Three body fragmentation of CO_2 in collisions with 5.9 MeV/u Xe¹⁸⁺ and Xe⁴³⁺ ions

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The multiple ionization and fragmentation of CO_2 by fast Xe^{18+} and Xe^{43+} ions was studied utilizing a position- and time-sensitive multi-particle detector which allows the coincident measurement of the momenta of correlated fragment ions. The experiment has been performed using the highly charged ion beam of the UNILAC at the GSI Darmstadt. The slow fragment ions and electrons generated in the collision process are separated by a weak electric field. Electrons were detected by a channeltron at one side of the interaction region; positive ions were accelerated towards the time- and position-sensitive multi-particle detector at the other side [1,2]. For each positive fragment ion the position and the time-of-flight relative to the electron signal were recorded. Of special interest are the Coulomb explosion processes where all fragments are positively charged. For these reaction channels the coincident measurement of the momenta of correlated fragment ions yields a kinematically complete image of the molecular break-up process, and the kinetic energy release as well as angular correlations can be derived for each individual event. In collisions of fast highly charged Xe-ions with CO₂ coincidences with a total charge of at least 6 are clearly separated. Among the various observed reaction channels the reactions $\tilde{C}^{q+} + O^{p+} + O^{r+}$ fulfill the conditions for a kinematically complete description of the fragmentation process. For these reactions the fragmentation dynamics may be analyzed in terms of three independent parameters. A practical choice of the characteristic variables consists of the kinetic energy release and the angles χ and θ_v in velocity space [3].

Fig. 1 shows the kinetic energy release spectrum and the measured distribution of the angles χ and θ_v observed in C⁺+O⁺+O⁺ fragmentation in collisions with 5.9MeV/u Xe¹⁸⁺ and Xe⁴³⁺. All three characteristic parameters are independent of the projectile charge measured here. The maximum of the measured kinetic energy distribution is in good agreement with the prediction of the point charge Coulomb explosion model.

The angle χ , defined by the relative velocity of the O⁺ions \vec{v}_{OO} and \vec{v}_C , is an indicator whether the molecular bonds break simultaneously or in a stepwise fashion [4]. The χ distribution shows a peak around 90 degrees which is consistent with a simultaneous break up of the molecular bonds. A break-up of the molecular bonds in a time short on a time scale defined by rotational and vibrational periods of the system leads to a strong angular correlation between the corresponding velocities which shows up as a narrow peak in the χ -distribution. In case of a two-step process the correlation would be lost resulting in a uniform χ -distribution.

The angle θ_v , defined by the two relative \vec{v}_{CO} velocities, is closely connected with the O-C-O bond angle. For Carbon-dioxide as a linear molecule the maximum of the O-C-O bond angle would be expected around 180



Figure 1: Kinetic energy release and angles χ and θ_v derived from coincident C⁺+O⁺+O⁺ fragments in collisions with 5.9 MeV/u Xe^{*q*+}. The energy release predicted by the Coulomb explosion model (CE) and the most probable angle θ_v expected for the bending mode $v_2 = 0$ are marked in the figure.

degrees. The θ_v -distribution observed in collisions with fast highly charged ions is clearly shifted to smaller angles with a broad maximum around 120 degrees. This can be qualitatively understood taking into account the vibration modes of CO₂. Using a harmonic oscillator potential to describe the bending-mode groundstate ($\nu_2 = 0$) leads to a most probable "bond angle" of $\beta \approx 172.5$ degree. In the Coulomb explosion model this angle corresponds to an angle $\theta_v \approx 142^\circ$ in velocity space which is in good qualitative agreement with the experimental results.

References

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