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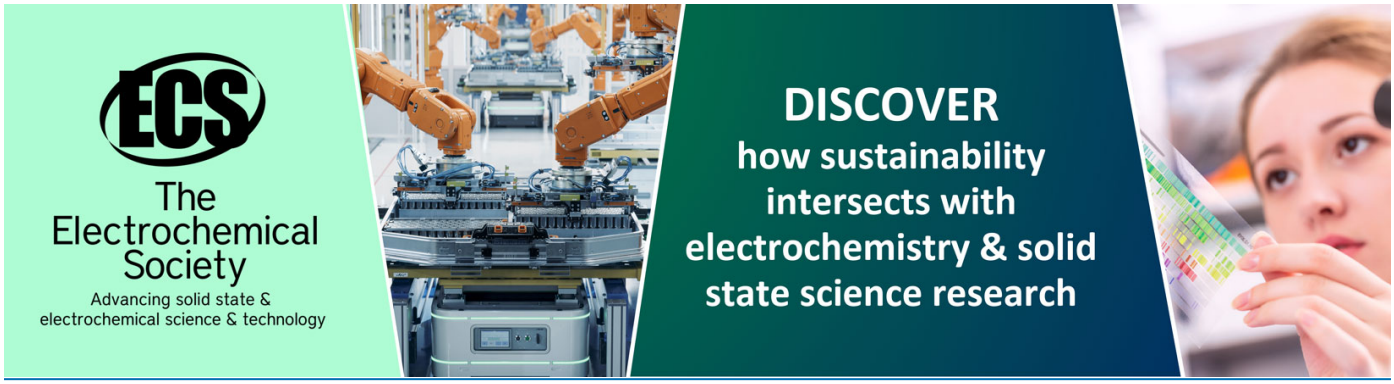

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Kinetic energy release in dissociation of NH_3^{q+} under ion impact

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Synopsis The dynamics of the dissociation of multiply charged ammonia ions is investigated. The pathways for sequential and concerted dissociation are separated, and the kinetic energy released along the different pathways is measured. The measured values are compared with *ab-initio* quantum chemical calculations to identify the repulsive states of the molecular ion which are responsible for the two pathways.

Dissociation of molecules under charged particle impact has been an active field of study. Concerted and sequential dissociation of multiply charged polyatomic molecular ions is being studied by several groups to understand the role of excited states in such processes. We have studied the dissociation of ammonia under energetic highly charged ion impact. The (multiply charged) projectile ion beam is obtained from an electron cyclotron resonance ion source. These ions are made to collide with an effusive jet of neutral NH_3 molecules at room temperature. The technique of recoil ion momentum spectrometry and multi-hit ion detection are used in unison [1] to measure the kinetic energy released in the dissociation of NH_3^{q+} (q=2,3). The measured data contains a mixed signature (black curve in Figure 1) for the events arising from the concerted and sequential dissociation dissociation of multiply ionized NH_3. We have used the technique of Dalitz plot [2] to disentangle the events arising from the symmetric concerted dissociation of NH_3^{3+} from the rest of the events.

The theoretical *ab initio* calculations using the quantum chemistry package GAMESS are performed to obtain the possible electronic states for the doubly and triply ionized ammonia molecule. The energy values for these states are found to be in reasonable agreement with our experimental results and are compared with earlier reported experimental result in literature [3]. These calculations further help in identifying the pathway of dissociation of doubly charged NH_3 when it dissociates sequentially.

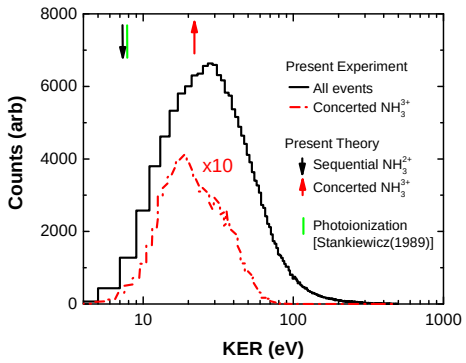

Figure 1. Kinetic energy release distribution for the dissociation of NH_3^{q+} (q=2,3)

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