Fullerene-cubane: X-ray experiments and Monte Carlo simulations

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Recently, macroscopic amounts of $C_{60}.C_8H_8$ (fullerene-cubane) have been synthesised [1]. By means of powder and single crystal x-ray diffraction the structure was inferred to be face-centered cubic at room temperature and orthorhombic below 140K [1]. It was concluded that the C_{60} molecules rotate freely in the cubic phase while the orthorhombic phase exhibits orientational ordering; the cubane molecules are orientationally ordered in both phases, an observation deduced from proton NMR measurements [1].

We report further single crystal x-ray studies of fullerene-cubane in the range 300K–20K. New results obtained concerning the phase transformation sequence will be presented. Moreover diffuse scattering features yielding information about the rotational or transalational motion of the C_{60} and/or C_8H_8 molecules will be discussed.

We also report on Monte Carlo simulations of fullerene-cubane aiming to reproduce the phase transitions and to provide insight into the precise rotational behaviour of the C_{60} molecules.

[1] S. Pekker, E. Kováts, G. Oszlányi, G. Bényei, G. Klupp, G. Bortel, I. Jalsovszky, E. Jakab, F. Borondics, K. Kamarás, M. Bokor, G. Kriza, K. Tompa, G. Faigel, *Nature Materials* **4**, 764 (2005).