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ESRF	**Experiment title:** Investigation of the dynamic Jahn-Teller effect in PrO_2 using powder diffraction	**Experiment number**: CH-1102
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Shifts: 9	**Local contact(s)**: W van Beek	*Received at ESRF:*

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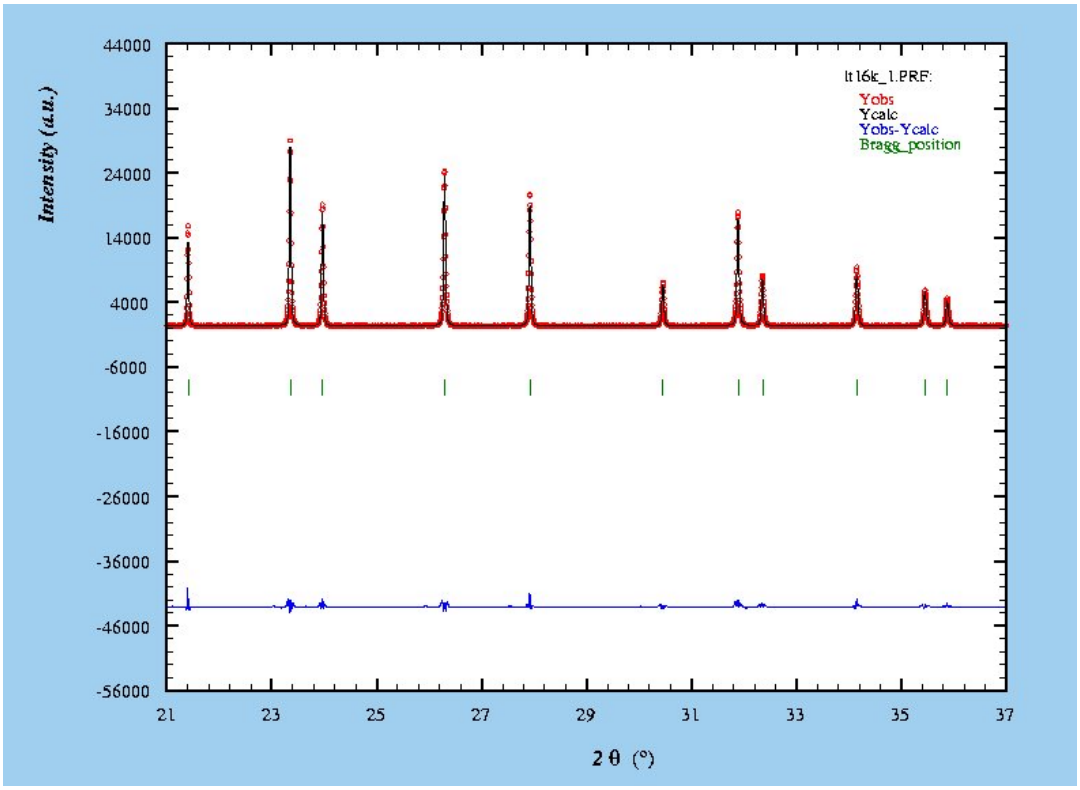
Report:

PrO_2 is an insulator with the fluorite structure type. It exhibits antiferromagnetic ordering below T_N = 14K. Polycrystalline samples of PrO_2 prepared in the Dept of Physics of the University of Oxford were first characterized by powder diffraction at room temperature using a wavelength of 0.50022Å. In addition to sharp diffraction peaks from PrO_2, it was also possible to identify impurity peaks from Pr_6O_{11} (lattice parameter 5.469Å) at about 1% concentration. We then proceeded to collect full diffraction patterns at a series of seven temperatures (8K, 12K, 16K, 20K, 70K, 150K and 293K). The patterns were analyzed using FULLPROF, and we extracted the refined lattice parameters and the temperature factors for the Pr and O atoms. We wished to probe for small tetragonal lattice distortions, which can often be revealed using high-resolution synchrotron data at levels far lower that those determined from neutron diffraction. In addition, we looked for any anomalies in the thermal displacement parameters of the oxygen atoms, particularly when passing through the magnetic ordering temperature of 14K. An increase in the displacement parameters below the transition would be a clear signature of electron-lattice interactions (dynamic Jahn-Teller effect).

The figure is an example of part of the diffraction pattern measured at 16K, showing the excellent full-pattern fit to the experimental data.



Despite the high quality of the Rietveld fit, it was difficult to extract precise values for the oxygen thermal parameters from the experimental data. The very strong scattering power of the praseodymium relative to oxygen leads to a domination of the high angle peaks by Pr. Within the experimental accuracy which could be achieved, the temperature dependence of the oxgen thermal parameters showed no anomalous behavior at or below 14K. No evidence of peak splitting or even peak broadening could be found in the diffraction pattern at any temperature.

Neutron powder diffraction results from recent experiments at ISIS and ILL indicate that there is a structural distortion at T=123K. Below this temperature, weak reflections with indices of the form (h+½, k, l) with k and l one even and one odd integer but not zero, e.g. (½, 1, 2) could be observed in the neutron patterns. We can confirm that a reflection with indices (½,1,2) could clearly be seen in the synchrotron data, confirming that there is a structural distortion at low temperature corresponding to a doubling of the crystal lattice in one direction. Although we only collected data at seven different temperatures, we can also confirm that the new peak was not present at 150K and 293K but could be observed at 70K and below.

Futher analysis of the origins of this structural distortion will require more experimental data, where attention should be concentrated upon establishing the temperature dependence of the additional diffraction peaks. In particular, low temperature synchrotron single crystal diffraction data collected with an area detector would be very helpful.