

**Experiment title:**High pressure powder studies of the  $C_{60}$  intercalation compound  $(CO)_x C_{60}$ **Experiment number:**

HS-502

**Beamline:**

ID30

**Date of experiment:**

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**Shifts:**

12

**Local contact(s):**

D. Häusermann

*Received at ESRF:***04 MAI 1999****Names and affiliations of applicants (\* indicates experimentalists):**Sander van Smaalen<sup>1</sup>, Robert E. Dinnebier\*<sup>1</sup>, Ronald Miletich\*<sup>2</sup>, Martin Kunz\*<sup>2</sup><sup>1</sup>Laboratory of Crystallography, University of Bayreuth, D-95440 Bayreuth, Germany<sup>2</sup>Laboratory of Crystallography, ETH Zentrum, CH-8092 Zuerich, Switzerland**Report:**

The compound  $(CO)_x C_{60}$  was shown to be an intercalation compound of  $C_{60}$ , for which the substructure formed by the  $C_{60}$  molecules was identical to the structure of  $C_{60}$  itself [1]. Studies of the lattice parameter and the crystal structure as a function of temperature have shown that the ordering transition ( $T_c$ ) and the glass transition ( $T_g$ ) occur at temperatures slightly lower than the corresponding transitions in pure  $C_{60}$  [2]. At any temperature below  $T_c$ , the occupation of the major orientation was found to be larger than in pure  $C_{60}$ , resulting in a saturated value of 93% at  $T=25K$ .

In the present experiment, the effect of pressure on the crystal structure of  $(CO)_x C_{60}$  was studied using a DAC at room temperature and at  $T=150K$ . An angle dispersive powder diffraction technique at  $\lambda=0.4246\text{\AA}$  with an image plate detector was used. Data reduction was performed using the program FIT2D (by Andy Hammersley, ESRF). The lattice constant of the cubic unit cell could be determined by LeBail-fits as a function of pressure (Fig. 1). From the almost linear relationship a Bulk modulus of  $B=29.4\text{ Gpa}$  was derived (Fig. 2). Unfortunately, the quality of the measured diffraction data was not sufficient to determine the ratio major:minor in its dependence on pressure.

[1] Van Smaalen *et al.*, Phys. Rev. B57, 1998, 11, 6321-6324.[2] Van Smaalen *et al.*, Europhys. Lett.Phys., 1998, 43(3), 302-307.

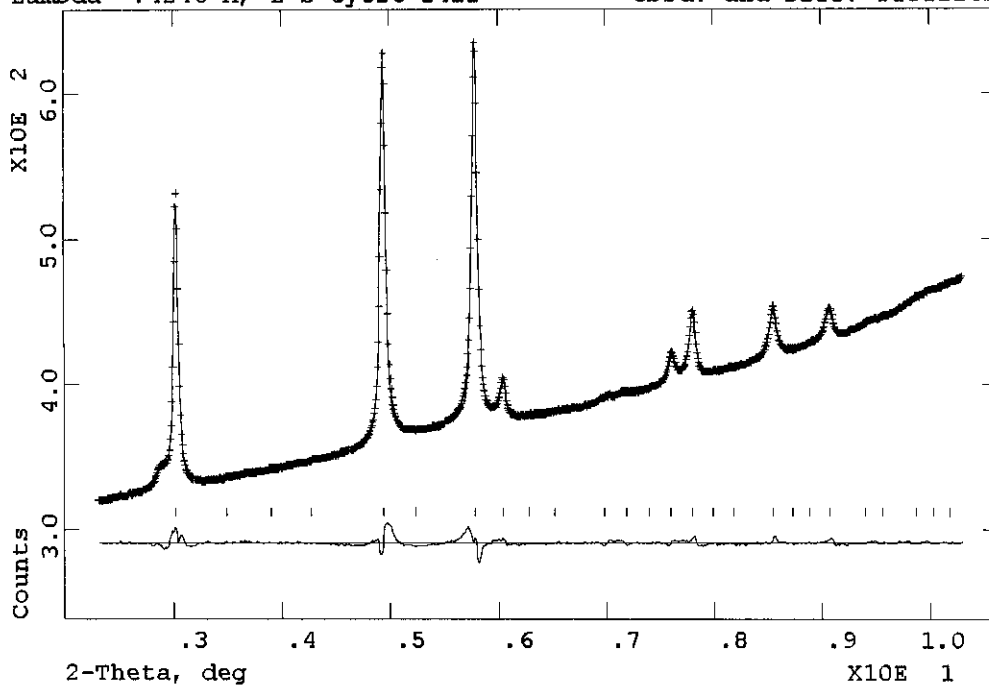


Fig. 1 LeBail plot of  $(\text{CO})_x\text{C}_{60}$  at 8.4 kbar.

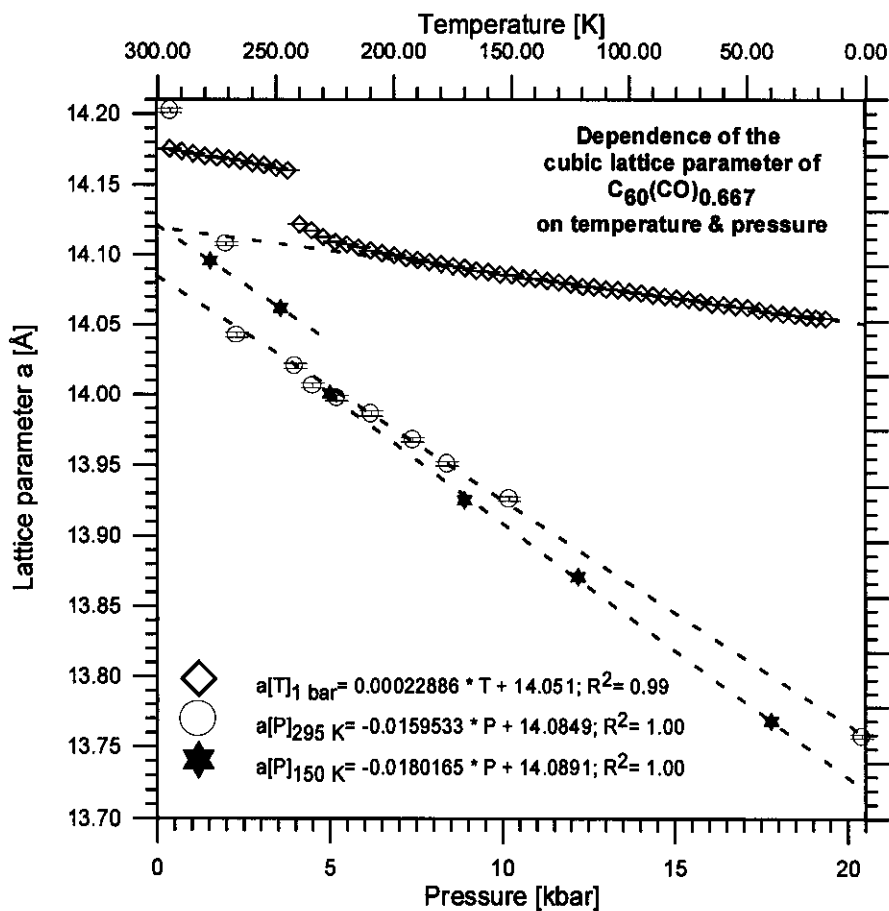


Fig. 2 Pressure (at  $T_1 = 295 \text{ K}$  and  $T_2 = 150 \text{ K}$ ) and temperature dependence of the lattice parameter of  $(\text{CO})_x\text{C}_{60}$ .