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Probing the Coulomb Barrier Towards Ionic Fragmentation

SHAUN ARD, NASRIN MIRSALEH-KOHAN, ROBERT COMPTON, University of Tennessee — Quintessential to understanding the stability of multiply charged anions (MCAs) is the characterization of the so-called “Coulomb Barrier” (CB) toward the loss of an excess electron and/or dissociation into charged fragments. The CB arises due to the superposition of the long-range Coulomb repulsion of the excess electron (or anion), and the short-range attractive polarization binding energy of the anion (or fragment). The CB adds to the stability of MCAs, often rendering thermodynamically unstable species to be metastable toward autodetachment or dissociation. The magnitude and shape of the CB is expected to depend heavily on the decay pathway. Whereas dissociation into charged fragments is often the lowest energy pathway for many MCAs, the vast majority of previous research has focused on electron loss. In this work, collision-induced dissociation (CID) is employed to study fragmentation of disulfonic dianions of increasing “length”. Energy threshold for the production of SO_3^- plus its conjugate anion are used to estimate the magnitude of the Coulomb barrier to dissociation. These measured thresholds are compared with *ab initio* calculations of the dissociation energy. The relationship between these magnitudes and the distance between the excess charges will then be discussed.

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