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Heptaaqua(4-nitrobenzoato-κ^2O,O')-strontium(II) 4-nitrobenzoate dihydrate

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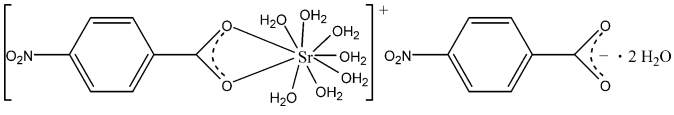
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.067; data-to-parameter ratio = 12.4.

The title compound, $[Sr(C_7H_4NO_4)(H_2O)_7](C_7H_4NO_4)\cdot 2H_2O$, was synthesized from the aqueous reaction of strontium carbonate with 4-nitrobenzoic acid. The structure consists of a nine-coordinate heptaaqua(4-nitrobenzoato-κ^2O,O')-strontium(II) complex cation, an uncoordinated 4-nitrobenzoate anion and two solvent water molecules. The cations, anions and solvent water molecules are linked with the aid of several O—H···O and C—H···O interactions, resulting in a three-dimensional hydrogen-bonding network. The hydrogen bonding between a solvent water molecule and a symmetry-related solvent water molecule results in the formation of a water dimer.

Related literature

For a recent review of the chemistry of metal carboxylates, see: Rao *et al.* (2004). The structures of the 4-nitrobenzoate (4-nba) complexes of the lighter alkali earths $[Mg(H_2O)_6](4\text{-nba})_2\cdot 2H_2O$ and $[Ca(H_2O)_4(4\text{-nba-}\kappa^2O,O')(4\text{-nba-}\kappa^1O]$ have been reported recently (Srinivasan *et al.*, 2006; Srinivasan, Sawant *et al.*, 2007). For related literature, see: Srinivasan, Sawant & Ragahavaiah (2007); Bondi (1964). For reviews of hydrogen-bonded water clusters in crystalline hydrates, see: Infantes & Motherwell (2002); Supriya & Das (2003).



Experimental

Crystal data

$[Sr(C_7H_4NO_4)(H_2O)_7](C_7H_4NO_4)\cdot 2H_2O$
M_r = 581.99
Monoclinic, $P2_1/c$
a = 6.7364 (7) Å
b = 11.1705 (12) Å
c = 31.738 (3) Å
β = 95.568 (2)°
V = 2377.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.35 mm^{-1}
T = 293 (2) K
0.42 × 0.36 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.375, T_{max} = 0.761
11962 measured reflections
4604 independent reflections
3777 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.067
S = 1.02
4604 reflections
370 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O9—H9B···O11^{i}	0.82	2.10	2.894 (2)	162
O10—H10A···O13^{ii}	0.82	2.04	2.841 (2)	165
O14—H14A···O5^{iii}	0.82	1.98	2.788 (2)	170
O9—H9A···O5^{i}	0.80 (3)	2.03 (3)	2.815 (2)	169 (3)
O11—H11A···O2^{ii}	0.80 (3)	1.95 (3)	2.707 (2)	160 (3)
O11—H11B···O16^{iv}	0.82 (3)	2.02 (3)	2.833 (3)	176 (3)
O15—H15B···O7^{v}	0.81 (4)	2.35 (4)	3.104 (3)	154 (4)
O15—H15A···O17^{vi}	0.73 (4)	2.17 (4)	2.881 (4)	165 (4)
O17—H17B···O16^{iv}	0.82 (4)	1.98 (4)	2.761 (4)	158 (4)
O17—H17A···O4^{vii}	0.78 (4)	2.37 (4)	3.087 (3)	153 (4)
O17—H17A···O3^{vii}	0.78 (4)	2.57 (4)	3.264 (3)	150 (4)
O14—H14B···O17	0.801 (17)	2.06 (2)	2.831 (3)	163 (3)
O13—H13A···O1^{i}	0.82 (3)	1.85 (3)	2.657 (2)	168 (3)
O13—H13B···O5^{iii}	0.81 (3)	1.94 (3)	2.732 (2)	164 (3)
O12—H12B···O9^{viii}	0.74 (3)	2.18 (3)	2.899 (3)	165 (3)
O12—H12A···O6	0.81 (3)	2.00 (3)	2.799 (2)	175 (3)
O16—H16B···O6	0.82 (3)	1.93 (3)	2.739 (3)	171 (3)
O16—H16A···O10^{i}	0.76 (4)	2.28 (4)	2.921 (3)	141 (4)
O16—H16A···O2	0.76 (4)	2.61 (4)	3.229 (3)	140 (4)
O10—H10B···O12^{vi}	0.806 (18)	2.15 (2)	2.915 (3)	158 (3)
C4—H4···O7^{ix}	0.93	2.60	3.476 (3)	158
C11—H11···O4^{ix}	0.93	2.53	3.396 (3)	155
C6—H6···O8^{x}	0.93	2.55	3.349 (3)	144

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg 1999); software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2092).

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supplementary materials

Acta Cryst. (2007). E**63**, m2251-m2252 [**doi:10.1107/S1600536807036872**]

Heptaaqua(4-nitrobenzoato-κ^2O,O')strontium(II) 4-nitrobenzoate dihydrate

B. R. Srinivasan, P. Raghavaiah and J. V. Sawant

Comment

The design of supramolecular architectures employing carboxylic acids as ambidentate and templating ligands with metals providing interesting connectivity, is an area of current research (Rao *et al.*, 2004). As part of our metal carboxylate research programme, we are curently investigating the synthesis, structure and thermal characterization of 4-nitrobenzoate (4-nba) complexes of alkali earth metals (Srinivasan, Sawant & Ragahavaiah, 2007). Recently we reported on the structures of $[Mg(H_2O)_6](4\text{-nba})_2\cdot 2H_2O$ (Srinivasan, Sawant *et al.*, 2007) and $[Ca(H_2O)_4(4\text{-nba-}\kappa^2O,O')(4\text{-nba-}\kappa^1O]$ (Srinivasan *et al.*, 2006). In continuation of this work, we describe the structure of a nine coordinated Sr(II) complex, heptaaquo(4-nitrobenzoato-κ^2O,O')strontium(II) 4-nitrobenzoate dihydrate (I).

(I) crystallizes in the monoclinic space group P 2_1/c with all atoms located in general positions (Fig. 1). The structure consists of a nine coordinated heptaaquo(4-nitrobenzoato-κ^2O,O')strontium(II) complex cation, an uncoordinated 4-nitrobenzoate and two lattice water molecules. It is interesting to note that the Sr compound contains coordinated and crystal water molecules, a bidentate 4-nba ligand as well as an uncoordinated 4-nba anion unlike the related $[Mg(H_2O)_6](4\text{-nba})_2\cdot 2H_2O$ compound where both the nitrobenzoates function as anions. The calcium 4-nitrobenzoate compound $[Ca(H_2O)_4(4\text{-nba-}\kappa^2O,O')(4\text{-nba-}\kappa^1O]$ exhibits both monodentate and bidentate 4-nba ligation and contains only coordinated water molecules. The geometric parameters of the coordinated and free 4-nba anions are comparable with the observed values in the aforementioned Mg and Ca complexes. The Sr—O bond lengths vary from 2.5702 (16) to 2.7893 (15) Å while the O—Sr—O angles scatter in a wide range between 47.56 (4) to 144.55 (6) °.

An analysis of the structure reveals that the title compound is involved in several hydrogen bonding interactions through all possible sites and the resulting hydrogen bonded network is displayed in Fig. 2. Each molecule of (I) is linked to ten others with the aid of O—H···O and and C—H···O bonds, with the O atoms of the coordinated and lattice water molecules, the nitro and carboxylate functionalities functioning as hydrogen bond acceptors. All the H atoms attached to the water molecules excepting H16A and H17A and three H atoms on the aromatic rings function function as singly shared H donors. A total of twenty O—H···O interactions ranging from 1.85 to 2.61 Å and three weak C—H···O contacts between 2.53 to 2.60 Å are observed (Table 1). All these O···H contacts are less than the sum of their van der Waals radii (Bondi, 1964). As a result of hydogen bonding, the cations and anions are organized into alternating layers in the crystallographic *ac* plane with the crystal waters situated in the space between them. The short O17—H17B···O16^{iv} contact at 1.98 Å acccompanied by a O···O distance of 2.761 (4) Å between O17 and a symmetry related crystal water O16^{iv} (for symmetry codes see Table 1) constitutes a water dimer (Infantes & Motherwell, 2002; Supriya & Das, 2003). The water dimer thus formed is further hydrogen bonded to four different complex cations and an uncoordinated 4-nba anion with the aid of eight O—H···O bonds (Fig. 3). The bifurcated acceptor nature of O16 and O17 results in a tetrahedral coordination around the O atoms of the crystal water molecules. In summary, we have described the synthesis and structural characterization of a nine coordinated strontium 4-nitrobenzoate complex, which functions as a molecular container for encapsulating a water dimer.

Experimental

A mixture of strontium carbonate (1.476 g, 10 mmol) and 4-nitrobenzoic acid (4-nbaH) (3.34 g, 20 mmol) was taken in water (50 ml) and heated on a steam bath. The insoluble starting materials slowly started dissolving accompanied with brisk effervescence of CO_2. The heating of the reaction mixture was stopped when there was no more evolution of CO_2. At this stage, the reaction mixture was almost clear and the pH was close to neutral. The hot solution was filtered and the filtrate was left undisturbed for 3–4 days. The colorless crystalline blocks that separated were filtered, washed thoroughly with ether and dried in air. Yield: 75%. The crystalline blocks thus obtained were suitable for X-ray diffraction studies.

Refinement

H atoms bonded to the O atoms were located in a difference map and refined with distance restraints of O—H = 0.82 (2) Å. The H atoms on the aromatic ring were positioned geometrically and refined using a riding model, C—H = 0.93 Å and U_{iso}(H) = 1.2U_{iso}(C). The largest peak in the residual electron density map of 0.32 e Å^{-3} is located at a distance of 1.01 Å from Sr1 and the deepest hole of −0.33 e Å^{-3} is located at a distance of 1.26 Å from C5.

Figures

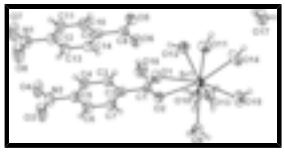


Fig. 1. A view of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

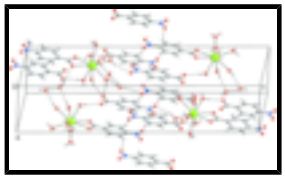


Fig. 2. The crystal packing diagram for (I) viewed along the *b* axis. O—H···O and C—H···O bonds are shown as dashed and dotted lines respectively. For symmetry codes see Table 2.

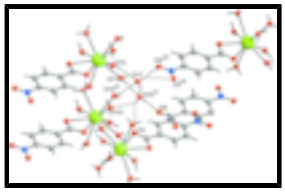


Fig. 3. A view of the surroundings of the water dimer showing it linking to four complex cations and an anion with the aid of O—H···O bonds (dashed lines). For symmetry codes see Table 2.

Heptaaqua(4-nitrobenzoato-κ^2*O*,*O*^{1})strontium(II) 4-nitrobenzoate dihydrate

Crystal data

$[Sr(C_7H_4NO_4)(H_2O)_7](C_7H_4NO_4)\cdot 2H_2O$	F_{000} = 1192
M_r = 581.99	D_x = 1.626 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6400 reflections
a = 6.7364 (7) Å	θ = 2.2–25.9º

b = 11.1705 (12) Å	μ = 2.35 mm^{-1}
c = 31.738 (3) Å	T = 293 (2) K
β = 95.568 (2)º	Block, colourless
V = 2377.0 (4) Å^3	0.42 × 0.36 × 0.12 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4604 independent reflections
Radiation source: fine-focus sealed tube	3777 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 293(2) K	θ_{max} = 25.9º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -7 \rightarrow 8$
T_{min} = 0.375, T_{max} = 0.761	$k = -13 \rightarrow 13$
11962 measured reflections	$l = -39 \rightarrow 30$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.067	$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.004
4604 reflections	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
370 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0025 (3)	0.65965 (18)	0.18550 (7)	0.0300 (4)
C2	−0.0562 (3)	0.66764 (18)	0.13846 (6)	0.0301 (5)
C3	−0.0877 (3)	0.77767 (18)	0.11883 (7)	0.0327 (5)
H3	−0.0742	0.8474	0.1349	0.039*
C4	−0.1389 (3)	0.7850 (2)	0.07570 (7)	0.0362 (5)
H4	−0.1614	0.8588	0.0625	0.043*
C5	−0.1557 (3)	0.6806 (2)	0.05288 (7)	0.0362 (5)
C6	−0.1257 (4)	0.5696 (2)	0.07123 (7)	0.0441 (6)
H6	−0.1391	0.5003	0.0550	0.053*
C7	−0.0754 (3)	0.56418 (19)	0.11419 (7)	0.0388 (5)
H7	−0.0538	0.4901	0.1272	0.047*
C8	0.4166 (3)	0.8073 (2)	0.14200 (7)	0.0339 (5)
C9	0.3714 (3)	0.80910 (18)	0.09441 (7)	0.0324 (5)
C10	0.3370 (4)	0.9169 (2)	0.07315 (7)	0.0459 (6)
H10	0.3425	0.9882	0.0883	0.055*
C11	0.2950 (4)	0.9193 (2)	0.02994 (8)	0.0517 (7)
H11	0.2727	0.9915	0.0157	0.062*
C12	0.2867 (4)	0.8128 (2)	0.00817 (7)	0.0431 (6)
C13	0.3197 (3)	0.7048 (2)	0.02820 (7)	0.0420 (6)
H13	0.3132	0.6339	0.0128	0.050*
C14	0.3625 (3)	0.7033 (2)	0.07153 (7)	0.0365 (5)
H14	0.3856	0.6307	0.0855	0.044*
N1	0.2398 (4)	0.8156 (2)	−0.03805 (7)	0.0609 (6)
N2	−0.2068 (3)	0.6866 (2)	0.00693 (6)	0.0498 (5)
O5	0.4273 (2)	0.90757 (14)	0.16036 (5)	0.0431 (4)
O6	0.4421 (2)	0.70920 (15)	0.15994 (5)	0.0461 (4)
O7	0.2177 (4)	0.9120 (2)	−0.05542 (6)	0.0964 (8)
O8	0.2234 (4)	0.7223 (2)	−0.05699 (6)	0.0997 (9)
O1	0.0180 (2)	0.75470 (13)	0.20659 (4)	0.0392 (4)
O2	0.0360 (2)	0.55860 (12)	0.20171 (5)	0.0402 (4)
O3	−0.2349 (4)	0.5945 (2)	−0.01283 (6)	0.0863 (7)
O4	−0.2209 (3)	0.78452 (18)	−0.01001 (6)	0.0704 (6)
O9	−0.2271 (2)	0.51563 (14)	0.27570 (6)	0.0403 (4)
H9B	−0.2154	0.4631	0.2581	0.060*
O10	−0.2163 (3)	0.80181 (16)	0.28840 (6)	0.0459 (4)
H10A	−0.2205	0.8522	0.2696	0.069*
O11	0.2215 (3)	0.87224 (15)	0.30012 (6)	0.0435 (4)
O12	0.4433 (3)	0.67180 (18)	0.24718 (6)	0.0427 (4)
O13	0.2293 (3)	0.43788 (14)	0.28746 (5)	0.0403 (4)
O14	0.4076 (3)	0.63574 (16)	0.34331 (6)	0.0612 (5)
H14A	0.4470	0.5662	0.3445	0.092*
O15	−0.0202 (4)	0.6336 (3)	0.35732 (7)	0.0664 (6)
O16	0.4203 (3)	0.4644 (2)	0.15802 (7)	0.0553 (5)
O17	0.6857 (4)	0.7745 (2)	0.39513 (8)	0.0719 (6)
Sr1	0.10618 (3)	0.655680 (16)	0.282763 (6)	0.02839 (7)

H9A	−0.269 (5)	0.483 (3)	0.2954 (9)	0.082 (11)*
H11A	0.142 (4)	0.922 (3)	0.3055 (9)	0.067 (10)*
H11B	0.326 (4)	0.895 (2)	0.3127 (9)	0.061 (9)*
H15B	0.072 (6)	0.626 (3)	0.3754 (13)	0.102 (15)*
H15A	−0.085 (6)	0.679 (3)	0.3650 (13)	0.108 (18)*
H17B	0.654 (7)	0.841 (4)	0.3855 (15)	0.13 (2)*
H17A	0.688 (6)	0.781 (4)	0.4196 (14)	0.125 (18)*
H14B	0.467 (4)	0.677 (2)	0.3609 (8)	0.079 (11)*
H13A	0.159 (5)	0.382 (3)	0.2930 (9)	0.075 (10)*
H13B	0.338 (4)	0.421 (2)	0.2993 (8)	0.055 (9)*
H12B	0.519 (4)	0.624 (3)	0.2511 (9)	0.059 (10)*
H12A	0.445 (4)	0.687 (2)	0.2224 (9)	0.059 (9)*
H16B	0.423 (5)	0.538 (3)	0.1557 (10)	0.082 (12)*
H16A	0.336 (6)	0.451 (3)	0.1718 (13)	0.113 (17)*
H10B	−0.321 (3)	0.767 (3)	0.2836 (9)	0.086 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0265 (10)	0.0321 (11)	0.0310 (11)	−0.0017 (9)	0.0018 (8)	0.0019 (10)
C2	0.0284 (11)	0.0337 (12)	0.0285 (11)	−0.0005 (9)	0.0039 (9)	0.0015 (9)
C3	0.0364 (12)	0.0293 (11)	0.0325 (12)	0.0022 (9)	0.0047 (9)	0.0006 (9)
C4	0.0380 (12)	0.0368 (12)	0.0337 (12)	0.0034 (10)	0.0037 (10)	0.0091 (10)
C5	0.0369 (12)	0.0455 (14)	0.0262 (12)	−0.0009 (10)	0.0027 (9)	0.0004 (9)
C6	0.0593 (16)	0.0380 (13)	0.0348 (13)	−0.0038 (11)	0.0034 (11)	−0.0054 (10)
C7	0.0521 (14)	0.0296 (12)	0.0343 (13)	−0.0019 (10)	0.0026 (11)	0.0014 (9)
C8	0.0271 (11)	0.0411 (13)	0.0337 (12)	−0.0045 (9)	0.0032 (9)	−0.0011 (10)
C9	0.0297 (11)	0.0365 (12)	0.0313 (12)	−0.0042 (9)	0.0039 (9)	−0.0004 (9)
C10	0.0643 (17)	0.0350 (13)	0.0372 (14)	−0.0051 (11)	−0.0009 (12)	−0.0025 (10)
C11	0.0748 (19)	0.0381 (14)	0.0403 (15)	−0.0098 (13)	−0.0032 (13)	0.0074 (11)
C12	0.0509 (15)	0.0492 (15)	0.0288 (12)	−0.0097 (11)	0.0015 (11)	0.0016 (10)
C13	0.0495 (15)	0.0411 (13)	0.0356 (13)	−0.0047 (11)	0.0058 (11)	−0.0069 (10)
C14	0.0382 (13)	0.0357 (12)	0.0356 (13)	−0.0017 (10)	0.0045 (10)	0.0029 (10)
N1	0.0832 (18)	0.0640 (16)	0.0341 (12)	−0.0151 (13)	−0.0012 (12)	0.0012 (11)
N2	0.0570 (14)	0.0632 (15)	0.0283 (11)	0.0036 (11)	−0.0002 (9)	0.0029 (10)
O5	0.0516 (10)	0.0400 (9)	0.0370 (9)	−0.0074 (8)	0.0007 (7)	−0.0082 (7)
O6	0.0618 (11)	0.0411 (9)	0.0351 (9)	0.0020 (8)	0.0028 (8)	0.0046 (7)
O7	0.177 (3)	0.0686 (15)	0.0390 (12)	−0.0140 (15)	−0.0123 (13)	0.0131 (11)
O8	0.185 (3)	0.0688 (15)	0.0414 (12)	−0.0109 (16)	−0.0064 (14)	−0.0147 (11)
O1	0.0497 (9)	0.0342 (8)	0.0325 (8)	0.0096 (7)	−0.0020 (7)	−0.0043 (7)
O2	0.0540 (10)	0.0303 (8)	0.0348 (9)	−0.0070 (7)	−0.0042 (7)	0.0078 (7)
O3	0.147 (2)	0.0734 (14)	0.0348 (11)	−0.0045 (15)	−0.0093 (12)	−0.0123 (10)
O4	0.1043 (16)	0.0692 (13)	0.0357 (10)	0.0078 (12)	−0.0026 (10)	0.0147 (10)
O9	0.0466 (10)	0.0359 (9)	0.0395 (10)	−0.0014 (7)	0.0098 (8)	−0.0003 (7)
O10	0.0447 (11)	0.0459 (10)	0.0472 (11)	−0.0064 (8)	0.0047 (8)	0.0012 (8)
O11	0.0421 (11)	0.0333 (9)	0.0537 (11)	0.0034 (8)	−0.0023 (9)	−0.0089 (8)
O12	0.0402 (10)	0.0512 (11)	0.0367 (10)	0.0046 (8)	0.0040 (8)	0.0055 (8)
O13	0.0430 (11)	0.0288 (9)	0.0465 (10)	−0.0039 (8)	−0.0091 (8)	0.0071 (7)

O14	0.0736 (13)	0.0458 (11)	0.0575 (12)	0.0136 (10)	−0.0279 (10)	−0.0138 (9)
O15	0.0657 (15)	0.0956 (18)	0.0375 (11)	0.0094 (13)	0.0033 (11)	0.0013 (11)
O16	0.0553 (13)	0.0501 (13)	0.0602 (13)	0.0011 (10)	0.0048 (10)	0.0121 (10)
O17	0.0935 (17)	0.0756 (17)	0.0451 (14)	0.0017 (13)	−0.0016 (12)	−0.0117 (12)
Sr1	0.03358 (12)	0.02477 (11)	0.02640 (11)	−0.00023 (8)	0.00075 (8)	0.00064 (8)

Geometric parameters (Å, °)

C1—O2	1.252 (2)	N1—O7	1.212 (3)
C1—O1	1.254 (2)	N2—O3	1.210 (3)
C1—C2	1.509 (3)	N2—O4	1.219 (2)
C1—Sr1	3.098 (2)	O1—Sr1	2.6723 (14)
C2—C3	1.385 (3)	O2—Sr1	2.7893 (15)
C2—C7	1.388 (3)	O9—Sr1	2.7277 (16)
C3—C4	1.381 (3)	O9—H9B	0.8200
C3—H3	0.9300	O9—H9A	0.80 (3)
C4—C5	1.372 (3)	O10—Sr1	2.7367 (17)
C4—H4	0.9300	O10—H10A	0.8200
C5—C6	1.376 (3)	O10—H10B	0.806 (18)
C5—N2	1.467 (3)	O11—Sr1	2.5838 (17)
C6—C7	1.374 (3)	O11—H11A	0.80 (3)
C6—H6	0.9300	O11—H11B	0.82 (3)
C7—H7	0.9300	O12—Sr1	2.6387 (18)
C8—O6	1.240 (3)	O12—H12B	0.74 (3)
C8—O5	1.261 (3)	O12—H12A	0.81 (3)
C8—C9	1.512 (3)	O13—Sr1	2.5702 (16)
C9—C14	1.385 (3)	O13—H13A	0.82 (3)
C9—C10	1.389 (3)	O13—H13B	0.81 (3)
C10—C11	1.373 (3)	O14—Sr1	2.6662 (18)
C10—H10	0.9300	O14—H14A	0.8200
C11—C12	1.374 (3)	O14—H14B	0.801 (17)
C11—H11	0.9300	O15—Sr1	2.603 (2)
C12—C13	1.371 (3)	O15—H15B	0.81 (4)
C12—N1	1.470 (3)	O15—H15A	0.73 (4)
C13—C14	1.377 (3)	O16—H16B	0.82 (3)
C13—H13	0.9300	O16—H16A	0.76 (4)
C14—H14	0.9300	O17—H17B	0.82 (4)
N1—O8	1.203 (3)	O17—H17A	0.78 (4)
O2—C1—O1	122.79 (19)	H11A—O11—H11B	104 (3)
O2—C1—C2	118.64 (18)	Sr1—O12—H12B	119 (2)
O1—C1—C2	118.57 (18)	Sr1—O12—H12A	122 (2)
O2—C1—Sr1	64.11 (11)	H12B—O12—H12A	104 (3)
O1—C1—Sr1	58.75 (10)	Sr1—O13—H13A	124 (2)
C2—C1—Sr1	176.64 (14)	Sr1—O13—H13B	121.3 (19)
C3—C2—C7	119.17 (19)	H13A—O13—H13B	103 (3)
C3—C2—C1	120.75 (18)	Sr1—O14—H14A	109.5
C7—C2—C1	120.07 (18)	Sr1—O14—H14B	138 (2)
C4—C3—C2	120.8 (2)	H14A—O14—H14B	112.1
C4—C3—H3	119.6	Sr1—O15—H15B	111 (3)

C2—C3—H3	119.6	Sr1—O15—H15A	120 (3)
C5—C4—C3	118.2 (2)	H15B—O15—H15A	106 (4)
C5—C4—H4	120.9	H16B—O16—H16A	106 (3)
C3—C4—H4	120.9	H17B—O17—H17A	106 (4)
C4—C5—C6	122.8 (2)	O13—Sr1—O11	141.74 (6)
C4—C5—N2	119.1 (2)	O13—Sr1—O15	89.42 (8)
C6—C5—N2	118.1 (2)	O11—Sr1—O15	90.74 (7)
C7—C6—C5	118.1 (2)	O13—Sr1—O12	78.64 (6)
C7—C6—H6	120.9	O11—Sr1—O12	76.93 (6)
C5—C6—H6	120.9	O15—Sr1—O12	140.05 (8)
C6—C7—C2	121.0 (2)	O13—Sr1—O14	70.13 (6)
C6—C7—H7	119.5	O11—Sr1—O14	74.47 (6)
C2—C7—H7	119.5	O15—Sr1—O14	68.30 (8)
O6—C8—O5	125.0 (2)	O12—Sr1—O14	71.78 (7)
O6—C8—C9	118.42 (19)	O13—Sr1—O1	119.10 (5)
O5—C8—C9	116.56 (19)	O11—Sr1—O1	80.86 (5)
C14—C9—C10	119.2 (2)	O15—Sr1—O1	142.93 (7)
C14—C9—C8	120.46 (19)	O12—Sr1—O1	73.11 (6)
C10—C9—C8	120.31 (19)	O14—Sr1—O1	140.66 (6)
C11—C10—C9	120.7 (2)	O13—Sr1—O9	73.76 (6)
C11—C10—H10	119.6	O11—Sr1—O9	141.49 (6)
C9—C10—H10	119.6	O15—Sr1—O9	71.40 (7)
C10—C11—C12	118.6 (2)	O12—Sr1—O9	137.70 (5)
C10—C11—H11	120.7	O14—Sr1—O9	125.06 (6)
C12—C11—H11	120.7	O1—Sr1—O9	93.11 (5)
C13—C12—C11	122.1 (2)	O13—Sr1—O10	144.55 (6)
C13—C12—N1	119.4 (2)	O11—Sr1—O10	69.62 (6)
C11—C12—N1	118.5 (2)	O15—Sr1—O10	70.45 (8)
C12—C13—C14	118.9 (2)	O12—Sr1—O10	135.13 (6)
C12—C13—H13	120.6	O14—Sr1—O10	123.81 (6)
C14—C13—H13	120.6	O1—Sr1—O10	72.79 (5)
C13—C14—C9	120.5 (2)	O9—Sr1—O10	72.26 (5)
C13—C14—H14	119.8	O13—Sr1—O2	73.16 (5)
C9—C14—H14	119.8	O11—Sr1—O2	125.53 (5)
O8—N1—O7	122.7 (2)	O15—Sr1—O2	139.50 (7)
O8—N1—C12	118.7 (2)	O12—Sr1—O2	73.00 (5)
O7—N1—C12	118.5 (2)	O14—Sr1—O2	132.94 (5)
O3—N2—O4	122.2 (2)	O1—Sr1—O2	47.45 (4)
O3—N2—C5	119.2 (2)	O9—Sr1—O2	68.71 (5)
O4—N2—C5	118.7 (2)	O10—Sr1—O2	103.16 (5)
C1—O1—Sr1	97.60 (12)	O13—Sr1—C1	96.41 (5)
C1—O2—Sr1	92.07 (12)	O11—Sr1—C1	103.48 (6)
Sr1—O9—H9B	109.5	O15—Sr1—C1	147.67 (7)
Sr1—O9—H9A	123 (2)	O12—Sr1—C1	72.11 (6)
H9B—O9—H9A	105.9	O14—Sr1—C1	143.28 (6)
Sr1—O10—H10A	109.5	O1—Sr1—C1	23.65 (4)
Sr1—O10—H10B	113 (2)	O9—Sr1—C1	79.76 (5)
H10A—O10—H10B	103.0	O10—Sr1—C1	87.30 (5)
Sr1—O11—H11A	120 (2)	O2—Sr1—C1	23.82 (4)

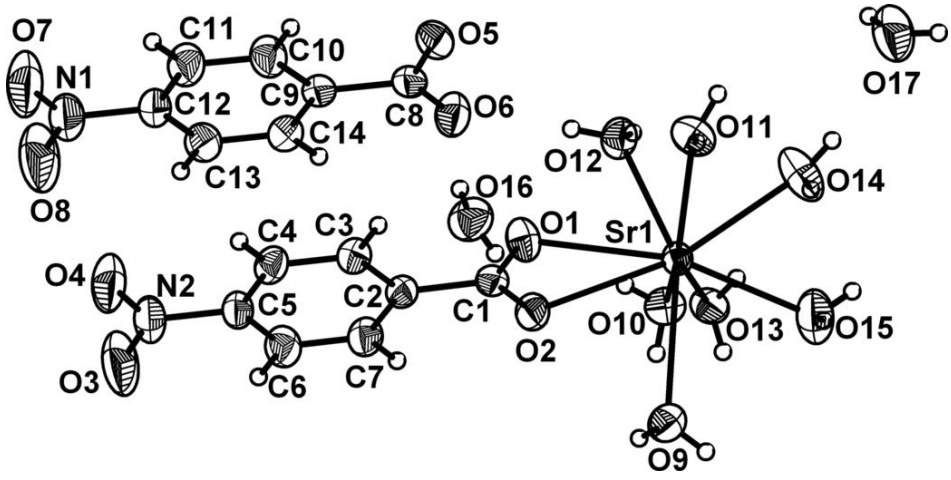
Sr1—O11—H11B	129 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9B···O11^{i}	0.82	2.10	2.894 (2)	162
O10—H10A···O13^{ii}	0.82	2.04	2.841 (2)	165
O14—H14A···O5^{iii}	0.82	1.98	2.788 (2)	170
O9—H9A···O5^{i}	0.80 (3)	2.03 (3)	2.815 (2)	169 (3)
O11—H11A···O2^{ii}	0.80 (3)	1.95 (3)	2.707 (2)	160 (3)
O11—H11B···O16^{iv}	0.82 (3)	2.02 (3)	2.833 (3)	176 (3)
O15—H15B···O7^{v}	0.81 (4)	2.35 (4)	3.104 (3)	154 (4)
O15—H15A···O17^{vi}	0.73 (4)	2.17 (4)	2.881 (4)	165 (4)
O17—H17B···O16^{iv}	0.82 (4)	1.98 (4)	2.761 (4)	158 (4)
O17—H17A···O4^{vii}	0.78 (4)	2.37 (4)	3.087 (3)	153 (4)
O17—H17A···O3^{vii}	0.78 (4)	2.57 (4)	3.264 (3)	150 (4)
O14—H14B···O17	0.801 (17)	2.06 (2)	2.831 (3)	163 (3)
O13—H13A···O1^{i}	0.82 (3)	1.85 (3)	2.657 (2)	168 (3)
O13—H13B···O5^{iii}	0.81 (3)	1.94 (3)	2.732 (2)	164 (3)
O12—H12B···O9^{viii}	0.74 (3)	2.18 (3)	2.899 (3)	165 (3)
O12—H12A···O6	0.81 (3)	2.00 (3)	2.799 (2)	175 (3)
O16—H16B···O6	0.82 (3)	1.93 (3)	2.739 (3)	171 (3)
O16—H16A···O10^{i}	0.76 (4)	2.28 (4)	2.921 (3)	141 (4)
O16—H16A···O2	0.76 (4)	2.61 (4)	3.229 (3)	140 (4)
O10—H10B···O12^{vi}	0.806 (18)	2.15 (2)	2.915 (3)	158 (3)
C4—H4···O7^{ix}	0.93	2.60	3.476 (3)	158
C11—H11···O4^{ix}	0.93	2.53	3.396 (3)	155
C6—H6···O8^{x}	0.93	2.55	3.349 (3)	144

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) −*x*, *y*+1/2, −*z*+1/2; (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2; (v) *x*, −*y*+3/2, *z*+1/2; (vi) *x*−1, *y*, *z*; (vii) *x*+1, −*y*+3/2, *z*+1/2; (viii) *x*+1, *y*, *z*; (ix) −*x*, −*y*+2, −*z*; (x) −*x*, −*y*+1, −*z*.

Fig. 1


O7
C11
C10
O5
N1
C12
C9
C8
O6
C14
C13
O8
O17
O12
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O14
O16
O1
Sr1
C4
C3
O4
N2
C5
C2
C1
O10
O13
O15
O2
O3
C6
C7
O9

Fig. 2

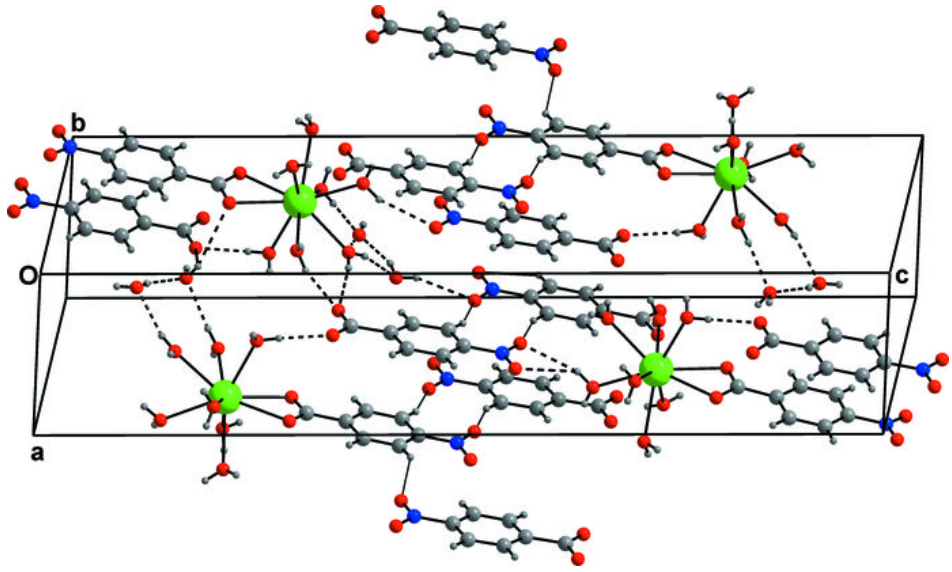

Fig. 3