List of Tables

Table	*Title*	*page*
3.1	Energies of stationary points on the 3-oxetanone dissociation pathways shown in Figure 3.1. Numbers are in units of kcal/mol and are relative to the reactant energy at a given level of theory.	17
3.2	Overall trajectory events following excitation of the 3-oxetanone molecule	20
3.3	Various different dissociation pathways observed for the 3-oxetanone molecule	22
3.4	Minor pathways observed in the dissociation of 3-oxetanone	25
4.1	Stationary point energies of CF_2Cl_2 dissociation profile computed using different levels of theory. The energies are in kcal/mol and relative to the reactant molecule.	33
4.2	Stationary point energies of CF_2Br_2 dissociation profile computed using different levels of theory. The energies are in kcal/mol and relative to the reactant molecule.	33
4.3	Stationary point energies of $CHBr_3$ dissociation profile computed using different levels of theory. The energies are in kcal/mol and relative to the reactant molecule.	34
4.4	Stationary point energies of CH_2BrCl dissociation profile computed using different levels of theory. The energies are in kcal/mol and relative to the reactant molecule.	35
4.5	Comparison of stationary point energies (in kcal/mol) on the dissociation energy profiles of halons computed using PBE0/6-31G* and CCSD(T)//MP2/aug-cc-pVTZ level of theories. Energies given are relative to respective reactants and zero point energy corrected.	36
4.6	Summary of trajectory events of CF_2Cl_2 and CF_2Br_2 dissociation.	39
4.7	Fractions of radical and molecular products (in percentage) produced in the unimolecular decompositions of halons.	45
5.1	Comparison of stationary point energies (in kcal/mol) on the dissociation energy profiles of $RC(O)N_3$ (R = CH_3 and F) computed using different methods with 6-31+G* basis set. Energies given are relative to the respective syn conformer without zero-point energy corrections.	51