Intra-molecular interactions during the fragmentation of small systems.

R. D. Thomas*

February 3, 2006

Abstract

Recent dissociative recombination (DR) experiments have investigated the role of the parent ion's structure, bonding and charge centre on the DR process. For examples, in the DR of the H_5^+ and $D_5O_2^+$[1] cluster ions, the dominant product channels greatly reflect the structure of the parent ion, $H_3^+ \cdot H_2$, and $D_2O \cdot D^+ \cdot D_2O$[1] respectively, and the question arises on the role played by the "neutral" constituent in the cluster, i.e. as spectator or participant. To investigate this question we have studied the DR of one of the simplest such systems, $Li^+ \cdot H_2$, which is a weakly bound cluster with the charge centre located on the lithium atom. All these systems represent excellent models for providing insight into the dynamics occurring in the fragmentation of small systems.

[1] Någård et al. J. Chem. Phys. 117, 5264 (2002)

*Molecular Physics, Stockholm University