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LIST OF SYMBOLS AND ABBREVIATIONS

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

Symbols

θ	Theta
°	Degree
α	Alpha
μ	Mu
Å	Armstrong
Ω	Ohm
υ	Nu
β	Beta
λ	Lambda
Δ	Delta

Abbreviations

acac	acetylacetone
acbo	2,3-anthrachinone-*bis*(oxamato)
aq.	Aqueous
B3LYP	Becke, 3-Parameter Lee Yang Par
BJH	Barrett-Joyner-Halenda
BP	Becke Perdew
bziz	benzimidazole
$^{\circ}C$	Degree celcius
ca.	Circa (approximately)
CASSCF	Complete Active Space Self Consistent Theory
CI	Configuration Interaction
cm	Centimetre
cm^{-1}	Per centimetre
cm^3g^{-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^3	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	High-Frequency Electron Paramagnetic Resonance
HFS	Hartree Fock Slater
HOMO	Highest Occupied Molecular Orbital
HPLC	High performance liquid chromatography
HREM	High-resolution electron microscopy

HRTEM	High-resolution transmission electron microscope
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
$kJmol^{-1}$	Kilojoule per mole
$kJmol^{-1}K^{-1}$	Kilojoule per mole per kelvin
KLMC	Knowledge Led Master Code
$Kmin^{-1}$	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 Unccupied Molecular Orbital
λ_{max}	$\lambda_{maximum}$
m	Metre
M	Molar
MAE	Magnetic Anisotropy Energy
$mAhg^{-1}$	milliampere-hour per gram
MB	Methylene blue
mg	Milligram
m^2g^{-1}	Metre square per gram
mg/g	Milligram per gram
mgL^{-1}	Milligram per litre
μm	Micrometre

$\mu g/dm^3$	Microgram per decimetre cube
MHz	Megahertz
min	Minute
$min^{-1}g^{-1}$	Perminute per gram
MLCT	Metal to Ligand Charge Transfer
mL	Millilitre
$mLmol^{-1}$	Millilitre per mole
mmol	Millimole
mmol/L	Millimole per litre
mol	Mole
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-*bis*(oxamato)
NESC	Normalized Elimination Of Spin Component
NEVPT	N-electron Valence Shell Perturbation Theory
NH_2pymd	2-aminopyrimidine
nm	Nanometre
NMR	Nuclear Magnetic Resonance
No.	Number
nΩ.m	Nanoohmmetre
NO_2dmiz	nitro-N-dimethylimizadole
NPs	Nanoparticles
npbo	1,8-naphthalene-*bis*(oxamato)
4-NP	4-nitrophenol
4-NT	4-nitrotoluene
ORR	Oxygen reduction reaction
obbo	o-benzyl-*bis*(oxamato).
opba	*o*-phenylene-*bis*(oxamato)
ox	oxalate
pba	propylene-*bis*(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 Singles
RSD	Relative standard deviation
s	Second
salen	*N*,*N*″-ethylene-bis(salicylideneiminate)
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	Zeroth Order Regular Approximation