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## LIST OF SYMBOLS AND ABBREVIATIONS

The symbols and abbreviations used in the thesis are listed below:

### Symbols

|              |           |
|--------------|-----------|
| $\theta$     | Theta     |
| $^{\circ}$   | Degree    |
| $\alpha$     | Alpha     |
| $\mu$        | Mu        |
| $\text{\AA}$ | Armstrong |
| $\Omega$     | Ohm       |
| $\nu$        | Nu        |
| $\beta$      | Beta      |
| $\lambda$    | Lambda    |
| $\Delta$     | Delta     |

### Abbreviations

|                            |  |
|----------------------------|--|
| acac                       | acetylacetone                                |
| acbo                       | 2,3-anthrachinone- <i>bis</i> (oxamato)      |
| aq.                        | Aqueous                                      |
| B3LYP                      | Becke, 3-Parameter Lee Yang Par              |
| BJH                        | Barrett-Joyner-Halenda                       |
| BP                         | Becke Perdew                                 |
| bziz                       | benzimidazole                                |
| $^{\circ}\text{C}$         | Degree celcius                               |
| <i>ca.</i>                 | Circa (approximately)                        |
| CASSCF                     | Complete Active Space Self Consistent Theory |
| CI                         | Configuration Interaction                    |
| cm                         | Centimetre                                   |
| $\text{cm}^{-1}$           | Per centimetre                               |
| $\text{cm}^3\text{g}^{-1}$ | Centimetre cube per gram                     |
| COMP                       | Composite                                    |
| CP                         | Coupled Pertrubed                            |

|                     |  |
|---------------------|--|
| dapbh               | diacetylpyridinebis(benzoylhydrazone)  |
| DFT                 | Density Functional Theory              |
| dmpz                | 3,5-dimethylpyrazole                   |
| DOMO                | Double Occupied Molecular Orbital      |
| DOS                 | Density of States                      |
| dtc                 | dithiocarbamate                        |
| ECP                 | Electron Core Potential                |
| en                  | ethylenediamine                        |
| EPR                 | Electron Paramagnetic Resonance        |
| eqn.                | Equation                               |
| eV                  | Electron volt                          |
| FC                  | Fermi Contact                          |
| FLU                 | Fluorescein                            |
| FMO                 | Frontier Molecular Orbital             |
| FTIR                | Fourier transform infrared             |
| FTO                 | Fluorine doped Tin Oxide               |
| FWHM                | Full width at half-maximum             |
| g                   | Gram                                   |
| g/mg.min            | Gram per milligram per minute          |
| g/cm <sup>3</sup>   | Gram per centimeter cube               |
| g/mol               | Gram per mole                          |
| g/L                 | Gram per litre                         |
| gly                 | glycine                                |
| GGA                 | General Gradient Approximation         |
| GMC                 | Gauge Mean Correction                  |
| GPa                 | Giga pascal                            |
| HF-EPR<br>Resonance | High-Frequency Electron Paramagnetic   |
| HFS                 | Hartree Fock Slater                    |
| HOMO                | Highest Occupied Molecular Orbital     |
| HPLC                | High performance liquid chromatography |
| HREM                | High-resolution electron microscopy    |

|                                  |   |
|----------------------------------|---|
| HRTEM<br>microscope              | High-resolution<br>transmission<br>electron |
| HS                               | High Spin                                   |
| IORA                             | Infinite Order Relativistic Approximation   |
| IR                               | Infrared                                    |
| J/(mol.K)                        | Joule per mole per kelvin                   |
| K                                | Kelvin                                      |
| $k_{app}$                        | $k_{apparent}$                              |
| kcal/mol                         | Kilocalori per mole                         |
| kHz                              | Kilohertz                                   |
| $\text{kJmol}^{-1}$              | Kilojoule per mole                          |
| $\text{kJmol}^{-1}\text{K}^{-1}$ | Kilojoule per mole per kelvin               |
| KLMC                             | Knowledge Led Master Code                   |
| $\text{Kmin}^{-1}$               | Kelvin per minute                           |
| KS                               | Kohn Sham                                   |
| kV                               | Kilovolt                                    |
| L                                | Litre                                       |
| L/mg                             | Litre per milligram                         |
| LDA                              | Local Density Approximation                 |
| LFT                              | Ligand Field Theory                         |
| LMCT                             | Ligand to Metal Charge Transfer             |
| LS                               | Low Spin                                    |
| LUMO                             | Lowest Unoccupied Molecular Orbital         |
| $\lambda_{max}$                  | $\lambda_{maximum}$                         |
| m                                | Metre                                       |
| M                                | Molar                                       |
| MAE                              | Magnetic Anisotropy Energy                  |
| $\text{mAhg}^{-1}$               | milliamper-hour per gram                    |
| MB                               | Methylene blue                              |
| mg                               | Milligram                                   |
| $\text{m}^2\text{g}^{-1}$        | Metre square per gram                       |
| mg/g                             | Milligram per gram                          |
| $\text{mgL}^{-1}$                | Milligram per litre                         |
| $\mu\text{m}$                    | Micrometre                                  |

|                                |  |
|--------------------------------|--|
| $\mu\text{g}/\text{dm}^3$      | Microgram per decimetre cube                 |
| MHz                            | Megahertz                                    |
| min                            | Minute                                       |
| $\text{min}^{-1}\text{g}^{-1}$ | Perminute per gram                           |
| MLCT                           | Metal to Ligand Charge Transfer              |
| mL                             | Millilitre                                   |
| $\text{mLmol}^{-1}$            | Millilitre per mole                          |
| mmol                           | Millimole                                    |
| mmol/L                         | Millimole per litre                          |
| mol                            | Mole   |
| $\text{mol}^{-1}$              | Per mole                                     |
| mol/L                          | Mole per litre                               |
| molecules/g/s                  | Molecules per gram per second                |
| MRCI                           | Multi Reference Configuration Interaction    |
| MW                             | Microwave                                    |
| nabo                           | 2,3-naphthalene- <i>bis</i> (oxamato)        |
| NESC                           | Normalized Elimination Of Spin Component     |
| NEVPT                          | N-electron Valence Shell Perturbation Theory |
| $\text{NH}_2\text{pymd}$       | 2-aminopyrimidine                            |
| nm                             | Nanometre                                    |
| NMR                            | Nuclear Magnetic Resonance                   |
| No.                            | Number                                       |
| $\text{n}\Omega.\text{m}$      | Nanoohmmetre                                 |
| $\text{NO}_2\text{dmiz}$       | nitro-N-dimethylimidazole                    |
| NPs                            | Nanoparticles                                |
| npbo                           | 1,8-naphthalene- <i>bis</i> (oxamato)        |
| 4-NP                           | 4-nitrophenol                                |
| 4-NT                           | 4-nitrotoluene                               |
| ORR                            | Oxygen reduction reaction                    |
| obbo                           | <i>o</i> -benzyl- <i>bis</i> (oxamato).      |
| opba                           | <i>o</i> -phenylene- <i>bis</i> (oxamato)    |
| ox                             | oxalate                                      |
| pba                            | propylene- <i>bis</i> (oxamato)              |



|              |  |
|--------------|--|
| ppm          | Parts-per million  |
| PK           | Pederson-Khanna  |
| py           | pyridine   |
| pterpy       | 4'-phenyl-,2':6',2''-terpyridine                           |
| $Q_{e,cal}$  | $Q_{e,calculated}$   |
| $Q_{e,exp}$  | $Q_{e,experimental}$                                       |
| quin         | quinoline  |
| QDPT         | Quasi Degenerate Perturbation Theory                       |
| QRO          | Quasi Restricted Orbital                                   |
| Ref.         | Reference  |
| RHF          | Restricted Hartree-Fock                                    |
| RKS          | Restricted Kohn Sham                                       |
| ROCIS        | Restricted Open-Shell Configuration Interaction<br>Singles |
| RSD          | Relative standard deviation                                |
| s            | Second   |
| <i>salen</i> | <i>N,N''-ethylene-bis(salicylideneiminate)</i>             |
| SAED         | Selected area electron diffraction                         |
| SCF          | Self Consistent Field                                      |
| SEM          | Scanning electron microscope                               |
| SIM          | Single Ion Magnet  |
| SMM          | Single Molecule Magnet                                     |
| SOC          | Spin Orbit Coupling  |
| SOMF         | Spin-Orbit Mean-Field                                      |
| SOMO         | Singly Occupied Molecular Orbital                          |
| SSC          | Spin-Spin Coupling   |
| SO/OZ        | Spin Orbit/ Orbital Zeeman                                 |
| STO          | Slater Type Orbital  |
| T            | Temperature  |
| t            | Time   |
| terpy        | 2,2':6'',2''-terpyridine                                   |
| tpp          | 5,10,15,20-tetraphenylporphyrin                            |
| TDDFT        | Time-dependent density functional theory                   |

|         |  |
|---------|--|
| UV      | Ultra violet                                   |
| UV-Vis  | Ultra violet visible                           |
| VMO     | Virtual Molecular Orbital                      |
| W       | Watt   |
| W/(m.K) | Watt per metre per kelvin                      |
| wt      | Weight   |
| XPS     | X-ray photoelectron spectroscopy               |
| XRD     | X-ray diffraction                              |
| ZFS     | Zero Field Splitting                           |
| ZORA    | Zero <sup>th</sup> Order Regular Approximation |