

**CRYSTAL STRUCTURE OF THE HIGH PRESSURE PHASE OF PbI<sub>2</sub>**

H. Iwasaki<sup>1</sup> H. Kawamura<sup>2</sup> Y. Akahama<sup>2</sup>  
<sup>1</sup>Ritsumeikan University Faculty of Science and Engineering Noji-Higashi 1-1-1 KUSATSU SHIGA 525-8577 JAPAN <sup>2</sup>Himeji Institute of Technology, Faculty of Science

The title compound has the layered CdCl<sub>2</sub> (C<sub>6</sub>)-type structure under normal pressure. On compression, phase transition was found to take place at 0.5 GPa with a volume contraction of 4 % (Bridgman, 1948), but the structure of the high pressure phase has remained undetermined.

We made X-ray diffraction measurements using powdered samples squeezed in a diamond-anvil cell at a pressure of 0.9 GPa on a synchrotron radiation source at Photon Factory. In the pattern taken using the radiation 0.06195 nm in wavelength, closely spaced 36 diffraction lines have been recorded up to  $1/2d = 2.55 \text{ nm}^{-1}$ . They could be indexed in terms of an orthorhombic unit cell of the sizes of  $a = 0.8419$ ,  $b = 1.190$  and  $c = 8.751$  nm, the longest axis being parallel to the c-axis of the original CdCl<sub>2</sub>-type structure. Analysis of the pattern on the basis of the intensities of the diffraction lines has led to the structure that can be interpreted as being formed by collapsing thirteen layers of the CdCl<sub>2</sub>-type structure in the c-axis direction. It is denser by 10 % than that of the normal pressure phase in agreement with the P-V relation determined by Bridgman (1948).

Discussion is given on the structural feature of the high pressure phase and suggestion to the possible structure model of phase which form on further compression of the compound.

References

Bridgman, P. W. (1948). Proc. Am. Acad. Arts Sci. 76, 71-87.

**Keywords:** HIGH PRESSURE, STRUCTURE ANALYSIS, LEAD IODIDE

**FIRST-PRINCIPLES STUDIES OF PHASE TRANSITIONS AT HIGH PRESSURE IN SiO<sub>2</sub>**

D. D. Klug<sup>1</sup> J.S. Tse<sup>1</sup> M. Geshi<sup>1</sup> x. Gonze<sup>2</sup>  
<sup>1</sup>Steele Institute For Molecular Sciences National Research Council of Canada 100 Sussex Drive OTTAWA ONTARIO K1A 0R6 CANADA <sup>2</sup>Universite' Catholique de Louvain

This study describe the application of first-principles linear response theory to the characterization of the mechanisms for pressure-induced phase transitions in SiO<sub>2</sub>. The pressure-induced transformations of cristobalite and post-stishovite phases are investigated by the calculation of phonon stabilities in these phases as a function of pressure. This work provides details of the origins and mechanisms of the phase transitions both observed experimentally and predicted by recent *ab initio* molecular dynamics studies on high-pressure SiO<sub>2</sub>[1].

References

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**LOW TEMPERATURE TRANSFORMATIONS OF ICE**

S. Klotz<sup>1</sup> F. Meducin<sup>1</sup> G. Hamel<sup>1</sup> J.S. Loveday<sup>2</sup> M. Guthrie<sup>2</sup> R.J. Nelmes<sup>2</sup>  
<sup>1</sup>University P&M Curie Physique Des Milieux Condenses (B77) 4 Place Jussieu PARIS 75252 FRANCE <sup>2</sup>Department of Physics and Astronomy and Centre of Science at Extreme Conditions, The University of Edinburgh, Edinburgh EH9 3JZ, UK

The transformations of ice when compressed at low temperatures are of long-standing interest. The transformation to high-density amorphous ice is a model for pressure amorphisation and there is interest in potential new crystalline phases made by low temperature compression. However, there is a dearth of diffraction information obtained under *in-situ* conditions.

The Paris-Edinburgh cell enables us to carry out high-pressure neutron diffraction studies down to 80 K and we have explored the behavior of all known low-pressure ice phases, with the exception of ice XI, but including high-density amorphous ice in the pressure range 0-5 GPa. On compression they all transform to a low-T form of ice VII. Warming at pressures in the range 0-1 GPa reveals complex and unexpected behavior.

**Keywords:** ICE, STRUCTURE, PRESSURE

**Cs<sub>2</sub>HgBr<sub>4</sub> : AMORPHIZATION UNDER PRESSURE**

D. Machon<sup>1</sup> P. Bouvier<sup>1</sup> V. Dmitriev<sup>1</sup> G. Lucazeau<sup>2</sup> H.P. Weber<sup>3</sup>  
<sup>1</sup>Swiss-Norwegian Beam Lines at ESRF SNBL, ESRF 6 Rue Jules Horowitz P.O. Box 220 GRENOBLE 38043 FRANCE <sup>2</sup>LEPMI, ENSEEG-INPG, BP 75, F-38402 Saint Martin d'Heres <sup>3</sup>Institut of Crystallography, University of Lausanne, CH-1015 lausanne

Why some compounds or compound classes amorphize under pressure, is a question of great import to crystallography. To answer it, we investigated the structural evolution of molecular ionic Cs<sub>2</sub>HgBr<sub>4</sub> with pressure, both on powder samples and single crystals, and using two complementary techniques, synchrotron radiation diffraction and Raman spectroscopy. In a previous study on compounds of the same structure A<sub>2</sub>BX<sub>4</sub> type, but of different chemistry, the authors proposed that the ratio of the size of the tetrahedral anionic BX<sub>4</sub> group to that of the A cations determined whether amorphization occurred or not. As a first step, we varied the degree of hydrostaticity during compression of powder samples of Cs<sub>2</sub>HgBr<sub>4</sub> (loading with a)nitrogen, b)paraffin oil and c)without any pressure transmitting medium;  $p < 33$  GPa). The compound was found to undergo a phase transition to a monoclinic phase at about 9 GPa; transition pressure, monoclinic distortion and volume jump were found to be strongly dependent on the degree of hydrostaticity. To obtain diffraction patterns typical of non-crystalline state, the cell had to be loaded without any pressure-transmitting medium or with paraffin oil instead. In contrast, if nitrogen was used as the pressure-transmitting medium, amorphization did not occur. Non-hydrostaticity, and not some structural parameter, is apparently the key factor for amorphization in this compound. In a second step we subjected single crystals to pressures varying between 0 and 5 GPa, using silicon oil as pressure-transmitting medium. The transition to a monoclinic phase was confirmed and displays a large region of coexistence.

**Keywords:** AMORPHIZATION, PHASE-TRANSITION, PRESSURE