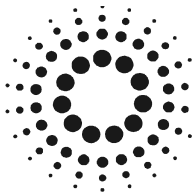
EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON



Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF. This double-page report will be reduced by ESRF to a one page, A4 format, and will be published in the Annex to the ESRF Annual Report.

Should you wish to make more general comments on the experiment, enclose these on a separate sheet, and send both the Report and comments to the User Office.

When preparing your report, please follow the instructions below:

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- make sure the report does not exceed the space available; tables and figures may be included if you wish.
- for work which is published or which is in press, you may simply include a copy of the abstract together with full reference details. If the abstract is in a language other than English, ensure that you include an English translation.
- bear in mind that the report will be reduced to 71% of its original size. A type-face such as “Times”, 14 points, with a 1.5 line spacing between lines for the text produces a report which can be read easily.

Note that requests for further beam time must always be accompanied by a report on previous measurements.

Postal address: User Office, ESRF, B.P. 220, F-38043 GRENOBLE Cedex, France.
Telephone: (33) 76 88 25 52; Fax: (33) 76 88 20 20; e-mail: useroff@esrf.fr.

ESRF	**Experiment title:** Structural Studies of Higher Fullerenes and Endohedral Metallofullerenes	**Experiment number:** CH-615
Beamlines: BM1/BM16	**Date of experiment:** from: 4/3/99 to 7/3/99 and 16/6/99 to: 21/6/99	**Date of report:** 19/8/00
Shifts: 9/15	**Local contact(s):** K Knudsen / A N Fitch	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Abstract of publication resulting from this proposal: *Europhys. Lett.* **51**, 314-319 (2000)

We report the results of a high-resolution synchrotron X-ray powder diffraction study of polymerised CsC_{60} in the temperature range 4 to 40 K. Its crystal structure is monoclinic (space group $I2/m$), isostructural with RbC_{60}. Below 14 K, a spontaneous thermal contraction is observed along both the polymer chain axis, a and the interchain separation along [111], d_1. This structural anomaly could trigger the occurrence of the spin-singlet ground state, observed by NMR at the same temperature.

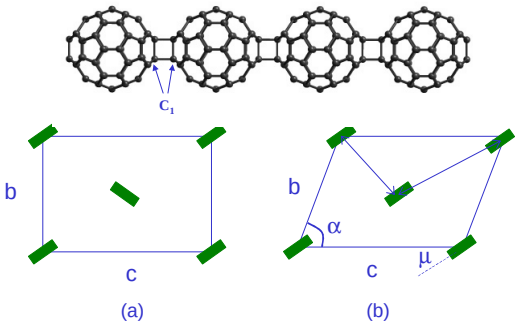

Fig. 1 Linear polymer chains formed by [2+2] cycloaddition in AC_{60} salts. Schematic drawing of chain orientations for (a) *Pmnn* space group and (b) *I*2/*m* space group. The shaded bars indicate the orientation of covalently bonded polymer chains along *a* by projection on the crystallographic *bc* plane.

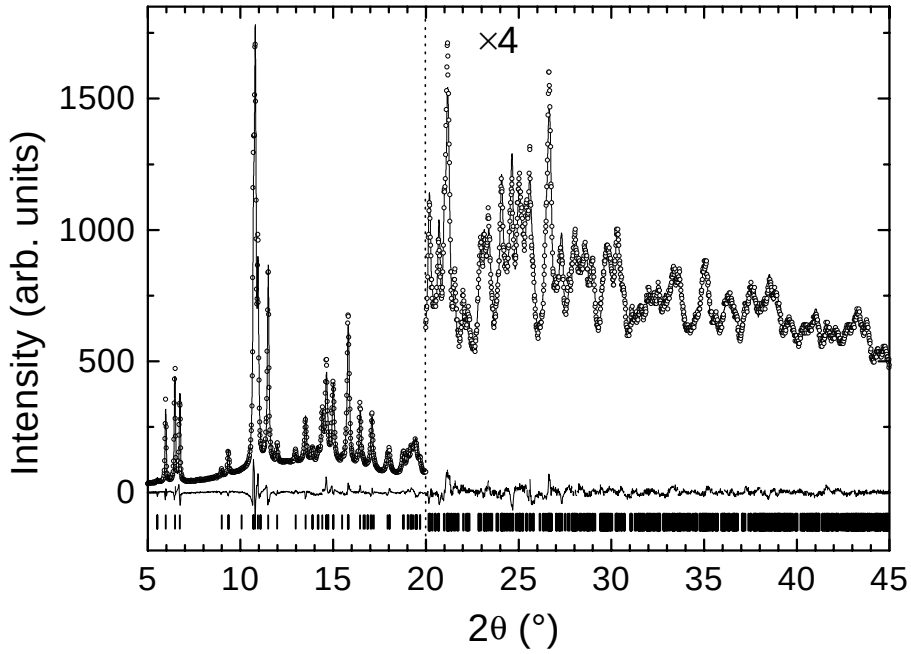

Fig. 2 Observed (points), calculated (solid line) and difference (lower panel) synchrotron X-ray (λ= 0.79972 Å) powder diffraction profiles of CsC_{60} at 20 K (space group *I*2/*m*). The positions of the reflections are shown as tick marks.

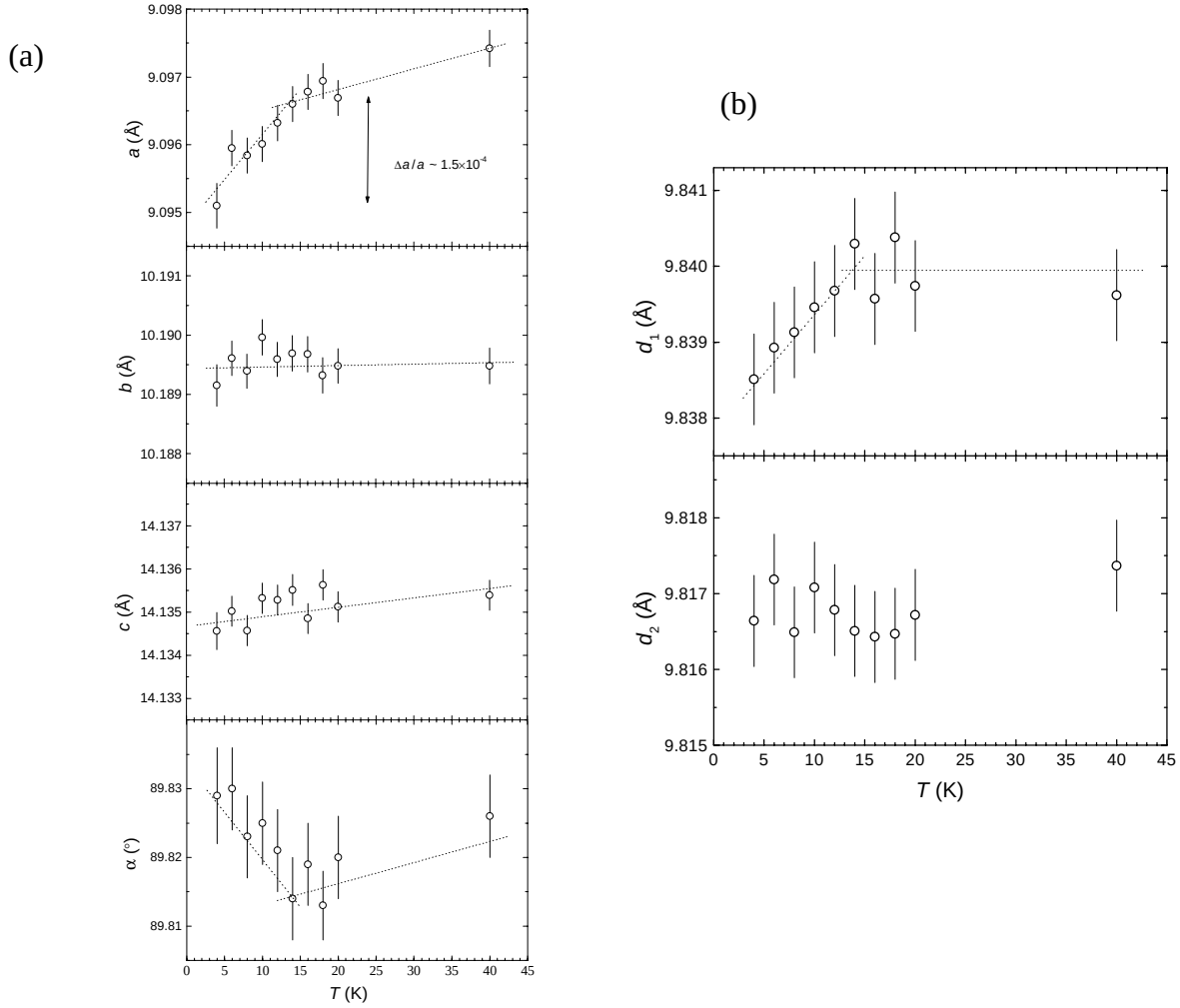

Fig. 3 Temperature dependence (a) of the monoclinic lattice parameters, *a*, *b*, *c* and α and (b) of the interchain distances, d_1 (along [111]) and d_2 (along [1-11])of polymerised CsC_{60}. The dotted lines are guides to the eye.