ESRF	Experiment title: STRUCTURAL STUDY OF NOVEL RARE-EARTH C60 INTERCALATED PHASES	Experiment number: CH- 140
Beamline: BM-16	Date of Experiment: from: 01 Aug. 96 to: 04 Aug. 96	Date of Report: 06 Fev. 98
Shifts: 9	Local contact(s): ANNE MICHEL	*i Received at ESRF* 05 MAR. 1998

Names and affiliations of applicants (*indicates experimentalists):

CHOUTEAU Gérard	LCMI - CNRS Grenoble
CLAVES Daniel	LEPMI - INPG Grenoble et LMI Clermond-Ferrand
COLLOMB Andre	Lab. Crist.- CNRS Grenoble
KSARI Younal	LCMI - CNRS Grenoble
TOUZAIN Philippe	LEPMI - INPG Grenoble

Report:

The proposal concerned crystal chemistry of rare earths-doped C_{60} fullerene and its links to the magnetic properties of these phases.

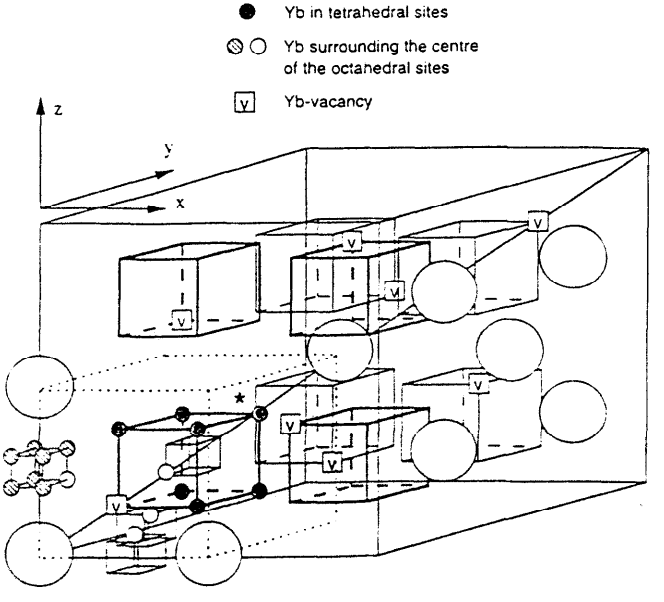
X-ray diffraction measurements at room temperature were performed on 6 samples of nominal compositions M_3C_{60} and M_6C_{60} (M = Sm, Eu, Yb). A Debye-Scherrer setting (highly air sensitive samples) equipped with a multianalyser system and a monochromatic beam λ = 0.35827 Å (nearly complete suppression of the incident beam absorption by the heavy element) were used. The high resolution powder diffraction patterns obtained display peak shapes whose FWHM ~ 0.04°, i.e. efficiencient reflection discrimination among the very strong peak density observed in some cases due to important cell parameters (~28 Å for the M_3C_{60} phases studied).

The structural analysis has revealed a similar structure for all phases of the M_3C_{60} type. The minimized peak overlap allowed for an invalidation of some structural features earlier proposed for a phase Yb_xC_{60} (x in the vicinity of 3) on the basis of law resolution data, i.e. no orthorhombic distortion was clearly evidenced ($Pa\bar{3}$ retained).

The most surprising feature is the probable decrease of the initial icosahedral symmetry of the fullerene molecule, responsible for the unusual peak shape observed (this phenomenon could be confirmed recently by Raman spectroscopy). The short carbon-metal distances systematically determined indicate a partial covalence trend, with consequences for the magnetic properties of the Eu-doped phases.

The higher metal concentration M_6C_{60} phases are characterized by a transition towards BCC symmetry. The slight carbon-metal orbitals hybridization also observed in these compounds allowed to invoke, for the first time in C_{60}-based compounds, a spin polarization mechanism via superexange in Eu_6C_{60}.

N.B.: Due to an incessant evolution of the subject from the proposal deposit to the experiments realization dates, the samples nature and priority may have changed compared to the initial program.



Simplified structural model for low concentration Yb_xC_{60} phases (x~3). Doted lin represent the unit cell of the fullerene sublattice. Yb in tetrahedral sites (grey spheres) a displaced ~0.4 Å away from the central position (not shown). Large spheres represent part the C_{60} molecules, white spheres Yb atoms in octahedral sites close to the Yb-vacancy (sing filled), and hatched spheres other Yb in octahedral sites partial and random occupancy