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Poly[potassium aquadi-μ-oxalato-neodymium(III) dihydrate]

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Key indicators

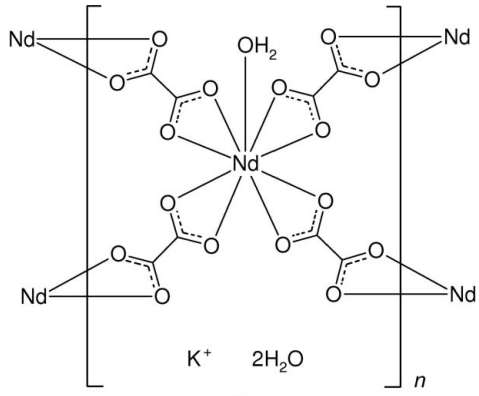
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.016 Å
R factor = 0.054
wR factor = 0.120
Data-to-parameter ratio = 12.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $\{K[Nd(C_2O_4)_2(H_2O)]\cdot 2H_2O\}_n$, has been prepared hydrothermally. Every Nd^{III} atom is linked to four others through oxalate anions lying on centres of inversion, generating a three-dimensional anionic network with channels that contain K^+ cations and water molecules.

Comment

Previously, some lanthanide oxalates have been reported with layered honeycomb network structures (Ollendorf & Weigel, 1969; Hansson, 1970, 1973; Trollet *et al.*, 1997). To produce open-framework lanthanide oxalates, the challenge is to connect layers of such complexes to construct three-dimensional architectures. We present here the structure of the title Nd^{III} complex, (I), which exhibits a three-dimensional network structure.



(I)

In (I), Nd^{III} is nine-coordinated by eight O atoms from four oxalate anions and one water molecule in a distorted monocapped square-antiprismatic geometry (Fig. 1). The Nd—O distances (Table 1) are closely comparable to the corresponding distances in $(NH_4)_2[Nd_2(C_2O_4)_3(CO_3)(H_2O)]\cdot H_2O$ (average Nd—O = 2.492 Å; Trombe *et al.*, 2002). Every Nd^{III} atom is linked to four others through oxalate anions lying on centres of inversion, generating a three-dimensional anionic network structure with formula $[Nd(C_2O_4)_2(H_2O)]^-$ (Fig. 2). This network exhibits channels running along [001], in which K^+ cations and water molecules reside.

Experimental

All reagents and solvents were used as obtained without further purification. $K_{10}[P_2W_{17}O_{61}]\cdot 20H_2O$ was synthesized according to the procedure given by Contant (1990). Hydrothermal reaction of $K_{10}[P_2W_{17}O_{61}]\cdot 20H_2O$ (0.10 mmol), Nd_2O_3 (0.50 mmol), $(NH_4)_2C_2O_4$

(0.37 mmol), edta (0.25 mmol) and water (15 ml) at 473 K for 60 h yielded pink crystals of (I).

Crystal data

$K[Nd(C_2O_4)_2(H_2O)]\cdot 2H_2O$
$M_r = 413.43$
Monoclinic, $C2/c$
$a = 23.085\ (5)$ Å
$b = 7.4913\ (15)$ Å
$c = 12.941\ (3)$ Å
$\beta = 99.286\ (3)^\circ$
$V = 2208.6\ (8)$ Å^3
$Z = 8$
$D_x = 2.487$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 5.13$ mm^{-1}
$T = 293\ (2)$ K
Block, pink
0.26 × 0.13 × 0.11 mm

Data collection

Rigaku R-AXIS-IV diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.330$, $T_{max} = 0.569$
5056 measured reflections
1985 independent reflections
1531 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 25.3^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.120$
$S = 1.28$
1985 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 55.1422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.87$ e Å^{-3}
$\Delta\rho_{min} = -2.08$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Nd1—O1^{i}	2.492 (8)	K1—O1^{iv}	3.161 (11)
Nd1—O2	2.502 (8)	K1—O3	2.781 (9)
Nd1—O3^{i}	2.527 (7)	K1—O5^{v}	2.936 (8)
Nd1—O4	2.514 (8)	K1—O6^{vi}	3.377 (9)
Nd1—O5	2.455 (7)	K1—O8^{vii}	2.857 (8)
Nd1—O6^{ii}	2.444 (7)	K1—O1W^{v}	3.336 (9)
Nd1—O7	2.505 (8)	K1—O2W	3.324 (13)
Nd1—O8^{iii}	2.472 (8)	K1—O3W	2.841 (11)
Nd1—O1W	2.432 (8)	K1—O3W^{vi}	2.803 (10)

Symmetry codes: (i) $x, -y+1, z-\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$; (iv) $x, y-1, z$; (v) $x, -y, z+\frac{1}{2}$; (vi) $-x+1, y, -z+\frac{3}{2}$; (vii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

H atoms of the water molecules were placed at calculated positions so as to form reasonable O—H···O contacts, with O—H = 0.85 Å, and refined as riding, with $U_{iso}(H) = 1.5U_{iso}(O)$. The resulting H-atom positions are approximate. The water O atoms were restrained to approximately isotropic behaviour. The deepest hole in the residual electron density is located 1.05 Å from K1.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

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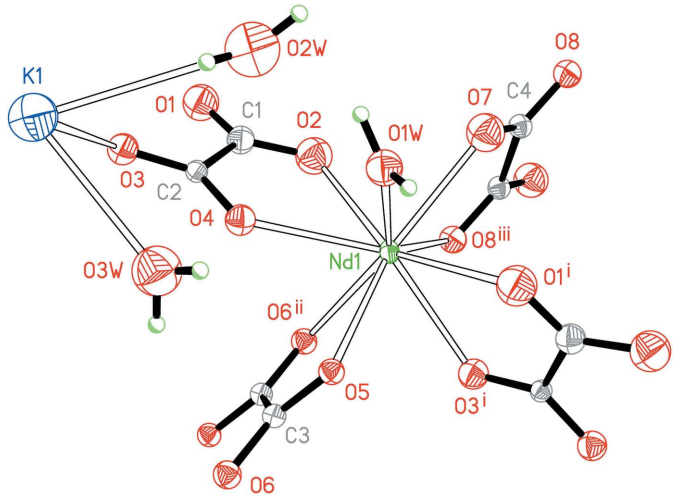

Figure 1
The asymmetric unit, expanded to show the complete coordination of the Nd^{III} atom, with displacement ellipsoids drawn at the 50% probability level. Symmetry codes as in Table 1.

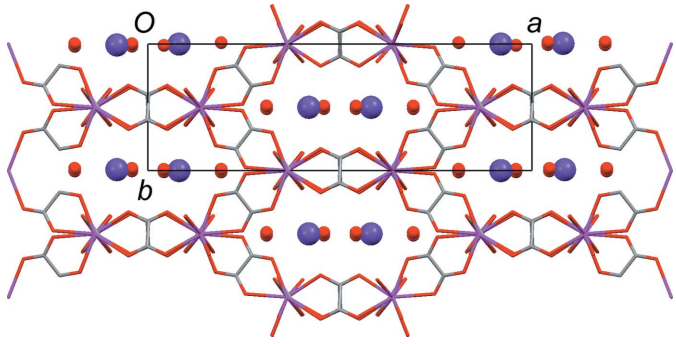

Figure 2
View of (I) along [001], showing the $[Nd(C_2O_4)_2(H_2O)]^-$ network structure, with K^+ cations (purple spheres) and water molecules (red spheres) residing in channels. H atoms have been omitted.

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