ESRF	**Experiment title:** STRUCTURAL ASPECTS OF THE (O-H) DISORDER ON MAGNETIC AND ELECTRONIC PROPERTIES OF *TM*$(OH)_2$ LAYERED COMPOUNDS	**Experiment number**: HS1838
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Report:

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Pressure Induced Self-Oxidation of Fe(OH)$_2$, **accepted for publication in Phys. Rev. Let**.

ABSTRACT

Mössbauer spectroscopy, x-ray diffraction (XRD), and electrical resistance (R(P,T)) studies in $Fe(OH)_2$ to 40 GPa revealed an unforeseen process by which a gradual Fe^{2+} oxidation takes place, starting at ~8 GPa reaching 70% Fe^{3+}-abundance at 40 GPa. Based on XRD and R(P,T) data it is unequivocally concluded that this non-reversible process, $Fe^{2+} \rightarrow Fe^{3+} + e^-$, results in Fe^{2+} converting into Fe^{3+} with no structural transition. The "ejected" electrons form a deep band within the $Fe(OH)_2$ high-pressure electronic-manifold becoming weakly-

localized at P > 50 GPa. This process is attributed to an effective ionization potential created by the pressure-induced orientationally deformed (OH) dipoles and the unusual small binding energy of the valence electron in $Fe^{2+}(OH)_2$.

Typical diffraction patterns illustrating the obtained results are shown in Fig. 1. As can be seen no new structural components are observed to the pressure ~30 GPa; the diffraction patterns are that of pure $Fe(OH)_2$.

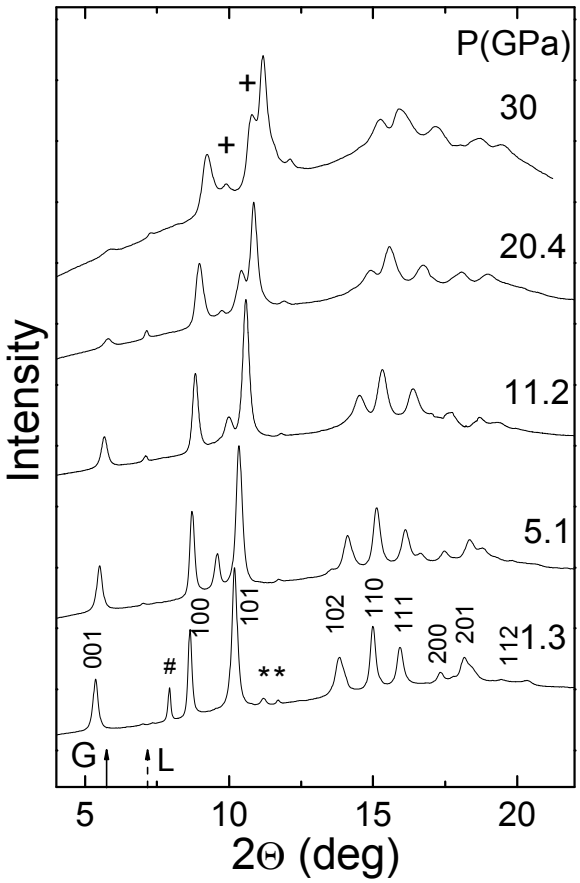

Fig. 1. X-ray powder diffraction patterns of $Fe(OH)_2$ at T = 298 K and various pressures. Indexes correspond to the diffraction peaks of the original CdI_2 type structure. Weak peaks corresponding to ruby are marked with (*). Peaks, which appear at ~5 GPa in addition to the CdI_2 type structure ones, are marked with (+), and can be accounted for as texture effects and consequent distortion of the original structure. The Ar (111) peak is marked with (#). Positions of the most intense peak of Goethite, or α-FeO(OH), and Lepidocrocite, or γ-FeO(OH), are marked with arrows.

Detailed HP-XRD analyses of several *TM*$(OH)_2$ (*TM*= Fe, Co, and Ni) compounds to pressures ~ 80 GPa will be published soon.