

## TABLE OF CONTENT

	Contents	Page No.
ABSTRACT		i-iv
LIST OF FIGURES		v-vi
LIST OF TABLES		vii-viii
LIST OF SYMBOLS AND ABBREVIATIONS		ix-xiv
<b>CHAPTER 1: INTRODUCTION</b>		<b>1-1-1-39</b>
	INTRODUCTION	1-1
1.1	Various magnetic parameters	1-5
1.1.1	g-Tensor	1-5
1.1.2	D-Tensor	1-9
1.1.3	Hyperfine coupling	1-12
1.2	Magnetic properties in metal clusters	1-14
1.3	Computational methods	1-16
1.3.1	Basis sets	1-16
1.3.2	Functionals	1-19
1.3.3	Quantum mechanical methods	1-21
1.3.3.1	<i>Ab Initio</i> method	1-21
1.3.3.2	Density functional theory	1-22
1.3.4	ORCA package	1-24
1.3.4.1	Treatment of spin-orbit coupling	1-24
1.3.4.2	Quasi-restricted orbitals approach	1-25
1.3.4.3	Pederson-Khanna approach (PK)	1-26
1.3.4.4	Coupled-Perturbed (CP) approach:	1-27
1.3.4.5	Spin-spin contribution	1-27
	REFERENCES	1-28-1-39
<b>CHAPTER 2: ZERO FIELD SPLITTING IN Mn (III) COMPLEXES: A COMPARATIVE STUDY OF DFT BASE COUPLED-PERTURBED AND PEDERSON-KHANNA APPROACHES</b>		<b>2-1-2-21</b>
	INTRODUCTION	2-1
2.1	Theory	2-3
2.2	Computational details	2-7
2.3	Results and discussion	2-8
	REFERENCES	2-16-2-21
<b>CHAPTER 3: A SYSTEMATIC APPROACH TO FIND SUITABLE BASIS SETS AND FUNCTIONALS FOR BETTER PREDICTION OF</b>		<b>3-1-3-25</b>

## MAGNETIC PARAMETERS USING Cu(II) COMPLEXES

INTRODUCTION	3-1
<b>Section 3a. Study of Mono and Bidentate Ligands Bound Cu(II) Complexes</b>	<b>3-2—3-9</b>
3A.1 Theory	3-2
3A.2 Computational details	3-3
3A.3 Results and discussion	3-5
<b>Section 3b. Study of Basis Sets and Functionals In Cu(II) Bis(Oxamato) Complexes</b>	<b>3-10—3-19</b>
3B.1 Theory	3-10
3B.2 Computational details	3-11
3B.3 Results and discussion	3-13
REFERENCES	3-20—3-25
<b>CHAPTER 4: REGULAR APPROXIMATION APPROACH FOR PREDICTION OF MAGNETIC PARAMETERS IN Co(II) COMPLEXES AND THEIR CORRELATION WITH CHEMICAL REACTIVITY</b>	<b>4-1—4-20</b>
INTRODUCTION	4-1
4.1 Theory	4-2
4.2 Computational details	4-3
4.3 Results and discussion	4-4
4.3.1 Calculation of g-Tensors in the Co[Cl <sub>2</sub> L <sub>2</sub> ] complexes	4-5
4.3.2 Calculation of D-Tensors in the Co[Cl <sub>2</sub> L <sub>2</sub> ] complexes	4-8
4.3.3 FMO Analysis done on cobalt complexes	4-11
REFERENCES	4-17—4-20
<b>CHAPTER 5: AN INVESTIGATIVE STUDY FOR ESTIMATION OF ZERO FIELD SPLITTING AND HYPERFINE COUPLING IN Co(II) COMPLEXES USING AB INITIO CASSCF METHOD</b>	<b>5-1—5-16</b>
INTRODUCTION	5-1
<b>Section 5a. Prediction of D-Tensor and Hyperfine Coupling in [CoN<sub>2</sub>X<sub>2</sub>] and [Co(PPh<sub>3</sub>)<sub>2</sub>X<sub>2</sub>]. using CASSCF Method</b>	<b>5-1—5-8</b>
5A.1 Theory	5-1
5A.2 Computational details	5-3
5A.3 Results and discussion	5-5
<b>Section 5b. Study Of D-Tensors in seven coordinated Co(II) complexes</b>	<b>5-9—5-13</b>
5B.1 Theory	5-9
5B.2 Computational details	5-9
5B.3 Results and discussion	5-10
REFERENCES	5-14—5-16

<b>CHAPTER 6: DENSITY FUNCTIONAL STUDY OF MAGNETIC PARAMETERS IN (NiO)<sub>n</sub> NANOCCLUSERS</b>	<b>6-1—6-15</b>
INTRODUCTION	6-1
6.1 Theory	6-2
6.2 Computational details	6-3
6.3 Results and discussion	6-4
REFERENCES	6-13—6-15
<b>CHAPTER 7: CONCLUSION AND FUTURE PROSPECTS</b>	<b>7-1—7-3</b>
7.1 Concluding Remarks and Outlook	7-1
Future Scope	7-3
<b>LIST OF PUBLICATIONS &amp; CONFERENCES ATTENDED</b>	<b>xiv</b>