



**Experiment title:** Compton profiles of hydrogen bonds in ice

**Experiment number:**  
HE454

**Beamline:**

ID15B

**Date of Experiment:**

from: 12.9.98 to: 18.9.98

**Date of Report:**

28.2.99

**Shifts:**

18

**Local contact(s):**

A. Shukla

*Received at ESRF:*

**Names and affiliations of applicants (\*indicates experimentalists):**

E. Isaacs, P. Platzman, B. Barbiellini, C. Tulk

## Report:

Abstract of the article:

Covalency of the Hydrogen bond in Ice: A direct X-ray measurement E. D. Isaacs, A. Shukla, P. M. Platzman, D. R. Hamann, B. Barbiellini and C. A. Tulk, Phys. Rev. Lett., **82**, 600, 1999

Periodic Intensity variations in the measured Compton profile anisotropies of ordinary ice Ih correspond to distances of 1.72 and 2.85 Å, which are close to the hydrogen bond length and the nearest neighbour O-O distance, respectively. We interpret this result as direct evidence for the substantial covalent nature of the hydrogen bond. Very good quantitative agreement between the data and a fully quantum mechanical bonding model for ice Ih and the disagreement with a purely electrostatic (classical) bonding model support this interpretation and demonstrate how exquisitely sensitive Compton scattering is to the phase of the electronic wave function.