Abstract Submitted
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Deterministic simulations of endohedral noble gas release from fullerene clusters[1] M.K. BALASUBRAMANYA, Texas A&M University - Corpus Christi, MICHAEL ROTH, University of Northern Iowa, PHILIP TILTON, Texas A&M University - Corpus Christi, BRYCE SUCHY, University of Northern Iowa — Molecular Dynamics computer simulations are conducted on small ($N = 5$) endohedral $X@C_{60}$ clusters, where X = He, Ne, Ar, Kr and Xe. The cluster dissociates at a temperature between $T = 1150$K and 1200K. As temperature is raised further, endohedral atoms begin leaving the cluster near $T = 4000$K. In the temperature range [4000K, 5000K] escape constants and half lives are calculated for release of the various gases. Helium exits much more quickly than any other noble gas examined, and larger species tend to exit more slowly not only because of their larger collision diameter but also because they stabilize the fullerene cage. Comparisons with and contrasts to experiment are mentioned.

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