LIST OF TABLES

Table no.	Title	Page no.
4.1	Selected bond lengths and bond angles of gemfibrozil by B3LYP/6-31G (d) in comparison with the XRD data.	39
4.2	Selected dihedral angles of gemfibrozil by B3LYP/6-31G (d) in comparison with the XRD data.	40
4.3	Second order perturbation theory analysis of Fock matrix in NBO basis.	42
4.4	Definition of internal valence coordinates of gemfibrozil.	43
4.5	Definition of local symmetry coordinates (much like the natural internal coordinates) and the corresponding force constant (mdyne/A°) of gemfibrozil with scale factors used.	47
4.6	Vibrational assignment of gemfibrozil by normal coordinate analysis based on SQM force field calculations.	51
4.7	Atomic charges for optimized geometry of gemfibrozil at B3LYP/6-31G (d) level.	59
5.1	Bond lengths of sulfasalazine monomer and dimer by B3LYP/6-311G (d, p) in comparison with the XRD data.	66
5.2	Bond angles of sulfasalazine monomer and dimer by B3LYP/6-311G (d, p) in comparison with the XRD data.	68
5.3	Dihedral angles of sulfasalazine monomer and dimer by B3LYP/6-311G (d, p) in comparison with the XRD data.	70
5.4	Optimized hydrogen-bond geometry of sulfasalazine.	72
5.5	Occupancies of interacting NBOs of sulfasalazine with their respective energies.	73
5.6	Second order perturbation theory analysis of Fock matrix in NBO basis.	74
5.7	Definition of internal valence coordinates of sulfasalazine.	76
5.8	Definition of local symmetry coordinates (much like the natural internal coordinates) and the corresponding force constant (mdyne/A°) of sulfasalazine with scale factors used.	80
5.9	Vibrational assignment of sulfasalazine by normal coordinate analysis based on SQM force field calculations.	86

Table no.	Title	Page no.
5.10	Aromaticity values of pyridine and phenyl rings in sulfasalazine.	94
6.1	Selected bond lengths and bond angles of sulfamerazine by B3LYP/6-311G (d, p) in comparison with the XRD data.	98
6.2	Selected dihedral angles of sulfamerazine by B3LYP/ 6-311G (d, p) in comparison with the XRD data.	99
6.3	Second order perturbation theory analysis of Fock matrix in NBO basis	101
6.4	Different types of electronic basins, ELF value at attractor (ELF), basin population (N), standard deviation (σ^2) and relative fluctuation (λ) of sulfamerazine.	104
6.5	Definition of internal valence coordinates of sulfamerazine.	105
6.6	Definition of local symmetry coordinates (much like the natural internal coordinates) and the corresponding force constant (mdyne/A°) of sulfamerazine with scale factors used.	108
6.7	Vibrational assignment of sulfamerazine by normal coordinate analysis based on SQM force field calculations.	111
7.1	Bond lengths and Bond angles of PNOC and PNMC by B3LYP/6-31G (d) in comparison with the XRD data.	121
7.2	Dihedral angles of PNOC and PNMC by B3LYP/6-31G (d) in comparison with the XRD data.	122
7.3	Second order perturbation theory analysis of Fock matrix in NBO basis.	126
7.4	Definition of internal valence coordinates of 2-methyl-4-nitrophenol.	127
7.5	Definition of internal valence coordinates of 3-methyl-4-nitrophenol.	128
7.6	Definition of local symmetry coordinates (much like the natural internal coordinates) of PNOC and the corresponding force constant (mdyne/A_) with scale factors used.	131
7.7	Definition of local symmetry coordinates (much like the natural internal coordinates) of PNMC and the corresponding force constant (mdyne/A_) with scale factors used.	133
7.8	Vibrational assignment of PNOC and PNMC by normal coordinate analysis based on SQM force field calculations.	136
8.1	Selected bond lengths and bond angles of ethyl centralite by B3LYP/6-31G(d) in comparison with the XRD data.	146

Table no.	Title	Page no.
8.2	Dihedral angles of ethyl centralite by B3LYP/6-31G(d) in comparison with the XRD data.	148
8.3	Second order perturbation theory analysis of Fock matrix in NBO basis.	152
8.4	Definition of internal valence coordinates of ethyl centralite.	153
8.5	Definition of local symmetry coordinates (much like the natural internal coordinates) and the corresponding force constant (mdyne/A°) of EC with scale factors used.	157
8.6	Vibrational assignment of ethyl centralite by normal coordinate analysis based on SQM force field calculations.	162
8.7	Experimental and calculated absorption wavelengths, energies, oscillator strengths of EC using TD-DFT method at the B3LYP/6-31G(d) level.	170

LIST OF FIGURES

Figure no.	Title	Page no.
2.1	Instrumentation of single beam Fourier transform infrared spectrometer.	12
2.2	Quantum energy transitions for Rayleigh and Raman scattering.	14
2.3	Instrumentation of Fourier transform-Raman spectrometer.	17
2.4	Electronic transitions.	20
2.5	Schematic of the double beam spectrophotometer for the UV-visible region.	21
4.1	Optimized molecular structure and atomic numbering of gemfibrozil.	38
4.2	(a) Experimental and (b) Simulated IR spectra of gemfibrozil.	46
4.3	(a) Experimental and (b) Simulated Raman spectra of gemfibrozil.	50
4.4	The atomic orbital components of the frontier molecular orbital of gemfibrozil.	58
4.5	Atomic charge distribution of gemfibrozil.	60
5.1	Optimized molecular structure and atomic numbering of sulfasalazine monomer.	64
5.2	Optimized molecular structure and atomic numbering of sulfasalazine dimer.	64
5.3	Bridging part (intra and intermolecular hydrogen bonding) of sulfasalazine dimer.	65
5.4	(a) Experimental and (b) simulated IR spectra of sulfasalazine.	84
5.5	(a) Experimental and (b) simulated Raman spectra of sulfasalazine (3600-2500 cm ⁻¹ region).	85
5.6	(a) Experimental and (b) simulated Raman spectra of sulfasalazine (2500-50 cm ⁻¹ region).	93
6.1	Optimized molecular structure and atomic numbering of sulfamerazine.	97
6.2	Electron localization function value defining the bonding isosurface $\eta(r)$ = 0.80 for sulfamerazine.	103
6.3	(a) Experimental and (b) simulated IR spectra of sulfamerazine.	111
6.4	(a) Experimental and (b) simulated Raman spectra of sulfamerazine (3600-2500 cm ⁻¹ region).	116

Figure no.	Title	Page no.
6.5	(a) Experimental and (b) simulated Raman spectra of sulfamerazine (2500-50 cm ⁻¹ region).	117
7.1	Optimized molecular structure and atomic numbering of (A) PNOC and (B) PNMC.	123
7.2	Experimental and simulated IR spectra of PNOC (A, B) and PNMC (C, D) respectively.	131
7.3	Experimental and simulated Raman spectra of PNOC (A, B) and PNMC (C, D) respectively (3600-2500 cm ⁻¹ region).	133
7.4	Experimental and simulated Raman spectra of PNOC (A, B) and PNMC (C, D) respectively (2500-50 cm ⁻¹ region).	142
8.1	Optimized molecular structure of ethyl centralite.	145
8.2	(a) Experimental and (b) simulated IR spectra of ethyl centralite.	160
8.3	(a) Experimental and (b) simulated Raman spectra of ethyl centralite.	161
8.4	(a) Experimental UV-visible spectrum of ethyl centralite in ethanol and (b) simulated UV-visible spectrum of ethyl centralite in gas phase and ethanol calculated using the PCM-TD-DFT method.	169
8.5	Molecular frontier orbitals of ethyl centralite.	170
8.6	Simultaneous strong bands both in (a) FT-Raman and (b) FT-IR spectra of ethyl centralite contributing to its NLO activity.	172