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Poly[μ_2 -hydroxido- μ_4 -sulfato-neodymium(III)]

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Nd}-\text{O}) = 0.004$ Å; R factor = 0.023; wR factor = 0.057; data-to-parameter ratio = 10.1.

The title compound, $[\text{Nd}(\text{OH})(\text{SO}_4)]_n$, was obtained hydrothermally from an aqueous solution of neodymium nitrate, 1,2-propanediamine and sulfuric acid. The structure features nonacoordinated neodymium with sulfate and hydroxide anions acting as bridging ligands. The OH group forms a weak $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond with an $\text{O}\cdots\text{O}$ distance of 3.224 (5) Å.

Related literature

For related literature, see: Doran *et al.* (2002); Xu, Ding, Zhou & Liu (2006); Xu, Ding, Feng *et al.* (2006); Xu *et al.* (2007); Yuan *et al.* (2004); Zhang *et al.* (2004); Ding *et al.* (2006).

Experimental

Crystal data

$[\text{Nd}(\text{OH})(\text{SO}_4)]$
 $M_r = 257.31$
 Monoclinic, $P2_1/n$
 $a = 4.4678$ (9) Å
 $b = 12.432$ (2) Å
 $c = 6.8575$ (13) Å
 $\beta = 106.324$ (3)°

$V = 365.53$ (12) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 14.66$ mm⁻¹
 $T = 293$ (2) K
 $0.10 \times 0.08 \times 0.06$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.322$, $T_{\max} = 0.473$
 (expected range = 0.282–0.415)

1837 measured reflections
 675 independent reflections
 669 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.056$
 $S = 1.24$
 675 reflections
 67 parameters
 1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.56$ e Å⁻³
 $\Delta\rho_{\text{min}} = -2.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|----------|-------------|-------------|---------------|
| $\text{O5}-\text{H1}\cdots\text{O1}^1$ | 0.83 (3) | 2.43 (3) | 3.224 (5) | 160 (6) |

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

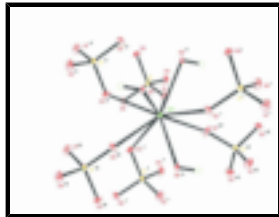
Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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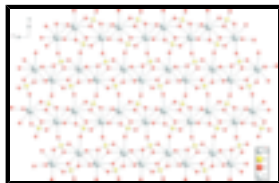
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2079).

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