ESRF	**Experiment title:** Study of correlations between pressure-induced structural changes and superconducting properties in bulk CaC_6	**Experiment number**: HS-3120
Beamline: ID09A	**Date of experiment**: from: 26/11/2006 to: 30/11/2006	**Date of report**: 03/08/2018
Shifts: 18	**Local contact(s)**: Michael Hanfland	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Geneviève Loupias*, Matteo d'Astuto*, Nedjma Bendiab*, Christophe Bellin*, Andrea Gauzzi* (UMR7590 IMPMC, Université Pierre et Marie Curie, Paris, France)

N. Emery*, C. Hérold*, P. Lagrange* (Laboratoire de Chimie du Solide Minéral-UMR 7555 CNRS, Université Henri Poincaré Nancy I, France)

Report:

See A. Gauzzi *et al.*, Phys. Rev. B **78**, 064506 (2008).

Abstract

In order to account for the large drop of superconducting critical temperature, T_c, and for the dramatic increase of residual resistivity, ρ_0, previously reported in CaC_6 at $P_{cr} \sim 9$ GPa, we studied the room temperature crystal structure of bulk CaC_6 samples as a function of pressure up to 13 GPa by means of synchrotron X-ray diffraction in diamond anvil cells. At P_{cr}, we found no change of the trigonal R-3m space group symmetry, but a large increase of isothermal compressibility, κ, from -0.0082 GPa^{-1} to -0.0215 GPa^{-1}, accompanied by a large broadening of Bragg peaks. Both effects being reversible, it follows that superconductivity in CaC_6 is maximized at the verge of a peculiar order-disorder phase transition concomitant to a large lattice softening. Space group symmetry considerations supported by *ab initio* calculations of the relaxed structure within the Density Functional Theory lead us to conclude that the disordered phase is presumably characterized by a random off-centering of the Ca atoms in the *ab*-plane with respect to the C honeycomb layers.