ESRF	**Experiment title: Structural, Electronic, and Magnetic Properties of High-Pressure Phases of Binary Transition-Metal Layered Compounds.**	**Experiment number**: HS1381
Beamline: ID30	**Date of experiment**: from: 23.11.00 to: 28.11.00	**Date of report**:
Shifts: 15	**Local contact(s)**: T. Le Bihan	*Received at ESRF:*

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Report:

This is an addendum to the report subbmitted 23.08.2001

G. Kh. Rozenberg, M. P. Pasternak, W. M. Xu, L. S. Dubrovinsky, R. Ahuja, and T. Le Bihan, *Pressure-Induced Structural Transformations in the Mott Insulator FeI_2,* submitted to Phys. Rev. B.

ABSTRACT

A full-profile refinement of the FeI_2 structures at pressures up to 70 GPa were performed combined with *ab* initio calculations to particularly elucidate the structural aspects of the pressure-induced Mott transition phenomenon and clear crystallographic features of the quenching of the orbital ordering induced by pressure. Synchrotron powder XRD diffraction studies have shown that at 17 GPa the substantial alteration of lattice parameters takes place attributed according to Mössbauer spectroscopy (MS) data (Pasternak et al., *Phys. Rev*. **B65**,

035106, 2002) to the sudden quench of the orbital term. Starting at P ~ 20 GPa a sluggish structural phase transition takes place related according to the resistance and MS studies, to the onset of *Mott* transition. In accordance with *ab initio* calculations the doubling of lattice parameters and a formation of a new Fe sublattice for the original CdI2-type structure could describe this structural transition. The latter alterations in the Fe sublattice may indicate a trend of the Fe sites to disorder in the new HP phase. This phase transition is characterized by a significant change of the unit cell parameters, reduction in volume and Fe-I distances. The transition is completed at ~ 35 GPa. The substantial reduction of Fe-I with minimal changes in the Fe-Fe bond lengths at the transition, suggests a *Charge-Transfer* gap closure mechanism involving the iodine *p*-bands. At P>40 GPa the reverse of the structural transition is observed resulting in the onset of the original CdI2-type structure.