List of Tables

3.1 The calculated formation energies (in hartrees) of the N^{q+} atomic ions 43

3.2 Theoretically calculated values of KER in case of N_2^{q+} ($3 \leq q \leq 6$) dissociating to the lowest possible states of $N^{m+} + N^{n+}$ with m+n=q. These values denote the upper limit of the KER. (see text) 45

3.3 The calculated formation energies (in hartrees) of the C^{q+} and O^{q+} atomic ions 48

3.4 Theoretically calculated values of KER in case of CO^{q+} ($4 \leq q \leq 6$) dissociating to the lowest possible states of $C^{m+} + O^{n+}$ with m+n=q. These values denote the upper limit of the kinetic energy release (KER). 49

4.1 This table shows the KER values obtained for the various fragmentation channels N^{r+} - N^{s+} in N_2 fragmentation induced by ion impact. The values calculated from pure Coulomb explosion model are also included. 54

4.2 Theoretically calculated values of KER in case of N_2^{q+} ($3 \leq q \leq 6$) dissociating to the lowest possible states of $N^{m+} + N^{n+}$ with m+n=q. These values denote the upper limit of the KER. 55

4.3 The possible molecular states of N_2^{2+} dissociating into $N^+(^3P) + N^+(^3P)$ along with the theoretically calculated values of KER taken from reference [4] 56

4.4 Results of theoretical calculations for N_2^{3+} dissociation taken from reference [6] 57

5.1 Observed most probable values in the KER spectra for the various fragmentation channels C^{r+} - O^{s+} in CO fragmentation induced by ion impact. The values calculated from pure Coulomb explosion model are also included. 74

5.2 The possible molecular states of CO^{3+} dissociating into $C^{2+}+O^{+}$ along with the theoretically calculated values of KER [14] 76

5.3 The possible molecular states of CO^{4+} dissociating into C^{m+} + O^{n+} $(m+n=4)$ along with the theoretically calculated (UHF calculation) values of KER 78

5.4 The possible molecular states of CO^{5+} dissociating into C^{m+} + O^{n+} $(m+n=5)$ along with the theoretically calculated (MP2 calculation) values of KER 80

5.5 The possible molecular states of CO^{6+} dissociating into C^{m+} + O^{n+} $(m+n=6)$ along with the theoretically calculated (UHF calculation) values of KER 82