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Report:

The recent synthesis and isolation in bulk quantities of the nitrogen-substituted fullerene solid,[1] $(C_{59}N)_2$, and its subsequent intercalation with alkali metals to afford azafulleride salts[2] with stoichiometry $A_6C_{59}N$ (A= K, Rb) opened the way to new opportunities in the quest for the synthesis of fullerene-based materials with novel structural, electronic and conducting properties. Unlike solid C_{60}, whose properties have been exhaustively studied in recent years, little is known at present about the physical properties of such condensed heterofullerene phases. As part of our present beam allocation on BMl, we performed X-ray diffraction measurements on a series of alkali metal intercalated $(C_{59}N)_2$ as a function of temperature. A preliminary acount of our results is currently in press.[3] In brief, $A_6C_{59}N$ (A= K, Rb) adopt bcc structures, comprising of quasi-spherical monomeric $(C_{59}N)^{6-}$ ions and are essentially isostructural with the corresponding salts of C_{60}, K_6C_{60} and Rb_6C_{60}. On the other hand, $Na_6C_{59}N$ adopts a hexagonal close packed (space group *P63/mmc*, a= 10.257(2) A, c= 16.745(11) A, c/a= 1.633) structure (Fig. l), reflecting the smaller size of the Na+ cation, in the same way that the same effect leads to Na_6C_{60} adopting a face centred cubic structure.

In addition, attempts to synthesise a series of Rb intercalates of (C59N)2 with varying Rb

content have resulted in weakly-doped pammagnetic hexagonal salts with stoichiometries $Rb_{2x}(C_{59}N)_2$ (x< 0.9) (Fig. 1). The structural data are consistent with charge transfer from Rb to the heterofullenes as the lattice dimensions show slight contraction upon intercalation (a= 9.81 Å, c= 16.06 Å for $Rb_{1.8}(C_{59}N)_2$).

References

[l] Hummelen, J.C. et al., Science 1995,269, 1554.

[2] Prassides, K. *et al., Science* **1996,271, 1833.**

[3] Kordatos, K. *et al.,* in Proceedings of International Winterschool on Novel Nanostructures, Eds. H. Kuzmany et al., 1997, in press.

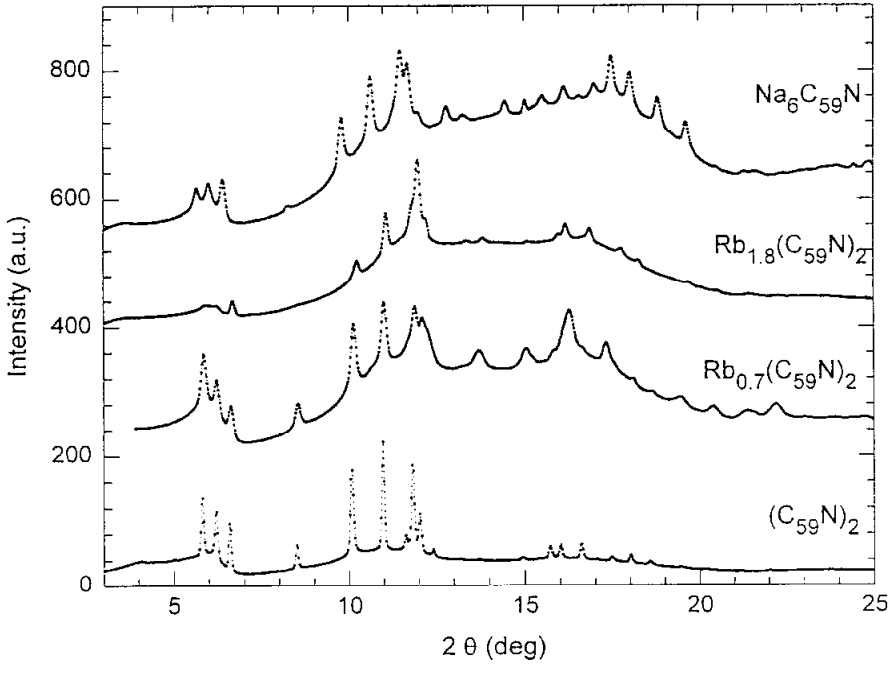

Fig. 1 Synchrotron X-ray diffraction profiles of hexagonal (a) $Na_6C_{59}N$, (b) $Rb_{0.7}(C_{59}N)_2$, (c) $Rb_{1.8}(C_{59}N)_2$, and (d) $(C_{59}N)_2$ in the range 3° to 25° at ambient temperature (λ= 0.873 Å).