FRAGMENTATION OF SMALL NEUTRAL CARBON CLUSTERS

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Recently a new experimental tool has been developed for fragmentation studies of high velocity clusters, based on shape analyses of current pulses delivered by semiconductor detectors [1]. Using this tool, branching ratios of de-excitation of neutral C_n clusters formed by electron capture in $Cn^+ \rightarrow$ He, Ne, Ar collisions at $v_p = 2.6$ a.u, have been measured for n = 5, 6, 7, 8, 9 and 10.

Theoretically we have adapted the Microcanonical Metropolis Monte-Carlo (MMMC) model presented in [2] for the study of metal clusters multifragmentation to the case of small carbon clusters. This model allows the quantitative study of the fragmentation in systems where a large number of fragmentation channels are possible. The basic ingredients introduced in this model (dissociation energies, geometries and density of states) have been obtained using DFT (B3LYP) and CCSD(T) ab initio calculations. In this model all the points of the phase-space are treated simultaneously to calculate the probability of each fragmentation channel at a given total energy of the system.

Therefore we are able to estimate the energy deposit in the capture process through the convolution of the calculated fragmentation probabilities with the right distribution function. In this communication we present and compare the experimental branching ratios with the theoretical results obtained and the calculated energy distribution for the C_5, C_7 and C_9 clusters fragmentation.

References

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