ESRF	**Experiment title:** Structural Studies of Superconducting Alkali and Alkaline Earth Fullerides	**Experiment number**: CH-731
Beamlines: BM16/BM1	**Date of experiment**: from: 17/11/99 to 22/11/99 and 26/1/00 to: 29/1/00	**Date of report**: 19/8/00
Shifts: 15/9	**Local contact(s)**: A N Fitch / K Knudsen	*Received at ESRF:*

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Report:

Abstract of publication resulting from this proposal: *Chem. Mater.* **12**, Sept. 2000, in press.

The crystal structure of the superconducting $K_3Ba_3C_{60}$ fulleride (T_c= 5.4 K) has been studied by synchrotron X-ray and neutron powder diffraction between 10 and 295 K. It is body-centered cubic (*bcc*) at all temperatures with an essentially half full t_{1g}-derived band. Close contacts between Ba^{2+} and K^+ ions and neighboring C_{60} units imply a strong orbital hybridization, which leads to broadening of the conduction band. We find that the Ba^{2+} and K^+ cations are disordered in the same distorted tetrahedral interstitial sites, (0, ½, ¼+δ) but they are displaced by a different distance, δ from the center of the site. The resulting local distortions may be responsible for the observed complex relationship between T_c and cubic lattice parameter in $A_3Ba_3C_{60}$ (*A*= Na, K, Rb, Cs) fullerides.

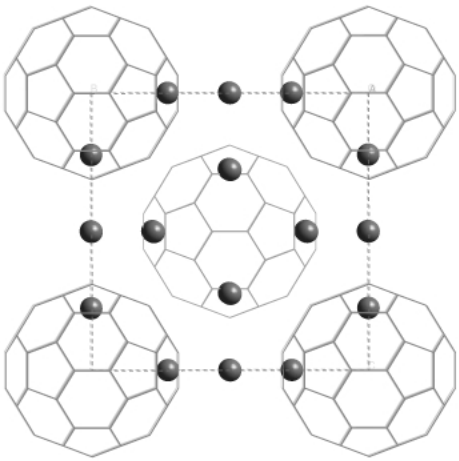

Fig. 1 Schematic view of the *bcc* structure of $K_3Ba_3C_{60}$ on the (001) plane. Shaded circles show the interstitial sites, which are randomly occupied by alkali and alkaline-earth metals.

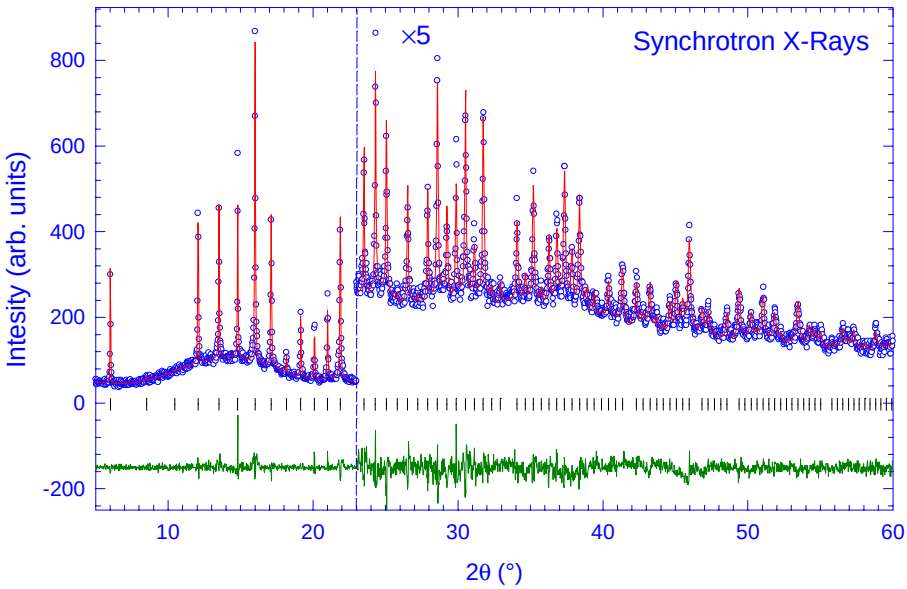

Fig. 2 Final observed (points) and calculated (solid line) synchrotron X-ray (λ= 0.83502 Å) powder diffraction profile for $K_3Ba_3C_{60}$ at 10 K. The lower line shows the difference profiles and the ticks mark the position of the Bragg reflections. The profile has been expanded for clarity by a factor of 5 at Bragg angles larger than 23°.

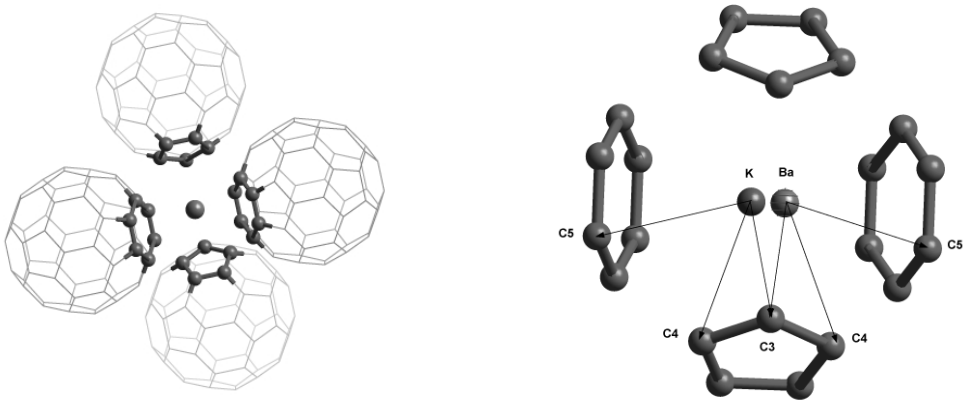

Fig. 3 Perspective view of the coordination of the Ba^{2+} and K^{+} cations in the *bcc* structure of $K_3Ba_3C_{60}$.