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The nuclear and magnetic structure of "white rust"—$Fe(OH_{0.86}D_{0.14})_2$

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ABSTRACT

The structure of $Fe(OH_{0.86},OD_{0.14})_2$ was refined by applying the Rietveld technique to neutron powder diffraction data collected at 300, 150, and 10 K. The nuclear structure, of the CdI_2 type ($P\bar{3}m1$) and isostructural with Mg, Ca, Mn, Ni, and β-$Co(OH)_2$, is maintained over the range of temperatures studied. At 10 K, the magnetic structure is ordered antiferromagnetically, with the magnetic moments aligned in the basal plane. The refined Fe^{2+} magnetic moment magnitude is 3.50(4) μ_B. This magnetic structure (space group $P_{2c}\bar{1}$) is unique amongst those encountered in the transition metal dihydroxides, for which the moment is either directed along the *c* axis [β-$Co(OH)_2$ and $Ni(OH)_2$], or at least has a considerable component along this direction [$Mn(OH)_2$]. The dependence of the strength of potential hydrogen bonds with temperature is discussed.