Fragment kinetic energy distributions in ion induced CO_2 fragmentation

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Fragment kinetic energy distributions in ion induced CO_2 fragmentation

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Synopsis The dissociation of CO_2^{3+} formed in heavy ion induced ionization of CO_2 has been studied using the technique of time of flight mass spectroscopy with position sensitive ion detector, with 5 MeV/u Si^{12+} ions as projectiles. The kinetic energy released in the $CO_2^{3+} \rightarrow C^+ + O^+ + O^+$ is measured and compared to theoretical *ab initio* calculations as well as photoionization results.

Several studies, both experimental as well as theoretical, have been carried out on multiply charged CO_2 molecular ions. Almost all accurate calculations to date pertain to properties of the neutral, singly and doubly charged CO_2 leaving the potential energy surfces of CO_2^{3+} unexplored. In the present article we report the results of study of ion-induced molecular dissociation of CO_2^{3+}, generated during the collision of neutral CO_2 molecules with a beam of 5 MeV/amu Si^{12+} ions, using the technique of time-of-flight mass spectrometry employing time and position sensitive detectors in multi-hit coincidence mode. The experiments were carried out using the Pelletron accelerator at the Inter University Accelerator Centre (IUAC), New Delhi, India. We have observed three fragmentation pathways of CO_2^{3+} (i) C^{2+}:O^+:**O**, (ii) **C**:O^{2+}:O^+ and (iii) C^+:O^+:O^+ .

Earlier studies [1] on the triple photoionization of CO_2 and subsequent dissociation into C^+:O^+:O^+ have indicated that the kinetic energy release (KER) in the fragmentation of CO_2^{3+} is about 44 eV attributed by the authors to multiple level crossings in the potential energy curves. The prediction from a simplistic Coulomb explosion model is about 30 eV. The fragmentation of CO_2^{3+} formed in the collisions of CO_2 with slow heavy ions (3.2 keV/u Ar^{8+}) [2] have indicated the possibility of multiple mechanisms being responsible for the different kinetic energy releases observed in those experiments including sequential, asymmetric stretch as well as direct dissociation.

In our experiments, the short interaction times mean that the transitions are vertical (Frank-Condon) and the molecule is "fixed-in-space". The kinetic energies of the fragments are plotted in figure 1 along with a momentum correlation map of all the three fragments. We find that the two O fragments have equal but not opposite momentum and the central C atom always carries some significant amount of momentum. The kinetic energy distributions of the two O^+ ions are also very similar. From momentum imaging we have determined that the O-C-O bond angle for this channel is around 170^o.

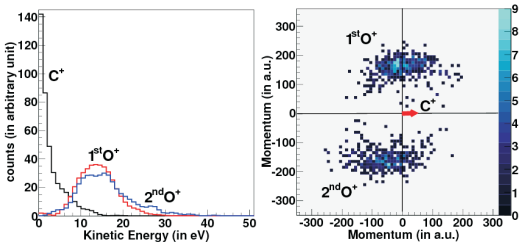

Figure 1. Kinetic Energy distributions of the fragments and momentum imaging for the dissociation of CO_2^{3+} into C^++O^++O^+.

We have also carried out *ab initio* quantum chemical calculations using the GAMESS package [3]. Theoretically calculated KER for $CO_2^{3+} \rightarrow C^+ + O^+ + O^+$ is in good agreement with the experimental result (31 eV). This can come from the decay of $^2\Pi$ molecular state of CO_2^{3+} into C^+ (^{2}P) + O^+ (^{4}S) + O^+ (^{4}S) releasing around 30.8 eV.

References

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