

## The crystal and magnetic structures of a high temperature polymorph of NiNb<sub>2</sub>O<sub>6</sub>

In contrast to the tri-rutile ( $P4_2/mnm$ ) materials, NiSb<sub>2</sub>O<sub>6</sub> and NiTa<sub>2</sub>O<sub>6</sub>, the thermodynamically stable form of NiNb<sub>2</sub>O<sub>6</sub> is that of columbite ( $Pbcn$ ). A high temperature polymorph, originally reported as a disordered simple rutile, actually crystallizes in  $P4_2/n$ , a sub-group of  $P4_2/mnm$ . [1,2] The lower symmetry is attributed to a second order Jahn-Teller effect associated with the Nb<sup>5+</sup> ion ( $4d^0$ ). The structure of this polymorph is very similar to tri-rutile with only slight distortions. The magnetic properties of the series NiB<sub>2</sub>O<sub>6</sub>, B = Sb, Ta and Nb, are also very similar, showing a broad susceptibility maximum between 20K – 30K, attributed to short range spin correlations, followed by long range antiferromagnetic order at much lower temperatures. The magnetic structures of NiSb<sub>2</sub>O<sub>6</sub> and NiTa<sub>2</sub>O<sub>6</sub> have been reported and are surprisingly different with  $\mathbf{k} = (1/2 \ 0 \ 1/2)$  for the former and  $\mathbf{k} = (1/4 \ -1/4 \ 1/2)$  for the latter in spite of the close similarity in unit cell dimensions, ( $\sim 1-2\%$ ). [3] The magnetic structure of NiNb<sub>2</sub>O<sub>6</sub> has been solved using powder and single crystal neutron diffraction and is quite different from those of the related tri-rutile phases, with  $\mathbf{k} = (1/2 \ 1/2 \ 1/2)$ . The ordered total moment is 1.54(9) B.M. much reduced from the expected value near 2 B.M, suggesting some residual spin dynamics below  $T_N$ .

[1]. Wichman and Muller-Buschbaum, Z. Anorg. Allg. Chem. 503(1983) 101.

[2] T.J.S. Munsie et al, J. Solid State Chem. 236 (2016) 19.

[3] Ehrenberg et al, J. Magn. Magn. Mat. 184 (1998) 111.

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