



| | | |
|--|--|--------------------------------------|
| | Experiment title: High pressure metallisation of halogens | Experiment number: HS 1490 |
| Beamline: | Date of experiment: from: 28 March 2001 to : 02 April 2001 | Date of report: 31/08/2006 |
| Shifts: | Local contact(s): Sakura Pascarelli | <i>Received at ESRF:</i> |
| Names and affiliations of applicants: -A. San Miguel Laboratoire de Physique de la Matière Condensée et Nanostructures Université Lyon 1 and CNRS, France -J.P. Itié, A. Polian, M. Gauthier Physique des Milieux Condensés, UPMC, Paris, France | | |

Report:

See also the ESRF Highlights 2000, "Metallisation of Halogens at High Pressure", pag.16-17 (2001)

Eur. Phys. J. B 17, 227–233 (2000)

THE EUROPEAN
PHYSICAL JOURNAL B

EDP Sciences
© Società Italiana di Fisica
Springer-Verlag 2000

Bromine metallization studied by X-ray absorption spectroscopy

A. San Miguel^{1,a}, H. Libotte², J.P. Gaspard², M. Gauthier³, J.P. Itié³, and A. Polian³

¹ Département de Physique des Matériaux, Université Claude Bernard-Lyon 1, 69622 Villeurbanne Cedex, France

² Physique de la Matière Condensée, Université de Liège, B5, 4000, Sart-Tilman, Belgique

³ Physique des Milieux Condensés, B77, Université P. et M. Curie, 4 place Jussieu, 75352 Paris Cedex 05, France

Received 20 March 2000

Abstract. Bromine has been studied up to a pressure of 110 GPa by X-ray absorption spectroscopy (XAS) at the bromine K-edge, that allows to measure the pressure evolution of the width of the unoccupied conduction band. At 25 ± 5 GPa we observe a slope change in the evolution of this width. Comparison with published calculations of the electronic density of states indicates that the physical origin of the slope change is compatible with the metallisation process. This is also confirmed by a simple tight binding calculation. In addition, the metallisation pressure value is in agreement with calculated ones. At 68 ± 5 GPa a discontinuity in the evolution of the width of the sigma antibonding band points out the onset of a phase transformation. This result is compatible with the observed phase transformation near 80 ± 5 GPa by X-ray diffraction that is associated with the molecular dissociation.