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Alkaline earth metal salts of 1-naphthoic acid

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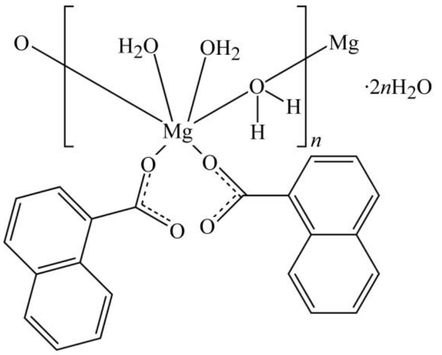
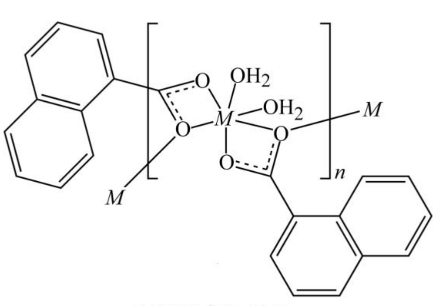
The structures of the Mg, Ca, Sr and Ba salts of 1-naphthoic acid are examined and compared with analogous structures of salts of benzoate derivatives. It is shown that *catena*-poly[[[diaquabis(1-naphthoato-κO)magnesium(II)]-μ-aqua] dihydrate], $\{[\mathrm{Mg(C_{11}H_7O_2)_2(H_2O)_3}]\cdot 2\mathrm{H_2O}\}_n$, exists as a one-dimensional coordination polymer that propagates only through Mg—OH$_2$—Mg interactions along the crystallographic *b* direction. In contrast with related benzoate salts, the naphthalene systems are large enough to prevent inorganic chain-to-chain interactions, and thus species with inorganic channels rather than layers are formed. The Ca, Sr and Ba salts all have metal centres that lie on a twofold axis ($Z' = \frac{1}{2}$) and all have the common name *catena*-poly[[diaquametal(II)]-bis(μ-1-naphthoato)-$\kappa^3O,O':O;\kappa^3O:O,O'$], $[M(\mathrm{C_{11}H_7O_2})_2(\mathrm{H_2O})_2]_n$, where M = Ca, Sr or Ba. The Ca and Sr salts are essentially isostructural, and all three species form one-dimensional coordination polymers through a carboxylate group that forms three M—O bonds. The polymeric chains propagate *via* *c*-glide planes and through *MOMO* four-membered rings. Again, inorganic channel structures are formed rather than layered structures, and the three structures are similar to those found for Ca and Sr salicylates and other substituted benzoates.

Comment

Salt forms of active pharmaceutical ingregients (APIs) are commonly investigated as a simple route to altering the physicochemical properties of the API (Stahl & Wermuth, 2002) whilst, it is hoped, not changing its fundamental underlying biological activity [see Zhao *et al.* (2010) for an example of possible unforeseen consequences resulting from salt choice]. Many of the performance-critical properties of an API (such as solubility, melting point and hygroscopicity) are dependant upon its solid-state structure, and thus a true understanding of structure–property relationships should allow the most appropriate counter-ion to be chosen for any given desired property. However, structure–property relationships of this type are poorly understood, and thus salt selection of API forms is currently undertaken using time-consuming trial-and-error methods (Stahl & Wermuth, 2002). One reason for the lack of understanding is a general dearth of large groups of systematically related crystal structures of salt forms with associated phase-specific physicochemical data. Some such studies do exist (for example, Collier *et al.*, 2006; Black *et al.*, 2007; Kennedy *et al.*, 2011) but they are relatively uncommon. As a contribution to this field, Arlin *et al.* (2011) showed that the Mg, Ca and Sr (but not Ba) salt forms of a set of simple benzoate-derived anions could be systematically structurally classified, and that these structural features helped to rationalize comparative aqueous solubility data. This work was later extended to phenylacetic acid (Arlin *et al.*, 2012). A major aim of this earlier work was to use the lessons learned from simple model compounds to predict behaviour in larger commercial APIs with similar functionality. Many APIs have carboxylate groups and six-membered aryl rings (*e.g.* profens, aspirin), as do the reported model benzoate structures. However, several important drug classes (*e.g.* naproxens, fluoroquinolones) have larger fused aromatic groups and this structural feature was not included in the model data set. To help fill this gap, the Mg, Ca, Sr and Ba complexes of 1-naphthoate (NPH) have now been investigated in order to investigate what effects the extra bulk of the aromatic region has on crystal stucture, and the results are presented here (Mg-, Ca-, Sr and BaNPH). Naphthalene derivatives with multiple carboxylate groups have been structurally examined (see, for example, Fitzgerald & Gerkin, 1994; Senkovska, 2006), but the only such simple Group 2 metal salt with a monocarboxylate naphthoate to have been structurally characterized to date is the Mg salt of 1-hydroxy-2-naphthoic acid (Huang & Song, 2008).



MgNPH



CaNPH (M = Ca)
SrNPH (M = Sr)
BaNPH (M = Ba)

doi:10.1107/S0108270112030399

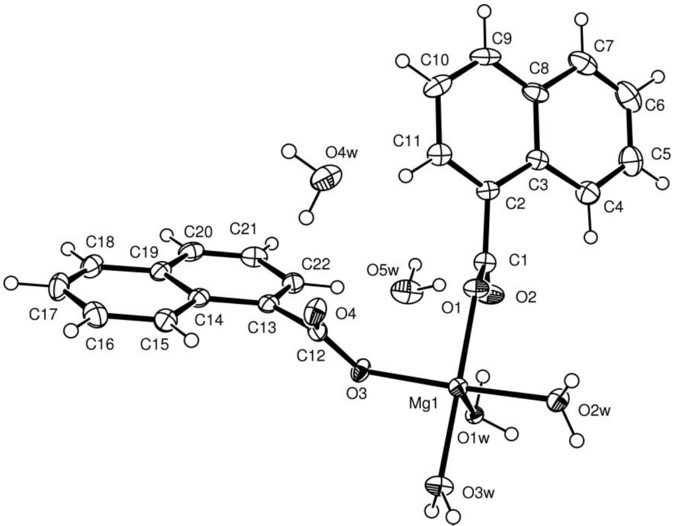


Figure 1
The contents of the asymmetric unit of MgNPH, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

MgNPH has the formula $\{[Mg(NPH)_2(H_2O)_3]\cdot 2H_2O\}_n$ (Fig. 1) and has an approximately octahedral metal centre. The NPH ligands are mutually *cis* [O3—Mg—O1 = 87.58 (8)°] and each bonds to Mg through only one of its carboxylate O atoms, with the other O atom taking part only in hydrogen-bonding interactions. The C—O distances involving the non-metal-bound O atoms are approximately 0.02 Å shorter than those of the metal-bound O atoms (Table 1). Such large variations in C—O bond lengths are not found for the Ca, Sr or Ba salts (see below), which all have η^2- rather than η^1-COO bonding modes. Two of the water ligands are also terminal but the third, O1*W*, acts as a bridge between metal centres. Table 1 shows that the bridging Mg—O bonds are approximately 0.17 Å longer than the terminal bonds. The bridging water ligands are *trans* to one another [O1—Mg—O1$W^{\rm i}$ = 177.47 (5)°; symmetry code: (i) $-x$, $y - \frac{1}{2}$, $-z + \frac{1}{2}$] and this results in a one-dimensional coordination chain based on $Mg—OH_2—Mg$ units which propagates along the crystallographic *b* direction (Fig. 2). In contrast, the Mg salt of 1-hydroxy-2-naphthoic acid reported by Huang & Song (2008) is a discrete $[Mg(L)_2(H_2O)_4]$ complex.

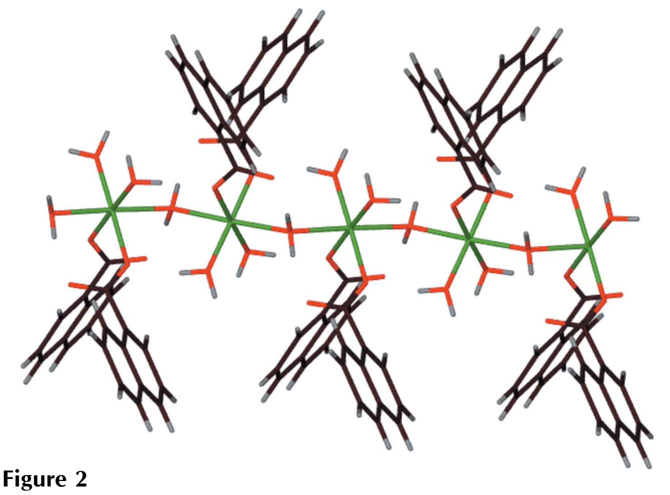


Figure 2
Part of the one-dimensional coordination polymer found in MgNPH. The polymer chain is parallel to the crystallographic *b* direction. The noncoordinated water molecules are not shown.

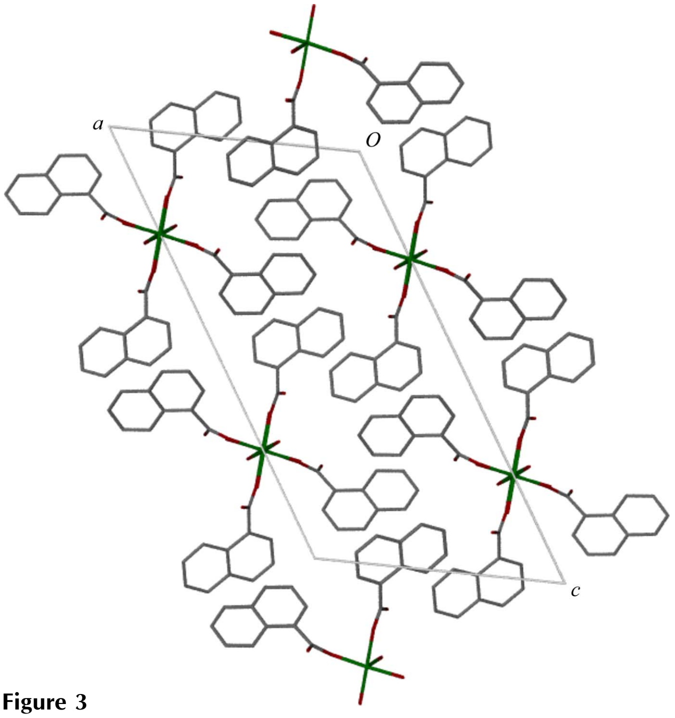


Figure 3
The packing mode of MgNPH, viewed down *b*, showing that each hydrophilic inorganic chain is separated from the others by hydrophobic organic groups.

Previous work has shown that a common motif for magnesium salts of carboxylate ions with no good hydrogen-bonding substituents (*e.g.* benzoate, halobenzoates and phenylacetate) is a one-dimensional coordination polymer that packs to give alternating inorganic layers and organic bilayers (Arlin *et al.*, 2011, 2012). Although also a one-dimensional polymer, the structure of MgNPH differs from those of these smaller anions in significant ways. Firstly, for the benzene-based species, the carboxylate group is found to be the bridging ligand, not water as in MgNPH. Indeed, a search of the Cambridge Structural Database (Version 5.33; Allen, 2002) found no other structure of an Mg salt of an aryl carboxylate anion that bridges through water and not through the carboxylate group. Secondly, as shown in Fig. 3, the structure of MgNPH does not contain an inorganic layer. Instead, the one-dimensional chains are isolated from each other by the organic groups. With smaller anions, the inorganic layers tend to be formed by hydrogen bonding between the inorganic chains. Here, the larger naphthalene group seems to have a fundamental effect on the packing structure by separating these chains. The presence of large nonpolar groups may also explain why two of the H atoms of the water molecules do not act as traditional hydrogen-bond donors (Table 2).

The structures of CaNPH and SrNPH were found to be essentially isostructural, with the composition $[M(NPH)_2(H_2O)_2]_n$ (Figs. 4 and 5). This reflects the structures of the benzoate and phenylacetate derivatives, where the Ca and Sr

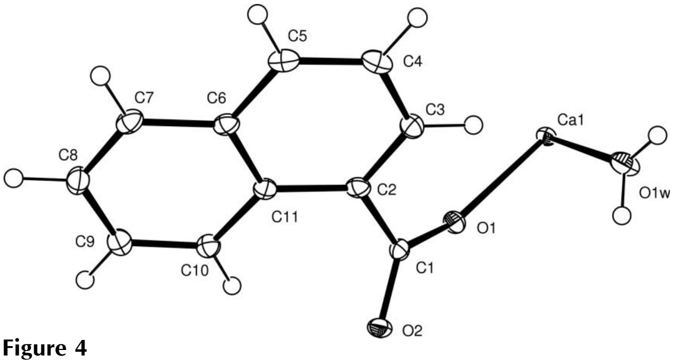


Figure 4
The contents of the asymmetric unit of CaNPH, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

structures were found to have similar structural types and even (for salicylate, 4-aminosalicylate, 4-aminobenzoate and phenylacetate) to form isostructural pairs. In both CaNPH and SrNPH, the metal centre lies on a twofold axis and is formally eight-coordinate though, as Cotton & Bergman (1964) classically showed, if each chelated group is assigned to one coordination site rather than two, then the structures can be described as distorted octahedral (Tables 3 and 5). The water ligands are terminal and *trans* to the chelated carboxylate groups [O1W—M···C1 = 168.66 (5) and 167.13 (8)° for CaNPH and SrNPH, respectively]. The NPH anions use both their O atoms to chelate to one metal centre, and one O atom of each ligand then bridges to a further metal centre. Thus, it is this coordination mode of the carboxylate (and not water as in MgNPH) that leads to the propagation of a one-dimensional coordination polymer based on perfectly planar $MOMO$ rings along the c-glide plane (Fig. 6). The aromatic rings form dihedral angles of 46.68 (5) and 44.59 (10)° with the CaOCaO and SrOSrO rings, respectively.

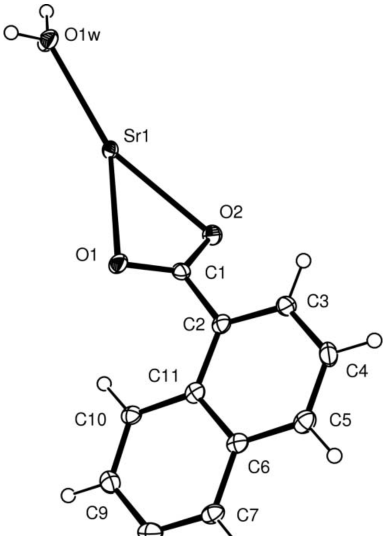


Figure 5
The contents of the asymmetric unit of SrNPH, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

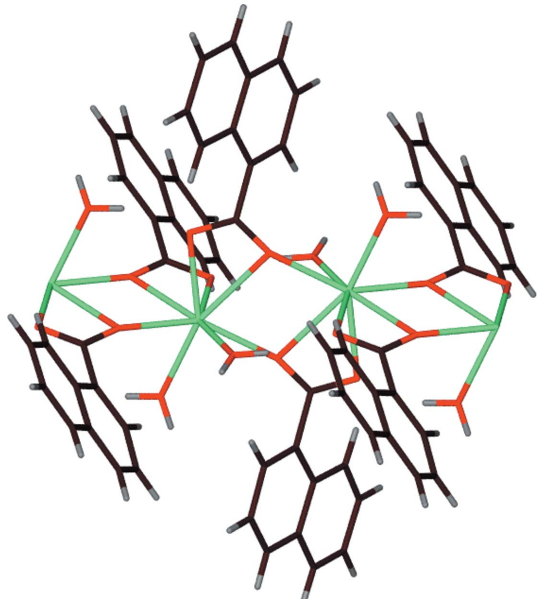


Figure 6
Part of the one-dimensional coordination polymer found in CaNPH. The polymer propagates in the crystallographic c direction. SrNPH is isostructural.

As with MgNPH above, the one-dimensional polymers in the Ca and Sr salts do not interact to form the two-dimensional sheets seen for the equivalent benzoate and phenylacetate structures (Senkovska & Thewalt, 2005; Arlin *et al.*, 2011, 2012). However, both the geometry of the coordination polymer and the packing motif with inorganic channels shown in Fig. 7 are the same as those found in a second class of Ca and Sr salt structures of benzoate derivatives, but oddly this

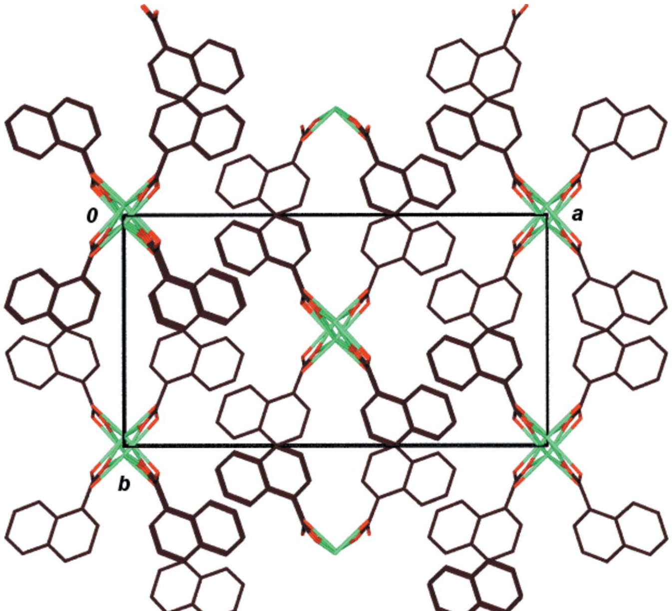


Figure 7
The packing structure of CaNPH, viewed along the length of the coordination polymer. SrNPH is isostructural. H atoms have been omitted for clarity.

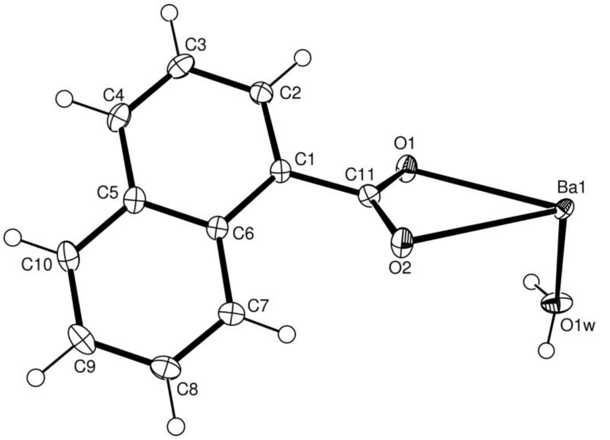


Figure 8
The contents of the asymmetric unit of BaNPH, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

class of structure was observed previously only with benzoates containing hydrogen-bonding substituents, especially salicylate and 2-nitrobenzoate (Debuyst *et al.*, 1979; Arlin *et al.*, 2011).

Crystals of BaNPH (Fig. 8) formed as very thin plates (approximately 0.005 mm) which required the use of synchrotron radiation for characterization. It was found to have the same [$M(\mathrm{NPH})_2(\mathrm{H_2O})_2$] composition, and indeed the same coordination geometry (Table 7), the same polymeric one-dimensional coordination arrangement and the same packing mode featuring inorganic channels, as the Ca and Sr salts, though it is not isostructural with them. The dihedral angle between the *MOMO* plane and the aromatic plane [39.48 (9) °] is slightly less than in the Ca or Sr salts. The Ba ions again lie on a twofold rotation axis and the coordination polymer propagates along the crystallographic *c* direction. The similarity of the structure of BaNPH to the structures of CaNPH and SrNPH is somewhat unusual as, of the nine families of Group 2 metal salts of benzoate anions described by Arlin *et al.*, (2011), only the Ba salt of 4-chlorobenzoate had a structure that was somewhat similar to its lighter analogues. All other Ba salts were found to be structurally varied and distinct. Finally, it is noted that each water molecule in the Ca, Sr and Ba salt structures uses only one H atom as a hydrogen-bond donor (Tables 4, 6 and 8).

In summary, whereas phenylacetate, with its additional Csp^3 atom between the aryl and –COO groups, was found to have Mg, Ca and Sr salt structures that were closely related to those found for analogous benzoate and halobenzoate salts (Arlin *et al.*, 2011, 2012), adding a larger aromatic fragment in the shape of naphthalene was found to give different structural types. The structure of MgNPH has an unusual motif based on Mg—OH$_2$—Mg bridging and a change to the packing structure that can be understood in terms of the large nonpolar parts of the naphthoate anions preventing the polar/inorganic chains from hydrogen bonding with each other. The Ca, Sr and Ba salts of naphthoate all have similar one-dimensional polymeric coordination structures and similar packing modes. Again, the large size of the naphthoate fragments appears to prevent the one-dimensional inorganic chains from aggregating, but intriguingly the resulting structures are now of a type previously seen for Ca and Sr salts of salicylate and other benzoate derivatives with extra (rather than fewer) polar or hydrogen-bond-forming substituents.

Experimental

All samples were prepared by slowly adding a slight excess of an aqueous solution of the appropriate metal carbonate to a stirred aqueous slurry of 1-naphthoic acid. The solutions were heated gently to achieve complete dissolution of the solids. The volumes of the resulting clear solutions were reduced until white precipitates were deposited; these were collected by filtration. Colourless crystals suitable for single-crystal diffraction studies were obtained by recrystallization of the samples from warm water.

MgNPH

Crystal data

$[\mathrm{Mg(C_{11}H_7O_2)_2(H_2O)_3}]\cdot 2\mathrm{H_2O}$
$M_r = 456.72$
Monoclinic, $P2_1/c$
$a = 12.8896\ (4)$ Å
$b = 8.0048\ (2)$ Å
$c = 24.5300\ (5)$ Å
$\beta = 121.190\ (1)°$

$V = 2165.13\ (10)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.13$ mm^{-1}
$T = 123$ K
$0.15 \times 0.13 \times 0.03$ mm

Data collection

Nonius KappaCCD area-detector diffractometer
8977 measured reflections

4968 independent reflections
2744 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.078$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.150$
$S = 1.02$
4968 reflections
319 parameters
15 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.43$ e Å^{-3}

Table 1
Selected bond lengths (Å) for MgNPH.

Mg1—O3*W*	2.016 (2)	Mg1—O1	2.069 (2)
Mg1—O2*W*	2.028 (2)	Mg1—O1*W*$^{\mathrm{i}}$	2.195 (2)
Mg1—O3	2.058 (2)	Mg1—O1*W*	2.200 (2)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2	0.88 (1)	1.76 (1)	2.621 (3)	164 (3)
O1*W*—H2*W*···O4$^{\mathrm{ii}}$	0.87 (1)	1.79 (1)	2.637 (3)	165 (3)
O2*W*—H3*W*···O4*W*$^{\mathrm{ii}}$	0.87 (1)	1.88 (1)	2.713 (3)	159 (3)
O2*W*—H4*W*···O3$^{\mathrm{i}}$	0.87 (1)	1.84 (1)	2.704 (3)	171 (3)
O3*W*—H5*W*···O1$^{\mathrm{ii}}$	0.87 (1)	1.83 (1)	2.693 (3)	167 (3)
O3*W*—H6*W*···O5*W*$^{\mathrm{i}}$	0.87 (1)	1.86 (1)	2.701 (3)	161 (3)
O4*W*—H7*W*···O4	0.88 (1)	1.90 (2)	2.691 (3)	149 (3)
O5*W*—H9*W*···O2	0.90 (1)	1.85 (2)	2.692 (3)	155 (3)

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

Table 3
Selected bond lengths (Å) for CaNPH.

Ca1—O1	2.3608 (11)	Ca1—O2^{ii}	2.4652 (12)
Ca1—O1^{i}	2.3608 (10)	Ca1—O2^{iii}	2.4652 (12)
Ca1—O1*W*^{i}	2.4143 (12)	Ca1—O1^{ii}	2.5765 (12)
Ca1—O1*W*	2.4143 (12)	Ca1—O1^{iii}	2.5765 (11)

Symmetry codes: (i) $-x, y, -z + \frac{5}{2}$; (ii) $-x, -y, -z + 2$; (iii) $x, -y, z + \frac{1}{2}$.

Table 4
Hydrogen-bond geometry (Å, °) for CaNPH.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*W*—H1*W*$\cdots$O2^{iv}	0.86 (1)	1.88 (1)	2.7120 (16)	160 (2)

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

CaNPH

Crystal data

$[Ca(C_{11}H_7O_2)_2(H_2O)_2]$
M_r = 418.44
Monoclinic, *C*2/*c*
a = 21.079 (1) Å
b = 11.4410 (6) Å
c = 7.7200 (3) Å
β = 93.994 (3)°
V = 1857.27 (15) Å^3
Z = 4
Mo *Kα* radiation
μ = 0.38 mm^{-1}
T = 123 K
0.28 × 0.12 × 0.06 mm

Data collection

Nonius KappaCCD area-detector diffractometer
4047 measured reflections
2108 independent reflections
1641 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.077
S = 1.07
2108 reflections
138 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

SrNPH

Crystal data

$[Sr(C_{11}H_7O_2)_2(H_2O)_2]$
M_r = 465.98
Monoclinic, *C*2/*c*
a = 21.2740 (19) Å
b = 11.3397 (10) Å
c = 7.9619 (5) Å
β = 94.520 (4)°
V = 1914.8 (3) Å^3
Z = 4
Mo *Kα* radiation
μ = 2.85 mm^{-1}
T = 123 K
0.20 × 0.20 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.922, T_{max} = 1.000
4336 measured reflections
2312 independent reflections
1853 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.100
S = 1.06
2312 reflections
138 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 5
Selected bond lengths (Å) for SrNPH.

Sr1—O2^{i}	2.495 (2)	Sr1—O1	2.621 (2)
Sr1—O2^{ii}	2.495 (2)	Sr1—O1^{iii}	2.621 (2)
Sr1—O1*W*^{iii}	2.581 (2)	Sr1—O2^{iii}	2.678 (2)
Sr1—O1*W*	2.581 (2)	Sr1—O2	2.678 (2)

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

Table 6
Hydrogen-bond geometry (Å, °) for SrNPH.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*W*—H1*W*$\cdots$O1^{iv}	0.87 (1)	1.89 (1)	2.715 (3)	160 (3)

Symmetry code: (iv) $-x, -y + 1, -z + 1$.

BaNPH

Crystal data

$[Ba(C_{11}H_7O_2)_2(H_2O)_2]$
M_r = 515.70
Orthorhombic, *Pbcn*
a = 20.464 (3) Å
b = 11.9699 (15) Å
c = 8.2812 (10) Å
V = 2028.5 (4) Å^3
Z = 4
Synchrotron radiation
λ = 0.82520 Å
μ = 1.99 mm^{-1}
T = 150 K
0.10 × 0.10 × 0.01 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.673, T_{max} = 1.000
14467 measured reflections
2355 independent reflections
2196 reflections with $I > 2\sigma(I)$
R_{int} = 0.172

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.126
S = 1.14
2355 reflections
139 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.44 e Å^{-3}
$\Delta\rho_{min}$ = −1.46 e Å^{-3}

Water H atoms were positioned as found by difference syntheses and were refined with restraints such that the O—H and H$\cdots$H distances approximated 0.88 (1) and 1.33 (2) Å, respectively; U_{iso}(H) values were set at $1.5U_{eq}$(O). This introduced 15 restraints for the Mg

Table 7
Selected bond lengths (Å) for BaNPH.

Ba1—O1^{i}	2.6536 (19)	Ba1—O2^{iii}	2.792 (2)
Ba1—O1^{ii}	2.6536 (19)	Ba1—O2	2.792 (2)
Ba1—O1*W*	2.769 (2)	Ba1—O1	2.8551 (18)
Ba1—O1*W*^{iii}	2.769 (2)	Ba1—O1^{iii}	2.8551 (18)

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

Table 8
Hydrogen-bond geometry (Å, °) for BaNPH.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*W*—H1*W*$\cdots$O2^{iv}	0.88 (1)	1.86 (1)	2.713 (3)	163 (3)

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

salt and three restraints for each of the other salts. H atoms bonded to C atoms were positioned geometrically and refined in riding mode, with C—H = 0.95 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Nonius, 1998) for MgNPH, CaNPH and SrNPH; *APEX2* (Bruker, 2007) for BaNPH. Cell refinement: *DENZO* and *COLLECT* for MgNPH, CaNPH and SrNPH; *SAINT* (Bruker, 2007) for BaNPH. Data reduction: *DENZO* for MgNPH, CaNPH and SrNPH; *SAINT* for BaNPH. For all compounds, program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008). Molecular graphics: *ORTEP-3* (Farrugia, 1997) and *X-SEED* (Barbour, 2001) for MgNPH and CaNPH; *ORTEP-3* for SrNPH and BaNPH. For all compounds, software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FN3109). Services for accessing these data are described at the back of the journal.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.

Arlin, J.-B., Florence, A. J., Johnston, A., Kennedy, A. R., Miller, G. J. & Patterson, K. (2011). *Cryst. Growth Des.* **11**, 1318–1327.

Arlin, J.-B., Kennedy, A. R. & Shankland, K. (2012). *Acta Cryst.* C**68**, m29–m33.

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.

Black, S. N., Collier, E. A., Davey, R. J. & Roberts, R. J. (2007). *J. Pharm. Sci.* **96**, 1053–1068.

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Collier, E. A., Davey, R. J., Black, S. N. & Roberts, R. J. (2006). *Acta Cryst.* B**62**, 498–505.

Cotton, F. A. & Bergman, J. G. (1964). *J. Am. Chem. Soc.* **86**, 2941–2942.

Debuyst, R., Dejehet, F., Dekandelaer, M.-C., Declercq, J. P., Germain, G. & van Meerssche, M. (1979). *J. Chim. Phys. Phys. Chim. Biol.* **76**, 1117–1124.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Fitzgerald, L. J. & Gerkin, R. E. (1994). *Acta Cryst.* C**50**, 185–188.

Huang, F. & Song, W.-D. (2008). *Acta Cryst.* E**64**, m552.

Kennedy, A. R., Morrison, C. A., Briggs, N. E. B. & Arbuckle, W. (2011). *Cryst. Growth Des.* **11**, 1821–1834.

Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Senkovska, I. (2006). *Z. Naturforsch. Teil B*, **61**, 1383–1390.

Senkovska, I. & Thewalt, U. (2005). *Acta Cryst.* C**61**, m448–m449.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Stahl, P. H. & Wermuth, C. G. (2002). In *Handbook of Pharmaceutical Salts. Properties, Selection and Uses*. Zurich: Wiley-VCH.

Zhao, P. *et al.* (2010). *Mol. Pharmacol.* **78**, 560–568.

supplementary materials

Acta Cryst. (2012). C**68**, m213–m218 [doi:10.1107/S0108270112030399]

Alkaline earth metal salts of 1-naphthoic acid

Jean-Baptiste Arlin and Alan R. Kennedy

(MgNPH) *catena*-poly[[[diaquabis(1-naphthoato-κO)magnesium(II)]-μ-aqua] dihydrate]

Crystal data

$[Mg(C_{11}H_7O_2)_2(H_2O)_3]\cdot 2H_2O$	$F(000) = 960$
$M_r = 456.72$	$D_x = 1.401$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5287 reflections
$a = 12.8896$ (4) Å	$\theta = 1.0$–$27.5°$
$b = 8.0048$ (2) Å	$\mu = 0.13$ mm^{-1}
$c = 24.5300$ (5) Å	$T = 123$ K
$\beta = 121.190$ (1)°	Plate, colourless
$V = 2165.13$ (10) Å^3	$0.15 \times 0.13 \times 0.03$ mm
$Z = 4$	

Data collection

Nonius KappaCCD area-detector diffractometer	2744 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.078$
Graphite monochromator	$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
φ and ω scans	$h = -16 \rightarrow 16$
8977 measured reflections	$k = -10 \rightarrow 10$
4968 independent reflections	$l = -31 \rightarrow 31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.150$	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 1.1013P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
4968 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
319 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
15 restraints	
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 (Å²)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Mg1	0.00172 (8)	0.76819 (11)	0.24870 (4)	0.0177 (2)
O1	0.10496 (17)	0.6870 (2)	0.34203 (8)	0.0231 (5)
O2	0.20189 (19)	0.9184 (2)	0.39368 (9)	0.0316 (5)
O1W	0.08195 (16)	1.0194 (2)	0.27487 (8)	0.0182 (4)
H1W	0.1309 (19)	1.001 (4)	0.3160 (5)	0.027*
H2W	0.1338 (18)	1.036 (4)	0.2627 (11)	0.027*
O3	−0.12473 (17)	0.8492 (2)	0.27004 (9)	0.0232 (5)
O2W	0.13182 (19)	0.6868 (2)	0.23202 (9)	0.0241 (5)
H3W	0.134 (3)	0.718 (3)	0.1986 (10)	0.036*
H4W	0.136 (3)	0.5784 (12)	0.2308 (13)	0.036*
O4	−0.21291 (17)	0.6144 (2)	0.27392 (9)	0.0268 (5)
O3W	−0.09957 (19)	0.8507 (2)	0.15824 (9)	0.0256 (5)
H5W	−0.105 (3)	0.9587 (13)	0.1520 (13)	0.038*
H6W	−0.116 (3)	0.813 (3)	0.1212 (8)	0.038*
O4W	−0.1462 (2)	0.3629 (3)	0.35837 (11)	0.0382 (6)
H7W	−0.191 (3)	0.443 (3)	0.3324 (14)	0.057*
H8W	−0.192 (3)	0.332 (4)	0.3731 (15)	0.057*
O5W	0.1341 (2)	1.1675 (3)	0.44229 (11)	0.0499 (7)
H9W	0.177 (3)	1.088 (4)	0.4373 (16)	0.075*
H10W	0.187 (3)	1.190 (5)	0.4833 (7)	0.075*
C1	0.1754 (3)	0.7674 (4)	0.39284 (13)	0.0230 (7)
C2	0.2250 (3)	0.6739 (3)	0.45441 (12)	0.0216 (7)
C3	0.3512 (3)	0.6791 (3)	0.50196 (13)	0.0228 (7)
C4	0.4398 (3)	0.7619 (4)	0.49337 (15)	0.0324 (8)
H4	0.4158	0.8176	0.4544	0.039*
C5	0.5587 (3)	0.7612 (5)	0.54091 (17)	0.0438 (9)
H5	0.6166	0.8177	0.5347	0.053*
C6	0.5974 (3)	0.6789 (5)	0.59874 (17)	0.0473 (10)
H6	0.6808	0.6800	0.6312	0.057*
C7	0.5165 (3)	0.5982 (4)	0.60841 (15)	0.0394 (9)
H7	0.5435	0.5432	0.6479	0.047*
C8	0.3909 (3)	0.5941 (4)	0.56028 (14)	0.0290 (7)
C9	0.3053 (3)	0.5072 (4)	0.56976 (14)	0.0336 (8)
H9	0.3320	0.4502	0.6088	0.040*
C10	0.1856 (3)	0.5048 (4)	0.52358 (14)	0.0322 (8)
H10	0.1291	0.4477	0.5307	0.039*
C11	0.1456 (3)	0.5872 (4)	0.46524 (14)	0.0269 (7)
H11	0.0622	0.5827	0.4329	0.032*
C12	−0.1851 (2)	0.7647 (4)	0.28802 (13)	0.0214 (6)
C13	−0.2203 (3)	0.8519 (3)	0.33046 (13)	0.0206 (6)
C14	−0.3384 (3)	0.8366 (3)	0.32240 (13)	0.0212 (7)
C15	−0.4348 (3)	0.7466 (4)	0.27194 (14)	0.0260 (7)

H15	−0.4221	0.6897	0.2419	0.031*
C16	−0.5468 (3)	0.7411 (4)	0.26617 (15)	0.0319 (8)
H16	−0.6107	0.6801	0.2321	0.038*
C17	−0.5680 (3)	0.8241 (4)	0.30977 (16)	0.0338 (8)
H17	−0.6457	0.8188	0.3052	0.041*
C18	−0.4776 (3)	0.9120 (4)	0.35840 (15)	0.0300 (8)
H18	−0.4929	0.9679	0.3877	0.036*
C19	−0.3605 (3)	0.9224 (4)	0.36655 (14)	0.0244 (7)
C20	−0.2664 (3)	1.0156 (4)	0.41677 (14)	0.0284 (7)
H20	−0.2814	1.0719	0.4461	0.034*
C21	−0.1550 (3)	1.0261 (4)	0.42391 (13)	0.0281 (7)
H21	−0.0924	1.0880	0.4583	0.034*
C22	−0.1322 (3)	0.9453 (4)	0.38020 (13)	0.0259 (7)
H22	−0.0544	0.9553	0.3851	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0203 (5)	0.0143 (5)	0.0192 (5)	−0.0003 (4)	0.0107 (4)	−0.0008 (4)
O1	0.0292 (12)	0.0185 (11)	0.0170 (10)	−0.0034 (9)	0.0087 (9)	−0.0018 (8)
O2	0.0417 (13)	0.0176 (11)	0.0245 (11)	−0.0063 (10)	0.0094 (10)	0.0007 (9)
O1W	0.0193 (10)	0.0178 (10)	0.0188 (10)	0.0003 (9)	0.0107 (8)	0.0014 (9)
O3	0.0274 (11)	0.0171 (11)	0.0339 (12)	−0.0018 (9)	0.0222 (10)	−0.0006 (9)
O2W	0.0330 (12)	0.0139 (10)	0.0333 (12)	0.0006 (10)	0.0228 (10)	0.0009 (9)
O4	0.0321 (12)	0.0161 (11)	0.0414 (13)	−0.0043 (9)	0.0257 (10)	−0.0042 (9)
O3W	0.0363 (12)	0.0165 (11)	0.0185 (10)	0.0011 (10)	0.0102 (10)	−0.0011 (9)
O4W	0.0580 (16)	0.0289 (13)	0.0409 (14)	0.0016 (12)	0.0350 (13)	0.0022 (11)
O5W	0.0619 (18)	0.0432 (16)	0.0392 (14)	0.0042 (13)	0.0223 (13)	0.0046 (13)
C1	0.0250 (16)	0.0202 (16)	0.0222 (16)	−0.0020 (13)	0.0112 (13)	−0.0025 (13)
C2	0.0286 (17)	0.0168 (15)	0.0189 (15)	−0.0020 (13)	0.0120 (13)	−0.0021 (12)
C3	0.0298 (17)	0.0177 (15)	0.0197 (15)	0.0019 (13)	0.0119 (13)	−0.0036 (13)
C4	0.0322 (19)	0.0306 (18)	0.0330 (18)	−0.0011 (15)	0.0159 (15)	0.0002 (15)
C5	0.0290 (19)	0.050 (2)	0.049 (2)	−0.0036 (18)	0.0174 (18)	−0.0054 (19)
C6	0.031 (2)	0.052 (2)	0.041 (2)	0.0093 (19)	0.0063 (17)	−0.0065 (19)
C7	0.044 (2)	0.037 (2)	0.0249 (18)	0.0118 (18)	0.0088 (16)	0.0004 (15)
C8	0.0401 (19)	0.0206 (16)	0.0209 (16)	0.0083 (15)	0.0120 (15)	0.0007 (13)
C9	0.057 (2)	0.0211 (17)	0.0224 (16)	0.0061 (16)	0.0206 (17)	0.0056 (14)
C10	0.053 (2)	0.0233 (18)	0.0324 (18)	−0.0064 (16)	0.0305 (17)	−0.0035 (15)
C11	0.0323 (17)	0.0231 (16)	0.0243 (16)	−0.0015 (14)	0.0140 (14)	−0.0034 (13)
C12	0.0193 (15)	0.0197 (16)	0.0247 (16)	0.0009 (13)	0.0111 (13)	0.0011 (13)
C13	0.0267 (16)	0.0130 (14)	0.0249 (16)	0.0026 (13)	0.0154 (13)	0.0042 (12)
C14	0.0261 (16)	0.0153 (15)	0.0245 (16)	0.0008 (13)	0.0146 (13)	0.0029 (12)
C15	0.0298 (18)	0.0186 (16)	0.0325 (17)	0.0033 (14)	0.0182 (15)	0.0020 (13)
C16	0.0282 (18)	0.0235 (17)	0.0404 (19)	0.0010 (14)	0.0152 (16)	0.0034 (15)
C17	0.0315 (18)	0.0296 (18)	0.052 (2)	0.0057 (16)	0.0297 (18)	0.0042 (17)
C18	0.0390 (19)	0.0247 (17)	0.0393 (19)	0.0082 (15)	0.0295 (17)	0.0042 (15)
C19	0.0328 (17)	0.0171 (15)	0.0317 (17)	0.0070 (14)	0.0226 (15)	0.0064 (13)
C20	0.043 (2)	0.0211 (16)	0.0267 (16)	0.0041 (15)	0.0223 (15)	0.0023 (14)
C21	0.0386 (19)	0.0206 (16)	0.0215 (15)	−0.0015 (14)	0.0130 (14)	−0.0032 (13)
C22	0.0268 (17)	0.0226 (16)	0.0288 (17)	0.0005 (14)	0.0149 (14)	0.0033 (14)

Geometric parameters (Å, º)

Mg1—O3W	2.016 (2)	C6—C7	1.349 (5)
Mg1—O2W	2.028 (2)	C6—H6	0.9500
Mg1—O3	2.058 (2)	C7—C8	1.427 (4)
Mg1—O1	2.069 (2)	C7—H7	0.9500
Mg1—O1W^{i}	2.195 (2)	C8—C9	1.421 (5)
Mg1—O1W	2.200 (2)	C9—C10	1.362 (4)
O1—C1	1.273 (3)	C9—H9	0.9500
O2—C1	1.253 (3)	C10—C11	1.409 (4)
O1W—Mg1^{ii}	2.195 (2)	C10—H10	0.9500
O1W—H1W	0.881 (10)	C11—H11	0.9500
O1W—H2W	0.873 (10)	C12—C13	1.505 (4)
O3—C12	1.270 (3)	C13—C22	1.379 (4)
O2W—H3W	0.871 (10)	C13—C14	1.435 (4)
O2W—H4W	0.872 (10)	C14—C15	1.415 (4)
O4—C12	1.252 (3)	C14—C19	1.430 (4)
O3W—H5W	0.874 (10)	C15—C16	1.377 (4)
O3W—H6W	0.874 (10)	C15—H15	0.9500
O4W—H7W	0.876 (10)	C16—C17	1.401 (4)
O4W—H8W	0.873 (10)	C16—H16	0.9500
O5W—H9W	0.896 (10)	C17—C18	1.355 (4)
O5W—H10W	0.894 (10)	C17—H17	0.9500
C1—C2	1.500 (4)	C18—C19	1.418 (4)
C2—C11	1.371 (4)	C18—H18	0.9500
C2—C3	1.430 (4)	C19—C20	1.414 (4)
C3—C8	1.419 (4)	C20—C21	1.356 (4)
C3—C4	1.427 (4)	C20—H20	0.9500
C4—C5	1.364 (4)	C21—C22	1.407 (4)
C4—H4	0.9500	C21—H21	0.9500
C5—C6	1.401 (5)	C22—H22	0.9500
C5—H5	0.9500		

O3W—Mg1—O2W	90.86 (9)	C6—C7—C8	121.0 (3)
O3W—Mg1—O3	91.72 (9)	C6—C7—H7	119.5
O2W—Mg1—O3	177.36 (10)	C8—C7—H7	119.5
O3W—Mg1—O1	179.08 (9)	C3—C8—C9	119.7 (3)
O2W—Mg1—O1	89.84 (8)	C3—C8—C7	119.0 (3)
O3—Mg1—O1	87.58 (8)	C9—C8—C7	121.3 (3)
O3W—Mg1—O1W^{i}	93.30 (8)	C10—C9—C8	120.8 (3)
O2W—Mg1—O1W^{i}	90.03 (8)	C10—C9—H9	119.6
O3—Mg1—O1W^{i}	90.40 (8)	C8—C9—H9	119.6
O1—Mg1—O1W^{i}	87.31 (8)	C9—C10—C11	120.0 (3)
O3W—Mg1—O1W	87.73 (8)	C9—C10—H10	120.0
O2W—Mg1—O1W	92.27 (8)	C11—C10—H10	120.0
O3—Mg1—O1W	87.27 (8)	C2—C11—C10	121.1 (3)
O1—Mg1—O1W	91.64 (8)	C2—C11—H11	119.5
O1W^{i}—Mg1—O1W	177.47 (5)	C10—C11—H11	119.5
C1—O1—Mg1	130.42 (18)	O4—C12—O3	123.7 (3)
Mg1^{ii}—O1W—Mg1	131.30 (8)	O4—C12—C13	119.4 (2)

Mg1^{ii}—O1W—H1W	114.4 (19)	O3—C12—C13	116.8 (2)
Mg1—O1W—H1W	97.7 (18)	C22—C13—C14	119.8 (3)
Mg1^{ii}—O1W—H2W	97.5 (19)	C22—C13—C12	117.3 (2)
Mg1—O1W—H2W	112 (2)	C14—C13—C12	122.9 (2)
H1W—O1W—H2W	101.2 (18)	C15—C14—C19	118.5 (3)
C12—O3—Mg1	129.00 (17)	C15—C14—C13	123.5 (3)
Mg1—O2W—H3W	122 (2)	C19—C14—C13	117.9 (3)
Mg1—O2W—H4W	113.7 (19)	C16—C15—C14	120.4 (3)
H3W—O2W—H4W	102.7 (19)	C16—C15—H15	119.8
Mg1—O3W—H5W	117.7 (18)	C14—C15—H15	119.8
Mg1—O3W—H6W	134.4 (19)	C15—C16—C17	121.0 (3)
H5W—O3W—H6W	101.9 (19)	C15—C16—H16	119.5
H7W—O4W—H8W	100.0 (19)	C17—C16—H16	119.5
H9W—O5W—H10W	97.4 (19)	C18—C17—C16	120.0 (3)
O2—C1—O1	123.6 (3)	C18—C17—H17	120.0
O2—C1—C2	119.6 (2)	C16—C17—H17	120.0
O1—C1—C2	116.7 (2)	C17—C18—C19	121.4 (3)
C11—C2—C3	120.3 (3)	C17—C18—H18	119.3
C11—C2—C1	118.4 (3)	C19—C18—H18	119.3
C3—C2—C1	121.2 (3)	C20—C19—C18	121.6 (3)
C8—C3—C4	118.3 (3)	C20—C19—C14	119.7 (3)
C8—C3—C2	118.1 (3)	C18—C19—C14	118.7 (3)
C4—C3—C2	123.6 (3)	C21—C20—C19	121.3 (3)
C5—C4—C3	120.2 (3)	C21—C20—H20	119.4
C5—C4—H4	119.9	C19—C20—H20	119.4
C3—C4—H4	119.9	C20—C21—C22	119.8 (3)
C4—C5—C6	121.4 (3)	C20—C21—H21	120.1
C4—C5—H5	119.3	C22—C21—H21	120.1
C6—C5—H5	119.3	C13—C22—C21	121.5 (3)
C7—C6—C5	120.1 (3)	C13—C22—H22	119.2
C7—C6—H6	120.0	C21—C22—H22	119.2
C5—C6—H6	120.0		

O2W—Mg1—O1—C1	98.8 (2)	C3—C8—C9—C10	−0.1 (4)
O3—Mg1—O1—C1	−80.6 (2)	C7—C8—C9—C10	179.7 (3)
O1W^{i}—Mg1—O1—C1	−171.1 (2)	C8—C9—C10—C11	0.9 (4)
O1W—Mg1—O1—C1	6.6 (2)	C3—C2—C11—C10	1.4 (4)
O3W—Mg1—O1W—Mg1^{ii}	47.12 (12)	C1—C2—C11—C10	−176.4 (3)
O2W—Mg1—O1W—Mg1^{ii}	137.89 (12)	C9—C10—C11—C2	−1.5 (4)
O3—Mg1—O1W—Mg1^{ii}	−44.71 (11)	Mg1—O3—C12—O4	−28.0 (4)
O1—Mg1—O1W—Mg1^{ii}	−132.21 (12)	Mg1—O3—C12—C13	149.89 (19)
O3W—Mg1—O3—C12	118.8 (2)	O4—C12—C13—C22	132.9 (3)
O1—Mg1—O3—C12	−61.8 (2)	O3—C12—C13—C22	−45.1 (4)
O1W^{i}—Mg1—O3—C12	25.4 (2)	O4—C12—C13—C14	−44.9 (4)
O1W—Mg1—O3—C12	−153.6 (2)	O3—C12—C13—C14	137.2 (3)
Mg1—O1—C1—O2	−5.7 (4)	C22—C13—C14—C15	178.5 (3)
Mg1—O1—C1—C2	172.46 (18)	C12—C13—C14—C15	−3.8 (4)
O2—C1—C2—C11	128.3 (3)	C22—C13—C14—C19	0.9 (4)
O1—C1—C2—C11	−50.0 (4)	C12—C13—C14—C19	178.6 (2)

O2—C1—C2—C3	−49.5 (4)	C19—C14—C15—C16	−0.6 (4)
O1—C1—C2—C3	132.3 (3)	C13—C14—C15—C16	−178.2 (3)
C11—C2—C3—C8	−0.6 (4)	C14—C15—C16—C17	0.1 (4)
C1—C2—C3—C8	177.1 (2)	C15—C16—C17—C18	0.2 (5)
C11—C2—C3—C4	177.9 (3)	C16—C17—C18—C19	0.0 (5)
C1—C2—C3—C4	−4.4 (4)	C17—C18—C19—C20	179.2 (3)
C8—C3—C4—C5	−1.4 (4)	C17—C18—C19—C14	−0.5 (4)
C2—C3—C4—C5	−179.9 (3)	C15—C14—C19—C20	−178.9 (3)
C3—C4—C5—C6	0.6 (5)	C13—C14—C19—C20	−1.2 (4)
C4—C5—C6—C7	−0.1 (5)	C15—C14—C19—C18	0.8 (4)
C5—C6—C7—C8	0.3 (5)	C13—C14—C19—C18	178.5 (3)
C4—C3—C8—C9	−178.6 (3)	C18—C19—C20—C21	−179.4 (3)
C2—C3—C8—C9	0.0 (4)	C14—C19—C20—C21	0.3 (4)
C4—C3—C8—C7	1.6 (4)	C19—C20—C21—C22	1.0 (4)
C2—C3—C8—C7	−179.8 (3)	C14—C13—C22—C21	0.3 (4)
C6—C7—C8—C3	−1.1 (5)	C12—C13—C22—C21	−177.5 (3)
C6—C7—C8—C9	179.1 (3)	C20—C21—C22—C13	−1.3 (4)

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) −*x*, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2	0.88 (1)	1.76 (1)	2.621 (3)	164 (3)
O1*W*—H2*W*···O4^{ii}	0.87 (1)	1.79 (1)	2.637 (3)	165 (3)
O2*W*—H3*W*···O4*W*^{ii}	0.87 (1)	1.88 (1)	2.713 (3)	159 (3)
O2*W*—H4*W*···O3^{i}	0.87 (1)	1.84 (1)	2.704 (3)	171 (3)
O3*W*—H5*W*···O1^{ii}	0.87 (1)	1.83 (1)	2.693 (3)	167 (3)
O3*W*—H6*W*···O5*W*^{i}	0.87 (1)	1.86 (1)	2.701 (3)	161 (3)
O4*W*—H7*W*···O4	0.88 (1)	1.90 (2)	2.691 (3)	149 (3)
O5*W*—H9*W*···O2	0.90 (1)	1.85 (2)	2.692 (3)	155 (3)

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) −*x*, *y*+1/2, −*z*+1/2.

(CaNPH) *catena*-poly[[diaquacalcium(II)]-bis(*μ*-1-naphthoato)- *κ*^{3}*O*,*O′*:*O*;*κ*^{3}*O*:*O*,*O′*]

Crystal data

$[Ca(C_{11}H_7O_2)_2(H_2O)_2]$
M_r = 418.44
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 21.079 (1) Å
b = 11.4410 (6) Å
c = 7.7200 (3) Å
β = 93.994 (3)°
V = 1857.27 (15) Å^3
Z = 4

F(000) = 872
D_x = 1.496 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 2196 reflections
θ = 1–27.5°
μ = 0.38 mm^{-1}
T = 123 K
Cut needle, colourless
0.28 × 0.12 × 0.06 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator

φ and *ω* scans
4047 measured reflections
2108 independent reflections
1641 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$
$\theta_{\max} = 27.5°$, $\theta_{\min} = 3.3°$
$h = -27 \rightarrow 27$
$k = -14 \rightarrow 14$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.077$
$S = 1.07$
2108 reflections
138 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0258P)^2 + 1.991P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.28$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

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}
Ca1	0.0000	0.03980 (4)	1.2500	0.01390 (13)
O1	0.04711 (5)	0.09489 (10)	0.99365 (14)	0.0170 (3)
O2	0.07864 (5)	0.11825 (10)	0.72994 (14)	0.0192 (3)
O1W	−0.07630 (6)	0.17367 (12)	1.11200 (15)	0.0240 (3)
H1W	−0.0827 (9)	0.1706 (18)	1.0004 (12)	0.036*
H2W	−0.0996 (9)	0.2304 (14)	1.143 (2)	0.036*
C1	0.07467 (7)	0.15460 (15)	0.8834 (2)	0.0152 (4)
C2	0.10026 (8)	0.27320 (15)	0.9348 (2)	0.0159 (4)
C3	0.06320 (8)	0.34445 (15)	1.0302 (2)	0.0184 (4)
H3	0.0238	0.3161	1.0656	0.022*
C4	0.08283 (8)	0.45869 (16)	1.0764 (2)	0.0215 (4)
H4	0.0560	0.5075	1.1391	0.026*
C5	0.14031 (8)	0.49945 (16)	1.0311 (2)	0.0197 (4)
H5	0.1532	0.5765	1.0628	0.024*
C6	0.18086 (8)	0.42798 (15)	0.9373 (2)	0.0162 (4)
C7	0.24163 (8)	0.46787 (16)	0.8961 (2)	0.0187 (4)
H7	0.2553	0.5438	0.9316	0.022*
C8	0.28081 (8)	0.39944 (16)	0.8064 (2)	0.0206 (4)
H8	0.3213	0.4277	0.7794	0.025*
C9	0.26091 (8)	0.28643 (16)	0.7541 (2)	0.0203 (4)
H9	0.2883	0.2389	0.6915	0.024*
C10	0.20274 (8)	0.24413 (15)	0.7919 (2)	0.0174 (4)

H10	0.1903	0.1677	0.7555	0.021*
C11	0.16068 (7)	0.31362 (15)	0.8851 (2)	0.0148 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0149 (2)	0.0161 (3)	0.0108 (2)	0.000	0.00190 (17)	0.000
O1	0.0183 (6)	0.0187 (7)	0.0143 (6)	−0.0020 (5)	0.0031 (4)	0.0022 (5)
O2	0.0228 (6)	0.0236 (7)	0.0115 (6)	−0.0064 (5)	0.0029 (5)	−0.0024 (5)
O1W	0.0272 (7)	0.0293 (8)	0.0154 (6)	0.0116 (6)	0.0017 (5)	−0.0017 (6)
C1	0.0116 (8)	0.0196 (9)	0.0142 (8)	0.0015 (6)	−0.0002 (6)	0.0007 (7)
C2	0.0197 (8)	0.0177 (9)	0.0101 (8)	−0.0007 (7)	−0.0005 (6)	0.0016 (7)
C3	0.0180 (8)	0.0220 (10)	0.0154 (8)	−0.0019 (7)	0.0026 (6)	0.0012 (7)
C4	0.0270 (9)	0.0205 (10)	0.0174 (8)	0.0043 (8)	0.0040 (7)	−0.0041 (8)
C5	0.0271 (9)	0.0162 (9)	0.0155 (8)	−0.0009 (7)	−0.0014 (7)	−0.0017 (7)
C6	0.0199 (8)	0.0167 (9)	0.0116 (8)	−0.0017 (7)	−0.0019 (6)	0.0015 (7)
C7	0.0224 (9)	0.0168 (9)	0.0163 (8)	−0.0056 (7)	−0.0024 (7)	0.0022 (7)
C8	0.0167 (8)	0.0251 (10)	0.0201 (9)	−0.0043 (7)	0.0009 (7)	0.0034 (8)
C9	0.0189 (9)	0.0224 (10)	0.0198 (9)	0.0015 (7)	0.0026 (7)	0.0020 (7)
C10	0.0188 (9)	0.0161 (9)	0.0171 (8)	−0.0012 (7)	0.0006 (7)	0.0005 (7)
C11	0.0163 (8)	0.0176 (9)	0.0103 (8)	−0.0002 (7)	−0.0010 (6)	0.0028 (7)

Geometric parameters (Å, º)

Ca1—O1	2.3608 (11)	C2—C3	1.378 (2)
Ca1—O1$^{\mathrm{i}}$	2.3608 (10)	C2—C11	1.432 (2)
Ca1—O1W$^{\mathrm{i}}$	2.4143 (12)	C3—C4	1.409 (2)
Ca1—O1W	2.4143 (12)	C3—H3	0.9500
Ca1—O2$^{\mathrm{ii}}$	2.4652 (12)	C4—C5	1.366 (2)
Ca1—O2$^{\mathrm{iii}}$	2.4652 (12)	C4—H4	0.9500
Ca1—O1$^{\mathrm{ii}}$	2.5765 (12)	C5—C6	1.417 (2)
Ca1—O1$^{\mathrm{iii}}$	2.5765 (11)	C5—H5	0.9500
Ca1—C1$^{\mathrm{ii}}$	2.8738 (17)	C6—C7	1.417 (2)
Ca1—C1$^{\mathrm{iii}}$	2.8738 (17)	C6—C11	1.425 (2)
O1—C1	1.2638 (19)	C7—C8	1.361 (2)
O1—Ca1$^{\mathrm{ii}}$	2.5765 (12)	C7—H7	0.9500
O2—C1	1.2640 (19)	C8—C9	1.410 (3)
O2—Ca1$^{\mathrm{ii}}$	2.4652 (12)	C8—H8	0.9500
O1W—H1W	0.863 (9)	C9—C10	1.368 (2)
O1W—H2W	0.856 (9)	C9—H9	0.9500
C1—C2	1.503 (2)	C10—C11	1.423 (2)
C1—Ca1$^{\mathrm{ii}}$	2.8738 (17)	C10—H10	0.9500

O1—Ca1—O1$^{\mathrm{i}}$	149.04 (6)	O1—Ca1—Ca1$^{\mathrm{iv}}$	154.92 (3)
O1—Ca1—O1W$^{\mathrm{i}}$	83.94 (4)	O1$^{\mathrm{i}}$—Ca1—Ca1$^{\mathrm{iv}}$	38.46 (3)
O1$^{\mathrm{i}}$—Ca1—O1W$^{\mathrm{i}}$	76.52 (4)	O1W$^{\mathrm{i}}$—Ca1—Ca1$^{\mathrm{iv}}$	76.19 (3)
O1—Ca1—O1W	76.52 (4)	O1W—Ca1—Ca1$^{\mathrm{iv}}$	122.00 (3)
O1$^{\mathrm{i}}$—Ca1—O1W	83.94 (4)	O2$^{\mathrm{ii}}$—Ca1—Ca1$^{\mathrm{iv}}$	74.03 (3)
O1W$^{\mathrm{i}}$—Ca1—O1W	101.25 (7)	O2$^{\mathrm{iii}}$—Ca1—Ca1$^{\mathrm{iv}}$	86.46 (3)
O1—Ca1—O2$^{\mathrm{ii}}$	124.92 (4)	O1$^{\mathrm{ii}}$—Ca1—Ca1$^{\mathrm{iv}}$	123.17 (3)

O1^{i}—Ca1—O2^{ii}	79.59 (4)
O1W^{i}—Ca1—O2^{ii}	150.20 (4)
O1W—Ca1—O2^{ii}	93.60 (4)
O1—Ca1—O2^{iii}	79.59 (4)
O1^{i}—Ca1—O2^{iii}	124.92 (4)
O1W^{i}—Ca1—O2^{iii}	93.60 (4)
O1W—Ca1—O2^{iii}	150.20 (4)
O2^{ii}—Ca1—O2^{iii}	85.64 (6)
O1—Ca1—O1^{ii}	73.19 (4)
O1^{i}—Ca1—O1^{ii}	127.48 (4)
O1W^{i}—Ca1—O1^{ii}	155.86 (4)
O1W—Ca1—O1^{ii}	81.15 (4)
O2^{ii}—Ca1—O1^{ii}	51.72 (4)
O2^{iii}—Ca1—O1^{ii}	75.05 (4)
O1—Ca1—O1^{iii}	127.48 (4)
O1^{i}—Ca1—O1^{iii}	73.19 (4)
O1W^{i}—Ca1—O1^{iii}	81.15 (4)
O1W—Ca1—O1^{iii}	155.86 (4)
O2^{ii}—Ca1—O1^{iii}	75.05 (4)
O2^{iii}—Ca1—O1^{iii}	51.72 (3)
O1^{ii}—Ca1—O1^{iii}	106.53 (5)
O1—Ca1—C1^{ii}	99.09 (4)
O1^{i}—Ca1—C1^{ii}	104.79 (4)
O1W^{i}—Ca1—C1^{ii}	168.66 (5)
O1W—Ca1—C1^{ii}	90.08 (4)
O2^{ii}—Ca1—C1^{ii}	25.97 (4)
O2^{iii}—Ca1—C1^{ii}	76.33 (4)
O1^{ii}—Ca1—C1^{ii}	26.09 (4)
O1^{iii}—Ca1—C1^{ii}	88.42 (4)
O1—Ca1—C1^{iii}	104.79 (4)
O1^{i}—Ca1—C1^{iii}	99.09 (4)
O1W^{i}—Ca1—C1^{iii}	90.08 (4)
O1W—Ca1—C1^{iii}	168.66 (5)
O2^{ii}—Ca1—C1^{iii}	76.33 (4)
O2^{iii}—Ca1—C1^{iii}	25.97 (4)
O1^{ii}—Ca1—C1^{iii}	88.42 (4)
O1^{iii}—Ca1—C1^{iii}	26.09 (4)
C1^{ii}—Ca1—C1^{iii}	78.59 (6)
O1—Ca1—Ca1^{ii}	38.46 (3)
O1^{i}—Ca1—Ca1^{ii}	154.92 (3)
O1W^{i}—Ca1—Ca1^{ii}	122.00 (3)
O1W—Ca1—Ca1^{ii}	76.19 (3)
O2^{ii}—Ca1—Ca1^{ii}	86.46 (3)
O2^{iii}—Ca1—Ca1^{ii}	74.03 (3)
O1^{ii}—Ca1—Ca1^{ii}	34.74 (2)
O1^{iii}—Ca1—Ca1^{ii}	123.17 (3)
C1^{ii}—Ca1—Ca1^{ii}	60.70 (3)
C1^{iii}—Ca1—Ca1^{ii}	97.70 (3)
O1^{iii}—Ca1—Ca1^{iv}	34.74 (2)
C1^{ii}—Ca1—Ca1^{iv}	97.70 (3)
C1^{iii}—Ca1—Ca1^{iv}	60.70 (3)
Ca1^{ii}—Ca1—Ca1^{iv}	153.45 (3)
C1—O1—Ca1	161.56 (11)
C1—O1—Ca1^{ii}	90.20 (9)
Ca1—O1—Ca1^{ii}	106.81 (4)
C1—O2—Ca1^{ii}	95.38 (9)
Ca1—O1W—H1W	117.9 (13)
Ca1—O1W—H2W	137.4 (13)
H1W—O1W—H2W	104.6 (15)
O1—C1—O2	121.12 (15)
O1—C1—C2	118.93 (14)
O2—C1—C2	119.88 (14)
O1—C1—Ca1^{ii}	63.71 (8)
O2—C1—Ca1^{ii}	58.65 (8)
C2—C1—Ca1^{ii}	166.08 (11)
C3—C2—C11	120.01 (15)
C3—C2—C1	117.95 (14)
C11—C2—C1	122.04 (14)
C2—C3—C4	121.10 (15)
C2—C3—H3	119.5
C4—C3—H3	119.5
C5—C4—C3	120.13 (16)
C5—C4—H4	119.9
C3—C4—H4	119.9
C4—C5—C6	120.72 (16)
C4—C5—H5	119.6
C6—C5—H5	119.6
C7—C6—C5	121.05 (16)
C7—C6—C11	119.25 (15)
C5—C6—C11	119.69 (15)
C8—C7—C6	121.26 (16)
C8—C7—H7	119.4
C6—C7—H7	119.4
C7—C8—C9	119.63 (16)
C7—C8—H8	120.2
C9—C8—H8	120.2
C10—C9—C8	121.08 (16)
C10—C9—H9	119.5
C8—C9—H9	119.5
C9—C10—C11	120.62 (16)
C9—C10—H10	119.7
C11—C10—H10	119.7
C10—C11—C6	118.16 (14)
C10—C11—C2	123.50 (15)
C6—C11—C2	118.30 (15)

O1^{i}—Ca1—O1—C1	19.5 (3)	O1—C1—C2—C3	−42.3 (2)
O1W^{i}—Ca1—O1—C1	−31.2 (3)	O2—C1—C2—C3	134.80 (16)
O1W—Ca1—O1—C1	71.9 (3)	Ca1^{ii}—C1—C2—C3	54.9 (5)
O2^{ii}—Ca1—O1—C1	156.8 (3)	O1—C1—C2—C11	138.69 (15)
O2^{iii}—Ca1—O1—C1	−126.0 (3)	O2—C1—C2—C11	−44.2 (2)
O1^{ii}—Ca1—O1—C1	156.6 (3)	Ca1^{ii}—C1—C2—C11	−124.0 (4)
O1^{iii}—Ca1—O1—C1	−105.2 (3)	C11—C2—C3—C4	1.9 (2)
C1^{ii}—Ca1—O1—C1	159.8 (3)	C1—C2—C3—C4	−177.15 (15)
C1^{iii}—Ca1—O1—C1	−119.7 (3)	C2—C3—C4—C5	−2.0 (3)
Ca1^{ii}—Ca1—O1—C1	156.6 (3)	C3—C4—C5—C6	0.1 (3)
Ca1^{iv}—Ca1—O1—C1	−68.8 (3)	C4—C5—C6—C7	−177.39 (16)
O1^{i}—Ca1—O1—Ca1^{ii}	−137.05 (4)	C4—C5—C6—C11	1.9 (2)
O1W^{i}—Ca1—O1—Ca1^{ii}	172.19 (5)	C5—C6—C7—C8	179.83 (16)
O1W—Ca1—O1—Ca1^{ii}	−84.68 (5)	C11—C6—C7—C8	0.5 (2)
O2^{ii}—Ca1—O1—Ca1^{ii}	0.25 (6)	C6—C7—C8—C9	−0.3 (3)
O2^{iii}—Ca1—O1—Ca1^{ii}	77.38 (5)	C7—C8—C9—C10	0.0 (3)
O1^{ii}—Ca1—O1—Ca1^{ii}	0.0	C8—C9—C10—C11	0.1 (2)
O1^{iii}—Ca1—O1—Ca1^{ii}	98.23 (7)	C9—C10—C11—C6	0.1 (2)
C1^{ii}—Ca1—O1—Ca1^{ii}	3.21 (5)	C9—C10—C11—C2	−177.50 (15)
C1^{iii}—Ca1—O1—Ca1^{ii}	83.71 (5)	C7—C6—C11—C10	−0.4 (2)
Ca1^{iv}—Ca1—O1—Ca1^{ii}	134.65 (7)	C5—C6—C11—C10	−179.72 (14)
Ca1—O1—C1—O2	−170.2 (2)	C7—C6—C11—C2	177.31 (14)
Ca1^{ii}—O1—C1—O2	−12.53 (15)	C5—C6—C11—C2	−2.0 (2)
Ca1—O1—C1—C2	6.9 (4)	C3—C2—C11—C10	177.74 (15)
Ca1^{ii}—O1—C1—C2	164.57 (13)	C1—C2—C11—C10	−3.3 (2)
Ca1—O1—C1—Ca1^{ii}	−157.6 (3)	C3—C2—C11—C6	0.1 (2)
Ca1^{ii}—O2—C1—O1	13.16 (16)	C1—C2—C11—C6	179.11 (14)
Ca1^{ii}—O2—C1—C2	−163.91 (12)		

Symmetry codes: (i) $-x, y, -z+5/2$; (ii) $-x, -y, -z+2$; (iii) $x, -y, z+1/2$; (iv) $-x, -y, -z+3$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2^{v}	0.86 (1)	1.88 (1)	2.7120 (16)	160 (2)

Symmetry code: (v) $-x, y, -z+3/2$.

(SrNPH) *catena*-poly[[diaquastrontium(II)]-bis(*μ*-1-naphthoato)- *κ*^{3}*O,O′*:*O*;*κ*^{3}*O*:*O,O′*]

Crystal data

$[Sr(C_{11}H_7O_2)_2(H_2O)_2]$
$M_r = 465.98$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 21.2740$ (19) Å
$b = 11.3397$ (10) Å
$c = 7.9619$ (5) Å
$\beta = 94.520$ (4)°
$V = 1914.8$ (3) Å^3
$Z = 4$

$F(000) = 944$
$D_x = 1.616$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 13743 reflections
$\theta = 1.0$–30.0°
$\mu = 2.85$ mm^{-1}
$T = 123$ K
Cut fragment, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer	4336 measured reflections
Radiation source: fine-focus sealed tube	2312 independent reflections
Graphite monochromator	1853 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\rm int} = 0.059$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$\theta_{\rm max} = 28.0°$, $\theta_{\rm min} = 3.2°$
$T_{\rm min} = 0.922$, $T_{\rm max} = 1.000$	$h = -27\rightarrow28$
	$k = -14\rightarrow14$
	$l = -10\rightarrow10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 1.1387P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\rm max} < 0.001$
2312 reflections	$\Delta\rho_{\rm max} = 0.62$ e Å^{-3}
138 parameters	$\Delta\rho_{\rm min} = -0.45$ e Å^{-3}
3 restraints	
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	$U_{\rm iso}$*/$U_{\rm eq}$
Sr1	0.0000	0.54911 (4)	0.7500	0.01586 (14)
O1	0.08138 (10)	0.3771 (2)	0.7297 (3)	0.0220 (5)
O2	0.04972 (10)	0.4005 (2)	0.9857 (2)	0.0203 (5)
O1W	−0.07903 (12)	0.6931 (2)	0.5967 (3)	0.0268 (6)
H1W	−0.0826 (18)	0.688 (3)	0.4875 (13)	0.040*
H2W	−0.0992 (17)	0.757 (2)	0.616 (4)	0.040*
C1	0.07734 (14)	0.3404 (3)	0.8781 (4)	0.0173 (7)
C2	0.10307 (14)	0.2211 (3)	0.9292 (4)	0.0171 (7)
C3	0.06709 (15)	0.1487 (3)	1.0219 (4)	0.0201 (7)
H3	0.0275	0.1759	1.0538	0.024*
C4	0.08798 (16)	0.0349 (3)	1.0702 (4)	0.0234 (8)
H4	0.0620	−0.0146	1.1317	0.028*
C5	0.14525 (16)	−0.0041 (3)	1.0292 (4)	0.0231 (7)
H5	0.1588	−0.0809	1.0629	0.028*
C6	0.18528 (15)	0.0676 (3)	0.9368 (4)	0.0182 (7)
C7	0.24615 (15)	0.0299 (3)	0.8987 (4)	0.0207 (7)

H7	0.2607	−0.0459	0.9343	0.025*
C8	0.28399 (15)	0.1004 (3)	0.8122 (4)	0.0234 (8)
H8	0.3244	0.0733	0.7870	0.028*
C9	0.26332 (15)	0.2138 (3)	0.7598 (4)	0.0223 (8)
H9	0.2902	0.2626	0.6999	0.027*
C10	0.20490 (14)	0.2543 (3)	0.7942 (4)	0.0186 (7)
H10	0.1918	0.3309	0.7579	0.022*
C11	0.16387 (15)	0.1830 (3)	0.8835 (4)	0.0172 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0168 (2)	0.0199 (2)	0.0109 (2)	0.000	0.00093 (14)	0.000
O1	0.0257 (12)	0.0265 (14)	0.0140 (11)	0.0098 (11)	0.0022 (9)	0.0021 (10)
O2	0.0215 (12)	0.0247 (13)	0.0148 (11)	0.0022 (10)	0.0018 (9)	−0.0023 (10)
O1W	0.0322 (14)	0.0322 (15)	0.0159 (12)	0.0128 (12)	0.0010 (10)	0.0011 (11)
C1	0.0128 (14)	0.0244 (19)	0.0146 (15)	0.0003 (13)	0.0002 (12)	−0.0001 (13)
C2	0.0190 (15)	0.0201 (18)	0.0116 (14)	0.0008 (14)	−0.0023 (12)	−0.0012 (13)
C3	0.0199 (16)	0.0240 (19)	0.0167 (16)	0.0037 (14)	0.0031 (13)	−0.0003 (14)
C4	0.0247 (17)	0.028 (2)	0.0182 (16)	−0.0041 (16)	0.0044 (13)	0.0043 (14)
C5	0.0286 (18)	0.0221 (17)	0.0181 (16)	0.0034 (16)	−0.0011 (14)	−0.0011 (15)
C6	0.0208 (15)	0.0221 (19)	0.0109 (14)	0.0029 (14)	−0.0035 (12)	−0.0054 (13)
C7	0.0222 (16)	0.021 (2)	0.0182 (15)	0.0047 (14)	−0.0030 (12)	−0.0026 (13)
C8	0.0195 (16)	0.029 (2)	0.0211 (17)	0.0054 (15)	−0.0016 (13)	−0.0065 (15)
C9	0.0218 (18)	0.026 (2)	0.0197 (16)	−0.0027 (15)	0.0026 (14)	−0.0006 (14)
C10	0.0172 (15)	0.0222 (18)	0.0157 (15)	0.0012 (14)	−0.0028 (12)	−0.0013 (13)
C11	0.0219 (16)	0.0184 (18)	0.0107 (15)	0.0003 (14)	−0.0022 (12)	−0.0050 (12)

Geometric parameters (Å, º)

Sr1—O2^{i}	2.495 (2)	C2—C11	1.438 (4)
Sr1—O2^{ii}	2.495 (2)	C3—C4	1.408 (5)
Sr1—O1W^{iii}	2.581 (2)	C3—H3	0.9500
Sr1—O1W	2.581 (2)	C4—C5	1.360 (5)
Sr1—O1	2.621 (2)	C4—H4	0.9500
Sr1—O1^{iii}	2.621 (2)	C5—C6	1.423 (5)
Sr1—O2^{iii}	2.678 (2)	C5—H5	0.9500
Sr1—O2	2.678 (2)	C6—C7	1.419 (4)
Sr1—C1^{iii}	3.014 (3)	C6—C11	1.439 (4)
Sr1—C1	3.014 (3)	C7—C8	1.360 (5)
O1—C1	1.262 (4)	C7—H7	0.9500
O2—C1	1.274 (4)	C8—C9	1.411 (5)
O2—Sr1^{i}	2.495 (2)	C8—H8	0.9500
O1W—H1W	0.868 (10)	C9—C10	1.373 (4)
O1W—H2W	0.865 (10)	C9—H9	0.9500
C1—C2	1.503 (4)	C10—C11	1.421 (4)
C2—C3	1.376 (4)	C10—H10	0.9500

O2^{i}—Sr1—O2^{ii}	153.50 (11)	O2^{i}—Sr1—Sr1^{i}	38.50 (5)
O2^{i}—Sr1—O1W^{iii}	76.10 (7)	O2^{ii}—Sr1—Sr1^{i}	154.98 (5)

O2^{ii}—Sr1—O1W^{iii}	87.14 (7)
O2^{i}—Sr1—O1W	87.14 (7)
O2^{ii}—Sr1—O1W	76.10 (7)
O1W^{iii}—Sr1—O1W	101.48 (12)
O2^{i}—Sr1—O1	123.26 (7)
O2^{ii}—Sr1—O1	78.03 (7)
O1W^{iii}—Sr1—O1	95.23 (8)
O1W—Sr1—O1	148.27 (7)
O2^{i}—Sr1—O1^{iii}	78.03 (7)
O2^{ii}—Sr1—O1^{iii}	123.26 (7)
O1W^{iii}—Sr1—O1^{iii}	148.27 (7)
O1W—Sr1—O1^{iii}	95.23 (8)
O1—Sr1—O1^{iii}	83.85 (11)
O2^{i}—Sr1—O2^{iii}	124.41 (8)
O2^{ii}—Sr1—O2^{iii}	73.95 (8)
O1W^{iii}—Sr1—O2^{iii}	159.48 (7)
O1W—Sr1—O2^{iii}	81.97 (8)
O1—Sr1—O2^{iii}	73.43 (7)
O1^{iii}—Sr1—O2^{iii}	49.34 (6)
O2^{i}—Sr1—O2	73.95 (8)
O2^{ii}—Sr1—O2	124.41 (8)
O1W^{iii}—Sr1—O2	81.97 (8)
O1W—Sr1—O2	159.48 (7)
O1—Sr1—O2	49.34 (6)
O1^{iii}—Sr1—O2	73.43 (7)
O2^{iii}—Sr1—O2	101.97 (10)
O2^{i}—Sr1—C1^{iii}	102.06 (8)
O2^{ii}—Sr1—C1^{iii}	98.69 (8)
O1W^{iii}—Sr1—C1^{iii}	167.13 (8)
O1W—Sr1—C1^{iii}	91.09 (8)
O1—Sr1—C1^{iii}	74.95 (8)
O1^{iii}—Sr1—C1^{iii}	24.64 (7)
O2^{iii}—Sr1—C1^{iii}	24.98 (7)
O2—Sr1—C1^{iii}	85.28 (8)
O2^{i}—Sr1—C1	98.69 (8)
O2^{ii}—Sr1—C1	102.06 (8)
O1W^{iii}—Sr1—C1	91.09 (8)
O1W—Sr1—C1	167.13 (9)
O1—Sr1—C1	24.64 (7)
O1^{iii}—Sr1—C1	74.95 (8)
O2^{iii}—Sr1—C1	85.28 (8)
O2—Sr1—C1	24.98 (7)
C1^{iii}—Sr1—C1	76.50 (12)
O2^{i}—Sr1—Sr1^{iv}	154.98 (5)
O2^{ii}—Sr1—Sr1^{iv}	38.50 (5)
O1W^{iii}—Sr1—Sr1^{iv}	125.21 (5)
O1W—Sr1—Sr1^{iv}	76.38 (5)
O1—Sr1—Sr1^{iv}	71.95 (5)
O1^{iii}—Sr1—Sr1^{iv}	84.78 (5)
O1W^{iii}—Sr1—Sr1^{i}	76.38 (5)
O1W—Sr1—Sr1^{i}	125.21 (5)
O1—Sr1—Sr1^{i}	84.78 (5)
O1^{iii}—Sr1—Sr1^{i}	71.95 (5)
O2^{iii}—Sr1—Sr1^{i}	118.39 (5)
O2—Sr1—Sr1^{i}	35.45 (5)
C1^{iii}—Sr1—Sr1^{i}	94.18 (6)
C1—Sr1—Sr1^{i}	60.26 (6)
Sr1^{iv}—Sr1—Sr1^{i}	148.74 (2)
C1—O1—Sr1	95.39 (18)
C1—O2—Sr1^{i}	159.8 (2)
C1—O2—Sr1	92.46 (18)
Sr1^{i}—O2—Sr1	106.05 (8)
Sr1—O1W—H1W	116 (2)
Sr1—O1W—H2W	140 (2)
H1W—O1W—H2W	103 (2)
O1—C1—O2	121.5 (3)
O1—C1—C2	120.0 (3)
O2—C1—C2	118.5 (3)
O1—C1—Sr1	59.97 (16)
O2—C1—Sr1	62.56 (16)
C2—C1—Sr1	167.3 (2)
C3—C2—C11	120.4 (3)
C3—C2—C1	118.4 (3)
C11—C2—C1	121.2 (3)
C2—C3—C4	121.1 (3)
C2—C3—H3	119.5
C4—C3—H3	119.5
C5—C4—C3	120.1 (3)
C5—C4—H4	119.9
C3—C4—H4	119.9
C4—C5—C6	121.5 (3)
C4—C5—H5	119.2
C6—C5—H5	119.2
C7—C6—C5	122.2 (3)
C7—C6—C11	118.9 (3)
C5—C6—C11	118.9 (3)
C8—C7—C6	121.2 (3)
C8—C7—H7	119.4
C6—C7—H7	119.4
C7—C8—C9	120.2 (3)
C7—C8—H8	119.9
C9—C8—H8	119.9
C10—C9—C8	120.8 (3)
C10—C9—H9	119.6
C8—C9—H9	119.6
C9—C10—C11	120.7 (3)
C9—C10—H10	119.6
C11—C10—H10	119.6

O2^{iii}—Sr1—Sr1^{iv}	35.45 (5)	C10—C11—C2	123.8 (3)
O2—Sr1—Sr1^{iv}	118.39 (5)	C10—C11—C6	118.2 (3)
C1^{iii}—Sr1—Sr1^{iv}	60.26 (6)	C2—C11—C6	118.0 (3)
C1—Sr1—Sr1^{iv}	94.18 (6)		

O2^{i}—Sr1—O1—C1	4.4 (2)	O2^{ii}—Sr1—C1—O2	155.47 (18)
O2^{ii}—Sr1—O1—C1	167.11 (19)	O1W^{iii}—Sr1—C1—O2	68.16 (18)
O1W^{iii}—Sr1—O1—C1	81.16 (19)	O1W—Sr1—C1—O2	−124.2 (3)
O1W—Sr1—O1—C1	−156.97 (19)	O1—Sr1—C1—O2	168.4 (3)
O1^{iii}—Sr1—O1—C1	−66.96 (18)	O1^{iii}—Sr1—C1—O2	−82.97 (18)
O2^{iii}—Sr1—O1—C1	−116.30 (19)	O2^{iii}—Sr1—C1—O2	−132.07 (17)
O2—Sr1—O1—C1	6.44 (17)	C1^{iii}—Sr1—C1—O2	−108.4 (2)
C1^{iii}—Sr1—O1—C1	−90.4 (2)	Sr1^{iv}—Sr1—C1—O2	−166.42 (17)
Sr1^{iv}—Sr1—O1—C1	−153.45 (19)	Sr1^{i}—Sr1—C1—O2	−5.45 (15)
Sr1^{i}—Sr1—O1—C1	5.39 (18)	O2^{i}—Sr1—C1—C2	90.0 (9)
O2^{i}—Sr1—O2—C1	171.8 (2)	O2^{ii}—Sr1—C1—C2	−106.6 (9)
O2^{ii}—Sr1—O2—C1	−29.5 (2)	O1W^{iii}—Sr1—C1—C2	166.1 (9)
O1W^{iii}—Sr1—O2—C1	−110.40 (19)	O1W—Sr1—C1—C2	−26.2 (12)
O1W—Sr1—O2—C1	148.3 (2)	O1—Sr1—C1—C2	−93.7 (10)
O1—Sr1—O2—C1	−6.36 (17)	O1^{iii}—Sr1—C1—C2	15.0 (9)
O1^{iii}—Sr1—O2—C1	89.85 (18)	O2^{iii}—Sr1—C1—C2	−34.1 (9)
O2^{iii}—Sr1—O2—C1	49.14 (17)	O2—Sr1—C1—C2	98.0 (10)
C1^{iii}—Sr1—O2—C1	67.8 (2)	C1^{iii}—Sr1—C1—C2	−10.4 (9)
Sr1^{iv}—Sr1—O2—C1	15.44 (19)	Sr1^{iv}—Sr1—C1—C2	−68.4 (9)
Sr1^{i}—Sr1—O2—C1	171.8 (2)	Sr1^{i}—Sr1—C1—C2	92.5 (9)
O2^{i}—Sr1—O2—Sr1^{i}	0.0	O1—C1—C2—C3	−135.5 (3)
O2^{ii}—Sr1—O2—Sr1^{i}	158.69 (8)	O2—C1—C2—C3	42.1 (4)
O1W^{iii}—Sr1—O2—Sr1^{i}	77.77 (9)	Sr1—C1—C2—C3	−49.2 (11)
O1W—Sr1—O2—Sr1^{i}	−23.5 (3)	O1—C1—C2—C11	44.8 (4)
O1—Sr1—O2—Sr1^{i}	−178.19 (13)	O2—C1—C2—C11	−137.7 (3)
O1^{iii}—Sr1—O2—Sr1^{i}	−81.98 (8)	Sr1—C1—C2—C11	131.1 (9)
O2^{iii}—Sr1—O2—Sr1^{i}	−122.69 (9)	C11—C2—C3—C4	−1.7 (5)
C1^{iii}—Sr1—O2—Sr1^{i}	−104.00 (9)	C1—C2—C3—C4	178.5 (3)
C1—Sr1—O2—Sr1^{i}	−171.8 (2)	C2—C3—C4—C5	1.7 (5)
Sr1^{iv}—Sr1—O2—Sr1^{i}	−156.39 (5)	C3—C4—C5—C6	−0.2 (5)
Sr1—O1—C1—O2	−12.1 (3)	C4—C5—C6—C7	177.5 (3)
Sr1—O1—C1—C2	165.4 (2)	C4—C5—C6—C11	−1.1 (5)
Sr1^{i}—O2—C1—O1	168.5 (4)	C5—C6—C7—C8	−179.1 (3)
Sr1—O2—C1—O1	11.8 (3)	C11—C6—C7—C8	−0.5 (5)
Sr1^{i}—O2—C1—C2	−9.0 (8)	C6—C7—C8—C9	0.6 (5)
Sr1—O2—C1—C2	−165.7 (2)	C7—C8—C9—C10	−0.3 (5)
Sr1^{i}—O2—C1—Sr1	156.7 (6)	C8—C9—C10—C11	0.0 (5)
O2^{i}—Sr1—C1—O1	−176.31 (18)	C9—C10—C11—C2	177.7 (3)
O2^{ii}—Sr1—C1—O1	−12.90 (19)	C9—C10—C11—C6	0.1 (4)
O1W^{iii}—Sr1—C1—O1	−100.21 (19)	C3—C2—C11—C10	−177.3 (3)
O1W—Sr1—C1—O1	67.5 (4)	C1—C2—C11—C10	2.5 (5)
O1^{iii}—Sr1—C1—O1	108.66 (19)	C3—C2—C11—C6	0.3 (4)
O2^{iii}—Sr1—C1—O1	59.56 (18)	C1—C2—C11—C6	−179.9 (3)
O2—Sr1—C1—O1	−168.4 (3)	C7—C6—C11—C10	0.2 (4)

C1^{iii}—Sr1—C1—O1	83.28 (19)	C5—C6—C11—C10	178.8 (3)
Sr1^{iv}—Sr1—C1—O1	25.22 (18)	C7—C6—C11—C2	−177.6 (3)
Sr1^{i}—Sr1—C1—O1	−173.8 (2)	C5—C6—C11—C2	1.0 (4)
O2^{i}—Sr1—C1—O2	−7.9 (2)		

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $x, -y+1, z-1/2$; (iii) $-x, y, -z+3/2$; (iv) $-x, -y+1, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O1^{iv}	0.87 (1)	1.89 (1)	2.715 (3)	160 (3)

Symmetry code: (iv) $-x, -y+1, -z+1$.

(BaNPH) *catena*-poly[[diaquabarium(II)]-bis(*μ*-1-naphthoato)- κ^3*O,O′*:*O*;κ^3*O*:*O,O′*]

Crystal data

[Ba($C_{11}H_7O_2$)$_2$(H_2O)$_2$]
M_r = 515.70
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
a = 20.464 (3) Å
b = 11.9699 (15) Å
c = 8.2812 (10) Å
V = 2028.5 (4) Å^3
Z = 4

F(000) = 1016
D_x = 1.689 Mg m^{-3}
Synchrotron radiation, λ = 0.82520 Å
Cell parameters from 8174 reflections
θ = 3.7–32.9°
μ = 1.99 mm^{-1}
T = 150 K
Plate, colourless
0.10 × 0.10 × 0.01 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: Daresbury SRS station 9.8
Silicon 111 monochromator
fine slice ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.673, T_{max} = 1.000

14467 measured reflections
2355 independent reflections
2196 reflections with $I > 2\sigma(I)$
R_{int} = 0.172
θ_{max} = 33.0°, θ_{min} = 3.7°
h = −26→26
k = −15→15
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.126
S = 1.14
2355 reflections
139 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 1.7007P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.44 e Å^{-3}
$\Delta\rho_{min}$ = −1.45 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0135 (10)

Special details

Experimental. SADABS `absorbtion correction′ also includes a correction for synchrotron beam decay.

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 (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Ba1	0.5000	1.058363 (17)	0.2500	0.01293 (18)
O1	0.55542 (9)	0.89902 (15)	0.0331 (2)	0.0202 (4)
O2	0.58514 (11)	0.87800 (18)	0.2876 (3)	0.0227 (5)
O1W	0.58616 (10)	1.20076 (18)	0.0948 (2)	0.0259 (5)
H1W	0.5914 (16)	1.186 (3)	−0.0081 (16)	0.039*
H2W	0.6251 (9)	1.225 (3)	0.120 (4)	0.039*
C1	0.60220 (12)	0.7246 (2)	0.1049 (3)	0.0150 (5)
C2	0.56422 (13)	0.6626 (2)	0.0018 (3)	0.0205 (6)
H2	0.5252	0.6939	−0.0404	0.025*
C3	0.58220 (15)	0.5532 (2)	−0.0425 (4)	0.0253 (6)
H3	0.5547	0.5107	−0.1117	0.030*
C4	0.63869 (19)	0.5084 (2)	0.0137 (3)	0.0235 (7)
H4	0.6506	0.4347	−0.0173	0.028*
C5	0.68027 (13)	0.5699 (2)	0.1178 (3)	0.0182 (6)
C6	0.66177 (12)	0.67921 (19)	0.1673 (3)	0.0143 (5)
C7	0.70534 (16)	0.7392 (3)	0.2701 (3)	0.0176 (6)
H7	0.6941	0.8123	0.3054	0.021*
C8	0.76338 (14)	0.6921 (2)	0.3186 (4)	0.0237 (6)
H8	0.7920	0.7336	0.3863	0.028*
C9	0.7814 (2)	0.5833 (4)	0.2697 (4)	0.0252 (7)
H9	0.8214	0.5514	0.3051	0.030*
C10	0.74053 (14)	0.5246 (2)	0.1709 (3)	0.0236 (6)
H10	0.7527	0.4517	0.1370	0.028*
C11	0.57986 (12)	0.8419 (2)	0.1458 (3)	0.0159 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0188 (2)	0.0109 (2)	0.0090 (3)	0.000	−0.00099 (6)	0.000
O1	0.0285 (10)	0.0176 (9)	0.0144 (9)	0.0065 (7)	−0.0021 (7)	0.0025 (7)
O2	0.0319 (11)	0.0228 (10)	0.0133 (9)	0.0106 (9)	−0.0041 (9)	−0.0014 (9)
O1W	0.0254 (10)	0.0344 (11)	0.0178 (10)	−0.0105 (9)	−0.0011 (8)	−0.0002 (8)
C1	0.0181 (12)	0.0165 (11)	0.0103 (11)	0.0019 (9)	0.0013 (9)	0.0011 (9)
C2	0.0196 (13)	0.0215 (12)	0.0204 (14)	0.0020 (10)	−0.0042 (10)	−0.0014 (10)
C3	0.0312 (16)	0.0218 (14)	0.0228 (16)	−0.0038 (11)	−0.0026 (13)	−0.0073 (10)
C4	0.0316 (18)	0.0184 (13)	0.0206 (16)	0.0019 (10)	0.0032 (10)	−0.0049 (12)

C5	0.0222 (13)	0.0179 (12)	0.0145 (14)	0.0024 (9)	0.0037 (10)	0.0016 (9)
C6	0.0185 (12)	0.0148 (11)	0.0097 (11)	0.0001 (9)	0.0030 (9)	0.0038 (8)
C7	0.0178 (15)	0.0219 (15)	0.0132 (12)	−0.0032 (12)	0.0021 (10)	0.0028 (10)
C8	0.0211 (13)	0.0313 (15)	0.0187 (16)	−0.0024 (11)	−0.0034 (11)	0.0021 (11)
C9	0.0177 (18)	0.0361 (17)	0.0219 (16)	0.0075 (17)	0.0008 (11)	0.0067 (13)
C10	0.0263 (14)	0.0255 (13)	0.0190 (14)	0.0105 (11)	0.0021 (11)	0.0008 (11)
C11	0.0171 (11)	0.0183 (12)	0.0124 (13)	0.0013 (9)	−0.0001 (10)	0.0017 (9)

Geometric parameters (Å, º)

Ba1—O1^{i}	2.6536 (19)	C1—C11	1.515 (3)
Ba1—O1^{ii}	2.6536 (19)	C2—C3	1.409 (3)
Ba1—O1W	2.769 (2)	C2—H2	0.9500
Ba1—O1W^{iii}	2.769 (2)	C3—C4	1.356 (5)
Ba1—O2^{iii}	2.792 (2)	C3—H3	0.9500
Ba1—O2	2.792 (2)	C4—C5	1.418 (4)
Ba1—O1	2.8551 (18)	C4—H4	0.9500
Ba1—O1^{iii}	2.8551 (18)	C5—C10	1.417 (4)
Ba1—C11^{iii}	3.183 (3)	C5—C6	1.422 (3)
Ba1—C11	3.183 (3)	C6—C7	1.427 (4)
O1—C11	1.260 (3)	C7—C8	1.375 (4)
O1—Ba1^{i}	2.6536 (19)	C7—H7	0.9500
O2—C11	1.256 (3)	C8—C9	1.413 (5)
O1W—H1W	0.878 (10)	C8—H8	0.9500
O1W—H2W	0.872 (10)	C9—C10	1.365 (5)
C1—C2	1.373 (4)	C9—H9	0.9500
C1—C6	1.431 (3)	C10—H10	0.9500
O1^{i}—Ba1—O1^{ii}	157.84 (8)	O1^{i}—Ba1—Ba1^{iv}	153.96 (4)
O1^{i}—Ba1—O1W	75.15 (6)	O1^{ii}—Ba1—Ba1^{iv}	39.15 (4)
O1^{ii}—Ba1—O1W	91.13 (6)	O1W—Ba1—Ba1^{iv}	129.55 (4)
O1^{i}—Ba1—O1W^{iii}	91.13 (6)	O1W^{iii}—Ba1—Ba1^{iv}	75.93 (4)
O1^{ii}—Ba1—O1W^{iii}	75.15 (6)	O2^{iii}—Ba1—Ba1^{iv}	81.86 (5)
O1W—Ba1—O1W^{iii}	104.01 (9)	O2—Ba1—Ba1^{iv}	69.33 (5)
O1^{i}—Ba1—O2^{iii}	77.49 (6)	O1—Ba1—Ba1^{iv}	112.50 (4)
O1^{ii}—Ba1—O2^{iii}	120.93 (6)	O1^{iii}—Ba1—Ba1^{iv}	35.93 (4)
O1W—Ba1—O2^{iii}	145.25 (7)	C11^{iii}—Ba1—Ba1^{iv}	58.85 (5)
O1W^{iii}—Ba1—O2^{iii}	97.49 (7)	C11—Ba1—Ba1^{iv}	89.81 (5)
O1^{i}—Ba1—O2	120.93 (6)	Ba1^{i}—Ba1—Ba1^{iv}	142.707 (12)
O1^{ii}—Ba1—O2	77.49 (6)	C11—O1—Ba1^{i}	158.12 (17)
O1W—Ba1—O2	97.49 (7)	C11—O1—Ba1	93.10 (16)
O1W^{iii}—Ba1—O2	145.25 (7)	Ba1^{i}—O1—Ba1	104.93 (6)
O2^{iii}—Ba1—O2	78.69 (10)	C11—O2—Ba1	96.20 (16)
O1^{i}—Ba1—O1	75.07 (6)	Ba1—O1W—H1W	114 (2)
O1^{ii}—Ba1—O1	120.96 (6)	Ba1—O1W—H2W	133 (2)
O1W—Ba1—O1	82.30 (6)	H1W—O1W—H2W	101 (2)
O1W^{iii}—Ba1—O1	163.01 (6)	C2—C1—C6	120.1 (2)
O2^{iii}—Ba1—O1	70.19 (6)	C2—C1—C11	118.0 (2)
O2—Ba1—O1	46.03 (6)	C6—C1—C11	121.9 (2)
O1^{i}—Ba1—O1^{iii}	120.96 (6)	C1—C2—C3	121.1 (2)

O1^{ii}—Ba1—O1^{iii}	75.07 (6)
O1W—Ba1—O1^{iii}	163.01 (6)
O1W^{iii}—Ba1—O1^{iii}	82.30 (6)
O2^{iii}—Ba1—O1^{iii}	46.03 (6)
O2—Ba1—O1^{iii}	70.19 (6)
O1—Ba1—O1^{iii}	96.17 (8)
O1^{i}—Ba1—C11^{iii}	100.17 (6)
O1^{ii}—Ba1—C11^{iii}	97.84 (6)
O1W—Ba1—C11^{iii}	162.56 (7)
O1W^{iii}—Ba1—C11^{iii}	92.77 (6)
O2^{iii}—Ba1—C11^{iii}	23.10 (6)
O2—Ba1—C11^{iii}	70.16 (7)
O1—Ba1—C11^{iii}	80.26 (6)
O1^{iii}—Ba1—C11^{iii}	23.29 (6)
O1^{i}—Ba1—C11	97.84 (6)
O1^{ii}—Ba1—C11	100.17 (6)
O1W—Ba1—C11	92.77 (6)
O1W^{iii}—Ba1—C11	162.56 (7)
O2^{iii}—Ba1—C11	70.16 (7)
O2—Ba1—C11	23.10 (6)
O1—Ba1—C11	23.29 (6)
O1^{iii}—Ba1—C11	80.26 (6)
C11^{iii}—Ba1—C11	71.00 (9)
O1^{i}—Ba1—Ba1^{i}	39.15 (4)
O1^{ii}—Ba1—Ba1^{i}	153.96 (4)
O1W—Ba1—Ba1^{i}	75.93 (4)
O1W^{iii}—Ba1—Ba1^{i}	129.55 (4)
O2^{iii}—Ba1—Ba1^{i}	69.33 (5)
O2—Ba1—Ba1^{i}	81.86 (5)
O1—Ba1—Ba1^{i}	35.93 (4)
O1^{iii}—Ba1—Ba1^{i}	112.50 (4)
C11^{iii}—Ba1—Ba1^{i}	89.81 (5)
C11—Ba1—Ba1^{i}	58.85 (5)
C1—C2—H2	119.4
C3—C2—H2	119.4
C4—C3—C2	120.0 (3)
C4—C3—H3	120.0
C2—C3—H3	120.0
C3—C4—C5	121.0 (2)
C3—C4—H4	119.5
C5—C4—H4	119.5
C10—C5—C4	120.8 (3)
C10—C5—C6	119.6 (3)
C4—C5—C6	119.5 (3)
C5—C6—C7	117.9 (2)
C5—C6—C1	118.2 (2)
C7—C6—C1	123.8 (2)
C8—C7—C6	120.5 (3)
C8—C7—H7	119.7
C6—C7—H7	119.7
C7—C8—C9	121.3 (3)
C7—C8—H8	119.3
C9—C8—H8	119.3
C10—C9—C8	119.1 (3)
C10—C9—H9	120.5
C8—C9—H9	120.5
C9—C10—C5	121.5 (3)
C9—C10—H10	119.3
C5—C10—H10	119.3
O2—C11—O1	122.7 (2)
O2—C11—C1	120.1 (2)
O1—C11—C1	117.2 (2)
O2—C11—Ba1	60.70 (14)
O1—C11—Ba1	63.61 (14)
C1—C11—Ba1	165.96 (16)

O1^{i}—Ba1—O1—C11	−167.48 (18)
O1^{ii}—Ba1—O1—C11	29.24 (17)
O1W—Ba1—O1—C11	115.91 (15)
O1W^{iii}—Ba1—O1—C11	−130.9 (2)
O2^{iii}—Ba1—O1—C11	−85.66 (16)
O2—Ba1—O1—C11	7.66 (14)
O1^{iii}—Ba1—O1—C11	−47.04 (14)
C11^{iii}—Ba1—O1—C11	−64.11 (17)
Ba1^{i}—Ba1—O1—C11	−167.48 (18)
Ba1^{iv}—Ba1—O1—C11	−13.84 (16)
O1^{i}—Ba1—O1—Ba1^{i}	0.0
O1^{ii}—Ba1—O1—Ba1^{i}	−163.28 (5)
O1W—Ba1—O1—Ba1^{i}	−76.61 (7)
O1W^{iii}—Ba1—O1—Ba1^{i}	36.6 (2)
O2^{iii}—Ba1—O1—Ba1^{i}	81.82 (7)
C8—C9—C10—C5	−0.6 (5)
C4—C5—C10—C9	179.2 (3)
C6—C5—C10—C9	0.4 (4)
Ba1—O2—C11—O1	15.1 (3)
Ba1—O2—C11—C1	−163.85 (19)
Ba1^{i}—O1—C11—O2	−160.5 (3)
Ba1—O1—C11—O2	−14.7 (3)
Ba1^{i}—O1—C11—C1	18.5 (6)
Ba1—O1—C11—C1	164.29 (19)
Ba1^{i}—O1—C11—Ba1	−145.8 (5)
C2—C1—C11—O2	139.5 (3)
C6—C1—C11—O2	−42.0 (4)
C2—C1—C11—O1	−39.5 (3)
C6—C1—C11—O1	139.0 (2)
C2—C1—C11—Ba1	50.2 (8)

O2—Ba1—O1—Ba1^{i}	175.14 (11)	C6—C1—C11—Ba1	−131.3 (6)
O1^{iii}—Ba1—O1—Ba1^{i}	120.44 (8)	O1^{i}—Ba1—C11—O2	178.06 (16)
C11^{iii}—Ba1—O1—Ba1^{i}	103.37 (7)	O1^{ii}—Ba1—C11—O2	11.03 (17)
C11—Ba1—O1—Ba1^{i}	167.48 (18)	O1W—Ba1—C11—O2	102.68 (17)
Ba1^{iv}—Ba1—O1—Ba1^{i}	153.64 (4)	O1W^{iii}—Ba1—C11—O2	−61.6 (3)
O1^{i}—Ba1—O2—C11	−2.24 (19)	O2^{iii}—Ba1—C11—O2	−108.33 (17)
O1^{ii}—Ba1—O2—C11	−168.87 (17)	O1—Ba1—C11—O2	165.9 (3)
O1W—Ba1—O2—C11	−79.38 (17)	O1^{iii}—Ba1—C11—O2	−61.73 (17)
O1W^{iii}—Ba1—O2—C11	152.44 (16)	C11^{iii}—Ba1—C11—O2	−83.83 (17)
O2^{iii}—Ba1—O2—C11	65.59 (15)	Ba1^{i}—Ba1—C11—O2	174.40 (18)
O1—Ba1—O2—C11	−7.72 (15)	Ba1^{iv}—Ba1—C11—O2	−26.92 (16)
O1^{iii}—Ba1—O2—C11	112.70 (17)	O1^{i}—Ba1—C11—O1	12.21 (18)
C11^{iii}—Ba1—O2—C11	87.91 (17)	O1^{ii}—Ba1—C11—O1	−154.82 (15)
Ba1^{i}—Ba1—O2—C11	−4.84 (16)	O1W—Ba1—C11—O1	−63.18 (15)
Ba1^{iv}—Ba1—O2—C11	151.06 (17)	O1W^{iii}—Ba1—C11—O1	132.5 (2)
C6—C1—C2—C3	1.1 (4)	O2^{iii}—Ba1—C11—O1	85.82 (16)
C11—C1—C2—C3	179.6 (2)	O2—Ba1—C11—O1	−165.9 (3)
C1—C2—C3—C4	−1.7 (4)	O1^{iii}—Ba1—C11—O1	132.42 (14)
C2—C3—C4—C5	0.4 (5)	C11^{iii}—Ba1—C11—O1	110.32 (17)
C3—C4—C5—C10	−177.4 (3)	Ba1^{i}—Ba1—C11—O1	8.55 (13)
C3—C4—C5—C6	1.5 (4)	Ba1^{iv}—Ba1—C11—O1	167.23 (14)
C10—C5—C6—C7	−0.2 (4)	O1^{i}—Ba1—C11—C1	−84.6 (7)
C4—C5—C6—C7	−179.1 (2)	O1^{ii}—Ba1—C11—C1	108.4 (7)
C10—C5—C6—C1	176.9 (2)	O1W—Ba1—C11—C1	−160.0 (7)
C4—C5—C6—C1	−2.0 (4)	O1W^{iii}—Ba1—C11—C1	35.7 (8)
C2—C1—C6—C5	0.7 (4)	O2^{iii}—Ba1—C11—C1	−11.0 (7)
C11—C1—C6—C5	−177.7 (2)	O2—Ba1—C11—C1	97.3 (7)
C2—C1—C6—C7	177.6 (3)	O1—Ba1—C11—C1	−96.8 (7)
C11—C1—C6—C7	−0.8 (4)	O1^{iii}—Ba1—C11—C1	35.6 (7)
C5—C6—C7—C8	0.3 (4)	C11^{iii}—Ba1—C11—C1	13.5 (7)
C1—C6—C7—C8	−176.6 (3)	Ba1^{i}—Ba1—C11—C1	−88.3 (7)
C6—C7—C8—C9	−0.6 (5)	Ba1^{iv}—Ba1—C11—C1	70.4 (7)
C7—C8—C9—C10	0.8 (5)		

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x, -y+2, z+1/2$; (iii) $-x+1, y, -z+1/2$; (iv) $-x+1, -y+2, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2^{v}	0.88 (1)	1.86 (1)	2.713 (3)	163 (3)

Symmetry code: (v) $x, -y+2, z-1/2$.