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Breakdown curves of carbon-based molecules for astrochemistry

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Synopsis: Breakdown curves (BDC), which are energy dependent fragmentation branching ratios, constitute a kind of "identity card" of an excited molecule or cluster. We developed a method for constructing semi-empirical BDC, based on fragmentation measurements and structural known quantities of the considered species. Calculations of BDC have been performed within the statistical M3C theory. We will present a comparison of the two methods for some species and discuss application of these results to astrochemistry.

Carbon-based molecules are ubiquitous in astrophysical environments. The study of the composition and evolution of the molecular material is called astrochemistry. It involves the knowledge of a huge amount of data including fragmentation branching ratios (BR). The experimental group in Orsay (France) has developed a dedicated set-up (AGAT) for fragmentation recording of molecules and clusters of known charge and internal energy. Recently they showed how these data could be used to provide, within a statistical fragmentation context, BR for numerous physical and chemical processes of astrophysical interest [1]. The method relies on the construction of Breakdown curves (BDC, which are energy dependent BR) constrained by the experimental measurements.

On the other hand, BDC have been calculated within the Microcanonical Metropolis Monte Carlo method (M3C), recently improved [2]. Figure 1 shows, for the C_7 cluster, a comparison between the semi-empirical BDC and those obtained through M3C. The very good agreement validates so far the semi-empirical approach.

Whereas BDC of some hydrocarbon molecules were so constructed and used to predict BR for various processes [1] we aim at continuing those studies on $C_nH_m^{q+}$ species with larger m and n (n≤5, m≤4 q≤2) and, in a longer term, on nitrogenated species. BR of processes derived from the BDC will be included in the international astrochemical database KIDA (http://kida.obs.u-bordeaux1.fr) [3]. The impact of so-extracted BR in some astrophysical environments (dark clouds and photo-dissociation regions) will be presented and discussed.

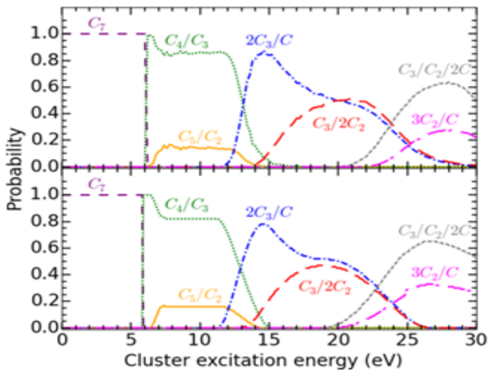

Figure 1 Breakdown curves for the C_7 cluster. Upper panel: theoretical M3C calculations. Lower panel: semi-empirical model.

References

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