Mutual Neutralization in sub-eV C_{60}^{+} + C_{60}^{-} collisions

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The detection of fullerenes in neutral and ionic forms in several extra-terrestrial environments [1][2][3] has been subsequently followed by extensive research, inquiring about the factors that constitute the molecule's formation and survival in these environments [4]. To advance the understanding of charge transfer processes involving fullerene molecules and their importance in e.g. space, we have performed mutual neutralization studies using the cryogenic storage ring facility, DESIREE [5]. With DESIREE, we are able to study sub-eV collisions between C_{60}^{+} and C_{60}^{-} ion beams, which marks the first-ever reported studies in this regime for molecular collisions. We detect neutral products formed in the process, that have an energy distribution with identifiable electronic excited states. The process is then modelled with the multi-state Landau-Zener method [6], using relevant interaction potentials [7][8] and coupling elements [9]. The excited states of C_{60} used in the model were computed using Time Dependent-Density Functional Theory at the PBE0/6-311++G(d,p) level of theory. The Landau Zener model predicts the total charge transfer cross section to be 5.52 x 10^{-11} cm^2, for a center-of-mass collision energy of 1 meV. This is a factor of 4-5 larger than for H^{+} + H^{-} collisions at the same collision energy [10]. The branching ratios subsequently obtained from the theoretical calculations follow the experimental trend observed for the same.

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