ESRF	**Experiment title:** **Structural studies of fullerenes at high pressures**	**Experiment number:** HS-500
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Report:

The study of the physical and chemical properties of fullerenes in the solid state has attracted considerable interest in recent years but most of the work has concentrated on the most abundant fullerenes, namely C_{60} and C_{70}. The main reason behind this bias is that the higher fullerenes are very difficult to extract from arc-processed soot and have been available only in very small quantities. As a consequence no experimental work on these systems has been performed at elevated pressures. C_{84} has 24 structural isomers obeying the isolated pentagon rule. ^{13}C NMR studies have revealed that the most abundant isomers are those with D_2(IV) and D_{2d}(II) symmetry (in a ratio 2:l) (Fig. 1). Our interest in these two isomers is due to their quasi-spherical shape, reminiscent of the shape of C_{60} itself. As part of our beam allocation on ID09 we have studied the pressure dependence at ambient temperature of the structure of C_{84} using a sublimed sample, which was a mixture of the two major isomers. We find that the structure remains strictly *fcc* up to a pressure -93 kbar (λ= 0.4995 A) in contrast with the behaviour of C_{60} and C_{70} (Fig. 2). The lack of a phase transition may be related to the presence of static structural disorder that arises from the coexistence of the two structural isomers.

Within the family of intercalated C_{60}, the focus has been on studying alkali metal fullerides, again due to difficulties in preparation of other materials such as the alkaline-earth fullerides. Our successful synthesis in bulk quantities of pure Ba_4C_{60} and Sr_4C_{60} has allowed the us to assign these compounds unequivocally to the superconducting stoichiometries. Synchrotron diffraction gave the structure of Ba_4C_{60} to be orthorhombic (space group ***Immm)*** with a very short c-axis[2]. Fig 2a shows the variation of lattice constants with pressure for Ba_4C_{60} where low compressibility along the c-axis is evident. The resulting volume dependence (scaled to ambient pressure) and a fit to the Munaghan equation of states is shown in Fig 2b. The compressibility is half that found for pristine C_{60}.

References

[1] S. Margadonna *et al., Chem. Mater.* 10, 1742 (1998).

[2] C. M. Brown *et al.,* in preparation.

Fig 1. Synchrotron X-ray diffraction profiles of C_{84} (λ= 0.4995 Å). Left panel: ambient pressure. Right panel: -44 kbar.

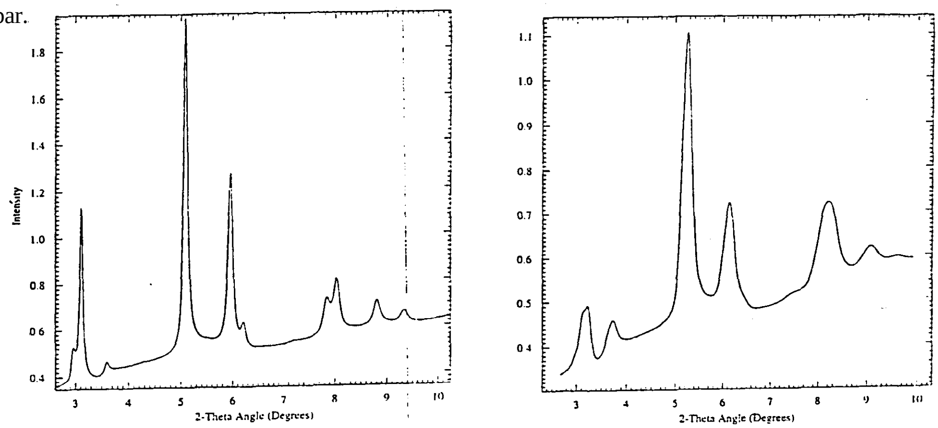

Fig2a. Variation of orthorhombic lattice constants for Ba_4C_{60} as a function of pressure.

Fig 2b. Pressure dependence of the scaled unit cell cell volume for Ba_4C_{60} (solid circles). The solid line is a fit to the Murnaghan equation of states.