	0.235089000
1	-8.458291000	-1.403528000	-0.612040000
6	-8.302022000	0.730395000	-0.235954000
1	-8.458461000	1.403360000	0.611150000
1	-9.072852000	0.941362000	-0.976911000
6	-6.890579000	0.922788000	-0.802381000
1	-6.536323000	1.951043000	-0.694726000
1	-6.841103000	0.649320000	-1.863311000
7	6.062464000	-0.000174000	-0.000311000
6	6.890700000	0.922642000	0.801675000
1	6.841396000	0.649188000	1.862616000
1	6.536419000	1.950893000	0.694062000
1	9.073000000	0.941219000	0.975862000
6	8.302054000	0.730243000	0.235028000
1	8.458360000	1.403196000	-0.612109000
6	8.301977000	-0.730715000	-0.235996000
1	8.458373000	-1.403678000	0.611118000
1	9.072797000	-0.941735000	-0.976947000
6	6.890525000	-0.923033000	-0.802427000
1	6.536202000	-1.951265000	-0.694763000
1	6.841074000	-0.649573000	-1.863360000

ii) [Fe(L2)2]2+

26	-0.000001000	0.000001000	-0.000626000
7	0.347343000	1.408822000	1.409913000
6	1.669507000	1.646730000	1.648324000
6	2.080280000	2.586907000	2.589694000
6	1.127059000	3.302140000	3.305594000
6	-0.219328000	3.056876000	3.059732000
6	-0.561934000	2.105508000	2.107178000
7	1.916991000	0.000675000	-0.000492000
6	2.588812000	0.826882000	0.827504000
6	3.971147000	0.857311000	0.858704000
6	4.718419000	0.000512000	0.000764000
6	3.971828000	-0.856474000	-0.857580000
6	2.589462000	-0.825870000	-0.827618000
7	0.348453000	-1.408629000	-1.410936000
6	1.670800000	-1.646025000	-1.648852000
6	2.082283000	-2.586003000	-2.590109000
6	1.129600000	-3.301606000	-3.306357000
6	-0.216974000	-3.056872000	-3.060984000
6	-0.560304000	-2.105630000	-2.108565000
7	-0.348466000	1.410400000	-1.409166000
6	-1.670815000	1.648173000	-1.646694000
6	-2.082306000	2.589398000	-2.586700000
6	-1.129629000	3.305877000	-3.302080000
6	0.216948000	3.060741000	-3.057120000
6	0.560285000	2.108247000	-2.105955000
7	-1.916992000	-0.000676000	-0.000481000
6	-2.589471000	0.826969000	-0.826501000
6	-3.971837000	0.857611000	-0.856413000
6	-4.718418000	-0.000538000	0.000774000
6	-3.971141000	-0.858482000	0.857563000
6	-2.588806000	-0.827991000	0.826413000
7	-0.347332000	-1.410578000	1.408157000
6	-1.669494000	-1.648870000	1.646194000
6	-2.080259000	-2.590281000	2.586334000
6	-1.127033000	-3.306367000	3.301373000
6	0.219352000	-3.060693000	3.055909000
6	0.561950000	-2.108088000	2.104589000
1	3.133699000	2.760640000	2.763769000
1	1.431388000	4.036642000	4.041031000
1	-0.995929000	3.589638000	3.592915000
1	-1.599517000	1.887903000	1.889106000
1	4.478579000	1.529377000	1.532424000
1	4.479768000	-1.528971000	-1.530482000
1	3.135833000	-2.759242000	-2.763886000
1	1.434482000	-4.035965000	-4.041707000
1	-0.993172000	-3.589919000	-3.594469000
1	-1.598044000	-1.888375000	-1.890889000
1	-3.135858000	2.762922000	-2.760184000
1	-1.434517000	4.041211000	-4.036453000
1	0.993141000	3.594431000	-3.589969000
1	1.598027000	1.890652000	-1.888629000
1	-4.479784000	1.531010000	-1.528407000
1	-4.478568000	-1.531450000	1.530386000
1	-3.133677000	-2.764305000	2.760127000
1	-1.431356000	-4.041833000	4.035848000
1	0.995958000	-3.594080000	3.588460000
1	1.599532000	-1.890139000	1.886853000
7	-6.071274000	-0.000677000	0.001238000
7	6.071278000	0.000639000	0.001236000
6	-6.814781000	-0.893476000	0.892799000

1	-7.879427000	-0.740226000	0.739172000
1	-6.591950000	-1.944090000	0.682465000
1	-6.592674000	-0.684081000	1.943761000
6	-6.815602000	0.891859000	-0.889858000
1	-6.593423000	1.942583000	-0.679358000
1	-6.593642000	0.682852000	-1.940926000
1	-7.880112000	0.737923000	-0.735940000
6	6.814787000	0.892243000	0.893990000
1	7.879433000	0.739090000	0.740264000
1	6.592069000	1.943145000	0.684972000
1	6.592567000	0.681531000	1.944663000
6	6.815610000	-0.890689000	-0.891067000
1	6.593502000	-1.941702000	-0.681935000
1	6.593582000	-0.680313000	-1.941846000
1	7.880119000	-0.736895000	-0.737002000

iii) [Fe(L3)2]2+

26	0.000027000	-0.491803000	0.000028000
7	0.250548000	-1.901433000	1.430085000
6	1.553189000	-2.139608000	1.758020000
6	1.899579000	-3.079982000	2.724636000
6	0.899959000	-3.795617000	3.373791000
6	-0.426593000	-3.550217000	3.037016000
6	-0.703947000	-2.598459000	2.063767000
7	1.913638000	-0.492003000	0.127991000
6	2.526503000	-1.320573000	1.002082000
6	3.901659000	-1.348824000	1.121188000
6	4.699793000	-0.494790000	0.311631000
6	4.022183000	0.368778000	-0.588209000
6	2.639308000	0.334803000	-0.651203000
7	0.441793000	0.917885000	-1.382348000
6	1.777128000	1.155637000	-1.530774000
6	2.251115000	2.095293000	-2.442401000
6	1.348663000	2.810996000	-3.221036000
6	-0.011263000	2.566163000	-3.066644000
6	-0.417934000	1.614749000	-2.139501000
7	-0.441844000	0.917327000	1.382932000
6	-1.777191000	1.154986000	1.531389000
6	-2.251246000	2.094239000	2.443397000
6	-1.348850000	2.809628000	3.222385000
6	0.011090000	2.564888000	3.067961000
6	0.417829000	1.613879000	2.140433000
7	-1.913581000	-0.492068000	-0.127970000
6	-2.639309000	0.334488000	0.651441000
6	-4.022173000	0.368532000	0.588314000
6	-4.699732000	-0.494709000	-0.311892000
6	-3.901528000	-1.348452000	-1.121692000
6	-2.526383000	-1.320275000	-1.002444000
7	-0.250396000	-1.900949000	-1.430532000
6	-1.553018000	-2.139046000	-1.758604000
6	-1.899345000	-3.079128000	-2.725526000
6	-0.899682000	-3.794548000	-3.374851000
6	0.426850000	-3.549233000	-3.037932000
6	0.704140000	-2.597769000	-2.064378000
1	2.938919000	-3.253604000	2.969429000
1	1.153656000	-4.530516000	4.127796000
1	-1.237644000	-4.083305000	3.515820000
1	-1.724429000	-2.380967000	1.775996000
1	4.383632000	-2.019466000	1.821011000
1	4.581064000	1.047267000	-1.214380000
1	3.314067000	2.267469000	-2.545385000

1	1.702207000	3.545043000	-3.934583000
1	-0.749920000	3.098872000	-3.651325000
1	-1.467955000	1.397268000	-1.992393000
1	-3.314208000	2.266333000	2.546413000
1	-1.702447000	3.543360000	3.936229000
1	0.749705000	3.097358000	3.652911000
1	1.467862000	1.396481000	1.993285000
1	-4.581083000	1.046869000	1.214624000
1	-4.383444000	-2.018829000	-1.821808000
1	-2.938670000	-3.252698000	-2.970416000
1	-1.153330000	-4.529221000	-4.129092000
1	1.237933000	-4.082164000	-3.516856000
1	1.724606000	-2.380347000	-1.776495000
7	-6.044529000	-0.537545000	-0.407071000
1	-6.431358000	-1.152323000	-1.107111000
7	6.044591000	-0.537616000	0.406707000
1	6.431552000	-1.152824000	1.106291000
6	-7.256346000	1.667190000	-0.295515000
1	-7.603810000	1.527606000	-1.325205000
1	-6.313050000	2.222809000	-0.361255000
6	-8.287038000	2.485892000	0.492117000
1	-9.224075000	1.921273000	0.555436000
1	-7.939342000	2.614719000	1.524416000
6	-8.559820000	3.857382000	-0.131095000
1	-7.649625000	4.462953000	-0.177300000
1	-8.947971000	3.760016000	-1.148735000
1	-9.297437000	4.412479000	0.451831000
6	-7.002431000	0.290377000	0.332258000
1	-6.658296000	0.389081000	1.365970000
1	-7.934890000	-0.276336000	0.378626000
6	7.002424000	0.290520000	-0.332517000
1	6.658448000	0.389135000	-1.366295000
1	7.934991000	-0.276024000	-0.378668000
6	7.256023000	1.667378000	0.295291000
1	7.603123000	1.527822000	1.325106000
6	8.286988000	2.486098000	-0.491959000
1	9.224128000	1.921590000	-0.554729000
1	7.939806000	2.614738000	-1.524452000
1	6.312689000	2.222972000	0.360698000
1	7.648993000	4.463174000	0.176864000
6	8.559288000	3.857713000	0.131197000
1	9.297124000	4.412818000	-0.451444000
1	8.946948000	3.760537000	1.149043000

iv) [Fe(L4)2]2+

26	-0.000063000	0.000109000	0.001309000
7	-0.341219000	1.392720000	-1.427236000
6	-1.662995000	1.629039000	-1.667798000
6	-2.079261000	2.555380000	-2.619628000
6	-1.127237000	3.260916000	-3.347739000
6	0.219317000	3.018174000	-3.101567000
6	0.565659000	2.079705000	-2.136591000
7	-1.917843000	-0.001659000	0.003134000
6	-2.580875000	0.821732000	-0.838110000
6	-3.965448000	0.850431000	-0.864345000
6	-4.674295000	0.003832000	0.003568000
6	-3.970788000	-0.845149000	0.870675000
6	-2.580215000	-0.820478000	0.842225000
7	-0.341189000	-1.396465000	1.426753000
6	-1.663109000	-1.632310000	1.668963000
6	-2.076924000	-2.563633000	2.617050000

6	-1.124148000	-3.275192000	3.338379000
6	0.221892000	-3.033601000	3.089229000
6	0.566402000	-2.089593000	2.128901000
7	0.341098000	1.428499000	1.394416000
6	1.662989000	1.670125000	1.631149000
6	2.076600000	2.623126000	2.557507000
6	1.123680000	3.351113000	3.262072000
6	-0.222307000	3.103687000	3.018449000
6	-0.566639000	2.137635000	2.080232000
7	1.917839000	0.001428000	0.003531000
6	2.580138000	0.839523000	0.823328000
6	3.970756000	0.865034000	0.851222000
6	4.674270000	-0.003796000	0.004113000
6	3.965486000	-0.870300000	-0.844040000
6	2.580946000	-0.841079000	-0.818595000
7	0.341382000	-1.425580000	-1.394761000
6	1.663162000	-1.667104000	-1.629761000
6	2.079636000	-2.614588000	-2.560478000
6	1.127747000	-3.336236000	-3.272808000
6	-0.218856000	-3.087962000	-3.032500000
6	-0.565374000	-2.128142000	-2.088811000
1	-3.133607000	2.725350000	-2.792708000
1	-1.433319000	3.985145000	-4.092512000
1	0.994768000	3.542854000	-3.644427000
1	1.604699000	1.866827000	-1.921289000
1	-4.522819000	1.498383000	-1.526450000
1	-4.505727000	-1.502564000	1.544442000
1	-3.130471000	-2.735295000	2.793235000
1	-1.429106000	-4.003731000	4.079393000
1	0.998190000	-3.563859000	3.625395000
1	1.605083000	-1.878237000	1.910443000
1	3.130115000	2.798897000	2.729801000
1	1.428512000	4.096611000	3.986072000
1	-0.998713000	3.646200000	3.542055000
1	-1.605280000	1.921104000	1.866719000
1	4.505551000	1.538064000	1.509502000
1	4.522994000	-1.533314000	-1.490945000
1	3.134008000	-2.788434000	-2.729486000
1	1.433981000	-4.076969000	-4.001106000
1	-0.994198000	-3.624609000	-3.563692000
1	-1.604454000	-1.910577000	-1.878443000
8	-6.007707000	0.067304000	-0.058334000
1	-6.433863000	-0.538281000	0.561309000
8	6.007677000	-0.068774000	-0.056299000
1	6.433818000	0.551046000	0.549118000

v) [Fe(L5)2]2+

26	0.000000000	0.042140000	0.000000000
7	-0.257035000	1.454544000	1.426962000
6	-1.562039000	1.692794000	1.743825000
6	-1.920994000	2.634631000	2.703925000
6	-0.927930000	3.354327000	3.359308000
6	0.401719000	3.110383000	3.034192000
6	0.690282000	2.155816000	2.066383000
7	-1.914138000	0.039852000	0.111517000
6	-2.527582000	0.872720000	0.983142000
6	-3.905385000	0.897838000	1.092082000
6	-4.672686000	0.039798000	0.278592000
6	-4.017904000	-0.818193000	-0.621235000
6	-2.626440000	-0.786946000	-0.674279000
7	-0.425465000	-1.366497000	-1.389085000

6	-1.759488000	-1.605058000	-1.548734000
6	-2.227813000	-2.542595000	-2.465029000
6	-1.319393000	-3.255852000	-3.239681000
6	0.038913000	-3.010049000	-3.075302000
6	0.439225000	-2.060802000	-2.142426000
7	0.425471000	-1.366384000	1.389198000
6	1.759495000	-1.604929000	1.548863000
6	2.227824000	-2.542389000	2.465235000
6	1.319407000	-3.255584000	3.239948000
6	-0.038900000	-3.009797000	3.075552000
6	-0.439215000	-2.060628000	2.142598000
7	1.914137000	0.039850000	-0.111519000
6	2.626443000	-0.786887000	0.674339000
6	4.017907000	-0.818139000	0.621289000
6	4.672685000	0.039778000	-0.278611000
6	3.905380000	0.897755000	-1.092163000
6	2.527578000	0.872647000	-0.983214000
7	0.257029000	1.454433000	-1.427074000
6	1.562031000	1.692661000	-1.743958000
6	1.920983000	2.634426000	-2.704130000
6	0.927917000	3.354069000	-3.359566000
6	-0.401731000	3.110148000	-3.034429000
6	-0.690291000	2.155654000	-2.066547000
1	-2.963317000	2.805859000	2.937831000
1	-1.189492000	4.091211000	4.108633000
1	1.207558000	3.647162000	3.517684000
1	1.714372000	1.941718000	1.789312000
1	-4.424314000	1.552081000	1.778823000
1	-4.577955000	-1.486452000	-1.257569000
1	-3.289801000	-2.716315000	-2.575923000
1	-1.667507000	-3.988402000	-3.957371000
1	0.782013000	-3.540268000	-3.656619000
1	1.488610000	-1.8444612000	-1.989610000
1	3.289813000	-2.716098000	2.576141000
1	1.667525000	-3.988073000	3.957698000
1	-0.781997000	-3.539969000	3.656914000
1	-1.488601000	-1.844453000	1.989767000
1	4.577961000	-1.486348000	1.257674000
1	4.424307000	1.551943000	-1.778959000
1	2.963305000	2.805638000	-2.938050000
1	1.189476000	4.090898000	-4.108948000
1	-1.207572000	3.646888000	-3.517961000
1	-1.714380000	1.941575000	-1.789459000
8	5.990108000	0.121185000	-0.439832000
6	6.871422000	-0.707879000	0.340858000
1	6.761056000	-0.491340000	1.406196000
1	6.686182000	-1.765478000	0.137880000
1	7.873497000	-0.443192000	0.015743000
8	-5.990110000	0.121215000	0.439804000
6	-6.871419000	-0.707921000	-0.340816000
1	-6.761052000	-0.491473000	-1.406172000
1	-6.686176000	-1.765501000	-0.137746000
1	-7.873496000	-0.443209000	-0.015725000

vi) [Fe(L6)2]2+

26	0.000000000	0.000103000	-0.000541000
7	0.339591000	1.408454000	1.411059000
6	1.661716000	1.645830000	1.649447000
6	2.075080000	2.581735000	2.593930000
6	1.122042000	3.293727000	3.313657000
6	-0.224568000	3.049817000	3.067753000

6	-0.569064000	2.102349000	2.111586000
7	1.912563000	-0.000636000	-0.000639000
6	2.578426000	0.831411000	0.825560000
6	3.967146000	0.850019000	0.848737000
6	4.699973000	-0.001656000	-0.000942000
6	3.966315000	-0.852458000	-0.850800000
6	2.577657000	-0.833049000	-0.827137000
7	0.338290000	-1.408557000	-1.412147000
6	1.660204000	-1.646816000	-1.650835000
6	2.072745000	-2.583049000	-2.595351000
6	1.119081000	-3.294459000	-3.314822000
6	-0.227313000	-3.049664000	-3.068608000
6	-0.570973000	-2.101920000	-2.112416000
7	-0.338435000	1.408886000	-1.411988000
6	-1.660372000	1.647061000	-1.650631000
6	-2.073001000	2.583364000	-2.595039000
6	-1.119404000	3.294937000	-3.314437000
6	0.227013000	3.050237000	-3.068257000
6	0.570764000	2.102412000	-2.112178000
7	-1.912563000	0.000786000	-0.000504000
6	-2.577743000	0.833156000	-0.826978000
6	-3.966402000	0.852413000	-0.850653000
6	-4.699973000	0.001496000	-0.000834000
6	-3.967059000	-0.850133000	0.848816000
6	-2.578341000	-0.831372000	0.825651000
7	-0.339447000	-1.408291000	1.411054000
6	-1.661550000	-1.645735000	1.649503000
6	-2.074824000	-2.581634000	2.594029000
6	-1.121719000	-3.293550000	3.313744000
6	0.224868000	-3.049567000	3.067782000
6	0.569273000	-2.102110000	2.111573000
1	3.129028000	2.753066000	2.767391000
1	1.426985000	4.024645000	4.052388000
1	-1.000797000	3.580131000	3.603881000
1	-1.607524000	1.887145000	1.895471000
1	4.492721000	1.497662000	1.536463000
1	4.491357000	-1.500102000	-1.538933000
1	3.126541000	-2.755105000	-2.769019000
1	1.423382000	-4.025617000	-4.053578000
1	-1.004011000	-3.579505000	-3.604525000
1	-1.609245000	-1.886024000	-1.896094000
1	-3.126814000	2.755354000	-2.768673000
1	-1.423775000	4.026151000	-4.053110000
1	1.003660000	3.580212000	-3.604116000
1	1.609056000	1.886573000	-1.895892000
1	-4.491510000	1.500020000	-1.538770000
1	-4.492570000	-1.497869000	1.536504000
1	-3.128756000	-2.753013000	2.767542000
1	-1.426592000	-4.024460000	4.052510000
1	1.001148000	-3.579817000	3.603900000
1	1.607713000	-1.886859000	1.895411000
6	6.172613000	-0.002625000	-0.000713000
6	6.894490000	-1.180186000	-0.249216000
6	6.896945000	1.176127000	0.249441000
6	8.283229000	-1.178294000	-0.240458000
6	8.282922000	1.172265000	0.242662000
6	9.006509000	-0.004896000	0.001461000
1	6.372820000	-2.116866000	-0.410495000
1	6.375446000	2.113061000	0.409882000
1	8.816545000	-2.105369000	-0.417364000
1	8.817570000	2.099039000	0.420038000
6	-6.172612000	0.002302000	-0.000620000

6	-6.894616000	1.179785000	-0.249122000
6	-6.896817000	-1.176532000	0.249518000
6	-8.283355000	1.177740000	-0.240378000
6	-8.282794000	-1.172822000	0.242724000
6	-9.006508000	0.004260000	0.001524000
1	-6.373047000	2.116523000	-0.410388000
1	-6.375215000	-2.113410000	0.409958000
1	-8.816771000	2.104757000	-0.417282000
1	-8.817342000	-2.099657000	0.420088000
6	10.511695000	0.004303000	0.005169000
1	10.921034000	-0.983875000	-0.206259000
1	10.899215000	0.699709000	-0.744939000
1	10.897414000	0.330465000	0.975460000
6	-10.511693000	-0.005105000	0.005217000
1	-10.921139000	0.983030000	-0.206207000
1	-10.899129000	-0.700547000	-0.744901000
1	-10.897386000	-0.331317000	0.975501000

vii) [Fe(L7)2]2+

26	0.000000000	0.034293000	0.000002000
7	-0.264338000	1.444576000	1.426440000
6	-1.572249000	1.683257000	1.732276000
6	-1.937591000	2.623460000	2.691854000
6	-0.948924000	3.339629000	3.357859000
6	0.383106000	3.094277000	3.044111000
6	0.678681000	2.141982000	2.075992000
7	-1.909556000	0.035024000	0.098621000
6	-2.528756000	0.864226000	0.961183000
6	-3.916140000	0.883358000	1.051611000
6	-4.688509000	0.033965000	0.239801000
6	-4.004098000	-0.817617000	-0.648354000
6	-2.617429000	-0.795369000	-0.697194000
7	-0.410845000	-1.375501000	-1.391276000
6	-1.742910000	-1.614037000	-1.562307000
6	-2.202853000	-2.553724000	-2.480871000
6	-1.286971000	-3.268818000	-3.244704000
6	0.070024000	-3.023251000	-3.068020000
6	0.461704000	-2.071781000	-2.134146000
7	0.410806000	-1.376270000	1.390512000
6	1.742866000	-1.614911000	1.561436000
6	2.202786000	-2.555108000	2.479490000
6	1.286885000	-3.270616000	3.242912000
6	-0.070105000	-3.024943000	3.066338000
6	-0.461762000	-2.072955000	2.132982000
7	1.909557000	0.035037000	-0.098606000
6	2.617408000	-0.795780000	0.696785000
6	4.004078000	-0.818003000	0.647970000
6	4.688514000	0.034053000	-0.239712000
6	3.916167000	0.883880000	-1.051088000
6	2.528780000	0.864700000	-0.960708000
7	0.264377000	1.445328000	-1.425683000
6	1.572294000	1.684148000	-1.731384000
6	1.937658000	2.624839000	-2.690475000
6	0.949008000	3.341366000	-3.356119000
6	-0.383029000	3.095875000	-3.042507000
6	-0.678626000	2.143085000	-2.074881000
1	-2.981207000	2.796481000	2.918254000
1	-1.215691000	4.074772000	4.107071000
1	1.185656000	3.627705000	3.536671000
1	1.705051000	1.927055000	1.808181000
1	-4.412864000	1.549653000	1.744737000

1	-4.556992000	-1.488091000	-1.291044000
1	-3.263800000	-2.727481000	-2.600894000
1	-1.628394000	-4.003290000	-3.963668000
1	0.818522000	-3.555665000	-3.640302000
1	1.509738000	-1.856091000	-1.971823000
1	3.263729000	-2.728941000	2.599435000
1	1.628288000	-4.005487000	3.961478000
1	-0.818619000	-3.557667000	3.638312000
1	-1.509791000	-1.857166000	1.970760000
1	4.556955000	-1.488817000	1.290320000
1	4.412909000	1.550547000	-1.743843000
1	2.981278000	2.797957000	-2.916781000
1	1.215792000	4.076889000	-4.104951000
1	-1.185566000	3.629570000	-3.534797000
1	-1.705002000	1.928037000	-1.807187000
6	6.150014000	0.075195000	-0.355325000
1	6.532725000	0.779285000	-1.087984000
6	7.022854000	-0.656418000	0.342952000
1	6.729123000	-1.381362000	1.093680000
1	8.087683000	-0.548062000	0.179595000
6	-6.150007000	0.075045000	0.355476000
1	-6.532696000	0.778721000	1.088543000
6	-7.022866000	-0.656167000	-0.343196000
1	-6.729156000	-1.380682000	-1.094346000
1	-8.087691000	-0.547901000	-0.179751000

viii) [Fe(L8)2]2+

26	0.000000000	0.000150000	0.000082000
7	-0.335411000	1.410132000	1.409920000
6	-1.657349000	1.648773000	1.647249000
6	-2.073692000	2.588499000	2.586243000
6	-1.121716000	3.305168000	3.303481000
6	0.224868000	3.060230000	3.059819000
6	0.571440000	2.108088000	2.108371000
7	-1.914605000	-0.001462000	-0.003647000
6	-2.573106000	0.830951000	0.828687000
6	-3.967303000	0.850276000	0.847312000
6	-4.659133000	-0.004593000	-0.008175000
6	-3.962527000	-0.857888000	-0.861348000
6	-2.568440000	-0.835397000	-0.838116000
7	-0.327505000	-1.410217000	-1.411327000
6	-1.648141000	-1.651195000	-1.653585000
6	-2.059346000	-2.591182000	-2.594574000
6	-1.103479000	-3.305688000	-3.308784000
6	0.241752000	-3.058341000	-3.060165000
6	0.583120000	-2.106078000	-2.106956000
7	0.329610000	-1.410201000	1.410997000
6	1.650592000	-1.650000000	1.652504000
6	2.063164000	-2.590088000	2.592796000
6	1.108330000	-3.305842000	3.307138000
6	-0.237263000	-3.059577000	3.059392000
6	-0.580014000	-2.107194000	2.106802000
7	1.914606000	0.001130000	0.003570000
6	2.569684000	-0.832678000	0.837192000
6	3.963803000	-0.853607000	0.859918000
6	4.659136000	0.001104000	0.007123000
6	3.966033000	0.855772000	-0.847531000
6	2.571865000	0.834830000	-0.828455000
7	0.333305000	1.411367000	-1.409039000
6	1.654897000	1.651992000	-1.646316000
6	2.069874000	2.592941000	-2.584688000

6	1.116864000	3.308770000	-3.301389000
6	-0.229362000	3.061778000	-3.057823000
6	-0.574550000	2.108528000	-2.106983000
1	-3.127825000	2.761007000	2.757691000
1	-1.427724000	4.040013000	4.037761000
1	1.000265000	3.593824000	3.593879000
1	1.610828000	1.894435000	1.895815000
1	-4.507756000	1.512682000	1.509713000
1	-5.742081000	-0.005842000	-0.009957000
1	-4.499285000	-1.521579000	-1.525465000
1	-3.112534000	-2.765503000	-2.769944000
1	-1.405478000	-4.040690000	-4.044566000
1	1.020071000	-3.590163000	-3.591736000
1	1.621354000	-1.890680000	-1.890566000
1	3.116605000	-2.763501000	2.767545000
1	1.411394000	-4.040950000	4.042376000
1	-1.014805000	-3.592345000	3.591154000
1	-1.618556000	-1.892660000	1.891030000
1	4.501545000	-1.517171000	1.523365000
1	5.742086000	0.001103000	0.008537000
1	4.505504000	1.519236000	-1.509675000
1	3.123756000	2.767045000	-2.756064000
1	1.421807000	4.044546000	-4.035180000
1	-1.005536000	3.594635000	-3.591491000
1	-1.613632000	1.893314000	-1.894508000

ix) [Fe(L9)2]2+

26	-0.000085000	0.000230000	-0.000245000
7	-0.352215000	1.266055000	1.554125000
6	-1.676909000	1.472712000	1.803259000
7	-2.171442000	2.246562000	2.754425000
6	-1.301425000	2.882842000	3.543583000
6	0.074378000	2.742181000	3.378542000
6	0.510349000	1.911779000	2.356072000
7	-1.921094000	0.002385000	-0.002373000
6	-2.590922000	0.741992000	0.901899000
6	-3.972948000	0.775688000	0.938399000
6	-4.683965000	0.008584000	-0.004713000
6	-3.976914000	-0.760732000	-0.945214000
6	-2.590165000	-0.732009000	-0.904780000
7	-0.354403000	-1.268869000	-1.553013000
6	-1.679693000	-1.469629000	-1.803194000
7	-2.177787000	-2.245434000	-2.751420000
6	-1.309857000	-2.892095000	-3.534922000
6	0.066234000	-2.760307000	-3.366501000
6	0.505462000	-1.925998000	-2.348345000
7	0.351602000	-1.552146000	1.268242000
6	1.676168000	-1.804847000	1.471178000
7	2.170304000	-2.754133000	2.247597000
6	1.299955000	-3.535964000	2.892408000
6	-0.075785000	-3.364998000	2.758313000
6	-0.511316000	-2.345886000	1.923567000
7	1.921034000	-0.001509000	-0.001965000
6	2.590554000	-0.908120000	0.735280000
6	3.972487000	-0.949012000	0.764142000
6	4.683913000	-0.007947000	-0.005227000
6	3.977319000	0.934994000	-0.771755000
6	2.590471000	0.898889000	-0.738283000
7	0.355081000	1.555224000	-1.266656000
6	1.680480000	1.802047000	-1.470747000
7	2.179023000	2.752331000	-2.243708000

6	1.311457000	3.543102000	-2.881973000
6	-0.064710000	3.380293000	-2.744118000
6	-0.504423000	2.358612000	-1.914366000
1	0.778442000	3.256840000	4.018644000
1	1.565014000	1.753398000	2.167301000
1	-4.496937000	1.374462000	1.671314000
1	-4.477144000	-1.367627000	-1.690407000
1	0.768336000	-3.285024000	-4.000555000
1	1.560734000	-1.774596000	-2.157256000
1	-0.780119000	-3.997791000	3.281571000
1	-1.565898000	-2.152533000	1.770246000
1	4.496404000	-1.683156000	1.361483000
1	4.477655000	1.679329000	-1.379609000
1	-0.766509000	4.021540000	-3.260430000
1	-1.559788000	2.171902000	-1.758212000
8	6.014317000	-0.076081000	0.046218000
1	6.438529000	0.596698000	-0.502314000
8	-6.014357000	0.064480000	0.059057000
1	-6.438258000	-0.484094000	-0.613885000
1	1.732717000	4.318617000	-3.512693000
1	1.718737000	-4.310463000	3.526090000
1	-1.730738000	-3.525261000	-4.308647000
1	-1.720528000	3.514305000	4.319719000

x) [Fe(L10)2]2+

26	0.000000000	0.000238000	0.000074000
7	-0.337114000	1.412116000	1.410975000
6	-1.658921000	1.651080000	1.649690000
6	-2.075700000	2.590562000	2.588327000
6	-1.123343000	3.307791000	3.304936000
6	0.222990000	3.063046000	3.060430000
6	0.569609000	2.110628000	2.108873000
7	-1.914440000	-0.000109000	-0.000535000
6	-2.573894000	0.831766000	0.831000000
6	-3.965423000	0.856775000	0.856284000
6	-4.657188000	-0.001085000	-0.000928000
6	-3.964564000	-0.858462000	-0.857924000
6	-2.573056000	-0.832470000	-0.832237000
7	-0.335691000	-1.411624000	-1.411230000
6	-1.657276000	-1.651170000	-1.650630000
6	-2.073170000	-2.590580000	-2.589731000
6	-1.120148000	-3.307126000	-3.306136000
6	0.225949000	-3.061769000	-3.060969000
6	0.571671000	-2.109469000	-2.108968000
7	0.336035000	-1.410755000	1.412158000
6	1.657673000	-1.650144000	1.651411000
6	2.073779000	-2.589045000	2.590926000
6	1.120917000	-3.305200000	3.307935000
6	-0.225237000	-3.059959000	3.062957000
6	-0.571174000	-2.108193000	2.110501000
7	1.914440000	0.000227000	0.000563000
6	2.573258000	-0.831782000	0.832459000
6	3.964771000	-0.857721000	0.857866000
6	4.657188000	-0.000664000	0.000381000
6	3.965216000	0.856818000	-0.857041000
6	2.573691000	0.831770000	-0.831462000
7	0.336771000	1.411580000	-1.411451000
6	1.658524000	1.650667000	-1.650349000
6	2.075090000	2.589918000	-2.589312000
6	1.122574000	3.306780000	-3.306074000
6	-0.223702000	3.061911000	-3.061387000

6	-0.570106000	2.109745000	-2.109501000
1	-3.129677000	2.763421000	2.760984000
1	-1.429257000	4.042727000	4.039205000
1	0.998645000	3.596986000	3.593906000
1	1.609075000	1.897566000	1.896060000
1	-4.511259000	1.516400000	1.515668000
1	-4.509742000	-1.518508000	-1.517430000
1	-3.126985000	-2.763879000	-2.762932000
1	-1.425375000	-4.041988000	-4.040764000
1	1.002113000	-3.595146000	-3.594270000
1	1.610945000	-1.895999000	-1.895635000
1	3.127633000	-2.762242000	2.763994000
1	1.426308000	-4.039667000	4.042890000
1	-1.001279000	-3.593029000	3.596743000
1	-1.610494000	-1.894844000	1.897268000
1	4.510108000	-1.517490000	1.517518000
1	4.510893000	1.516178000	-1.516821000
1	3.129029000	2.762892000	-2.762089000
1	1.428324000	4.041534000	-4.040594000
1	-0.999480000	3.595566000	-3.594971000
1	-1.609526000	1.896598000	-1.896549000
17	6.384417000	-0.001226000	0.000265000
17	-6.384417000	-0.001704000	-0.001172000

xi) [Fe(L11)2]2+

26	0.000000000	-0.000003000	0.002829000
7	0.324859000	1.412030000	1.415259000
6	1.644958000	1.656991000	1.654408000
6	2.057997000	2.596360000	2.595023000
6	1.101764000	3.306573000	3.313236000
6	-0.243595000	3.055344000	3.068549000
6	-0.585954000	2.103703000	2.114827000
7	1.911018000	0.007589000	0.002101000
6	2.564109000	0.844746000	0.836225000
6	3.954618000	0.872657000	0.857212000
6	4.657073000	0.021542000	0.002630000
6	3.966510000	-0.837932000	-0.853188000
6	2.572599000	-0.822103000	-0.830538000
7	0.337994000	-1.410587000	-1.407734000
6	1.660257000	-1.644412000	-1.647162000
6	2.079595000	-2.583530000	-2.585294000
6	1.129011000	-3.305173000	-3.299554000
6	-0.218182000	-3.065565000	-3.053760000
6	-0.567432000	-2.113309000	-2.103227000
7	-0.338000000	1.410825000	-1.407494000
6	-1.660263000	1.644680000	-1.646885000
6	-2.079605000	2.583955000	-2.584859000
6	-1.129025000	3.305732000	-3.298989000
6	0.218169000	3.066096000	-3.053227000
6	0.567423000	2.113677000	-2.102858000
7	-1.911018000	-0.007598000	0.002101000
6	-2.572602000	0.822230000	-0.830400000
6	-3.966513000	0.838063000	-0.853044000
6	-4.657073000	-0.021551000	0.002638000
6	-3.954614000	-0.872802000	0.857081000
6	-2.564106000	-0.844889000	0.836093000
7	-0.324854000	-1.412263000	1.415029000
6	-1.644951000	-1.657263000	1.654144000
6	-2.057987000	-2.596781000	2.594613000
6	-1.101750000	-3.307102000	3.312714000
6	0.243607000	-3.055829000	3.068065000

6	0.585962000	-2.104041000	2.114489000
1	3.111775000	2.772196000	2.766227000
1	1.403912000	4.041198000	4.049395000
1	-1.021785000	3.583637000	3.603920000
1	-1.624426000	1.885734000	1.902165000
1	4.514361000	1.528741000	1.510660000
1	4.516595000	-1.494509000	-1.512161000
1	3.134382000	-2.751544000	-2.757694000
1	1.436709000	-4.040067000	-4.033139000
1	-0.992343000	-3.603597000	-3.585242000
1	-1.607467000	-1.904394000	-1.889182000
1	-3.134393000	2.751989000	-2.757236000
1	-1.436726000	4.040747000	-4.032450000
1	0.992327000	3.604227000	-3.584613000
1	1.607460000	1.904734000	-1.888844000
1	-4.516601000	1.494746000	-1.511909000
1	-4.514355000	-1.528996000	1.510421000
1	-3.111764000	-2.772648000	2.765791000
1	-1.403894000	-4.041841000	4.048761000
1	1.021801000	-3.584204000	3.603353000
1	1.624434000	-1.886039000	1.901856000
6	6.161090000	0.079235000	0.052982000
8	6.757939000	0.817705000	0.788077000
8	6.723847000	-0.779658000	-0.808050000
1	7.688820000	-0.701490000	-0.734268000
6	-6.161090000	-0.079257000	0.052982000
8	-6.757937000	-0.817870000	0.787931000
8	-6.723849000	0.779778000	-0.807909000
1	-7.688822000	0.701581000	-0.734155000

xii) [Fe(L12)2]2+

26	0.000000000	0.000000000	-0.060753000
7	-0.293160000	1.422614000	-1.471387000
6	-1.607113000	1.689161000	-1.722852000
6	-1.992969000	2.642051000	-2.661545000
6	-1.018523000	3.343707000	-3.363296000
6	0.319852000	3.071508000	-3.104174000
6	0.635677000	2.107228000	-2.154188000
7	-1.913823000	0.049166000	-0.070427000
6	-2.548512000	0.885443000	-0.918969000
6	-3.942346000	0.910691000	-0.977957000
6	-4.648262000	0.058287000	-0.131703000
6	-3.985067000	-0.805395000	0.732412000
6	-2.593355000	-0.784250000	0.744996000
7	-0.372953000	-1.400495000	1.349975000
6	-1.701054000	-1.615821000	1.573145000
6	-2.148046000	-2.546496000	2.506917000
6	-1.217109000	-3.278103000	3.236803000
6	0.136599000	-3.055678000	3.010343000
6	0.512847000	-2.111870000	2.061433000
7	0.372965000	1.400313000	1.350152000
6	1.701068000	1.615612000	1.573338000
6	2.148068000	2.546169000	2.507222000
6	1.217138000	3.277686000	3.237207000
6	-0.136573000	3.055289000	3.010730000
6	-0.512829000	2.111600000	2.061706000
7	1.913823000	-0.049167000	-0.070448000
6	2.593362000	0.784144000	0.745077000
6	3.985074000	0.805286000	0.732488000
6	4.648262000	-0.058288000	-0.131739000
6	3.942338000	-0.910585000	-0.978096000

6	2.548505000	-0.885340000	-0.919098000
7	0.293148000	-1.422430000	-1.471576000
6	1.607099000	-1.688952000	-1.723079000
6	1.992947000	-2.641722000	-2.661897000
6	1.018495000	-3.343282000	-3.363736000
6	-0.319877000	-3.071109000	-3.104575000
6	-0.635694000	-2.106950000	-2.154463000
1	-3.041110000	2.837734000	-2.844892000
1	-1.301021000	4.088585000	-4.096944000
1	1.112337000	3.593585000	-3.624432000
1	1.668167000	1.873354000	-1.929798000
1	-4.458575000	1.561793000	-1.672601000
1	-4.582998000	-1.475628000	1.342321000
1	-3.208056000	-2.698421000	2.662292000
1	-1.544953000	-4.006712000	3.967926000
1	0.895476000	-3.600928000	3.556363000
1	1.558321000	-1.915991000	1.861620000
1	3.208079000	2.698074000	2.662607000
1	1.544988000	4.006202000	3.968419000
1	-0.895445000	3.600471000	3.556825000
1	-1.558304000	1.915745000	1.861878000
1	4.583011000	1.475435000	1.342484000
1	4.458561000	-1.561603000	-1.672823000
1	3.041086000	-2.837387000	-2.845271000
1	1.300987000	-4.088067000	-4.097481000
1	-1.112367000	-3.593113000	-3.624899000
1	-1.668182000	-1.873100000	-1.930040000
16	6.486596000	0.154067000	-0.186915000
8	6.747140000	1.300304000	0.749158000
6	6.911462000	-1.391007000	0.713342000
1	6.580449000	-2.260171000	0.142950000
1	6.464679000	-1.359737000	1.706541000
1	7.998740000	-1.392346000	0.791375000
16	-6.486594000	-0.154076000	-0.186908000
8	-6.747137000	-1.300301000	0.749179000
6	-6.911472000	1.391002000	0.713335000
1	-6.580429000	2.260160000	0.142951000
1	-7.998753000	1.392353000	0.791334000
1	-6.464716000	1.359735000	1.706546000

xiii) [Fe(L13)2]2+

26	0.000037000	0.000009000	-0.001561000
7	-0.343395000	-1.430290000	1.382817000
6	-1.665358000	-1.669553000	1.612333000
6	-2.051383000	-2.632796000	2.546193000
7	-1.169285000	-3.346524000	3.241474000
6	0.119576000	-3.105225000	3.011450000
6	0.539122000	-2.150117000	2.084844000
7	-1.922497000	0.002366000	-0.004609000
6	-2.587872000	-0.843995000	0.811738000
6	-3.971770000	-0.873639000	0.838024000
6	-4.680897000	-0.000158000	-0.006428000
6	-3.974980000	0.874147000	-0.849264000
6	-2.585113000	0.845301000	-0.819216000
7	-0.339481000	1.433867000	-1.382493000
6	-1.661262000	1.673809000	-1.615754000
6	-2.042828000	2.641385000	-2.546465000
7	-1.159020000	3.360068000	-3.234321000
6	0.128980000	3.119636000	-2.999046000
6	0.544964000	2.159296000	-2.076019000
7	0.341353000	-1.385306000	-1.430811000

6	1.663447000	-1.616486000	-1.671155000
6	2.046170000	-2.551845000	-2.633749000
7	1.163199000	-3.247409000	-3.346039000
6	-0.125088000	-3.015852000	-3.103585000
6	-0.542235000	-2.087443000	-2.148942000
7	1.922500000	-0.001774000	-0.002797000
6	2.586213000	-0.815191000	-0.845979000
6	3.976119000	-0.841675000	-0.876550000
6	4.680885000	0.003437000	-0.003537000
6	3.970623000	0.846284000	0.870603000
6	2.586804000	0.816284000	0.842830000
7	0.341534000	1.380273000	1.433027000
6	1.663206000	1.612384000	1.671510000
6	2.048021000	2.542168000	2.639144000
7	1.165028000	3.229795000	3.359165000
6	-0.123521000	2.995518000	3.120333000
6	-0.541873000	2.073742000	2.160039000
1	-3.099316000	-2.835047000	2.739969000
1	0.843616000	-3.683051000	3.575671000
1	1.590326000	-1.963811000	1.907852000
1	-4.529482000	-1.540525000	1.481294000
1	-4.507823000	1.552119000	-1.504197000
1	-3.089662000	2.845042000	-2.744835000
1	0.855049000	3.702420000	-3.555466000
1	1.595557000	1.974130000	-1.894305000
1	3.093240000	-2.748147000	-2.838202000
1	-0.850442000	-3.580010000	-3.679786000
1	-1.593050000	-1.909033000	-1.961820000
1	4.509728000	-1.495969000	-1.554548000
1	4.527706000	1.490735000	1.536894000
1	3.095709000	2.738421000	2.840274000
1	-0.848298000	3.552063000	3.704645000
1	-1.592849000	1.893056000	1.976016000
8	6.009598000	0.068488000	0.060793000
1	6.445365000	-0.530787000	-0.559346000
8	-6.009738000	-0.065850000	0.055039000
1	-6.444459000	0.555101000	-0.544184000

xiv) [Fe (L14) 2] 2+

26	0.000002000	0.097440000	-0.000001000
7	0.261303000	-1.320389000	1.423603000
6	1.570362000	-1.587982000	1.697650000
6	1.942795000	-2.540687000	2.641582000
6	0.956350000	-3.241307000	3.328194000
6	-0.377372000	-2.966014000	3.049771000
6	-0.678534000	-2.002038000	2.093985000
7	1.911369000	0.079329000	0.076313000
6	2.524867000	-0.788928000	0.907715000
6	3.916430000	-0.882247000	0.927836000
6	4.637597000	-0.054852000	0.074088000
6	3.999779000	0.834975000	-0.783560000
6	2.606294000	0.881222000	-0.757927000
7	0.398375000	1.503551000	-1.395851000
6	1.730007000	1.716457000	-1.599551000
6	2.191042000	2.643144000	-2.530408000
6	1.271974000	3.375402000	-3.274625000
6	-0.085119000	3.158843000	-3.064027000
6	-0.476062000	2.217219000	-2.118962000
7	-0.398372000	1.503599000	1.395799000
6	-1.730005000	1.716513000	1.599490000
6	-2.191040000	2.643229000	2.530317000

6	-1.271973000	3.375511000	3.274512000
6	0.085121000	3.158943000	3.063924000
6	0.476064000	2.217289000	2.118890000
7	-1.911365000	0.079327000	-0.076317000
6	-2.606291000	0.881250000	0.757893000
6	-3.999777000	0.835007000	0.783523000
6	-4.637595000	-0.054851000	-0.074093000
6	-3.916426000	-0.882275000	-0.927811000
6	-2.524863000	-0.788958000	-0.907690000
7	-0.261297000	-1.320442000	-1.423552000
6	-1.570357000	-1.588042000	-1.697593000
6	-1.942789000	-2.540781000	-2.641492000
6	-0.956343000	-3.241429000	-3.328075000
6	0.377378000	-2.966130000	-3.049657000
6	0.678540000	-2.002119000	-2.093906000
1	2.988257000	-2.736851000	2.839637000
1	1.226772000	-3.987228000	4.065321000
1	-1.178784000	-3.485501000	3.558939000
1	-1.708075000	-1.768870000	1.855946000
1	4.436469000	-1.606072000	1.541862000
1	4.584060000	1.424646000	-1.478051000
1	3.252762000	2.792476000	-2.675855000
1	1.611504000	4.100046000	-4.004342000
1	-0.835143000	3.706132000	-3.620124000
1	-1.524540000	2.024029000	-1.933013000
1	-3.252760000	2.792566000	2.675757000
1	-1.611504000	4.100178000	4.004205000
1	0.835143000	3.706250000	3.620005000
1	1.524542000	2.024092000	1.932949000
1	-4.584058000	1.424702000	1.477993000
1	-4.436464000	-1.606122000	-1.541812000
1	-2.988251000	-2.736950000	-2.839542000
1	-1.226765000	-3.987377000	-4.065175000
1	1.178790000	-3.485638000	-3.558803000
1	1.708081000	-1.768944000	-1.855873000
16	-6.455284000	-0.288385000	0.073308000
8	-6.785178000	0.172140000	1.417999000
6	-7.169351000	0.855587000	-1.121511000
1	-6.836522000	0.588874000	-2.123425000
1	-6.898550000	1.875767000	-0.853847000
1	-8.248811000	0.719374000	-1.036266000
16	6.455285000	-0.288385000	-0.073301000
8	6.785153000	0.172089000	-1.418016000
6	7.169336000	0.855635000	1.121482000
1	6.836509000	0.588957000	2.123406000
1	8.248795000	0.719421000	1.036242000
1	6.898534000	1.875806000	0.853783000
8	6.697119000	-1.653310000	0.381824000
8	-6.697142000	-1.653321000	-0.381774000

xv) [Fe(L15)2]2+

26	0.000000000	0.000166000	0.000074000
7	-0.344974000	1.415040000	1.414197000
6	-1.669821000	1.649202000	1.646872000
6	-2.098188000	2.585994000	2.582610000
6	-1.152167000	3.307265000	3.304306000
6	0.196577000	3.068459000	3.066955000
6	0.554244000	2.117629000	2.117141000
7	-1.901812000	-0.001484000	-0.003821000
6	-2.568462000	0.825821000	0.822967000
6	-3.967433000	0.807040000	0.803313000

7	-4.644420000	-0.004597000	-0.008685000
6	-3.962710000	-0.814708000	-0.818245000
6	-2.563630000	-0.830320000	-0.832933000
7	-0.336710000	-1.415144000	-1.415710000
6	-1.660220000	-1.651738000	-1.653564000
6	-2.083227000	-2.588930000	-2.591334000
6	-1.133105000	-3.308058000	-3.309770000
6	0.214260000	-3.066734000	-3.067219000
6	0.566486000	-2.115659000	-2.115617000
7	0.338878000	-1.414498000	1.415964000
6	1.662739000	-1.649666000	1.653251000
6	2.087151000	-2.586446000	2.590800000
6	1.138102000	-3.306581000	3.309645000
6	-0.209625000	-3.066618000	3.067752000
6	-0.563277000	-2.115917000	2.116308000
7	1.901813000	0.001185000	0.003738000
6	2.564899000	-0.827071000	0.832419000
6	3.963954000	-0.809792000	0.817263000
7	4.644424000	0.001319000	0.007661000
6	3.966196000	0.812328000	-0.803927000
6	2.567195000	0.829432000	-0.823122000
7	0.342804000	1.415689000	-1.413946000
6	1.667301000	1.651761000	-1.646708000
6	2.094263000	2.589370000	-2.582270000
6	1.147167000	3.309468000	-3.303724000
6	-0.201216000	3.068703000	-3.066309000
6	-0.557457000	2.117170000	-2.116665000
1	-3.154723000	2.751996000	2.747426000
1	-1.464901000	4.040849000	4.037079000
1	0.966765000	3.605942000	3.604799000
1	1.596704000	1.911349000	1.912089000
1	-4.556272000	1.450980000	1.446869000
1	-4.547799000	-1.460012000	-1.463850000
1	-3.138808000	-2.756847000	-2.760266000
1	-1.441650000	-4.041902000	-4.044057000
1	0.987527000	-3.602455000	-3.602396000
1	1.607778000	-1.907539000	-1.906537000
1	3.142984000	-2.753247000	2.759265000
1	1.447745000	-4.040134000	4.043761000
1	-0.982086000	-3.603122000	3.603311000
1	-1.604877000	-1.908876000	1.907685000
1	4.550027000	-1.454579000	1.462492000
1	4.554052000	1.457119000	-1.447529000
1	3.150549000	2.756906000	-2.747132000
1	1.458804000	4.043661000	-4.036356000
1	-0.972212000	3.605207000	-3.603974000
1	-1.599611000	1.909396000	-1.911569000

xvi) [Fe(L16)2]2+

26	0.000039000	0.000317000	0.000118000
7	-0.345790000	1.436305000	1.379688000
6	-1.667895000	1.679267000	1.612012000
6	-2.055467000	2.640723000	2.535609000
6	-1.046112000	3.333360000	3.201844000
6	0.538311000	2.163838000	2.079468000
7	-1.920711000	-0.001246000	-0.003829000
6	-2.583576000	0.845637000	0.809956000
6	-3.977403000	0.866777000	0.829476000
6	-3.972627000	-0.873877000	-0.844031000
6	-2.578995000	-0.849622000	-0.819773000
7	-0.337825000	-1.436299000	-1.381381000

6	-1.658835000	-1.681438000	-1.618692000
6	-2.041080000	-2.643092000	-2.544110000
6	-1.027879000	-3.333493000	-3.207034000
6	0.550045000	-2.161690000	-2.078250000
7	0.339546000	-1.380094000	1.437217000
6	1.660829000	-1.614941000	1.683273000
6	2.044136000	-2.539478000	2.645351000
6	1.031696000	-3.204094000	3.335235000
6	-0.547532000	-2.078163000	2.162447000
7	1.920721000	0.001034000	0.003848000
6	2.580033000	-0.814293000	0.852081000
6	3.973665000	-0.836394000	0.876706000
6	3.976409000	0.837674000	-0.863374000
6	2.582567000	0.816004000	-0.842636000
7	0.344011000	1.381188000	-1.435173000
6	1.666020000	1.616591000	-1.676622000
6	2.052371000	2.541811000	-2.636887000
6	1.042111000	3.206549000	-3.329776000
6	-0.540818000	2.079736000	-2.162795000
1	-3.096662000	2.852422000	2.738228000
1	-1.279917000	4.097376000	3.935891000
1	1.587721000	1.968686000	1.892722000
1	-4.516034000	1.543244000	1.479593000
1	-4.507305000	-1.551657000	-1.496008000
1	-3.081039000	-2.856837000	-2.750927000
1	-1.257751000	-4.097617000	-3.942238000
1	3.084334000	-2.744344000	2.859812000
1	1.262401000	-3.938729000	4.099654000
1	4.509168000	-1.487808000	1.554376000
1	4.514170000	1.488564000	-1.539784000
1	3.093278000	2.747000000	-2.847538000
1	1.275096000	3.941770000	-4.092934000
6	-4.671258000	-0.004198000	-0.008495000
6	4.671278000	0.000605000	0.007568000
1	-5.754185000	-0.005283000	-0.010420000
1	5.754206000	0.000443000	0.009109000
7	0.264344000	-3.093143000	-2.974464000
7	0.247553000	3.095205000	2.974031000
7	-0.260798000	-2.973711000	3.094205000
7	-0.251154000	2.975855000	-3.093012000
1	-1.596121000	-1.889640000	1.964706000
1	1.598419000	-1.964863000	-1.887588000
1	-1.590013000	1.890543000	-1.968945000

xvii) [Fe(L17)2]2+

26	-0.000112000	-0.000125000	0.000262000
7	-0.334098000	-1.360543000	-1.452759000
6	-1.656115000	-1.589017000	-1.694831000
6	-2.040130000	-2.506718000	-2.674400000
6	0.131806000	-2.956613000	-3.157802000
6	0.549753000	-2.045953000	-2.185912000
7	-1.920535000	-0.000704000	0.002889000
6	-2.578121000	-0.805184000	-0.856298000
6	-3.972771000	-0.826676000	-0.878354000
6	-3.970585000	0.825772000	0.887992000
6	-2.576125000	0.804310000	0.863543000
7	-0.330782000	1.359563000	1.454275000
6	-1.652042000	1.587765000	1.699758000
6	-2.033887000	2.504971000	2.680811000
6	0.139176000	2.954637000	3.159188000
6	0.554855000	2.044647000	2.185835000

7	0.329774000	1.453758000	-1.360592000
6	1.650499000	1.698488000	-1.590366000
6	2.031693000	2.679330000	-2.508463000
6	-0.141858000	3.158116000	-2.955577000
6	-0.556699000	2.185434000	-2.044955000
7	1.920530000	0.001014000	-0.002811000
6	2.575399000	0.861628000	-0.807951000
6	3.969949000	0.886261000	-0.831402000
6	3.973389000	-0.880645000	0.820396000
6	2.578894000	-0.858743000	0.800910000
7	0.335720000	-1.453700000	1.359382000
6	1.657204000	-1.696858000	1.585370000
6	2.042319000	-2.677853000	2.501854000
6	-0.129362000	-3.159721000	2.954529000
6	-0.548006000	-2.187075000	2.045754000
1	-3.087265000	-2.701045000	-2.880085000
1	0.857081000	-3.507489000	-3.746842000
1	1.600999000	-1.869706000	-1.999062000
1	-4.511568000	-1.467622000	-1.563101000
1	-4.508795000	1.466709000	1.573318000
1	-3.080608000	2.698789000	2.889049000
1	0.865764000	3.505207000	3.746890000
1	1.605635000	1.868608000	1.996285000
1	3.078306000	2.887050000	-2.703558000
1	-0.868526000	3.746030000	-3.505735000
1	-1.607219000	1.995977000	-1.867327000
1	4.506667000	1.572163000	-1.472875000
1	4.513859000	-1.565173000	1.460304000
1	3.089807000	-2.884145000	2.693739000
1	-0.853656000	-3.748986000	3.506362000
1	-1.599220000	-1.998777000	1.871109000
6	-4.665023000	-0.000281000	0.005419000
6	4.664989000	0.003490000	-0.006288000
1	5.748131000	0.004456000	-0.007344000
1	-5.748168000	0.000165000	0.006461000
7	-1.156371000	-3.186344000	-3.401177000
7	-1.148507000	3.184143000	3.405894000
7	1.145844000	3.404406000	-3.186539000
7	1.159351000	-3.404454000	3.181874000

xviii) [Fe(L18)2]2+

26	-0.000014000	0.000008000	0.000073000
7	-0.338030000	1.427757000	1.346693000
6	-1.651888000	1.680068000	1.584206000
7	-2.099426000	2.590623000	2.442916000
6	-1.172963000	3.280020000	3.093390000
7	0.590903000	2.114263000	1.994308000
7	-1.914367000	-0.000879000	-0.002191000
6	-2.574829000	0.846809000	0.797612000
6	-3.966614000	0.877864000	0.826258000
6	-3.963813000	-0.882046000	-0.835096000
6	-2.572105000	-0.849354000	-0.803458000
7	-0.333431000	-1.427458000	-1.347799000
6	-1.646522000	-1.681329000	-1.588240000
7	-2.091075000	-2.592070000	-2.448262000
6	-1.162339000	-3.279921000	-3.097189000
7	0.597643000	-2.112292000	-1.993991000
7	0.334298000	-1.346899000	1.428209000
6	1.647444000	-1.585999000	1.682610000
7	2.092557000	-2.445289000	2.593818000
6	1.164190000	-3.094645000	3.281711000

7	1.914356000	0.000280000	0.002246000
6	2.572587000	-0.800433000	0.850864000
6	3.964313000	-0.830748000	0.884025000
6	3.966120000	0.830748000	-0.875743000
6	2.574329000	0.800764000	-0.845163000
7	0.337218000	1.347645000	-1.426921000
6	1.650958000	1.586647000	-1.678604000
6	1.171103000	3.096224000	-3.277938000
1	-1.505830000	4.031353000	3.801975000
1	-4.478118000	1.571457000	1.480737000
1	-4.473175000	-1.576180000	-1.490667000
1	-1.492813000	-4.031396000	-3.806733000
1	1.495054000	-3.803705000	4.033481000
1	4.474057000	-1.485874000	1.578298000
1	4.477218000	1.485796000	-1.569094000
1	1.503589000	3.805442000	-4.028844000
6	-4.660579000	-0.002502000	-0.005155000
6	4.660587000	-0.000071000	0.004778000
6	0.199486000	-3.033520000	-2.863992000
6	0.189735000	3.035434000	2.862941000
6	-0.197803000	-2.862527000	3.035073000
7	-0.592053000	1.994906000	-2.113223000
6	-0.191421000	2.864540000	-3.033732000
7	2.097948000	2.446223000	-2.588545000
1	-0.974711000	3.377987000	-3.578122000
7	-0.596462000	-1.993384000	2.113319000
1	-0.982259000	-3.375271000	3.578435000
1	0.984273000	-3.576645000	-3.376476000
1	0.972681000	3.580056000	3.376669000
1	5.743503000	-0.000203000	0.005782000
1	-5.743494000	-0.003139000	-0.006320000

xix) [Fe(L19)2]2+

26	0.000124000	0.000042000	0.000027000
7	0.343660000	-1.415439000	1.409778000
6	1.668717000	-1.646917000	1.639398000
6	2.064626000	-2.595637000	2.583765000
6	-0.103829000	-3.073252000	3.060694000
6	-0.532443000	-2.130674000	2.122418000
7	1.908864000	0.000935000	-0.001875000
6	2.573885000	-0.827967000	0.823457000
6	3.974208000	-0.811154000	0.806354000
6	3.971580000	0.815752000	-0.814013000
6	2.571455000	0.830880000	-0.828611000
7	0.339331000	1.415602000	-1.410355000
6	1.663538000	1.648509000	-1.642716000
6	2.056512000	2.597469000	-2.588197000
6	-0.113453000	3.072475000	-3.060814000
6	-0.539076000	2.129694000	-2.121498000
7	-0.340925000	1.409908000	1.415918000
6	-1.664890000	1.640713000	1.648908000
6	-2.059136000	2.585756000	2.598210000
6	0.110506000	3.060299000	3.072926000
6	0.537144000	2.121881000	2.130169000
7	-1.908815000	-0.000759000	0.001765000
6	-2.572266000	0.825563000	0.831456000
6	-3.972341000	0.809541000	0.816384000
6	-3.973366000	-0.811252000	-0.810034000
6	-2.573056000	-0.826965000	-0.826887000
7	-0.342475000	-1.410631000	-1.415036000
6	-1.666845000	-1.642115000	-1.645728000

6	-2.062219000	-2.587815000	-2.593776000
6	0.106815000	-3.061838000	-3.071790000
6	0.534639000	-2.122658000	-2.130217000
1	3.114327000	-2.790581000	2.777089000
1	-0.823612000	-3.648177000	3.633408000
1	-1.586289000	-1.955871000	1.948995000
1	4.563120000	-1.456547000	1.448783000
1	4.558833000	1.461840000	-1.457258000
1	3.105633000	2.793482000	-2.783556000
1	-0.835013000	3.646408000	-3.632282000
1	-1.592353000	1.953772000	-1.945841000
1	-3.108525000	2.779758000	2.794066000
1	0.831110000	3.632569000	3.647241000
1	1.590450000	1.946980000	1.953833000
1	-4.560302000	1.452363000	1.462256000
1	-4.561720000	-1.454344000	-1.455287000
1	-3.111815000	-2.782436000	-2.787917000
1	0.826739000	-3.634189000	-3.646880000
1	1.588184000	-1.947259000	-1.955743000
7	1.186216000	-3.304237000	3.289642000
7	1.175923000	3.304788000	-3.292556000
7	-1.179399000	3.290777000	3.305240000
7	-1.183315000	-3.292870000	-3.301915000
7	4.649275000	0.002791000	-0.004309000
7	-4.649227000	-0.000947000	0.003595000

xx) [Fe(L20)2]2+

26	-0.007732000	0.005015000	-0.006057000
7	0.308941000	-0.336206000	1.959270000
6	1.621188000	-0.421033000	2.307380000
6	2.022762000	-0.652474000	3.620610000
6	1.083568000	-0.808379000	4.644150000
6	-0.261555000	-0.716540000	4.257862000
6	-0.599682000	-0.484777000	2.935275000
7	1.904376000	-0.035114000	0.010397000
6	2.553642000	-0.245937000	1.174120000
6	3.942277000	-0.278733000	1.211103000
6	4.691308000	-0.092263000	0.036144000
6	3.977279000	0.123577000	-1.148968000
6	2.582864000	0.147678000	-1.136260000
7	0.356938000	0.331051000	-1.965558000
6	1.682787000	0.361082000	-2.288643000
6	2.114467000	0.574539000	-3.590256000
6	1.199874000	0.769824000	-4.635914000
6	-0.150544000	0.733936000	-4.277812000
6	-0.521959000	0.516008000	-2.956486000
7	-0.310373000	1.974595000	0.324835000
6	-1.620935000	2.337552000	0.368552000
6	-2.015039000	3.655373000	0.586666000
6	-1.069684000	4.668499000	0.771448000
6	0.273190000	4.267065000	0.721933000
6	0.603782000	2.940473000	0.501414000
7	-1.919149000	0.046836000	-0.023559000
6	-2.559414000	1.214474000	0.165521000
6	-3.952947000	1.271025000	0.156195000
6	-4.705928000	0.108595000	-0.051185000
6	-3.996106000	-1.089279000	-0.244825000
6	-2.606599000	-1.095890000	-0.226937000
7	-0.388384000	-1.950066000	-0.342706000
6	-1.711682000	-2.257531000	-0.412034000
6	-2.156251000	-3.557835000	-0.637662000

6	-1.250943000	-4.609940000	-0.803510000
6	0.106440000	-4.265379000	-0.727713000
6	0.487880000	-2.953714000	-0.501046000
1	3.078248000	-0.710737000	3.841736000
1	-1.058088000	-0.824483000	4.982040000
1	-1.638245000	-0.413982000	2.637780000
1	4.447941000	-0.448869000	2.151204000
1	4.503969000	0.272588000	-2.079375000
1	3.176332000	0.589238000	-3.794479000
1	-0.929383000	0.873569000	-5.013667000
1	-1.568768000	0.488614000	-2.680698000
1	-3.069361000	3.888009000	0.611872000
1	1.074006000	4.982410000	0.854370000
1	1.640738000	2.631515000	0.463391000
1	-4.448425000	2.217692000	0.309911000
1	-4.532789000	-2.013117000	-0.408992000
1	-3.218672000	-3.746458000	-0.683113000
1	0.878909000	-5.013896000	-0.844165000
1	1.535894000	-2.688414000	-0.442423000
6	1.465578000	-1.064300000	6.105668000
6	0.848687000	-2.410921000	6.555343000
6	0.900296000	0.082810000	6.978008000
1	1.314279000	1.049431000	6.679433000
1	-0.188596000	0.146156000	6.919924000
1	1.164351000	-0.087319000	8.024161000
1	-0.241408000	-2.408100000	6.486396000
1	1.111564000	-2.605249000	7.597569000
1	1.226054000	-3.241236000	5.952785000
6	6.225005000	-0.130123000	0.088191000
6	6.676029000	-1.512620000	0.618550000
6	6.723293000	0.981094000	1.043707000
1	6.415644000	1.970724000	0.696056000
1	6.352505000	0.847793000	2.062692000
1	7.814514000	0.965505000	1.088075000
1	6.302911000	-1.711242000	1.625988000
1	7.766754000	-1.552412000	0.659901000
1	6.335333000	-2.319117000	-0.035946000
6	-1.681141000	-6.058940000	-1.053793000
6	-3.211667000	-6.211595000	-1.098694000
6	-1.127851000	-6.948986000	0.085507000
1	-0.036926000	-6.925255000	0.134091000
1	-1.519081000	-6.638038000	1.057694000
1	-1.426843000	-7.986280000	-0.080976000
1	-3.681691000	-5.922419000	-0.154344000
1	-3.466037000	-7.257832000	-1.277402000
1	-3.659667000	-5.628414000	-1.908332000
6	-6.240785000	0.104681000	-0.072447000
6	-6.829267000	1.508015000	0.157594000
6	-6.756607000	-0.834420000	1.044773000
1	-6.419168000	-1.864509000	0.908186000
1	-6.427621000	-0.496161000	2.030788000
1	-7.848785000	-0.844767000	1.040990000
1	-6.549197000	1.917347000	1.132280000
1	-7.918932000	1.451043000	0.134064000
1	-6.526881000	2.214077000	-0.620884000
6	1.689746000	1.004253000	-6.068869000
6	2.523280000	-0.219188000	-6.520982000
6	2.573868000	2.274483000	-6.096342000
1	2.012371000	3.155547000	-5.775235000
1	3.454159000	2.179631000	-5.455935000
1	2.927193000	2.453883000	-7.114197000
1	3.402139000	-0.376299000	-5.890928000

1	2.876221000	-0.065469000	-7.543171000
1	1.925313000	-1.133982000	-6.505763000
6	-1.443229000	6.134470000	1.014020000
6	-0.864507000	6.579188000	2.379088000
6	-2.966540000	6.351510000	1.030854000
1	-3.430882000	6.083397000	0.077548000
1	-3.453649000	5.786813000	1.830941000
1	-3.179866000	7.407380000	1.206621000
1	-1.274352000	5.981643000	3.197545000
1	-1.122408000	7.624344000	2.564123000
1	0.224340000	6.498843000	2.410958000
6	0.522555000	1.195697000	-7.053374000
1	-0.124526000	0.315559000	-7.099427000
1	-0.088787000	2.066455000	-6.801305000
1	0.918706000	1.358540000	-8.057330000
6	-1.096524000	-6.526641000	-2.408715000
1	-0.004884000	-6.490838000	-2.420578000
1	-1.393692000	-7.560281000	-2.599486000
1	-1.466547000	-5.912465000	-3.233810000
6	-6.723404000	-0.411590000	-1.449587000
1	-6.384808000	-1.430484000	-1.651658000
1	-7.815264000	-0.418198000	-1.477456000
1	-6.370906000	0.231478000	-2.260189000
6	-0.832055000	6.998897000	-0.115448000
1	-1.218629000	6.703777000	-1.094402000
1	-1.089505000	8.048180000	0.045256000
1	0.257574000	6.928341000	-0.144179000
6	2.989900000	-1.129822000	6.305800000
1	3.481309000	-0.191616000	6.032652000
1	3.209215000	-1.312758000	7.359219000
1	3.444919000	-1.944895000	5.735756000
6	6.859996000	0.093870000	-1.295734000
1	6.602860000	1.071360000	-1.713387000
1	7.947012000	0.059383000	-1.204275000
1	6.572437000	-0.681660000	-2.011207000

xxi) [Fe (L21) 2] 2+

26	0.000000000	0.000118000	0.000364000
7	0.339056000	1.408692000	1.412381000
6	1.661094000	1.646295000	1.651109000
6	2.074678000	2.581464000	2.596088000
6	1.121643000	3.293110000	3.316405000
6	-0.224840000	3.049224000	3.070232000
6	-0.569398000	2.102225000	2.113440000
7	1.912748000	-0.000109000	0.000215000
6	2.577615000	0.832331000	0.826823000
6	3.966816000	0.851500000	0.849579000
6	4.697601000	-0.000208000	-0.000235000
6	3.966479000	-0.851855000	-0.849818000
6	2.577285000	-0.832586000	-0.826616000
7	0.338492000	-1.408631000	-1.411627000
6	1.660444000	-1.646470000	-1.650622000
6	2.073678000	-2.581829000	-2.595564000
6	1.120381000	-3.293443000	-3.315566000
6	-0.226008000	-3.049336000	-3.069111000
6	-0.570212000	-2.102151000	-2.112377000
7	-0.338633000	1.408868000	-1.411592000
6	-1.660606000	1.646602000	-1.650564000
6	-2.073927000	2.581949000	-2.595481000
6	-1.120696000	3.293664000	-3.315469000
6	0.225717000	3.049674000	-3.069023000

6	0.570009000	2.102490000	-2.112320000
7	-1.912748000	0.000289000	0.000345000
6	-2.577368000	0.832653000	-0.826534000
6	-3.966564000	0.851770000	-0.849751000
6	-4.697601000	0.000084000	-0.000134000
6	-3.966731000	-0.851506000	0.849725000
6	-2.577531000	-0.832189000	0.826980000
7	-0.338915000	-1.408375000	1.412497000
6	-1.660931000	-1.646025000	1.651303000
6	-2.074428000	-2.581107000	2.596407000
6	-1.121328000	-3.292614000	3.316774000
6	0.225132000	-3.048677000	3.070526000
6	0.569601000	-2.101772000	2.113611000
1	3.128514000	2.752913000	2.770219000
1	1.426574000	4.023484000	4.055666000
1	-1.001035000	3.579170000	3.606794000
1	-1.607979000	1.887378000	1.897688000
1	4.492403000	1.499216000	1.537356000
1	4.491797000	-1.499594000	-1.537779000
1	3.127450000	-2.753464000	-2.769896000
1	1.425041000	-4.023966000	-4.054791000
1	-1.002404000	-3.579251000	-3.605413000
1	-1.608717000	-1.887127000	-1.896439000
1	-3.127715000	2.753503000	-2.769797000
1	-1.425423000	4.024179000	-4.054674000
1	1.002063000	3.579677000	-3.605311000
1	1.608533000	1.887542000	-1.896396000
1	-4.491944000	1.499413000	-1.537753000
1	-4.492253000	-1.499254000	1.537521000
1	-3.128248000	-2.752588000	2.770601000
1	-1.426191000	-4.022917000	4.056132000
1	1.001377000	-3.578513000	3.607125000
1	1.608163000	-1.886898000	1.897795000
6	6.172100000	-0.000265000	-0.000471000
6	6.892067000	-1.185511000	-0.223273000
6	6.892231000	1.184925000	0.222104000
6	8.279438000	-1.192409000	-0.217926000
6	8.279601000	1.191713000	0.216317000
6	8.969907000	-0.000376000	-0.000914000
1	6.370011000	-2.124822000	-0.363888000
1	6.370296000	2.124277000	0.362888000
1	8.827081000	-2.112818000	-0.372027000
1	8.827366000	2.112077000	0.370246000
6	-6.172100000	-0.000021000	-0.000386000
6	-6.892193000	1.185146000	-0.223203000
6	-6.892106000	-1.185287000	0.222188000
6	-8.279565000	1.191894000	-0.217871000
6	-8.279476000	-1.192224000	0.216387000
6	-8.969907000	-0.000212000	-0.000859000
1	-6.370238000	2.124513000	-0.363816000
1	-6.370072000	-2.124582000	0.362983000
1	-8.827306000	2.112243000	-0.371982000
1	-8.827143000	-2.112647000	0.370316000
17	10.708798000	-0.000444000	-0.001189000
17	-10.708798000	-0.000331000	-0.001153000
xxii) [Fe (L22) 2]2+			
26	0.000018000	-0.043948000	-0.000135000
7	0.510537000	-1.453683000	-1.360284000
6	1.844762000	-1.700249000	-1.440165000
6	2.385866000	-2.638834000	-2.312700000

6	1.528921000	-3.367011000	-3.149209000
6	0.150776000	-3.108079000	-3.063483000
6	-0.300201000	-2.160802000	-2.170775000
7	1.903449000	-0.046535000	0.231511000
6	2.660982000	-0.883314000	-0.514883000
6	4.035383000	-0.916377000	-0.368943000
6	4.646111000	-0.065710000	0.572717000
6	3.844616000	0.794764000	1.338908000
6	2.466581000	0.773335000	1.136433000
7	0.173627000	1.362886000	1.446989000
6	1.461816000	1.596266000	1.844940000
6	1.775289000	2.519116000	2.823708000
6	0.751824000	3.253499000	3.445929000
6	-0.566779000	3.013448000	3.037966000
6	-0.792375000	2.068960000	2.047045000
7	-0.509701000	-1.458892000	1.354908000
6	-1.843800000	-1.706435000	1.433940000
6	-2.384376000	-2.648546000	2.302992000
6	-1.527017000	-3.379433000	3.136714000
6	-0.149010000	-3.119479000	3.051880000
6	0.301434000	-2.168633000	2.162702000
7	-1.903416000	-0.046691000	-0.231715000
6	-2.660485000	-0.886496000	0.511735000
6	-4.034898000	-0.919604000	0.365875000
6	-4.646122000	-0.065745000	-0.572568000
6	-3.845108000	0.797901000	-1.335686000
6	-2.467035000	0.776299000	-1.133504000
7	-0.174375000	1.367933000	-1.442225000
6	-1.462717000	1.602249000	-1.839125000
6	-1.776702000	2.528547000	-2.814468000
6	-0.753621000	3.265601000	-3.434151000
6	0.565150000	3.024523000	-3.027333000
6	0.791266000	2.076521000	-2.039894000
1	3.453517000	-2.798202000	-2.336716000
1	-0.534971000	-3.655074000	-3.696549000
1	-1.358598000	-1.949238000	-2.090651000
1	4.667626000	-1.573741000	-0.949250000
1	4.281014000	1.457973000	2.070237000
1	2.795088000	2.699197000	3.134930000
1	-1.406510000	3.538242000	3.469940000
1	-1.804444000	1.868632000	1.718087000
1	-3.451947000	-2.808523000	2.326481000
1	0.537052000	-3.668492000	3.682855000
1	1.359719000	-1.956226000	2.083337000
1	-4.666792000	-1.579346000	0.943860000
1	-4.281886000	1.463641000	-2.064486000
1	-2.796618000	2.709359000	-3.124881000
1	1.404613000	3.551169000	-3.457571000
1	1.803465000	1.875366000	-1.711840000
8	-5.973402000	-0.156956000	-0.656274000
6	-6.695272000	0.666284000	-1.588894000
1	-6.556897000	1.725505000	-1.357946000
1	-6.385752000	0.451270000	-2.614761000
1	-7.739806000	0.397466000	-1.458753000
8	5.973418000	-0.156653000	0.656271000
6	6.694812000	0.663464000	1.592012000
1	6.555976000	1.723468000	1.364968000
1	6.385280000	0.444507000	2.617040000
1	7.739482000	0.395609000	1.460985000
8	1.908095000	-4.292533000	-4.027135000
6	3.300297000	-4.620611000	-4.172013000
1	3.871182000	-3.749242000	-4.502842000

1	3.704601000	-5.014393000	-3.236028000
1	3.334776000	-5.391240000	-4.937008000
8	1.135368000	4.121737000	4.379061000
6	0.148958000	4.911407000	5.068609000
1	-0.392285000	5.550809000	4.367154000
1	-0.543815000	4.269207000	5.617636000
1	0.710887000	5.525764000	5.766450000
8	-1.137660000	4.137142000	-4.363991000
6	-0.151672000	4.929778000	-5.050731000
1	0.389508000	5.566690000	-4.346964000
1	0.541198000	4.289908000	-5.602349000
1	-0.713964000	5.546587000	-5.746110000
8	-1.905683000	-4.308428000	4.011186000
6	-3.297723000	-4.637681000	4.154966000
1	-3.868971000	-3.767812000	4.489100000
1	-3.701935000	-5.028148000	3.217555000
1	-3.331781000	-5.411174000	4.917084000

xxiii) [Fe(L23)2]2+

26	0.004244000	0.030672000	0.036427000
7	0.692064000	1.226993000	1.513473000
6	2.050626000	1.281235000	1.616596000
6	2.701688000	2.037874000	2.574374000
6	1.971636000	2.815511000	3.510699000
6	0.560225000	2.743467000	3.379216000
6	-0.005307000	1.958722000	2.398112000
7	1.892664000	-0.198651000	-0.199345000
6	2.755602000	0.446784000	0.612215000
6	4.125362000	0.311306000	0.467493000
6	4.658419000	-0.529986000	-0.547565000
6	3.712813000	-1.194200000	-1.376385000
6	2.356497000	-1.003130000	-1.177791000
7	0.012120000	-1.250995000	-1.527666000
6	1.253233000	-1.620892000	-1.954484000
6	1.456124000	-2.484225000	-3.016181000
6	0.359374000	-3.043066000	-3.722655000
6	-0.920402000	-2.643352000	-3.256901000
6	-1.030494000	-1.773742000	-2.193888000
7	-0.314369000	1.610507000	-1.184269000
6	-1.609819000	2.031995000	-1.243991000
6	-2.018264000	3.095618000	-2.028625000
6	-1.088544000	3.816430000	-2.822638000
6	0.252266000	3.358071000	-2.740887000
6	0.570613000	2.286988000	-1.934860000
7	-1.883529000	0.260832000	0.272501000
6	-2.531215000	1.239316000	-0.392613000
6	-3.895603000	1.428310000	-0.255041000
6	-4.651309000	0.592500000	0.612513000
6	-3.930781000	-0.437159000	1.277971000
6	-2.565216000	-0.565860000	1.091704000
7	-0.373198000	-1.466700000	1.341223000
6	-1.678659000	-1.576839000	1.719256000
6	-2.124453000	-2.537127000	2.609702000
6	-1.226686000	-3.477179000	3.179444000
6	0.124799000	-3.341809000	2.767417000
6	0.482528000	-2.351623000	1.878709000
1	3.779391000	2.014702000	2.610160000
1	-0.096206000	3.305043000	4.026354000
1	-1.083486000	1.912335000	2.304993000
1	4.783690000	0.862390000	1.119443000
1	4.045104000	-1.863044000	-2.153750000

1	2.467273000	-2.715272000	-3.311863000
1	-1.827058000	-3.016849000	-3.708061000
1	-2.012043000	-1.477081000	-1.844718000
1	-3.063241000	3.362430000	-2.038952000
1	1.047809000	3.840178000	-3.288377000
1	1.597516000	1.947235000	-1.877025000
1	-4.378245000	2.213849000	-0.813058000
1	-4.441626000	-1.127473000	1.929009000
1	-3.168501000	-2.550366000	2.879919000
1	0.893079000	-4.010956000	3.123877000
1	1.516261000	-2.258325000	1.568831000
7	-5.988294000	0.775661000	0.805201000
7	5.999393000	-0.690398000	-0.716694000
6	-6.756771000	-0.098358000	1.704883000
1	-7.633792000	0.466998000	2.022399000
1	-6.172651000	-0.272465000	2.612756000
6	-6.722723000	1.838565000	0.101854000
1	-6.121634000	2.751980000	0.114256000
1	-7.608027000	2.059996000	0.699134000
6	6.978245000	-0.088414000	0.199616000
1	7.855863000	-0.738050000	0.199881000
1	6.586137000	-0.123588000	1.218419000
6	6.556731000	-1.475260000	-1.827337000
1	5.946705000	-1.318966000	-2.719768000
1	7.533905000	-1.047587000	-2.060673000
6	-7.200156000	-1.428001000	1.085281000
1	-7.744686000	-2.018504000	1.826604000
1	-7.864935000	-1.265951000	0.235046000
1	-6.349847000	-2.019484000	0.737940000
6	6.705000000	-2.967458000	-1.516778000
1	7.148671000	-3.486435000	-2.370080000
1	7.356948000	-3.125864000	-0.654672000
1	5.741196000	-3.432528000	-1.296797000
6	7.388325000	1.336537000	-0.183044000
1	8.134708000	1.714308000	0.520160000
1	7.828598000	1.363104000	-1.182456000
1	6.534947000	2.018662000	-0.175605000
6	-7.143722000	1.489038000	-1.329569000
1	-7.663444000	2.338329000	-1.780488000
1	-6.284815000	1.243712000	-1.958522000
1	-7.824234000	0.635930000	-1.344395000
7	0.523608000	-3.895850000	-4.766882000
6	1.848779000	-4.375658000	-5.181391000
6	2.549460000	-3.458674000	-6.188026000
6	-0.618788000	-4.396819000	-5.546000000
6	-1.248591000	-5.666959000	-4.968176000
1	-1.361235000	-3.602403000	-5.644619000
1	-2.071255000	-6.000719000	-5.605304000
1	-0.254624000	-4.589505000	-6.557252000
1	-0.518394000	-6.477766000	-4.912855000
1	1.707235000	-5.365937000	-5.619029000
1	2.468532000	-4.531026000	-4.295370000
1	1.951883000	-3.343190000	-7.095128000
1	3.514378000	-3.883559000	-6.475904000
1	2.723070000	-2.462726000	-5.773689000
1	-1.642022000	-5.499571000	-3.963031000
7	-1.455636000	4.866368000	-3.602102000
6	-2.827807000	5.390984000	-3.608888000
6	-3.750618000	4.690117000	-4.610023000
6	-0.497936000	5.548129000	-4.485905000
6	0.270416000	6.682503000	-3.802827000
1	0.187476000	4.810695000	-4.908287000

1	0.942979000	7.163186000	-4.517460000
1	-1.067910000	5.941112000	-5.330332000
1	-0.412063000	7.445329000	-3.420767000
1	-2.761891000	6.454324000	-3.847956000
1	-3.237137000	5.341383000	-2.597338000
1	-3.366625000	4.782796000	-5.628470000
1	-4.745136000	5.142670000	-4.585811000
1	-3.852735000	3.625361000	-4.387348000
7	-1.631612000	-4.433588000	4.054629000
6	-0.676718000	-5.342742000	4.706319000
6	-0.378144000	-6.606518000	3.895479000
6	-3.045963000	-4.623492000	4.403435000
6	-3.514343000	-3.754258000	5.573988000
1	-3.661206000	-4.452051000	3.517225000
1	-4.563304000	-3.961341000	5.800418000
1	-3.174637000	-5.679002000	4.651561000
1	-2.931526000	-3.961919000	6.474249000
1	-1.104796000	-5.614218000	5.673497000
1	0.241524000	-4.796634000	4.931301000
1	-1.289953000	-7.178996000	3.709655000
1	0.314236000	-7.249317000	4.444583000
1	0.071777000	-6.367693000	2.929226000
7	2.579398000	3.570860000	4.461840000
6	1.810178000	4.301032000	5.480818000
6	1.379201000	5.702325000	5.039947000
6	4.040122000	3.710327000	4.531746000
6	4.724475000	2.620429000	5.361767000
1	4.447235000	3.745015000	3.518672000
1	5.802738000	2.795360000	5.396783000
1	4.246834000	4.690648000	4.965835000
1	4.353293000	2.618931000	6.389133000
1	2.441940000	4.368667000	6.368893000
1	0.946893000	3.701374000	5.776046000
1	2.245274000	6.319365000	4.789268000
1	0.837101000	6.199382000	5.848123000
1	0.727426000	5.665894000	4.164184000
1	4.551630000	1.626202000	4.943013000
1	0.868202000	6.316220000	-2.965215000
1	-3.415369000	-2.689353000	5.350604000

xxiv) [Fe(L24)2]2+

26	-0.000044000	-0.000252000	0.000370000
7	0.365693000	-1.481244000	1.314563000
7	1.716036000	-1.686096000	1.496062000
6	1.937124000	-2.695983000	2.391994000
7	1.927415000	0.001466000	-0.001150000
6	2.592866000	-0.868205000	0.770366000
6	3.980675000	-0.906992000	0.804770000
6	4.662035000	0.003964000	-0.003174000
6	3.977804000	0.913669000	-0.810121000
6	2.590125000	0.872370000	-0.773649000
7	0.361065000	1.481488000	-1.314391000
7	1.710734000	1.688547000	-1.498137000
6	1.928556000	2.699047000	-2.394241000
7	-0.363664000	1.313772000	1.481893000
7	-1.713710000	1.496573000	1.687496000
6	0.237031000	2.097476000	2.367237000
7	-1.927457000	-0.001507000	0.000998000
6	-2.591699000	0.771197000	0.870578000
6	-3.979427000	0.806931000	0.910113000
6	-4.662052000	-0.001040000	0.000098000

6	-3.979119000	-0.809036000	-0.909600000
6	-2.591357000	-0.773712000	-0.869280000
7	-0.363066000	-1.315326000	-1.480585000
1	2.932048000	-3.005564000	2.666426000
1	4.516914000	-1.609005000	1.427535000
1	5.745008000	0.004958000	-0.003981000
1	4.511851000	1.616664000	-1.433658000
1	2.922555000	3.010366000	-2.670078000
1	0.497636000	3.945032000	-3.499433000
1	1.313897000	2.139173000	2.414685000
1	-4.514722000	1.430781000	1.611883000
1	-5.745026000	-0.000923000	-0.000205000
1	-4.514154000	-1.432523000	-1.611892000
7	-1.713040000	-1.498810000	-1.686128000
6	-1.932243000	-2.395643000	-2.695732000
6	0.238008000	-2.100176000	-2.364632000
6	-0.703227000	-2.799189000	-3.151166000
1	1.314899000	-2.141677000	-2.411795000
1	-0.503122000	-3.502306000	-3.942208000
1	-2.926578000	-2.671163000	-3.006232000
6	-0.704576000	2.795107000	3.154571000
6	-1.933375000	2.391795000	2.698357000
1	-2.927802000	2.667041000	3.008575000
1	-0.504810000	3.496682000	3.947055000
6	0.698954000	3.153420000	-2.797316000
6	-0.241203000	2.365446000	-2.098628000
1	-1.318154000	2.411463000	-2.139730000
6	0.708970000	-3.152241000	2.797242000
1	0.510441000	-3.944070000	3.499917000
6	-0.233740000	-2.365966000	2.099934000
1	-1.310545000	-2.413848000	2.142828000

xxv) [Fe (L25) 2] 2+

26	0.000000000	-0.000022000	0.017731000
7	0.312035000	1.414930000	1.428899000
6	1.628973000	1.680717000	1.665910000
6	2.022290000	2.625406000	2.610369000
6	1.054663000	3.315953000	3.331254000
6	-0.286664000	3.042672000	3.086759000
6	-0.611126000	2.088390000	2.130586000
7	1.912115000	0.039032000	0.016947000
6	2.562391000	0.886312000	0.840642000
6	3.949015000	0.936850000	0.861563000
6	4.704538000	0.102829000	0.009830000
6	3.983859000	-0.765303000	-0.837848000
6	2.596390000	-0.778191000	-0.809794000
7	0.369138000	-1.401545000	-1.393532000
6	1.695688000	-1.612201000	-1.632379000
6	2.126533000	-2.540980000	-2.576257000
6	1.187549000	-3.272595000	-3.294474000
6	-0.163645000	-3.055554000	-3.047986000
6	-0.526118000	-2.114298000	-2.092580000
7	-0.369112000	1.401482000	-1.393559000
6	-1.695658000	1.612140000	-1.632425000
6	-2.126488000	2.540898000	-2.576332000
6	-1.187492000	3.272487000	-3.294560000
6	0.163698000	3.055443000	-3.048052000
6	0.526156000	2.114210000	-2.092618000
7	-1.912116000	-0.039067000	0.016922000
6	-2.596376000	0.778158000	-0.809830000
6	-3.983846000	0.765295000	-0.837883000

6	-4.704538000	-0.102811000	0.009811000
6	-3.949032000	-0.936832000	0.861556000
6	-2.562407000	-0.886321000	0.840632000
7	-0.312060000	-1.414960000	1.428905000
6	-1.629002000	-1.680728000	1.665913000
6	-2.022335000	-2.625404000	2.610379000
6	-1.054719000	-3.315957000	3.331273000
6	0.286612000	-3.042696000	3.086781000
6	0.611090000	-2.088426000	2.130601000
1	3.072386000	2.819832000	2.782756000
1	1.344303000	4.053119000	4.069945000
1	-1.073717000	3.555528000	3.624083000
1	-1.644635000	1.850064000	1.914866000
1	4.457066000	1.596269000	1.550922000
1	4.518001000	-1.399217000	-1.531499000
1	3.183576000	-2.691580000	-2.749993000
1	1.506519000	-3.998140000	-4.032590000
1	-0.929455000	-3.601930000	-3.582958000
1	-1.568345000	-1.919446000	-1.875271000
1	-3.183528000	2.691498000	-2.750083000
1	-1.506450000	3.998014000	-4.032699000
1	0.929517000	3.601799000	-3.583031000
1	1.568379000	1.919357000	-1.875293000
1	-4.517979000	1.399208000	-1.531541000
1	-4.457097000	-1.596228000	1.550927000
1	-3.072434000	-2.819816000	2.782762000
1	-1.344372000	-4.053114000	4.069970000
1	1.073657000	-3.555558000	3.624111000
1	1.644602000	-1.850115000	1.914882000
6	6.170443000	0.140554000	0.005986000
6	6.929163000	-0.997285000	-0.312696000
6	6.870715000	1.323527000	0.326382000
6	8.316378000	-0.975273000	-0.308978000
6	8.248062000	1.364945000	0.320373000
6	8.993384000	0.213357000	0.005680000
1	6.434740000	-1.937634000	-0.528068000
1	6.328341000	2.236642000	0.542515000
1	8.862032000	-1.879718000	-0.538765000
1	8.786077000	2.277184000	0.544788000
6	-6.170445000	-0.140508000	0.005968000
6	-6.929143000	0.997347000	-0.312705000
6	-6.870738000	-1.323471000	0.326360000
6	-8.316360000	0.975361000	-0.308984000
6	-8.248086000	-1.364863000	0.320354000
6	-8.993386000	-0.213259000	0.005668000
1	-6.434702000	1.937688000	-0.528071000
1	-6.328377000	-2.236596000	0.542485000
1	-8.861998000	1.879817000	-0.538763000
1	-8.786117000	-2.277092000	0.544764000
8	-10.325114000	-0.355925000	0.034834000
6	-11.167068000	0.759736000	-0.281430000
1	-11.014118000	1.578359000	0.427230000
1	-10.990269000	1.105513000	-1.303628000
1	-12.184565000	0.387829000	-0.193598000
8	10.325109000	0.356047000	0.034843000
6	11.167083000	-0.759597000	-0.281431000
1	11.014149000	-1.578227000	0.427225000
1	10.990286000	-1.105371000	-1.303630000
1	12.184573000	-0.387672000	-0.193600000

i) [Fe(L1)2]3+

26	-0.000010000	-0.061389000	0.000004000
7	0.287713000	1.342034000	1.434797000
6	1.600942000	1.651339000	1.648184000
6	1.967332000	2.623384000	2.572140000
6	0.981765000	3.288994000	3.295468000
6	-0.352441000	2.962765000	3.077111000
6	-0.657011000	1.984936000	2.139367000
7	1.907523000	-0.022333000	0.025369000
6	2.548807000	0.858377000	0.835376000
6	3.920902000	0.933405000	0.867498000
6	4.706777000	0.070574000	0.031684000
6	3.986478000	-0.844322000	-0.805862000
6	2.611998000	-0.859494000	-0.779098000
7	0.389507000	-1.500630000	-1.349377000
6	1.717015000	-1.720083000	-1.579349000
6	2.137164000	-2.681402000	-2.492486000
6	1.189749000	-3.430125000	-3.183906000
6	-0.160759000	-3.199255000	-2.942856000
6	-0.519482000	-2.227972000	-2.017501000
7	-0.287730000	1.341811000	-1.435008000
6	-1.600960000	1.651082000	-1.648446000
6	-1.967349000	2.622980000	-2.572556000
6	-0.981782000	3.288480000	-3.295985000
6	0.352424000	2.962287000	-3.077573000
6	0.656994000	1.984605000	-2.139676000
7	-1.907542000	-0.022340000	-0.025371000
6	-2.548824000	0.858245000	-0.835516000
6	-3.920919000	0.933267000	-0.867650000
6	-4.706782000	0.070565000	-0.031702000
6	-3.986496000	-0.844195000	0.805994000
6	-2.612016000	-0.859373000	0.779232000
7	-0.389526000	-1.500417000	1.349613000
6	-1.717033000	-1.719836000	1.579618000
6	-2.137183000	-2.681012000	2.492907000
6	-1.189767000	-3.429624000	3.184446000
6	0.160740000	-3.198789000	2.943362000
6	0.519463000	-2.227651000	2.017854000
1	3.010605000	2.860798000	2.731078000
1	1.253871000	4.047635000	4.019359000
1	-1.149118000	3.453063000	3.621313000
1	-1.682755000	1.706075000	1.940092000
1	4.410956000	1.625555000	1.534809000
1	4.524202000	-1.509538000	-1.463817000
1	3.192297000	-2.846545000	-2.664725000
1	1.502555000	-4.181344000	-3.899006000
1	-0.929358000	-3.758822000	-3.460012000
1	-1.559127000	-2.018875000	-1.803847000
1	-3.010623000	2.860367000	-2.731534000
1	-1.253888000	4.047006000	-4.019996000
1	1.149101000	3.452502000	-3.621850000
1	1.682737000	1.705777000	-1.940355000
1	-4.410978000	1.625316000	-1.535065000
1	-4.524225000	-1.509304000	1.464054000
1	-3.192316000	-2.846129000	2.665170000
1	-1.502573000	-4.180731000	3.899664000
1	0.929340000	-3.758273000	3.460607000
1	1.559108000	-2.018585000	1.804168000
7	-6.036480000	0.116088000	-0.036954000
6	-6.910785000	-0.799230000	0.742165000
1	-6.853961000	-0.537967000	1.804528000
1	-6.585703000	-1.833763000	0.614980000
1	-9.089055000	-0.746987000	0.904207000

6	-8.309418000	-0.544012000	0.170881000
1	-8.485262000	-1.190958000	-0.692035000
6	-8.258034000	0.927966000	-0.259572000
1	-8.394266000	1.585648000	0.602415000
1	-9.017841000	1.183375000	-0.997316000
6	-6.842092000	1.087045000	-0.823003000
1	-6.448714000	2.097514000	-0.695583000
1	-6.797368000	0.820086000	-1.884493000
7	6.036530000	0.116094000	0.036935000
6	6.842169000	1.086674000	0.823422000
1	6.797470000	0.819219000	1.884788000
1	6.448782000	2.097200000	0.696482000
1	9.017927000	1.182926000	0.997738000
6	8.258104000	0.927863000	0.259892000
1	8.394320000	1.585946000	-0.601792000
6	8.309479000	-0.543911000	-0.171248000
1	8.485337000	-1.191259000	0.691364000
1	9.089105000	-0.746543000	-0.904680000
6	6.910830000	-0.798855000	-0.742626000
1	6.585742000	-1.833443000	-0.615917000
1	6.853993000	-0.537096000	-1.804865000

ii) [Fe(L2)2]3+

26	-0.031068000	0.000000000	0.000000000
7	-0.335892000	1.997190000	0.000001000
6	-1.656101000	2.342503000	0.000001000
6	-2.054137000	3.674510000	0.000001000
6	-1.087482000	4.676891000	0.000002000
6	0.255385000	4.317760000	0.000002000
6	0.588587000	2.967970000	0.000001000
7	-1.903775000	0.000000000	0.000000000
6	-2.577536000	1.185048000	0.000000000
6	-3.949437000	1.222721000	0.000000000
6	-4.702022000	0.000000000	0.000000000
6	-3.949437000	-1.222721000	0.000000000
6	-2.577536000	-1.185048000	0.000000000
7	-0.335892000	-1.997190000	-0.000001000
6	-1.656101000	-2.342503000	-0.000001000
6	-2.054137000	-3.674510000	-0.000001000
6	-1.087482000	-4.676891000	-0.000002000
6	0.255384000	-4.317760000	-0.000002000
6	0.588587000	-2.967970000	-0.000001000
7	0.343692000	-0.000001000	1.983142000
6	1.663874000	-0.000001000	2.329320000
6	2.055620000	-0.000001000	3.663642000
6	1.088312000	-0.000002000	4.663603000
6	-0.254553000	-0.000002000	4.301660000
6	-0.585418000	-0.000001000	2.953206000
7	1.906580000	0.000000000	0.000000000
6	2.581762000	0.000000000	1.174017000
6	3.958274000	0.000000000	1.216336000
6	4.713552000	0.000000000	0.000000000
6	3.958274000	0.000000000	-1.216336000
6	2.581762000	0.000000000	-1.174017000
7	0.343692000	0.000001000	-1.983142000
6	1.663874000	0.000001000	-2.329320000
6	2.055620000	0.000001000	-3.663642000
6	1.088312000	0.000002000	-4.663603000
6	-0.254553000	0.000002000	-4.301660000
6	-0.585418000	0.000001000	-2.953206000
1	-3.104263000	3.934475000	0.000001000

1	-1.381234000	5.719591000	0.000002000
1	1.038201000	5.065185000	0.000002000
1	1.622898000	2.650886000	0.000001000
1	-4.460264000	2.172544000	0.000001000
1	-4.460264000	-2.172544000	-0.000001000
1	-3.104263000	-3.934475000	-0.000001000
1	-1.381234000	-5.719591000	-0.000002000
1	1.038201000	-5.065185000	-0.000002000
1	1.622898000	-2.650886000	-0.000001000
1	3.105745000	-0.000001000	3.923192000
1	1.379910000	-0.000002000	5.706911000
1	-1.039707000	-0.000002000	5.046549000
1	-1.619352000	-0.000001000	2.636519000
1	4.464188000	-0.000001000	2.168842000
1	4.464188000	0.000001000	-2.168842000
1	3.105745000	0.000001000	-3.923192000
1	1.379910000	0.000002000	-5.706911000
1	-1.039707000	0.000002000	-5.046549000
1	-1.619352000	0.000001000	-2.636519000
7	6.053140000	0.000000000	0.000000000
7	-6.038492000	0.000000000	0.000000000
6	6.806254000	0.000000000	-1.264517000
1	7.868855000	0.000000000	-1.041053000
1	6.584574000	-0.893769000	-1.853666000
1	6.584574000	0.893771000	-1.853665000
6	6.806254000	0.000000000	1.264517000
1	6.584574000	0.893769000	1.853666000
1	6.584574000	-0.893771000	1.853665000
1	7.868855000	0.000000000	1.041053000
6	-6.797056000	1.264180000	0.000000000
1	-7.858542000	1.036627000	0.000000000
1	-6.575027000	1.851649000	0.894165000
1	-6.575027000	1.851650000	-0.894164000
6	-6.797056000	-1.264180000	0.000000000
1	-6.575027000	-1.851649000	-0.894165000
1	-6.575028000	-1.851650000	0.894164000
1	-7.858542000	-1.036627000	0.000000000

iii) [Fe(L3)2]3+

26	0.001437000	0.472872000	0.025431000
7	0.177556000	1.778167000	-1.516770000
6	1.464872000	1.958744000	-1.937625000
6	1.758947000	2.792216000	-3.010418000
6	0.726249000	3.458297000	-3.664957000
6	-0.580458000	3.274759000	-3.225931000
6	-0.812162000	2.427630000	-2.150035000
7	1.899768000	0.485037000	-0.153731000
6	2.470166000	1.216349000	-1.146776000
6	3.832568000	1.234996000	-1.318132000
6	4.675927000	0.478944000	-0.441953000
6	4.035395000	-0.285327000	0.581029000
6	2.663489000	-0.249946000	0.692886000
7	0.494146000	-0.750819000	1.541844000
6	1.834577000	-0.969579000	1.681590000
6	2.325584000	-1.798673000	2.684236000
6	1.436330000	-2.417012000	3.558412000
6	0.072565000	-2.188058000	3.408345000
6	-0.357922000	-1.347626000	2.389643000
7	-0.392150000	-1.082890000	-1.214693000
6	-1.724939000	-1.310607000	-1.410563000
6	-2.162333000	-2.313543000	-2.267751000

6	-1.228545000	-3.102544000	-2.934181000
6	0.125934000	-2.868650000	-2.723574000
6	0.502310000	-1.850650000	-1.856968000
7	-1.909011000	0.460337000	0.122647000
6	-2.612068000	-0.420294000	-0.630495000
6	-3.988535000	-0.447585000	-0.607982000
6	-4.699607000	0.479006000	0.216394000
6	-3.919231000	1.383268000	1.003124000
6	-2.547534000	1.345839000	0.930966000
7	-0.283491000	1.941876000	1.368623000
6	-1.591759000	2.206851000	1.655410000
6	-1.940399000	3.205189000	2.558622000
6	-0.939987000	3.947192000	3.179396000
6	0.390260000	3.669848000	2.881335000
6	0.676940000	2.659175000	1.973142000
1	2.782060000	2.926166000	-3.335299000
1	0.941727000	4.111674000	-4.501813000
1	-1.411579000	3.777061000	-3.703706000
1	-1.815118000	2.258398000	-1.782648000
1	4.282954000	1.829520000	-2.102391000
1	4.624084000	-0.887819000	1.255764000
1	3.390155000	-1.962014000	2.785667000
1	1.804262000	-3.066127000	4.343816000
1	-0.652212000	-2.649510000	4.066503000
1	-1.410407000	-1.146177000	2.241371000
1	-3.220301000	-2.482505000	-2.416759000
1	-1.556120000	-3.887950000	-3.604612000
1	0.884223000	-3.461273000	-3.218667000
1	1.546108000	-1.637430000	-1.670857000
1	-4.530503000	-1.170743000	-1.197896000
1	-4.419862000	2.095846000	1.645785000
1	-2.980854000	3.404644000	2.777962000
1	-1.196812000	4.728793000	3.884200000
1	1.198317000	4.223904000	3.341187000
1	1.698966000	2.415925000	1.715485000
7	-6.031864000	0.526218000	0.262580000
1	-6.442379000	1.189546000	0.906396000
7	6.000506000	0.519214000	-0.590774000
1	6.356189000	1.061315000	-1.367159000
6	-7.332019000	-1.629111000	0.286221000
1	-7.712081000	-1.376424000	1.281933000
1	-6.420759000	-2.220258000	0.441508000
6	-8.375202000	-2.466633000	-0.467173000
1	-9.278521000	-1.865620000	-0.617369000
1	-7.997676000	-2.707407000	-1.468311000
6	-8.738474000	-3.758303000	0.270089000
1	-7.863974000	-4.401252000	0.407472000
1	-9.159460000	-3.547566000	1.256662000
1	-9.482233000	-4.327348000	-0.290195000
6	-6.987791000	-0.333579000	-0.460003000
1	-6.588415000	-0.539724000	-1.455994000
1	-7.886539000	0.267701000	-0.609180000
6	7.016729000	-0.194162000	0.205137000
1	6.687716000	-0.222419000	1.246670000
1	7.913209000	0.428234000	0.183634000
6	7.332168000	-1.600075000	-0.322273000
1	7.641132000	-1.526434000	-1.370532000
6	8.436990000	-2.285119000	0.494721000
1	9.337861000	-1.662440000	0.474297000
1	8.130537000	-2.346090000	1.545936000
1	6.422660000	-2.213666000	-0.307495000
1	7.902261000	-4.347101000	0.013469000

6	8.772702000	-3.685392000	-0.025373000
1	9.561643000	-4.141833000	0.574732000
1	9.123721000	-3.651263000	-1.060070000

iv) [Fe(L4)2]3+

26	-0.026005000	-0.001418000	0.000818000
7	-0.329990000	1.996911000	-0.005661000
6	-1.651903000	2.340876000	-0.006055000
6	-2.057369000	3.669863000	-0.012534000
6	-1.093607000	4.676860000	-0.019558000
6	0.249785000	4.321613000	-0.020037000
6	0.589475000	2.972054000	-0.012914000
7	-1.914522000	-0.004374000	0.001414000
6	-2.572806000	1.186593000	-0.001031000
6	-3.950105000	1.219664000	0.000133000
6	-4.661235000	-0.001769000	0.003483000
6	-3.955451000	-1.224588000	0.005541000
6	-2.572466000	-1.190717000	0.004315000
7	-0.329752000	-2.001765000	0.003445000
6	-1.651698000	-2.346549000	0.004579000
6	-2.054722000	-3.676135000	0.004109000
6	-1.090109000	-4.682678000	0.001619000
6	0.252543000	-4.326202000	-0.000498000
6	0.590267000	-2.975774000	0.000558000
7	0.340701000	0.006150000	1.986561000
6	1.661100000	0.005949000	2.334989000
6	2.055073000	0.012674000	3.667662000
6	1.087028000	0.020681000	4.668966000
6	-0.254938000	0.021991000	4.306353000
6	-0.587437000	0.014557000	2.956732000
7	1.915836000	-0.002134000	0.004963000
6	2.578054000	0.000435000	1.181223000
6	3.964696000	-0.000755000	1.218786000
6	4.673675000	-0.004445000	0.002268000
6	3.958804000	-0.006385000	-1.213051000
6	2.578445000	-0.004985000	-1.176474000
7	0.341339000	-0.002934000	-1.982667000
6	1.661922000	-0.004672000	-2.329294000
6	2.059198000	-0.003965000	-3.661138000
6	1.092628000	-0.000526000	-4.663616000
6	-0.250287000	0.002357000	-4.303145000
6	-0.585686000	0.001040000	-2.954495000
1	-3.109185000	3.924314000	-0.012807000
1	-1.391550000	5.718489000	-0.025114000
1	1.030659000	5.071329000	-0.026340000
1	1.626517000	2.664080000	-0.013815000
1	-4.513224000	2.143108000	-0.001808000
1	-4.493469000	-2.164037000	0.007731000
1	-3.105566000	-3.934164000	0.004989000
1	-1.387029000	-5.724605000	0.000770000
1	1.034325000	-5.074999000	-0.003465000
1	1.626938000	-2.666528000	-0.001733000
1	3.105182000	0.012426000	3.928428000
1	1.378848000	0.026452000	5.712329000
1	-1.040643000	0.029208000	5.050956000
1	-1.622623000	0.016179000	2.644346000
1	4.496645000	0.001446000	2.161679000
1	4.515928000	-0.008496000	-2.140149000
1	3.110450000	-0.005355000	-3.917726000
1	1.386182000	0.000525000	-5.706518000
1	-1.034609000	0.006144000	-5.049230000

1	-1.621421000	0.004026000	-2.643979000
8	-5.975745000	0.095109000	0.004327000
1	-6.437812000	-0.756268000	0.006038000
8	5.991757000	-0.006078000	-0.095980000
1	6.450942000	-0.004014000	0.756127000

v) [Fe (L5) 2] 3+

26	0.000000000	0.041939000	-0.000007000
7	-0.234688000	1.445129000	1.414298000
6	-1.543229000	1.688802000	1.737111000
6	-1.879424000	2.634392000	2.698417000
6	-0.870284000	3.345841000	3.342822000
6	0.456559000	3.092727000	3.008083000
6	0.732936000	2.136386000	2.040471000
7	-1.912339000	0.038039000	0.109836000
6	-2.518452000	0.874880000	0.983905000
6	-3.893149000	0.900150000	1.092088000
6	-4.664927000	0.037772000	0.274525000
6	-4.004631000	-0.824518000	-0.629563000
6	-2.616954000	-0.792384000	-0.680637000
7	-0.399480000	-1.358583000	-1.384105000
6	-1.737267000	-1.603671000	-1.549315000
6	-2.182347000	-2.544035000	-2.470290000
6	-1.255953000	-3.247120000	-3.237431000
6	0.100121000	-2.990762000	-3.063541000
6	0.487226000	-2.040226000	-2.127956000
7	0.399489000	-1.358359000	1.384321000
6	1.737278000	-1.603410000	1.549568000
6	2.182366000	-2.543613000	2.470704000
6	1.255978000	-3.246571000	3.237969000
6	-0.100098000	-2.990251000	3.064040000
6	-0.487211000	-2.039879000	2.128292000
7	1.912339000	0.038039000	-0.109843000
6	2.616958000	-0.792265000	0.680750000
6	4.004634000	-0.824418000	0.629660000
6	4.664924000	0.037721000	-0.274577000
6	3.893141000	0.899977000	-1.092263000
6	2.518445000	0.874736000	-0.984055000
7	0.234679000	1.444918000	-1.414517000
6	1.543217000	1.688546000	-1.737373000
6	1.879406000	2.634003000	-2.698813000
6	0.870262000	3.345363000	-3.343310000
6	-0.456579000	3.092296000	-3.008526000
6	-0.732949000	2.136089000	-2.040780000
1	-2.917206000	2.817477000	2.944211000
1	-1.118855000	4.086277000	4.093828000
1	1.269466000	3.625015000	3.485040000
1	1.751882000	1.913859000	1.754356000
1	-4.414967000	1.554153000	1.777590000
1	-4.567154000	-1.491644000	-1.265637000
1	-3.240896000	-2.730612000	-2.593536000
1	-1.590891000	-3.982496000	-3.959276000
1	0.851515000	-3.514459000	-3.640422000
1	1.532340000	-1.813954000	-1.966078000
1	3.240917000	-2.730160000	2.593981000
1	1.590924000	-3.981819000	3.959941000
1	-0.851486000	-3.513853000	3.641013000
1	-1.532327000	-1.813642000	1.966377000
1	4.567162000	-1.491446000	1.265833000
1	4.414953000	1.553867000	-1.777877000
1	2.917186000	2.817055000	-2.944639000

1	1.118828000	4.085695000	-4.094419000
1	-1.269489000	3.624519000	-3.485550000
1	-1.751893000	1.913600000	-1.754630000
8	5.966036000	0.120401000	-0.435629000
6	6.882776000	-0.700556000	0.334249000
1	6.782379000	-0.479694000	1.398482000
1	6.707538000	-1.757414000	0.124938000
1	7.870961000	-0.413374000	-0.011816000
8	-5.966040000	0.120476000	0.435558000
6	-6.882773000	-0.700639000	-0.334161000
1	-6.782374000	-0.479982000	-1.398436000
1	-6.707528000	-1.757455000	-0.124646000
1	-7.870960000	-0.413397000	0.011846000

vi) [Fe(L6)2]3+

26	0.000000000	0.000024000	0.001349000
7	-0.317963000	1.399617000	-1.400639000
6	-1.643791000	1.642978000	-1.644422000
6	-2.032801000	2.582568000	-2.592571000
6	-1.062559000	3.284372000	-3.302513000
6	0.281788000	3.030452000	-3.046733000
6	0.612690000	2.081810000	-2.089500000
7	-1.911315000	-0.000239000	0.001240000
6	-2.571810000	0.835818000	-0.826692000
6	-3.956178000	0.856202000	-0.849817000
6	-4.699810000	-0.000948000	0.000913000
6	-3.955922000	-0.857261000	0.852283000
6	-2.571619000	-0.836460000	0.829271000
7	-0.317642000	-1.399521000	1.403346000
6	-1.643410000	-1.643189000	1.647168000
6	-2.032174000	-2.582755000	2.595453000
6	-1.061753000	-3.284200000	3.305489000
6	0.282536000	-3.029983000	3.049651000
6	0.613194000	-2.081393000	2.092294000
7	0.317682000	1.399591000	1.403321000
6	1.643458000	1.643238000	1.647123000
6	2.032250000	2.582817000	2.595383000
6	1.061849000	3.284299000	3.305412000
6	-0.282447000	3.030105000	3.049592000
6	-0.613134000	2.081499000	2.092260000
7	1.911315000	0.000289000	0.001184000
6	2.571643000	0.836481000	0.829226000
6	3.955946000	0.857234000	0.852246000
6	4.699810000	0.000899000	0.000876000
6	3.956154000	-0.856224000	-0.849859000
6	2.571786000	-0.835792000	-0.826743000
7	0.317922000	-1.399550000	-1.400661000
6	1.643743000	-1.642922000	-1.644474000
6	2.032725000	-2.582490000	-2.592656000
6	1.062462000	-3.284258000	-3.302605000
6	-0.281877000	-3.030326000	-3.046797000
6	-0.612751000	-2.081709000	-2.089529000
1	-3.082607000	2.766409000	-2.778292000
1	-1.353738000	4.018338000	-4.044379000
1	1.065818000	3.555055000	-3.577246000
1	1.645924000	1.856110000	-1.862997000
1	-4.476844000	1.505209000	-1.539288000
1	-4.476443000	-1.506071000	1.542057000
1	-3.081931000	-2.766853000	2.781206000
1	-1.352745000	-4.018124000	4.047470000
1	1.066698000	-3.554310000	3.580239000

1	1.646370000	-1.855446000	1.865772000
1	3.082012000	2.766901000	2.781121000
1	1.352864000	4.018234000	4.047373000
1	-1.066593000	3.554462000	3.580174000
1	-1.646316000	1.855564000	1.865755000
1	4.476486000	1.506021000	1.542028000
1	4.476801000	-1.505251000	-1.539326000
1	3.082526000	-2.766338000	-2.778402000
1	1.353619000	-4.018206000	-4.044498000
1	-1.065923000	-3.554901000	-3.577313000
1	-1.645978000	-1.856005000	-1.863002000
6	-6.158330000	-0.001707000	0.000282000
6	-6.885752000	-1.145195000	0.388354000
6	-6.888187000	1.142187000	-0.390451000
6	-8.270382000	-1.145449000	0.375508000
6	-8.270238000	1.139185000	-0.381143000
6	-8.995267000	-0.005266000	-0.003475000
1	-6.371514000	-2.060966000	0.655896000
1	-6.374364000	2.058638000	-0.656465000
1	-8.804794000	-2.045377000	0.656160000
1	-8.806354000	2.038336000	-0.662962000
6	6.158330000	0.001609000	0.000253000
6	6.885787000	1.145075000	0.388328000
6	6.888152000	-1.142308000	-0.390475000
6	8.270417000	1.145284000	0.375490000
6	8.270203000	-1.139351000	-0.381158000
6	8.995267000	0.005077000	-0.003487000
1	6.371577000	2.060862000	0.655866000
1	6.374301000	-2.058743000	-0.656490000
1	8.804857000	2.045195000	0.656144000
1	8.806292000	-2.038520000	-0.662974000
6	-10.495796000	0.003772000	-0.009616000
1	-10.909991000	-0.950562000	0.314323000
1	-10.880049000	0.786850000	0.650996000
1	-10.876617000	0.220117000	-1.012483000
6	10.495796000	-0.004010000	-0.009621000
1	10.910021000	0.950309000	0.314326000
1	10.880021000	-0.787105000	0.650988000
1	10.876615000	-0.220361000	-1.012487000

vii) [Fe(L7)2]3+

26	0.000001000	0.034496000	0.000013000
7	-0.242874000	1.435615000	1.416176000
6	-1.554842000	1.679726000	1.726927000
6	-1.898465000	2.622804000	2.688143000
6	-0.894407000	3.330351000	3.345255000
6	0.435060000	3.075935000	3.023266000
6	0.719375000	2.122405000	2.054691000
7	-1.911455000	0.035151000	0.096931000
6	-2.522025000	0.867268000	0.962377000
6	-3.906881000	0.886563000	1.052831000
6	-4.683066000	0.033677000	0.237644000
6	-3.995655000	-0.820892000	-0.653898000
6	-2.610509000	-0.798267000	-0.702181000
7	-0.387373000	-1.366174000	-1.383512000
6	-1.723842000	-1.610182000	-1.560761000
6	-2.160792000	-2.552883000	-2.483852000
6	-1.227731000	-3.259235000	-3.239096000
6	0.127356000	-3.004576000	-3.052092000
6	0.506458000	-2.051946000	-2.116125000
7	0.387328000	-1.367095000	1.382608000

6	1.723790000	-1.611236000	1.559728000
6	2.160708000	-2.554554000	2.482204000
6	1.227621000	-3.261401000	3.236951000
6	-0.127459000	-3.006608000	3.050078000
6	-0.506528000	-2.053349000	2.114739000
7	1.911456000	0.035147000	-0.096912000
6	2.610485000	-0.798771000	0.701698000
6	3.995633000	-0.821361000	0.653450000
6	4.683072000	0.033775000	-0.237527000
6	3.906912000	0.887174000	-1.052202000
6	2.522053000	0.867817000	-0.961808000
7	0.242918000	1.436498000	-1.415278000
6	1.554894000	1.680762000	-1.725873000
6	1.898547000	2.624404000	-2.686525000
6	0.894510000	3.332369000	-3.343219000
6	-0.434965000	3.077796000	-3.021390000
6	-0.719309000	2.123696000	-2.053385000
1	-2.937868000	2.807448000	2.925354000
1	-1.149152000	4.068374000	4.096572000
1	1.244287000	3.604317000	3.510734000
1	1.741082000	1.898991000	1.779084000
1	-4.404954000	1.552261000	1.745616000
1	-4.549013000	-1.490905000	-1.296802000
1	-3.218389000	-2.738276000	-2.616627000
1	-1.556318000	-3.996547000	-3.961896000
1	0.883796000	-3.531815000	-3.619050000
1	1.550383000	-1.827590000	-1.944268000
1	3.218300000	-2.740046000	2.614880000
1	1.556182000	-3.999198000	3.959269000
1	-0.883918000	-3.534221000	3.616663000
1	-1.550446000	-1.828867000	1.943007000
1	4.548972000	-1.491775000	1.295952000
1	4.405007000	1.553315000	-1.744545000
1	2.937956000	2.809159000	-2.923623000
1	1.149279000	4.070832000	-4.094096000
1	-1.244175000	3.606492000	-3.508545000
1	-1.741023000	1.900147000	-1.777912000
6	6.137877000	0.077954000	-0.356076000
1	6.522088000	0.784201000	-1.085140000
6	7.010849000	-0.660303000	0.341608000
1	6.720897000	-1.389721000	1.089688000
1	8.076005000	-0.551036000	0.177825000
6	-6.137867000	0.077774000	0.356273000
1	-6.522056000	0.783553000	1.085801000
6	-7.010860000	-0.660041000	-0.341853000
1	-6.720931000	-1.388978000	-1.090410000
1	-8.076011000	-0.550884000	-0.177964000

viii) [Fe(L8)2]3+

26	-0.000112000	-0.000081000	-0.000037000
7	-0.309786000	1.403957000	1.399345000
6	-1.635671000	1.649353000	1.643211000
6	-2.029353000	2.593567000	2.583754000
6	-1.060140000	3.302746000	3.290709000
6	0.283820000	3.047686000	3.037182000
6	0.617845000	2.092392000	2.085621000
7	-1.918949000	-0.000184000	-0.001170000
6	-2.563833000	0.837458000	0.833770000
6	-3.958270000	0.857654000	0.853815000
6	-4.648916000	-0.000953000	-0.002098000
6	-3.957227000	-0.859192000	-0.857506000

6	-2.562804000	-0.838225000	-0.836490000
7	-0.308062000	-1.404022000	-1.399732000
6	-1.633617000	-1.649663000	-1.645162000
6	-2.026035000	-2.593586000	-2.586525000
6	-1.055882000	-3.302180000	-3.292759000
6	0.287738000	-3.046838000	-3.037693000
6	0.620488000	-2.091892000	-2.085337000
7	0.308217000	-1.399669000	1.404060000
6	1.633816000	-1.644548000	1.650007000
6	2.026385000	-2.585612000	2.594169000
6	1.056353000	-3.292009000	3.302761000
6	-0.287312000	-3.037390000	3.047201000
6	-0.620227000	-2.085400000	2.091959000
7	1.918902000	0.000145000	0.001203000
6	2.562873000	-0.835485000	0.838822000
6	3.957306000	-0.856398000	0.859756000
6	4.648934000	-0.000631000	0.001842000
6	3.958184000	0.855475000	-0.856460000
6	2.563738000	0.835313000	-0.836224000
7	0.309666000	1.399683000	-1.403689000
6	1.635526000	1.644713000	-1.648061000
6	2.029091000	2.586328000	-2.591257000
6	1.059806000	3.293195000	-3.300408000
6	-0.284131000	3.038482000	-3.046378000
6	-0.618056000	2.085860000	-2.092121000
1	-3.079605000	2.778607000	2.767618000
1	-1.353109000	4.041885000	4.026965000
1	1.067214000	3.576815000	3.564686000
1	1.653018000	1.870281000	1.864901000
1	-4.501412000	1.520312000	1.514380000
1	-5.732583000	-0.001256000	-0.002453000
1	-4.499535000	-1.522222000	-1.518387000
1	-3.076048000	-2.778784000	-2.771607000
1	-1.347856000	-4.041068000	-4.029661000
1	1.071843000	-3.575500000	-3.564607000
1	1.655370000	-1.869659000	-1.863384000
1	3.076426000	-2.770254000	2.779631000
1	1.348451000	-4.028645000	4.041865000
1	-1.071332000	-3.564376000	3.575916000
1	-1.655149000	-1.863853000	1.869501000
1	4.499667000	-1.517552000	1.522470000
1	5.732600000	-0.000937000	0.002091000
1	4.501236000	1.516212000	-1.519023000
1	3.079326000	2.771130000	-2.775462000
1	1.352690000	4.030306000	-4.038727000
1	-1.067587000	3.565855000	-3.575545000
1	-1.653206000	1.864124000	-1.870922000

ix) [Fe(L9)2]3+

26	0.000000000	-0.000012000	0.000516000
7	-0.329746000	-1.405568000	-1.408489000
6	-1.658460000	-1.642273000	-1.641761000
7	-2.127934000	-2.510392000	-2.512759000
6	-1.247430000	-3.218053000	-3.228998000
6	0.129203000	-3.050966000	-3.068321000
6	0.553627000	-2.120507000	-2.133231000
7	-1.920562000	-0.000701000	0.003208000
6	-2.583299000	-0.830852000	-0.825321000
6	-3.962439000	-0.868274000	-0.858963000
6	-4.678480000	-0.005765000	0.005607000
6	-3.967604000	0.858505000	0.867958000

6	-2.583381000	0.823930000	0.829636000
7	-0.332222000	1.410978000	1.408904000
6	-1.661328000	1.642079000	1.643202000
7	-2.134861000	2.512070000	2.510502000
6	-1.256524000	3.229856000	3.220147000
6	0.120288000	3.071434000	3.055586000
6	0.548144000	2.136969000	2.125536000
7	0.329683000	1.406049000	-1.407997000
6	1.658386000	1.642835000	-1.641244000
7	2.127823000	2.511239000	-2.511979000
6	1.247289000	3.219098000	-3.227984000
6	-0.129338000	3.051909000	-3.067352000
6	-0.553721000	2.121169000	-2.132525000
7	1.920564000	0.000650000	0.003101000
6	2.583263000	0.831153000	-0.825109000
6	3.962400000	0.868658000	-0.858728000
6	4.678478000	0.005825000	0.005490000
6	3.967643000	-0.858768000	0.867546000
6	2.583417000	-0.824217000	0.829262000
7	0.332286000	-1.411523000	1.408372000
6	1.661401000	-1.642652000	1.642584000
7	2.134973000	-2.512894000	2.509610000
6	1.256665000	-3.230902000	3.219069000
6	-0.120153000	-3.072443000	3.054602000
6	-0.548049000	-2.137722000	2.124828000
1	0.841970000	-3.622587000	-3.648638000
1	1.605186000	-1.936272000	-1.953975000
1	-4.490316000	-1.537190000	-1.527108000
1	-4.469244000	1.537518000	1.547793000
1	0.830950000	3.652889000	3.628675000
1	1.600404000	1.959573000	1.943323000
1	-0.842128000	3.623654000	-3.647519000
1	-1.605272000	1.936845000	-1.953315000
1	4.490255000	1.537852000	-1.526612000
1	4.469316000	-1.537979000	1.547159000
1	-0.830791000	-3.654049000	3.627570000
1	-1.600318000	-1.960279000	1.942705000
8	5.994006000	0.075035000	-0.060245000
1	6.452141000	-0.528509000	0.543207000
8	-5.994010000	-0.074919000	-0.060136000
1	-6.452130000	0.528388000	0.543565000
1	1.668450000	-3.942212000	3.927750000
1	1.656986000	3.928785000	-3.939590000
1	-1.668277000	3.940983000	3.929030000
1	-1.657157000	-3.927523000	-3.940802000

x) [Fe(L10)2]3+

26	0.000004000	0.000002000	0.000041000
7	0.333379000	1.433272000	1.387418000
6	1.655978000	1.692970000	1.613022000
6	2.058874000	2.659431000	2.526577000
6	1.094749000	3.380099000	3.229297000
6	-0.248469000	3.110110000	2.996556000
6	-0.587877000	2.130482000	2.068789000
7	1.919979000	-0.000088000	-0.000016000
6	2.573636000	0.860883000	0.813199000
6	3.961203000	0.883065000	0.836343000
6	4.659052000	-0.000139000	-0.000172000
6	3.961076000	-0.883315000	-0.836606000
6	2.573511000	-0.861081000	-0.813304000
7	0.333166000	-1.433383000	-1.387275000

6	1.655732000	-1.693144000	-1.613009000
6	2.058497000	-2.659673000	-2.526551000
6	1.094272000	-3.380353000	-3.229121000
6	-0.248910000	-3.110312000	-2.996240000
6	-0.588184000	-2.130617000	-2.068495000
7	-0.333179000	1.433363000	-1.387297000
6	-1.655746000	1.693134000	-1.613008000
6	-2.058518000	2.659661000	-2.526549000
6	-1.094299000	3.380330000	-3.229139000
6	0.248885000	3.110279000	-2.996280000
6	0.588167000	2.130584000	-2.068538000
7	-1.919979000	0.000104000	0.000017000
6	-2.573517000	0.861077000	-0.813287000
6	-3.961082000	0.883295000	-0.836596000
6	-4.659053000	0.000125000	-0.000151000
6	-3.961199000	-0.883069000	0.836368000
6	-2.573631000	-0.860870000	0.813231000
7	-0.333371000	-1.433252000	1.387431000
6	-1.655967000	-1.692943000	1.613058000
6	-2.058854000	-2.659383000	2.526639000
6	-1.094721000	-3.380035000	3.229365000
6	0.248494000	-3.110051000	2.996604000
6	0.587893000	-2.130448000	2.068808000
1	3.110285000	2.852846000	2.694617000
1	1.392035000	4.136251000	3.946080000
1	-1.030236000	3.643124000	3.522619000
1	-1.625042000	1.897713000	1.868788000
1	4.507778000	1.558773000	1.479582000
1	4.507553000	-1.559044000	-1.479906000
1	3.109883000	-2.853134000	-2.694690000
1	1.391456000	-4.136557000	-3.945893000
1	-1.030753000	-3.643337000	-3.522178000
1	-1.625321000	-1.897805000	-1.868401000
1	-3.109905000	2.853132000	-2.694670000
1	-1.391489000	4.136533000	-3.945909000
1	1.030724000	3.643294000	-3.522235000
1	1.625305000	1.897763000	-1.868462000
1	-4.507563000	1.559006000	-1.479912000
1	-4.507769000	-1.558785000	1.479602000
1	-3.110263000	-2.852792000	2.694696000
1	-1.392000000	-4.136170000	3.946170000
1	1.030267000	-3.643051000	3.522672000
1	1.625056000	-1.897687000	1.868788000
17	-6.368650000	0.000121000	-0.000273000
17	6.368648000	-0.000168000	-0.000268000

xi) [Fe(L11)2]3+

26	0.000032000	-0.035077000	0.000272000
7	-0.257266000	1.352323000	1.444844000
6	-1.573961000	1.643341000	1.684613000
6	-1.941861000	2.596724000	2.625601000
6	-0.952569000	3.270449000	3.340350000
6	0.382448000	2.968185000	3.094461000
6	0.688450000	2.003928000	2.141703000
7	-1.919424000	0.000013000	0.036146000
6	-2.529066000	0.860065000	0.878353000
6	-3.917533000	0.922027000	0.914660000
6	-4.650622000	0.083531000	0.069886000
6	-3.997297000	-0.800026000	-0.791422000
6	-2.602132000	-0.820612000	-0.786464000
7	-0.378626000	-1.461883000	-1.357927000

6	-1.710400000	-1.665340000	-1.598923000
6	-2.138814000	-2.603444000	-2.530922000
6	-1.194836000	-3.350568000	-3.232279000
6	0.156832000	-3.139882000	-2.979561000
6	0.524544000	-2.188998000	-2.035052000
7	0.378884000	-1.461630000	1.358479000
6	1.710681000	-1.665011000	1.599431000
6	2.139188000	-2.603062000	2.531438000
6	1.195277000	-3.350235000	3.232833000
6	-0.156413000	-3.139647000	2.980144000
6	-0.524223000	-2.188783000	2.035654000
7	1.919434000	0.000000000	-0.035974000
6	2.602297000	-0.820343000	0.786795000
6	3.997458000	-0.799612000	0.791634000
6	4.650603000	0.083771000	-0.069986000
6	3.917353000	0.921916000	-0.914977000
6	2.528895000	0.859835000	-0.878537000
7	0.256966000	1.351945000	-1.444901000
6	1.573657000	1.642751000	-1.685010000
6	1.941493000	2.595619000	-2.626544000
6	0.952154000	3.269061000	-3.341501000
6	-0.382843000	2.967047000	-3.095236000
6	-0.688778000	2.003311000	-2.141921000
1	-2.986738000	2.815206000	2.803944000
1	-1.224395000	4.016958000	4.077267000
1	1.181101000	3.466572000	3.628924000
1	1.717009000	1.747352000	1.928047000
1	-4.458507000	1.591490000	1.571941000
1	-4.576190000	-1.445957000	-1.437396000
1	-3.195434000	-2.753341000	-2.710716000
1	-1.512671000	-4.085176000	-3.962630000
1	0.921818000	-3.699939000	-3.502147000
1	1.567147000	-2.001183000	-1.816479000
1	3.195825000	-2.752887000	2.711195000
1	1.513178000	-4.084808000	3.963191000
1	-0.921345000	-3.699748000	3.502762000
1	-1.566845000	-2.000991000	1.817150000
1	4.576477000	-1.445286000	1.437754000
1	4.458220000	1.591230000	-1.572497000
1	2.986360000	2.813923000	-2.805158000
1	1.223935000	4.015160000	-4.078848000
1	-1.181547000	3.465239000	-3.629806000
1	-1.717334000	1.746987000	-1.927948000
6	-6.161579000	0.186631000	0.145609000
8	-6.700831000	0.952632000	0.892434000
8	-6.750457000	-0.658838000	-0.699492000
1	-7.716803000	-0.571011000	-0.628590000
6	6.161544000	0.187051000	-0.145841000
8	6.700641000	0.952887000	-0.892947000
8	6.750589000	-0.658071000	0.699487000
1	7.716918000	-0.570138000	0.628500000

xii) [Fe(L12)2]3+

26	0.000037000	0.000106000	-0.003530000
7	-0.211274000	1.460614000	-1.388769000
6	-1.517611000	1.733140000	-1.695330000
6	-1.847339000	2.690609000	-2.646621000
6	-0.832621000	3.388138000	-3.299400000
6	0.491594000	3.110086000	-2.978946000
6	0.759716000	2.141770000	-2.019274000
7	-1.917372000	0.099777000	-0.051236000

6	-2.502285000	0.943104000	-0.929291000
6	-3.891538000	0.985150000	-1.034619000
6	-4.641074000	0.142143000	-0.209914000
6	-4.017490000	-0.724306000	0.685776000
6	-2.628873000	-0.720202000	0.750960000
7	-0.429282000	-1.337988000	1.426519000
6	-1.768076000	-1.546103000	1.612912000
6	-2.234548000	-2.461124000	2.549785000
6	-1.318333000	-3.177917000	3.316226000
6	0.042043000	-2.956787000	3.125082000
6	0.447029000	-2.029082000	2.172707000
7	0.429557000	1.338235000	1.426395000
6	1.768385000	1.546074000	1.612841000
6	2.235013000	2.460983000	2.549748000
6	1.318915000	3.177953000	3.316164000
6	-0.041498000	2.957118000	3.124949000
6	-0.446640000	2.029511000	2.172538000
7	1.917374000	-0.099743000	-0.051390000
6	2.629035000	0.720066000	0.750847000
6	4.017650000	0.723932000	0.685626000
6	4.641048000	-0.142561000	-0.210151000
6	3.891341000	-0.985364000	-1.034921000
6	2.502104000	-0.943097000	-0.929551000
7	0.210969000	-1.460134000	-1.389146000
6	1.517274000	-1.732878000	-1.695676000
6	1.846867000	-2.690291000	-2.647066000
6	0.832050000	-3.387540000	-3.299997000
6	-0.492126000	-3.109259000	-2.979595000
6	-0.760109000	-2.141009000	-2.019815000
1	-2.883349000	2.897604000	-2.880153000
1	-1.076138000	4.137672000	-4.043026000
1	1.309854000	3.631795000	-3.458593000
1	1.778906000	1.902968000	-1.748011000
1	-4.375160000	1.641948000	-1.747477000
1	-4.649568000	-1.383840000	1.275828000
1	-3.298085000	-2.613324000	2.681848000
1	-1.664004000	-3.895250000	4.051060000
1	0.785588000	-3.491509000	3.702211000
1	1.496868000	-1.834710000	1.998817000
1	3.298577000	2.612964000	2.681852000
1	1.664703000	3.895202000	4.051025000
1	-0.784957000	3.491994000	3.702047000
1	-1.496512000	1.835360000	1.998595000
1	4.649860000	1.383308000	1.275712000
1	4.374836000	-1.642162000	-1.747864000
1	2.882848000	-2.897460000	-2.880571000
1	1.075466000	-4.137028000	-4.043702000
1	-1.310462000	-3.630736000	-3.459364000
1	-1.779270000	-1.902039000	-1.748590000
16	6.479127000	0.118602000	-0.349437000
8	6.734432000	1.248230000	0.601166000
6	7.005137000	-1.439470000	0.472879000
1	6.685272000	-2.300250000	-0.116300000
1	6.615522000	-1.463294000	1.489682000
1	8.094546000	-1.391687000	0.490102000
16	-6.479121000	-0.119343000	-0.349150000
8	-6.734195000	-1.248933000	0.601563000
6	-7.005362000	1.438703000	0.473062000
1	-6.685666000	2.299490000	-0.116199000
1	-8.094763000	1.390741000	0.490334000
1	-6.615712000	1.462680000	1.489849000

xiii) [Fe(L13)2]3+

26	0.000002000	-0.002076000	-0.000023000
7	0.336114000	1.436635000	-1.382749000
6	1.657731000	1.692927000	-1.600228000
6	2.030802000	2.676919000	-2.518445000
7	1.134549000	3.384191000	-3.201883000
6	-0.150473000	3.125483000	-2.984107000
6	-0.562867000	2.148769000	-2.070458000
7	1.917839000	-0.004823000	0.000066000
6	2.580443000	0.862971000	-0.808994000
6	3.958620000	0.888546000	-0.836565000
6	4.674432000	-0.002465000	-0.003250000
6	3.965829000	-0.894348000	0.831950000
6	2.581615000	-0.868082000	0.805306000
7	0.338166000	-1.438221000	1.388638000
6	1.660527000	-1.696606000	1.602192000
6	2.033341000	-2.677497000	2.522903000
7	1.138349000	-3.378838000	3.214515000
6	-0.146502000	-3.116259000	3.002512000
6	-0.559380000	-2.142933000	2.084744000
7	-0.338471000	-1.438052000	-1.388780000
6	-1.660878000	-1.696287000	-1.602212000
6	-2.033887000	-2.677047000	-2.522985000
7	-1.139035000	-3.378395000	-3.214772000
6	0.145864000	-3.115949000	-3.002897000
6	0.558936000	-2.142761000	-2.085069000
7	-1.917840000	-0.004508000	-0.000024000
6	-2.581795000	-0.867712000	-0.805176000
6	-3.966014000	-0.893875000	-0.831625000
6	-4.674433000	-0.001950000	0.003687000
6	-3.958436000	0.888990000	0.836917000
6	-2.580264000	0.863314000	0.809149000
7	-0.335812000	1.436759000	1.382650000
6	-1.657381000	1.693198000	1.600256000
6	-2.030257000	2.677299000	2.518436000
7	-1.133862000	3.384550000	3.201709000
6	0.151111000	3.125712000	2.983800000
6	0.563309000	2.148880000	2.070190000
1	3.075276000	2.901345000	-2.708882000
1	-0.880781000	3.700521000	-3.544109000
1	-1.611884000	1.946587000	-1.901151000
1	4.518164000	1.562284000	-1.472231000
1	4.500483000	-1.578288000	1.479320000
1	3.077240000	-2.906105000	2.711038000
1	-0.876121000	-3.684311000	3.570487000
1	-1.608432000	-1.936631000	1.920430000
1	-3.077827000	-2.905541000	-2.711026000
1	0.875366000	-3.684003000	-3.571020000
1	1.608025000	-1.936576000	-1.920838000
1	-4.500810000	-1.577768000	-1.478927000
1	-4.517840000	1.562758000	1.472676000
1	-3.074689000	2.901841000	2.708967000
1	0.881537000	3.700740000	3.543657000
1	1.612289000	1.946584000	1.900791000
8	-5.986096000	0.071962000	0.072859000
1	-6.457624000	-0.547887000	-0.504190000
8	5.986111000	0.071349000	-0.072238000
1	6.457512000	-0.548554000	0.504856000

xiv) [Fe(L14)2]3+

26	-0.000545000	0.089531000	-0.002921000
7	0.257972000	-1.339200000	1.383004000
6	1.568175000	-1.572423000	1.703544000
6	1.919926000	-2.522103000	2.655481000
6	0.919598000	-3.250461000	3.296395000
6	-0.409543000	-3.008805000	2.964798000
6	-0.699542000	-2.047998000	2.003091000
7	1.917802000	0.106604000	0.103115000
6	2.527217000	-0.752851000	0.944589000
6	3.920700000	-0.819999000	0.979527000
6	4.636508000	0.017476000	0.129412000
6	3.991277000	0.898868000	-0.735634000
6	2.597576000	0.923354000	-0.727621000
7	0.375108000	1.465185000	-1.427922000
6	1.709889000	1.725222000	-1.590967000
6	2.153627000	2.660433000	-2.517435000
6	1.223328000	3.347535000	-3.295806000
6	-0.130356000	3.077338000	-3.126188000
6	-0.513471000	2.129577000	-2.184855000
7	-0.369614000	1.476016000	1.414093000
6	-1.704177000	1.735664000	1.580376000
6	-2.145643000	2.675374000	2.503291000
6	-1.213378000	3.367688000	3.274776000
6	0.139958000	3.098176000	3.101767000
6	0.520738000	2.145798000	2.164104000
7	-1.918231000	0.108309000	-0.105372000
6	-2.594844000	0.929359000	0.723807000
6	-3.988426000	0.905383000	0.736216000
6	-4.636716000	0.020180000	-0.122838000
6	-3.924119000	-0.821334000	-0.971602000
6	-2.530477000	-0.754624000	-0.941286000
7	-0.262640000	-1.341583000	-1.384696000
6	-1.573721000	-1.577178000	-1.699767000
6	-1.928054000	-2.530913000	-2.646734000
6	-0.929319000	-3.260922000	-3.288216000
6	0.400759000	-3.016654000	-2.962318000
6	0.693323000	-2.051675000	-2.005508000
1	2.960512000	-2.696850000	2.896442000
1	1.177357000	-3.994732000	4.040550000
1	-1.217119000	-3.552937000	3.437986000
1	-1.723663000	-1.839961000	1.724129000
1	4.447874000	-1.541627000	1.591732000
1	4.575146000	1.488227000	-1.432127000
1	3.211602000	2.854176000	-2.637372000
1	1.554691000	4.079205000	-4.023183000
1	-0.884250000	3.587265000	-3.712230000
1	-1.557703000	1.894848000	-2.029849000
1	-3.203373000	2.868798000	2.625837000
1	-1.543056000	4.102914000	3.999329000
1	0.895355000	3.612193000	3.682270000
1	1.564688000	1.911516000	2.006607000
1	-4.570050000	1.498252000	1.431599000
1	-4.453559000	-1.545238000	-1.579148000
1	-2.969334000	-2.707418000	-2.883409000
1	-1.188978000	-4.008368000	-4.028515000
1	1.207154000	-3.561878000	-3.436267000
1	1.718230000	-1.841482000	-1.730998000
16	-6.462701000	-0.271768000	0.104637000
8	-6.703994000	0.181623000	1.467756000
6	-7.292152000	0.829422000	-1.049297000
1	-7.010788000	0.568897000	-2.068594000
1	-7.058416000	1.863262000	-0.799188000

1	-8.357621000	0.641203000	-0.897427000
16	6.463040000	-0.276235000	-0.090819000
8	6.709111000	0.170959000	-1.455125000
6	7.289142000	0.829826000	1.060881000
1	7.004292000	0.574038000	2.080410000
1	8.355028000	0.640490000	0.913409000
1	7.056677000	1.862616000	0.805314000
8	6.634203000	-1.653616000	0.350681000
8	-6.635766000	-1.651076000	-0.330050000

xv) [Fe (L15) 2] 3+

26	-0.003508000	0.008735000	0.004747000
7	-0.583304000	1.327536000	1.404777000
6	-1.943473000	1.462558000	1.515401000
6	-2.512270000	2.328549000	2.441502000
6	-1.682010000	3.076182000	3.275485000
6	-0.303165000	2.935645000	3.157425000
6	0.207269000	2.053103000	2.211334000
7	-1.900287000	-0.120226000	-0.208854000
6	-2.698231000	0.622392000	0.576411000
6	-4.085784000	0.503507000	0.401639000
7	-4.595453000	-0.318124000	-0.512736000
6	-3.779896000	-1.042214000	-1.278835000
6	-2.387570000	-0.957227000	-1.140505000
7	-0.056785000	-1.343514000	-1.499930000
6	-1.334061000	-1.666248000	-1.885560000
6	-1.573250000	-2.585221000	-2.898632000
6	-0.493675000	-3.194224000	-3.539236000
6	0.798093000	-2.863310000	-3.145793000
6	0.974221000	-1.935377000	-2.125048000
7	0.246528000	-1.413252000	1.415439000
6	1.560297000	-1.636409000	1.741764000
6	1.920291000	-2.602501000	2.672478000
6	0.925804000	-3.361373000	3.289306000
6	-0.404531000	-3.128172000	2.957704000
6	-0.703159000	-2.146394000	2.019395000
7	1.902742000	0.086525000	0.187315000
6	2.508172000	-0.762480000	1.034483000
6	3.905580000	-0.702488000	1.136656000
7	4.613153000	0.167454000	0.417821000
6	3.987297000	1.000165000	-0.411239000
6	2.591023000	0.976866000	-0.546335000
7	0.387142000	1.526723000	-1.259482000
6	1.722897000	1.809238000	-1.390619000
6	2.170542000	2.808596000	-2.245578000
6	1.242359000	3.540620000	-2.985235000
6	-0.111126000	3.252348000	-2.844938000
6	-0.498662000	2.241284000	-1.972478000
1	-3.588246000	2.422847000	2.515327000
1	-2.108420000	3.756294000	4.003488000
1	0.376119000	3.498226000	3.785478000
1	1.275418000	1.924377000	2.098107000
1	-4.792908000	1.070504000	0.997552000
1	-4.248853000	-1.693837000	-2.008047000
1	-2.586833000	-2.828468000	-3.190716000
1	-0.664166000	-3.913520000	-4.331719000
1	1.663487000	-3.311869000	-3.617129000
1	1.968397000	-1.660272000	-1.800166000
1	2.961743000	-2.765658000	2.918807000
1	1.190022000	-4.119202000	4.017548000
1	-1.206860000	-3.693181000	3.415234000

1	-1.729297000	-1.944462000	1.743563000
1	4.463769000	-1.354390000	1.799899000
1	4.609049000	1.691622000	-0.969682000
1	3.228587000	3.018788000	-2.336891000
1	1.574577000	4.323435000	-3.656988000
1	-0.863971000	3.798657000	-3.399104000
1	-1.544454000	1.996637000	-1.844137000

xvi) [Fe (L16) 2] 3+

26	0.001033000	-0.011303000	0.000368000
7	-0.154766000	1.360003000	1.471954000
6	-1.448253000	1.643518000	1.826549000
6	-1.708592000	2.592056000	2.801861000
6	-0.610945000	3.225953000	3.394228000
6	0.824934000	2.029527000	2.106357000
7	-1.918000000	0.007457000	0.206133000
6	-2.465034000	0.856162000	1.100392000
6	-3.848685000	0.906922000	1.258466000
6	-4.056071000	-0.807821000	-0.439751000
6	-2.666268000	-0.816509000	-0.555359000
7	-0.493592000	-1.440969000	-1.314888000
6	-1.840284000	-1.654683000	-1.443266000
6	-2.311915000	-2.599755000	-2.340680000
6	-1.364182000	-3.307316000	-3.086666000
6	0.330713000	-2.178813000	-2.080438000
7	0.524301000	-1.435427000	1.309606000
6	1.874659000	-1.629727000	1.429281000
6	2.365569000	-2.572267000	2.319038000
6	1.432731000	-3.297323000	3.067019000
6	-0.284474000	-2.188813000	2.076323000
7	1.917460000	0.043237000	-0.210226000
6	2.682842000	-0.773258000	0.542434000
6	4.071726000	-0.740521000	0.420399000
6	3.827355000	0.982619000	-1.264854000
6	2.445626000	0.907753000	-1.100828000
7	0.124979000	1.379796000	-1.456605000
6	1.412560000	1.684749000	-1.815814000
6	1.653982000	2.644877000	-2.784447000
6	0.544140000	3.268431000	-3.365327000
6	-0.867274000	2.041048000	-2.079762000
1	-2.717104000	2.840161000	3.105824000
1	-0.744617000	3.975692000	4.168045000
1	1.845545000	1.803033000	1.822203000
1	-4.307426000	1.579034000	1.972070000
1	-4.672814000	-1.462639000	-1.041702000
1	-3.369262000	-2.793152000	-2.466472000
1	-1.664115000	-4.063164000	-3.805936000
1	3.426396000	-2.750478000	2.437810000
1	1.747976000	-4.052010000	3.780935000
1	4.702334000	-1.388646000	1.015191000
1	4.271688000	1.667614000	-1.975303000
1	2.657115000	2.909982000	-3.091837000
1	0.663146000	4.026679000	-4.133239000
6	-4.642657000	0.065630000	0.476237000
6	4.638966000	0.148895000	-0.492394000
1	-5.720885000	0.089254000	0.584233000
1	5.716124000	0.191433000	-0.605281000
7	-0.053540000	-3.092576000	-2.951402000
7	0.644910000	2.941082000	3.043582000
7	0.118349000	-3.101120000	2.940539000
7	-0.705546000	2.963138000	-3.010223000

1	-1.352090000	-2.031169000	1.977432000
1	1.395265000	-2.005859000	-1.974700000
1	-1.883016000	1.797770000	-1.792138000
xvii) [Fe (L17) 2] 3+			
26	-0.000505000	-0.016832000	0.000092000
7	-0.523046000	-1.449973000	1.310123000
6	-1.871127000	-1.640166000	1.414097000
6	-2.366525000	-2.594134000	2.307709000
6	-0.254490000	-3.141162000	2.958676000
6	0.281011000	-2.197184000	2.075118000
7	-1.913166000	0.031839000	-0.220710000
6	-2.678400000	-0.790206000	0.529153000
6	-4.067188000	-0.760791000	0.400187000
6	-3.819733000	0.967548000	-1.283419000
6	-2.438224000	0.898226000	-1.113873000
7	-0.118743000	1.380625000	-1.468778000
6	-1.405790000	1.674272000	-1.820753000
6	-1.649195000	2.643940000	-2.796381000
6	0.583713000	3.004248000	-3.058841000
6	0.868922000	2.039869000	-2.085249000
7	0.511209000	-1.453723000	-1.310506000
6	1.857900000	-1.651717000	-1.417444000
6	2.345770000	-2.607969000	-2.312788000
6	0.229172000	-3.142385000	-2.959422000
6	-0.298893000	-2.195917000	-2.074140000
7	1.913384000	0.018203000	0.219111000
6	2.672023000	-0.807687000	-0.533111000
6	4.061212000	-0.787468000	-0.406579000
6	3.828046000	0.939817000	1.279900000
6	2.445771000	0.879621000	1.112652000
7	0.130274000	1.374924000	1.472986000
6	1.419579000	1.660618000	1.822879000
6	1.670357000	2.626940000	2.800040000
6	-0.560017000	2.998809000	3.067991000
6	-0.852583000	2.038138000	2.092997000
1	-3.432912000	-2.766656000	2.411976000
1	0.396818000	-3.745812000	3.581556000
1	1.349384000	-2.047921000	1.993402000
1	-4.699826000	-1.411487000	0.989954000
1	-4.264558000	1.650642000	-1.995345000
1	-2.660313000	2.900317000	-3.095406000
1	1.385044000	3.537940000	-3.559617000
1	1.888642000	1.807644000	-1.809353000
1	3.410907000	-2.786591000	-2.419492000
1	-0.426977000	-3.742925000	-3.581192000
1	-1.366187000	-2.040494000	-1.990048000
1	4.688498000	-1.441580000	-0.998279000
1	4.278413000	1.618844000	1.992240000
1	2.683521000	2.877096000	3.097420000
1	-1.357335000	3.535779000	3.571657000
1	-1.874127000	1.812104000	1.818705000
6	-4.630652000	0.129039000	-0.514545000
6	4.632177000	0.097371000	0.508335000
1	5.709443000	0.129293000	0.624788000
1	-5.707483000	0.168172000	-0.632859000
7	-1.565263000	-3.333156000	3.069716000
7	-0.664338000	3.299661000	-3.405873000
7	1.538588000	-3.341808000	-3.073519000
7	0.690411000	3.286728000	3.412930000

xviii) [Fe (L18) 2] 3+

26	-0.001209000	-0.021165000	-0.000576000
7	-0.077852000	1.358742000	1.463216000
6	-1.336885000	1.677423000	1.854715000
7	-1.612776000	2.581786000	2.786799000
6	-0.573239000	3.180387000	3.349092000
7	0.970259000	1.941036000	2.021157000
7	-1.908017000	0.053167000	0.275872000
6	-2.402158000	0.923183000	1.168073000
6	-3.773787000	1.031462000	1.376396000
6	-4.092077000	-0.694699000	-0.298528000
6	-2.707009000	-0.742560000	-0.446842000
7	-0.591510000	-1.437968000	-1.265396000
6	-1.933520000	-1.614382000	-1.344017000
7	-2.514760000	-2.498446000	-2.145896000
6	-1.704527000	-3.235080000	-2.891267000
7	0.230920000	-2.170994000	-1.993299000
7	0.563537000	-1.445287000	1.269009000
6	1.902548000	-1.639695000	1.355421000
7	2.467184000	-2.529085000	2.163350000
6	1.642883000	-3.252585000	2.906032000
7	1.908694000	0.020941000	-0.271887000
6	2.692584000	-0.782522000	0.458700000
6	4.078930000	-0.755795000	0.317054000
6	3.794510000	0.965637000	-1.368240000
6	2.420261000	0.878504000	-1.166102000
7	0.104546000	1.343123000	-1.476028000
6	1.369582000	1.642861000	-1.862999000
6	0.632653000	3.144273000	-3.372286000
1	-0.770118000	3.927199000	4.112677000
1	-4.158621000	1.735777000	2.103663000
1	-4.724177000	-1.346913000	-0.888516000
1	-2.152865000	-3.964251000	-3.559588000
1	2.077513000	-3.985446000	3.579367000
1	4.698286000	-1.414506000	0.913316000
1	4.192951000	1.660055000	-2.097697000
1	0.842943000	3.883491000	-4.139676000
6	-4.620887000	0.208072000	0.626138000
6	4.625755000	0.134307000	-0.609458000
6	-0.305317000	-3.069760000	-2.808274000
6	0.742655000	2.848139000	2.960636000
6	0.246351000	-3.069399000	2.813877000
7	-0.933329000	1.933276000	-2.044502000
6	-0.689419000	2.830574000	-2.989327000
7	1.661648000	2.537078000	-2.799953000
1	-1.553974000	3.301630000	-3.442358000
7	-0.273028000	-2.165853000	1.993504000
1	-0.457188000	-3.649076000	3.400039000
1	0.387025000	-3.659845000	-3.397369000
1	1.615404000	3.312322000	3.404977000
1	5.700058000	0.179422000	-0.744829000
1	-5.693724000	0.269765000	0.766585000

xix) [Fe (L19) 2] 3+

26	0.000635000	-0.015580000	0.000302000
7	0.541415000	-1.447755000	1.314300000
6	1.894339000	-1.629691000	1.407836000
6	2.407120000	-2.576441000	2.298991000
6	0.304693000	-3.137135000	2.971605000
6	-0.248158000	-2.198800000	2.089564000

7	1.907645000	0.035915000	-0.230366000
6	2.680127000	-0.776858000	0.512612000
6	4.072227000	-0.708019000	0.336265000
6	3.824578000	0.927840000	-1.268779000
6	2.429315000	0.894216000	-1.125828000
7	0.115351000	1.384136000	-1.474469000
6	1.404692000	1.672543000	-1.833629000
6	1.651910000	2.637354000	-2.812651000
6	-0.580618000	3.009204000	-3.068413000
6	-0.869330000	2.047730000	-2.090126000
7	-0.135312000	1.375886000	1.480341000
6	-1.428467000	1.650638000	1.835801000
6	-1.688456000	2.610613000	2.816434000
6	0.539533000	3.003343000	3.080704000
6	0.840981000	2.047257000	2.101144000
7	-1.907990000	0.012421000	0.227811000
6	-2.442247000	0.862933000	1.123206000
6	-3.838275000	0.880506000	1.262188000
6	-4.062401000	-0.755306000	-0.346060000
6	-2.669138000	-0.807969000	-0.518421000
7	-0.520807000	-1.455648000	-1.313646000
6	-1.871373000	-1.651362000	-1.412045000
6	-2.371243000	-2.602944000	-2.305447000
6	-0.260756000	-3.142090000	-2.970483000
6	0.279281000	-2.198613000	-2.086158000
1	3.476303000	-2.740169000	2.393066000
1	-0.336690000	-3.744904000	3.602149000
1	-1.319083000	-2.061202000	2.020073000
1	4.757415000	-1.333296000	0.899563000
1	4.317625000	1.591787000	-1.971314000
1	2.664160000	2.886659000	-3.115520000
1	-1.381310000	3.545954000	-3.567498000
1	-1.890999000	1.824276000	-1.813656000
1	-2.704163000	2.849241000	3.116329000
1	1.333206000	3.546503000	3.584048000
1	1.865673000	1.834341000	1.827563000
1	-4.340723000	1.537491000	1.964621000
1	-4.738664000	-1.387697000	-0.912193000
1	-3.438363000	-2.777415000	-2.403477000
1	0.389008000	-3.743227000	-3.598797000
1	1.348463000	-2.050160000	-2.012692000
7	1.617135000	-3.318767000	3.070542000
7	0.667153000	3.296240000	-3.420403000
7	-0.712276000	3.277457000	3.429051000
7	-1.570982000	-3.336843000	-3.074367000
7	4.610542000	0.135393000	-0.540600000
7	-4.613071000	0.080594000	0.530379000

xx) [Fe(L20)2]3+

26	0.000000000	0.000000000	0.010668000
7	1.394883000	0.314818000	-1.385242000
6	1.643801000	1.635589000	-1.634014000
6	2.584620000	2.030103000	-2.575864000
6	3.317769000	1.086725000	-3.310360000
6	3.036462000	-0.261280000	-3.029248000
6	2.089980000	-0.602665000	-2.081726000
7	-0.000756000	1.913863000	0.011589000
6	0.832821000	2.566543000	-0.822123000
6	0.850358000	3.954658000	-0.839373000
6	0.000000000	4.689324000	0.011377000
6	-0.848102000	3.959833000	0.859684000

6	-0.830546000	2.566584000	0.841782000
7	-1.396558000	0.313578000	1.406351000
6	-1.644385000	1.639461000	1.654935000
6	-2.583044000	2.031731000	2.593174000
6	-3.321223000	1.086588000	3.329948000
6	-3.042959000	-0.257348000	3.050691000
6	-2.092121000	-0.598782000	2.100371000
7	1.396558000	-0.313578000	1.406351000
6	1.644385000	-1.639461000	1.654935000
6	2.583044000	-2.031731000	2.593174000
6	3.321223000	-1.086588000	3.329948000
6	3.042959000	0.257348000	3.050691000
6	2.092121000	0.598782000	2.100371000
7	0.000756000	-1.913863000	0.011589000
6	0.830546000	-2.566584000	0.841782000
6	0.848102000	-3.959833000	0.859684000
6	0.000000000	-4.689324000	0.011377000
6	-0.850358000	-3.954658000	-0.839373000
6	-0.832821000	-2.566543000	-0.822123000
7	-1.394883000	-0.314818000	-1.385242000
6	-1.643801000	-1.635589000	-1.634014000
6	-2.584620000	-2.030103000	-2.575864000
6	-3.317769000	-1.086725000	-3.310360000
6	-3.036462000	0.261280000	-3.029248000
6	-2.089980000	0.602665000	-2.081726000
1	2.749323000	3.084860000	-2.740477000
1	3.554188000	-1.056749000	-3.548052000
1	1.873734000	-1.640448000	-1.865824000
1	1.520117000	4.475008000	-1.509309000
1	-1.517298000	4.479207000	1.529123000
1	-2.747935000	3.087491000	2.758656000
1	-3.560753000	-1.052761000	3.567227000
1	-1.878455000	-1.637661000	1.885772000
1	2.747935000	-3.087491000	2.758656000
1	3.560753000	1.052761000	3.567227000
1	1.878455000	1.637661000	1.885772000
1	1.517298000	-4.479207000	1.529123000
1	-1.520117000	-4.475008000	-1.509309000
1	-2.749323000	-3.084860000	-2.740477000
1	-3.554188000	1.056749000	-3.548052000
1	-1.873734000	1.640448000	-1.865824000
6	4.363025000	1.469191000	-4.356871000
6	3.936295000	0.871854000	-5.722378000
6	5.729085000	0.872156000	-3.931461000
1	6.055203000	1.267627000	-2.966206000
1	5.704356000	-0.217906000	-3.867156000
1	6.483977000	1.138195000	-4.673838000
1	3.872414000	-0.218227000	-5.697487000
1	4.677740000	1.138066000	-6.478124000
1	2.970534000	1.266939000	-6.047457000
6	0.026154000	6.221019000	-0.014602000
6	-0.337683000	6.700128000	-1.442812000
6	1.454587000	6.699788000	0.348962000
1	1.743668000	6.371520000	1.350560000
1	2.206837000	6.346051000	-0.360115000
1	1.483532000	7.790948000	0.334840000
1	0.371149000	6.346529000	-2.195359000
1	-0.323474000	7.791292000	-1.471544000
1	-1.339391000	6.372026000	-1.731732000
6	-4.363025000	-1.469191000	-4.356871000
6	-4.509869000	-2.993681000	-4.504152000
6	-3.936295000	-0.871854000	-5.722378000

1	-3.872414000	0.218227000	-5.697487000
1	-2.970534000	-1.266939000	-6.047457000
1	-4.677740000	-1.138066000	-6.478124000
1	-3.581786000	-3.468581000	-4.835536000
1	-5.265300000	-3.210818000	-5.260584000
1	-4.842365000	-3.468815000	-3.576588000
6	-0.026154000	-6.221019000	-0.014602000
6	0.970770000	-6.837110000	0.982677000
6	0.337683000	-6.700128000	-1.442812000
1	-0.371149000	-6.346529000	-2.195359000
1	1.339391000	-6.372026000	-1.731732000
1	0.323474000	-7.791292000	-1.471544000
1	2.005218000	-6.561942000	0.757725000
1	0.911691000	-7.924763000	0.923574000
1	0.745450000	-6.561962000	2.017043000
6	-4.354207000	1.536637000	4.361982000
6	-5.430396000	2.392112000	3.645722000
6	-3.639430000	2.392447000	5.438843000
1	-2.866691000	1.819134000	5.956884000
1	-3.180083000	3.291450000	5.020538000
1	-4.369603000	2.716783000	6.182748000
1	-5.011568000	3.290963000	3.186545000
1	-6.175166000	2.716612000	4.374945000
1	-5.947478000	1.818522000	2.872547000
6	4.354207000	-1.536637000	4.361982000
6	5.430396000	-2.392112000	3.645722000
6	3.639430000	-2.392447000	5.438843000
1	2.866691000	-1.819134000	5.956884000
1	3.180083000	-3.291450000	5.020538000
1	4.369603000	-2.716783000	6.182748000
1	5.011568000	-3.290963000	3.186545000
1	6.175166000	-2.716612000	4.374945000
1	5.947478000	-1.818522000	2.872547000
6	-5.042084000	0.344113000	5.049323000
1	-5.590591000	-0.281540000	4.339833000
1	-4.332912000	-0.281689000	5.598076000
1	-5.767357000	0.716351000	5.774255000
6	-5.729085000	-0.872156000	-3.931461000
1	-5.704356000	0.217906000	-3.867156000
1	-6.483977000	-1.138195000	-4.673838000
1	-6.055203000	-1.267627000	-2.966206000
6	-1.454587000	-6.699788000	0.348962000
1	-2.206837000	-6.346051000	-0.360115000
1	-1.483532000	-7.790948000	0.334840000
1	-1.743668000	-6.371520000	1.350560000
6	5.042084000	-0.344113000	5.049323000
1	4.332912000	0.281689000	5.598076000
1	5.767357000	-0.716351000	5.774255000
1	5.590591000	0.281540000	4.339833000
6	4.509869000	2.993681000	-4.504152000
1	4.842365000	3.468815000	-3.576588000
1	5.265300000	3.210818000	-5.260584000
1	3.581786000	3.468581000	-4.835536000
6	-0.970770000	6.837110000	0.982677000
1	-0.745450000	6.561962000	2.017043000
1	-0.911691000	7.924763000	0.923574000
1	-2.005218000	6.561942000	0.757725000

xxi) [Fe(L21)2]3+

26	-0.000001000	0.000049000	0.000168000
7	0.317781000	1.399439000	1.402766000

6	1.643743000	1.642599000	1.646957000
6	2.033249000	2.581039000	2.595856000
6	1.063279000	3.282698000	3.306732000
6	-0.281009000	3.029333000	3.050625000
6	-0.612296000	2.081504000	2.092469000
7	1.912026000	-0.000087000	0.000117000
6	2.571565000	0.835966000	0.828527000
6	3.956577000	0.856550000	0.851112000
6	4.698082000	-0.000117000	-0.000124000
6	3.956412000	-0.856757000	-0.851242000
6	2.571404000	-0.836139000	-0.828419000
7	0.317505000	-1.399423000	-1.402391000
6	1.643420000	-1.642725000	-1.646708000
6	2.032739000	-2.581274000	-2.595576000
6	1.062632000	-3.282904000	-3.306290000
6	-0.281606000	-3.029404000	-3.050052000
6	-0.612705000	-2.081467000	-2.091937000
7	-0.317572000	1.399800000	-1.402104000
6	-1.643499000	1.643105000	-1.646353000
6	-2.032863000	2.581836000	-2.595022000
6	-1.062789000	3.283651000	-3.305600000
6	0.281461000	3.030151000	-3.049427000
6	0.612605000	2.082024000	-2.091516000
7	-1.912027000	0.000184000	0.000205000
6	-2.571444000	0.836333000	-0.828204000
6	-3.956453000	0.856878000	-0.851035000
6	-4.698082000	0.000056000	-0.000063000
6	-3.956538000	-0.856713000	0.851035000
6	-2.571527000	-0.836049000	0.828464000
7	-0.317716000	-1.399555000	1.402561000
6	-1.643667000	-1.642775000	1.646757000
6	-2.033127000	-2.581343000	2.595549000
6	-1.063124000	-3.283067000	3.306314000
6	0.281152000	-3.029639000	3.050204000
6	0.612393000	-2.081685000	2.092156000
1	3.083027000	2.764585000	2.782176000
1	1.354765000	4.015814000	4.049357000
1	-1.064885000	3.553695000	3.581679000
1	-1.645788000	1.856653000	1.866351000
1	4.477319000	1.505056000	1.541143000
1	4.477020000	-1.505262000	-1.541375000
1	3.082481000	-2.764932000	-2.781987000
1	1.353972000	-4.016107000	-4.048887000
1	-1.065586000	-3.553742000	-3.580975000
1	-1.646154000	-1.856506000	-1.865738000
1	-3.082614000	2.765498000	-2.781382000
1	-1.354164000	4.016998000	-4.048041000
1	1.065416000	3.554631000	-3.580246000
1	1.646065000	1.857047000	-1.865378000
1	-4.477093000	1.505463000	-1.541068000
1	-4.477252000	-1.505369000	1.540947000
1	-3.082897000	-2.764931000	2.781876000
1	-1.354574000	-4.016281000	4.048856000
1	1.065054000	-3.554048000	3.581174000
1	1.645875000	-1.856787000	1.866038000
6	6.159048000	-0.000137000	-0.000244000
6	6.884860000	-1.152655000	-0.367325000
6	6.884955000	1.152357000	0.366719000
6	8.268026000	-1.160377000	-0.359503000
6	8.268121000	1.160037000	0.358672000
6	8.962738000	-0.000181000	-0.000472000
1	6.370587000	-2.073109000	-0.616669000

1	6.370752000	2.072828000	0.616149000
1	8.816414000	-2.056150000	-0.619882000
1	8.816579000	2.055793000	0.618963000
6	-6.159047000	-0.000003000	-0.000197000
6	-6.884916000	1.152484000	-0.367257000
6	-6.884894000	-1.152546000	0.366733000
6	-8.268083000	1.160132000	-0.359447000
6	-8.268059000	-1.160300000	0.358671000
6	-8.962735000	-0.000111000	-0.000452000
1	-6.370688000	2.072972000	-0.616574000
1	-6.370641000	-2.072993000	0.616147000
1	-8.816517000	2.055882000	-0.619809000
1	-8.816471000	-2.056092000	0.618935000
17	10.687431000	-0.000207000	-0.000612000
17	-10.687429000	-0.000178000	-0.000608000

xxii) [Fe(L22)2]3+

26	-0.000078000	-0.015548000	-0.000268000
7	0.270743000	-1.389444000	-1.435598000
6	1.581054000	-1.697931000	-1.672775000
6	1.962078000	-2.648106000	-2.604846000
6	0.971927000	-3.327946000	-3.342797000
6	-0.375943000	-2.995651000	-3.094446000
6	-0.672105000	-2.040748000	-2.153449000
7	1.917582000	-0.051273000	-0.025115000
6	2.540378000	-0.919214000	-0.857026000
6	3.916185000	-0.998298000	-0.879580000
6	4.671128000	-0.162412000	-0.021789000
6	3.996166000	0.731667000	0.834098000
6	2.607520000	0.755836000	0.801568000
7	0.376988000	1.404884000	1.357177000
6	1.711458000	1.607381000	1.611922000
6	2.142903000	2.529943000	2.537434000
6	1.203414000	3.300247000	3.256886000
6	-0.160679000	3.088957000	2.986014000
6	-0.512846000	2.144166000	2.039569000
7	-0.264902000	-1.394635000	1.431316000
6	-1.574112000	-1.707562000	1.668907000
6	-1.951514000	-2.661186000	2.598913000
6	-0.958723000	-3.340025000	3.334254000
6	0.387947000	-3.003284000	3.085429000
6	0.680461000	-2.045161000	2.146564000
7	-1.917379000	-0.057995000	0.025367000
6	-2.536621000	-0.929911000	0.855808000
6	-3.912125000	-1.013515000	0.879268000
6	-4.670490000	-0.178121000	0.023973000
6	-3.999180000	0.720080000	-0.830472000
6	-2.610603000	0.748709000	-0.798998000
7	-0.382612000	1.405750000	-1.355155000
6	-1.717895000	1.604791000	-1.608258000
6	-2.152960000	2.527912000	-2.531536000
6	-1.216426000	3.302396000	-3.250340000
6	0.148536000	3.094526000	-2.981228000
6	0.504395000	2.148890000	-2.036991000
1	3.009538000	-2.860215000	-2.760709000
1	-1.157761000	-3.498347000	-3.648230000
1	-1.700907000	-1.777295000	-1.950456000
1	4.452585000	-1.675498000	-1.529736000
1	4.543151000	1.382700000	1.499477000
1	3.193518000	2.689984000	2.738429000
1	-0.937085000	3.641505000	3.495377000

1	-1.557319000	1.966480000	1.818821000
1	-2.998206000	-2.876770000	2.755164000
1	1.171734000	-3.505160000	3.637169000
1	1.708314000	-1.778270000	1.943271000
1	-4.445826000	-1.693987000	1.528228000
1	-4.548841000	1.370742000	-1.494006000
1	-3.204235000	2.685208000	-2.731251000
1	0.922831000	3.650325000	-3.490270000
1	1.549594000	1.973815000	-1.817583000
8	-5.977731000	-0.319752000	0.107099000
6	-6.873197000	0.471692000	-0.712366000
1	-6.753686000	1.533061000	-0.486423000
1	-6.697275000	0.267540000	-1.770295000
1	-7.870308000	0.144499000	-0.433748000
8	5.978910000	-0.299561000	-0.104163000
6	6.871082000	0.493018000	0.717777000
1	6.748287000	1.554484000	0.494056000
1	6.694960000	0.285983000	1.775114000
1	7.869496000	0.169712000	0.439287000
8	1.192608000	-4.251082000	-4.252659000
6	2.537026000	-4.673292000	-4.587521000
1	3.107762000	-3.834228000	-4.990160000
1	3.026667000	-5.105464000	-3.712699000
1	2.409438000	-5.433459000	-5.352239000
8	1.699838000	4.156268000	4.124103000
6	0.828442000	4.998919000	4.920398000
1	0.241358000	5.652429000	4.272724000
1	0.184797000	4.384459000	5.552347000
1	1.498067000	5.590971000	5.536711000
8	-1.716181000	4.158697000	-4.115386000
6	-0.847986000	5.005379000	-4.910887000
1	-0.262111000	5.659291000	-4.262524000
1	-0.203224000	4.393996000	-5.544682000
1	-1.519903000	5.596731000	-5.525376000
8	-1.175915000	-4.266051000	4.242006000
6	-2.518805000	-4.692929000	4.577092000
1	-3.091545000	-3.856496000	4.982351000
1	-3.008040000	-5.124331000	3.701664000
1	-2.388317000	-5.454620000	5.339802000
xxiii)	[Fe(L23)2]3+		
26	0.003208000	0.009278000	0.006136000
7	0.363962000	1.384659000	1.408861000
6	1.696937000	1.609380000	1.645434000
6	2.140456000	2.513695000	2.582635000
6	1.222208000	3.277972000	3.364831000
6	-0.154009000	3.021967000	3.092859000
6	-0.513910000	2.100836000	2.142723000
7	1.912291000	-0.023864000	-0.030092000
6	2.601559000	0.784767000	0.804153000
6	3.979653000	0.793515000	0.809538000
6	4.710609000	-0.065192000	-0.071212000
6	3.931504000	-0.901746000	-0.929940000
6	2.554455000	-0.851567000	-0.883198000
7	0.287291000	-1.364408000	-1.406671000
6	1.596996000	-1.642765000	-1.692844000
6	1.968037000	-2.563671000	-2.647341000
6	0.988984000	-3.285969000	-3.393016000
6	-0.363727000	-2.971616000	-3.068784000
6	-0.649224000	-2.037395000	-2.104828000
7	-0.341611000	1.379527000	-1.399596000
6	-1.657854000	1.725994000	-1.561283000

6	-2.067489000	2.674826000	-2.470349000
6	-1.126814000	3.354150000	-3.301893000
6	0.231703000	2.962201000	-3.114690000
6	0.557332000	2.005062000	-2.187680000
7	-1.911045000	0.090998000	0.098424000
6	-2.579541000	0.965415000	-0.682687000
6	-3.953187000	1.075002000	-0.620242000
6	-4.700032000	0.266860000	0.292499000
6	-3.944441000	-0.660366000	1.075685000
6	-2.571024000	-0.712344000	0.958996000
7	-0.327593000	-1.429540000	1.346117000
6	-1.641849000	-1.604862000	1.693988000
6	-2.042955000	-2.531407000	2.629330000
6	-1.095785000	-3.371293000	3.289050000
6	0.260251000	-3.170424000	2.895225000
6	0.577682000	-2.223741000	1.954781000
1	3.202354000	2.626720000	2.732234000
1	-0.937475000	3.552568000	3.611349000
1	-1.561497000	1.918479000	1.942954000
1	4.503947000	1.465044000	1.469626000
1	4.415058000	-1.588125000	-1.605842000
1	3.018207000	-2.719773000	-2.836778000
1	-1.187986000	-3.467228000	-3.557882000
1	-1.679560000	-1.809338000	-1.863757000
1	-3.121203000	2.886080000	-2.559862000
1	1.030434000	3.416736000	-3.680055000
1	1.592285000	1.720714000	-2.049247000
1	-4.458144000	1.771141000	-1.269472000
1	-4.442842000	-1.329314000	1.757702000
1	-3.091750000	-2.605084000	2.869167000
1	1.059879000	-3.762884000	3.312112000
1	1.609840000	-2.081495000	1.662341000
7	-6.039684000	0.379324000	0.414947000
7	6.057742000	-0.083322000	-0.089954000
6	-6.801908000	-0.466308000	1.357478000
1	-7.719294000	0.074000000	1.589934000
1	-6.248535000	-0.528617000	2.297868000
6	-6.811814000	1.336547000	-0.404744000
1	-6.263367000	2.280766000	-0.449855000
1	-7.726785000	1.552634000	0.146361000
6	6.871347000	0.708455000	0.854200000
1	7.801793000	0.158191000	1.001809000
1	6.378342000	0.721261000	1.828022000
6	6.821835000	-0.896716000	-1.056805000
1	6.300684000	-0.895379000	-2.015960000
1	7.762592000	-0.372404000	-1.231073000
6	-7.143175000	-1.861762000	0.827781000
1	-7.692347000	-2.417697000	1.591255000
1	-7.775326000	-1.806283000	-0.059538000
1	-6.249037000	-2.433893000	0.568411000
6	7.098940000	-2.321569000	-0.572972000
1	7.696927000	-2.854649000	-1.315401000
1	7.660250000	-2.318100000	0.363740000
1	6.176225000	-2.883766000	-0.409813000
6	7.174006000	2.125086000	0.361637000
1	7.807555000	2.641387000	1.086232000
1	7.708062000	2.106078000	-0.590684000
1	6.262961000	2.712637000	0.224095000
6	-7.159374000	0.835777000	-1.809260000
1	-7.715256000	1.608628000	-2.345188000
1	-6.267522000	0.592972000	-2.392111000
1	-7.787242000	-0.055412000	-1.769218000

7	1.318231000	-4.192811000	-4.330442000
6	2.717199000	-4.574185000	-4.602599000
6	3.401478000	-3.683337000	-5.641580000
6	0.298415000	-4.875096000	-5.153506000
6	-0.243603000	-6.154988000	-4.514709000
1	-0.505591000	-4.172769000	-5.379273000
1	-0.964427000	-6.626070000	-5.186496000
1	0.771325000	-5.104409000	-6.109692000
1	0.557104000	-6.874203000	-4.329184000
1	2.697829000	-5.607683000	-4.951710000
1	3.273237000	-4.589647000	-3.663136000
1	2.866624000	-3.705402000	-6.593340000
1	4.417804000	-4.039554000	-5.824148000
1	3.456927000	-2.642834000	-5.312049000
1	-0.744719000	-5.953831000	-3.565029000
7	-1.495208000	4.289037000	-4.195099000
6	-2.890603000	4.751076000	-4.325630000
6	-3.719662000	3.917612000	-5.305007000
6	-0.524703000	4.924569000	-5.110473000
6	0.147819000	6.164667000	-4.518966000
1	0.212570000	4.181996000	-5.419513000
1	0.824277000	6.603826000	-5.255381000
1	-1.076114000	5.191475000	-6.013331000
1	-0.589349000	6.924347000	-4.250190000
1	-2.846555000	5.788139000	-4.661737000
1	-3.351950000	4.779618000	-3.336670000
1	-3.278688000	3.928246000	-6.303900000
1	-4.727387000	4.331667000	-5.383303000
1	-3.800800000	2.875810000	-4.985191000
7	-1.456361000	-4.282933000	4.209050000
6	-0.461401000	-5.093234000	4.941992000
6	-0.084837000	-6.390466000	4.224091000
6	-2.867779000	-4.543596000	4.552264000
6	-3.402584000	-3.636240000	5.662148000
1	-3.475722000	-4.468654000	3.648619000
1	-4.436045000	-3.903542000	5.893646000
1	-2.926439000	-5.587884000	4.862515000
1	-2.818470000	-3.747243000	6.578043000
1	-0.898207000	-5.316819000	5.916507000
1	0.418750000	-4.480384000	5.142617000
1	-0.961103000	-7.021882000	4.062127000
1	0.624362000	-6.955920000	4.832420000
1	0.377575000	-6.197488000	3.253335000
7	1.626307000	4.168724000	4.286617000
6	0.669221000	4.896103000	5.146405000
6	0.162526000	6.199051000	4.525483000
6	3.050111000	4.489157000	4.506415000
6	3.730888000	3.571158000	5.523755000
1	3.571622000	4.477987000	3.547507000
1	4.767493000	3.883327000	5.668886000
1	3.087952000	5.523282000	4.852030000
1	3.231794000	3.618406000	6.493821000
1	1.187654000	5.103628000	6.083727000
1	-0.156406000	4.230383000	5.402386000
1	0.987337000	6.881365000	4.308958000
1	-0.510569000	6.702148000	5.223029000
1	-0.382314000	6.020362000	3.595646000
1	3.729219000	2.528694000	5.195909000
1	0.727702000	5.924222000	-3.624899000
1	-3.377389000	-2.582534000	5.373488000

xxiv) [Fe(L24)2]3+

26	-0.000001000	0.000325000	-0.000219000
7	-0.337193000	1.380201000	-1.369542000
7	-1.687427000	1.595258000	-1.582789000
6	-1.866184000	2.554500000	-2.534393000
7	-1.925973000	-0.001219000	0.001523000
6	-2.583133000	0.828238000	-0.821528000
6	-3.969401000	0.863851000	-0.856788000
6	-4.647911000	-0.003652000	0.003995000
6	-3.966264000	-0.869946000	0.863548000
6	-2.580147000	-0.831848000	0.825771000
7	-0.332197000	-1.379920000	1.369993000
7	-1.681705000	-1.597315000	1.585455000
6	-1.857248000	-2.556724000	2.537453000
7	0.335162000	1.370696000	1.379123000
7	1.685100000	1.584678000	1.595304000
6	-0.302126000	2.198128000	2.211222000
7	1.925974000	0.000716000	-0.001212000
6	2.581921000	0.824121000	0.828854000
6	3.968128000	0.860341000	0.865541000
6	4.647915000	0.000159000	-0.001572000
6	3.967541000	-0.859786000	-0.868465000
6	2.581362000	-0.823011000	-0.831400000
7	0.334226000	-1.368786000	-1.381053000
1	-2.849052000	2.870936000	-2.848116000
1	-4.510900000	1.528487000	-1.516325000
1	-5.731797000	-0.004630000	0.004988000
1	-4.505386000	-1.535543000	1.524062000
1	-2.839055000	-2.874845000	2.852800000
1	-0.382870000	-3.715992000	3.689048000
1	-1.380372000	2.228509000	2.240986000
1	4.508661000	1.520163000	1.530681000
1	5.731801000	-0.000050000	-0.001732000
1	4.507631000	-1.519847000	-1.533728000
7	1.684032000	-1.583299000	-1.597539000
6	1.860886000	-2.534772000	-2.557243000
6	-0.303571000	-2.194930000	-2.214059000
6	0.611693000	-2.943510000	-2.969613000
1	-1.381834000	-2.224709000	-2.243765000
1	0.388081000	-3.686098000	-3.718760000
1	2.843127000	-2.849318000	-2.874814000
6	0.613607000	2.947530000	2.965408000
6	1.862545000	2.536993000	2.554069000
1	2.844979000	2.851354000	2.871217000
1	0.390451000	3.691452000	3.713366000
6	-0.607488000	-2.967610000	2.945994000
6	0.306732000	-2.212033000	2.196200000
1	1.385035000	-2.240921000	2.225324000
6	-0.617815000	2.967827000	-2.944620000
1	-0.395667000	3.716858000	-3.687764000
6	0.298963000	2.213529000	-2.196571000
1	1.377168000	2.244301000	-2.227415000

xxv) [Fe (L25) 2] 3+

26	-0.000001000	0.000014000	0.023075000
7	-0.346161000	1.393709000	-1.378511000
6	-1.676133000	1.612615000	-1.622473000
6	-2.080307000	2.546855000	-2.570184000
6	-1.122522000	3.266682000	-3.277906000
6	0.226340000	3.036979000	-3.021457000
6	0.573025000	2.093431000	-2.065442000

7	-1.909416000	-0.034975000	0.022729000
6	-2.589206000	0.787369000	-0.806052000
6	-3.971317000	0.779945000	-0.832761000
6	-4.706796000	-0.093842000	0.015944000
6	-3.938749000	-0.934729000	0.869380000
6	-2.557694000	-0.884366000	0.848997000
7	-0.294154000	-1.405048000	1.424797000
6	-1.615178000	-1.673212000	1.667965000
6	-1.985333000	-2.620035000	2.617035000
6	-1.001962000	-3.302016000	3.327236000
6	0.337607000	-3.022385000	3.071639000
6	0.649891000	-2.068435000	2.114039000
7	0.294171000	1.404893000	1.424978000
6	1.615198000	1.673015000	1.668174000
6	1.985366000	2.619713000	2.617363000
6	1.002003000	3.301612000	3.327656000
6	-0.337569000	3.022025000	3.072030000
6	-0.649865000	2.068200000	2.114309000
7	1.909414000	0.035003000	0.022710000
6	2.557704000	0.884269000	0.849096000
6	3.938759000	0.934611000	0.869487000
6	4.706797000	0.093832000	0.015935000
6	3.971304000	-0.779830000	-0.832888000
6	2.589194000	-0.787239000	-0.806181000
7	0.346141000	-1.393482000	-1.378712000
6	1.676109000	-1.612362000	-1.622713000
6	2.080271000	-2.546467000	-2.570563000
6	1.122477000	-3.266184000	-3.278384000
6	-0.226382000	-3.036507000	-3.021895000
6	-0.573055000	-2.093097000	-2.065739000
1	-3.133030000	2.712149000	-2.756332000
1	-1.426120000	3.996372000	-4.018948000
1	1.001087000	3.576567000	-3.550442000
1	1.609525000	1.885212000	-1.837070000
1	-4.496995000	1.419430000	-1.526768000
1	-4.440457000	-1.596541000	1.559967000
1	-3.031344000	-2.824104000	2.802666000
1	-1.278918000	-4.040936000	4.069577000
1	1.131397000	-3.531319000	3.602769000
1	1.678108000	-1.821758000	1.886448000
1	3.031380000	2.823750000	2.803016000
1	1.278969000	4.040434000	4.070091000
1	-1.131352000	3.530898000	3.603229000
1	-1.678085000	1.821560000	1.886691000
1	4.440474000	1.596319000	1.560168000
1	4.496972000	-1.419231000	-1.526981000
1	3.132991000	-2.711740000	-2.756742000
1	1.426065000	-3.995768000	-4.019535000
1	-1.001137000	-3.576012000	-3.550955000
1	-1.609552000	-1.884905000	-1.837331000
6	-6.155767000	-0.130890000	0.012360000
6	-6.866464000	-1.258571000	0.500727000
6	-6.921459000	0.953583000	-0.472976000
6	-8.237888000	-1.300341000	0.494950000
6	-8.301904000	0.935100000	-0.468928000
6	-8.985039000	-0.200683000	0.013625000
1	-6.334630000	-2.136112000	0.847347000
1	-6.433496000	1.856389000	-0.820127000
1	-8.779539000	-2.169933000	0.844488000
1	-8.848353000	1.796795000	-0.825767000
6	6.155770000	0.130856000	0.012356000
6	6.866489000	1.258525000	0.500724000

6	6.921446000	-0.953626000	-0.472984000
6	8.237913000	1.300271000	0.494949000
6	8.301892000	-0.935166000	-0.468939000
6	8.985046000	0.200602000	0.013621000
1	6.334672000	2.136075000	0.847344000
1	6.433470000	-1.856423000	-0.820142000
1	8.779579000	2.169854000	0.844488000
1	8.848326000	-1.796868000	-0.825784000
8	10.301412000	0.336829000	0.059325000
6	11.170229000	-0.713903000	-0.411549000
1	11.024671000	-1.622623000	0.176481000
1	10.998536000	-0.905134000	-1.472963000
1	12.177600000	-0.336162000	-0.262920000
8	-10.301403000	-0.336931000	0.059332000
6	-11.170238000	0.713788000	-0.411539000
1	-11.024706000	1.622504000	0.176503000
1	-10.998537000	0.905035000	-1.472949000
1	-12.177602000	0.336024000	-0.262926000

Optimized Cartesian coordinates (Å) of the DFT calculations in CH₃CN phase:

i) [Fe(L1)₂]²⁺

26	0.000001000	0.000076000	0.000240000
7	0.342647000	1.406247000	1.406848000
6	1.663999000	1.647006000	1.645041000
6	2.073523000	2.588890000	2.584974000
6	1.116978000	3.301110000	3.299052000
6	-0.228858000	3.052393000	3.053694000
6	-0.570131000	2.099773000	2.102017000
7	1.914030000	-0.000148000	0.000078000
6	2.584248000	0.828833000	0.825792000
6	3.965808000	0.859604000	0.857440000
6	4.705985000	-0.000262000	-0.000376000
6	3.965459000	-0.860059000	-0.857958000
6	2.583911000	-0.829170000	-0.825865000
7	0.342076000	-1.406257000	-1.406358000
6	1.663337000	-1.647246000	-1.644840000
6	2.072498000	-2.589289000	-2.584770000
6	1.115682000	-3.301458000	-3.298535000
6	-0.230057000	-3.052532000	-3.052864000
6	-0.570963000	-2.099751000	-2.101217000
7	-0.342233000	1.406870000	-1.405856000
6	-1.663518000	1.647797000	-1.644257000
6	-2.072781000	2.590076000	-2.583906000
6	-1.116040000	3.302569000	-3.297448000
6	0.229726000	3.053736000	-3.051831000
6	0.570734000	2.100698000	-2.100478000
7	-1.914030000	0.000243000	0.000233000
6	-2.584003000	0.829409000	-0.825491000
6	-3.965554000	0.860165000	-0.857563000
6	-4.705985000	0.000069000	-0.000200000
6	-3.965712000	-0.859958000	0.857372000
6	-2.584155000	-0.829034000	0.825723000
7	-0.342491000	-1.406495000	1.406489000
6	-1.663818000	-1.647344000	1.644735000
6	-2.073241000	-2.589413000	2.584525000

6	-1.116622000	-3.301733000	3.298402000
6	0.229188000	-3.052932000	3.052986000
6	0.570359000	-2.100125000	2.101460000
1	3.126398000	2.764752000	2.757555000
1	1.419928000	4.036778000	4.033460000
1	-1.008145000	3.582277000	3.585150000
1	-1.606943000	1.880194000	1.884512000
1	4.479431000	1.523394000	1.535403000
1	4.478805000	-1.523876000	-1.536106000
1	3.125309000	-2.765324000	-2.757573000
1	1.418350000	-4.037252000	-4.032933000
1	-1.009552000	-3.582374000	-3.584058000
1	-1.607695000	-1.880008000	-1.883492000
1	-3.125610000	2.766045000	-2.756663000
1	-1.418787000	4.038546000	-4.031631000
1	1.009163000	3.583840000	-3.582848000
1	1.607489000	1.881011000	-1.882804000
1	-4.478972000	1.524101000	-1.535540000
1	-4.479260000	-1.523998000	1.535148000
1	-3.126099000	-2.765330000	2.757160000
1	-1.419494000	-4.037540000	4.032704000
1	1.008532000	-3.582888000	3.584287000
1	1.607150000	-1.880484000	1.883911000
7	-6.054419000	-0.000009000	-0.000408000
6	-6.877548000	-0.922998000	0.800315000
1	-6.830065000	-0.652933000	1.862089000
1	-6.522623000	-1.950678000	0.693592000
1	-9.059021000	-0.944906000	0.974619000
6	-8.288475000	-0.731087000	0.233487000
1	-8.440623000	-1.400264000	-0.617739000
6	-8.288483000	0.730819000	-0.235006000
1	-8.440973000	1.399981000	0.616171000
1	-9.058819000	0.944551000	-0.976382000
6	-6.877399000	0.922885000	-0.801392000
1	-6.522617000	1.950604000	-0.694562000
1	-6.829556000	0.652823000	-1.863149000
7	6.054419000	-0.000324000	-0.000596000
6	6.877651000	0.922387000	0.800342000
1	6.830163000	0.652066000	1.862050000
1	6.522824000	1.950128000	0.693878000
1	9.059131000	0.944041000	0.974614000
6	8.288551000	0.730475000	0.233443000
1	8.440748000	1.399842000	-0.617625000
6	8.288407000	-0.731319000	-0.235401000
1	8.440839000	-1.400700000	0.615613000
1	9.058712000	-0.944951000	-0.976839000
6	6.877295000	-0.923106000	-0.801815000
1	6.522411000	-1.950815000	-0.695232000
1	6.829467000	-0.652780000	-1.863506000

ii) [Fe(L2)2]2+

26	0.000000000	-0.000012000	0.000057000
7	-0.342937000	-1.407065000	1.405881000
6	-1.664339000	-1.647933000	1.643695000
6	-2.074070000	-2.590170000	2.583096000
6	-1.117616000	-3.303104000	3.296614000
6	0.228227000	-3.054486000	3.051477000
6	0.569721000	-2.101116000	2.100615000
7	-1.913420000	0.000070000	-0.000067000
6	-2.583820000	-0.828436000	0.824919000
6	-3.965829000	-0.859911000	0.855253000

6	-4.707867000	0.000107000	-0.000336000
6	-3.965643000	0.860086000	-0.855803000
6	-2.583641000	0.828573000	-0.825202000
7	-0.342629000	1.407091000	-1.405798000
6	-1.663983000	1.648030000	-1.643816000
6	-2.073520000	2.590313000	-2.583258000
6	-1.116920000	3.303234000	-3.296591000
6	0.228872000	3.054560000	-3.051231000
6	0.570169000	2.101141000	-2.100348000
7	0.342787000	-1.407005000	-1.405868000
6	1.664167000	-1.647922000	-1.643762000
6	2.073807000	-2.590150000	-2.583215000
6	1.117286000	-3.303035000	-3.296690000
6	-0.228533000	-3.054379000	-3.051460000
6	-0.569935000	-2.101016000	-2.100557000
7	1.913420000	-0.000083000	0.000137000
6	2.583734000	-0.828508000	-0.825001000
6	3.965740000	-0.859988000	-0.855479000
6	4.707867000	-0.000062000	0.000124000
6	3.965733000	0.859872000	0.855713000
6	2.583727000	0.828373000	0.825248000
7	0.342779000	1.406928000	1.406035000
6	1.664155000	1.647795000	1.643995000
6	2.073783000	2.589969000	2.583505000
6	1.117250000	3.302837000	3.296983000
6	-0.228565000	3.054216000	3.051700000
6	-0.569955000	2.100912000	2.100735000
1	-3.126869000	-2.765848000	2.756188000
1	-1.420755000	-4.039170000	4.030527000
1	1.007400000	-3.584864000	3.582583000
1	1.606625000	-1.881520000	1.883655000
1	-4.473455000	-1.533114000	1.527237000
1	-4.473121000	1.533263000	-1.527924000
1	-3.126284000	2.766039000	-2.756513000
1	-1.419907000	4.039337000	-4.030531000
1	1.008157000	3.584929000	-3.582183000
1	1.607030000	1.881498000	-1.883226000
1	3.126590000	-2.765865000	-2.756367000
1	1.420354000	-4.039095000	-4.030638000
1	-1.007759000	-3.584721000	-3.582525000
1	-1.606819000	-1.881388000	-1.883535000
1	4.473296000	-1.533102000	-1.527605000
1	4.473281000	1.533038000	1.527793000
1	3.126563000	2.765647000	2.756710000
1	1.420309000	4.038855000	4.030979000
1	-1.007798000	3.584543000	3.582771000
1	-1.606835000	1.881315000	1.883662000
7	6.063289000	-0.000049000	0.000116000
7	-6.063289000	0.000121000	-0.000461000
6	6.802794000	0.904659000	0.878748000
1	7.867442000	0.766954000	0.710520000
1	6.558279000	1.950786000	0.670596000
1	6.593937000	0.698706000	1.933344000
6	6.802786000	-0.904735000	-0.878550000
1	6.558265000	-1.950864000	-0.670414000
1	6.593915000	-0.698760000	-1.933139000
1	7.867435000	-0.767035000	-0.710326000
6	-6.802884000	-0.904663000	0.878016000
1	-7.867514000	-0.766973000	0.709661000
1	-6.558317000	-1.950769000	0.669821000
1	-6.594164000	-0.698779000	1.932654000
6	-6.802699000	0.904923000	-0.879080000

1	-6.558130000	1.951020000	-0.670841000
1	-6.593795000	0.699031000	-1.933679000
1	-7.867361000	0.767266000	-0.710910000
iii) [Fe (L3) 2]2+			
26	0.000004000	0.491182000	0.000003000
7	-0.244990000	1.897415000	1.427843000
6	-1.546514000	2.136499000	1.757665000
6	-1.891796000	3.074099000	2.726993000
6	-0.888983000	3.785648000	3.375264000
6	0.436876000	3.540042000	3.035794000
6	0.712855000	2.590524000	2.060078000
7	-1.909943000	0.492671000	0.127514000
6	-2.520772000	1.322368000	1.000367000
6	-3.895506000	1.356193000	1.117117000
6	-4.689890000	0.505075000	0.304513000
6	-4.017665000	-0.360328000	-0.593852000
6	-2.634373000	-0.331020000	-0.653313000
7	-0.437483000	-0.916304000	-1.378334000
6	-1.772284000	-1.153803000	-1.529146000
6	-2.245262000	-2.095823000	-2.438425000
6	-1.339267000	-2.813090000	-3.211213000
6	0.020321000	-2.568602000	-3.054111000
6	0.425939000	-1.614542000	-2.129265000
7	0.437520000	-0.916159000	1.378478000
6	1.772324000	-1.153640000	1.529291000
6	2.245320000	-2.095571000	2.438653000
6	1.339340000	-2.812764000	3.211528000
6	-0.020251000	-2.568292000	3.054427000
6	-0.425887000	-1.614324000	2.129495000
7	1.909951000	0.492693000	-0.127512000
6	2.634396000	-0.330934000	0.653370000
6	4.017687000	-0.360245000	0.593886000
6	4.689895000	0.505085000	-0.304560000
6	3.895496000	1.356135000	-1.117220000
6	2.520764000	1.322320000	-1.000441000
7	0.244971000	1.897286000	-1.427969000
6	1.546492000	2.136382000	-1.757796000
6	1.891758000	3.073932000	-2.727177000
6	0.888932000	3.785412000	-3.375505000
6	-0.436924000	3.539786000	-3.036038000
6	-0.712887000	2.590322000	-2.060264000
1	-2.930851000	3.246511000	2.972362000
1	-1.140977000	4.518356000	4.131531000
1	1.250411000	4.069806000	3.513218000
1	1.732474000	2.373440000	1.770697000
1	-4.377419000	2.026864000	1.816112000
1	-4.574915000	-1.036747000	-1.223256000
1	-3.307650000	-2.267799000	-2.543116000
1	-1.691504000	-3.549224000	-3.922785000
1	0.761648000	-3.102511000	-3.633620000
1	1.475365000	-1.397978000	-1.980575000
1	3.307710000	-2.267534000	2.543342000
1	1.691590000	-3.548828000	3.923165000
1	-0.761567000	-3.102145000	3.634003000
1	-1.475316000	-1.397776000	1.980802000
1	4.574947000	-1.036616000	1.223333000
1	4.377396000	2.026747000	-1.816281000
1	2.930811000	3.246360000	-2.972543000
1	1.140915000	4.518083000	-4.131811000
1	-1.250468000	4.069494000	-3.513508000

1	-1.732503000	2.373225000	-1.770883000
7	6.038241000	0.555300000	-0.398052000
1	6.422783000	1.165694000	-1.102735000
7	-6.038237000	0.555295000	0.397980000
1	-6.422795000	1.165759000	1.102593000
6	7.221556000	-1.658674000	-0.297796000
1	7.571869000	-1.518753000	-1.326619000
1	6.270061000	-2.198426000	-0.361568000
6	8.236770000	-2.495320000	0.488417000
1	9.182475000	-1.944931000	0.557295000
1	7.880851000	-2.623540000	1.517513000
6	8.490692000	-3.869161000	-0.138373000
1	7.568533000	-4.456168000	-0.189841000
1	8.880260000	-3.772048000	-1.156343000
1	9.217933000	-4.441326000	0.443717000
6	6.987419000	-0.279054000	0.333348000
1	6.648669000	-0.382371000	1.368283000
1	7.928124000	0.274526000	0.372073000
6	-6.987403000	-0.279077000	-0.333415000
1	-6.648611000	-0.382458000	-1.368331000
1	-7.928092000	0.274524000	-0.372211000
6	-7.221607000	-1.658657000	0.297793000
1	-7.571982000	-1.518671000	1.326585000
6	-8.236790000	-2.495324000	-0.488438000
1	-9.182480000	-1.944920000	-0.557403000
1	-7.880810000	-2.623603000	-1.517506000
1	-6.270129000	-2.198427000	0.361655000
1	-7.568633000	-4.456151000	0.189958000
6	-8.490777000	-3.869128000	0.138405000
1	-9.217995000	-4.441307000	-0.443700000
1	-8.880405000	-3.771956000	1.156347000

iv) [Fe(L4)2]2+

26	0.000025000	-0.000663000	-0.000233000
7	-0.325797000	1.366031000	1.448213000
6	-1.644579000	1.602557000	1.701270000
6	-2.051304000	2.517299000	2.667608000
6	-1.090196000	3.209104000	3.396063000
6	0.253502000	2.965582000	3.136890000
6	0.590658000	2.038959000	2.157674000
7	-1.913962000	0.001832000	0.009005000
6	-2.569163000	0.810400000	0.866770000
6	-3.954219000	0.839574000	0.902272000
6	-4.663150000	0.008550000	0.024138000
6	-3.969363000	-0.825441000	-0.861970000
6	-2.580443000	-0.801739000	-0.840675000
7	-0.345842000	-1.364288000	-1.446665000
6	-1.668103000	-1.597047000	-1.686036000
6	-2.086786000	-2.509446000	-2.649460000
6	-1.134894000	-3.202258000	-3.389185000
6	0.211923000	-2.962102000	-3.144143000
6	0.561447000	-2.037841000	-2.166901000
7	0.341002000	-1.449040000	1.362283000
6	1.662559000	-1.695354000	1.592059000
6	2.078397000	-2.661074000	2.503308000
6	1.124376000	-3.395979000	3.198294000
6	-0.221698000	-3.143893000	2.961282000
6	-0.568346000	-2.164795000	2.037918000
7	1.913905000	-0.002120000	-0.007901000
6	2.577589000	-0.854397000	0.795257000
6	3.966413000	-0.881314000	0.817684000

6	4.663207000	0.002029000	-0.016723000
6	3.957121000	0.883551000	-0.846614000
6	2.571974000	0.853463000	-0.816459000
7	0.330536000	1.446058000	-1.367813000
6	1.650075000	1.692434000	-1.607112000
6	2.059698000	2.656584000	-2.522852000
6	1.100760000	3.390020000	-3.212427000
6	-0.243705000	3.137798000	-2.965890000
6	-0.583789000	2.160146000	-2.038670000
1	-3.103647000	2.687759000	2.848910000
1	-1.388534000	3.924571000	4.151789000
1	1.036038000	3.479878000	3.678572000
1	1.626926000	1.826322000	1.931846000
1	-4.501036000	1.479156000	1.580264000
1	-4.511053000	-1.468151000	-1.543242000
1	-3.140963000	-2.678309000	-2.821107000
1	-1.442935000	-3.915833000	-4.142791000
1	0.987503000	-3.477092000	-3.695090000
1	1.600494000	-1.827707000	-1.951749000
1	3.132095000	-2.838095000	2.669568000
1	1.430177000	-4.151197000	3.911125000
1	-0.998942000	-3.690707000	3.478164000
1	-1.606789000	-1.944158000	1.830562000
1	4.505821000	-1.564146000	1.460676000
1	4.506175000	1.560683000	-1.485209000
1	3.112555000	2.832380000	-2.695880000
1	1.401386000	4.144252000	-3.928514000
1	-1.024606000	3.683689000	-3.478219000
1	-1.620705000	1.939547000	-1.823696000
8	-6.004178000	0.061045000	0.084208000
1	-6.403585000	-0.541860000	-0.556182000
8	6.004535000	0.056400000	-0.070123000
1	6.401469000	-0.584837000	0.533511000

v) [Fe(L5)2]2+

26	0.000005000	0.045005000	0.000141000
7	0.247624000	1.456541000	-1.421472000
6	1.550342000	1.695936000	-1.744311000
6	1.904390000	2.635980000	-2.707212000
6	0.905996000	3.351950000	-3.357768000
6	-0.421576000	3.106984000	-3.026003000
6	-0.705431000	2.153834000	-2.055619000
7	1.909712000	0.044603000	-0.116772000
6	2.518600000	0.878856000	-0.986798000
6	3.896789000	0.906688000	-1.097437000
6	4.659872000	0.048916000	-0.285709000
6	4.012725000	-0.809751000	0.614330000
6	2.622202000	-0.781639000	0.667754000
7	0.423612000	-1.365324000	1.378596000
6	1.757147000	-1.603678000	1.537892000
6	2.226366000	-2.546315000	2.447655000
6	1.315604000	-3.264174000	3.214695000
6	-0.042512000	-3.019366000	3.049718000
6	-0.443774000	-2.064373000	2.123344000
7	-0.423847000	-1.357207000	-1.386511000
6	-1.757399000	-1.594769000	-1.546821000
6	-2.226790000	-2.532260000	-2.461781000
6	-1.316169000	-3.245672000	-3.233127000
6	0.041968000	-3.001607000	-3.067200000
6	0.443398000	-2.051846000	-2.135533000
7	-1.909694000	0.044176000	0.117073000

6	-2.622297000	-0.777721000	-0.671888000
6	-4.012796000	-0.806210000	-0.618410000
6	-4.659834000	0.047408000	0.286497000
6	-3.896637000	0.900745000	1.102787000
6	-2.518463000	0.873613000	0.991746000
7	-0.247390000	1.448321000	1.429859000
6	-1.550105000	1.686546000	1.753593000
6	-1.904036000	2.621900000	2.721100000
6	-0.905511000	3.334063000	3.375631000
6	0.422071000	3.089988000	3.043247000
6	0.705803000	2.141690000	2.068086000
1	2.945399000	2.806577000	-2.945285000
1	1.163099000	4.087326000	-4.109543000
1	-1.231759000	3.640045000	-3.505264000
1	-1.727642000	1.939356000	-1.774178000
1	4.407652000	1.564430000	-1.786123000
1	4.572731000	-1.476976000	1.250788000
1	3.287960000	-2.719293000	2.557953000
1	1.663658000	-4.001038000	3.927375000
1	-0.787331000	-3.553753000	3.624132000
1	-1.492824000	-1.849983000	1.970365000
1	-3.288412000	-2.704705000	-2.572717000
1	-1.664344000	-3.978559000	-3.949839000
1	0.786670000	-3.532626000	-3.644879000
1	1.492457000	-1.838114000	-1.981694000
1	-4.572811000	-1.469963000	-1.258480000
1	-4.407412000	1.554634000	1.795186000
1	-2.945042000	2.791877000	2.959643000
1	-1.162518000	4.065811000	4.130970000
1	1.232347000	3.620099000	3.525613000
1	1.728014000	1.927943000	1.786093000
8	-5.986929000	0.123387000	0.446106000
6	-6.841016000	-0.720781000	-0.344609000
1	-6.721325000	-0.505289000	-1.408633000
1	-6.635679000	-1.774786000	-0.144536000
1	-7.853197000	-0.478092000	-0.032706000
8	5.986990000	0.125759000	-0.444776000
6	6.840993000	-0.722960000	0.341137000
1	6.721086000	-0.513665000	1.406366000
1	6.635748000	-1.775798000	0.134928000
1	7.853217000	-0.478415000	0.030828000

vi) [Fe(L6)2]2+

26	0.000000000	-0.000192000	0.001250000
7	0.332405000	1.406205000	1.408248000
6	1.652903000	1.648501000	1.647048000
6	2.064219000	2.589083000	2.586681000
6	1.106794000	3.299799000	3.301499000
6	-0.238368000	3.050146000	3.056102000
6	-0.580652000	2.098004000	2.103704000
7	1.908842000	0.000232000	0.001397000
6	2.570144000	0.833524000	0.827647000
6	3.959453000	0.852995000	0.851522000
6	4.682970000	0.000662000	0.001704000
6	3.959842000	-0.851836000	-0.848330000
6	2.570567000	-0.832820000	-0.824777000
7	0.333164000	-1.406368000	-1.405765000
6	1.653787000	-1.648104000	-1.644382000
6	2.065631000	-2.588423000	-2.584049000
6	1.108600000	-3.299444000	-3.299087000
6	-0.236702000	-3.050355000	-3.053876000

6	-0.579517000	-2.098452000	-2.101431000
7	-0.332912000	1.405978000	-1.405836000
6	-1.653494000	1.647881000	-1.644519000
6	-2.065176000	2.588214000	-2.584242000
6	-1.108025000	3.299058000	-3.299294000
6	0.237234000	3.049773000	-3.054047000
6	0.579885000	2.097878000	-2.101535000
7	-1.908842000	-0.000495000	0.001176000
6	-2.570418000	0.832720000	-0.824955000
6	-3.959690000	0.851987000	-0.848502000
6	-4.682971000	-0.000410000	0.001503000
6	-3.959606000	-0.852907000	0.851286000
6	-2.570293000	-0.833687000	0.827406000
7	-0.332656000	-1.406686000	1.408085000
6	-1.653195000	-1.648847000	1.646788000
6	-2.064674000	-2.589495000	2.586284000
6	-1.107370000	-3.300440000	3.301037000
6	0.237836000	-3.050952000	3.055708000
6	0.580285000	-2.098722000	2.103458000
1	3.117080000	2.765145000	2.758682000
1	1.409192000	4.034963000	4.036422000
1	-1.017992000	3.578777000	3.588044000
1	-1.618212000	1.880340000	1.889013000
1	4.482743000	1.504817000	1.536445000
1	4.483574000	-1.503542000	-1.533043000
1	3.118588000	-2.764041000	-2.755909000
1	1.411407000	-4.034409000	-4.034040000
1	-1.016026000	-3.579246000	-3.586000000
1	-1.617194000	-1.881225000	-1.886864000
1	-3.118104000	2.763968000	-2.756145000
1	-1.410706000	4.034030000	-4.034293000
1	1.016650000	3.578508000	-3.586190000
1	1.617525000	1.880512000	-1.886936000
1	-4.483304000	1.503823000	-1.533181000
1	-4.483010000	-1.504649000	1.536198000
1	-3.117564000	-2.765444000	2.758217000
1	-1.409893000	-4.035661000	4.035850000
1	1.017367000	-3.579776000	3.587594000
1	1.617880000	-1.881172000	1.888824000
6	6.162491000	0.000554000	0.001166000
6	6.883387000	-1.186109000	-0.200188000
6	6.884412000	1.185924000	0.205756000
6	8.273176000	-1.183635000	-0.193790000
6	8.274322000	1.181719000	0.202167000
6	8.996173000	-0.000878000	0.001974000
1	6.357736000	-2.124921000	-0.330615000
1	6.359711000	2.124271000	0.343149000
1	8.805429000	-2.118196000	-0.335046000
1	8.807572000	2.114102000	0.353868000
6	-6.162491000	-0.000016000	0.000988000
6	-6.883158000	1.186788000	-0.200343000
6	-6.884641000	-1.185247000	0.205584000
6	-8.272948000	1.184586000	-0.193919000
6	-8.274548000	-1.180770000	0.202023000
6	-8.996173000	0.001971000	0.001852000
1	-6.357327000	2.125498000	-0.330773000
1	-6.360123000	-2.123698000	0.342960000
1	-8.805020000	2.119253000	-0.335159000
1	-8.807979000	-2.113050000	0.353728000
6	10.503593000	0.002898000	-0.026980000
1	10.910269000	-0.948919000	0.320731000
1	10.870330000	0.162192000	-1.046840000

1	10.911573000	0.801913000	0.595278000
6	-10.503595000	-0.001517000	-0.027069000
1	-10.910078000	0.950485000	0.320358000
1	-10.870384000	-0.161061000	-1.046871000
1	-10.911717000	-0.800263000	0.595444000

vii) [Fe(L7)2]2+

26	0.000018000	-0.000993000	0.033097000
7	-0.255299000	-1.422567000	1.441198000
6	-1.561054000	-1.732698000	1.682065000
6	-1.922754000	-2.692316000	2.622746000
6	-0.928985000	-3.352681000	3.336384000
6	0.401240000	-3.034474000	3.088557000
6	0.693134000	-2.066384000	2.135309000
7	-1.905198000	-0.104078000	0.033709000
6	-2.519740000	-0.965712000	0.864915000
6	-3.906888000	-1.058072000	0.887034000
6	-4.674982000	-0.246512000	0.037649000
6	-3.998602000	0.641055000	-0.817194000
6	-2.612349000	0.690063000	-0.796874000
7	-0.408248000	1.383209000	-1.376267000
6	-1.739534000	1.552878000	-1.616497000
6	-2.200478000	2.467109000	-2.558905000
6	-1.282454000	3.227770000	-3.273937000
6	0.074056000	3.052734000	-3.026466000
6	0.466716000	2.122326000	-2.072150000
7	0.410197000	-1.390059000	-1.370482000
6	1.741841000	-1.562147000	-1.606799000
6	2.203648000	-2.482843000	-2.542727000
6	1.286429000	-3.246713000	-3.255347000
6	-0.070399000	-3.068569000	-3.012206000
6	-0.463947000	-2.132451000	-2.063938000
7	1.905194000	0.103501000	0.035149000
6	2.613654000	-0.694603000	-0.790600000
6	4.000005000	-0.643442000	-0.810474000
6	4.674771000	0.249771000	0.039717000
6	3.905332000	1.065443000	0.883809000
6	2.518337000	0.971321000	0.861176000
7	0.253387000	1.425392000	1.437465000
6	1.558524000	1.741433000	1.673863000
6	1.918993000	2.709275000	2.606456000
6	0.924686000	3.370994000	3.317970000
6	-0.404849000	3.044986000	3.076794000
6	-0.695509000	2.069317000	2.130905000
1	-2.965347000	-2.920797000	2.796258000
1	-1.191862000	-4.101857000	4.072335000
1	1.207750000	-3.522165000	3.619475000
1	1.717879000	-1.795632000	1.919350000
1	-4.399968000	-1.751278000	1.554841000
1	-4.551086000	1.282599000	-1.488187000
1	-3.261127000	2.584465000	-2.733278000
1	-1.623585000	3.943711000	-4.010878000
1	0.824149000	3.622342000	-3.558540000
1	1.514283000	1.962330000	-1.855922000
1	3.264298000	-2.603049000	-2.714350000
1	1.628481000	-3.967527000	-3.987085000
1	-0.820030000	-3.640328000	-3.542630000
1	-1.511752000	-1.970083000	-1.850856000
1	4.554472000	-1.287178000	-1.477640000
1	4.397259000	1.762343000	1.548808000
1	2.961194000	2.943450000	2.774588000

1	1.186659000	4.127059000	4.047168000
1	-1.211864000	3.532657000	3.606953000
1	-1.719811000	1.792940000	1.920255000
6	6.139052000	0.365507000	0.082900000
1	6.516997000	1.106721000	0.780848000
6	7.012942000	-0.341945000	-0.638090000
1	6.716220000	-1.100577000	-1.353260000
1	8.077423000	-0.176258000	-0.527221000
6	-6.139469000	-0.360111000	0.080471000
1	-6.519197000	-1.098817000	0.780139000
6	-7.011752000	0.347258000	-0.642527000
1	-6.713225000	1.103854000	-1.359104000
1	-8.076591000	0.183710000	-0.531921000

viii) [Fe(L8)2]2+

26	0.000001000	0.000053000	0.000052000
7	-0.330062000	1.407287000	1.404175000
6	-1.650488000	1.647510000	1.644098000
6	-2.063461000	2.587842000	2.583218000
6	-1.106890000	3.301844000	3.295831000
6	0.238475000	3.055101000	3.048753000
6	0.582103000	2.102274000	2.097428000
7	-1.911048000	-0.001473000	-0.002987000
6	-2.567917000	0.831081000	0.828397000
6	-3.961098000	0.851362000	0.848107000
6	-4.651538000	-0.004265000	-0.006641000
6	-3.957071000	-0.858486000	-0.859526000
6	-2.563994000	-0.835386000	-0.836089000
7	-0.323449000	-1.407555000	-1.405468000
6	-1.642769000	-1.649934000	-1.649351000
6	-2.051438000	-2.590474000	-2.590146000
6	-1.091623000	-3.302412000	-3.300466000
6	0.252595000	-3.053389000	-3.049467000
6	0.591847000	-2.100514000	-2.096619000
7	0.325423000	-1.404487000	1.408117000
6	1.645075000	-1.646378000	1.650663000
6	2.055027000	-2.586328000	2.591489000
6	1.096178000	-3.297764000	3.303612000
6	-0.248383000	-3.048619000	3.054584000
6	-0.588940000	-2.096554000	2.101393000
7	1.911051000	0.000989000	0.002831000
6	2.565169000	-0.831674000	0.836264000
6	3.958281000	-0.853275000	0.859240000
6	4.651542000	0.000976000	0.005405000
6	3.959897000	0.855205000	-0.849766000
6	2.566748000	0.833579000	-0.829443000
7	0.328089000	1.405534000	-1.406348000
6	1.648183000	1.648279000	-1.645581000
6	2.059867000	2.589274000	-2.584603000
6	1.102326000	3.300978000	-3.298213000
6	-0.242695000	3.051151000	-3.052364000
6	-0.585013000	2.098020000	-2.100871000
1	-3.116768000	2.760489000	2.755963000
1	-1.409932000	4.037160000	4.030248000
1	1.017529000	3.586408000	3.578753000
1	1.620050000	1.887261000	1.882287000
1	-4.499202000	1.514746000	1.510416000
1	-5.733875000	-0.005370000	-0.008071000
1	-4.492023000	-1.523006000	-1.523239000
1	-3.103965000	-2.764814000	-2.765978000
1	-1.391291000	-4.037838000	-4.036153000

1	1.034108000	-3.582958000	-3.577579000
1	1.628823000	-1.883848000	-1.878444000
1	3.107788000	-2.760586000	2.765975000
1	1.396853000	-4.032821000	4.039259000
1	-1.029163000	-3.577571000	3.584397000
1	-1.626208000	-1.879793000	1.884711000
1	4.494177000	-1.516653000	1.523336000
1	5.733880000	0.000971000	0.006414000
1	4.497061000	1.518497000	-1.512928000
1	3.112941000	2.764220000	-2.756480000
1	1.404359000	4.036853000	-4.032484000
1	-1.022485000	3.580391000	-3.583347000
1	-1.622668000	1.880666000	-1.886669000

ix) [Fe(L9)2]2+

26	0.000000000	-0.000424000	-0.000509000
7	-0.341080000	-1.275239000	1.538811000
6	-1.661683000	-1.485152000	1.797480000
7	-2.145453000	-2.270408000	2.746896000
6	-1.260373000	-2.911809000	3.516629000
6	0.110447000	-2.768485000	3.337177000
6	0.533912000	-1.926332000	2.319539000
7	-1.917266000	-0.001323000	0.007586000
6	-2.580276000	-0.746173000	0.909565000
6	-3.962564000	-0.776734000	0.952116000
6	-4.672553000	-0.002512000	0.020433000
6	-3.973296000	0.771953000	-0.917537000
6	-2.587815000	0.741532000	-0.886521000
7	-0.356015000	1.273549000	-1.537683000
6	-1.679350000	1.481479000	-1.783644000
7	-2.174018000	2.264836000	-2.728971000
6	-1.297664000	2.906585000	-3.508464000
6	0.075050000	2.765094000	-3.342583000
6	0.510054000	1.924812000	-2.328122000
7	0.344051000	-1.538586000	-1.275935000
6	1.665166000	-1.791023000	-1.490251000
7	2.150796000	-2.738704000	-2.276456000
6	1.267249000	-3.513422000	-2.913967000
6	-0.103915000	-3.340746000	-2.765720000
6	-0.529374000	-2.324362000	-1.923061000
7	1.917279000	0.000466000	-0.007804000
6	2.582085000	-0.898716000	-0.754482000
6	3.964383000	-0.935491000	-0.789006000
6	4.672563000	-0.000664000	-0.016812000
6	3.971450000	0.934330000	0.759670000
6	2.586078000	0.897414000	0.733175000
7	0.353077000	1.537950000	1.272819000
6	1.675923000	1.790118000	1.476359000
7	2.168757000	2.737203000	2.258726000
6	1.290886000	3.511807000	2.904309000
6	-0.081497000	3.339176000	2.767741000
6	-0.514545000	2.323414000	1.928019000
1	0.823431000	-3.288513000	3.961168000
1	1.585168000	-1.764908000	2.120895000
1	-4.482124000	-1.380305000	1.682725000
1	-4.484564000	1.381373000	-1.651467000
1	0.781117000	3.285089000	-3.974408000
1	1.563513000	1.765147000	-2.140040000
1	-0.815693000	-3.968909000	-3.282363000
1	-1.581011000	-2.130860000	-1.757964000
1	4.485269000	-1.664272000	-1.393653000

1	4.481216000	1.670345000	1.367849000
1	-0.788755000	3.966883000	3.291097000
1	-1.567642000	2.130216000	1.772061000
8	6.010747000	-0.056731000	-0.066104000
1	6.407102000	0.621976000	0.496065000
8	-6.010960000	-0.048630000	0.081139000
1	-6.408385000	0.514580000	-0.596021000
1	1.701882000	4.285507000	3.542921000
1	1.672652000	-4.287542000	-3.555683000
1	-1.710173000	3.546108000	-4.280603000
1	-1.664244000	-3.552745000	4.292196000

x) [Fe (L10) 2]2+

26	0.000000000	0.000330000	0.000117000
7	-0.331189000	1.408163000	1.406413000
6	-1.651292000	1.649295000	1.647283000
6	-2.065337000	2.588982000	2.585840000
6	-1.108529000	3.302862000	3.298712000
6	0.236346000	3.055625000	3.051603000
6	0.580547000	2.102869000	2.100064000
7	-1.910475000	-0.000163000	-0.000656000
6	-2.566994000	0.831926000	0.830827000
6	-3.958754000	0.857776000	0.856952000
6	-4.638351000	-0.001389000	-0.001219000
6	-3.957626000	-0.859963000	-0.859083000
6	-2.565901000	-0.832885000	-0.832366000
7	-0.329347000	-1.407507000	-1.406679000
6	-1.649151000	-1.649477000	-1.648398000
6	-2.062022000	-2.589155000	-2.587478000
6	-1.104333000	-3.302103000	-3.300100000
6	0.240228000	-3.053935000	-3.052225000
6	0.583235000	-2.101277000	-2.100156000
7	0.329817000	-1.406117000	1.408180000
6	1.649696000	-1.647939000	1.649618000
6	2.062866000	-2.586929000	2.589255000
6	1.105400000	-3.299230000	3.302824000
6	-0.239241000	-3.051079000	3.055362000
6	-0.582551000	-2.099171000	2.102653000
7	1.910476000	0.000278000	0.000692000
6	2.566180000	-0.831872000	0.832754000
6	3.957914000	-0.858844000	0.859114000
6	4.638352000	-0.000789000	0.000501000
6	3.958467000	0.857751000	-0.858066000
6	2.566716000	0.831827000	-0.831552000
7	0.330719000	1.407203000	-1.407261000
6	1.650746000	1.648521000	-1.648377000
6	2.064492000	2.587797000	-2.587476000
6	1.107461000	3.301046000	-3.300679000
6	-0.237335000	3.053588000	-3.053357000
6	-0.581232000	2.101281000	-2.101261000
1	-3.118200000	2.762883000	2.759611000
1	-1.411524000	4.038126000	4.033073000
1	1.015432000	3.586638000	3.581812000
1	1.618764000	1.888554000	1.885931000
1	-4.501478000	1.518016000	1.516699000
1	-4.499466000	-1.520725000	-1.519033000
1	-3.114674000	-2.763724000	-2.761880000
1	-1.406410000	-4.037330000	-4.034876000
1	1.019990000	-3.584152000	-3.582235000
1	1.621193000	-1.886308000	-1.885427000
1	3.115571000	-2.761454000	2.763371000

1	1.407710000	-4.033925000	4.038036000
1	-1.018831000	-3.580760000	3.586161000
1	-1.620575000	-1.884231000	1.888210000
1	4.499979000	-1.519141000	1.519344000
1	4.500966000	1.517572000	-1.518417000
1	3.117302000	2.761885000	-2.761390000
1	1.410222000	4.035993000	-4.035453000
1	-1.016593000	3.584101000	-3.583814000
1	-1.619383000	1.886817000	-1.886958000
17	6.381906000	-0.001437000	0.000411000
17	-6.381905000	-0.002156000	-0.001589000

xi) [Fe(L11)2]2+

26	0.000000000	0.005651000	0.000033000
7	-0.315995000	1.413358000	1.408534000
6	-1.633736000	1.655706000	1.658508000
6	-2.040571000	2.595416000	2.600158000
6	-1.077934000	3.307790000	3.306524000
6	0.265046000	3.059004000	3.050149000
6	0.601877000	2.106265000	2.095919000
7	-1.906099000	0.005503000	0.012332000
6	-2.555625000	0.840239000	0.849334000
6	-3.945389000	0.862419000	0.879560000
6	-4.647374000	0.006986000	0.029899000
6	-3.959206000	-0.850377000	-0.829756000
6	-2.567060000	-0.827809000	-0.815499000
7	-0.334897000	-1.401788000	-1.403577000
6	-1.655904000	-1.644427000	-1.636206000
6	-2.074141000	-2.585175000	-2.571858000
6	-1.120393000	-3.297697000	-3.290075000
6	0.225662000	-3.048331000	-3.051373000
6	0.574306000	-2.094827000	-2.102170000
7	0.335019000	-1.400522000	1.404879000
6	1.656044000	-1.643092000	1.637472000
6	2.074359000	-2.583204000	2.573729000
6	1.120670000	-3.295097000	3.292649000
6	-0.225404000	-3.045724000	3.054059000
6	-0.574127000	-2.092894000	2.104207000
7	1.906098000	0.005609000	-0.012317000
6	2.567131000	-0.827085000	0.816078000
6	3.959279000	-0.849617000	0.830259000
6	4.647372000	0.007115000	-0.030083000
6	3.945314000	0.861901000	-0.880334000
6	2.555552000	0.839730000	-0.849986000
7	0.315873000	1.412214000	-1.409642000
6	1.633594000	1.654572000	-1.659711000
6	2.040354000	2.593739000	-2.601935000
6	1.077658000	3.305529000	-3.308813000
6	-0.265301000	3.056687000	-3.052387000
6	-0.602054000	2.104515000	-2.097564000
1	-3.092626000	2.768862000	2.779697000
1	-1.374927000	4.043187000	4.043248000
1	1.048487000	3.588739000	3.575179000
1	1.638446000	1.891115000	1.874910000
1	-4.492769000	1.520395000	1.539231000
1	-4.503131000	-1.511966000	-1.487080000
1	-3.128046000	-2.759951000	-2.738407000
1	-1.426720000	-4.033733000	-4.022324000
1	1.002422000	-3.578139000	-3.586169000
1	1.613518000	-1.879132000	-1.894624000
1	3.128276000	-2.757975000	2.740204000

1	1.427057000	-4.030649000	4.025358000
1	-1.002118000	-3.575025000	3.589422000
1	-1.613353000	-1.877205000	1.896732000
1	4.503260000	-1.510699000	1.488045000
1	4.492637000	1.519376000	-1.540553000
1	3.092394000	2.767229000	-2.781512000
1	1.374591000	4.040518000	-4.045967000
1	-1.048787000	3.585956000	-3.577819000
1	-1.638607000	1.889327000	-1.876516000
6	-6.144872000	0.047158000	0.078718000
8	-6.768922000	0.776434000	0.811388000
8	-6.706120000	-0.814510000	-0.779683000
1	-7.670253000	-0.740513000	-0.700165000
6	6.144866000	0.047256000	-0.079057000
8	6.768853000	0.776101000	-0.812208000
8	6.706188000	-0.813935000	0.779775000
1	7.670313000	-0.740003000	0.700114000

xii) [Fe(L12)2]2+

26	0.000001000	0.000021000	-0.098676000
7	-0.336128000	1.404678000	-1.505129000
6	-1.657065000	1.640163000	-1.746337000
6	-2.074238000	2.577454000	-2.685953000
6	-1.119938000	3.294023000	-3.399466000
6	0.225850000	3.052300000	-3.151830000
6	0.573425000	2.101923000	-2.199061000
7	-1.909968000	-0.010193000	-0.097278000
6	-2.570202000	0.820406000	-0.929734000
6	-3.963272000	0.833133000	-0.956639000
6	-4.633639000	-0.026872000	-0.092074000
6	-3.949492000	-0.890174000	0.752145000
6	-2.557721000	-0.854151000	0.730262000
7	-0.317155000	-1.411161000	1.306228000
6	-1.635228000	-1.665831000	1.542503000
6	-2.044102000	-2.612852000	2.475899000
6	-1.082923000	-3.320337000	3.189178000
6	0.260390000	-3.058615000	2.947753000
6	0.599019000	-2.099118000	2.000715000
7	0.317200000	1.410886000	1.306536000
6	1.635278000	1.665550000	1.542779000
6	2.044179000	2.612447000	2.476290000
6	1.083021000	3.319800000	3.189728000
6	-0.260299000	3.058062000	2.948355000
6	-0.598954000	2.098697000	2.001193000
7	1.909970000	0.010219000	-0.097320000
6	2.557747000	0.854005000	0.730377000
6	3.949519000	0.889986000	0.752264000
6	4.633640000	0.026826000	-0.092121000
6	3.963249000	-0.832994000	-0.956851000
6	2.570178000	-0.820240000	-0.929936000
7	0.336086000	-1.404294000	-1.505482000
6	1.657017000	-1.639813000	-1.746695000
6	2.074162000	-2.576965000	-2.686462000
6	1.119842000	-3.293335000	-3.400147000
6	-0.225940000	-3.051546000	-3.152538000
6	-0.573487000	-2.101324000	-2.199603000
1	-3.127776000	2.747366000	-2.859882000
1	-1.425706000	4.027281000	-4.134725000
1	1.003126000	3.585680000	-3.682331000
1	1.612406000	1.891908000	-1.984486000
1	-4.503575000	1.484720000	-1.630484000

1	-4.510841000	-1.563545000	1.387572000
1	-3.096696000	-2.794943000	2.643498000
1	-1.381121000	-4.061412000	3.919701000
1	1.042877000	-3.583606000	3.478992000
1	1.635911000	-1.873896000	1.791443000
1	3.096778000	2.794549000	2.643850000
1	1.381239000	4.060784000	3.920335000
1	-1.042770000	3.582944000	3.479725000
1	-1.635852000	1.873458000	1.791965000
1	4.510888000	1.563221000	1.387819000
1	4.503536000	-1.484460000	-1.630825000
1	3.127696000	-2.746923000	-2.860375000
1	1.425588000	-4.026488000	-4.135519000
1	-1.003232000	-3.584761000	-3.683180000
1	-1.612462000	-1.891262000	-1.985048000
16	6.464232000	0.134709000	-0.095833000
8	6.800857000	1.337343000	0.766612000
6	6.765415000	-1.349850000	0.933403000
1	6.378147000	-2.230181000	0.420723000
1	6.287879000	-1.208115000	1.902305000
1	7.846806000	-1.425487000	1.041892000
16	-6.464226000	-0.134827000	-0.095818000
8	-6.800805000	-1.337558000	0.766507000
6	-6.765484000	1.349618000	0.933559000
1	-6.378245000	2.230010000	0.420962000
1	-7.846882000	1.425201000	1.042034000
1	-6.287959000	1.207820000	1.902457000

xiii) [Fe(L13)2]2+

26	0.001842000	0.000802000	-0.000694000
7	-0.336628000	1.984420000	-0.024308000
6	-1.656192000	2.318814000	-0.028009000
6	-2.039540000	3.658993000	-0.043270000
7	-1.154566000	4.655641000	-0.054919000
6	0.134114000	4.314157000	-0.051850000
6	0.550163000	2.984492000	-0.036583000
7	-1.917167000	-0.000800000	-0.002437000
6	-2.580543000	1.172534000	-0.015006000
6	-3.964713000	1.212754000	-0.014881000
6	-4.667889000	-0.001565000	-0.001132000
6	-3.965444000	-1.215136000	0.011073000
6	-2.578109000	-1.172329000	0.010294000
7	-0.334239000	-1.982773000	0.021741000
6	-1.653598000	-2.318511000	0.023630000
6	-2.035453000	-3.659094000	0.037488000
7	-1.149547000	-4.654930000	0.049359000
6	0.138723000	-4.312156000	0.048046000
6	0.553389000	-2.981980000	0.034247000
7	0.330396000	0.025135000	1.983287000
6	1.649058000	0.029099000	2.321092000
6	2.029574000	0.045805000	3.662181000
7	1.141927000	0.058676000	4.656386000
6	-0.145980000	0.055425000	4.311603000
6	-0.558978000	0.038663000	2.980884000
7	1.918504000	0.000486000	0.002150000
6	2.574979000	0.014498000	1.177642000
6	3.964791000	0.015539000	1.216243000
6	4.663225000	0.000367000	0.006286000
6	3.968438000	-0.010758000	-1.205854000
6	2.578513000	-0.011107000	-1.171418000
7	0.336338000	-0.020940000	-1.983764000

6	1.655986000	-0.022787000	-2.317658000
6	2.040486000	-0.035237000	-3.657659000
7	1.155799000	-0.045693000	-4.654526000
6	-0.133124000	-0.044302000	-4.313555000
6	-0.550072000	-0.031977000	-2.984019000
1	-3.087666000	3.932577000	-0.045323000
1	0.866862000	5.112416000	-0.060944000
1	1.600452000	2.728569000	-0.033660000
1	-4.516352000	2.142152000	-0.024820000
1	-4.498395000	-2.156523000	0.021038000
1	-3.083069000	-3.934628000	0.038023000
1	0.872230000	-5.109704000	0.057405000
1	1.603387000	-2.724924000	0.032827000
1	3.077033000	0.047967000	3.938337000
1	-0.880551000	0.065733000	5.108166000
1	-1.608463000	0.035764000	2.721675000
1	4.515413000	0.033652000	2.146405000
1	4.521756000	-0.013025000	-2.134604000
1	3.088753000	-0.035971000	-3.930711000
1	-0.865328000	-0.052349000	-5.112317000
1	-1.600318000	-0.030446000	-2.727877000
8	6.026168000	0.071383000	0.008175000
1	6.414601000	-0.813236000	0.005131000
8	-6.004622000	0.073210000	-0.001269000
1	-6.407144000	-0.805366000	0.014374000

xiv) [Fe(L14) 2] 2+

26	0.000003000	0.003058000	0.000130000
7	-0.335648000	1.414593000	1.399679000
6	-1.656485000	1.670978000	1.617635000
6	-2.077231000	2.621333000	2.541860000
6	-1.124790000	3.330187000	3.265719000
6	0.220987000	3.065967000	3.043928000
6	0.571759000	2.103087000	2.104527000
7	-1.907667000	0.006670000	-0.019439000
6	-2.566050000	0.854822000	0.796126000
6	-3.958851000	0.893816000	0.795274000
6	-4.626642000	0.026568000	-0.061285000
6	-3.945924000	-0.842683000	-0.905206000
6	-2.552988000	-0.826212000	-0.860575000
7	-0.312827000	-1.404334000	-1.408552000
6	-1.629928000	-1.644048000	-1.665220000
6	-2.035387000	-2.581992000	-2.608848000
6	-1.071178000	-3.296967000	-3.310771000
6	0.270795000	-3.052083000	-3.047216000
6	0.605974000	-2.100152000	-2.091200000
7	0.313205000	-1.402861000	1.410200000
6	1.630377000	-1.642716000	1.666356000
6	2.036074000	-2.580057000	2.610484000
6	1.072033000	-3.294040000	3.313647000
6	-0.270017000	-3.048707000	3.050904000
6	-0.605437000	-2.097525000	2.094228000
7	1.907672000	0.006950000	0.019438000
6	2.553229000	-0.825469000	0.860852000
6	3.946183000	-0.841946000	0.905073000
6	4.626660000	0.026823000	0.060455000
6	3.958622000	0.893620000	-0.796366000
6	2.565825000	0.854667000	-0.796765000
7	0.335269000	1.413991000	-1.400122000
6	1.656041000	1.670522000	-1.618315000
6	2.076533000	2.620863000	-2.542669000

6	1.123903000	3.329555000	-3.266434000
6	-0.221805000	3.065151000	-3.044452000
6	-0.572320000	2.102286000	-2.104941000
1	-3.131078000	2.806929000	2.696549000
1	-1.432319000	4.074099000	3.989336000
1	0.996837000	3.591552000	3.584102000
1	1.611467000	1.877159000	1.911480000
1	-4.508360000	1.580577000	1.423158000
1	-4.488079000	-1.490805000	-1.578851000
1	-3.086637000	-2.753298000	-2.794843000
1	-1.366652000	-4.031047000	-4.049296000
1	1.055436000	-3.583945000	-3.568239000
1	1.642217000	-1.888444000	-1.865801000
1	3.087373000	-2.751639000	2.795943000
1	1.367696000	-4.027658000	4.052556000
1	-1.054530000	-3.579688000	3.573017000
1	-1.641740000	-1.885475000	1.869418000
1	4.488549000	-1.489638000	1.578965000
1	4.507926000	1.580029000	-1.424813000
1	3.130334000	2.806610000	-2.697493000
1	1.431234000	4.073489000	-3.990112000
1	-0.997804000	3.590593000	-3.584552000
1	-1.611971000	1.876178000	-1.911816000
16	6.445363000	0.065831000	0.112989000
8	6.846172000	-0.478963000	1.416174000
6	6.955917000	-1.077255000	-1.178178000
1	6.587525000	-0.716067000	-2.136575000
1	6.569580000	-2.068040000	-0.947178000
1	8.045887000	-1.075237000	-1.159680000
16	-6.445314000	0.065534000	-0.114422000
8	-6.845704000	-0.479585000	-1.417600000
6	-6.956278000	-1.077245000	1.176858000
1	-6.588122000	-0.715844000	2.135265000
1	-8.046244000	-1.075170000	1.158077000
1	-6.569934000	-2.068109000	0.946200000
8	-6.853822000	1.423517000	0.266333000
8	6.853722000	1.423730000	-0.268233000

xv) [Fe(L15)2]2+

26	0.000001000	0.000119000	0.000064000
7	-0.341052000	1.412081000	1.407740000
6	-1.664310000	1.647701000	1.642460000
6	-2.090757000	2.584373000	2.577541000
6	-1.141178000	3.303295000	3.295444000
6	0.206135000	3.063090000	3.055535000
6	0.562534000	2.111892000	2.106050000
7	-1.897453000	-0.001955000	-0.004076000
6	-2.563096000	0.825269000	0.820838000
6	-3.960062000	0.807642000	0.801923000
7	-4.640070000	-0.005489000	-0.009302000
6	-3.954839000	-0.816888000	-0.817877000
6	-2.557777000	-0.830946000	-0.831494000
7	-0.331992000	-1.412408000	-1.409430000
6	-1.653733000	-1.651020000	-1.649685000
6	-2.074150000	-2.588249000	-2.586957000
6	-1.119973000	-3.304541000	-3.301396000
6	0.225773000	-3.061186000	-3.055949000
6	0.576041000	-2.109653000	-2.104526000
7	0.334684000	-1.408117000	1.413144000
6	1.656878000	-1.645343000	1.652247000
6	2.079090000	-2.581361000	2.589918000

6	1.126279000	-3.297621000	3.306204000
6	-0.219937000	-3.055102000	3.062505000
6	-0.572029000	-2.104795000	2.110528000
7	1.897456000	0.001415000	0.003876000
6	2.559362000	-0.825113000	0.832487000
6	3.956399000	-0.808708000	0.818579000
7	4.640077000	0.001802000	0.007807000
6	3.958515000	0.812085000	-0.804968000
6	2.561519000	0.828061000	-0.822895000
7	0.338359000	1.409470000	-1.410933000
6	1.661164000	1.648046000	-1.645241000
6	2.085814000	2.585344000	-2.580520000
6	1.134865000	3.301588000	-3.299288000
6	-0.211981000	3.057881000	-3.060291000
6	-0.566552000	2.106311000	-2.110497000
1	-3.146655000	2.749440000	2.742226000
1	-1.451660000	4.037040000	4.028156000
1	0.979335000	3.598442000	3.589894000
1	1.603871000	1.905345000	1.899774000
1	-4.540099000	1.455722000	1.447461000
1	-4.530751000	-1.466454000	-1.465591000
1	-3.128975000	-2.755757000	-2.756050000
1	-1.425748000	-4.038640000	-4.035729000
1	1.002435000	-3.594339000	-3.587475000
1	1.616060000	-1.900744000	-1.893950000
1	3.134238000	-2.748015000	2.757821000
1	1.433454000	-4.031031000	4.040641000
1	-0.995570000	-3.588042000	3.595744000
1	-1.612443000	-1.896436000	1.901381000
1	4.533538000	-1.455686000	1.467796000
1	4.537327000	1.459179000	-1.452585000
1	3.141392000	2.753058000	-2.744597000
1	1.443944000	4.035990000	-4.031934000
1	-0.986212000	3.590877000	-3.595510000
1	-1.607496000	1.897024000	-1.904980000

xvi) [Fe (L16) 2] 2+

26	-0.000030000	0.000070000	-0.000088000
7	-0.337836000	-1.270909000	1.531587000
6	-1.658278000	-1.487653000	1.788724000
6	-2.045154000	-2.341902000	2.811717000
6	-1.035681000	-2.952426000	3.546821000
6	0.550262000	-1.911322000	2.303626000
7	-1.916267000	0.000114000	0.000302000
6	-2.575681000	-0.750787000	0.903118000
6	-3.968198000	-0.771958000	0.928658000
6	-3.968400000	0.771825000	-0.927882000
6	-2.576004000	0.751009000	-0.902492000
7	-0.338320000	1.270811000	-1.531582000
6	-1.658622000	1.487725000	-1.788265000
6	-2.045766000	2.342022000	-2.811284000
6	-1.036636000	2.952240000	-3.546904000
6	0.549585000	1.911236000	-2.304106000
7	0.337928000	-1.531485000	-1.270938000
6	1.658188000	-1.788619000	-1.487596000
6	2.045160000	-2.811901000	-2.341649000
6	1.035916000	-3.547334000	-2.951889000
6	-0.550125000	-2.303809000	-1.911425000
7	1.916219000	0.000031000	-0.000182000
6	2.575763000	-0.902929000	-0.751026000
6	3.968164000	-0.928437000	-0.772051000

6	3.968381000	0.928433000	0.771278000
6	2.575852000	0.902929000	0.750435000
7	0.338228000	1.531701000	1.270724000
6	1.658550000	1.788624000	1.487319000
6	2.045728000	2.811633000	2.341597000
6	1.036643000	3.547010000	2.952159000
6	-0.549631000	2.304030000	1.911495000
1	-3.085638000	-2.530434000	3.034270000
1	-1.274346000	-3.630585000	4.358481000
1	1.597210000	-1.733900000	2.093522000
1	-4.501445000	-1.372857000	1.651826000
1	-4.501950000	1.372825000	-1.650737000
1	-3.086383000	2.530573000	-3.033277000
1	-1.275214000	3.630311000	-4.358589000
1	3.085742000	-3.034220000	-2.529996000
1	1.274368000	-4.359193000	-3.629796000
1	4.501563000	-1.651443000	-1.373003000
1	4.501830000	1.651761000	1.371804000
1	3.086349000	3.033812000	2.529867000
1	1.275274000	4.358652000	3.630260000
6	-4.662547000	-0.000114000	0.000698000
6	4.662515000	0.000269000	-0.000450000
1	-5.744530000	-0.000032000	0.000808000
1	5.744498000	0.000326000	-0.000721000
7	0.259932000	2.740600000	-3.298535000
7	0.260764000	-2.740800000	3.298021000
7	-0.260618000	-3.298482000	-2.740570000
7	-0.259935000	3.298408000	2.740896000
1	-1.597067000	-2.093410000	-1.733886000
1	1.596557000	1.733314000	-2.094200000
1	-1.596611000	2.093977000	1.733868000

xvii) [Fe(L17)2]2+

26	-0.000054000	-0.000017000	-0.000011000
7	-0.329088000	-1.499367000	-1.297195000
6	-1.648187000	-1.752479000	-1.518307000
6	-2.029616000	-2.766472000	-2.396490000
6	0.145788000	-3.261403000	-2.819300000
6	0.559852000	-2.255073000	-1.948768000
7	-1.916258000	0.001243000	0.000131000
6	-2.572504000	-0.887196000	-0.770168000
6	-3.965412000	-0.910898000	-0.791224000
6	-3.963861000	0.916092000	0.792488000
6	-2.571240000	0.890647000	0.770796000
7	-0.326694000	1.499886000	1.297057000
6	-1.645371000	1.754781000	1.518533000
6	-2.025102000	2.769432000	2.396697000
6	0.151088000	3.261719000	2.818485000
6	0.563492000	2.254547000	1.948161000
7	0.328753000	1.296841000	-1.499699000
6	1.647715000	1.517446000	-1.753427000
6	2.029203000	2.395481000	-2.767696000
6	-0.146352000	2.818736000	-3.261680000
6	-0.560400000	1.948685000	-2.255137000
7	1.916134000	-0.001267000	-0.000076000
6	2.572219000	0.768930000	-0.888744000
6	3.965123000	0.789528000	-0.913148000
6	3.963948000	-0.794285000	0.913773000
6	2.571317000	-0.772208000	0.888963000
7	0.326997000	-1.297520000	1.499459000
6	1.645624000	-1.519625000	1.753485000

6	2.025800000	-2.398282000	2.767721000
6	-0.150339000	-2.819319000	3.260906000
6	-0.563117000	-1.948553000	2.254482000
1	-3.077246000	-2.973987000	-2.578710000
1	0.879851000	-3.865137000	-3.339628000
1	1.609620000	-2.061388000	-1.778642000
1	-4.502106000	-1.620059000	-1.405612000
1	-4.499354000	1.626086000	1.406908000
1	-3.072373000	2.978686000	2.578950000
1	0.886135000	3.864556000	3.338460000
1	1.612949000	2.059373000	1.777837000
1	3.076853000	2.577095000	-2.975643000
1	-0.880395000	3.339680000	-3.864920000
1	-1.610113000	1.779100000	-2.060691000
1	4.501628000	1.403840000	-1.622516000
1	4.499572000	-1.408956000	1.623445000
1	3.073166000	-2.581148000	2.975975000
1	-0.885129000	-3.339533000	3.863864000
1	-1.612590000	-1.777621000	2.059903000
6	-4.656397000	0.002798000	0.000820000
6	4.656298000	-0.002819000	0.000141000
1	5.738380000	-0.003751000	0.000144000
1	-5.738479000	0.003334000	0.001403000
7	-1.142244000	-3.519682000	-3.045760000
7	-1.136524000	3.521768000	3.045312000
7	1.141883000	3.044752000	-3.520580000
7	1.137562000	-3.046795000	3.520148000

xviii) [Fe(L18)2]2+

26	-0.000399000	0.000084000	0.000079000
7	-0.332112000	1.186965000	-1.555072000
6	-1.642893000	1.397434000	-1.835417000
7	-2.086833000	2.156879000	-2.832670000
6	-1.153768000	2.729729000	-3.579273000
7	0.601573000	1.758461000	-2.298291000
7	-1.908905000	-0.003456000	0.001724000
6	-2.567271000	0.702484000	-0.926061000
6	-3.958417000	0.725369000	-0.958824000
6	-3.953510000	-0.739687000	0.967186000
6	-2.562983000	-0.711749000	0.931048000
7	-0.324225000	-1.188765000	1.554980000
6	-1.634083000	-1.403819000	1.838105000
7	-2.072727000	-2.165227000	2.835835000
6	-1.136310000	-2.735675000	3.580028000
7	0.612645000	-1.758017000	2.295454000
7	0.325223000	1.556196000	1.187587000
6	1.635473000	1.839619000	1.399876000
7	2.075414000	2.838471000	2.159337000
6	1.140244000	3.584610000	2.728904000
7	1.908776000	0.003393000	-0.000959000
6	2.563559000	0.932899000	0.706431000
6	3.954095000	0.969812000	0.732103000
6	3.957554000	-0.956039000	-0.733139000
6	2.566515000	-0.923978000	-0.707977000
7	0.330409000	-1.554583000	-1.188828000
6	1.641497000	-1.833689000	-1.401811000
6	1.151041000	-3.578191000	-2.733064000
1	-1.475967000	3.356441000	-4.402643000
1	-4.472381000	1.300680000	-1.716267000
1	-4.463365000	-1.316988000	1.725754000
1	-1.454959000	-3.363643000	4.403825000

1	1.459863000	4.410917000	3.353111000
1	4.464458000	1.728581000	1.308681000
1	4.470949000	-1.713023000	-1.309573000
1	1.472774000	-4.400578000	-3.361244000
6	-4.649842000	-0.008058000	0.004810000
6	4.649704000	0.007891000	-0.000746000
6	0.221785000	-2.528173000	3.302571000
6	0.205710000	2.526738000	-3.305010000
6	-0.218678000	3.307367000	2.523189000
7	-0.603025000	-2.297697000	-1.759490000
6	-0.208025000	-3.306343000	-2.525975000
7	2.084461000	-2.830015000	-2.162605000
1	-0.991518000	-3.892852000	-2.987617000
7	-0.610739000	2.296879000	1.758264000
1	-1.003542000	3.900133000	2.974365000
1	1.007528000	-2.981780000	3.892404000
1	0.988705000	2.982098000	-3.897129000
1	5.731900000	0.009980000	-0.000713000
1	-5.732039000	-0.009853000	0.006394000

xix) [Fe(L19)2]2+

26	0.000018000	-0.000012000	0.000047000
7	0.338462000	-1.327780000	-1.482025000
6	1.659924000	-1.551865000	-1.725404000
6	2.052131000	-2.446652000	-2.719563000
6	-0.119436000	-2.883083000	-3.219214000
6	-0.543377000	-1.994443000	-2.231091000
7	1.904673000	0.000081000	0.000254000
6	2.567638000	-0.782734000	-0.867555000
6	3.965207000	-0.768686000	-0.851777000
6	3.965008000	0.768918000	0.852794000
6	2.567344000	0.782885000	0.868179000
7	0.338029000	1.327941000	1.482089000
6	1.659437000	1.552052000	1.725779000
6	2.051403000	2.447021000	2.719879000
6	-0.120278000	2.883699000	3.218778000
6	-0.543966000	1.994833000	2.230757000
7	-0.338292000	-1.482256000	1.327762000
6	-1.659815000	-1.725859000	1.551731000
6	-2.051872000	-2.720158000	2.446337000
6	0.119690000	-3.219568000	2.882991000
6	0.543523000	-2.231224000	1.994436000
7	-1.904692000	-0.000135000	-0.000102000
6	-2.567527000	-0.867990000	0.782637000
6	-3.965191000	-0.852322000	0.768692000
6	-3.965054000	0.852312000	-0.768849000
6	-2.567476000	0.867837000	-0.782858000
7	-0.338160000	1.482018000	-1.327851000
6	-1.659654000	1.725568000	-1.551984000
6	-2.051624000	2.719653000	-2.446857000
6	0.119981000	3.219023000	-2.883367000
6	0.543733000	2.230843000	-1.994585000
1	3.101663000	-2.629524000	-2.916602000
1	-0.848954000	-3.415506000	-3.817748000
1	-1.595547000	-1.826304000	-2.049755000
1	4.544299000	-1.381497000	-1.531471000
1	4.543758000	1.381773000	1.532732000
1	3.100890000	2.630007000	2.917075000
1	-0.849948000	3.416306000	3.816963000
1	-1.596080000	1.826749000	2.049109000
1	-3.101362000	-2.917551000	2.629095000

1	0.849342000	-3.817809000	3.415552000
1	1.595705000	-2.049678000	1.826612000
1	-4.544103000	-1.532145000	1.381521000
1	-4.544007000	1.532134000	-1.381647000
1	-3.101098000	2.916969000	-2.629790000
1	0.849680000	3.817210000	-3.415926000
1	1.595900000	2.049404000	-1.826516000
7	1.169783000	-3.111479000	-3.465202000
7	1.168881000	3.112041000	3.465136000
7	-1.169426000	-3.465906000	3.111091000
7	-1.169113000	3.465257000	-3.111694000
7	4.645217000	0.000139000	0.000640000
7	-4.645231000	-0.000003000	-0.000061000

xx) [Fe(L20)2]2+

26	-0.007506000	0.002749000	-0.007259000
7	0.316611000	0.577782000	1.896211000
6	1.630081000	0.658240000	2.238557000
6	2.037907000	1.040336000	3.513751000
6	1.099927000	1.359027000	4.498220000
6	-0.246593000	1.268620000	4.120539000
6	-0.590565000	0.881979000	2.835787000
7	1.901920000	-0.025581000	0.013466000
6	2.556616000	0.307057000	1.143598000
6	3.944914000	0.293143000	1.184517000
6	4.682662000	-0.069143000	0.045610000
6	3.965539000	-0.406845000	-1.107272000
6	2.571897000	-0.377107000	-1.096973000
7	0.340739000	-0.582729000	-1.903421000
6	1.663664000	-0.702116000	-2.214919000
6	2.085703000	-1.095531000	-3.477025000
6	1.159436000	-1.387538000	-4.487569000
6	-0.187673000	-1.257501000	-4.143819000
6	-0.548745000	-0.858971000	-2.862225000
7	-0.309172000	1.907761000	-0.590035000
6	-1.619519000	2.253472000	-0.705332000
6	-2.014026000	3.530427000	-1.095598000
6	-1.065415000	4.513334000	-1.386109000
6	0.277167000	4.132151000	-1.260352000
6	0.607749000	2.845715000	-0.867471000
7	-1.916241000	0.032201000	-0.029913000
6	-2.557064000	1.160232000	-0.380424000
6	-3.950022000	1.207203000	-0.409257000
6	-4.696969000	0.073394000	-0.071074000
6	-3.989053000	-1.084402000	0.290772000
6	-2.600100000	-1.080152000	0.303074000
7	-0.380259000	-1.892443000	0.569094000
6	-1.702340000	-2.199471000	0.652106000
6	-2.143717000	-3.463501000	1.034009000
6	-1.232002000	-4.473026000	1.350466000
6	0.124027000	-4.131734000	1.257443000
6	0.501716000	-2.856489000	0.870643000
1	3.094689000	1.086251000	3.728942000
1	-1.043040000	1.496666000	4.816134000
1	-1.629891000	0.812316000	2.543335000
1	4.453418000	0.562874000	2.099130000
1	4.482827000	-0.692626000	-2.010070000
1	3.146174000	-1.174159000	-3.671802000
1	-0.975441000	-1.460311000	-4.854466000
1	-1.592864000	-0.757615000	-2.596665000
1	-3.068728000	3.748471000	-1.168593000

1	1.081043000	4.826565000	-1.464540000
1	1.644210000	2.551045000	-0.769508000
1	-4.443407000	2.123228000	-0.695233000
1	-4.521056000	-1.985456000	0.560907000
1	-3.205848000	-3.650434000	1.081546000
1	0.901989000	-4.848725000	1.483156000
1	1.548597000	-2.593246000	0.797492000
6	1.487151000	1.786951000	5.918288000
6	0.871843000	0.789474000	6.928274000
6	0.927670000	3.204669000	6.184386000
1	1.345930000	3.929330000	5.480805000
1	-0.160657000	3.236761000	6.099382000
1	1.193370000	3.520594000	7.196592000
1	-0.218086000	0.762793000	6.863794000
1	1.139226000	1.085290000	7.946077000
1	1.248278000	-0.222718000	6.758084000
6	6.216792000	-0.084426000	0.102028000
6	6.670424000	-1.085401000	1.191104000
6	6.722355000	1.333805000	0.457889000
1	6.408444000	2.061582000	-0.294906000
1	6.353738000	1.668792000	1.429868000
1	7.814742000	1.335006000	0.497658000
1	6.298833000	-0.811245000	2.180927000
1	7.762237000	-1.105767000	1.239226000
1	6.320983000	-2.095952000	0.963786000
6	-1.657035000	-5.882654000	1.777234000
6	-3.186816000	-6.045123000	1.809308000
6	-1.100807000	-6.167106000	3.192679000
1	-0.010404000	-6.113523000	3.221351000
1	-1.496247000	-5.453040000	3.919911000
1	-1.394563000	-7.171756000	3.507888000
1	-3.655135000	-5.362218000	2.523150000
1	-3.434424000	-7.063363000	2.117458000
1	-3.635169000	-5.880581000	0.825847000
6	-6.232073000	0.057329000	-0.085287000
6	-6.824732000	1.413678000	-0.506027000
6	-6.745792000	-0.284028000	1.333626000
1	-6.400583000	-1.264014000	1.670234000
1	-6.413751000	0.462146000	2.060207000
1	-7.838818000	-0.297610000	1.335018000
1	-6.540613000	2.214868000	0.181387000
1	-7.914826000	1.346446000	-0.499561000
1	-6.518769000	1.697313000	-1.516511000
6	1.638153000	-1.820511000	-5.877945000
6	2.476407000	-3.113894000	-5.742432000
6	2.513168000	-0.696485000	-6.481742000
1	1.943000000	0.230369000	-6.586106000
1	3.392510000	-0.487845000	-5.868330000
1	2.861904000	-0.995185000	-7.473749000
1	3.355901000	-2.967821000	-5.111399000
1	2.823117000	-3.432029000	-6.729101000
1	1.880297000	-3.923719000	-5.313661000
6	-1.437560000	5.935827000	-1.819281000
6	-0.856509000	6.939707000	-0.795444000
6	-2.960519000	6.140932000	-1.898195000
1	-3.424898000	5.473000000	-2.628633000
1	-3.443948000	5.986571000	-0.929830000
1	-3.170071000	7.166426000	-2.210530000
1	-1.267519000	6.763876000	0.202223000
1	-1.112950000	7.959414000	-1.094297000
1	0.231793000	6.874037000	-0.731809000
6	0.463381000	-2.094951000	-6.833211000

1	-0.178179000	-2.901528000	-6.468636000
1	-0.152713000	-1.205184000	-6.987432000
1	0.854014000	-2.398674000	-7.807024000
6	-1.073448000	-6.907486000	0.775722000
1	0.017574000	-6.870920000	0.742569000
1	-1.365095000	-7.918291000	1.072613000
1	-1.451341000	-6.727089000	-0.234137000
6	-6.715093000	-1.020130000	-1.085068000
1	-6.369815000	-2.019260000	-0.810459000
1	-7.807817000	-1.039175000	-1.104643000
1	-6.360431000	-0.802999000	-2.096026000
6	-0.829941000	6.210015000	-3.215492000
1	-1.222865000	5.510399000	-3.957969000
1	-1.085274000	7.223878000	-3.534616000
1	0.258944000	6.125676000	-3.210865000
6	3.011893000	1.814835000	6.123375000
1	3.501134000	2.525633000	5.452069000
1	3.231881000	2.124884000	7.147362000
1	3.461839000	0.829719000	5.973830000
6	6.844606000	-0.504200000	-1.238716000
1	6.582032000	0.184307000	-2.046321000
1	7.932551000	-0.498418000	-1.142737000
1	6.545656000	-1.514221000	-1.531337000

xxi) [Fe(L21)2]2+

26	-0.000001000	0.000086000	0.000231000
7	0.332093000	1.406384000	1.407156000
6	1.652521000	1.648766000	1.645905000
6	2.064383000	2.589053000	2.585414000
6	1.107077000	3.299780000	3.300484000
6	-0.238011000	3.050160000	3.055273000
6	-0.580723000	2.098098000	2.102830000
7	1.908640000	-0.000052000	0.000121000
6	2.569172000	0.833709000	0.826476000
6	3.958911000	0.853621000	0.849408000
6	4.678605000	-0.000136000	-0.000151000
6	3.958692000	-0.853848000	-0.849568000
6	2.568959000	-0.833849000	-0.826369000
7	0.331732000	-1.406326000	-1.406678000
6	1.652102000	-1.648843000	-1.645624000
6	2.063734000	-2.589226000	-2.585138000
6	1.106254000	-3.299931000	-3.299998000
6	-0.238772000	-3.050197000	-3.054568000
6	-0.581250000	-2.098035000	-2.102140000
7	-0.331832000	1.406472000	-1.406676000
6	-1.652219000	1.648916000	-1.645604000
6	-2.063915000	2.589274000	-2.585113000
6	-1.106483000	3.300040000	-3.299978000
6	0.238560000	3.050392000	-3.054554000
6	0.581103000	2.098245000	-2.102135000
7	-1.908641000	0.000175000	0.000210000
6	-2.569019000	0.833888000	-0.826317000
6	-3.958754000	0.853788000	-0.849519000
6	-4.678605000	0.000058000	-0.000068000
6	-3.958852000	-0.853614000	0.849526000
6	-2.569114000	-0.833606000	0.826594000
7	-0.331994000	-1.406143000	1.407253000
6	-1.652406000	-1.648572000	1.646048000
6	-2.064203000	-2.588810000	2.585634000
6	-1.106847000	-3.299429000	3.300747000
6	0.238222000	-3.049750000	3.055501000

6	0.580868000	-2.097746000	2.102976000
1	3.117221000	2.765101000	2.757470000
1	1.409659000	4.034815000	4.035416000
1	-1.017527000	3.578722000	3.587407000
1	-1.618439000	1.880841000	1.888703000
1	4.483402000	1.505939000	1.533005000
1	4.483007000	-1.506196000	-1.533272000
1	3.116530000	-2.765370000	-2.757351000
1	1.408656000	-4.035041000	-4.034928000
1	-1.018421000	-3.578744000	-3.586521000
1	-1.618914000	-1.880690000	-1.887858000
1	-3.116723000	2.765359000	-2.757315000
1	-1.408935000	4.035133000	-4.034905000
1	1.018172000	3.578994000	-3.586507000
1	1.618782000	1.880962000	-1.887859000
1	-4.483116000	1.506069000	-1.533251000
1	-4.483299000	-1.505947000	1.533143000
1	-3.117029000	-2.764899000	2.757722000
1	-1.409380000	-4.034423000	4.035740000
1	1.017775000	-3.578222000	3.587670000
1	1.618570000	-1.880449000	1.888820000
6	6.159901000	-0.000177000	-0.000297000
6	6.876378000	-1.195514000	-0.156515000
6	6.876476000	1.195120000	0.155777000
6	8.266590000	-1.203040000	-0.153840000
6	8.266688000	1.202567000	0.152826000
6	8.948024000	-0.000255000	-0.000575000
1	6.350835000	-2.137616000	-0.254508000
1	6.351006000	2.137251000	0.253874000
1	8.810771000	-2.131799000	-0.262607000
1	8.810944000	2.131296000	0.261483000
6	-6.159901000	-0.000012000	-0.000222000
6	-6.876466000	1.195266000	-0.156480000
6	-6.876384000	-1.195359000	0.155884000
6	-8.266679000	1.202686000	-0.153812000
6	-8.266596000	-1.202912000	0.152925000
6	-8.948022000	-0.000146000	-0.000514000
1	-6.350994000	2.137404000	-0.254500000
1	-6.350841000	-2.137446000	0.254013000
1	-8.810930000	2.131400000	-0.262611000
1	-8.810782000	-2.131679000	0.261608000
17	10.708588000	-0.000304000	-0.000749000
17	-10.708586000	-0.000230000	-0.000697000

xxii) [Fe(L22)2]2+

26	-0.000001000	-0.056268000	0.000005000
7	0.566070000	-1.465840000	-1.330485000
6	1.903241000	-1.708131000	-1.353337000
6	2.482370000	-2.647473000	-2.199072000
6	1.661295000	-3.376715000	-3.065919000
6	0.282008000	-3.124385000	-3.040604000
6	-0.210338000	-2.175379000	-2.169391000
7	1.888080000	-0.054171000	0.313660000
6	2.678212000	-0.885742000	-0.400031000
6	4.047113000	-0.907538000	-0.203963000
6	4.609767000	-0.047436000	0.755172000
6	3.776840000	0.809029000	1.487810000
6	2.408682000	0.774299000	1.234798000
7	0.103582000	1.350554000	1.446523000
6	1.371159000	1.591947000	1.898126000
6	1.636956000	2.519697000	2.887527000

6	0.581124000	3.245949000	3.457347000
6	-0.716192000	2.998411000	2.996387000
6	-0.894252000	2.049676000	1.999782000
7	-0.566073000	-1.465793000	1.330543000
6	-1.903245000	-1.708081000	1.353405000
6	-2.482374000	-2.647397000	2.199167000
6	-1.661298000	-3.376618000	3.066031000
6	-0.282011000	-3.124291000	3.040706000
6	0.210336000	-2.175310000	2.169467000
7	-1.888083000	-0.054175000	-0.313647000
6	-2.678215000	-0.885721000	0.400073000
6	-4.047116000	-0.907521000	0.204007000
6	-4.609769000	-0.047451000	-0.755156000
6	-3.776842000	0.808987000	-1.487825000
6	-2.408684000	0.774262000	-1.234814000
7	-0.103581000	1.350497000	-1.446571000
6	-1.371159000	1.591881000	-1.898176000
6	-1.636954000	2.519596000	-2.887611000
6	-0.581119000	3.245817000	-3.457465000
6	0.716198000	2.998283000	-2.996507000
6	0.894256000	2.049586000	-1.999865000
1	3.550165000	-2.801915000	-2.176818000
1	-0.380165000	-3.671387000	-3.697868000
1	-1.271508000	-1.968099000	-2.134182000
1	4.701308000	-1.562727000	-0.761580000
1	4.178231000	1.480803000	2.230398000
1	2.643032000	2.703207000	3.238131000
1	-1.578307000	3.517514000	3.387900000
1	-1.889956000	1.843102000	1.629521000
1	-3.550170000	-2.801834000	2.176923000
1	0.380163000	-3.671277000	3.697984000
1	1.271505000	-1.968032000	2.134251000
1	-4.701312000	-1.562690000	0.761647000
1	-4.178232000	1.480735000	-2.230437000
1	-2.643030000	2.703100000	-3.238216000
1	1.578316000	3.517359000	-3.388048000
1	1.889961000	1.843018000	-1.629602000
8	-5.940697000	-0.120577000	-0.893641000
6	-6.595857000	0.725051000	-1.854028000
1	-6.443871000	1.778928000	-1.610242000
1	-6.238702000	0.513566000	-2.864443000
1	-7.651894000	0.479986000	-1.779493000
8	5.940694000	-0.120560000	0.893661000
6	6.595856000	0.725105000	1.854014000
1	6.443870000	1.778973000	1.610186000
1	6.238704000	0.513660000	2.864438000
1	7.651893000	0.480036000	1.779486000
8	2.088309000	-4.307775000	-3.928435000
6	3.491509000	-4.613671000	-3.994197000
1	4.067106000	-3.735328000	-4.295030000
1	3.851274000	-4.992857000	-3.035005000
1	3.582182000	-5.387808000	-4.751478000
8	0.912984000	4.127492000	4.409070000
6	-0.124159000	4.906234000	5.030197000
1	-0.637499000	5.526349000	4.291954000
1	-0.838608000	4.259776000	5.544629000
1	0.384301000	5.539511000	5.752273000
8	-0.912978000	4.127328000	-4.409218000
6	0.124171000	4.906020000	-5.030398000
1	0.637531000	5.526164000	-4.292193000
1	0.838603000	4.259522000	-5.544805000
1	-0.384287000	5.539268000	-5.752500000

8	-2.088312000	-4.307656000	3.928571000
6	-3.491510000	-4.613558000	3.994334000
1	-4.067110000	-3.735217000	4.295167000
1	-3.851274000	-4.992746000	3.035143000
1	-3.582180000	-5.387695000	4.751615000

xxiii) [Fe(L23)2]2+

26	0.005924000	0.029393000	0.044021000
7	0.714067000	1.189941000	1.536391000
6	2.073758000	1.213685000	1.641472000
6	2.739567000	1.942759000	2.610360000
6	2.022514000	2.720549000	3.555145000
6	0.610385000	2.680443000	3.423874000
6	0.029035000	1.921855000	2.430357000
7	1.887010000	-0.242072000	-0.188910000
6	2.762400000	0.378850000	0.627102000
6	4.129124000	0.223189000	0.477687000
6	4.642349000	-0.613785000	-0.550119000
6	3.685747000	-1.254288000	-1.383812000
6	2.334108000	-1.042693000	-1.177199000
7	-0.015085000	-1.234959000	-1.530619000
6	1.218315000	-1.630662000	-1.957796000
6	1.403239000	-2.493217000	-3.023337000
6	0.293641000	-3.020142000	-3.732415000
6	-0.977759000	-2.594934000	-3.268053000
6	-1.069957000	-1.728820000	-2.199515000
7	-0.262878000	1.627914000	-1.160730000
6	-1.548265000	2.079444000	-1.226815000
6	-1.926238000	3.157796000	-2.006340000
6	-0.972693000	3.860722000	-2.786214000
6	0.357453000	3.375305000	-2.696323000
6	0.645215000	2.289937000	-1.896423000
7	-1.874822000	0.304445000	0.271952000
6	-2.494276000	1.302789000	-0.389055000
6	-3.854413000	1.523329000	-0.260453000
6	-4.633147000	0.696267000	0.593880000
6	-3.944272000	-0.355630000	1.256546000
6	-2.581018000	-0.512781000	1.078460000
7	-0.412978000	-1.470061000	1.329374000
6	-1.722737000	-1.549538000	1.701455000
6	-2.196926000	-2.505341000	2.581871000
6	-1.324615000	-3.472864000	3.142770000
6	0.031412000	-3.371010000	2.737837000
6	0.419095000	-2.381247000	1.859955000
1	3.816472000	1.897285000	2.644176000
1	-0.036791000	3.243224000	4.079185000
1	-1.049636000	1.899328000	2.336504000
1	4.797321000	0.754456000	1.135905000
1	4.003001000	-1.916220000	-2.173260000
1	2.409797000	-2.748142000	-3.314751000
1	-1.893010000	-2.942919000	-3.722143000
1	-2.045073000	-1.412483000	-1.850246000
1	-2.964404000	3.448750000	-2.020167000
1	1.169633000	3.841974000	-3.232616000
1	1.663710000	1.927410000	-1.833318000
1	-4.313934000	2.325532000	-0.814240000
1	-4.474222000	-1.040243000	1.898239000
1	-3.242347000	-2.493066000	2.846250000
1	0.782463000	-4.061184000	3.090701000
1	1.456164000	-2.312195000	1.555518000
7	-5.968460000	0.907837000	0.776729000

7	5.981168000	-0.791782000	-0.727844000
6	-6.762915000	0.042515000	1.660070000
1	-7.629829000	0.623910000	1.975900000
1	-6.190049000	-0.159858000	2.568390000
6	-6.671401000	1.990565000	0.073856000
1	-6.049680000	2.889168000	0.092134000
1	-7.557581000	2.227307000	0.663669000
6	6.971455000	-0.207441000	0.185778000
1	7.842191000	-0.865893000	0.176357000
1	6.585585000	-0.238611000	1.206350000
6	6.519516000	-1.572791000	-1.849015000
1	5.903424000	-1.406991000	-2.734720000
1	7.500325000	-1.156240000	-2.086219000
6	-7.231052000	-1.269251000	1.020341000
1	-7.792621000	-1.854940000	1.753077000
1	-7.884083000	-1.079296000	0.166294000
1	-6.389896000	-1.875208000	0.676397000
6	6.650998000	-3.068793000	-1.548978000
1	7.079350000	-3.585767000	-2.411622000
1	7.307692000	-3.238032000	-0.692132000
1	5.681457000	-3.520447000	-1.327506000
6	7.393560000	1.215000000	-0.193916000
1	8.146662000	1.580562000	0.508987000
1	7.826652000	1.238259000	-1.196900000
1	6.546005000	1.903802000	-0.174515000
6	-7.086009000	1.657239000	-1.363535000
1	-7.578085000	2.523497000	-1.813814000
1	-6.225133000	1.397401000	-1.983555000
1	-7.786058000	0.819865000	-1.386898000
7	0.439981000	-3.871581000	-4.782814000
6	1.754388000	-4.375949000	-5.199963000
6	2.468810000	-3.468230000	-6.205397000
6	-0.711878000	-4.338075000	-5.565605000
6	-1.371773000	-5.596522000	-4.994735000
1	-1.437566000	-3.528047000	-5.657819000
1	-2.201065000	-5.906654000	-5.635857000
1	-0.351823000	-4.535206000	-6.577250000
1	-0.657193000	-6.421620000	-4.941930000
1	1.593279000	-5.361719000	-5.640835000
1	2.375231000	-4.541260000	-4.317539000
1	1.867288000	-3.337281000	-7.108244000
1	3.424317000	-3.912587000	-6.496062000
1	2.666330000	-2.480423000	-5.782963000
1	-1.764047000	-5.421760000	-3.990440000
7	-1.312184000	4.923856000	-3.563644000
6	-2.676353000	5.466858000	-3.588579000
6	-3.590269000	4.782610000	-4.609373000
6	-0.331806000	5.593783000	-4.428065000
6	0.443613000	6.710488000	-3.723216000
1	0.351149000	4.850573000	-4.843188000
1	1.135055000	7.184977000	-4.424446000
1	-0.881804000	6.003693000	-5.277372000
1	-0.235661000	7.478453000	-3.344994000
1	-2.592633000	6.530097000	-3.821619000
1	-3.106291000	5.413741000	-2.586659000
1	-3.183686000	4.874270000	-5.619534000
1	-4.578244000	5.250278000	-4.597893000
1	-3.713367000	3.720002000	-4.388240000
7	-1.759425000	-4.428387000	4.007576000
6	-0.833158000	-5.374094000	4.643980000
6	-0.572546000	-6.631974000	3.810252000
6	-3.177845000	-4.573061000	4.359050000

6	-3.608506000	-3.700092000	5.541427000
1	-3.791694000	-4.366012000	3.480484000
1	-4.663993000	-3.872383000	5.767681000
1	-3.342431000	-5.625718000	4.597073000
1	-3.026909000	-3.939312000	6.435104000
1	-1.269735000	-5.651267000	5.605446000
1	0.102760000	-4.862616000	4.875678000
1	-1.503347000	-7.170073000	3.614469000
1	0.100595000	-7.303777000	4.349255000
1	-0.113030000	-6.387171000	2.850078000
7	2.646219000	3.450882000	4.518230000
6	1.890785000	4.183167000	5.543034000
6	1.489461000	5.597673000	5.114941000
6	4.109114000	3.554626000	4.592089000
6	4.763324000	2.438205000	5.411318000
1	4.521010000	3.586296000	3.581711000
1	5.845756000	2.586685000	5.446507000
1	4.338731000	4.524037000	5.038761000
1	4.388198000	2.436262000	6.437661000
1	2.521775000	4.230479000	6.432635000
1	1.012744000	3.601314000	5.828804000
1	2.370754000	6.195991000	4.870873000
1	0.955629000	6.096261000	5.928195000
1	0.837213000	5.580362000	4.238971000
1	4.567763000	1.455277000	4.976832000
1	1.022943000	6.324717000	-2.881432000
1	-3.475142000	-2.637875000	5.324328000

xxiv) [Fe(L24) 2] 2+

26	-0.000001000	-0.000028000	0.000017000
7	-0.357245000	1.394618000	-1.396025000
7	-1.704207000	1.591511000	-1.594263000
6	-1.920182000	2.543232000	-2.548671000
7	-1.922346000	-0.000224000	0.000217000
6	-2.584925000	0.820485000	-0.821971000
6	-3.971297000	0.859158000	-0.860880000
6	-4.652227000	-0.000521000	0.000466000
6	-3.970949000	-0.860048000	0.861689000
6	-2.584587000	-0.821074000	0.822534000
7	-0.356681000	-1.394739000	1.396149000
7	-1.703565000	-1.591894000	1.594674000
6	-1.919149000	-2.543610000	2.549176000
7	0.356963000	1.396170000	1.394586000
7	1.703885000	1.594582000	1.591579000
6	-0.252280000	2.229988000	2.225499000
7	1.922347000	0.000063000	-0.000076000
6	2.584755000	0.822261000	0.820757000
6	3.971123000	0.861155000	0.859723000
6	4.652227000	-0.000176000	0.000166000
6	3.971123000	-0.861377000	-0.859520000
6	2.584757000	-0.822220000	-0.820824000
7	0.356964000	-1.396009000	-1.394767000
1	-2.914532000	2.834793000	-2.841584000
1	-4.503269000	1.523150000	-1.526155000
1	-5.734399000	-0.000644000	0.000563000
1	-4.502664000	-1.524152000	1.527054000
1	-2.913373000	-2.835365000	2.842326000
1	-0.482434000	-3.716940000	3.724666000
1	-1.329320000	2.267141000	2.263299000
1	4.502963000	1.526397000	1.523851000
1	5.734399000	-0.000290000	0.000280000

1	4.502970000	-1.526745000	-1.523519000
7	1.703887000	-1.594343000	-1.591841000
6	1.919667000	-2.548539000	-2.543818000
6	-0.252279000	-2.229180000	-2.226329000
6	0.686793000	-2.975737000	-2.970806000
1	-1.329319000	-2.266255000	-2.264203000
1	0.483191000	-3.723856000	-3.717614000
1	2.913952000	-2.841461000	-2.835589000
6	0.686794000	2.977018000	2.969500000
6	1.919666000	2.549491000	2.542840000
1	2.913954000	2.842642000	2.834373000
1	0.483194000	3.725656000	3.715789000
6	-0.686189000	-2.970358000	2.976363000
6	0.252730000	-2.225995000	2.229500000
1	1.329777000	-2.263748000	2.266493000
6	-0.687396000	2.970237000	-2.976103000
1	-0.483946000	3.716891000	-3.724418000
6	0.251830000	2.226035000	-2.229462000
1	1.328863000	2.264000000	-2.266655000

xxv) [Fe (L25) 2] 2+

26	0.000000000	0.000087000	0.007154000
7	-0.296812000	-1.415418000	1.413708000
6	-1.610750000	-1.691399000	1.652272000
6	-1.997810000	-2.644019000	2.590193000
6	-1.022683000	-3.331484000	3.303762000
6	0.315767000	-3.047291000	3.058747000
6	0.633561000	-2.085202000	2.107951000
7	-1.908209000	-0.049135000	0.008055000
6	-2.548753000	-0.898259000	0.834562000
6	-3.936478000	-0.950994000	0.861649000
6	-4.685352000	-0.117642000	0.012563000
6	-3.981288000	0.751290000	-0.839280000
6	-2.592604000	0.767213000	-0.816562000
7	-0.370568000	1.396549000	-1.400240000
6	-1.697128000	1.604636000	-1.637971000
6	-2.132858000	2.533334000	-2.578501000
6	-1.194505000	3.267313000	-3.295014000
6	0.156885000	3.052395000	-3.050665000
6	0.524031000	2.110474000	-2.097437000
7	0.370465000	-1.396373000	-1.400271000
6	1.697010000	-1.604498000	-1.638059000
6	2.132673000	-2.533164000	-2.578651000
6	1.194269000	-3.267065000	-3.295176000
6	-0.157105000	-3.052103000	-3.050777000
6	-0.524182000	-2.110220000	-2.097486000
7	1.908210000	0.049261000	0.007963000
6	2.592546000	-0.767137000	-0.816654000
6	3.981232000	-0.751315000	-0.839368000
6	4.685359000	0.117559000	0.012481000
6	3.936545000	0.950963000	0.861570000
6	2.548816000	0.898331000	0.834478000
7	0.296912000	1.415643000	1.413631000
6	1.610869000	1.691542000	1.652185000
6	1.997993000	2.644165000	2.590076000
6	1.022911000	3.331730000	3.303611000
6	-0.315559000	3.047638000	3.058588000
6	-0.633417000	2.085532000	2.107830000
1	-3.045935000	-2.847125000	2.761560000
1	-1.306215000	-4.075479000	4.037333000

1	1.108641000	-3.556888000	3.589683000
1	1.665186000	-1.840663000	1.893366000
1	-4.439751000	-1.614642000	1.549988000
1	-4.519537000	1.388694000	-1.526006000
1	-3.189970000	2.682509000	-2.749792000
1	-1.516191000	3.993636000	-4.030564000
1	0.922225000	3.600114000	-3.584069000
1	1.566872000	1.919336000	-1.883196000
1	3.189773000	-2.682369000	-2.749988000
1	1.515903000	-3.993361000	-4.030777000
1	-0.922484000	-3.599757000	-3.584191000
1	-1.567010000	-1.919053000	-1.883203000
1	4.519436000	-1.388760000	-1.526092000
1	4.439865000	1.614568000	1.549915000
1	3.046132000	2.847200000	2.761442000
1	1.306494000	4.075730000	4.037158000
1	-1.108397000	3.557323000	3.589491000
1	-1.665059000	1.841064000	1.893241000
6	-6.161108000	-0.154377000	0.015712000
6	-6.915763000	0.996354000	-0.247955000
6	-6.858005000	-1.347532000	0.285472000
6	-8.306834000	0.975391000	-0.242041000
6	-8.240233000	-1.384842000	0.285916000
6	-8.981337000	-0.222103000	0.024013000
1	-6.417827000	1.940637000	-0.433455000
1	-6.313036000	-2.265974000	0.468138000
1	-8.849070000	1.890166000	-0.436516000
1	-8.773251000	-2.307824000	0.478620000
6	6.161118000	0.154178000	0.015641000
6	6.915686000	-0.996617000	-0.248002000
6	6.858106000	1.347283000	0.285390000
6	8.306759000	-0.975761000	-0.242076000
6	8.240336000	1.384485000	0.285846000
6	8.981352000	0.221685000	0.023967000
1	6.417679000	-1.940864000	-0.433492000
1	6.313206000	2.265769000	0.468039000
1	8.848925000	-1.890581000	-0.436535000
1	8.773425000	2.307428000	0.478542000
8	10.328371000	0.359240000	0.051174000
6	11.143947000	-0.786040000	-0.216773000
1	10.974054000	-1.573140000	0.523130000
1	10.958396000	-1.175876000	-1.221460000
1	12.171616000	-0.436937000	-0.146269000
8	-10.328346000	-0.359763000	0.051212000
6	-11.144011000	0.785447000	-0.216767000
1	-10.974195000	1.572571000	0.523127000
1	-10.958475000	1.175283000	-1.221457000
1	-12.171653000	0.436261000	-0.146277000

Appendix B

- **Supplementary material associated with article J. Mol. Graph. Model. (submitted 31.09.2023) Manuscript ID JMGM-D-23-01121: Optimized coordinates of the DFT calculations, Table S1, Figures S1 – S9.**

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3.1	$[\text{Fe}(\text{L}^1)_2]^{2+}$ -	269
3.2	$[\text{Fe}(\text{L}^2)_2]^{2+}$	271
3.3	$[\text{Fe}(\text{L}^3)_2]^{2+}$	272
3.4	$[\text{Fe}(\text{L}^4)_2]^{2+}$	273
3.5	$[\text{Fe}(\text{L}^5)_2]^{2+}$	275
3.6	$[\text{Fe}(\text{L}^6)_2]^{2+}$	276
3.7	$[\text{Fe}(\text{L}^7)_2]^{2+}$	278
3.8	$[\text{Fe}(\text{L}^8)_2]^{2+}$	279
3.9	$[\text{Fe}(\text{L}^9)_2]^{2+}$	280
3.10	$[\text{Fe}(\text{L}^{10})_2]^{2+}$	282
3.11	$[\text{Fe}(\text{L}^{11})_2]^{2+}$	283
3.12	$[\text{Fe}(\text{L}^{12})_2]^{2+}$	284
3.13	$[\text{Fe}(\text{L}^{13})_2]^{2+}$	285
3.14	$[\text{Fe}(\text{L}^{14})_2]^{2+}$	286
3.15	$[\text{Fe}(\text{L}^{15})_2]^{2+}$	288
3.16	$[\text{Fe}(\text{L}^{16})_2]^{2+}$	289
3.17	$[\text{Fe}(\text{L}^{17})_2]^{2+}$	291
3.18	$[\text{Fe}(\text{L}^{18})_2]^{2+}$	292
3.19	$[\text{Fe}(\text{L}^{19})_2]^{2+}$	295

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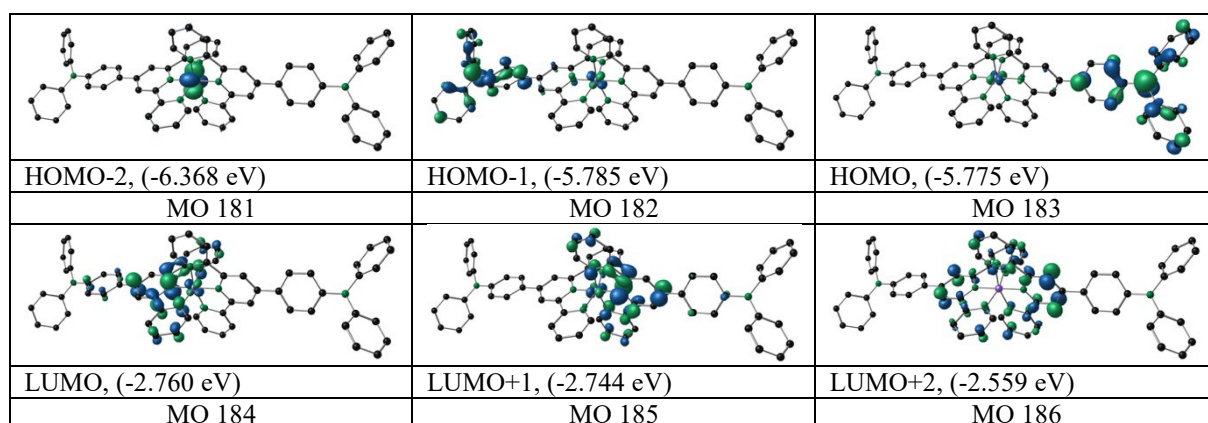


Figure S 1. Selected MOs of complex 18, containing an amide group, energy given in eV in brackets, calculated at the M06-D3/CEP-121G* level in MeCN solution.

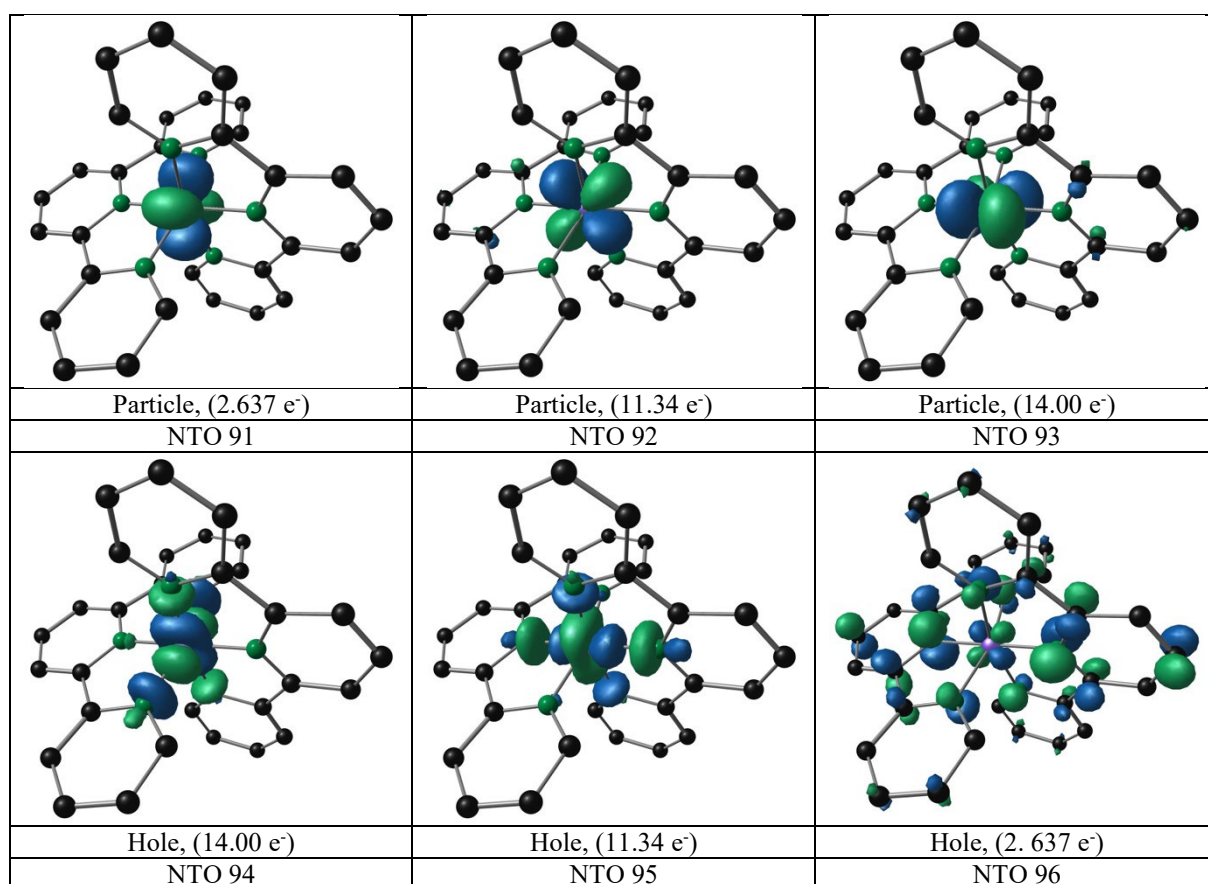


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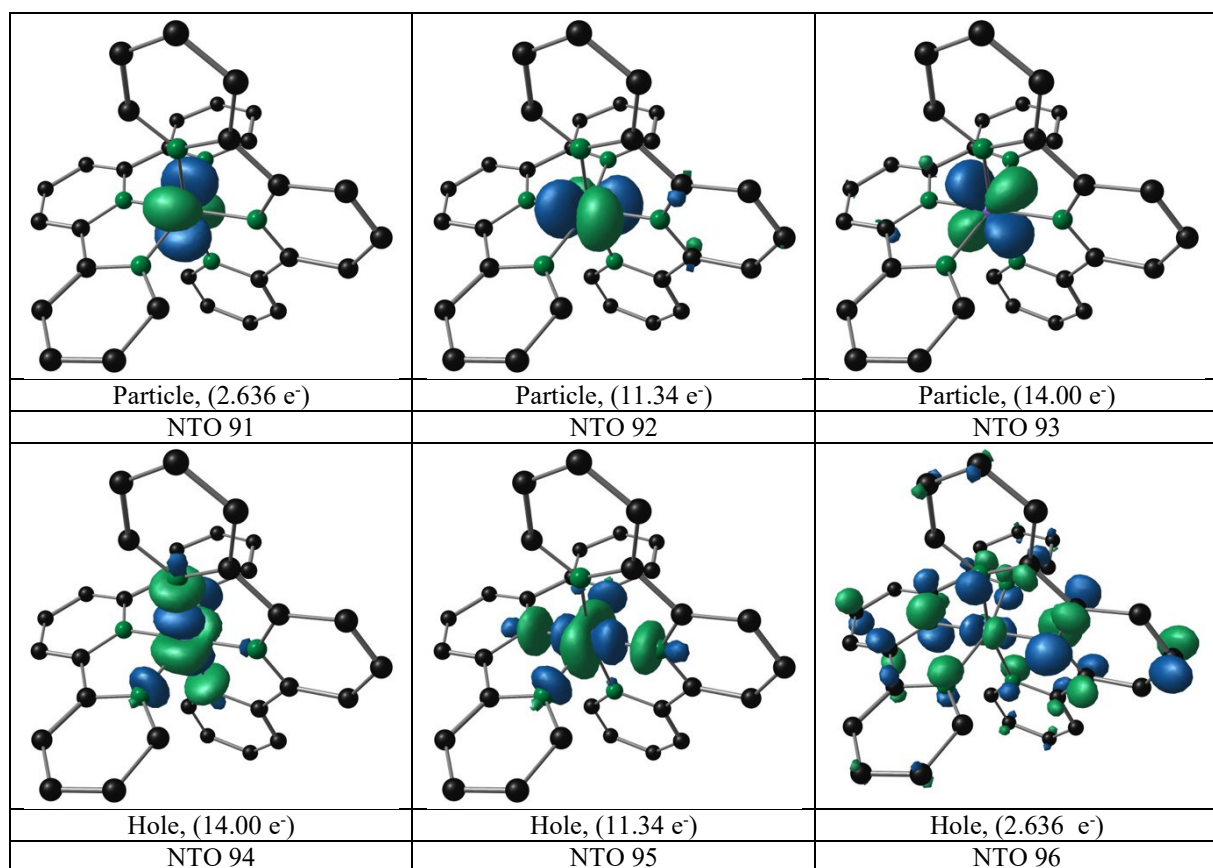


Figure S 3. NTOs of excited state 3 (contr. value 0.05), peak at 592.2 nm of 10. The electron occupation of the occupied (particle) and unoccupied (hole) NTO pairs are indicated. A contour of 0.05 e/Å³ was used for the orbital plot. Atoms are colour coded (online version) as follows: Fe (purple), C (black), N (green).

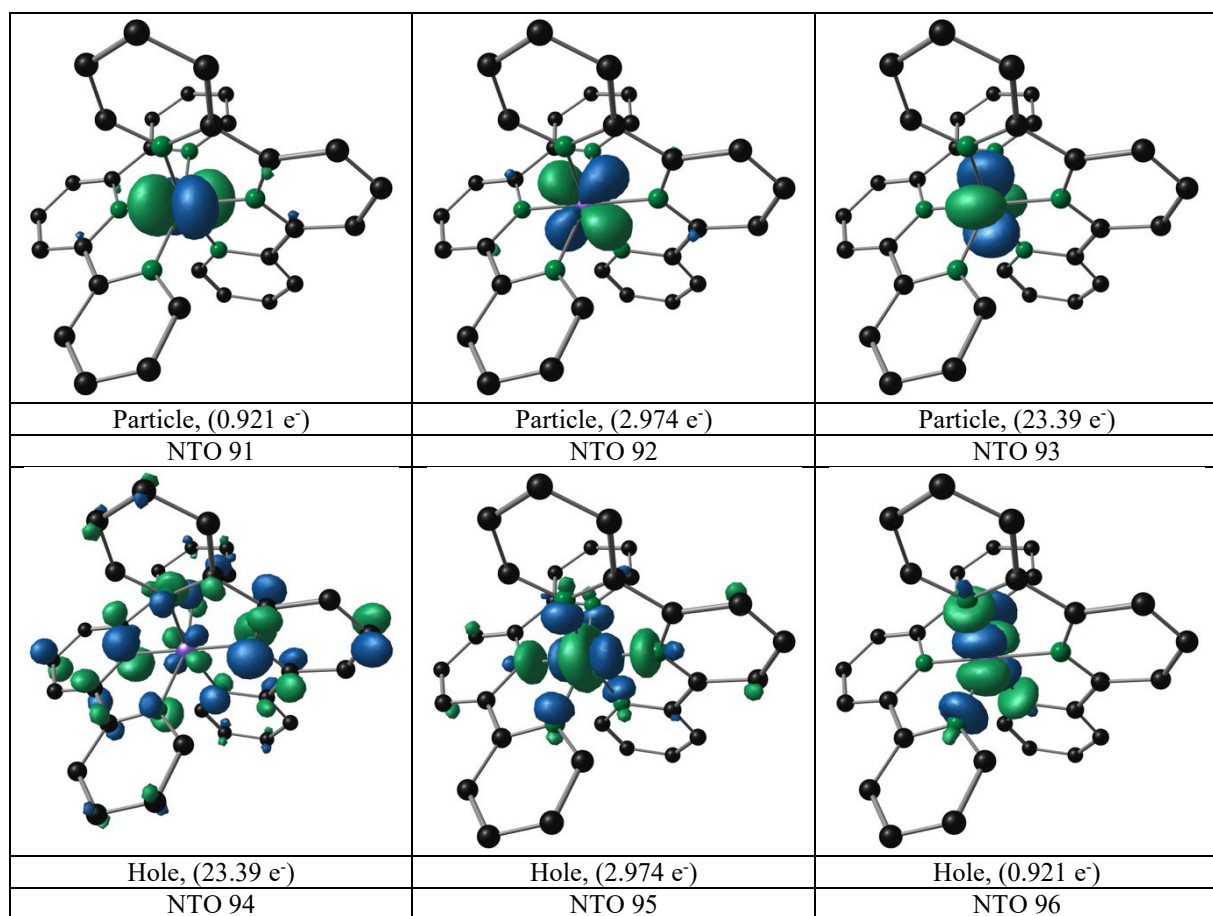


Figure S 4. NTOs of excited state 4 (contr. value 0.05), peak at 545.5 nm of 10. The electron occupation of the occupied (particle) and unoccupied (hole) NTO pairs are indicated. A contour of $0.05 \text{ e}/\text{\AA}^3$ was used for the orbital plot. Atoms are colour coded (online version) as follows: Fe (purple), C (black), N (green).

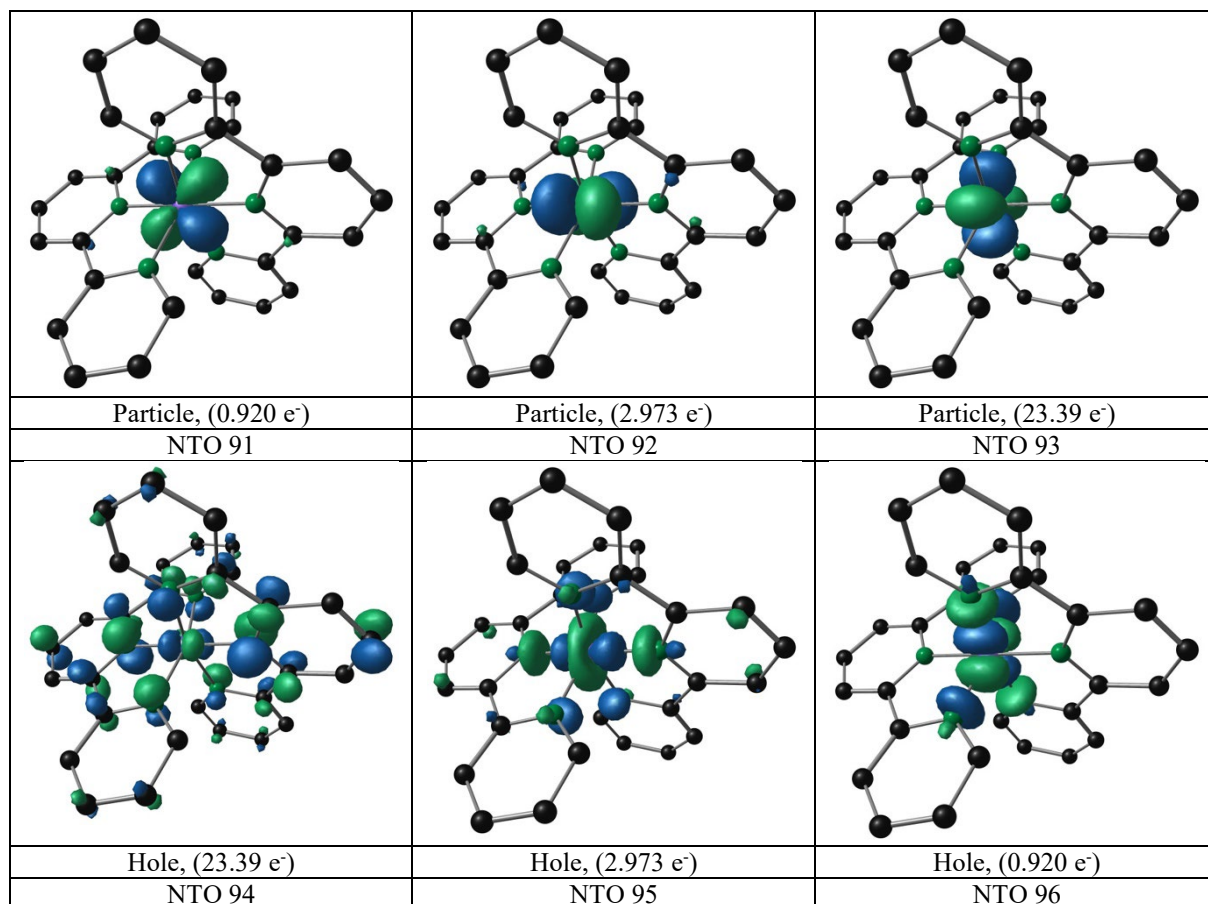


Figure S 5. NTOs of excited state 5 (contr. value 0.05), peak at 545.5 nm of 10. The electron occupation of the occupied (particle) and unoccupied (hole) NTO pairs are indicated. A contour of $0.05 \text{ e}/\text{\AA}^3$ was used for the orbital plot. Atoms are colour coded (online version) as follows: Fe (purple), C (black), N (green).

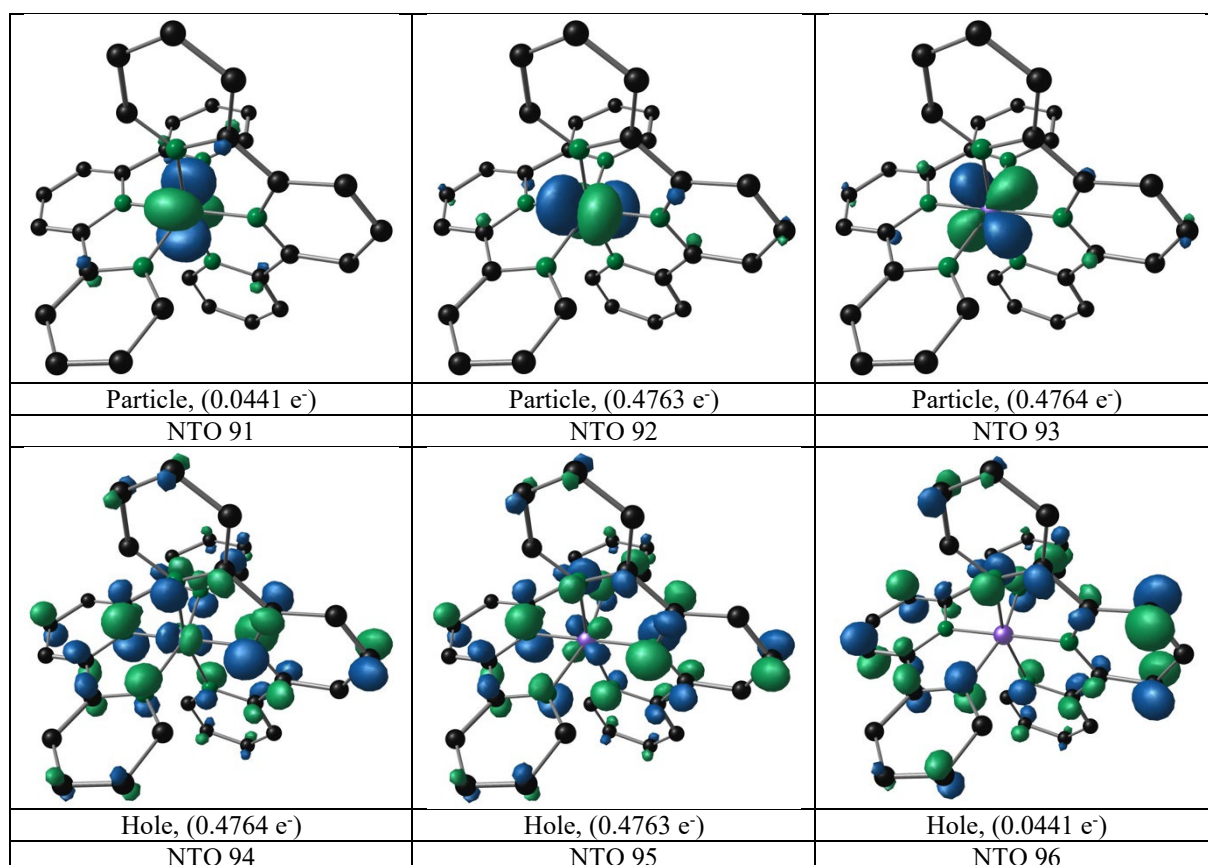


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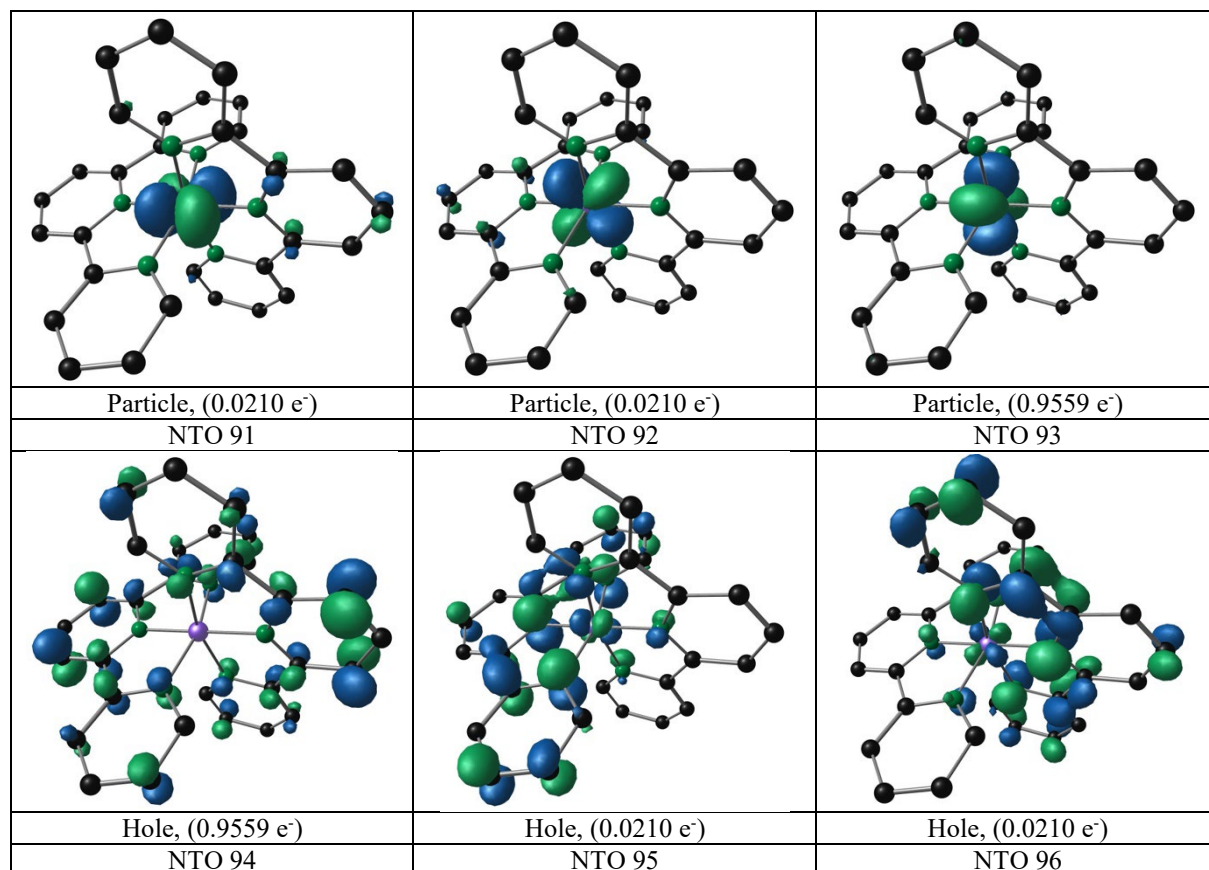
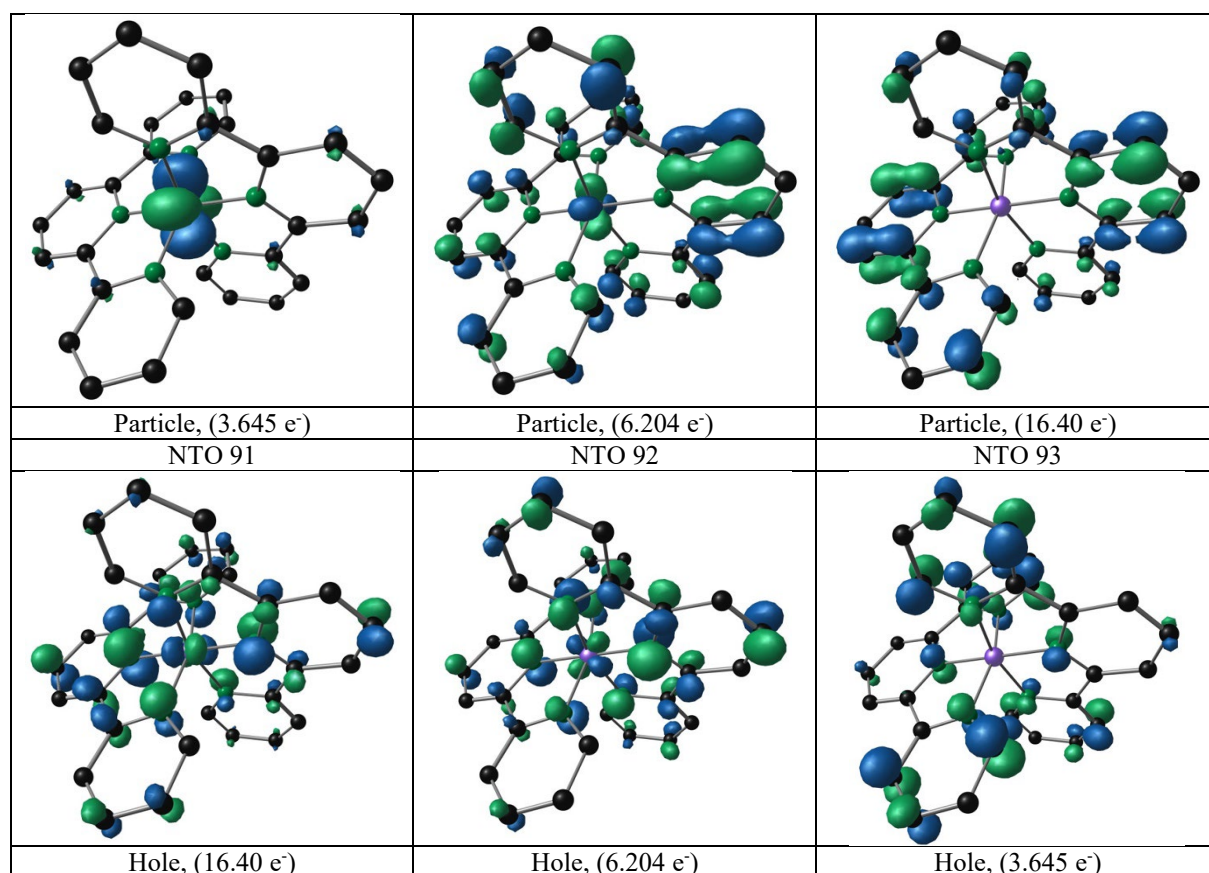


Figure S 7. NTOs of excited S12 (contr. value 0.05), peak at 436 NTOs, of 10. The electron occupation of the occupied (particle) and unoccupied (hole) NTO pairs are indicated. A contour of $0.05 \text{ e}/\text{\AA}^3$ was used for the orbital plot. Atoms are colour coded (online version) as follows: Fe (purple), C (black), N (green).



NTO 94	NTO 95	NTO 96
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Figure S 8. NTOs of excited 30 (contr. value 0.05), peak at 306.6 nm of 10. The electron occupation of the occupied (particle) and unoccupied (hole) NTO pairs are indicated. A contour of $0.05 \text{ e}/\text{\AA}^3$ was used for the orbital plot. Atoms are colour coded (online version) as follows: Fe (purple), C (black), N (green).

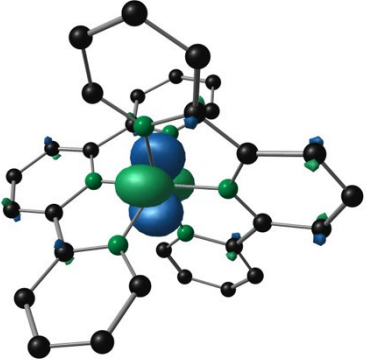
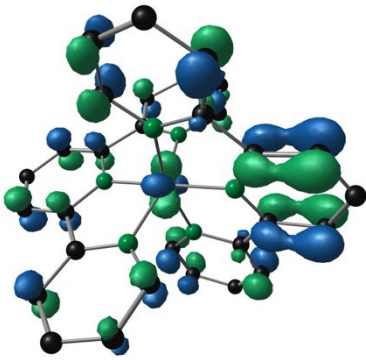
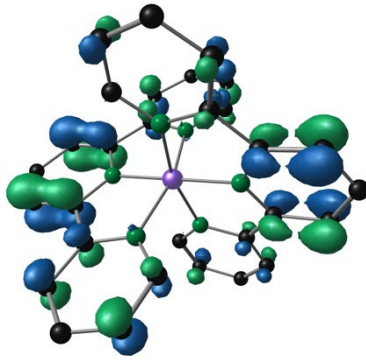
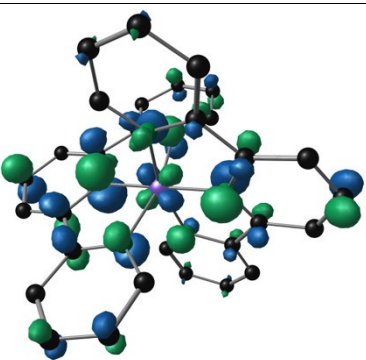
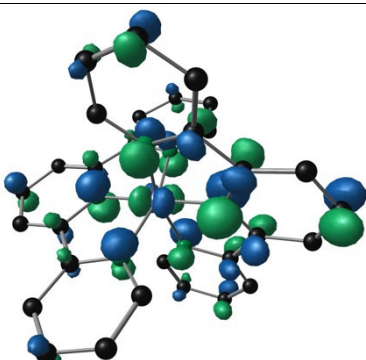
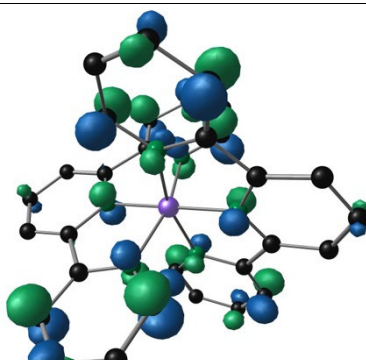
		
Particle, (3.645 e ⁻)	Particle, (6.205 e ⁻)	Particle, (16.40 e ⁻)
NTO 91	NTO 92	NTO 93
		
Hole, (16.40 e ⁻)	Hole, (6.205 e ⁻)	Hole, (3.645 e ⁻)
NTO 94	NTO 95	NTO 96

Figure S 9. NTOs of excited 31 (contr. value 0.05), peak at 306.6 nm of 10. The electron occupation of the occupied (particle) and unoccupied (hole) NTO pairs are indicated. A contour of $0.05 \text{ e}/\text{\AA}^3$ was used for the orbital plot. Atoms are colour coded (online version) as follows: Fe (purple), C (black), N (green).

2 Tables

Table S 1: Computed maximum wavelengths ($\lambda_{\text{max}}/\text{nm}$), transition energy (E in eV), oscillator strength (f), percentage (%) contribution, and type of transitions involved in the excitation of complexes L^1 - L^{19} .

L(n)	(N) State	E/eV	$\lambda_{\text{max}}/\text{nm}$	f	From	To	% contribution	Type of Transition
L¹	2	2.028	611.3	0.0009	HOMO-2	LUMO+11	41.5	MMCT
					HOMO-1	LUMO+10	49.2	MMCT
					HOMO	LUMO+1	2.4	MLCT
	3	2.028	611.3	0.0009	HOMO-2	LUMO+10	49.1	MMCT
					HOMO-1	LUMO+11	41.6	MMCT
					HOMO-2	LUMO+3	9.4	MLCT
	5	2.336	530.8	0.0074	HOMO-2	LUMO+11	2.2	MMCT
					HOMO	LUMO+1	82.1	MLCT
					HOMO	LUMO+3	2.1	MLCT
	6	2.337	530.5	0.0066	HOMO-2	LUMO+2	4.7	MLCT
					HOMO-1	LUMO+1	3.2	MLCT
					HOMO-1	LUMO+3	10.8	MLCT
					HOMO	LUMO	17.8	MLCT
					HOMO	LUMO+2	56.6	MLCT
	8	2.57	481.7	0.0432	HOMO-2	LUMO	5.3	MLCT
					HOMO-2	LUMO+2	17.3	MLCT
					HOMO-2	LUMO+10	10.0	MMCT
					HOMO-1	LUMO+1	28.7	MLCT
					HOMO-1	LUMO+3	16.5	MLCT
					HOMO-1	LUMO+11	11.4	MMCT
	12	2.72	455.8	0.0991	HOMO	LUMO+2	6.0	MLCT
					HOMO-2	LUMO	2.7	MLCT
					HOMO-2	LUMO+2	2.7	MLCT
					HOMO-1	LUMO+1	5.3	MLCT
					HOMO	LUMO	68.7	MLCT
	31	4.179	296.7	0.4074	HOMO	LUMO+2	18.2	MLCT
					HOMO-4	LUMO	6.5	LLCT
					HOMO-4	LUMO + 2	24.4	LLCT
					HOMO-3	LUMO + 1	51.2	LLCT
					HOMO-3	LUMO + 3	2.4	LLCT
	32	4.179	296.7	0.4073	HOMO	LUMO + 6	4.3	MLCT
					HOMO-4	LUMO + 1	29.5	LLCT
					HOMO-3	LUMO	11.6	LLCT
					HOMO-3	LUMO + 1	2.1	LLCT
					HOMO-3	LUMO + 2	42.0	LLCT
	48	5.002	247.9	0.4707	HOMO	LUMO + 5	4.2	MLCT
					HOMO-9	LUMO + 3	4.5	LLCT
					HOMO-8	LUMO + 1	12.4	LLCT
					HOMO-7	LUMO	5.4	LLCT
					HOMO-7	LUMO + 2	7.1	LLCT
					HOMO-6	LUMO + 1	17.2	MLCT

					HOMO-5	LUMO	5.4	MLCT
					HOMO-5	LUMO + 2	12.4	LLCT
					HOMO-4	LUMO + 4	6.9	LLCT
					HOMO-3	LUMO + 7	6.1	LLCT
					HOMO-2	LUMO + 8	4.0	MLCT
					HOMO-1	LUMO + 9	4.0	MLCT
					HOMO-2	LUMO + 10	14.4	MMCT
					HOMO-1	LUMO + 11	7.4	MMCT
					HOMO	LUMO + 1	75.6	MLCT
					HOMO-2	LUMO + 11	7.4	MMCT
L²	2	2.094	592.1	0.0035	HOMO-1	LUMO + 10	14.4	MMCT
					HOMO	LUMO	75.6	MLCT
					HOMO-2	LUMO + 11	7.4	MMCT
	3	2.094	592.1	0.0035	HOMO-1	LUMO + 10	14.4	MMCT
					HOMO	LUMO	75.6	MLCT
					HOMO-2	LUMO + 10	4.7	MMCT
	5	2.241	553.2	0.0002	HOMO-2	LUMO + 11	33.1	MMCT
					HOMO-1	LUMO + 10	33.3	MMCT
					HOMO-1	LUMO + 11	4.9	MMCT
					HOMO	LUMO	18.7	MLCT
					HOMO	LUMO + 1	2.7	MLCT
	6	2.241	553.2	0.0002	HOMO-2	LUMO + 10	33.3	MMCT
					HOMO-2	LUMO + 11	4.9	MMCT
					HOMO-1	LUMO + 10	4.7	MMCT
					HOMO-1	LUMO + 11	33.1	MMCT
					HOMO	LUMO	2.7	MLCT
	8	2.61	475.6	0.0941	HOMO	LUMO + 1	18.7	MLCT
					HOMO-2	LUMO + 1	47.5	MLCT
					HOMO-1	LUMO	47.5	MLCT
					HOMO	LUMO + 2	3.6	MLCT
					HOMO	LUMO + 2	95.3	MLCT
	13	2.934	422.7	0.0745	HOMO	LUMO + 2	95.3	MLCT
	21	3.791	327.1	0.1755	HOMO-4	LUMO + 1	34.4	LLCT
					HOMO-3	LUMO	46.4	LLCT
					HOMO	LUMO + 4	16.5	MLCT
	22	3.791	327.1	0.1756	HOMO-4	LUMO	34.4	LLCT
					HOMO-3	LUMO + 1	46.4	LLCT
					HOMO	LUMO + 5	16.5	MLCT
	28	4.041	306.8	0.3109	HOMO-4	LUMO + 1	30.0	LLCT
					HOMO	LUMO + 4	67.8	MLCT
	29	4.041	306.8	0.3109	HOMO-4	LUMO	29.9	LLCT
					HOMO	LUMO + 5	67.8	MLCT
	44	4.462	277.8	0.3934	HOMO-4	LUMO + 2	38.8	LLCT
					HOMO-3	LUMO + 3	41.7	LLCT
					HOMO-2	LUMO + 4	3.9	MLCT
					HOMO-2	LUMO + 9	3.4	MLCT
					HOMO-1	LUMO + 5	3.9	MLCT
					HOMO-1	LUMO + 8	3.4	MLCT
					HOMO-1	LUMO + 8	3.4	MLCT
L³	2	2.09	593.4	0.0025	HOMO-2	LUMO + 12	2.5	MLCT
					HOMO-2	LUMO + 14	36.6	MMCT
					HOMO-1	LUMO + 15	27.7	MMCT
	3	2.09	592.6	0.0028	HOMO	LUMO + 1	28.1	MLCT
					HOMO-2	LUMO + 15	28.4	MMCT
					HOMO-1	LUMO + 12	2.4	MLCT
	5	2.21	561.03	0.003	HOMO-1	LUMO + 14	35.7	MMCT
					HOMO	LUMO	28.6	MLCT
					HOMO-2	LUMO + 15	17.0	MMCT

					HOMO-1	LUMO + 14	11.6	MMCT
					HOMO	LUMO	65.1	MLCT
6	2.21	559.9	0.0029		HOMO-2	LUMO + 14	12.0	MMCT
					HOMO-1	LUMO + 15	16.4	MMCT
					HOMO	LUMO + 1	65.6	MLCT
8	2.50	495	0.266		HOMO-2	LUMO + 1	47.2	MLCT
					HOMO-1	LUMO	47.3	MLCT
					HOMO	LUMO + 2	2.4	MLCT
12	2.814	440.7	0.123		HOMO	LUMO + 2	96.2	MLCT
28	3.90	317.8	0.2112		HOMO-4	LUMO + 1	16.7	LLCT
					HOMO-3	LUMO	30.9	LLCT
					HOMO-2	LUMO + 8	15.3	MLCT
					HOMO-1	LUMO + 9	10.3	MLCT
					HOMO-1	LUMO + 11	2.0	MLCT
					HOMO	LUMO + 4	7.1	MLCT
					HOMO	LUMO + 6	9.1	MLCT
					HOMO	LUMO + 11	3.5	MLCT
29	3.90	317.7	0.2153		HOMO-4	LUMO	18.3	LLCT
					HOMO-3	LUMO + 1	28.1	LLCT
					HOMO-2	LUMO + 9	10.7	MLCT
					HOMO-1	LUMO + 8	14.8	MLCT
					HOMO	LUMO + 5	8.6	MLCT
					HOMO	LUMO + 7	8.7	MLCT
					HOMO	LUMO + 10	4.2	MLCT
48	4.43	279.7	1.087		HOMO-4	LUMO + 2	52.4	LLCT
					HOMO-3	LUMO + 3	39.1	LLCT
					HOMO-2	LUMO + 14	35.9	MMCT
L⁴	2	2.104	589.2	0.0022	HOMO-2	LUMO + 15	3.4	MMCT
					HOMO-1	LUMO + 14	7.1	MMCT
					HOMO-1	LUMO + 15	28.2	MMCT
					HOMO	LUMO + 1	18.6	MLCT
3	2.109	588	0.0023		HOMO-2	LUMO + 14	6.9	MMCT
					HOMO-2	LUMO + 15	29.7	MMCT
					HOMO-1	LUMO + 14	36.0	MMCT
					HOMO-1	LUMO + 15	3.4	MMCT
					HOMO	LUMO	17.7	MLCT
4	2.245	552.2	0.0045		HOMO-2	LUMO + 14	7.8	MMCT
					HOMO-1	LUMO + 3	2.2	MLCT
					HOMO-1	LUMO + 15	11.3	MMCT
					HOMO	LUMO	23.9	MLCT
					HOMO	LUMO + 1	50.1	MLCT
5	2.248	551.7	0.0047		HOMO-2	LUMO + 1	3.1	MLCT
					HOMO-2	LUMO + 3	2.3	MLCT
					HOMO-2	LUMO + 15	9.2	MMCT
					HOMO-1	LUMO	3.0	MLCT
					HOMO-1	LUMO + 14	5.2	MMCT
					HOMO	LUMO	50.7	MLCT
					HOMO	LUMO + 1	21.6	MLCT
6	2.262	548.1	0.0002		HOMO-2	LUMO	13.2	MLCT
					HOMO-2	LUMO + 1	30.6	MLCT
					HOMO-1	LUMO	31.5	MLCT
					HOMO-1	LUMO + 1	11.1	MLCT
					HOMO-1	LUMO + 14	2.4	MMCT

	8	2.55	485.8	0.1636	HOMO	LUMO + 1	4.0	MLCT
					HOMO-2	LUMO	9.4	MLCT
					HOMO-2	LUMO + 1	36.8	MLCT
					HOMO-1	LUMO	37.7	MLCT
	12	2.805	442	0.1171	HOMO-1	LUMO + 1	9.9	MLCT
					HOMO	LUMO + 2	3.6	MLCT
					HOMO	LUMO + 2	94.3	MLCT
					30	4.009	309.3	0.4226
	31	4.012	309	0.4272	HOMO-4	LUMO	21.9	LLCT
					HOMO-3	LUMO	49.7	LLCT
					HOMO-3	LUMO + 1	3.8	LLCT
					HOMO	LUMO + 4	12.5	MLCT
	42	4.401	281.7	0.8823	HOMO-4	LUMO + 1	22.6	LLCT
					HOMO-3	LUMO	3.9	LLCT
					HOMO-3	LUMO + 1	49.2	LLCT
					HOMO	LUMO + 5	12.4	MLCT
					HOMO-6	LUMO	14.0	LLCT
					HOMO-7	LUMO + 1	16.0	LLCT
					HOMO-5	LUMO	13.9	LLCT
					HOMO-5	LUMO + 1	14.1	LLCT
					HOMO-4	LUMO + 2	10.8	LLCT
					HOMO-3	LUMO + 2	3.2	LLCT
					HOMO-3	LUMO + 3	20.8	LLCT
L⁵	2	2.087	594.1	0.0022	HOMO-2	LUMO + 12	43.2	MMCT
					HOMO-1	LUMO + 15	30.5	MMCT
					HOMO	LUMO + 1	20.6	MLCT
					3	2.09	593.4	0.0024
	5	2.22	558.4	0.0038	HOMO-2	LUMO + 15	31.4	MMCT
					HOMO-1	LUMO + 12	42.4	MMCT
					HOMO	LUMO	20.7	MLCT
					HOMO-2	LUMO + 3	2.2	MLCT
	6	2.224	557.4	0.0038	HOMO-2	LUMO + 15	12.5	MMCT
					HOMO-1	LUMO + 12	8.5	MMCT
					HOMO	LUMO	73.1	MLCT
					HOMO-2	LUMO + 12	8.9	MMCT
	8	2.51	494.8	0.2752	HOMO-1	LUMO + 15	12.2	MMCT
					HOMO	LUMO + 1	73.3	MLCT
					HOMO-2	LUMO + 1	47.6	MLCT
					HOMO-1	LUMO	47.6	MLCT
	12	2.821	439.5	0.1233	HOMO	LUMO + 2	2.2	MLCT
					HOMO	LUMO + 2	96.7	MLCT
					30	3.942	314.6	0.2747
					HOMO-4	LUMO + 1	21.4	LLCT
	31	3.944	314.4	0.2998	HOMO-3	LUMO	41.1	LLCT
					HOMO-1	LUMO + 7	15.2	MLCT
					HOMO	LUMO + 4	15.4	MLCT
					HOMO-4	LUMO	24.4	LLCT
	37	4.15	298.8	0.1883	HOMO-3	LUMO + 1	38.9	LLCT
					HOMO-2	LUMO + 7	13.4	MLCT
					HOMO	LUMO + 5	16.0	MLCT
					HOMO-2	LUMO + 4	7.4	MLCT
L⁶	2	2.09	593.15	0.0021	HOMO-2	LUMO + 8	43.9	MLCT
					HOMO-1	LUMO + 5	6.5	MLCT
					HOMO-1	LUMO + 9	39.1	MLCT
					HOMO-2	LUMO + 12	44.4	MMCT
					HOMO-1	LUMO + 13	7.2	MLCT

					HOMO-1	LUMO + 15	24.8	MMCT
					HOMO	LUMO + 1	18.0	MLCT
3	2.093	592.25	0.0022		HOMO-2	LUMO + 13	7.5	MLCT
					HOMO-2	LUMO + 15	25.5	MMCT
					HOMO-1	LUMO + 12	43.8	MMCT
					HOMO	LUMO	17.7	MLCT
5	2.232	555.62	0.0042		HOMO-2	LUMO + 3	2.5	MLCT
					HOMO-2	LUMO + 13	2.2	MLCT
					HOMO-2	LUMO + 15	8.6	MMCT
					HOMO-1	LUMO + 12	7.0	MMCT
					HOMO	LUMO	75.0	MLCT
6	2.235	554.73	0.0042		HOMO-2	LUMO + 12	7.6	MMCT
					HOMO-1	LUMO + 3	2.1	MLCT
					HOMO-1	LUMO + 13	2.5	MLCT
					HOMO-1	LUMO + 15	8.4	MMCT
					HOMO	LUMO + 1	76.4	MLCT
8	2.52	492.84	0.2497		HOMO-2	LUMO + 1	47.6	MLCT
					HOMO-1	LUMO	47.8	MLCT
					HOMO	LUMO + 2	2.5	MLCT
12	2.812	440.88	0.1216		HOMO	LUMO + 2	96.1	MLCT
30	3.976	311.86	0.3762		HOMO-4	LUMO + 1	23.5	LLCT
					HOMO-3	LUMO	51.1	LLCT
					HOMO-1	LUMO + 7	2.3	MLCT
					HOMO	LUMO + 4	14.9	MLCT
31	3.979	311.63	0.4019		HOMO-4	LUMO	26.4	LLCT
					HOMO-3	LUMO + 1	48.0	LLCT
					HOMO-2	LUMO + 7	2.1	MLCT
					HOMO	LUMO + 5	15.2	MLCT
41	4.349	285.07	0.9685		HOMO-6	LUMO	43.1	LLCT
					HOMO-5	LUMO + 1	41.1	LLCT
					HOMO-4	LUMO + 2	2.4	LLCT
					HOMO-3	LUMO + 3	5.9	LLCT
L7	2	1.97	630.82	0.0005	HOMO-9	LUMO + 10	2.3	LMCT
					HOMO-2	LUMO + 11	37.8	MMCT
					HOMO-1	LUMO + 10	56.0	MMCT
					HOMO-1	LUMO + 10	2.4	MMCT
3	1.97	630.8	0.0005		HOMO-10	LUMO + 10	2.3	LMCT
					HOMO-2	LUMO + 10	55.5	MMCT
					HOMO-1	LUMO + 11	38.3	MMCT
					HOMO-2	LUMO + 10	2.4	MMCT
5	2.39	519.84	0.0061		HOMO-2	LUMO + 3	7.5	MLCT
					HOMO	LUMO + 1	87.5	MLCT
					HOMO-1	LUMO + 3	7.4	MLCT
					HOMO	LUMO	8.6	MLCT
6	2.39	519.78	0.0061		HOMO	LUMO + 2	79.0	MLCT
					HOMO-2	LUMO	3.9	MLCT
					HOMO-2	LUMO + 2	37.3	MLCT
					HOMO-2	LUMO + 10	2.8	MMCT
					HOMO-1	LUMO + 1	40.7	MLCT
					HOMO-1	LUMO + 3	3.9	MLCT

					HOMO-1	LUMO + 11	3.6	MMCT
					HOMO	LUMO	5.8	MLCT
14	2.75	450.73	0.0768		HOMO-2	LUMO + 2	3.0	MLCT
					HOMO-1	LUMO + 1	3.2	MLCT
					HOMO-1	LUMO + 3	5.5	MLCT
					HOMO	LUMO	79.8	MLCT
					HOMO	LUMO + 2	4.2	MLCT
35	4.31	287.7	0.2093		HOMO-10	LUMO	5.3	LLCT
					HOMO-9	LUMO + 3	4.1	LLCT
					HOMO-6	LUMO + 2	16.9	LLCT
					HOMO-3	LUMO + 1	62.3	LLCT
36	4.31	287.7	0.2094		HOMO-10	LUMO + 3	4.0	LLCT
					HOMO-9	LUMO	5.3	LLCT
					HOMO-6	LUMO + 1	17.9	LLCT
					HOMO-5	LUMO	2.5	LLCT
					HOMO-3	LUMO	4.4	LLCT
					HOMO-3	LUMO + 2	58.6	LLCT
L ⁸	2	2.06	600.63	0.0021	HOMO-2	LUMO + 10	46.9	MMCT
					HOMO-1	LUMO + 11	36.0	MMCT
					HOMO	LUMO + 1	12.1	MLCT
3	2.06	600.62	0.0021		HOMO-2	LUMO + 11	36.0	MMCT
					HOMO-1	LUMO + 10	46.9	MMCT
					HOMO	LUMO	12.1	MLCT
5	2.23	557.21	0.0061		HOMO-2	LUMO + 3	2.1	MLCT
					HOMO-2	LUMO + 11	7.0	MMCT
					HOMO-1	LUMO + 10	4.1	MMCT
					HOMO	LUMO	75.3	MLCT
					HOMO	LUMO + 1	7.9	MLCT
6	2.23	557.21	0.0061		HOMO-2	LUMO + 10	4.1	MMCT
					HOMO-1	LUMO + 3	2.1	MLCT
					HOMO-1	LUMO + 11	7.0	MMCT
					HOMO	LUMO	7.9	MLCT
					HOMO	LUMO + 1	75.3	MLCT
8	2.49	497.62	0.0828		HOMO-2	LUMO + 1	47.5	MLCT
					HOMO-1	LUMO	47.5	MLCT
					HOMO	LUMO + 2	2.9	MLCT
12	2.77	447.13	0.0729		HOMO	LUMO + 2	96.5	MLCT
35	4.12	300.75	0.4894		HOMO-4	LUMO + 1	27.6	LLCT
					HOMO-3	LUMO	55.1	LLCT
					HOMO	LUMO + 5	9.9	MLCT
36	4.12	300.75	0.4894		HOMO-4	LUMO	27.6	LLCT
					HOMO-3	LUMO + 1	55.1	LLCT
					HOMO	LUMO + 6	9.9	MLCT
L ⁹	2	2.09	593.33	0.0022	HOMO-2	LUMO + 14	43.7	MMCT
					HOMO-1	LUMO + 15	30.3	MMCT
					HOMO	LUMO + 3	19.1	MLCT
3	2.09	592.51	0.0023		HOMO-2	LUMO + 15	31.2	MMCT
					HOMO-1	LUMO + 14	43.1	MMCT
					HOMO	LUMO + 2	18.9	MLCT
5	2.23	556.82	0.0029		HOMO-2	LUMO + 3	14.4	MLCT

				HOMO-2	LUMO + 15	8.5	MMCT
				HOMO-1	LUMO + 2	13.7	MLCT
				HOMO-1	LUMO + 14	5.7	MMCT
				HOMO	LUMO + 2	52.4	MLCT
6	2.23	555.8	0.0039	HOMO-2	LUMO + 14	8.1	MMCT
				HOMO-1	LUMO + 15	11.1	MMCT
				HOMO	LUMO + 3	74.5	MLCT
8	2.51	493.45	0.2544	HOMO-2	LUMO	2.1	MLCT
				HOMO-2	LUMO + 3	45.6	MLCT
				HOMO-1	LUMO + 1	2.1	MLCT
				HOMO-1	LUMO + 2	45.5	MLCT
				HOMO	LUMO + 4	2.4	MLCT
18	2.82	440.25	0.1232	HOMO	LUMO + 4	95.4	MLCT
46	3.98	311.89	0.3344	HOMO-4	LUMO + 3	23.3	LLCT
				HOMO-3	LUMO + 2	49.6	LLCT
				HOMO-1	LUMO + 9	4.4	MLCT
				HOMO	LUMO + 6	15.6	MLCT
47	3.98	311.62	0.4012	HOMO-4	LUMO + 2	26.1	LLCT
				HOMO-3	LUMO + 3	47.4	LLCT
				HOMO-2	LUMO + 9	4.0	MLCT
				HOMO	LUMO + 7	15.9	MLCT
49	4.12	300.85	0.4752	HOMO-8	LUMO + 1	45.0	LLCT
				HOMO-7	LUMO	45.2	LLCT
				HOMO-5	LUMO	2.1	LLCT
50	4.13	300.3	0.3181	HOMO-8	LUMO	44.1	LLCT
				HOMO-7	LUMO + 1	44.2	LLCT
				HOMO-5	LUMO + 1	2.0	LLCT
2	2.09	592.21	0.0016	HOMO-2	LUMO + 10	48.1	MMCT
				HOMO-1	LUMO + 11	38.8	MMCT
				HOMO	LUMO + 1	9.5	MLCT
3	2.09	592.2	0.0016	HOMO-2	LUMO + 11	38.8	MMCT
				HOMO-1	LUMO + 10	48.1	MMCT
				HOMO	LUMO	9.5	MLCT
4	2.27	545.47	0.0066	HOMO-2	LUMO + 10	3.2	MMCT
				HOMO-1	LUMO + 3	2.8	MLCT
				HOMO-1	LUMO + 11	7.0	MMCT
				HOMO	LUMO + 1	85.2	MLCT
5	2.27	545.47	0.0066	HOMO-2	LUMO + 3	2.8	MLCT
				HOMO-2	LUMO + 11	7.0	MMCT
				HOMO-1	LUMO + 10	3.2	MMCT
				HOMO	LUMO	85.3	MLCT
8	2.59	478.55	0.0731	HOMO-2	LUMO + 1	47.4	MLCT
				HOMO-1	LUMO	47.4	MLCT
				HOMO	LUMO+2	4.0	MLCT
12	2.84	436.5	0.0787	HOMO	LUMO+2	94.9	MLCT
30	4.04	306.64	0.4794	HOMO-4	LUMO + 1	22.7	LLCT
				HOMO-3	LUMO	59.6	LLCT
				HOMO	LUMO + 5	13.4	MLCT
31	4.04	306.64	0.4793	HOMO-4	LUMO	22.7	LLCT
				HOMO-3	LUMO + 1	59.6	LLCT

					HOMO	LUMO + 6	13.4	MLCT
L¹¹	2	2.01	615.61	0.0007	HOMO-10	LUMO + 8	2.7	LMCT
					HOMO-9	LUMO + 11	2.2	LMCT
					HOMO-1	LUMO + 8	51.9	MMCT
					HOMO	LUMO + 11	40.0	MMCT
					HOMO-1	LUMO + 8	2.2	MMCT
	3	2.01	615.57	0.0007	HOMO-10	LUMO + 11	2.2	LMCT
					HOMO-9	LUMO + 8	2.7	LMCT
					HOMO-1	LUMO + 11	40.0	MMCT
					HOMO	LUMO + 8	51.6	MMCT
					HOMO	LUMO + 8	2.2	MMCT
	5	2.36	524.43	0.0047	HOMO-2	LUMO + 1	64.9	MLCT
					HOMO	LUMO + 1	2.8	MLCT
					HOMO	LUMO + 3	26.2	MLCT
					HOMO	LUMO + 5	2.2	MLCT
	6	2.37	524.2	0.0048	HOMO-2	LUMO	66.3	MLCT
					HOMO-1	LUMO + 3	26.6	MLCT
					HOMO-1	LUMO + 5	2.2	MLCT
	8	2.51	494.31	0.0574	HOMO-1	LUMO + 1	48.1	MLCT
					HOMO	LUMO	47.7	MLCT
	16	2.94	422.39	0.0704	HOMO-2	LUMO + 2	96.8	MLCT
	35	4.01	309.48	0.3602	HOMO-6	LUMO	16.1	LLCT
					HOMO-3	LUMO + 1	64.8	LLCT
					HOMO-2	LUMO + 6	12.5	MLCT
	36	4.01	309.44	0.3544	HOMO-6	LUMO + 1	15.8	LLCT
					HOMO-3	LUMO	64.0	LLCT
					HOMO-2	LUMO + 7	13.5	MLCT
L¹²	2	2.1405	579.22	0.0015	HOMO-2	LUMO + 10	47.3	MMCT
					HOMO-1	LUMO + 11	34.4	MMCT
					HOMO	LUMO	10.7	MLCT
					HOMO	LUMO + 1	3.0	MLCT
	3	2.1405	579.22	0.0015	HOMO-2	LUMO + 11	34.4	MMCT
					HOMO-1	LUMO + 10	47.3	MMCT
					HOMO	LUMO	3.0	MLCT
					HOMO	LUMO + 1	10.7	MLCT
	5	2.3039	538.15	0.0037	HOMO-2	LUMO + 10	5.5	MMCT
					HOMO-1	LUMO + 2	2.8	MLCT
					HOMO-1	LUMO + 11	8.8	MMCT
					HOMO	LUMO	62.7	MLCT
					HOMO	LUMO + 1	18.0	MLCT
	6	2.3039	538.14	0.0037	HOMO-2	LUMO + 2	2.8	MLCT
					HOMO-2	LUMO + 11	8.8	MMCT
					HOMO-1	LUMO + 10	5.5	MMCT
					HOMO	LUMO	18.0	MLCT
					HOMO	LUMO + 1	62.7	MLCT
	8	2.6274	471.89	0.0655	HOMO-2	LUMO	36.7	MLCT
					HOMO-2	LUMO + 1	11.4	MLCT
					HOMO-1	LUMO	11.4	MLCT
					HOMO-1	LUMO + 1	36.7	MLCT
	15	3.1176	397.69	0.0651	HOMO	LUMO + 3	96.2	MLCT

L ¹³	25	3.6996	335.13	0.1469	HOMO-6	LUMO + 1	29.0	LLCT
					HOMO-5	LUMO	12.7	LLCT
					HOMO-5	LUMO + 1	34.3	LLCT
					HOMO	LUMO + 5	5.4	MLCT
					HOMO	LUMO + 6	15.6	MLCT
	26	3.6996	335.13	0.1469	HOMO-6	LUMO	29.0	LLCT
					HOMO-5	LUMO	34.3	LLCT
					HOMO-5	LUMO + 1	12.7	LLCT
					HOMO	LUMO + 5	15.6	MLCT
					HOMO	LUMO + 6	5.4	MLCT
	40	3.945	314.29	0.2714	HOMO-6	LUMO	28.4	LLCT
					HOMO-6	LUMO + 1	10.3	LLCT
					HOMO-1	LUMO + 7	4.3	MLCT
					HOMO	LUMO + 5	50.5	MLCT
					HOMO	LUMO + 5	50.5	MLCT
	41	3.945	314.28	0.2714	HOMO-6	LUMO	10.3	LLCT
					HOMO-6	LUMO + 1	28.4	LLCT
					HOMO-2	LUMO + 7	4.3	MLCT
					HOMO	LUMO + 6	50.5	MLCT
					HOMO	LUMO + 6	50.5	MLCT
L ¹³	2	2.0799	596.09	0.0009	HOMO-2	LUMO + 10	15.6	MMCT
					HOMO-2	LUMO + 11	3.6	MMCT
					HOMO-1	LUMO + 10	36.3	MMCT
					HOMO-1	LUMO + 11	37.5	MMCT
					HOMO	LUMO	3.5	MLCT
	3	2.08	596.09	0.0009	HOMO-2	LUMO + 10	36.3	MMCT
					HOMO-2	LUMO + 11	37.5	MMCT
					HOMO-1	LUMO + 10	15.6	MMCT
					HOMO-1	LUMO + 11	3.6	MMCT
					HOMO	LUMO + 1	3.5	MLCT
					HOMO	LUMO + 1	3.5	MLCT
	5	2.3423	529.33	0.0083	HOMO-2	LUMO + 2	3.4	MLCT
					HOMO-1	LUMO + 2	4.7	MLCT
					HOMO-1	LUMO + 11	2.6	MMCT
					HOMO	LUMO	77.1	MLCT
					HOMO	LUMO + 1	8.5	MLCT
					HOMO	LUMO + 1	8.5	MLCT
	6	2.3423	529.33	0.0083	HOMO-2	LUMO + 2	4.7	MLCT
					HOMO-2	LUMO + 11	2.6	MMCT
					HOMO-1	LUMO + 2	3.4	MLCT
					HOMO	LUMO	8.5	MLCT
					HOMO	LUMO + 1	77.1	MLCT
					HOMO	LUMO + 1	77.1	MLCT
	8	2.5552	485.23	0.0502	HOMO-2	LUMO	43.3	MLCT
					HOMO-2	LUMO + 1	5.3	MLCT
					HOMO-1	LUMO	5.3	MLCT
					HOMO-1	LUMO + 1	43.3	MLCT
					HOMO-1	LUMO + 1	43.3	MLCT
	16	3.038	408.11	0.0697	HOMO	LUMO + 3	96.5	MLCT
	34	3.9058	317.43	0.3136	HOMO-3	LUMO	36.9	LLCT
					HOMO-3	LUMO + 1	23.7	LLCT
					HOMO-2	LUMO + 7	4.0	MLCT
					HOMO	LUMO + 5	15.0	MLCT
					HOMO	LUMO + 6	15.3	MLCT
					HOMO	LUMO + 6	15.3	MLCT
	35	3.9059	317.43	0.3136	HOMO-3	LUMO	23.7	LLCT
					HOMO-3	LUMO + 1	36.9	LLCT
					HOMO-3	LUMO + 1	36.9	LLCT

					HOMO-1	LUMO + 7	4.0	MLCT
					HOMO	LUMO + 5	15.3	MLCT
					HOMO	LUMO + 6	15.0	MLCT
L ¹⁴	2	2.0492	605.05	0.0031	HOMO-2	LUMO + 14	19.6	MMCT
					HOMO-1	LUMO + 15	11.5	MMCT
					HOMO	LUMO + 1	35.5	MLCT
					HOMO	LUMO + 3	29.8	MLCT
3	2.05	604.79	0.0034	HOMO-2	LUMO + 15	11.0	MMCT	
					HOMO-1	LUMO + 14	18.2	MMCT
					HOMO	LUMO	36.9	MLCT
					HOMO	LUMO + 2	30.4	MLCT
5	2.1624	573.36	0.0004	HOMO-2	LUMO + 15	33.2	MMCT	
					HOMO-1	LUMO + 14	32.6	MMCT
					HOMO	LUMO	18.1	MLCT
					HOMO	LUMO + 2	11.7	MLCT
6	2.1645	572.81	0.0005	HOMO-2	LUMO + 14	32.5	MMCT	
					HOMO-1	LUMO + 15	31.5	MMCT
					HOMO	LUMO + 1	19.2	MLCT
					HOMO	LUMO + 3	12.5	MLCT
8	2.3583	525.73	0.5029	HOMO-2	LUMO + 1	35.1	MLCT	
					HOMO-2	LUMO + 3	14.0	MLCT
					HOMO-1	LUMO	35.4	MLCT
					HOMO-1	LUMO + 2	13.9	MLCT
14	2.8205	439.58	0.1427	HOMO-1	LUMO	2.0	MLCT	
					HOMO	LUMO + 4	92.2	MLCT
					HOMO-6	LUMO	43.0	LLCT
					HOMO-5	LUMO + 1	43.1	LLCT
38	3.8727	320.15	1.3631	HOMO-2	LUMO + 8	2.9	MLCT	
					HOMO-1	LUMO + 7	3.1	MLCT
					HOMO	LUMO + 6	4.9	MLCT
L ¹⁵	2	2.0395	607.93	0.0012	HOMO-4	LUMO + 12	35.8	MMCT
					HOMO-4	LUMO + 13	25.9	MMCT
					HOMO-3	LUMO + 12	5.0	MMCT
					HOMO-2	LUMO + 1	5.1	MLCT
					HOMO-1	LUMO + 12	11.7	LMCT
					HOMO-1	LUMO + 13	3.4	LMCT
					HOMO	LUMO + 13	5.2	LMCT
3	2.044	606.57	0.0012	HOMO-4	LUMO + 12	4.7	MMCT	
					HOMO-3	LUMO + 12	37.2	MMCT
					HOMO-3	LUMO + 13	26.9	MMCT
					HOMO-2	LUMO	4.8	MLCT
					HOMO-1	LUMO + 13	5.0	LMCT
					HOMO	LUMO + 12	11.1	LMCT
					HOMO	LUMO + 13	2.8	LMCT
5	2.2709	545.97	0.0058	HOMO-4	LUMO + 13	2.7	MMCT	
					HOMO-3	LUMO + 3	4.2	MLCT
					HOMO-2	LUMO	23.1	MLCT
					HOMO-2	LUMO + 1	60.9	MLCT
					HOMO	LUMO + 3	2.3	LLCT
6	2.2764	544.66	0.0056	HOMO-4	LUMO + 3	4.3	MLCT	

8	2.3313	531.81	0.892	HOMO-3	LUMO + 13	2.6	MMCT
				HOMO-2	LUMO	60.6	MLCT
				HOMO-2	LUMO + 1	22.7	MLCT
				HOMO-1	LUMO + 3	2.8	LLCT
				HOMO-4	LUMO	8.8	MLCT
				HOMO-4	LUMO + 1	2.7	MLCT
				HOMO-3	LUMO	2.4	MLCT
				HOMO-3	LUMO + 1	9.7	MLCT
				HOMO-1	LUMO	6.8	MLCT
				HOMO-1	LUMO + 1	31.4	LLCT
				HOMO	LUMO	31.2	LLCT
				HOMO	LUMO + 1	5.9	LLCT
				HOMO-3	LUMO + 1	2.1	MLCT
				HOMO-2	LUMO + 2	91.9	MLCT
				HOMO-4	LUMO	27.2	MLCT
16	2.7748	446.82	0.2207	HOMO-4	LUMO + 1	7.6	MLCT
				HOMO-3	LUMO + 1	32.2	MLCT
				HOMO-2	LUMO + 2	5.8	MLCT
				HOMO-1	LUMO	6.4	LLCT
				HOMO-1	LUMO + 1	11.9	LLCT
				HOMO	LUMO	2.7	LLCT
				HOMO	LUMO + 1	2.1	LLCT
				HOMO-4	LUMO + 5	13.3	MLCT
19	2.9445	421.07	0.2198	HOMO-1	LUMO + 5	48.7	LLCT
				HOMO	LUMO + 5	25.3	LLCT
				HOMO	LUMO + 6	7.5	LLCT
				HOMO-4	LUMO + 5	4.6	MLCT
29	3.5162	352.61	0.3301	HOMO-4	LUMO + 8	4.6	MLCT
				HOMO-2	LUMO + 7	3.9	MLCT
				HOMO-1	LUMO + 8	54.3	LLCT
				HOMO	LUMO + 8	28.2	LLCT
				HOMO-4	LUMO + 13	2.9	LMCT
38	3.8691	320.44	0.5754	HOMO-3	LUMO + 12	3.9	LMCT
				HOMO-2	LUMO + 12	46.9	MMCT
				HOMO-1	LUMO + 13	32.3	MMCT
				HOMO	LUMO + 1	9.4	MLCT
3	2.076	597.3	0.0016	HOMO-4	LUMO + 12	4.0	LMCT
				HOMO-3	LUMO + 13	2.9	LMCT
				HOMO-2	LUMO + 13	33.5	MMCT
				HOMO-1	LUMO + 12	46.1	MMCT
5	2.256	549.6	0.0058	HOMO	LUMO	9.1	MLCT
				HOMO-2	LUMO + 3	3.4	MLCT
				HOMO-2	LUMO + 13	5.8	MMCT
				HOMO-1	LUMO + 12	3.0	MMCT
6	2.26	548.7	0.0057	HOMO	LUMO	84.7	MMCT
				HOMO-2	LUMO + 12	3.5	MLCT
				HOMO-1	LUMO + 3	3.2	MLCT
				HOMO-1	LUMO + 13	5.8	MMCT
8	2.504	495.11	0.3005	HOMO	LUMO + 1	84.4	MLCT
				HOMO-2	LUMO + 1	47.8	MLCT

					HOMO-1	LUMO	47.6	MLCT
	13	2.811	441.07	0.1294	HOMO	LUMO + 2	97.0	MLCT
	24	3.781	327.95	0.497	HOMO-4	LUMO	11.1	LLCT
					HOMO-3	LUMO + 1	10.5	LLCT
					HOMO-2	LUMO + 4	32.0	MLCT
					HOMO-1	LUMO + 5	41.8	MLCT
L ¹⁷	2	2.069	599.39	0.0014	HOMO-4	LUMO + 13	7.3	LMCT
					HOMO-3	LUMO + 12	9.9	LMCT
					HOMO-2	LUMO + 1	8.5	MLCT
					HOMO-1	LUMO + 12	41.4	MMCT
					HOMO	LUMO + 13	28.5	MMCT
	3	2.072	598.5	0.0016	HOMO-4	LUMO + 12	10.0	LMCT
					HOMO-3	LUMO + 13	7.3	LMCT
					HOMO-2	LUMO	8.1	MLCT
					HOMO-1	LUMO + 13	29.6	MMCT
					HOMO	LUMO + 12	40.7	MMCT
	5	2.26	548.7	0.006	HOMO-2	LUMO	85.3	MLCT
					HOMO-1	LUMO + 3	3.5	MLCT
					HOMO-1	LUMO + 13	4.6	MMCT
					HOMO	LUMO + 12	2.3	MMCT
	6	2.263	547.78	0.0058	HOMO-2	LUMO + 1	84.9	MLCT
					HOMO-1	LUMO + 12	2.7	MMCT
					HOMO	LUMO + 3	3.2	MLCT
					HOMO	LUMO + 13	4.7	MMCT
	8	2.487	498.64	0.366	HOMO-4	LUMO	2.7	LLCT
					HOMO-3	LUMO + 1	2.8	LLCT
					HOMO-1	LUMO + 1	46.0	MLCT
					HOMO	LUMO	45.5	MLCT
	14	2.803	442.27	0.14	HOMO-2	LUMO + 2	97.2	MLCT
	19	3.51	353.19	0.7222	HOMO-4	LUMO	45.7	LLCT
					HOMO-3	LUMO + 1	42.6	LLCT
					HOMO-2	LUMO + 4	2.1	MLCT
					HOMO-1	LUMO + 1	2.7	MLCT
					HOMO	LUMO	3.0	MLCT
	38	4.04	306.86	0.3913	HOMO-6	LUMO + 1	24.2	LLCT
					HOMO-5	LUMO	60.9	LLCT
					HOMO-2	LUMO + 5	8.8	MLCT
	39	4.044	306.56	0.426	HOMO-6	LUMO	27.6	LLCT
					HOMO-5	LUMO + 1	57.4	LLCT
					HOMO-2	LUMO + 6	8.9	MLCT
					HOMO-3	LUMO + 3	39.1	LLCT
L ¹⁸	2	2.063	601.09	0.0015	HOMO-4	LUMO + 14	41.7	MMCT
					HOMO-4	LUMO + 21	28.9	MMCT
					HOMO-2	LUMO + 1	8.6	MLCT
					HOMO-1	LUMO + 14	6.7	LMCT
					HOMO-1	LUMO + 21	4.0	LMCT
	3	2.069	599.17	0.0015	HOMO-3	LUMO + 14	44.1	MMCT
					HOMO-3	LUMO + 21	30.3	MMCT
					HOMO-2	LUMO	8.3	MLCT
					HOMO	LUMO + 14	5.0	LMCT

				HOMO	LUMO + 21	2.8	LMCT
5	2.253	550.34	0.0055	HOMO-4	LUMO + 14	2.8	MMCT
				HOMO-4	LUMO + 21	4.7	MMCT
				HOMO-3	LUMO + 3	3.4	MLCT
				HOMO-2	LUMO + 1	83.7	MLCT
6	2.258	549.05	0.0053	HOMO-4	LUMO + 3	3.4	MLCT
				HOMO-3	LUMO + 14	3.0	MMCT
				HOMO-3	LUMO + 21	4.8	MMCT
				HOMO-2	LUMO	83.3	MLCT
7	2.317	535.15	1.1572	HOMO-4	LUMO	12.8	MLCT
				HOMO-3	LUMO + 1	13.3	MLCT
				HOMO-1	LUMO	36.8	LLCT
				HOMO-1	LUMO + 1	4.0	LLCT
				HOMO	LUMO	3.8	LLCT
				HOMO	LUMO + 1	26.7	LLCT
15	2.741	452.26	0.2745	HOMO-4	LUMO	34.6	MLCT
				HOMO-3	LUMO + 1	5.5	MLCT
				HOMO-2	LUMO + 2	30.1	MLCT
				HOMO-2	LUMO + 3	8.0	MLCT
				HOMO-1	LUMO	16.0	LLCT
27	3.461	358.28	0.6322	HOMO-4	LUMO + 4	6.8	MLCT
				HOMO-1	LUMO + 4	76.0	LLCT
				HOMO-1	LUMO + 8	5.5	LLCT
				HOMO	LUMO + 4	2.2	LLCT
				HOMO	LUMO + 5	3.0	LLCT
2	2.084	594.83	0.0017	HOMO-2	LUMO + 10	27.8	MMCT
				HOMO-2	LUMO + 13	14.7	MMCT
				HOMO-1	LUMO + 10	17.4	MMCT
				HOMO-1	LUMO + 13	15.4	MMCT
				HOMO	LUMO + 1	12.3	MLCT
3	2.086	594.26	0.0019	HOMO-2	LUMO + 10	17.9	MMCT
				HOMO-2	LUMO + 13	16.6	MMCT
				HOMO-1	LUMO + 10	26.3	MMCT
				HOMO-1	LUMO + 13	14.5	MMCT
				HOMO	LUMO	12.0	MLCT
5	2.247	551.86	0.0053	HOMO-2	LUMO + 10	2.2	MMCT
				HOMO-2	LUMO + 13	4.4	MMCT
				HOMO-1	LUMO + 10	2.1	MMCT
				HOMO-1	LUMO + 13	2.7	MMCT
				HOMO	LUMO	82.0	MLCT
6	2.251	550.83	0.0051	HOMO-2	LUMO + 10	2.5	MMCT
				HOMO-2	LUMO + 13	2.7	MMCT
				HOMO-1	LUMO + 10	2.2	MMCT
				HOMO-1	LUMO + 13	4.2	MMCT
				HOMO	LUMO + 1	81.8	MLCT
8	2.512	493.53	0.2674	HOMO-2	LUMO	18.1	MLCT
				HOMO-2	LUMO + 1	28.3	MLCT
				HOMO-1	LUMO	28.9	MLCT
				HOMO-1	LUMO + 1	18.8	MLCT
				HOMO	LUMO + 2	2.2	MLCT

12	2.814	440.58	0.1242	HOMO	LUMO + 2	95.5	MLCT
38	3.996	310.24	0.3951	HOMO-8	LUMO	5.1	LLCT
				HOMO-8	LUMO + 1	15.5	LLCT
				HOMO-7	LUMO	2.1	LLCT
				HOMO-7	LUMO + 1	2.5	LLCT
				HOMO-6	LUMO	2.3	LLCT
				HOMO-6	LUMO + 2	2.6	LLCT
				HOMO-6	LUMO + 3	2.1	LLCT
				HOMO-5	LUMO	33.2	LLCT
				HOMO-5	LUMO + 1	15.6	LLCT
				HOMO	LUMO + 5	11.6	MLCT
39	4.003	309.71	0.4094	HOMO-8	LUMO	19.4	LLCT
				HOMO-8	LUMO + 1	6.0	LLCT
				HOMO-7	LUMO + 2	2.3	LLCT
				HOMO-6	LUMO	4.1	LLCT
				HOMO-6	LUMO + 1	5.2	LLCT
				HOMO-5	LUMO	14.2	LLCT
				HOMO-5	LUMO + 1	29.3	LLCT
				HOMO	LUMO + 4	11.2	MLCT
41	4.157	298.23	0.5274	HOMO-7	LUMO	11.2	LLCT
				HOMO-6	LUMO	27.4	LLCT
				HOMO-6	LUMO + 1	40.0	LLCT
				HOMO-5	LUMO	4.7	LLCT
				HOMO-5	LUMO + 1	3.8	LLCT
				HOMO-2	LUMO + 9	3.2	MLCT

3 Optimized coordinates of the DFT calculations.

Density functional theory (DFT) computations were conducted on the Fe(II) ($Q = 2$) molecules with spin $S = 0$ using the Gaussian 16 software package [1]. The M06 [2] functional with the Grimme's D3 empirical dispersion correction [3] and the CEP-121G basis set [4–6] was used. Optimizations were performed in Acetonitrile (MeCN) as implicit solvent using the IEFPCM solvent model [7] [8].

3.1 $[Fe(L^1)_2]^{2+}$

26	-0.000001000	0.000171000	-0.000225000
7	-0.291430000	-1.377713000	-1.398321000
6	-1.624315000	-1.645810000	-1.671063000
6	-2.005306000	-2.597351000	-2.633663000
6	-1.005183000	-3.295997000	-3.339816000
6	0.349300000	-3.021914000	-3.062204000
6	0.666456000	-2.057262000	-2.085818000
7	-1.897505000	0.000585000	-0.005868000
6	-2.564985000	-0.839901000	-0.857714000

6	-3.966049000	-0.868646000	-0.889634000
6	-4.668588000	-0.003059000	-0.014670000
6	-3.975211000	0.865459000	0.865040000
6	-2.570475000	0.838146000	0.839936000
7	-0.301341000	1.377100000	1.396010000
6	-1.636267000	1.645279000	1.659905000
6	-2.022935000	2.596767000	2.620389000
6	-1.027312000	3.294674000	3.333689000
6	0.328825000	3.019959000	3.065274000
6	0.652075000	2.055712000	2.090439000
7	0.301496000	1.397231000	-1.376263000
6	1.636490000	1.664983000	-1.640308000
6	2.023346000	2.626587000	-2.590584000
6	1.027851000	3.336833000	-3.291781000
6	-0.328352000	3.064315000	-3.021472000
6	-0.651794000	2.088673000	-2.058105000
7	1.897503000	0.000077000	0.005304000
6	2.570577000	0.847286000	-0.830734000
6	3.975324000	0.875047000	-0.855157000
6	4.668587000	-0.003603000	0.014517000
6	3.965934000	-0.879773000	0.878798000
6	2.564881000	-0.850460000	0.847214000
7	0.291274000	-1.397166000	1.378487000
6	1.624092000	-1.666165000	1.650598000
6	2.004901000	-2.627793000	2.603199000
6	1.004651000	-3.337023000	3.298538000
6	-0.349772000	-3.063380000	3.020190000
6	-0.666736000	-2.087665000	2.054801000
1	-3.059286000	-2.787598000	-2.826515000
1	-1.279499000	-4.036095000	-4.088419000
1	1.149586000	-3.539185000	-3.585237000
1	1.700607000	-1.816903000	-1.842155000
1	-4.522973000	-1.524646000	-1.554473000
1	-4.519079000	1.528887000	1.535783000
1	-3.077876000	2.788130000	2.807049000
1	-1.306482000	4.034486000	4.080758000
1	1.125825000	3.536303000	3.594198000
1	1.687709000	1.814720000	1.853790000
1	3.078337000	2.816316000	-2.778627000
1	1.307170000	4.084608000	-4.030823000
1	-1.125264000	3.590596000	-3.540645000
1	-1.687492000	1.848725000	-1.820677000
1	4.519282000	1.546656000	-1.517633000
1	4.522766000	-1.543896000	1.535601000
1	3.058834000	-2.817667000	2.796669000
1	1.278822000	-4.085038000	4.039284000
1	-1.150148000	-3.589064000	3.534626000
1	-1.700826000	-1.847216000	1.810972000
8	-6.042335000	-0.060057000	-0.073860000
1	-6.483134000	0.553788000	0.548587000
8	6.042323000	-0.060741000	0.073793000
1	6.483214000	0.561711000	-0.539981000

3.2 $[Fe(L^2)_2]^{2+}$

26	0.000000000	0.000085000	-0.000037000
7	0.298710000	-1.391138000	1.387822000
6	1.633873000	-1.657564000	1.654031000
6	2.023818000	-2.613197000	2.608004000
6	1.027806000	-3.319703000	3.312830000
6	-0.327853000	-3.048703000	3.041715000
6	-0.653741000	-2.078369000	2.073183000
7	1.880980000	0.000607000	-0.001055000
6	2.556240000	-0.841979000	0.839914000
6	3.968670000	-0.828192000	0.825869000
7	4.663855000	0.001511000	-0.002366000
6	3.967340000	0.830744000	-0.829949000
6	2.554888000	0.843624000	-0.842665000
7	0.296496000	1.391332000	-1.388471000
6	1.631250000	1.658545000	-1.655992000
6	2.019731000	2.614212000	-2.610537000
6	1.022644000	3.319905000	-3.314653000
6	-0.332594000	3.048050000	-3.042296000
6	-0.656984000	2.077757000	-2.073222000
7	-0.297140000	1.387987000	1.391565000
6	-1.632013000	1.654894000	1.658781000
6	-2.020920000	2.609009000	2.614702000
6	-1.024145000	3.313223000	3.320739000
6	0.331216000	3.041331000	3.049029000
6	0.656041000	2.072717000	2.078422000
7	-1.880980000	-0.000186000	0.000874000
6	-2.555281000	0.841205000	0.843798000
6	-3.967727000	0.827819000	0.830937000
7	-4.663855000	-0.000213000	0.001826000
6	-3.968283000	-0.828260000	-0.827739000
6	-2.555847000	-0.841606000	-0.841573000
7	-0.298066000	-1.388373000	-1.390838000
6	-1.633110000	-1.655458000	-1.657000000
6	-2.022629000	-2.610099000	-2.612142000
6	-1.026304000	-3.314786000	-3.318344000
6	0.329233000	-3.042891000	-3.047513000
6	0.654684000	-2.073671000	-2.077720000
1	3.078823000	-2.800434000	2.795249000
1	1.307389000	-4.063509000	4.055385000
1	-1.124592000	-3.572001000	3.563625000
1	-1.690698000	-1.843989000	1.838745000
1	4.553961000	-1.478061000	1.474349000
1	4.551595000	1.480995000	-1.478972000
1	3.074450000	2.802078000	-2.798783000
1	1.301090000	4.063715000	-4.057630000
1	-1.130144000	3.570664000	-3.563650000
1	-1.693594000	1.842792000	-1.837859000
1	-3.075722000	2.796811000	2.802538000
1	-1.302922000	4.055876000	4.064750000
1	1.128530000	3.562706000	3.571983000
1	1.692752000	1.837709000	1.843540000
1	-4.552284000	1.476682000	1.481080000
1	-4.553274000	-1.477127000	-1.477491000
1	-3.077550000	-2.797994000	-2.799203000
1	-1.305555000	-4.057858000	-4.061758000

1	1.126208000	-3.564707000	-3.570544000
1	1.691540000	-1.838595000	-1.843539000

3.3 $[Fe(L^3)_2]^{2+}$

26	0.000001000	-0.033181000	-0.000104000
7	0.278778000	1.352232000	1.392986000
6	1.609576000	1.627131000	1.667665000
6	1.984022000	2.582648000	2.628918000
6	0.978838000	3.276939000	3.332061000
6	-0.373462000	2.994846000	3.052891000
6	-0.684130000	2.027041000	2.077573000
7	1.890302000	-0.028388000	0.014225000
6	2.551809000	0.823478000	0.856750000
6	3.956465000	0.855909000	0.881080000
6	4.684207000	-0.003935000	0.017714000
6	3.974084000	-0.878236000	-0.845825000
6	2.568927000	-0.869538000	-0.825528000
7	0.306415000	-1.419640000	-1.384634000
6	1.642417000	-1.683786000	-1.644030000
6	2.035285000	-2.638075000	-2.598965000
6	1.043523000	-3.344000000	-3.309628000
6	-0.314117000	-3.074655000	-3.043884000
6	-0.643597000	-2.106346000	-2.075191000
7	-0.278850000	1.352366000	-1.393045000
6	-1.609662000	1.627199000	-1.667719000
6	-1.984158000	2.582742000	-2.628926000
6	-0.979009000	3.277135000	-3.332020000
6	0.373305000	2.995121000	-3.052843000
6	0.684024000	2.027282000	-2.077574000
7	-1.890300000	-0.028456000	-0.014402000
6	-2.551852000	0.823463000	-0.856837000
6	-3.956509000	0.855890000	-0.881099000
6	-4.684208000	-0.004010000	-0.017751000
6	-3.974037000	-0.878372000	0.845688000
6	-2.568882000	-0.869667000	0.825324000
7	-0.306341000	-1.419846000	1.384240000
6	-1.642331000	-1.683985000	1.643711000
6	-2.035150000	-2.638351000	2.598589000
6	-1.043352000	-3.344387000	3.309092000
6	0.314274000	-3.075081000	3.043240000
6	0.643705000	-2.106678000	2.074625000
1	3.036364000	2.779167000	2.824124000
1	1.248098000	4.019587000	4.079834000
1	-1.177437000	3.508107000	3.573971000
1	-1.717126000	1.781775000	1.834802000
1	4.478210000	1.515256000	1.572323000
1	4.509112000	-1.527069000	-1.537015000
1	3.091353000	-2.825015000	-2.783007000
1	1.327046000	-4.086202000	-4.052567000
1	-1.107960000	-3.597887000	-3.570587000
1	-1.680892000	-1.869789000	-1.842036000
1	-3.036510000	2.779203000	-2.824135000
1	-1.248307000	4.019802000	-4.079762000
1	1.177254000	3.508466000	-3.573880000

1	1.717031000	1.782075000	-1.834793000
1	-4.478285000	1.515286000	-1.572271000
1	-4.509027000	-1.527255000	1.536859000
1	-3.091209000	-2.825270000	2.782706000
1	-1.326838000	-4.086648000	4.051986000
1	1.108145000	-3.598408000	3.569808000
1	1.680989000	-1.870145000	1.841399000
6	6.176044000	0.015677000	0.014055000
6	6.912812000	-1.171035000	-0.198518000
6	6.878455000	1.229730000	0.222083000
6	8.323732000	-1.138443000	-0.199728000
6	8.283525000	1.239583000	0.213688000
6	9.027505000	0.059347000	0.003894000
1	6.395779000	-2.122073000	-0.336153000
1	6.334434000	2.162546000	0.363998000
6	-6.176045000	0.015621000	-0.013993000
6	-6.878454000	1.229685000	-0.221965000
6	-6.912818000	-1.171078000	0.198636000
6	-8.283523000	1.239562000	-0.213461000
6	-8.323738000	-1.138462000	0.199957000
6	-9.027508000	0.059340000	-0.003610000
1	-6.334432000	2.162495000	-0.363919000
1	-6.395794000	-2.122126000	0.336232000
1	10.116807000	0.075801000	0.000336000
1	-10.116809000	0.075812000	0.000033000
6	-9.045301000	2.521822000	-0.424287000
9	-8.225900000	3.624102000	-0.618484000
9	-9.892860000	2.457091000	-1.534720000
9	-9.876135000	2.830789000	0.657174000
6	-9.060012000	-2.433350000	0.421279000
9	-10.439161000	-2.292424000	0.403827000
9	-8.746118000	-3.393706000	-0.545801000
9	-8.735917000	-3.024076000	1.646863000
6	9.045309000	2.521830000	0.424568000
9	8.225912000	3.624112000	0.618766000
9	9.892835000	2.457065000	1.535024000
9	9.876179000	2.830816000	-0.656863000
6	9.060003000	-2.433344000	-0.420987000
9	10.439153000	-2.292441000	-0.403418000
9	8.746011000	-3.393693000	0.546069000
9	8.736002000	-3.024067000	-1.646596000

3.4 $[Fe(L^4)_2]^{2+}$

26	-0.007191000	0.531376000	0.030352000
7	-0.410080000	1.890168000	-1.354923000
6	-1.761253000	2.148715000	-1.524465000
6	-2.221934000	3.089964000	-2.461825000
6	-1.283218000	3.788814000	-3.247479000
6	0.090518000	3.525207000	-3.073041000
6	0.488837000	2.569779000	-2.117493000
7	-1.890492000	0.533010000	0.186082000
6	-2.627504000	1.338060000	-0.639502000
6	-4.032691000	1.300214000	-0.602157000
6	-4.670541000	0.405510000	0.293233000

6	-3.887121000	-0.396885000	1.159562000
6	-2.485753000	-0.316573000	1.078271000
7	-0.177660000	-0.816562000	1.475252000
6	-1.484695000	-1.088762000	1.848231000
6	-1.787003000	-2.023768000	2.854110000
6	-0.731779000	-2.699474000	3.499765000
6	0.596654000	-2.421742000	3.118978000
6	0.834207000	-1.475042000	2.103291000
7	0.432631000	1.950932000	1.339760000
6	1.789233000	2.198653000	1.481136000
6	2.272992000	3.178500000	2.365905000
6	1.352453000	3.927899000	3.126248000
6	-0.026592000	3.674907000	2.980220000
6	-0.448562000	2.678933000	2.077613000
7	1.874431000	0.487961000	-0.137130000
6	2.633132000	1.334706000	0.624882000
6	4.036660000	1.295181000	0.549590000
6	4.651792000	0.357166000	-0.317584000
6	3.844876000	-0.494472000	-1.112931000
6	2.446132000	-0.410246000	-0.996435000
7	0.125747000	-0.898634000	-1.338869000
6	1.424967000	-1.214096000	-1.705397000
6	1.703398000	-2.213783000	-2.654328000
6	0.632005000	-2.909114000	-3.250553000
6	-0.688476000	-2.585429000	-2.878618000
6	-0.902240000	-1.576126000	-1.919521000
1	-3.288837000	3.272752000	-2.573140000
1	-1.618929000	4.521603000	-3.977989000
1	0.844363000	4.043470000	-3.660042000
1	1.540107000	2.337239000	-1.952320000
1	-4.630230000	1.917249000	-1.271651000
1	-4.367710000	-1.070285000	1.866148000
1	-2.822512000	-2.218864000	3.125886000
1	-0.944443000	-3.426012000	4.280939000
1	1.437318000	-2.922954000	3.591681000
1	1.846955000	-1.235248000	1.780491000
1	3.343409000	3.351744000	2.456958000
1	1.706126000	4.691060000	3.816053000
1	-0.766646000	4.231750000	3.549139000
1	-1.504306000	2.451900000	1.935353000
1	4.651567000	1.951131000	1.163994000
1	4.305468000	-1.200365000	-1.800786000
1	2.733452000	-2.444307000	-2.919100000
1	0.826270000	-3.685772000	-3.987027000
1	-1.541378000	-3.099351000	-3.314419000
1	-1.909378000	-1.302629000	-1.605152000
6	-6.165466000	0.322027000	0.304644000
6	-6.881145000	-0.860414000	-0.041638000
6	-6.902295000	1.476436000	0.656345000
6	-8.292566000	-0.886292000	0.003974000
6	-8.312178000	1.451438000	0.700610000
6	-9.008126000	0.267250000	0.382387000
1	-6.360686000	2.387395000	0.912686000
1	-8.859181000	2.349674000	0.982945000
6	6.146426000	0.298256000	-0.389371000
6	6.841292000	1.458763000	-0.802540000
6	6.904630000	-0.859378000	-0.048645000

6	8.247740000	1.463665000	-0.911302000
6	8.312761000	-0.855286000	-0.158761000
6	8.984346000	0.303343000	-0.597187000
1	6.268444000	2.351014000	-1.056966000
1	8.760220000	2.366297000	-1.240453000
1	-10.095649000	0.240379000	0.416128000
1	10.069507000	0.298968000	-0.680504000
1	8.878050000	-1.744968000	0.111922000
1	-8.825921000	-1.794673000	-0.269622000
6	-6.158512000	-2.105261000	-0.492793000
9	-5.579488000	-2.832377000	0.561588000
9	-6.992931000	-3.009079000	-1.141956000
9	-5.110813000	-1.850461000	-1.384798000
6	6.234592000	-2.108281000	0.467084000
9	5.607492000	-2.865782000	-0.537599000
9	7.123335000	-2.984624000	1.080731000
9	5.237907000	-1.855440000	1.415744000

3.5 $[Fe(L^5)_2]^{2+}$

26	0.000001000	-0.015277000	-0.000019000
7	-0.294563000	-1.401608000	1.388020000
6	-1.628417000	-1.669603000	1.654810000
6	-2.012742000	-2.624435000	2.612943000
6	-1.015019000	-3.325953000	3.319503000
6	0.340430000	-3.052002000	3.046797000
6	0.661328000	-2.084010000	2.075060000
7	-1.890814000	-0.014664000	-0.001228000
6	-2.562508000	-0.859757000	0.840040000
6	-3.967365000	-0.879299000	0.861828000
6	-4.688676000	-0.011146000	-0.000389000
6	-3.965673000	0.854955000	-0.863230000
6	-2.560852000	0.831897000	-0.842306000
7	-0.291935000	1.370762000	-1.389081000
6	-1.625295000	1.640242000	-1.656865000
6	-2.007887000	2.595233000	-2.615550000
6	-1.008903000	3.295125000	-3.321928000
6	0.346039000	3.019421000	-3.048505000
6	0.665164000	2.051527000	-2.076098000
7	0.294577000	-1.401447000	-1.388216000
6	1.628433000	-1.669444000	-1.654994000
6	2.012765000	-2.624194000	-2.613205000
6	1.015047000	-3.325611000	-3.319872000
6	-0.340403000	-3.051643000	-3.047195000
6	-0.661308000	-2.083744000	-2.075367000
7	1.890818000	-0.014657000	0.001197000
6	2.562518000	-0.859679000	-0.840136000
6	3.967376000	-0.879221000	-0.861913000
6	4.688676000	-0.011144000	0.000389000
6	3.965669000	0.854887000	0.863294000
6	2.560847000	0.831835000	0.842353000
7	0.291926000	1.370627000	1.389179000
6	1.625283000	1.640109000	1.656973000
6	2.007867000	2.595036000	2.615726000
6	1.008877000	3.294851000	3.322172000

6	-0.346063000	3.019134000	3.048749000
6	-0.665180000	2.051312000	2.076268000
1	-3.067304000	-2.814722000	2.802364000
1	-1.292172000	-4.068232000	4.064830000
1	1.138805000	-3.571546000	3.570346000
1	1.696604000	-1.843992000	1.836312000
1	-4.497611000	-1.533782000	1.551270000
1	-4.494552000	1.511238000	-1.551993000
1	-3.062094000	2.786857000	-2.805611000
1	-1.284713000	4.037461000	-4.067697000
1	1.145367000	3.537602000	-3.571947000
1	1.700043000	1.810348000	-1.836844000
1	3.067329000	-2.814492000	-2.802606000
1	1.292207000	-4.067826000	-4.065262000
1	-1.138774000	-3.571105000	-3.570831000
1	-1.696586000	-1.843717000	-1.836635000
1	4.497631000	-1.533641000	-1.551408000
1	4.494546000	1.511109000	1.552117000
1	3.062072000	2.786668000	2.805787000
1	1.284681000	4.037136000	4.067994000
1	-1.145395000	3.537253000	3.572246000
1	-1.700057000	1.810125000	1.837013000
6	-6.180863000	-0.007987000	0.001327000
6	-6.895542000	1.198601000	-0.223419000
6	-6.900413000	-1.208753000	0.226927000
6	-8.300083000	1.204738000	-0.219653000
6	-8.308018000	-1.211677000	0.228060000
6	-8.998797000	-0.003293000	0.005505000
1	-6.357942000	2.134771000	-0.371455000
1	-6.367147000	-2.147699000	0.373531000
1	-8.854474000	-2.138174000	0.393127000
6	6.180862000	-0.007987000	-0.001305000
6	6.900414000	-1.208754000	-0.226891000
6	6.895534000	1.198601000	0.223462000
6	8.308020000	-1.211679000	-0.227985000
6	8.300075000	1.204737000	0.219730000
6	8.998793000	-0.003297000	-0.005402000
1	6.367147000	-2.147697000	-0.373511000
1	6.357926000	2.134768000	0.371490000
1	8.854481000	-2.138176000	-0.393035000
1	8.845019000	2.134871000	0.382870000
1	-8.845031000	2.134871000	-0.382781000
6	10.500493000	0.038422000	-0.000314000
9	11.095371000	-1.193476000	-0.241457000
9	11.018253000	0.916541000	-0.962628000
9	11.023311000	0.491132000	1.219372000
6	-10.500497000	0.038417000	0.000424000
9	-11.095364000	-1.193429000	0.241863000
9	-11.018253000	0.916762000	0.962529000
9	-11.023332000	0.490829000	-1.219369000

3.6 $[Fe(L^6)_2]^{2+}$

26	-0.000001000	0.425070000	0.000012000
7	-0.238990000	1.810559000	-1.399628000

6	-1.561371000	2.084024000	-1.714030000
6	-1.906833000	3.038958000	-2.686939000
6	-0.881266000	3.734250000	-3.358886000
6	0.462463000	3.454178000	-3.038347000
6	0.744059000	2.486670000	-2.054064000
7	-1.889164000	0.428552000	-0.070100000
6	-2.527313000	1.279165000	-0.931532000
6	-3.930660000	1.308888000	-0.997433000
6	-4.685649000	0.447114000	-0.157786000
6	-3.996400000	-0.425008000	0.726534000
6	-2.591590000	-0.413876000	0.748168000
7	-0.345298000	-0.962358000	1.373824000
6	-1.688196000	-1.228610000	1.592137000
6	-2.108021000	-2.186765000	2.531659000
6	-1.137204000	-2.893310000	3.269920000
6	0.227653000	-2.621232000	3.046358000
6	0.584770000	-1.649829000	2.090723000
7	0.239005000	1.810661000	1.399547000
6	1.561390000	2.084128000	1.713933000
6	1.906863000	3.039115000	2.686786000
6	0.881305000	3.734466000	3.358687000
6	-0.462427000	3.454397000	3.038158000
6	-0.744035000	2.486832000	2.053935000
7	1.889160000	0.428540000	0.070116000
6	2.527321000	1.279211000	0.931482000
6	3.930668000	1.308939000	0.997363000
6	4.685650000	0.447107000	0.157769000
6	3.996388000	-0.425077000	-0.726480000
6	2.591577000	-0.413943000	-0.748104000
7	0.345279000	-0.962473000	-1.373692000
6	1.688174000	-1.228734000	-1.592008000
6	2.107989000	-2.186953000	-2.531469000
6	1.137163000	-2.893562000	-3.269657000
6	-0.227692000	-2.621485000	-3.046082000
6	-0.584798000	-1.650012000	-2.090514000
1	-2.952978000	3.234139000	-2.914391000
1	-1.128282000	4.476386000	-4.114894000
1	1.281238000	3.968643000	-3.534642000
1	1.769154000	2.242231000	-1.778391000
1	-4.434334000	1.968446000	-1.701673000
1	-4.550344000	-1.075295000	1.401402000
1	-3.168979000	-2.375847000	2.682282000
1	-1.441906000	-3.638380000	4.001601000
1	1.005881000	-3.145164000	3.595303000
1	1.628236000	-1.411041000	1.888729000
1	2.953011000	3.234291000	2.914231000
1	1.128331000	4.476643000	4.114652000
1	-1.281195000	3.968909000	3.534416000
1	-1.769132000	2.242396000	1.778270000
1	4.434346000	1.968551000	1.701550000
1	4.550319000	-1.075414000	-1.401310000
1	3.168945000	-2.376036000	-2.682100000
1	1.441857000	-3.638683000	-4.001290000
1	-1.005926000	-3.145469000	-3.594967000
1	-1.628262000	-1.411220000	-1.888516000
6	-6.176687000	0.461689000	-0.201121000
6	-6.910824000	-0.727401000	0.013906000

6	-6.883684000	1.667222000	-0.455795000
6	-8.320728000	-0.697488000	-0.029422000
6	-8.290999000	1.685670000	-0.492190000
6	-9.023170000	0.498864000	-0.278980000
1	-6.394448000	-1.673822000	0.185124000
1	-6.333309000	2.597536000	-0.598024000
1	-8.816860000	2.620117000	-0.678567000
6	6.176689000	0.461686000	0.201082000
6	6.883690000	1.667223000	0.455724000
6	6.910828000	-0.727403000	-0.013944000
6	8.291006000	1.685675000	0.492094000
6	8.320733000	-0.697485000	0.029348000
6	9.023177000	0.498870000	0.278887000
1	6.333321000	2.597541000	0.597947000
1	6.394456000	-1.673831000	-0.185135000
1	8.816867000	2.620127000	0.678447000
1	-10.111099000	0.504302000	-0.306008000
1	10.111107000	0.504311000	0.305892000
6	9.054077000	-1.990151000	-0.194172000
9	10.435886000	-1.863681000	-0.144763000
9	8.718147000	-2.971081000	0.749584000
9	8.759027000	-2.568914000	-1.436501000
6	-9.054076000	-1.990142000	0.194148000
9	-10.435879000	-1.863735000	0.144397000
9	-8.717884000	-2.971226000	-0.749347000
9	-8.759298000	-2.568674000	1.436655000

3.7 $[Fe(L^7)_2]^{2+}$

26	0.000000000	0.001992000	-0.000046000
7	-0.305913000	1.388338000	-1.392478000
6	-1.642427000	1.647784000	-1.655516000
7	-2.101452000	2.543211000	-2.554449000
6	-1.165895000	3.246057000	-3.256840000
6	0.217164000	3.052580000	-3.059529000
6	0.615190000	2.099639000	-2.103407000
7	-1.902086000	0.000414000	-0.001767000
6	-2.578155000	0.836961000	-0.844230000
6	-3.976351000	0.868050000	-0.880048000
6	-4.679235000	-0.003746000	-0.007043000
6	-3.978873000	-0.874322000	0.868879000
6	-2.577692000	-0.836464000	0.835808000
7	-0.307040000	-1.383732000	1.392787000
6	-1.643954000	-1.645318000	1.651029000
7	-2.105545000	-2.540441000	2.548920000
6	-1.171841000	-3.240595000	3.256390000
6	0.211686000	-3.044065000	3.065151000
6	0.612254000	-2.091848000	2.109280000
7	0.306007000	1.394863000	1.385835000
6	1.642532000	1.654581000	1.648531000
7	2.101607000	2.553163000	2.544288000
6	1.166088000	3.259259000	3.243463000
6	-0.216979000	3.066282000	3.045714000
6	-0.615057000	2.109942000	2.093013000
7	1.902085000	0.000380000	0.001599000

6	2.578210000	0.840372000	0.840581000
6	3.976407000	0.871494000	0.876298000
6	4.679235000	-0.003841000	0.006795000
6	3.978817000	-0.877827000	-0.865678000
6	2.577637000	-0.839909000	-0.832598000
7	0.306945000	-1.390506000	-1.386132000
6	1.643849000	-1.652307000	-1.644226000
7	2.105393000	-2.550797000	-2.538770000
6	1.171651000	-3.254573000	-3.242586000
6	-0.211869000	-3.058752000	-3.050582000
6	-0.612387000	-2.102855000	-2.098369000
1	0.954045000	3.616349000	-3.622690000
1	1.664412000	1.894752000	-1.895486000
1	-4.509490000	1.535796000	-1.552219000
1	-4.491544000	-1.553301000	1.548387000
1	0.947161000	-3.605101000	3.632847000
1	1.662027000	-1.884824000	1.906366000
1	-0.953824000	3.632896000	3.606059000
1	-1.664285000	1.905417000	1.884763000
1	4.509588000	1.541853000	1.545831000
1	4.491442000	-1.559469000	-1.542549000
1	-0.947381000	-3.622993000	-3.615046000
1	-1.662157000	-1.896338000	-1.894920000
8	6.049625000	0.050315000	0.065033000
1	6.492478000	-0.569097000	-0.550843000
8	-6.049622000	0.050273000	-0.065485000
1	-6.492514000	-0.566261000	0.553245000
1	1.551581000	-3.977127000	-3.962137000
1	1.544481000	3.981701000	3.963967000
1	-1.551807000	-3.960709000	3.978364000
1	-1.544251000	3.966207000	-3.979654000

3.8 $[Fe(L^8)_2]^{2+}$

26	0.000000000	0.000004000	-0.000005000
7	0.298700000	-1.384969000	-1.386872000
6	1.634130000	-1.653284000	-1.653062000
6	1.991731000	-2.613891000	-2.612595000
6	0.945345000	-3.281269000	-3.281551000
6	-0.637889000	-2.082593000	-2.086443000
7	1.898432000	-0.000037000	0.000002000
6	2.570000000	-0.843644000	-0.843157000
6	3.977804000	-0.866707000	-0.866053000
6	3.977833000	0.866569000	0.866050000
6	2.570030000	0.843547000	0.843161000
7	0.298748000	1.384932000	1.386893000
6	1.634186000	1.653204000	1.653080000
6	1.991820000	2.613776000	2.612637000
6	0.945457000	3.281162000	3.281619000
6	-0.637818000	2.082547000	2.086505000
7	-0.298771000	-1.386869000	1.384945000
6	-1.634213000	-1.653053000	1.653197000
6	-1.991863000	-2.612599000	2.613773000
6	-0.945510000	-3.281562000	3.281196000
6	0.637785000	-2.086452000	2.082602000

7	-1.898432000	0.000049000	-0.000024000
6	-2.570043000	-0.843120000	0.843539000
6	-3.977847000	-0.865987000	0.866560000
6	-3.977790000	0.866168000	-0.866664000
6	-2.569987000	0.843245000	-0.843606000
7	-0.298677000	1.386901000	-1.384952000
6	-1.634103000	1.653144000	-1.653236000
6	-1.991689000	2.612713000	-2.613813000
6	-0.945292000	3.281644000	-3.281199000
6	0.637923000	2.086458000	-2.082576000
1	3.031512000	-2.837902000	-2.834633000
1	1.151757000	-4.037356000	-4.036442000
1	-1.683531000	-1.865732000	-1.872068000
1	4.513792000	-1.535978000	-1.534891000
1	4.513844000	1.535823000	1.534887000
1	3.031609000	2.837751000	2.834672000
1	1.151893000	4.037216000	4.036536000
1	-3.031655000	-2.834636000	2.837730000
1	-1.151959000	-4.036476000	4.037250000
1	-4.513869000	-1.534835000	1.535796000
1	-4.513767000	1.535036000	-1.535914000
1	-3.031466000	2.834794000	-2.837796000
1	-1.151691000	4.036570000	-4.037255000
6	4.680104000	-0.000079000	-0.000004000
6	-4.680105000	0.000104000	-0.000062000
1	5.767237000	-0.000094000	-0.000006000
1	-5.767237000	0.000126000	-0.000076000
7	-0.369781000	3.021219000	3.024499000
7	-0.369884000	-3.021300000	-3.024412000
7	0.369732000	-3.024430000	3.021286000
7	0.369932000	3.024458000	-3.021256000
1	1.683438000	-1.872068000	1.865799000
1	-1.683468000	1.865713000	1.872135000
1	1.683562000	1.872035000	-1.865746000

3.9 $[Fe(L^9)_2]^{2+}$

26	0.000001000	0.314229000	-0.000047000
7	0.259461000	1.699121000	1.396473000
6	1.586193000	1.968447000	1.695769000
6	1.945891000	2.921425000	2.665352000
6	0.930332000	3.619484000	3.349571000
6	-0.417788000	3.344013000	3.044049000
6	-0.713757000	2.378046000	2.062434000
7	1.890092000	0.314830000	0.045401000
6	2.540546000	1.161094000	0.901952000
6	3.944720000	1.182622000	0.956046000
6	4.686091000	0.317359000	0.108551000
6	3.985213000	-0.548222000	-0.772342000
6	2.580328000	-0.530338000	-0.780502000
7	0.325667000	-1.072735000	-1.379897000
6	1.665216000	-1.341391000	-1.615135000
6	2.071754000	-2.299040000	-2.561022000
6	1.090653000	-3.002408000	-3.288687000
6	-0.270720000	-2.727640000	-3.048312000

6	-0.614187000	-1.757032000	-2.086879000
7	-0.259529000	1.699646000	-1.396037000
6	-1.586266000	1.968810000	-1.695446000
6	-1.946005000	2.921957000	-2.664849000
6	-0.930479000	3.620419000	-3.348705000
6	0.417647000	3.345213000	-3.042969000
6	0.713656000	2.379031000	-2.061579000
7	-1.890090000	0.314786000	-0.045474000
6	-2.540583000	1.161208000	-0.901841000
6	-3.944758000	1.182732000	-0.955881000
6	-4.686090000	0.317318000	-0.108502000
6	-3.985170000	-0.548422000	0.772201000
6	-2.580283000	-0.530544000	0.780295000
7	-0.325589000	-1.073305000	1.379249000
6	-1.665136000	-1.341841000	1.614652000
6	-2.071639000	-2.299687000	2.560353000
6	-1.090508000	-3.003442000	3.287603000
6	0.270862000	-2.728881000	3.046979000
6	0.614294000	-1.758026000	2.085783000
1	2.995188000	3.113020000	2.880977000
1	1.188376000	4.360196000	4.103263000
1	-1.229229000	3.860765000	3.549924000
1	-1.742683000	2.137140000	1.798372000
1	4.458099000	1.837495000	1.657736000
1	4.529966000	-1.201560000	-1.451679000
1	3.130368000	-2.490302000	-2.724831000
1	1.384969000	-3.747026000	-4.025038000
1	-1.056727000	-3.248879000	-3.588640000
1	-1.654753000	-1.516715000	-1.872556000
1	-2.995307000	3.113382000	-2.880600000
1	-1.188553000	4.361251000	-4.102268000
1	1.229062000	3.862319000	-3.548523000
1	1.742588000	2.138317000	-1.797366000
1	-4.458171000	1.837732000	-1.657427000
1	-4.529893000	-1.201884000	1.451442000
1	-3.130253000	-2.490813000	2.724330000
1	-1.384798000	-3.748209000	4.023814000
1	1.056895000	-3.250450000	3.586951000
1	1.654858000	-1.517836000	1.871306000
6	6.177722000	0.317037000	0.143379000
6	6.893218000	-0.883920000	-0.064222000
6	6.900492000	1.516224000	0.385900000
6	8.299483000	-0.850638000	-0.023102000
6	8.310446000	1.522375000	0.419825000
6	9.030996000	0.330488000	0.214834000
1	6.384135000	-1.831933000	-0.227836000
1	6.360675000	2.453248000	0.523304000
1	8.844932000	2.453095000	0.597883000
6	-6.177725000	0.317009000	-0.143248000
6	-6.900499000	1.516228000	-0.385599000
6	-6.893220000	-0.883963000	0.064274000
6	-8.310455000	1.522394000	-0.419441000
6	-8.299487000	-0.850664000	0.023247000
6	-9.031003000	0.330493000	-0.214527000
1	-6.360685000	2.453263000	-0.522935000
1	-6.384133000	-1.831997000	0.227757000
1	-8.844945000	2.453136000	-0.597371000

1	10.117565000	0.307515000	0.235747000
1	-10.117573000	0.307532000	-0.235376000
7	9.038021000	-2.114147000	-0.233571000
8	8.373845000	-3.181766000	-0.456351000
8	10.313028000	-2.091429000	-0.186062000
7	-9.038024000	-2.114186000	0.233642000
8	-8.373847000	-3.181814000	0.456374000
8	-10.313030000	-2.091466000	0.186139000

3.10 $[Fe(L^{10})_2]^{2+}$

26	0.000000000	0.000030000	-0.000013000
7	0.292135000	-1.388418000	1.385536000
6	1.625675000	-1.656540000	1.653047000
6	2.008672000	-2.614441000	2.609186000
6	1.010197000	-3.318538000	3.311973000
6	-0.345172000	-3.044353000	3.038234000
6	-0.664682000	-2.073407000	2.069155000
7	1.894686000	0.000717000	-0.001441000
6	2.562481000	-0.845163000	0.842888000
6	3.970927000	-0.866228000	0.863592000
6	4.670914000	0.001920000	-0.003234000
6	3.969044000	0.869445000	-0.869157000
6	2.560633000	0.847175000	-0.846645000
7	0.289096000	1.388549000	-1.386221000
6	1.622060000	1.657704000	-1.655621000
6	2.002968000	2.615720000	-2.612494000
6	1.002968000	3.318824000	-3.314101000
6	-0.351802000	3.043541000	-3.038511000
6	-0.669191000	2.072564000	-2.068769000
7	-0.289959000	1.385662000	1.388875000
6	-1.623087000	1.654025000	1.658238000
6	-2.004587000	2.610343000	2.616568000
6	-1.005019000	3.312392000	3.319845000
6	0.349921000	3.037738000	3.044464000
6	0.667912000	2.068547000	2.073132000
7	-1.894686000	-0.000372000	0.001301000
6	-2.561159000	0.844450000	0.847728000
6	-3.969580000	0.866036000	0.870066000
6	-4.670914000	-0.000418000	0.002637000
6	-3.970392000	-0.866874000	-0.865447000
6	-2.561956000	-0.845227000	-0.844467000
7	-0.291272000	-1.386140000	-1.388048000
6	-1.624648000	-1.654848000	-1.655804000
6	-2.007053000	-2.611687000	-2.613246000
6	-1.008145000	-3.314009000	-3.317191000
6	0.347054000	-3.039145000	-3.043294000
6	0.665962000	-2.069375000	-2.072841000
1	3.063025000	-2.804950000	2.799334000
1	1.286402000	-4.063248000	4.055313000
1	-1.144119000	-3.566020000	3.558866000
1	-1.699537000	-1.832897000	1.829068000
1	4.509152000	-1.535215000	1.531341000
1	5.758686000	0.002403000	-0.003926000
1	4.505868000	1.538890000	-1.537560000

1	3.056897000	2.807081000	-2.804138000
1	1.277563000	4.063597000	-4.057973000
1	-1.151884000	3.564389000	-3.558214000
1	-1.703535000	1.831279000	-1.827277000
1	-3.058637000	2.801189000	2.808062000
1	-1.280071000	4.055852000	4.064862000
1	1.149681000	3.557752000	3.565496000
1	1.702401000	1.827791000	1.831729000
1	-4.506804000	1.534177000	1.539456000
1	-5.758687000	-0.000414000	0.003139000
1	-4.508218000	-1.535012000	-1.534363000
1	-3.061285000	-2.802755000	-2.803501000
1	-1.283892000	-4.057880000	-4.061541000
1	1.146324000	-3.559426000	-3.564816000
1	1.700673000	-1.828383000	-1.832617000

3.11 $[Fe(L^{II})_2]^{2+}$

26	0.000000000	0.000539000	0.000007000
7	-0.292853000	1.379391000	-1.384910000
6	-1.626330000	1.645473000	-1.655025000
6	-1.976506000	2.608546000	-2.622138000
7	-1.037412000	3.305487000	-3.319111000
6	0.266123000	3.033137000	-3.042639000
6	0.647248000	2.072321000	-2.077847000
7	-1.902327000	-0.000222000	-0.002663000
6	-2.572049000	0.842053000	-0.850489000
6	-3.971770000	0.870605000	-0.882150000
6	-4.673566000	0.000180000	-0.008979000
6	-3.977732000	-0.871476000	0.867697000
6	-2.574419000	-0.840921000	0.839981000
7	-0.297592000	-1.376798000	1.384679000
6	-1.632214000	-1.644245000	1.649175000
6	-1.985061000	-2.607110000	2.615473000
7	-1.048220000	-3.301732000	3.317802000
6	0.256106000	-3.027041000	3.047756000
6	0.640206000	-2.066914000	2.083357000
7	0.293414000	1.385750000	1.378392000
6	1.626982000	1.652423000	1.647427000
6	1.977493000	2.619246000	2.610672000
7	1.038639000	3.319790000	3.304346000
6	-0.264994000	3.047401000	3.028367000
6	-0.646458000	2.082599000	2.067697000
7	1.902327000	-0.000697000	0.002389000
6	2.572395000	0.845383000	0.846151000
6	3.972124000	0.873845000	0.877356000
6	4.673572000	-0.000784000	0.008107000
6	3.977382000	-0.876174000	-0.864550000
6	2.574077000	-0.845210000	-0.836698000
7	0.297034000	-1.383946000	-1.377690000
6	1.631566000	-1.652046000	-1.642023000
6	1.984075000	-2.618932000	-2.604421000
7	1.046988000	-3.317796000	-3.302201000
6	-0.257243000	-3.043477000	-3.031327000
6	-0.641000000	-2.078822000	-2.071320000

1	-3.019752000	2.827868000	-2.844638000
1	1.020605000	3.587175000	-3.596470000
1	1.693257000	1.861909000	-1.864097000
1	-4.530835000	1.527772000	-1.543447000
1	-4.519567000	-1.538080000	1.536193000
1	-3.028767000	-2.828673000	2.833772000
1	1.008855000	-3.578628000	3.606358000
1	1.686870000	-1.854647000	1.874768000
1	3.020811000	2.838758000	2.832637000
1	-1.019272000	3.604525000	3.579371000
1	-1.692528000	1.872183000	1.854247000
1	4.531461000	1.534001000	1.535442000
1	4.518929000	-1.545962000	-1.530085000
1	3.027709000	-2.840397000	-2.823169000
1	-1.010202000	-3.598856000	-3.585875000
1	-1.687602000	-1.866772000	-1.862212000
8	6.042332000	0.056700000	0.067888000
1	6.490214000	-0.560902000	-0.546245000
8	-6.042306000	0.057807000	-0.069131000
1	-6.490417000	-0.556323000	0.548309000

3.12 $[Fe(L^{12})_2]^{2+}$

26	0.000000000	-0.000001000	0.000026000
7	-0.297808000	1.384763000	-1.386598000
6	-1.633561000	1.649753000	-1.649520000
6	-1.994192000	2.613224000	-2.611764000
6	0.244611000	3.042302000	-3.045283000
6	0.635609000	2.079886000	-2.083708000
7	-1.888770000	-0.000149000	0.000065000
6	-2.562266000	0.841338000	-0.840869000
6	-3.975457000	0.829257000	-0.828659000
6	-3.975302000	-0.829794000	0.828935000
6	-2.562108000	-0.841720000	0.841042000
7	-0.297549000	-1.384892000	1.386597000
6	-1.633254000	-1.650061000	1.649594000
6	-1.993709000	-2.613659000	2.611777000
6	0.245170000	-3.042562000	3.045060000
6	0.635992000	-2.080006000	2.083553000
7	0.297572000	1.386677000	1.384804000
6	1.633281000	1.649753000	1.649870000
6	1.993752000	2.612078000	2.613321000
6	-0.245120000	3.045382000	3.042240000
6	-0.635958000	2.083721000	2.079844000
7	1.888770000	0.000142000	0.000036000
6	2.562122000	0.841163000	0.841551000
6	3.975316000	0.829074000	0.829584000
6	3.975443000	-0.828573000	-0.829412000
6	2.562252000	-0.840803000	-0.841451000
7	0.297785000	-1.386546000	-1.384824000
6	1.633534000	-1.649451000	-1.649854000
6	1.994149000	-2.611636000	-2.613389000
6	-0.244661000	-3.045090000	-3.042496000
6	-0.635643000	-2.083577000	-2.080011000
1	-3.039579000	2.829438000	-2.825497000

1	0.995117000	3.597941000	-3.602507000
1	1.684602000	1.875626000	-1.881643000
1	-4.560355000	1.478419000	-1.477763000
1	-4.560082000	-1.479016000	1.478085000
1	-3.039056000	-2.830014000	2.825564000
1	0.995780000	-3.598183000	3.602162000
1	1.684949000	-1.875633000	1.881423000
1	3.039104000	2.825943000	2.829580000
1	-0.995720000	3.602542000	3.597816000
1	-1.684918000	1.881536000	1.875543000
1	4.560106000	1.478242000	1.478780000
1	4.560330000	-1.477685000	-1.478577000
1	3.039532000	-2.825370000	-2.829622000
1	-0.995177000	-3.602246000	-3.598189000
1	-1.684633000	-1.881496000	-1.875750000
7	-1.060109000	3.312598000	-3.312556000
7	-1.059499000	-3.313008000	3.312425000
7	1.059554000	3.312807000	3.312604000
7	1.060054000	-3.312373000	-3.312803000
7	-4.668234000	-0.000304000	0.000167000
7	4.668234000	0.000283000	0.000107000

3.13 $[Fe(L^1)_2]^{2+}$

26	-0.000001000	-0.000006000	-0.000027000
7	-0.290201000	1.380389000	1.383011000
6	-1.623844000	1.647889000	1.649096000
6	-1.974591000	2.613349000	2.614560000
6	0.267860000	3.034893000	3.039741000
6	0.649696000	2.072482000	2.077136000
7	-1.900563000	-0.000227000	-0.000137000
6	-2.567427000	0.844443000	0.844766000
6	-3.975456000	0.867117000	0.867359000
6	-3.975160000	-0.867969000	-0.867936000
6	-2.567139000	-0.845029000	-0.845137000
7	-0.289729000	-1.380540000	-1.383045000
6	-1.623284000	-1.648315000	-1.649306000
6	-1.973715000	-2.613907000	-2.614756000
6	0.268872000	-3.035099000	-3.039548000
6	0.650391000	-2.072538000	-2.076968000
7	0.290071000	-1.382952000	1.380496000
6	1.623683000	-1.649043000	1.648115000
6	1.974343000	-2.614445000	2.613676000
6	-0.268148000	-3.039484000	3.035147000
6	-0.649893000	-2.076965000	2.072621000
7	1.900563000	0.000193000	0.000029000
6	2.567345000	-0.844740000	0.844734000
6	3.975372000	-0.867352000	0.867524000
6	3.975243000	0.868002000	-0.867504000
6	2.567221000	0.845216000	-0.844685000
7	0.289867000	1.383127000	-1.380411000
6	1.623440000	1.649439000	-1.648004000
6	1.973962000	2.615022000	-2.613436000
6	-0.268588000	3.039883000	-3.034762000
6	-0.650195000	2.077163000	-2.072384000

1	-3.017946000	2.834627000	2.834367000
1	1.021765000	3.588321000	3.594881000
1	1.696061000	1.860809000	1.866878000
1	-4.513930000	1.534997000	1.535294000
1	-4.513412000	-1.535950000	-1.535946000
1	-3.016998000	-2.835392000	-2.834699000
1	1.022961000	-3.588442000	-3.594522000
1	1.696691000	-1.860669000	-1.866581000
1	3.017679000	-2.834263000	2.835034000
1	-1.022100000	-3.594540000	3.588593000
1	-1.696239000	-1.866684000	1.860871000
1	4.513783000	-1.535315000	1.535425000
1	4.513560000	1.536031000	-1.535415000
1	3.017267000	2.834993000	-2.834788000
1	-1.022620000	3.594954000	-3.588085000
1	-1.696512000	1.866729000	-1.860643000
6	-4.674848000	-0.000491000	-0.000342000
6	4.674848000	0.000364000	-0.000002000
1	5.762142000	0.000428000	-0.000019000
1	-5.762142000	-0.000592000	-0.000427000
7	-1.036157000	3.309490000	3.312456000
7	-1.035054000	-3.309941000	-3.312452000
7	1.035848000	-3.312241000	3.309825000
7	1.035369000	3.312817000	-3.309453000

3.14 $[Fe(L^{14})_2]^{2+}$

26	0.000000000	0.000088000	0.000126000
7	0.292868000	1.385877000	1.389095000
6	1.626311000	1.654558000	1.656597000
6	2.009935000	2.608825000	2.615512000
6	1.011504000	3.308848000	3.322549000
6	-0.343598000	3.033967000	3.049430000
6	-0.663692000	2.066711000	2.076659000
7	1.890178000	0.000011000	-0.000092000
6	2.560824000	0.845832000	0.841554000
6	3.965636000	0.867572000	0.862516000
6	4.686422000	-0.000065000	-0.000434000
6	3.965376000	-0.867658000	-0.863211000
6	2.560569000	-0.845841000	-0.841909000
7	0.292444000	-1.385772000	-1.388884000
6	1.625810000	-1.654521000	-1.656717000
6	2.009152000	-2.608828000	-2.615707000
6	1.010515000	-3.308839000	-3.322466000
6	-0.344506000	-3.033907000	-3.048995000
6	-0.664312000	-2.066606000	-2.076175000
7	-0.292730000	1.385909000	-1.388853000
6	-1.626151000	1.654616000	-1.656454000
6	-2.009689000	2.608912000	-2.615376000
6	-1.011196000	3.308961000	-3.322300000
6	0.343881000	3.034079000	-3.049058000
6	0.663887000	2.066783000	-2.076298000
7	-1.890178000	0.000128000	0.000268000
6	-2.560742000	0.845913000	-0.841478000
6	-3.965552000	0.867646000	-0.862581000

6	-4.686422000	0.000033000	0.000322000
6	-3.965461000	-0.867527000	0.863203000
6	-2.560652000	-0.845705000	0.842040000
7	-0.292582000	-1.385619000	1.389246000
6	-1.625971000	-1.654348000	1.656974000
6	-2.009398000	-2.608574000	2.616011000
6	-1.010823000	-3.308490000	3.322950000
6	0.344223000	-3.033541000	3.049619000
6	0.664117000	-2.066340000	2.076729000
1	3.064243000	2.799855000	2.805422000
1	1.287904000	4.050661000	4.068586000
1	-1.142497000	3.552243000	3.573390000
1	-1.698821000	1.826534000	1.837772000
1	4.495396000	1.522871000	1.551432000
1	4.494936000	-1.522984000	-1.552255000
1	3.063403000	-2.799904000	-2.805884000
1	1.286695000	-4.050682000	-4.068554000
1	-1.143560000	-3.552176000	-3.572724000
1	-1.699375000	-1.826399000	-1.837037000
1	-3.063980000	2.799952000	-2.805369000
1	-1.287529000	4.050798000	-4.068338000
1	1.142828000	3.552382000	-3.572917000
1	1.698998000	1.826608000	-1.837333000
1	-4.495248000	1.522915000	-1.551575000
1	-4.495085000	-1.522837000	1.552213000
1	-3.063667000	-2.799650000	2.806093000
1	-1.287069000	-4.050268000	4.069078000
1	1.143229000	-3.551728000	3.573502000
1	1.699199000	-1.826119000	1.837680000
6	6.177914000	-0.000113000	-0.000601000
6	6.894187000	-1.207824000	-0.218053000
6	6.894315000	1.207547000	0.216708000
6	8.298295000	-1.217048000	-0.219118000
6	8.298423000	1.216669000	0.217510000
6	8.976476000	-0.000214000	-0.000865000
1	6.357018000	-2.144934000	-0.359266000
1	6.357240000	2.144695000	0.358026000
1	8.858395000	2.135102000	0.373968000
6	-6.177914000	-0.000032000	0.000330000
6	-6.894305000	1.207615000	-0.217082000
6	-6.894197000	-1.207744000	0.217737000
6	-8.298413000	1.216725000	-0.218023000
6	-8.298304000	-1.216982000	0.218663000
6	-8.976475000	-0.000159000	0.000317000
1	-6.357224000	2.144765000	-0.358370000
1	-6.357033000	-2.144846000	0.359025000
1	-8.858378000	2.135149000	-0.374557000
1	-8.858187000	-2.135458000	0.375188000
1	8.858170000	-2.135523000	-0.375675000
7	10.452414000	-0.000271000	-0.000971000
8	11.064787000	-1.104049000	-0.196473000
8	11.064898000	1.103448000	0.194516000
7	-10.452414000	-0.000228000	0.000293000
8	-11.064796000	-1.104006000	0.195768000
8	-11.064891000	1.103481000	-0.195274000

3.15 $[Fe(L^{15})_2]^{2+}$

26	-0.002690000	0.000228000	0.000015000
7	0.297040000	1.552827000	1.199009000
6	1.631752000	1.851704000	1.428978000
6	2.014120000	2.921662000	2.258333000
6	1.016518000	3.708759000	2.867923000
6	-0.339470000	3.403486000	2.631282000
6	-0.659347000	2.318725000	1.792045000
7	1.888399000	0.000181000	-0.000070000
6	2.566620000	0.942631000	0.723780000
6	3.968096000	0.969161000	0.739590000
6	4.713362000	0.000052000	-0.000133000
6	3.967976000	-0.969043000	-0.739746000
6	2.566502000	-0.942353000	-0.723917000
7	0.296846000	-1.552342000	-1.199075000
6	1.631526000	-1.851327000	-1.429098000
6	2.013778000	-2.921279000	-2.258514000
6	1.016094000	-3.708255000	-2.868125000
6	-0.339861000	-3.402863000	-2.631446000
6	-0.659621000	-2.318119000	-1.792143000
7	-0.300545000	1.199733000	-1.551989000
6	-1.634883000	1.436501000	-1.846578000
6	-2.016976000	2.270275000	-2.913213000
6	-1.018869000	2.876405000	-3.702378000
6	0.336917000	2.631975000	-3.402279000
6	0.656294000	1.789387000	-2.319936000
7	-1.894569000	0.000194000	0.000094000
6	-2.570797000	0.733362000	-0.937278000
6	-3.973067000	0.749812000	-0.963931000
6	-4.712767000	-0.000047000	0.000068000
6	-3.972957000	-0.749785000	0.964075000
6	-2.570688000	-0.733096000	0.937448000
7	-0.300366000	-1.199205000	1.552112000
6	-1.634672000	-1.436091000	1.846754000
6	-2.016652000	-2.269817000	2.913466000
6	-1.018465000	-2.875769000	3.702666000
6	0.337287000	-2.631205000	3.402528000
6	0.656550000	-1.788679000	2.320104000
1	3.068715000	3.133674000	2.423297000
1	1.293681000	4.540397000	3.512346000
1	-1.137852000	3.986882000	3.082887000
1	-1.693977000	2.047866000	1.583542000
1	4.476238000	1.727953000	1.329998000
1	4.476033000	-1.727927000	-1.330113000
1	3.068350000	-3.133373000	-2.423514000
1	1.293167000	-4.539887000	-3.512593000
1	-1.138307000	-3.986157000	-3.083069000
1	-1.694225000	-2.047187000	-1.583607000
1	-3.071494000	2.441462000	-3.120769000
1	-1.295428000	3.524005000	-4.531739000
1	1.135609000	3.080383000	-3.987713000
1	1.690724000	1.575047000	-2.052958000
1	-4.491960000	1.312886000	-1.737264000
1	-4.491772000	-1.312973000	1.737378000
1	-3.071147000	-2.441092000	3.121065000
1	-1.294938000	-3.523328000	4.532089000

1	1.136042000	-3.079466000	3.987991000
1	1.690954000	-1.574257000	2.053090000
6	6.195695000	-0.000126000	-0.000069000
6	6.945210000	-1.032750000	-0.634532000
6	6.945459000	1.032336000	0.634372000
6	8.344704000	-1.045465000	-0.638565000
6	8.344955000	1.044713000	0.638408000
6	9.092303000	-0.000467000	-0.000074000
1	6.437591000	-1.860417000	-1.130814000
1	6.438051000	1.860149000	1.130621000
1	8.859186000	-1.866053000	-1.135353000
1	8.859636000	1.865188000	1.135177000
6	-6.193173000	-0.000180000	0.000048000
6	-6.937513000	1.042146000	-0.622486000
6	-6.937341000	-1.042636000	0.622568000
6	-8.337991000	1.055202000	-0.623627000
6	-8.337817000	-1.055945000	0.623671000
6	-9.083513000	-0.000442000	0.000009000
1	-6.418771000	1.880900000	-1.089596000
1	-6.418458000	-1.881289000	1.089704000
1	-8.854384000	1.886408000	-1.100459000
1	-8.854074000	-1.887238000	1.100500000
7	-10.469641000	-0.000571000	0.000004000
7	10.477254000	-0.000621000	-0.000082000
6	-11.206504000	1.089343000	-0.654788000
1	-10.968752000	1.149582000	-1.729773000
1	-12.281330000	0.908187000	-0.551191000
1	-10.975840000	2.065951000	-0.197740000
6	-11.206288000	-1.090648000	0.654767000
1	-12.281150000	-0.909697000	0.551186000
1	-10.975435000	-2.067197000	0.197687000
1	-10.968513000	-1.150873000	1.729746000
6	11.214388000	1.083591000	0.664504000
1	12.289139000	0.906710000	0.553549000
1	10.978325000	2.064431000	0.219862000
1	10.981337000	1.130127000	1.741127000
6	11.214150000	-1.085052000	-0.664578000
1	10.981046000	-1.131654000	-1.741185000
1	12.288939000	-0.908365000	-0.553692000
1	10.977915000	-2.065802000	-0.219824000

3.16 $[Fe(L^{16})_2]^{2+}$

26	0.000000000	0.000150000	-0.001553000
7	0.295268000	1.386274000	1.386584000
6	1.629297000	1.654826000	1.652843000
6	2.012566000	2.610481000	2.610924000
6	1.014636000	3.311605000	3.317425000
6	-0.340953000	3.036820000	3.045114000
6	-0.661074000	2.068452000	2.073720000
7	1.891626000	-0.000325000	-0.001584000
6	2.564587000	0.845028000	0.838090000
6	3.968722000	0.865199000	0.860322000
6	4.697565000	-0.001491000	-0.001149000
6	3.968270000	-0.867472000	-0.862971000

6	2.564166000	-0.846148000	-0.841171000
7	0.294524000	-1.386186000	-1.389639000
6	1.628418000	-1.655413000	-1.655943000
6	2.011165000	-2.611332000	-2.613969000
6	1.012860000	-3.312035000	-3.320359000
6	-0.342580000	-3.036593000	-3.047979000
6	-0.662178000	-2.067988000	-2.076648000
7	-0.294730000	1.386700000	-1.389368000
6	-1.628660000	1.655814000	-1.655594000
6	-2.011541000	2.611833000	-2.613467000
6	-1.013331000	3.312777000	-3.319753000
6	0.342148000	3.037480000	-3.047417000
6	0.661881000	2.068752000	-2.076254000
7	-1.891627000	0.000538000	-0.001387000
6	-2.564292000	0.846348000	-0.840888000
6	-3.968398000	0.867484000	-0.862675000
6	-4.697565000	0.001313000	-0.000935000
6	-3.968596000	-0.865349000	0.860456000
6	-2.564463000	-0.844992000	0.838208000
7	-0.295063000	-1.386105000	1.386510000
6	-1.629056000	-1.654770000	1.652847000
6	-2.012192000	-2.610501000	2.610906000
6	-1.014166000	-3.311568000	3.317327000
6	0.341384000	-3.036650000	3.044960000
6	0.661370000	-2.068223000	2.073581000
1	3.067197000	2.801270000	2.799786000
1	1.291445000	4.054341000	4.062539000
1	-1.139490000	3.556154000	3.568748000
1	-1.696001000	1.826888000	1.834325000
1	4.496114000	1.520783000	1.550875000
1	4.495423000	-1.523230000	-1.553549000
1	3.065692000	-2.802665000	-2.802869000
1	1.289275000	-4.054959000	-4.065432000
1	-1.141399000	-3.555599000	-3.571508000
1	-1.696977000	-1.825907000	-1.837225000
1	-3.066094000	2.803063000	-2.802321000
1	-1.289848000	4.055780000	-4.064710000
1	1.140893000	3.556688000	-3.570859000
1	1.696710000	1.826762000	-1.836867000
1	-4.495646000	1.523235000	-1.553189000
1	-4.495896000	-1.521071000	1.550947000
1	-3.066796000	-2.801385000	2.799822000
1	-1.290872000	-4.054356000	4.062428000
1	1.139995000	-3.555928000	3.568537000
1	1.696266000	-1.826570000	1.834147000
6	6.186821000	-0.002558000	-0.000280000
6	6.912828000	-1.183378000	-0.303839000
6	6.914716000	1.179313000	0.305468000
6	8.321946000	-1.182227000	-0.297016000
6	8.321316000	1.176097000	0.303139000
6	9.049676000	-0.004793000	0.004252000
1	6.382064000	-2.113206000	-0.514336000
1	6.383630000	2.109379000	0.514076000
1	8.864001000	-2.102733000	-0.521297000
1	8.864690000	2.095841000	0.528514000
6	-6.186820000	0.002151000	-0.000088000
6	-6.913003000	1.182858000	-0.303665000

6	-6.914538000	-1.179840000	0.305617000
6	-8.322121000	1.181482000	-0.296896000
6	-8.321138000	-1.176848000	0.303235000
6	-9.049674000	0.003929000	0.004330000
1	-6.382376000	2.112769000	-0.514140000
1	-6.383312000	-2.109826000	0.514231000
1	-8.864315000	2.101903000	-0.521193000
1	-8.864375000	-2.096682000	0.528576000
6	10.566064000	0.005250000	0.010588000
1	10.972582000	-0.981934000	-0.246027000
1	10.958206000	0.736781000	-0.711817000
1	10.954305000	0.289676000	1.000148000
6	-10.566061000	-0.006358000	0.010596000
1	-10.972725000	0.980769000	-0.246012000
1	-10.958051000	-0.737932000	-0.711847000
1	-10.954303000	-0.290872000	1.000130000

3.17 $[Fe(L^{17})_2]^{2+}$

26	-0.000001000	0.047255000	0.000135000
7	0.284359000	1.433516000	1.390490000
6	1.616274000	1.702926000	1.666759000
6	1.991447000	2.658574000	2.628129000
6	0.987701000	3.358661000	3.327403000
6	-0.365632000	3.082926000	3.044928000
6	-0.677629000	2.114662000	2.070787000
7	1.891522000	0.047590000	0.014865000
6	2.558227000	0.893987000	0.858463000
6	3.961835000	0.916214000	0.890110000
6	4.699494000	0.051174000	0.033045000
6	3.975267000	-0.815577000	-0.833740000
6	2.571404000	-0.797308000	-0.819797000
7	0.306096000	-1.339024000	-1.385220000
6	1.642191000	-1.607630000	-1.641207000
6	2.032584000	-2.563615000	-2.596068000
6	1.040068000	-3.264815000	-3.310089000
6	-0.317576000	-2.989844000	-3.048282000
6	-0.645027000	-2.021249000	-2.079540000
7	-0.284201000	1.433311000	-1.390468000
6	-1.616088000	1.702776000	-1.666825000
6	-1.991161000	2.658351000	-2.628308000
6	-0.987343000	3.358309000	-3.327608000
6	0.365960000	3.082519000	-3.045045000
6	0.677855000	2.114333000	-2.070794000
7	-1.891523000	0.047728000	-0.014672000
6	-2.558131000	0.893984000	-0.858487000
6	-3.961737000	0.916201000	-0.890298000
6	-4.699492000	0.051302000	-0.033175000
6	-3.975364000	-0.815299000	0.833843000
6	-2.571501000	-0.797036000	0.820049000
7	-0.306257000	-1.338624000	1.385843000
6	-1.642378000	-1.607204000	1.641713000
6	-2.032869000	-2.562988000	2.596735000
6	-1.040427000	-3.263961000	3.311081000
6	0.317245000	-2.988961000	3.049443000

6	0.644797000	-2.020598000	2.080502000
1	3.044458000	2.850240000	2.825104000
1	1.258410000	4.101331000	4.074836000
1	-1.168474000	3.601416000	3.562794000
1	-1.710525000	1.872291000	1.823459000
1	4.481825000	1.572414000	1.585548000
1	4.505907000	-1.469667000	-1.523220000
1	3.088636000	-2.754493000	-2.776761000
1	1.322550000	-4.007751000	-4.052894000
1	-1.112122000	-3.509183000	-3.577987000
1	-1.681693000	-1.779321000	-1.848002000
1	-3.044151000	2.850067000	-2.825344000
1	-1.257975000	4.100924000	-4.075123000
1	1.168858000	3.600909000	-3.562926000
1	1.710728000	1.871925000	-1.823410000
1	-4.481650000	1.572274000	-1.585912000
1	-4.506080000	-1.469272000	1.523376000
1	-3.088939000	-2.753876000	2.777311000
1	-1.322986000	-4.006738000	4.054015000
1	1.111733000	-3.508111000	3.579419000
1	1.681484000	-1.778659000	1.849063000
6	6.186549000	0.053544000	0.043374000
6	6.919806000	-1.114562000	-0.285996000
6	6.912762000	1.230109000	0.385656000
6	8.328991000	-1.127621000	-0.275593000
6	8.313829000	1.236558000	0.394018000
6	9.027069000	0.056431000	0.064644000
1	6.394406000	-2.040370000	-0.524304000
1	6.381112000	2.154008000	0.616598000
1	8.856957000	-2.047057000	-0.521605000
1	8.874838000	2.136994000	0.641379000
6	-6.186546000	0.053653000	-0.043693000
6	-6.912734000	1.230144000	-0.386281000
6	-6.919828000	-1.114407000	0.285787000
6	-8.313800000	1.236567000	-0.394835000
6	-8.329011000	-1.127493000	0.275195000
6	-9.027063000	0.056485000	-0.065350000
1	-6.381068000	2.154012000	-0.617316000
1	-6.394444000	-2.040163000	0.524331000
1	-8.874790000	2.136949000	-0.642433000
1	-8.856996000	-2.046894000	0.521297000
8	-10.410966000	0.163947000	-0.106003000
6	-11.203841000	-1.010605000	0.228395000
1	-10.998805000	-1.833820000	-0.472390000
1	-11.001189000	-1.338878000	1.258902000
1	-12.246983000	-0.697690000	0.137384000
8	10.410974000	0.163927000	0.105089000
6	11.203827000	-1.010669000	-0.229211000
1	10.998896000	-1.833767000	0.471741000
1	11.001046000	-1.339121000	-1.259636000
1	12.246975000	-0.697719000	-0.138390000

3.18 $[Fe(L^{18})_2]^{2+}$

26	0.007184000	-0.000001000	-0.000044000
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7	0.301800000	-0.872995000	-1.756230000
6	1.635591000	-1.049459000	-2.091694000
6	2.017283000	-1.655026000	-3.302439000
6	1.018408000	-2.093148000	-4.195127000
6	-0.336990000	-1.912048000	-3.851997000
6	-0.655771000	-1.298216000	-2.625127000
7	1.898408000	0.000009000	-0.000040000
6	2.571704000	-0.540874000	-1.061945000
6	3.975286000	-0.556696000	-1.088235000
6	4.706649000	0.000023000	-0.000035000
6	3.975276000	0.556736000	1.088162000
6	2.571695000	0.540900000	1.061866000
7	0.301786000	0.872993000	1.756146000
6	1.635573000	1.049473000	2.091614000
6	2.017253000	1.655041000	3.302361000
6	1.018370000	2.093147000	4.195048000
6	-0.337025000	1.912031000	3.851913000
6	-0.655794000	1.298198000	2.625040000
7	-0.290358000	-1.757594000	0.870482000
6	-1.624703000	-2.098160000	1.034073000
6	-2.006681000	-3.313414000	1.630306000
6	-1.008525000	-4.204589000	2.073014000
6	0.347147000	-3.855376000	1.906439000
6	0.666585000	-2.624643000	1.300844000
7	-1.882650000	-0.000011000	-0.000050000
6	-2.559278000	-1.066329000	0.525744000
6	-3.961560000	-1.093048000	0.539316000
6	-4.703028000	-0.000027000	-0.000062000
6	-3.961568000	1.093003000	-0.539432000
6	-2.559286000	1.066298000	-0.525851000
7	-0.290371000	1.757596000	-0.870559000
6	-1.624718000	2.098144000	-1.034166000
6	-2.006706000	3.313398000	-1.630393000
6	-1.008556000	4.204592000	-2.073077000
6	0.347119000	3.855399000	-1.906483000
6	0.666566000	2.624664000	-1.300897000
1	3.071551000	-1.780300000	-3.541283000
1	1.294252000	-2.564172000	-5.136229000
1	-1.136216000	-2.235596000	-4.513939000
1	-1.690232000	-1.138428000	-2.322584000
1	4.501641000	-0.966411000	-1.948599000
1	4.501624000	0.966453000	1.948529000
1	3.071519000	1.780326000	3.541210000
1	1.294205000	2.564171000	5.136153000
1	-1.136257000	2.235566000	4.513854000
1	-1.690252000	1.138399000	2.322493000
1	-3.061008000	-3.556928000	1.745371000
1	-1.285231000	-5.148963000	2.536949000
1	1.145928000	-4.515518000	2.234722000
1	1.701313000	-2.317223000	1.152357000
1	-4.469491000	-1.959325000	0.956288000
1	-4.469505000	1.959278000	-0.956401000
1	-3.061035000	3.556898000	-1.745470000
1	-1.285269000	5.148967000	-2.537007000
1	1.145895000	4.515557000	-2.234746000
1	1.701296000	2.317258000	-1.152397000
6	6.191829000	0.000023000	-0.000027000

6	6.924889000	1.018128000	0.668333000
6	6.924898000	-1.018084000	-0.668373000
6	8.328275000	1.023940000	0.670904000
6	8.328283000	-1.023906000	-0.670912000
6	9.054261000	0.000013000	0.000006000
1	6.397791000	1.826830000	1.176658000
1	6.397806000	-1.826786000	-1.176705000
1	8.867280000	1.816158000	1.189948000
1	8.867295000	-1.816130000	-1.189939000
6	-6.190832000	-0.000026000	-0.000048000
6	-6.934431000	-1.033856000	0.635894000
6	-6.934442000	1.033808000	-0.635970000
6	-8.335874000	-1.038526000	0.643707000
6	-8.335886000	1.038488000	-0.643739000
6	-9.066423000	-0.000015000	-0.000003000
1	-6.426424000	-1.843222000	1.159636000
1	-6.426445000	1.843173000	-1.159723000
1	-8.870674000	-1.837749000	1.155966000
1	-8.870695000	1.837719000	-1.155977000
7	-10.483313000	-0.000003000	0.000029000
7	10.474744000	0.000002000	0.000031000
6	11.210221000	1.237956000	0.045358000
6	12.311162000	1.372629000	0.927126000
6	10.853011000	2.312963000	-0.806563000
1	12.579714000	0.540853000	1.580109000
1	10.012538000	2.197785000	-1.492607000
6	13.048767000	2.574576000	0.952021000
6	11.583738000	3.518234000	-0.761349000
1	13.895822000	2.670100000	1.631745000
1	11.302206000	4.341459000	-1.418432000
6	12.686316000	3.653507000	0.113471000
1	13.254590000	4.583124000	0.139710000
6	11.210201000	-1.237965000	-0.045258000
6	10.852930000	-2.312962000	0.806649000
6	12.311182000	-1.372660000	-0.926973000
1	10.012426000	-2.197766000	1.492652000
1	12.579781000	-0.540891000	-1.579946000
6	11.583636000	-3.518246000	0.761474000
6	13.048766000	-2.574621000	-0.951827000
1	11.302057000	-4.341464000	1.418546000
1	13.895853000	-2.670162000	-1.631510000
6	12.686255000	-3.653542000	-0.113292000
1	13.254514000	-4.583170000	-0.139500000
6	-11.221318000	-1.237188000	0.053858000
6	-12.314784000	-1.366777000	0.945156000
6	-10.874522000	-2.313098000	-0.800641000
1	-12.575234000	-0.533048000	1.598927000
1	-10.040063000	-2.200437000	-1.494325000
6	-13.055467000	-2.566651000	0.977850000
6	-11.608330000	-3.516181000	-0.747973000
1	-13.896964000	-2.659154000	1.664774000
1	-11.335410000	-4.340782000	-1.406869000
6	-12.703255000	-3.647153000	0.137001000
1	-13.273999000	-4.575051000	0.169149000
6	-11.221296000	1.237198000	-0.053755000
6	-12.314809000	1.366813000	-0.944992000
6	-10.874430000	2.313096000	0.800729000

1	-12.575313000	0.533092000	-1.598751000
1	-10.039934000	2.200414000	1.494367000
6	-13.055469000	2.566703000	-0.977638000
6	-11.608214000	3.516196000	0.748108000
1	-13.897002000	2.659226000	-1.664515000
1	-11.335241000	4.340787000	1.406991000
6	-12.703187000	3.647194000	-0.136804000
1	-13.273913000	4.575104000	-0.168917000

3.19 $[Fe(L^{19})_2]^{2+}$

26	-0.043328000	-0.045843000	0.045248000
7	0.406195000	-1.339326000	-1.389881000
6	1.762231000	-1.448805000	-1.657235000
6	2.251496000	-2.319328000	-2.647402000
6	1.338825000	-3.099681000	-3.385474000
6	-0.039462000	-2.986737000	-3.112120000
6	-0.467368000	-2.096588000	-2.107817000
7	1.836170000	0.162589000	0.059215000
6	2.599750000	-0.571047000	-0.807747000
6	3.997668000	-0.432780000	-0.823239000
6	4.620313000	0.477233000	0.074053000
6	3.800659000	1.224253000	0.963525000
6	2.407263000	1.046871000	0.933535000
7	0.090173000	1.313629000	1.483644000
6	1.385176000	1.718536000	1.768949000
6	1.656723000	2.677838000	2.760779000
6	0.584440000	3.240439000	3.482089000
6	-0.731334000	2.826817000	3.190861000
6	-0.938723000	1.862103000	2.185738000
7	-0.188650000	-1.503982000	1.381960000
6	-1.485993000	-1.925101000	1.631032000
6	-1.765485000	-2.946759000	2.556195000
6	-0.698556000	-3.556653000	3.246481000
6	0.619589000	-3.126651000	2.991970000
6	0.834807000	-2.098518000	2.053536000
7	-1.922990000	-0.252220000	0.031572000
6	-2.501552000	-1.193855000	0.838768000
6	-3.896173000	-1.362368000	0.855276000
6	-4.709563000	-0.545031000	0.023576000
6	-4.078981000	0.421895000	-0.806156000
6	-2.679920000	0.547211000	-0.780955000
7	-0.481704000	1.350635000	-1.293668000
6	-1.835845000	1.481584000	-1.560552000
6	-2.318088000	2.423867000	-2.486401000
6	-1.400198000	3.255907000	-3.158524000
6	-0.023862000	3.121870000	-2.884894000
6	0.396943000	2.158832000	-1.947087000
1	3.321178000	-2.385211000	-2.835992000
1	1.697704000	-3.779063000	-4.155595000
1	-0.774297000	-3.571200000	-3.659762000
1	-1.523268000	-1.979631000	-1.866877000
1	4.598183000	-0.998287000	-1.533641000
1	4.253079000	1.909861000	1.677654000
1	2.682861000	2.977552000	2.964051000

1	0.774259000	3.984003000	4.253172000
1	-1.584364000	3.236725000	3.725504000
1	-1.939892000	1.515369000	1.931821000
1	-2.793426000	-3.257108000	2.733402000
1	-0.894377000	-4.348472000	3.966316000
1	1.468529000	-3.571696000	3.504561000
1	1.837667000	-1.736930000	1.829173000
1	-4.354737000	-2.093584000	1.518581000
1	-4.674468000	1.044366000	-1.471852000
1	-3.386380000	2.504012000	-2.677585000
1	-1.753568000	3.990716000	-3.878687000
1	0.714766000	3.745007000	-3.382497000
1	1.451145000	2.023783000	-1.708268000
6	6.102217000	0.648277000	0.082383000
6	6.682450000	1.905918000	0.406471000
6	6.943498000	-0.441143000	-0.236709000
6	8.081815000	2.053491000	0.404295000
6	8.348275000	-0.282268000	-0.229151000
6	8.930481000	0.967322000	0.089902000
1	6.047975000	2.764851000	0.625860000
1	6.540184000	-1.429357000	-0.460480000
1	8.523108000	3.021154000	0.641978000
6	-6.193177000	-0.699619000	0.024144000
6	-6.782851000	-1.970662000	0.227868000
6	-7.018966000	0.439235000	-0.180710000
6	-8.190219000	-2.103271000	0.222850000
6	-8.422745000	0.290244000	-0.178573000
6	-9.013491000	-0.981986000	0.022544000
1	-6.155494000	-2.852964000	0.356407000
1	-6.563882000	1.421340000	-0.302646000
1	-8.641525000	-3.084080000	0.369457000
8	9.075453000	-1.427387000	-0.545411000
6	10.527366000	-1.336530000	-0.550680000
1	10.907463000	-1.059811000	0.444560000
1	10.884679000	-2.334231000	-0.818511000
1	10.872674000	-0.604887000	-1.296918000
8	-9.317100000	1.342282000	-0.359155000
6	-8.776118000	2.673468000	-0.584354000
1	-8.157591000	2.697490000	-1.494773000
1	-9.642903000	3.327556000	-0.708927000
1	-8.180082000	3.007182000	0.278918000
1	-10.100044000	-1.062318000	0.018121000
1	10.010307000	1.104363000	0.097421000

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