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Reinvestigation of layered poly[aqua-sodium(I) [[aquasamarium(III)]-di-μ-aqua-μ_3-pyridine-2,6-dicarboxylato-μ_2-pyridine-2,6-dicarboxylato] trihydrate]

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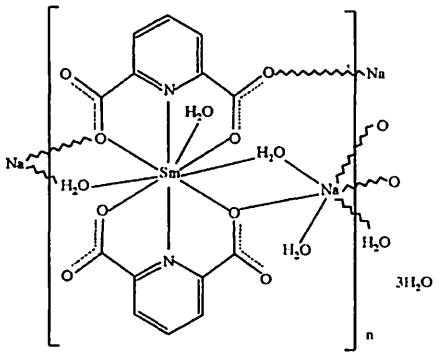
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.081; data-to-parameter ratio = 18.1.

The crystal structure of the title compound, $\{[NaSm(C_7H_3NO_4)_2(H_2O)_4]\cdot 3H_2O\}_n$, was first reported by van Albada, Gorter & Reedijk [(1999), *Polyhedron*, **18**, 1821–1824]. It has now been reinvestigated and confirmed from single-crystal data, giving greater understanding of the role of the water molecules. The two-dimensional layers found in the compound are built up from six-coordinate NaO_6 polyhedra and nine-coordinate SmN_2O_7 polyhedra. The former share edges with each other along the c axis and the latter are bridged by carboxylate groups of pyridine-2,6-dicarboxylate anions along the b axis. Eight-membered rings of water molecules, connected to one another by hydrogen bonding, are formed in the interlayer spaces.

Related literature

For related literature, see: van Albada *et al.* (1999); Benelli & Gatteschi (2002); Brouca-Cabarrecq *et al.* (2002); Duan *et al.* (2004); Ghosh & Bharadwaj (2003).



Experimental

Crystal data

$[NaSm(C_7H_3NO_4)_2(H_2O)_4]\cdot 3H_2O$
M_r = 629.66
Monoclinic, $P2_1/c$
a = 11.2065 (4) Å
b = 17.4485 (3) Å
c = 11.3728 (4) Å
β = 98.163 (1)° [98.163 (1)°
V = 2201.27 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.77 mm^{-1}
T = 296 K
0.30 × 0.18 × 0.04 mm

Data collection

Rigaku R-AXIS-IV diffractometer
Absorption correction: numerical (*ABSCOR*; Higashi, 1999)
T_{min} = 0.558, T_{max} = 0.895
22103 measured reflections
6163 independent reflections
5944 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.081
S = 1.17
6163 reflections
341 parameters
21 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −1.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sm1—O14	2.4144 (19)	Sm1—O2W	2.562 (2)
Sm1—O12	2.4213 (19)	Na1—O21	2.392 (2)
Sm1—O23	2.437 (2)	Na1—O5W	2.394 (3)
Sm1—O21	2.4460 (19)	Na1—O2W	2.434 (3)
Sm1—O3W	2.478 (2)	Na1—O24^{i}	2.445 (3)
Sm1—N11	2.533 (2)	Na1—O14^{ii}	2.456 (2)
Sm1—N21	2.540 (2)	Na1—O1W^{ii}	2.610 (3)
Sm1—O1W	2.547 (2)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O22^{iii}	0.851	1.931	2.753 (3)	162
O1W—H2W···O5W^{iv}	0.854	1.961	2.794 (3)	165
O2W—H3W···O11^{iii}	0.848	1.954	2.790 (3)	169
O2W—H4W···O13^{ii}	0.849	1.884	2.725 (3)	170
O3W—H5W···O24^{i}	0.851	2.019	2.853 (3)	166
O3W—H6W···O12^{iii}	0.845	1.885	2.725 (3)	173
O4W—H7W···O22^{iv}	0.856	2.077	2.907 (4)	163
O4W—H8W···O23	0.855	1.938	2.779 (3)	168
O5W—H9W···O4W^{ii}	0.848	1.961	2.784 (4)	163
O5W—H10W···O7W	0.852	1.939	2.791 (5)	177
O6W—H11W···O13^{ii}	0.854	1.947	2.789 (5)	168
O6W—H12W···O4W^{v}	0.854	2.03	2.858 (5)	163
O7W—H13W···O11^{iii}	0.851	2.22	2.989 (4)	151
O7W—H14W···O6W	0.852	1.96	2.754 (7)	155

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YM2055).

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