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:*

Names and affiliations of applicants (* indicates experimentalists):

Moshe P. Pasternak

Gregory Kh. Rozenberg

School of Physics and Astronomy, Tel Aviv University, ISRAEL

Report:

G. Kh. Rozenberg, M. P. Pasternak, L. S. Dubrovinsky, W. M. Xu, and T. Le Bihan, ***Structural aspects of Mott transition in FeI_2 compound under high pressure*****,. accepted for publication to High Pressure Research**.

ABSTRACT

Structural aspects of the pressure-induced *Mott* transition (*MT*) phenomenon have been studied in the layered transition metal compound FeI_2. X-ray diffraction studies performed at pressures up to 60 GPa, combined with data of resistance and Mössbauer spectroscopy (MS) studies to be published elsewhere have shown that starting at P ~ 20 GPa a sluggish *Mott* transition takes place, concurrent with a significant alteration of the unit cell parameters with indication of possible Fe positions disorder, reduction in volume, and in the 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.

M. P. Pasternak, W. M. Xu, G. Kh. Rozenberg, and R. D. Taylor, *Pressure-Induced Magnetic, and Electronic Transitions in the layered Mott-Insulator FeI2*, submitted to Phys. Rev. B

ABSTRACT

Powder-XRD, electrical resistance, and ^{57}Fe Mössbauer spectroscopy at pressures to 40 GPa in diamond anvil cells, have been employed to investigate the pressure evolution of the structural, electrical-transport, and magnetic properties of the antiferromagnetic insulator FeI_2. Up to 18 GPa, the volume decreases by 25%, resistivity decreases by ten orders of magnitude, T_N increases tenfold ,and the Fe^{2+} moments remain parallel to the *c*-axis. The isomer shift (IS) which is proportional to $-\rho_s(0)$ (*s*-electron density at the nucleus) decreases from 1.0 to 0.8 mm/s in accordance with the volume shrinkage, the quadrupole splitting (QS) increases monotonically to 12 GPa reaching 1.70 mm/s, and the magnetic hyperfine field (H_{hf}), composed of c*ontact* and *orbital* terms increases from 8 to 12 T. Close to 20 GPa an isostructural, first-order phase transition occurs accompanied by a 6% decrease in volume, 9% decrease in the *c*-axis and a considerable contraction in the Fe-I bonding length. At 20 GPa a new Mössbauer spectral component is observed characterized by H_{hf} = 32 T attributed to the quenching of the *orbital magnetic term* of the low pressure phase, T_N increases to 300 K and moments tilt to 55° with respect to *c*-axis. A slight increase in pressure results in a diamagnetic state first detected 20 GPa and characterized by a considerably lower IS (i.e., large density) and QS. The abundance of this diamagnetic phase increase with rising pressure to reach 100% at ~ 35 GPa. This state is also metallic, as shown by the R(P,T) data. The observation of diamagnetism, metallic behavior, and the considerable reduction in Fe-I distances establishes unequivocally that a *Charge Transfer* transition occurs in which the iodine ligand 5*p*-band overlaps with the" empty" iron 3*d* upper Hubbard sub-band resulting in total collapse of electron correlation.