Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Polymeric diaquatetrakis(μ-1,2-benzene-dicarboxylato)di-μ-nitrato-pentastrontium(II)

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Received 3 December 2004
Accepted 10 December 2004
Online 18 December 2004

Colourless crystals of polymeric diaquatetrakis(μ-1,2-benzenedicarboxylato)di-μ-nitrato-pentastrontium(II), $[Sr_5(C_8H_4O_4)_4(NO_3)_2(H_2O)_2]_n$, crystallized at the phase boundary of an aqueous silica gel containing sodium phthalate (1,2-benzenedicarboxylate) and an aqueous solution of $Sr(NO_3)_2$. Three crystallographically distinct Sr^{II} ions, one located on a centre of symmetry, are connected by two crystallographically distinct phthalate anions, one nitrate anion and a water molecule, to form a layered coordination polymer. These layers, perpendicular to [001], are held together by weak interatomic forces, as no interlayer hydrogen bonds were found.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.034
wR factor = 0.091
Data-to-parameter ratio = 17.1

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

Comment

During our studies of coordination polymers with dicarboxylate anions (*e.g.* Billetter *et al.*, 2004) colourless crystals of $[Sr_5(o\text{-}C_6H_4(COO)_2)_4(NO_3)_2(H_2O)_2]_n$, (I), were obtained. The crystal structure contains three crystallographically distinct Sr^{II} cations, with coordination numbers 12 (Sr1, placed on an inversion centre), 10 (Sr2) and 8 (Sr3), taking Sr—O distances up to 3.1 Å into account. The next nearest Sr—O distances start at 3.55 (3) Å (Sr3—O6).

$$^{2}_{\infty}[Sr_5\{o\text{-}C_6H_4(COO)_2\}_4(NO_3)_2(H_2O)_2]$$

(I)

The Sr^{II} cations are connected by two crystallographically distinct phthalate (1,2-benzenedicarboxylate) anions, one nitrate anion and one water molecule, to form a two-dimensional coordination polymer with layers perpendicular to [001]. Atom Sr1 is coordinated by six chelating bidentate carboxylate groups of four phthalate anions [Sr—O 2.564 (3)–2.967 (3) Å] (Fig. 1). The coordination sphere of atom Sr2 is composed of one chelating bidentate carboxylate group [Sr—O 2.768 (3) and 3.070 (3) Å], one chelating nitrate group [Sr—O 2.637 (3) and 2.705 (4) Å] and six monodentate carboxylate groups of four different phthalate anions [Sr—O 2.622 (3)–2.740 (3) Å] (Fig. 1). Atom Sr3 is coordinated by six monodentate carboxylate groups of five different phthalate anions [Sr—O 2.539 (3)–2.695 (3) Å], one monodentate nitrate group [Sr—O 2.579 (3) Å] and one water molecule [Sr—O 2.568 (4) Å] (Fig. 1). All these Sr—O distances agree well with those found in $Sr(NO_3)_2$ [Nowotny & Heger, 1983; Sr—O 2.7153 (5) Å (6 ×) and 2.8381 (5) Å (6 ×)] and $[Sr\{o\text{-}C_6H_4$-

$(COO)(COOH)\}_2(H_2O)_2]$ [Bats *et al.*, 1978; Sr—O 2.566 (2)–2.730 (2) Å (6 ×) and $Sr—OH_2$ 2.488 (3)–2.762 (3) Å (3 ×)].

The C—C and C—O distances within the phthalate anions are as expected (Table 1). In the nitrate anion, the N—O11 distance is about 0.04 Å longer than N—O9 and N—O10 (Table 1). This might be due to the fact that atom O11 coordinates to atoms Sr2 and Sr3, whereas atom O10 only coordinates to atom Sr2 and atom O9 is non-coordinating.

The irregular coordination polyhedra of atoms Sr1, Sr2 and Sr3 are connected into layers (Fig. 2). The nitrate anion connects atoms Sr2 and Sr3, whereas the two crystallographically distinct phthalates connect atoms Sr1, Sr2 (3 ×) and Sr3 (3 ×), and Sr1 (2 ×), Sr2 (2 ×) and Sr3 (2 ×).

Surprisingly, no hydrogen bonds were found between the layers. The only hydrogen bond which could be assigned is between water atom O12 and nitrate atom O9 [2.710 (5) Å; Table 2] within the layers. Thus, weak interatomic forces, *i.e.* van der Waals interactions, hold the layers together.

Experimental

1,2-Benzenedicarboxylic acid (1.66 g, 1 mmol) was suspended in deionized water (10 ml). The pH was adjusted to 3 with NaOH, which led to an almost clear solution. After filtration, an aqueous solution of $Na_2Si_3O_7$ (sodium waterglass) was added. At a pH of approximately 5.5, a gel was formed, which was layered with an aqueous solution (10 ml) of $Sr(NO_3)_2$ (2.12 g, 1 mmol). At the phase boundary, colourless crystals of (I) grew within a few days. No yield was determined.

Crystal data

$[Sr_5(C_8H_4O_4)_4(NO_3)_2(H_2O)_2]$
M_r = 1254.60
Triclinic, $P\overline{1}$
a = 7.0624 (11) Å
b = 10.3895 (16) Å
c = 12.7945 (19) Å
α = 91.557 (12)°
β = 91.519 (12)°
γ = 104.011 (12)°
V = 910.0 (2) $Å^3$

Z = 1
D_x = 2.289 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 9407 reflections
θ = 1.1–29.8°
μ = 7.39 mm^{-1}
T = 293 (2) K
Trigonal plate, colourless
0.2 × 0.2 × 0.05 mm

Data collection

Stoe IPDS-II diffractometer
ω and *φ* scans
Absorption correction: numerical, [*X-RED* (Stoe & Cie, 2001), after optimizing the crystal shape using *X-SHAPE* (Stoe & Cie, 1999)]
T_{min} = 0.253, T_{max} = 0.696
13 318 measured reflections

5061 independent reflections
3779 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 29.7°
h = −9 → 9
k = −14 → 14
l = −17 → 16

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.03
5061 reflections
296 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.2372P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.88 e $Å^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0106 (9)

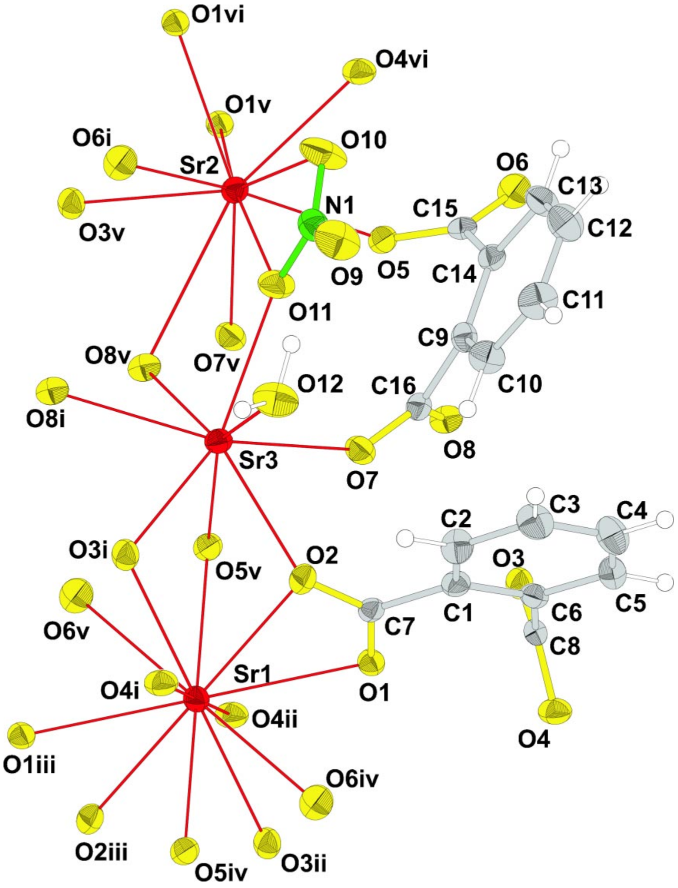

Figure 1
A view of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H-atom radii are arbitrary. For the nitrate and phthalate anions not belonging to the asymmetric unit, only the coordinating O atoms are displayed, for clarity. [Symmetry codes: (i) *x* − 1, *y*, *z*; (ii) 1 − *x*, −*y*, −*z*; (iii) −*x*, −*y*, −*z*; (iv) *x* − 1, *y* − 1, *z*; (v) 1 − *x*, 1 − *y*, −*z*; (vi) *x*, 1 + *y*, *z*.]

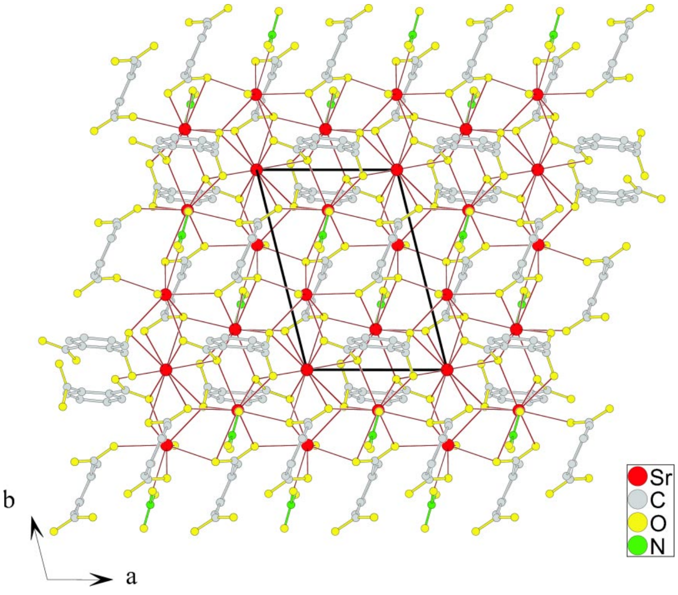

Figure 2
A polymeric layer in the crystal structure of (I), viewed in a projection along [001]. H atoms have been omitted for clarity.

Table 1
Selected bond lengths (Å).

Sr1—O4^{i}	2.564 (3)	C1—C2	1.390 (5)
Sr1—O4^{ii}	2.564 (3)	C1—C6	1.402 (5)
Sr1—O2^{iii}	2.650 (3)	C1—C7	1.496 (5)
Sr1—O2	2.650 (3)	C2—C3	1.386 (6)
Sr1—O6^{iv}	2.736 (3)	C3—C4	1.384 (6)
Sr1—O6^{v}	2.736 (3)	C4—C5	1.385 (6)
Sr1—O1^{iii}	2.794 (3)	C5—C6	1.394 (5)
Sr1—O1	2.794 (3)	C6—C8	1.493 (5)
Sr1—O5^{iv}	2.908 (3)	C7—O2	1.255 (4)
Sr1—O5^{v}	2.908 (3)	C7—O1	1.275 (4)
Sr1—O3^{ii}	2.967 (3)	C8—O4	1.258 (4)
Sr1—O3^{i}	2.967 (3)	C8—O3	1.268 (5)
Sr2—O1^{v}	2.622 (3)	C9—C10	1.387 (6)
Sr2—O11	2.637 (3)	C9—C14	1.411 (5)
Sr2—O6^{i}	2.650 (3)	C9—C16	1.517 (5)
Sr2—O4^{vi}	2.676 (3)	C10—C11	1.396 (6)
Sr2—O5	2.680 (3)	C11—C12	1.386 (7)
Sr2—O3^{v}	2.697 (3)	C12—C13	1.394 (6)
Sr2—O10	2.705 (4)	C13—C14	1.389 (5)
Sr2—O1^{vi}	2.740 (3)	C14—C15	1.494 (5)
Sr2—O7^{v}	2.768 (3)	C15—O6	1.253 (5)
Sr2—O8^{v}	3.070 (3)	C15—O5	1.275 (4)
Sr3—O5^{v}	2.539 (3)	C16—O7	1.247 (5)
Sr3—O12	2.568 (4)	C16—O8	1.272 (5)
Sr3—O11	2.579 (3)	N1—O10	1.232 (5)
Sr3—O2	2.598 (3)	N1—O9	1.233 (5)
Sr3—O7	2.663 (3)	N1—O11	1.277 (4)
Sr3—O3^{i}	2.671 (3)	O12—H121	0.88 (8)
Sr3—O8^{v}	2.677 (3)	O12—H122	0.90 (7)
Sr3—O8^{i}	2.695 (3)		

Symmetry codes: (i) $x-1, y, z$; (ii) $1-x, -y, -z$; (iii) $-x, -y, -z$; (iv) $x-1, y-1, z$; (v) $1-x, 1-y, -z$; (vi) $x, y+1, z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O12—H122···O9	0.90 (7)	1.82 (7)	2.710 (5)	169 (6)

The H-atom positions of the phthalate anions were calculated and refined as riding, with fixed C—H distances (0.93 Å) and one common isotropic displacement parameter. The H atoms of the water molecule were located in difference Fourier maps at the end of the refinement and refined isotropically without constraints.

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, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

We thank Dr Ingo Pantenburg for help with data collection and refinement.

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