

## Dineodymium(III) ditungstate(VI), Nd<sub>2</sub>W<sub>2</sub>O<sub>9</sub>

Peter Held\* and Petra Becker

Institut für Kristallographie, Universität zu Köln, Zùlpicher Strasse 49b, D-50674 Köln, Germany

Correspondence e-mail: peter.held@uni-koeln.de

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Key indicators: single-crystal X-ray study;  $T = 290$  K; mean  $\sigma(W-O) = 0.007$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.093; data-to-parameter ratio = 19.6.

Single crystals of monoclinic Nd<sub>2</sub>W<sub>2</sub>O<sub>9</sub> were obtained by growth from tungsten borate flux in an atmosphere of air. The crystal structure consists of chains of distorted [WO<sub>6</sub>] octahedra that run along the  $c$  axis of the structure, and of [NdO<sub>9</sub>] polyhedra that are connected *via* common faces and common edges to form a three-dimensional framework.

### Related literature

For literature on related structures, see: Lacorre *et al.* (2000), Goutenoire *et al.* (2000) and Evans *et al.* (2005) for La<sub>2</sub>Mo<sub>2</sub>O<sub>9</sub>; Laligant *et al.* (2001) for La<sub>2</sub>W<sub>2</sub>O<sub>9</sub>; Yoshimura *et al.* (1976) for Ce<sub>2</sub>W<sub>2</sub>O<sub>9</sub>; Borisov & Klevtsova (1970) for Pr<sub>2</sub>W<sub>2</sub>O<sub>9</sub>; Aruga *et al.* (2005) for Eu<sub>2</sub>W<sub>2</sub>O<sub>9</sub>.

### Experimental

#### Crystal data

Nd <sub>2</sub> W <sub>2</sub> O <sub>9</sub>	$V = 663.69$ (15) Å <sup>3</sup>
$M_r = 800.17$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 7.6501$ (11) Å	$\mu = 49.96$ mm <sup>-1</sup>
$b = 9.8547$ (10) Å	$T = 290$ (1) K
$c = 9.2326$ (13) Å	$0.25 \times 0.15 \times 0.13$ mm
$\beta = 107.538$ (11)°	

#### Data collection

Stoe IPDSII diffractometer	15723 measured reflections
Absorption correction: numerical	2330 independent reflections
[ <i>X-SHAPE</i> (Stoe & Cie, 1999)	2072 reflections with $I > 2\sigma(I)$
and <i>X-RED</i> (Stoe & Cie, 2001)]	$R_{int} = 0.088$
$T_{min} = 0.080$ , $T_{max} = 0.469$	

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	119 parameters
$wR(F^2) = 0.093$	$\Delta\rho_{max} = 2.34$ e Å <sup>-3</sup>
$S = 1.09$	$\Delta\rho_{min} = -1.62$ e Å <sup>-3</sup>
2330 reflections	

Data collection: *X-Area* (Stoe & Cie, 2001); cell refinement: *X-Area*; data reduction: *X-Area*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2082).

### References

- Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
- Aruga, A., Matsuda, T., Hasegawa, T. & Shioi, K. (2005). *Nippon Kagakkai Koen Yokoshu (Preprints of the Conference of the Chemical Society of Japan)*, **85**, 689.
- Borisov, S. V. & Klevtsova, R. F. (1970). *Sov. Phys. Crystallogr.* **15**, 28–31.
- Dowty, E. (2002). *ATOMS for Windows*. Shape Software, Kingsport, Tennessee, USA.
- Evans, I. R., Howard, J. A. K. & Evans, J. S. O. (2005). *Chem. Mater.* **17**, 4074–4077.
- Goutenoire, F., Isnard, O., Retoux, R. & Lacorre, P. (2000). *Chem. Mater.* **12**, 2575–2580.
- Lacorre, P., Goutenoire, F., Bohnke, O., Retoux, R. & Laligant, Y. (2000). *Nature*, **404**, 856–858.
- Laligant, Y., Le Bail, A. & Goutenoire, F. (2001). *J. Solid State Chem.* **159**, 223–227.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Stoe & Cie (1999). *X-SHAPE*. Stoe & Cie, Darmstadt, Germany.
- Stoe & Cie (2001). *X-RED* and *X-Area*. Stoe & Cie, Darmstadt, Germany.
- Yoshimura, M., Sibieude, F., Rouanet, A. & Foex, M. (1976). *J. Solid State Chem.* **16**, 219–232.























