

LIST OF FIGURES AND SCHEMES

Figure 1.1 Diethyldithiocarbamate-Fe (III) compounds	3
Figure 1.2 Mn ₁₂ (acetate) molecule	4
Figure 1.3 Examples of organic radicals	5
Figure 1.4 Examples of polyradicals	8
Figure 1.5 The Electrode–Molecule–Electrode transport structure	10
Figure 3.1 Molecular wires without radical substitution	35
Figure 3.2 Diradicals based on molecular wire 1	35
Figure 3.3 Diradicals based on molecular wire 2	35
Figure 3.4 Au-molecule-Au structures	36
Figure 3.5 Molecular wire1 and molecular wire 2	37
Figure 3.6 Transmission spectra of molecular wire without radical substitution	39
Figure 3.7 Molecular orbitals of the wire 1 under different electric fields	40
Figure 3.8 Molecular orbitals of the wire 2 under different electric fields	40
Figure 3.9 Plot of J vs. distance between the radical centers	42
Figure 3.10 Spin density distribution of radical substituted molecular wire 1	43
Figure 3.11 Spin density distribution of radical substituted molecular wire 2	43
Figure 3.12 Transmission spectra of diradical substituted molecular wire 1	44
Figure 3.13 Transmission spectra of diradical substituted molecular wire 2	45
Figure 4.1 Allene and cumulene based diradicals	50
Figure 4.2 R and S configuration of the diradicals	52
Figure 4.3 VCD spectra of two enantiomers of series 2	52
Figure 4.4 Spin density plot of all the diradicals	55
Figure 4.5 Spin density plot for the diradicals of series 1	56
Figure 4.6 Spin polarization of π electron within the coupler	57
Figure 4.7 Plot of J vs. distance between radical centers	57
Figure 4.8 Molecular orbitals of all the diradicals	60
Figure 4.9 Molecular orbitals of the diradicals with varying geometry	61
Figure 4.10 Molecular orbital of the diradicals in broken symmetry state	62
Figure 4.11 Allene and cumulenes based diradical with phases of HOMO-2	63
Figure 4.12 Plot of energy vs. distance between radical centers	64
Figure 5.1 Designed diradicals	70
Figure 5.2 Designed diradical for transport calculations	73
Figure 5.3 Plot of J vs. number of carbon atoms within the coupler	74
Figure 5.4 Regression analyses for odd cumulene series	78
Figure 5.5 Regression analyses for even cumulene series	79
Figure 5.6 Spin density plot for even cumulene systems	80
Figure 5.7 Spin density plot for conjugated systems	81
Figure 5.8 π -interaction of diradicals	82
Figure 5.9 Representation for the radical based systems	84
Figure 5.10 Transmission spectra (for α spin)	85
Figure 5.11 Transmission spectra (for β spin)	86
Figure 5.12 Representation for systems without radical centers	86
Figure 5.13 Transmission spectra of molecular wires without radical centers	87

Figure 5.14 Designed even cumulene based molecular wires	90
Figure 5.15 Designed even conjugated system based molecular wires	91
Figure 5.16 Designed odd cumulene based molecular wires	91
Figure 5.17 Spin polarization within the odd cumulene systems	92
Figure 5.18 Spin polarization within the even cumulene systems	92
Figure 5.19 Spin polarization within conjugated systems	93
Figure 6.1 Heteroallene and heterocumulene based diradicals	100
Figure 6.2 Dihedral angles in heterocumulene and heteroallene systems	105
Figure 6.3 Nitronyl nitroxide diradicals (with P-substitution)	107
Figure 6.4 Delocalization of unpaired electron in <i>Z</i> -isomer of heterocumulene based diradical	109
Figure 6.5 Spin density plot for the P-substituted allene and cumulene based <i>tert</i> -butyl nitroxide diradicals	110
Figure 6.6 Spin density plot for the As-substituted allene and cumulene based <i>tert</i> -butyl nitroxide diradicals	110
Figure 6.7 Delocalization of unpaired electron in heteroallene based diradicals	111
Figure 6.8 <i>J</i> values of P-substituted cumulene based diradicals at different dihedral angle	112
Figure 6.9 Spatial distribution of SOMOs of the P-substituted cumulene based diradicals	113
Figure 6.10 Spatial distribution of molecular orbitals of the P-substituted nitronyl nitroxide diradicals	114
Figure 6.11 Spatial distribution of molecular orbitals of the As-substituted <i>tert</i> -butyl nitroxide diradicals	115
Figure 6.12 Spatial distribution of SOMOs of the allene based diradicals with P-substitution	116