Ammonia Content and Superconductivity in the Ammoniated Fullerides $(NH_3)_xNaA_2C_{60}$

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The properties displayed by the series of ammoniated fullerides, $(NH_3)_xNaA_2C_{60}$ ($0.5 \leq x \leq 1$, A= K, Rb) have been quite puzzling. In these systems, the *fcc* structure is maintained with the ammonia coordinated to the sodium ions and the Na^+-NH_3 pairs residing in the octahedral sites. However, the T_cs are dramatically lower than expected and, in addition, they decrease with increasing lattice constant, showing a trend which is completely different from the conventional one. Suppression of superconductivity was associated with the presence of Na^+ ions displaced from the center of the octahedral sites which leads to a non-cubic local potential on C_{60}^{3-} and could lift the triple degeneracy of the t_{1u} LUMO.

In an attempt to obtain a better understanding of the structure of these ammoniated fullerides and its implications for superconductivity, we have undertaken a systematic combined high resolution synchrotron X-ray and neutron diffraction study of the series of perdeuterated superconductors, $(ND_3)_xNaKRbC_{60}$ and $(ND_3)_xNaRb_2C_{60}$ ($0.7 < x < 1$). By combining the complementary advantages of the two techniques, we have been able to monitor the structural properties as a function of ND_3 content, x and determine the exact stoichiometric compositions and the geometry of the Na^+-ND_3 pairs, factors which alter the local potential on the C_{60} units and/or the electronic states. We find that the displacement of the Na^+ ions from the center of the octahedral interstices is much larger than reported before (in excess of 2.0 Å).