

Structure, Ionization and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: $C_nH_m^{q+}$ ($n = 1 - 5, m = 1 - 4, q = 0 - 3$)

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Synopsis The $C_nH_m^{q+}$ family was studied at the DFT-B3LYP//CCSD(T) level of theory. Dissociation energies, ionization potentials, geometries and frequencies were obtained. Different trends for these properties have been observed and analyzed. The fragmentation behaviour has been studied within a combinatorial point of view.

Partially hydrogenated carbon clusters have been widely and heterogeneously studied. Theoretical modeling of their properties and their fragmentation behaviour provides valuable information to study the evolution of new molecules and ions detected in the Interstellar Medium (ISM). It also helps to understand the composition and chemical processes taking place in the ISM[1]. Previously we have only considered bare carbon clusters [2], when hydrogen atoms are added, the complexity of the studied systems increases. In general, only a few works have considered this family of molecules systematically but only on small sequences[3]. This work intends to homogenize all the sparse data available in bibliography for the hydrogenated carbon clusters. From this study we obtain trends that they may be extrapolated to bigger and more complex molecules of the same family.

In this work the calculation of several properties for species of the $C_nH_m^{q+}$ family (for $n=1-5$; $m=1-4$; $q=0-3$) are carried out at DFT-B3LYP/6-311++G(3df,2dp)//CCSD(T)/6-311++G(3df,2dp) level of theory. The studied properties are: relative energies between isomers, ionization potentials, dissociation energies, vibrational frequencies and fragmentation reactions.

The results are interpreted in terms of both, energetic and entropic contributions. The energetic contributions are the values obtained for the relative energy of the isomers. For instance, Fig. 1 shows the distribution of all the considered molecules, note the scaling of the problem by increasing the system size on the top panel. The entropic contribution comes from the combinatorial choices of all possible reaction channels. Fig. 2 shows the combinatorial probability density for the dissociation processes leading to 1, 2, 3 and 4 fragments.

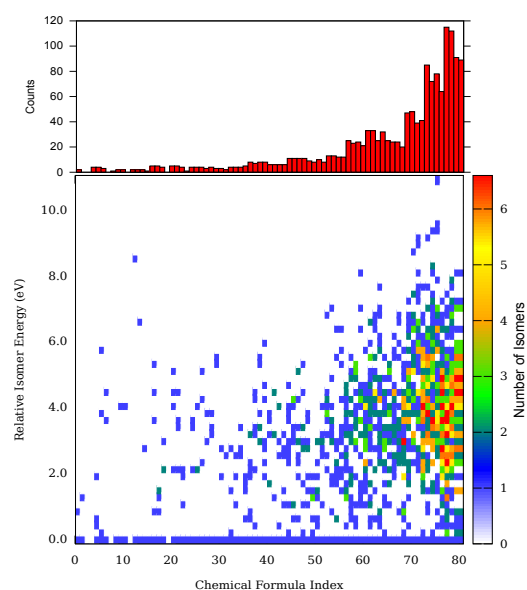


Figure 1. Bivariate histogram with the number of isomers as a function of the Chemical Formula Index $CFI[C_nH_m^{q+}] = (q + 1) + 4(m - 1) + 4(n - 1)$, and the relative isomer energy (from their ground state).

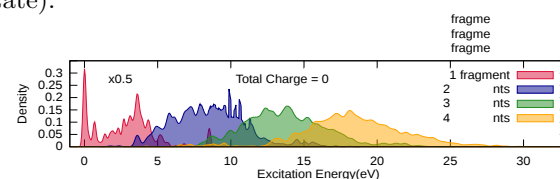


Figure 2. Combinatorial probability density to break down a $C_nH_m^{q+}$ molecule(or cation) into different number of fragments as a function of its internal energy

References

- [1] M. Chabot *et al* 2010 *A&A* **A39** 524
- [2] S. Díaz-Tendero *et al* 2005 *Phys. Rev. A* **71** 033202
- [3] K.-C. Lau *et al* 2005 *J. Chem. Phys* **22** 122

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