The search for non-IPR isomers of C_{60} in DESIREE

José E. Navarro Navarrete, Paul Martini, Suvasthika Indrajith, Michael Gatchell, Mark H. Stockett, Henrik Cederquist, Henning Schmidt, Henning Zettergren.

Stockholm University (SU), Department of Physics, AlbaNova University Center, S10691 Stockholm, Sweden

After the accidental discovery of fullerenes [1] and its unequivocally identification in the interstellar media (ISM) [2], extensive studies were made to elucidate their specific molecular geometries. These were found to be closed cages with an even number of carbon atoms arranged as 12 pentagons and zero, two or more hexagons. C₆₀ is the smallest member of the fullerene family that obeys the so-called isolated pentagon rule (IPR) [3], where each pentagon is surrounded by 5 hexagons for the most stable isomer. This geometry gives the molecule its exceptional stability and chemical inertness, making it the most abundant of the fullerenes. Every other C₆₀ isomer has at least two pairs of adjacent pentagons. For the first non-IPR isomer of the C₆₀- fullerene, the two adjacent pentagon configuration leads to an enhanced reactivity and a significantly higher electron affinity [4]. The latter suggests that this isomer could have a significant survival probability in astrophysical environments.

A previous study performed in the cryogenic electrostatic ion storage ring facility DESIREE also supports this idea. In this storage ring, the spontaneous decay of hot molecules can be followed on timescales up to hundreds of seconds owing to its excellent vacuum conditions (10^4 cm⁻³ of residual gas density [5]). The observed decay in the case of C₆₀- at timescales exceeding milliseconds could not be explained by the presence of the IPR isomer alone (Figure 1), which suggests that a small population of the first non-IPR isomer of C₆₀-, which do not cool efficiently, is being produced. The presence of this isomer could be measured in DESIREE by laser probing the depletion of neutral yield as a function of storage time.



Figure 1.- The left panel shows the significant rate constants as a function of internal excitation energy for the IPR C₆₀-. The blue curve describes the electron emission from vibrationally hot anions while the orange curve shows the recurrent fluorescence emission rate. The blue shaded region indicates the time window of the measurement ($100\mu s - 500 \text{ ms}$). The right panel shows the measured neutral yield as a function of storage time (black data points) together with the corresponding results from our simulation.

References:

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