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Evidence of nanosegregation and Jahn-Teller effect in Na_2C_{60}
KATALIN KAMARÁS, , GYÖNGYI KLUPP, PÉTER MATUS, LÁSZLO F. KISS, SÁNDOR PEKKER, Research Institute for Solid State Physics and Optics, Budapest, Hungary, DARIO QUINTAVALLE, ANDRÁS JÁNOSSY, Budapest University of Technology and Economics, Budapest, Hungary, NORBERT M. NEMES, CRAIG M. BROWN, JUSCELINO LEAO, NIST Center for Neutron Research, Gaithersburg, MD — Na_2C_{60} is the only known solid fulleride salt containing the divalent fulleride ion C_{60}^{2-}. Calculations predict a Jahn-Teller distortion of this ion, similar to the A_4C_{60} compounds, to which they are related by electron-hole symmetry. However, by combining various experimental methods, we found that divalent ions exist only above 450 K in solids with composition Na_2C_{60}; at room temperature and below, methods sensitive to molecular symmetry and charge (infrared absorption, ESR, NMR) detect at least two phases, most probably C_{60} and Na_3C_{60}. We explain our data by a model where nanosegregated regions of the size 3-30 nm with different Na concentration coexist. The concentration gradient disappears at higher temperature by diffusion of sodium, observed by neutron scattering. High temperature infrared spectra show evidence of a uniaxial (D_{3d}/D_{5d}) distortion of the fullerene balls.

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