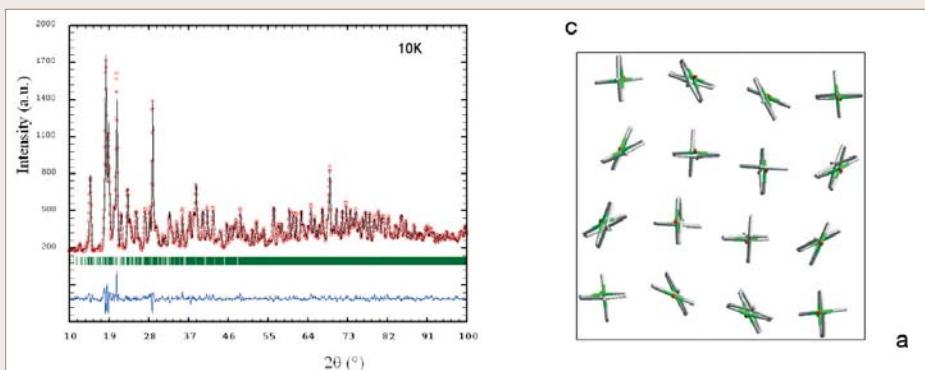


[C13. F. Damay] Synchrotron and neutron diffraction structural study of 4-methylpyridine-N-oxide (4MPNO) at 10K
 Combined synchrotron and neutron powder diffraction have been used to solve the structure of fully deuterated 4MPNO at 10 K. Using a simulated annealing algorithm on the synchrotron data, we were able to propose a structural model for 4MPNO, which involves a tetragonal cell with space group $P4_1$ ($a = b = 15.410(2)\text{\AA}$, $c = 19.680(3)\text{\AA}$). This model gives an excellent fit to both sets of diffraction data (Figure 1, left), even though it is impossible to rule out entirely other molecular arrangements. In our model, the asymmetric unit contains 8 molecules exhibiting a complex pattern of reorientations around the three cell axes (Figure 1, right). Along c , two columns of roughly perpendicular molecules alternate with two columns of molecules tilted by about 40° . This pattern is actually reminiscent of a combination of the 250 K and 100 K structures of 4MPNO, respectively [1]. Moreover, in sharp contrast with the simpler structure of parent compound 4-methylpyridine (4MP) at 10 K, the fourfold symmetry for methyl pairs and the translational invariance of the methyl sites are destroyed, as the molecular site symmetry in $P4_1$ is 1. The thermal ellipsoids calculated from the TLS matrix also show that the methyl groups are now largely localised. As a consequence, unlike 4MP, rotational dynamics in 4MPNO cannot be described by the quantum sine-Gordon model in 1D. Our results suggest two kinds of methyl-methyl interaction: along infinite chains parallel to a and b on the one hand, and between perpendicular chains through pairs of face to face methyl groups along c on the other [1].

[1] F. Damay et al, Acta Crystallogr. B 62, 627-633 (2006).

[Collaborations: F. Damay, A. Carretero-Genevrier, A. Cousson, J. Rodriguez-Carvajal, LLB, F. Filliaux, LADIR, W. Van Beek, ESRF].



Rietveld refinement of the neutron diffraction pattern of 4MPNO at 10K (left) and [001] projection of the structure (right)

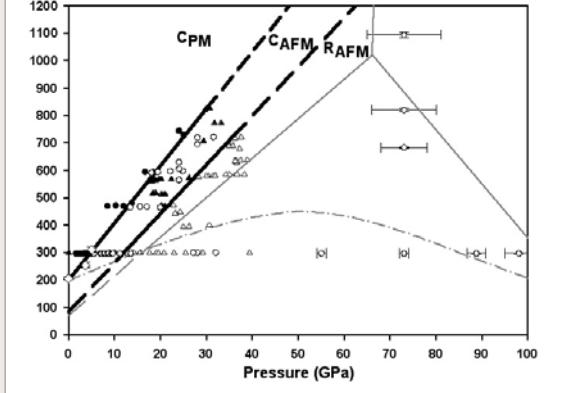
[C14. L. S. Dubrovinsky] High-pressure magnetism in geophysicaly important materials FeO and MnO

Magnetic ordering influences the density, bulk modulus, and elastic constants of materials. Developments of models of the Earth and analysis of the acoustic data, which provide the main experimental information on the Earth's interior, require direct information on magnetic properties of geophysical materials. Wüstite (FeO), the end-member of the magnesiowüstite MgO-FeO solid solution and the second abundant mineral in the Earth's lower mantle, is a good example of such a "geomaterial". Our combined Mössbauer, acoustic and neutron diffraction studies [1] show that the magnetic ordering temperature rapidly increases with pressure (Figure) and that pressure results in a considerable softening of the elastic modulus. The study established the existence of a magnetically ordered cubic phase of wüstite (Figure). This behavior differs from the other prototype antiferromagnetic oxide, MnO [2]. Below 3.5 GPa the magnetic ordering transition coincides with the structural transition, whereas at higher pressures the two transitions decouple, and the lattice distortion occurs at higher temperatures than the magnetic transition. Our results show that the structural transition (rhombohedral distortion) in transition metal monoxides is not directly coupled with the long-range magnetic ordering.

[1] A. P. Kantor, S. D. Jacobsen, I. K. Kantor, L. S. Dubrovinsky, C. A. Mc. Cammon, H. J. Reichman, I. N. Goncharenko, Phys. Rev. Lett. 93, 215502 (2004).

[2] A.P. Kantor, L. S. Dubrovinsky, N. A. Dubrovinskaia, I. Y. Kantor, I. Goncharenko, J Alloys Compounds 401, 42-45 (2005).

[Collaboration : L.S. Dubrovinsky, I.Yu. Kantor, A.P. Kantor, (Bayerisches Geoinstitut), N. A. Dubrovinskaia (Lehrstuhl für Kristallographie, Universität Bayreuth), I.N. Goncharenko (LLB)]



Phase diagram of non-stoichiometric wüstite. Black lines – phase boundaries between cubic paramagnetic (C_{PM}), cubic antiferromagnetic (C_{AFM}), and rhombohedral antiferromagnetic (R_{AFM}) phases obtained in this study. Circles – Mössbauer spectroscopic runs: solid circles – paramagnetic phase, open circles – magnetically ordered phase. Triangles – X-ray diffraction studies: solid triangles – cubic phase, open triangles – rhombohedral phase. Diamonds are T_N values obtained from neutron diffraction studies. The structural phase boundary of Fei and Mao (Fei and Mao, 1994) and the magnetic phase boundary proposed by Badro et al. (Badro et al., 1999) are also shown for comparison in gray color. Letters C, R, and B8 designate cubic, rhombohedral and NiAs-like hexagonal phases, PM and AFM – paramagnetic and antiferromagnetic phases, respectively.