## LIST OF TABLES

1.1 Commonly used methods in Gaussian calculation. ............................................. 51
1.2 Commonly used basis functions with their basis criteria and field of usefulness. ........ 52

2.1 Specifications of delay generator employed in experimental set-up. ......................... 72
2.2 (2+1) REMPI transitions of atomic species of chlorine and bromine. ....................... 81
2.3 Specifications of nozzle-skimmer assembly employed in experimental set-up. ............ 85
2.4 Laser emission characteristics of Nd:YAG Laser employed. ................................ 96
2.5 Specifications of second harmonic of Seeded Nd:YAG and the dye laser systems employed. 99
2.6 Specifications of excimer laser employed. ....................................................... 102
2.7 Specifications of boxcar employed in experimental set-up. ................................... 109

3.1 Comparison of results on photodissociation of oximes at 193 nm. All energies are reported in kcal/mol. ............................................................ 136

4.1 Different transition type in CHD and their vertical excitation energies in eV and corresponding values in kcal/mol, nm and respective oscillator strength, (given in parentheses) of various excited states of both the conformers of enolic-1,2-cyclohexanedione, namely H-bonded conformer (\textit{a}) and non-H-bonded conformer (\textit{c}). Table also reports the relative energy in units of kcal/mol and nm of different stationary points in the excited states of both the conformers. .............................................. 155

5.1 Vertical excitation energies (eV) and oscillator strengths (given in parentheses) of low-lying singlet states of CINT and NCP with respective designation. The nature of transition and MO’s involved in the transitions are also given. ................................................................. 187

6.1 Comparison of experimental and literature REMPI lines for Cl. ............................ 202
7.1 Comparison of experimental and literature REMPI lines for Br. ............................ 222
7.2 Various mass fragments observed in multiphotonic processes of 2-chloro-thiophene and 2-bromo-5-chlorothiophene at 235 nm. ................................. 231
7.3 Vertical excitation energies (eV) and oscillator strengths (given in parentheses) of low-lying singlet states of thiophene, 2-chlorothiophene and 2-bromo-5-chlorothiophene with respective designation. The $C_{2v}$, $C_s$ and $C_s$ symmetry designation of thiophenes, nature of transition and MO’s involved in the transitions are also indicated in the heading for thiophene, 2-chlorothiophene and 2-bromo-5-chlorothiophene.

7.4 The average translational energy, $\langle E_T \rangle$, available energy ($E_{avl}$), $f_T$ value, and the relative quantum yield of spin-orbit states ($\Phi$) for photodissociation of 2-chlorothiophene and 2-bromo-5-chlorothiophene at $h\nu=235$ nm. The excitation energy is 122 kcal/mol. The $D_0^0$ (C–X) for Cl and Br elimination channel is taken as 99.0 and 91.0 kcal/mol, respectively. All energies are in kcal/mol.