Two metal–organic frameworks based on Sr²⁺ and 1,2,4,5-tetrakis(4-carboxyphenyl)benzene linkers

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Two structurally different metal–organic frameworks based on Sr²⁺ ions and 1,2,4,5-tetrakis(4-carboxyphenyl)benzene linkers have been synthesized solvothermally in different solvent systems and studied with single-crystal X-ray diffraction technique. These are poly[[μ_{12}-4,4′,4″,4‴-(benzene-1,2,4,5-tetrayl)tetrabenzoato](dimethylformamide)distrontium(II)], [Sr$_2$(C$_{34}$H$_{18}$O$_8$)(C$_3$H$_7$NO)$_2$]$_n$, and poly[tetraaqua{μ_2-4,4′-[4,5-bis(4-carboxyphenyl)benzene-1,2-diyl]dibenzoato}tristrontium(II)], [Sr$_3$(C$_{34}$H$_{20}$O$_8$)$_2$(H$_2$O)$_4$]. The differences are noted between the crystal structures and coordination modes of these two MOFs, which are responsible for their semiconductor properties, where structural control over the bandgap is desirable. Hydrogen bonding is present in only one of the compounds, suggesting it has a slightly higher structural stability.

1. Chemical context

Porous crystalline networks based on metal ion-coordinated organic ligands, known as metal–organic frameworks (MOFs), have been an object of extensive studies for the past two decades. Such interest in these materials can be attributed to their fascinating properties and potential applications in a wide range of areas – from luminescent lighting and sensing to gas storage, to semiconductors (Kreno *et al.* 2012; Zhou *et al.* 2012; Furukawa *et al.* 2013; Gassensmith *et al.* 2014). Their intrinsically unlimited structural and compositional diversity allows the design of structures with virtually any desirable properties. Belonging to the class of coordination compounds, MOFs naturally tend to work particularly well when synthesized with transition-metal-ion centers, yet they still suffer from several drawbacks, namely the decreased stability, toxicity and relatively high cost of manufacture. In recent years, a new class of alkaline-metal-based MOFs has arisen, providing a solution for the aforementioned problems. Abundant in Earth's crust and generally non-toxic, ions of Ca, Sr and Ba, for example, have been reported to provide a structurally rich array of compounds with increased stability and unique properties (Kundu *et al.* 2012). Strontium to date has been a more 'exotic' choice in MOF design, with very few structures synthesized and studied. Still, several reports have recently indicated the possibility of Sr–MOF design, which yields structures with unique luminescent (Jia *et al.* 2017) and semiconducting (Usman *et al.* 2015) properties, the latter being relatively rare for MOFs and of great interest.
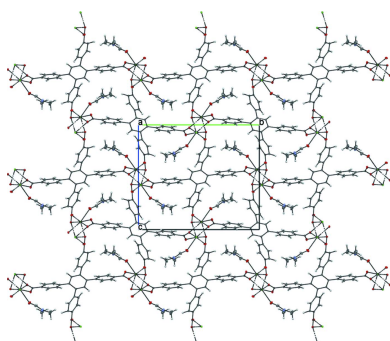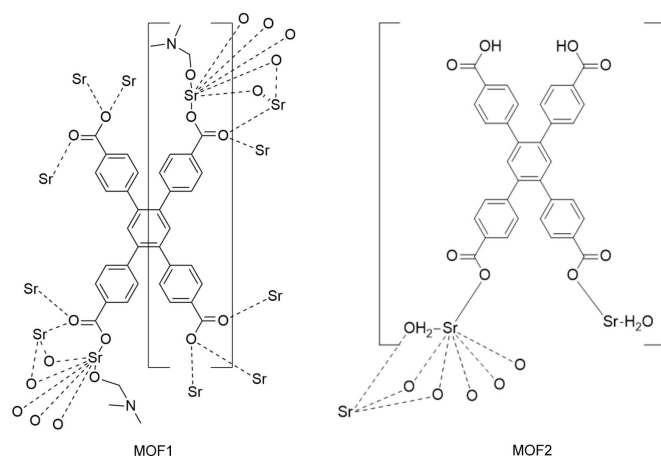
In this work two metal–organic complexes have been synthesized from strontium nitrate as metal ion source and 1,2,4,5-tetrakis(4-carboxyphenyl)benzene as linker under slightly different synthetic conditions (see *Synthesis and crystallization*). For reference purposes these are labeled as **MOF1** and **MOF2**, for the dimethylformamide (DMF) and non-DMF containing products, poly[[μ_{12}-4,4′,4″,4‴-(benzene-1,2,4,5-tetrayl)tetrabenzoato](dimethylformamide)distrontium(II)] and poly[tetraaqua[μ_{2}-4,5-bis(4-carboxyphenyl)-4,4′-(benzene-1,2-diyl)dibenzoato]tristrontium(II)], respectively.

2. Structural commentary

Fig. 1 illustrates the molecular structures of **MOF1** and **MOF2**, specifically their asymmetric units. Selected bond lengths are summarized in Tables 1 and 2. In both complexes, an Sr atom with an O$_7$ coordination set is present; however, in **MOF2** the asymmetric unit contains two Sr atoms, one seven- and the other eight-coordinated. In **MOF1**, the O$_7$ set comprises six O atoms belonging to the carboxyl groups of the ligands (O1–O4) and one atom (O5) belonging to a DMF molecule. In **MOF2**, the seven-coordinated Sr atom is surrounded by five oxygens of carboxyl groups (O4–O7, O9) and two oxygens of water molecules (O8 and O10). The other Sr atom coordinates eight oxygen atoms somewhat similarly: two from water (O8) and six from the carboxyl groups of the ligands (O5–O7). The multidentate nature of the 1,2,4,5-tetrakis(4-carboxyphenyl)benzene ligand, together with the high coordination number of the Sr atom, results in an interesting structure for both complexes.

The coordination environments of the Sr ions for both complexes are presented in Fig. 2. It can be seen that in **MOF1** all available oxygen atoms are coordinated to a metal center, thus all carboxyl groups in the ligands participate in the coordination.

In **MOF2**, atoms O1–O3 are not involved in coordination. While this fact leaves one of the four carboxyl groups (the O1–C1–O2 group) uncoordinated, it does receive some degree of additional stability from hydrogen bonding *via* the O1 atom

Figure 1
A view of the asymmetric units of **MOF1** (top) and **MOF2** (bottom) with the atom-labeling schemes. Displacement ellipsoids are drawn at the 50% probability level.

Table 3
Hydrogen-bond geometry (Å, °) for **MOF2**.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1$\cdots$O4^i	0.84	1.79	2.6051 (18)	164
O10—H10A$\cdots$O2^v	0.84 (3)	1.97 (3)	2.795 (2)	168 (3)
O10—H10B$\cdots$O6^{vi}	0.78 (3)	2.01 (3)	2.787 (2)	173 (3)
O8—H8B$\cdots$O3^{vii}	0.83 (3)	1.77 (3)	2.5948 (19)	170 (3)

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

(see *Supramolecular features* for more details). The remaining O2 atom shows some degree of disorder due to vibration.

3. Supramolecular features

. The packing of **MOF1** is shown in Fig. 3. While the abundance of carboxyl groups in the ligand provides a lot of potential for hydrogen-bonding sites, only **MOF2** exhibits such interactions (Table 3). Four inequivalent hydrogen bonds of the type O—H$\cdots$O are found in the crystal packing (Fig. 4), which are likely to contribute to additional structural stability compared to **MOF1**, which is lacking these or any other specific interactions. That said, three out of the four hydrogen bonds in **MOF2** stabilize the water molecule rather than the crystal structure directly

4. Database survey

No entries were found in the Cambridge Structural Database (CSD version 5.40, update of September 2019; Groom *et al.*, 2016) for metal–organic frameworks with the same metal–ligand combination as in the title compounds. For MOFs based on the title ligand, shown in the scheme below, and different metal ions, the search yielded eleven matches, among which ions of such metals as Cu, Mg, Zn, Co and Bi were present. The crystal structure of the pure ligand (ZARXOI; Hisaki *et al.* 2017), shown below, was also found during the search.
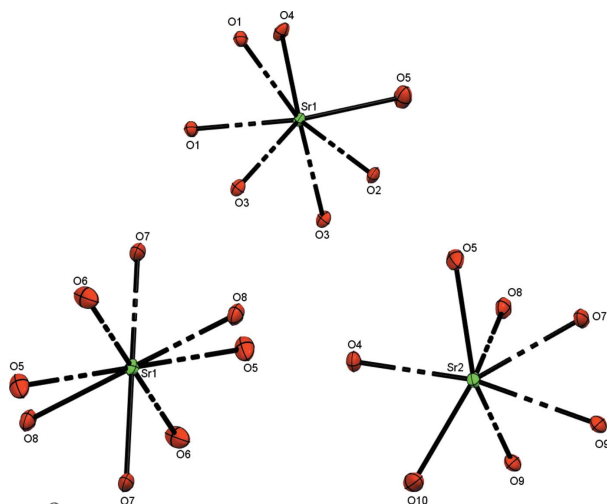
Figure 2
Coordination environments of the Sr atoms in **MOF1** (top) with an O_7 set and **MOF2** (bottom) with O_8 and O_7 sets.
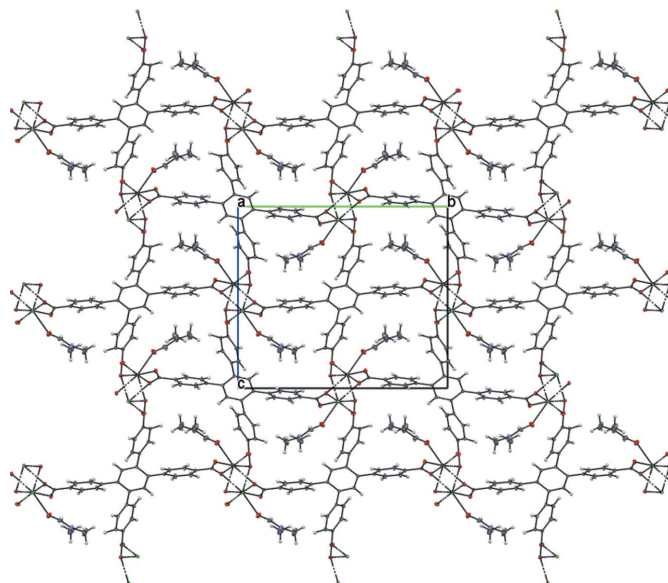
Figure 3
A view along the *a* axis of **MOF1**. Large channel-like pores are occupied by the DMF solvent molecules.
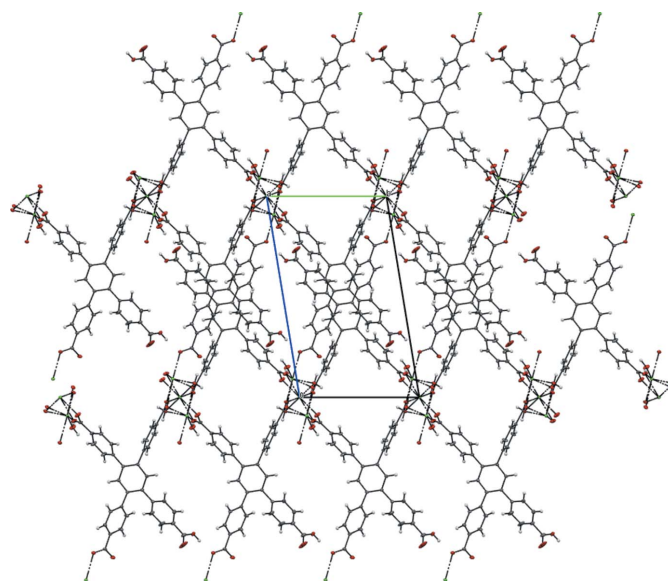
Figure 4
A view along the *a* axis of **MOF2**.

The ligand crystallizes in the orthorhombic system in space group *Pbcn*. MOFs with this linker, however, prefer the triclinic space group $P\bar{1}$, with some exceptions (see Table 4).
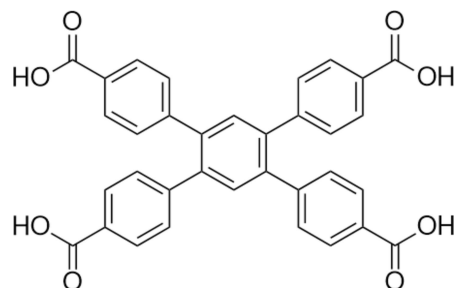
Table 4
Selected CSD data for title ligand-derived MOFs.

CSD code	Cation	Coordination number	Space group	Crystal system	Reference
ATIBUD	Zn^{2+}	6	$P\bar{1}$	triclinic	(Dissem *et al.* 2021)
ATICAK	Zn^{2+}	6	$P\bar{1}$	triclinic	(Dissem *et al.* 2021)
ATICEO	Zn^{2+}	6	$P\bar{1}$	triclinic	(Dissem *et al.* 2021)
ATICIS	Cu^{2+}	6	$P\bar{1}$	triclinic	(Dissem *et al.* 2021)
ATICOY	Cu^{2+}	6	$P\bar{1}$	triclinic	(Dissem *et al.* 2021)
ATICUE	Cu^{2+}	6	$P\bar{1}$	triclinic	(Dissem *et al.* 2021)
FIYDEZ	Co^{2+}	6	$I2/a$	monoclinic	(Dhankhar & Nagaraja 2019)
MIFKUJ	Zn^{2+}	4	$P\bar{1}$	triclinic	(Karra *et al.* 2013)
MIFLIY	Mg^{2+}	6	$C2/c$	monoclinic	(Karra, *et al.* 2013)
MIFMIZ	Ni^{2+}	6	$P\bar{1}$	triclinic	(Karra *et al.* 2013)
MIHMOI	Bi^{2+}	5	$C2/c$	monoclinic	(Köppen *et al.* 2018)

The dihedral angles between the phenyl rings and the central benzene moiety in the ligand are nearly equal: two pairs of 52.66 (18)° and two pairs of 51.05 (18)°. In **MOF1**, the pairwise equality of these angles is conserved; however, both sets of phenyl rings experience significant twists, being 38.08 (11) and 57.88 (11)°, respectively, for each pair. In **MOF2**, an even larger difference is observed, with dihedral angles of 47.44 (8), 60.17 (8), 60.49 (8) and 70.64 (8)° being found between the rings.

5. Synthesis and crystallization

MOF1 was synthesized as follows. Strontium nitrate (0.0212 g, 0.1 mmol), and 1,2,4,5-tetrakis(4-carboxyphenyl) benzene (0.0558 g, 0.1 mmol) were measured, placed in a beaker and dissolved in a mixture of DMF (3 mL) and water (3 mL). The solution was stirred, transferred to a Teflon-lined autoclave and sealed in a reactor, which was placed in the oven at 393 K for 120 h. The autoclave was removed from the oven and allowed to cool to room temperature.

The procedure for **MOF2** differed slightly. The same amounts of the metal precursor and ligand were placed in a beaker and dissolved in a mixture of ethanol (3 mL) and water (3 mL). The solution was stirred, transferred to a Teflon-lined autoclave and sealed in a reactor, which was placed in the oven at 393 K for 120 h. The autoclave was removed from the oven and allowed to cool to room temperature.

After each synthesis, the white crystals of the products were washed with methanol and collected by means of vacuum
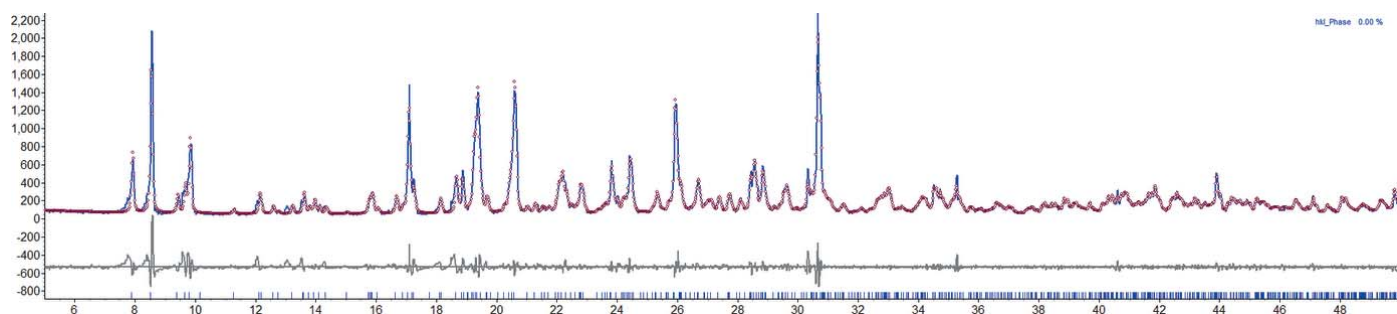
Figure 5
Pawley fit for **MOF2**. The initial parameters were taken from the cif file.
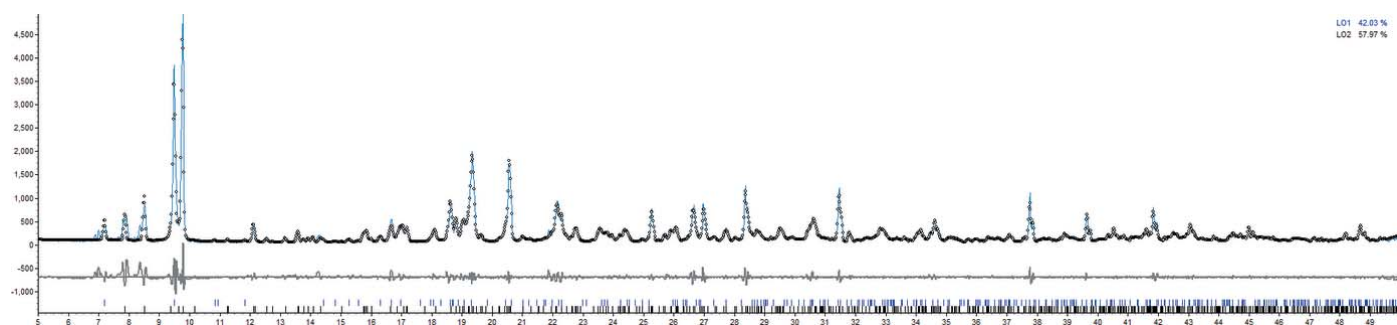
Figure 6
Pawley fit for the bulk solid obtained in the synthesis of **MOF1**. The thick blue lines indicate the crystalline phase for **MOF2** while the thick black lines indicate the crystalline phase for **MOF1**. The initial parameters were taken from the cif files for both MOFs.

Table 5
Experimental details.

	MOF1	MOF2
Crystal data		
Chemical formula	$[Sr_2(C_{34}H_{18}O_8)(C_3H_7NO)_2]$	$[Sr_3(C_{34}H_{20}O_8)_2(H_2O)_4]$
M_r	875.92	1445.91
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$
Temperature (K)	173	100
a, b, c (Å)	5.9350 (2), 18.6130 (8), 16.1256 (7)	9.240 (3), 11.330 (4), 19.414 (7)
α, β, γ (°)	90, 91.853 (2), 90	80.147 (6), 81.815 (7), 85.494 (7)
V (Å³)	1780.43 (12)	1979.1 (12)
Z	2	1
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm⁻¹)	3.06	2.08
Crystal size (mm)	$0.41 \times 0.12 \times 0.10$	$0.4 \times 0.3 \times 0.2$
Data collection		
Diffractometer	Bruker D8 VENTURE diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.63, 0.75	0.636, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	91152, 5387, 4453	33795, 10986, 9468
R_{int}	0.092	0.027
$(\sin \theta/\lambda)_{max}$ (Å⁻¹)	0.713	0.694
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.113, 0.87	0.030, 0.085, 1.08
No. of reflections	5387	10986
No. of parameters	246	429
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å⁻³)	0.94, −0.79	0.58, −0.40

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020) and *OLEX2* (Dolomanov *et al.*, 2009).

filtration into a capped vial. An important aspect of this study is the demonstrated possibility of structural control over Sr-based MOFs *via* slight changes in the synthesis conditions. This may be particularly important for semiconducting MOFs, where a structurally tuned bandgap may be desirable.

6. Powder X-ray diffraction

In order to identify any potential byproducts or starting materials within the bulk material of **MOF2**, PXRD was conducted using a conventional Bragg–Brentano PXRD instrument. A Pawley fit shows only one crystalline phase (Fig. 5), and this crystalline phase corresponds to the desired product as it has similar lattice parameters to the single crystal with only a minor increase of 7 Å³ of the total unit-cell volume from the single crystal to bulk solid at RT. The resulting lattice parameters for **MOF2** from PXRD are $a = 9.274$ (1), $b = 11.391$ (1), $c = 19.274$ (3) Å, $\alpha = 80.38$ (1), $\beta = 82.04$ (1), $\gamma = 86.11$ (1)°, $V = 1986.3$ Å³. Unfortunately, in the case of **MOF1**, an analysis by PXRD reveals the phases for **MOF1** and **MOF2** in the same bulk material (Fig. 6), as in order to do a Pawley fit for this sample both structures are needed. It is possible that for the bulk solid of **MOF1** other additional impurities are present as a few peaks below 10° were not indexed for either **MOF1** or **MOF2** (Fig. 6).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. All C-bound H atoms were positioned geometrically (C—H = 0.95–0.98 Å) and refined using a riding model, $U_{iso}(H) = 1.2U_{eq}(C)$. All O-bound H atoms were found from difference Fourier maps and freely refined. For **MOF2**, it was not possible to localize the H atoms at O3 and O6.

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Two metal–organic frameworks based on Sr^{2+} and 1,2,4,5-tetrakis(4-carboxyphenyl)benzene linkers

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Computing details

For both structures, data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* Bruker, 2017); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b). Molecular graphics: *Mercury* (Macrae *et al.*, 2020) for MOF1; *OLEX2* (Dolomanov *et al.*, 2009) for MOF2. For both structures, software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Poly[[μ_{12}-4,4′,4″,4‴-(benzene-1,2,4,5-tetrayl)tetrabenzoato](dimethylformamide)distrontium(II)] (MOF1)

Crystal data

[Sr$_2$(C$_{34}$H$_{18}$O$_8$)(C$_3$H$_7$NO)$_2$]	$F(000) = 884$
$M_r = 875.92$	$D_x = 1.634$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 5.9350$ (2) Å	Cell parameters from 9912 reflections
$b = 18.6130$ (8) Å	$\theta = 2.5–30.3°$
$c = 16.1256$ (7) Å	$\mu = 3.06$ mm^{-1}
$\beta = 91.853$ (2)°	$T = 173$ K
$V = 1780.43$ (12) Å^3	Needle, colourless
$Z = 2$	$0.41 \times 0.12 \times 0.10$ mm

Data collection

Bruker D8 VENTURE diffractometer	$T_{min} = 0.63$, $T_{max} = 0.75$
Radiation source: microfocus sealed tube, sealed tube	91152 measured reflections
Multilayer mirror monochromator	5387 independent reflections
Detector resolution: 10.4167 pixels mm^{-1}	4453 reflections with $I > 2\sigma(I)$
ω and φ scans, narrow frame width, shutterless	$R_{int} = 0.092$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$\theta_{max} = 30.4°$, $\theta_{min} = 2.5°$
	$h = -8\rightarrow8$
	$k = -26\rightarrow26$
	$l = -22\rightarrow22$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.033$	
$wR(F^2) = 0.113$	
$S = 0.87$	Hydrogen site location: inferred from neighbouring sites
5387 reflections	H-atom parameters constrained
246 parameters	
0 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ e Å^{-3}

Special details

Experimental. Crystal suitable for X–ray structure determination was selected under the polarizing microscope, covered with Paratone oil and mounted on a goniometer head using Mitegen cryoloop. Experiment was performed at the low temperature. QUINN software was used to calculate optimal data collection strategy. Data were collected till resolution of 0.71 A and were truncated with XPREP till actual observed resolution.

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

Refinement. The systematic absences in the diffraction data were consistent for the stated space group. The position of almost all non—hydrogen atoms were found by direct methods. The remaining atoms were located in an alternating series of least–squares cycles on difference Fourier map.

All non–hydrogen atoms were refined in full–matrix anisotropic approximation. All hydrogen atoms were placed in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

Final results were tested with CHECKCIF routine and all A–warnings (if any) were addressed on the very top of this file.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr1	1.26769 (3)	0.02155 (2)	0.57357 (2)	0.00827 (8)
O1	−0.0949 (3)	0.55858 (9)	0.06890 (10)	0.0112 (3)
O2	−0.4151 (3)	0.55104 (9)	0.13843 (10)	0.0136 (3)
O3	0.6267 (2)	0.07945 (8)	0.52809 (10)	0.0109 (3)
O4	0.9519 (3)	0.10863 (9)	0.59477 (11)	0.0134 (3)
O5	1.3861 (3)	0.09879 (10)	0.70033 (12)	0.0221 (4)
N1	1.3944 (4)	0.20500 (12)	0.76924 (15)	0.0237 (5)
C1	−0.2063 (3)	0.55326 (11)	0.13488 (13)	0.0087 (4)
C2	−0.0700 (3)	0.54814 (12)	0.21498 (13)	0.0091 (4)
C3	0.1403 (3)	0.58190 (12)	0.22287 (13)	0.0100 (4)
H3	0.132344	0.633313	0.205003	0.012*
C4	0.2716 (3)	0.57343 (12)	0.29489 (14)	0.0104 (4)
H4	0.412954	0.597216	0.300185	0.013*
C5	0.1993 (4)	0.53065 (11)	0.35938 (14)	0.0094 (4)
C6	−0.0111 (4)	0.49740 (14)	0.35140 (14)	0.0131 (4)
H6	−0.06246	0.468151	0.395216	0.016*
C7	−0.1471 (4)	0.50652 (13)	0.27989 (15)	0.0127 (4)
H7	−0.29139	0.484462	0.275591	0.015*
C8	0.3496 (4)	0.51761 (11)	0.43368 (14)	0.0094 (4)
C9	0.4097 (4)	0.44680 (12)	0.45112 (14)	0.0106 (4)
H9	0.34665	0.409848	0.417002	0.013*
C10	0.5582 (3)	0.42735 (11)	0.51635 (13)	0.0097 (4)
C11	0.6141 (4)	0.35008 (11)	0.52796 (13)	0.0096 (4)
C12	0.8328 (4)	0.32679 (12)	0.54984 (15)	0.0123 (4)
H12	0.950402	0.361023	0.557342	0.015*
C13	0.8791 (3)	0.25430 (12)	0.56065 (15)	0.0119 (4)

H13	1.027204	0.239731	0.577266	0.014*
C14	0.7129 (3)	0.20260 (11)	0.54761 (14)	0.0097 (4)
C15	0.4962 (4)	0.22504 (12)	0.52379 (16)	0.0150 (4)
H15	0.381025	0.190494	0.513177	0.018*
C16	0.4483 (4)	0.29796 (12)	0.51552 (15)	0.0142 (4)
H16	0.298689	0.312497	0.501034	0.017*
C17	0.7695 (3)	0.12412 (12)	0.55842 (13)	0.0089 (4)
C18	1.2917 (4)	0.15257 (14)	0.72679 (16)	0.0202 (5)
H18	1.133968	0.156933	0.71609	0.024*
C19	1.2757 (6)	0.27042 (18)	0.7921 (2)	0.0426 (9)
H19A	1.343578	0.311797	0.764847	0.064*
H19B	1.287327	0.276823	0.852445	0.064*
H19C	1.116626	0.266555	0.774482	0.064*
C20	1.6365 (5)	0.20386 (19)	0.7840 (2)	0.0397 (8)
H20A	1.702782	0.247421	0.760936	0.06*
H20B	1.700094	0.161503	0.757298	0.06*
H20C	1.670376	0.20188	0.843878	0.06*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00658 (11)	0.00830 (11)	0.00978 (12)	0.00054 (6)	−0.00196 (7)	−0.00102 (7)
O1	0.0118 (7)	0.0121 (8)	0.0096 (7)	−0.0008 (6)	0.0000 (6)	−0.0014 (6)
O2	0.0084 (7)	0.0193 (9)	0.0128 (8)	0.0002 (6)	−0.0036 (6)	−0.0017 (6)
O3	0.0109 (7)	0.0073 (7)	0.0142 (8)	−0.0020 (6)	−0.0014 (6)	−0.0011 (6)
O4	0.0104 (7)	0.0106 (8)	0.0188 (8)	0.0039 (6)	−0.0041 (6)	−0.0012 (6)
O5	0.0218 (9)	0.0208 (10)	0.0232 (10)	0.0048 (7)	−0.0053 (7)	−0.0092 (7)
N1	0.0247 (11)	0.0178 (11)	0.0283 (12)	0.0004 (9)	−0.0026 (9)	−0.0089 (9)
C1	0.0104 (9)	0.0064 (10)	0.0092 (9)	−0.0007 (7)	−0.0022 (7)	−0.0014 (7)
C2	0.0094 (9)	0.0091 (10)	0.0088 (9)	0.0023 (8)	−0.0018 (7)	−0.0026 (8)
C3	0.0099 (9)	0.0086 (9)	0.0115 (10)	0.0006 (7)	−0.0021 (8)	−0.0002 (8)
C4	0.0080 (9)	0.0099 (10)	0.0131 (10)	−0.0008 (7)	−0.0038 (7)	−0.0013 (8)
C5	0.0111 (10)	0.0072 (10)	0.0096 (10)	0.0017 (7)	−0.0038 (8)	−0.0007 (7)
C6	0.0143 (10)	0.0132 (10)	0.0118 (11)	−0.0032 (9)	−0.0015 (8)	0.0030 (9)
C7	0.0094 (9)	0.0141 (11)	0.0146 (11)	−0.0023 (8)	−0.0010 (8)	−0.0003 (9)
C8	0.0094 (9)	0.0090 (10)	0.0095 (10)	0.0017 (7)	−0.0030 (8)	0.0020 (7)
C9	0.0134 (9)	0.0083 (10)	0.0098 (10)	0.0002 (8)	−0.0048 (8)	−0.0007 (8)
C10	0.0114 (9)	0.0083 (10)	0.0093 (10)	0.0000 (7)	−0.0017 (7)	0.0001 (7)
C11	0.0121 (9)	0.0053 (9)	0.0112 (10)	0.0017 (7)	−0.0031 (7)	0.0004 (7)
C12	0.0113 (10)	0.0063 (10)	0.0193 (11)	−0.0017 (8)	−0.0015 (8)	0.0009 (8)
C13	0.0071 (9)	0.0090 (10)	0.0195 (11)	0.0022 (7)	−0.0032 (8)	−0.0004 (8)
C14	0.0095 (9)	0.0074 (9)	0.0122 (10)	0.0015 (7)	−0.0011 (8)	0.0001 (8)
C15	0.0110 (10)	0.0090 (10)	0.0246 (12)	−0.0023 (8)	−0.0047 (9)	0.0012 (9)
C16	0.0091 (9)	0.0083 (10)	0.0249 (12)	−0.0004 (7)	−0.0045 (8)	0.0020 (9)
C17	0.0115 (9)	0.0085 (10)	0.0067 (9)	−0.0005 (7)	0.0007 (7)	−0.0009 (7)
C18	0.0186 (11)	0.0243 (13)	0.0172 (12)	0.0013 (10)	−0.0056 (9)	−0.0056 (10)
C19	0.0467 (19)	0.0247 (16)	0.056 (2)	0.0092 (14)	−0.0039 (16)	−0.0189 (16)
C20	0.0273 (15)	0.0388 (19)	0.053 (2)	−0.0104 (13)	−0.0019 (14)	−0.0190 (16)

Geometric parameters (Å, º)

Sr1—O4	2.5094 (15)	C5—C8	1.490 (3)
Sr1—O2ⁱ	2.5170 (16)	C6—C7	1.396 (3)
Sr1—O3ⁱⁱ	2.5180 (15)	C6—H6	0.95
Sr1—O5	2.5780 (18)	C7—H7	0.95
Sr1—O1ⁱⁱⁱ	2.5792 (16)	C8—C9	1.392 (3)
Sr1—O3^{iv}	2.5848 (16)	C8—C10^{vii}	1.403 (3)
Sr1—O1^v	2.6176 (16)	C9—C10	1.398 (3)
Sr1—C3^v	3.193 (2)	C9—H9	0.95
Sr1—C1^v	3.318 (2)	C10—C11	1.487 (3)
Sr1—C2^v	3.346 (2)	C11—C16	1.392 (3)
Sr1—Sr1^{vi}	3.7817 (4)	C11—C12	1.402 (3)
Sr1—Sr1^{iv}	3.9854 (4)	C12—C13	1.387 (3)
O1—C1	1.274 (3)	C12—H12	0.95
O2—C1	1.243 (2)	C13—C14	1.389 (3)
O3—C17	1.274 (3)	C13—H13	0.95
O4—C17	1.248 (2)	C14—C15	1.394 (3)
O5—C18	1.230 (3)	C14—C17	1.508 (3)
N1—C18	1.329 (3)	C15—C16	1.392 (3)
N1—C20	1.449 (4)	C15—H15	0.95
N1—C19	1.460 (4)	C16—H16	0.95
C1—C2	1.505 (3)	C18—H18	0.95
C2—C7	1.391 (3)	C19—H19A	0.98
C2—C3	1.399 (3)	C19—H19B	0.98
C3—C4	1.387 (3)	C19—H19C	0.98
C3—H3	1.0	C20—H20A	0.98
C4—C5	1.389 (3)	C20—H20B	0.98
C4—H4	0.95	C20—H20C	0.98
C5—C6	1.396 (3)		
O4—Sr1—O2ⁱ	147.34 (5)	C20—N1—C19	117.0 (2)
O4—Sr1—O3ⁱⁱ	113.95 (5)	O2—C1—O1	125.8 (2)
O2ⁱ—Sr1—O3ⁱⁱ	73.87 (5)	O2—C1—C2	117.87 (19)
O4—Sr1—O5	73.58 (5)	O1—C1—C2	116.28 (18)
O2ⁱ—Sr1—O5	77.82 (6)	O2—C1—Sr1^{ix}	148.85 (15)
O3ⁱⁱ—Sr1—O5	77.34 (6)	O1—C1—Sr1^{ix}	46.87 (10)
O4—Sr1—O1ⁱⁱⁱ	70.83 (5)	C2—C1—Sr1^{ix}	77.98 (11)
O2ⁱ—Sr1—O1ⁱⁱⁱ	141.62 (5)	C7—C2—C3	119.7 (2)
O3ⁱⁱ—Sr1—O1ⁱⁱⁱ	86.67 (5)	C7—C2—C1	120.01 (19)
O5—Sr1—O1ⁱⁱⁱ	130.36 (5)	C3—C2—C1	120.18 (19)
O4—Sr1—O3^{iv}	138.90 (5)	C7—C2—Sr1^{ix}	121.05 (15)
O2ⁱ—Sr1—O3^{iv}	71.32 (5)	C3—C2—Sr1^{ix}	71.58 (12)
O3ⁱⁱ—Sr1—O3^{iv}	84.36 (5)	C1—C2—Sr1^{ix}	75.93 (11)
O5—Sr1—O3^{iv}	147.47 (5)	C4—C3—C2	120.0 (2)
O1ⁱⁱⁱ—Sr1—O3^{iv}	74.15 (5)	C4—C3—Sr1^{ix}	115.00 (14)
O4—Sr1—O1^v	75.82 (5)	C2—C3—Sr1^{ix}	83.85 (13)
O2ⁱ—Sr1—O1^v	108.02 (5)	C4—C3—H3	111.7

O3ⁱⁱ—Sr1—O1ᵛ	159.75 (5)	C2—C3—H3	111.7
O5—Sr1—O1ᵛ	122.91 (6)	Sr1ⁱˣ—C3—H3	111.7
O1ⁱⁱⁱ—Sr1—O1ᵛ	79.85 (5)	C3—C4—C5	120.90 (19)
O3ⁱᵛ—Sr1—O1ᵛ	77.49 (5)	C3—C4—H4	119.5
O4—Sr1—C3ᵛ	95.21 (6)	C5—C4—H4	119.5
O2ⁱ—Sr1—C3ᵛ	63.58 (5)	C4—C5—C6	118.8 (2)
O3ⁱⁱ—Sr1—C3ᵛ	134.51 (5)	C4—C5—C8	120.27 (19)
O5—Sr1—C3ᵛ	78.67 (6)	C6—C5—C8	120.8 (2)
O1ⁱⁱⁱ—Sr1—C3ᵛ	137.38 (5)	C5—C6—C7	120.9 (2)
O3ⁱᵛ—Sr1—C3ᵛ	96.19 (5)	C5—C6—H6	119.5
O1ᵛ—Sr1—C3ᵛ	57.55 (5)	C7—C6—H6	119.5
O4—Sr1—C1ᵛ	65.57 (5)	C2—C7—C6	119.6 (2)
O2ⁱ—Sr1—C1ᵛ	106.31 (5)	C2—C7—H7	120.2
O3ⁱⁱ—Sr1—C1ᵛ	179.38 (5)	C6—C7—H7	120.2
O5—Sr1—C1ᵛ	102.11 (6)	C9—C8—C10ᵛⁱⁱ	118.86 (19)
O1ⁱⁱⁱ—Sr1—C1ᵛ	93.50 (5)	C9—C8—C5	117.35 (19)
O3ⁱᵛ—Sr1—C1ᵛ	96.26 (5)	C10ᵛⁱⁱ—C8—C5	123.70 (18)
O1ᵛ—Sr1—C1ᵛ	20.81 (5)	C8—C9—C10	123.3 (2)
C3ᵛ—Sr1—C1ᵛ	45.45 (5)	C8—C9—H9	118.4
O4—Sr1—C2ᵛ	72.01 (5)	C10—C9—H9	118.4
O2ⁱ—Sr1—C2ᵛ	88.00 (5)	C9—C10—C8ᵛⁱⁱ	117.9 (2)
O3ⁱⁱ—Sr1—C2ᵛ	153.58 (5)	C9—C10—C11	118.56 (19)
O5—Sr1—C2ᵛ	80.19 (6)	C8ᵛⁱⁱ—C10—C11	123.55 (19)
O1ⁱⁱⁱ—Sr1—C2ᵛ	118.76 (5)	C16—C11—C12	117.72 (19)
O3ⁱᵛ—Sr1—C2ᵛ	108.25 (5)	C16—C11—C10	120.14 (19)
O1ᵛ—Sr1—C2ᵛ	44.66 (5)	C12—C11—C10	122.13 (19)
C3ᵛ—Sr1—C2ᵛ	24.57 (5)	C13—C12—C11	120.7 (2)
C1ᵛ—Sr1—C2ᵛ	26.10 (5)	C13—C12—H12	119.7
O4—Sr1—Sr1ᵛⁱ	141.76 (4)	C11—C12—H12	119.7
O2ⁱ—Sr1—Sr1ᵛⁱ	66.18 (4)	C12—C13—C14	121.19 (19)
O3ⁱⁱ—Sr1—Sr1ᵛⁱ	42.86 (4)	C12—C13—H13	119.4
O5—Sr1—Sr1ᵛⁱ	115.48 (4)	C14—C13—H13	119.4
O1ⁱⁱⁱ—Sr1—Sr1ᵛⁱ	76.98 (3)	C13—C14—C15	118.6 (2)
O3ⁱᵛ—Sr1—Sr1ᵛⁱ	41.50 (3)	C13—C14—C17	119.93 (18)
O1ᵛ—Sr1—Sr1ᵛⁱ	118.46 (4)	C15—C14—C17	121.48 (19)
C3ᵛ—Sr1—Sr1ᵛⁱ	122.72 (4)	C16—C15—C14	120.1 (2)
C1ᵛ—Sr1—Sr1ᵛⁱ	137.76 (4)	C16—C15—H15	119.9
C2ᵛ—Sr1—Sr1ᵛⁱ	144.14 (4)	C14—C15—H15	119.9
O4—Sr1—Sr1ⁱᵛ	68.07 (4)	C11—C16—C15	121.6 (2)
O2ⁱ—Sr1—Sr1ⁱᵛ	135.27 (4)	C11—C16—H16	119.2
O3ⁱⁱ—Sr1—Sr1ⁱᵛ	125.35 (4)	C15—C16—H16	119.2
O5—Sr1—Sr1ⁱᵛ	140.89 (4)	O4—C17—O3	125.9 (2)
O1ⁱⁱⁱ—Sr1—Sr1ⁱᵛ	40.28 (4)	O4—C17—C14	117.70 (19)
O3ⁱᵛ—Sr1—Sr1ⁱᵛ	71.39 (3)	O3—C17—C14	116.42 (18)
O1ᵛ—Sr1—Sr1ⁱᵛ	39.57 (3)	O5—C18—N1	124.8 (2)
C3ᵛ—Sr1—Sr1ⁱᵛ	97.11 (4)	O5—C18—H18	117.6
C1ᵛ—Sr1—Sr1ⁱᵛ	54.94 (4)	N1—C18—H18	117.6
C2ᵛ—Sr1—Sr1ⁱᵛ	81.03 (4)	N1—C19—H19A	109.5

Sr1^{vi}—Sr1—Sr1^{iv}	99.625 (9)	N1—C19—H19B	109.5
C1—O1—Sr1^{viii}	121.40 (13)	H19A—C19—H19B	109.5
C1—O1—Sr1^{ix}	112.32 (13)	N1—C19—H19C	109.5
Sr1^{viii}—O1—Sr1^{ix}	100.15 (5)	H19A—C19—H19C	109.5
C1—O2—Sr1^{x}	137.05 (15)	H19B—C19—H19C	109.5
C17—O3—Sr1^{xi}	136.59 (14)	N1—C20—H20A	109.5
C17—O3—Sr1^{iv}	123.11 (13)	N1—C20—H20B	109.5
Sr1^{xi}—O3—Sr1^{iv}	95.64 (5)	H20A—C20—H20B	109.5
C17—O4—Sr1	136.51 (15)	N1—C20—H20C	109.5
C18—O5—Sr1	127.84 (16)	H20A—C20—H20C	109.5
C18—N1—C20	120.6 (2)	H20B—C20—H20C	109.5
C18—N1—C19	121.7 (2)		

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

Poly[tetraaqua{μ_2-4,4′-[4,5-bis(4-carboxyphenyl)benzene-1,2-diyl]dibenzoato}tristrontium(II)] (MOF2)

Crystal data

[Sr$_3$(C$_{34}$H$_{20}$O$_8$)$_2$(H$_2$O)$_4$]	$Z = 1$
$M_r = 1445.91$	$F(000) = 728$
Triclinic, $P\bar{1}$	$D_x = 1.213$ Mg m^{-3}
$a = 9.240$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.330$ (4) Å	Cell parameters from 6851 reflections
$c = 19.414$ (7) Å	$\theta = 2.2$–29.5°
$\alpha = 80.147$ (6)°	$\mu = 2.08$ mm^{-1}
$\beta = 81.815$ (7)°	$T = 100$ K
$\gamma = 85.494$ (7)°	Block, colourless
$V = 1979.1$ (12) Å^3	0.4 × 0.3 × 0.2 mm

Data collection

Bruker APEXII CCD diffractometer	10986 independent reflections
φ and ω scans	9468 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$R_{int} = 0.027$
	$\theta_{max} = 29.6°$, $\theta_{min} = 1.1°$
$T_{min} = 0.636$, $T_{max} = 0.746$	$h = -12 \rightarrow 12$
33795 measured reflections	$k = -15 \rightarrow 15$
	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.030$	
$wR(F^2) = 0.085$	$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.5586P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
10986 reflections	$(\Delta/\sigma)_{max} = 0.003$
429 parameters	$\Delta\rho_{max} = 0.58$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.40$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr1	0.500000	0.000000	1.000000	0.01031 (5)
Sr2	0.15862 (2)	0.96611 (2)	0.90833 (2)	0.01075 (5)
O4	0.77813 (13)	0.93490 (11)	0.22606 (6)	0.0152 (2)
O9	0.96489 (13)	0.12177 (11)	0.95084 (6)	0.0146 (2)
O7	0.72246 (13)	0.11703 (11)	0.97587 (6)	0.0160 (2)
O8	0.68307 (14)	−0.14150 (11)	1.06935 (7)	0.0162 (2)
O1	0.76027 (14)	0.07521 (11)	0.32051 (7)	0.0181 (3)
H1	0.782266	0.034447	0.287841	0.027*
O3	0.66572 (15)	0.77992 (12)	0.20373 (6)	0.0200 (3)
O5	0.43315 (14)	0.91708 (13)	0.88233 (7)	0.0227 (3)
O6	0.65612 (14)	0.87652 (13)	0.91244 (7)	0.0234 (3)
O10	−0.06290 (16)	0.93714 (14)	0.85044 (8)	0.0241 (3)
H10A	−0.043 (3)	0.902 (3)	0.8154 (17)	0.048 (8)*
H10B	−0.144 (4)	0.926 (3)	0.8668 (17)	0.055 (10)*
C24	0.72064 (18)	0.70771 (15)	0.81898 (9)	0.0136 (3)
H24	0.784204	0.706162	0.853560	0.016*
C32	0.83640 (18)	0.15159 (14)	0.93521 (8)	0.0111 (3)
C28	0.77431 (18)	0.37379 (14)	0.73685 (8)	0.0113 (3)
C8	0.76849 (18)	0.44315 (15)	0.53917 (8)	0.0119 (3)
C22	0.59333 (18)	0.78304 (15)	0.82027 (9)	0.0141 (3)
C26	0.75375 (18)	0.44479 (15)	0.66608 (8)	0.0121 (3)
C9	0.72867 (18)	0.56715 (15)	0.52837 (8)	0.0126 (3)
C31	0.81624 (18)	0.23133 (14)	0.86662 (8)	0.0111 (3)
C3	0.7261 (2)	0.20327 (16)	0.43041 (9)	0.0172 (3)
H3	0.665755	0.138070	0.433079	0.021*
O2	0.9557 (2)	0.1732 (2)	0.26628 (10)	0.0622 (7)
C25	0.75471 (18)	0.63506 (15)	0.76738 (9)	0.0136 (3)
H25	0.840320	0.582839	0.767753	0.016*
C23	0.55765 (18)	0.86423 (15)	0.87496 (8)	0.0141 (3)
C27	0.78312 (18)	0.38512 (15)	0.60765 (8)	0.0122 (3)
H27	0.813999	0.302461	0.614792	0.015*
C19	0.66454 (19)	0.63775 (15)	0.71480 (8)	0.0137 (3)
C10	0.72208 (19)	0.63780 (15)	0.45634 (8)	0.0131 (3)
C2	0.83334 (19)	0.22956 (16)	0.37336 (9)	0.0167 (3)
C4	0.7072 (2)	0.27333 (15)	0.48400 (9)	0.0178 (3)
H4	0.633945	0.254908	0.523206	0.021*
C14	0.71919 (18)	0.83331 (15)	0.24491 (8)	0.0132 (3)
C5	0.79416 (18)	0.36995 (15)	0.48094 (8)	0.0123 (3)
C29	0.91564 (19)	0.33494 (16)	0.75236 (9)	0.0173 (3)

H29	0.997989	0.355855	0.718369	0.021*
C15	0.81029 (19)	0.80003 (15)	0.36476 (9)	0.0150 (3)
H15	0.872451	0.864866	0.349027	0.018*
C13	0.71811 (18)	0.76987 (15)	0.31994 (8)	0.0123 (3)
C18	0.70443 (18)	0.56721 (15)	0.65602 (8)	0.0134 (3)
C16	0.8109 (2)	0.73478 (15)	0.43264 (9)	0.0155 (3)
H16	0.872478	0.756600	0.463100	0.019*
C30	0.93634 (19)	0.26586 (16)	0.81727 (9)	0.0172 (3)
H30	1.032707	0.242259	0.827861	0.021*
C34	0.65490 (19)	0.34253 (17)	0.78723 (9)	0.0185 (4)
H34	0.558826	0.370510	0.777976	0.022*
C12	0.62771 (19)	0.67390 (16)	0.34409 (9)	0.0156 (3)
H12	0.564385	0.653273	0.314045	0.019*
C17	0.69599 (19)	0.62599 (15)	0.58677 (9)	0.0143 (3)
H17	0.666923	0.709008	0.579356	0.017*
C11	0.62918 (19)	0.60830 (16)	0.41139 (9)	0.0162 (3)
H11	0.567156	0.543338	0.426989	0.019*
C33	0.67545 (19)	0.27033 (17)	0.85127 (9)	0.0178 (4)
H33	0.592974	0.247482	0.884745	0.021*
C21	0.5004 (2)	0.78371 (19)	0.76956 (10)	0.0247 (4)
H21	0.412135	0.832720	0.770910	0.030*
C1	0.8559 (2)	0.15670 (18)	0.31465 (10)	0.0227 (4)
C20	0.5364 (2)	0.71297 (19)	0.71694 (10)	0.0251 (4)
H20	0.473320	0.715635	0.682029	0.030*
C6	0.9027 (2)	0.3952 (2)	0.42362 (10)	0.0250 (4)
H6	0.963271	0.460333	0.420742	0.030*
C7	0.9219 (2)	0.3245 (2)	0.37053 (11)	0.0321 (5)
H7	0.996586	0.341418	0.331808	0.039*
H8A	0.737 (3)	−0.194 (2)	1.0494 (13)	0.032 (7)*
H8B	0.672 (3)	−0.173 (2)	1.1116 (15)	0.034 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01136 (10)	0.01259 (10)	0.00711 (9)	−0.00104 (7)	−0.00067 (7)	−0.00224 (7)
Sr2	0.01190 (7)	0.01228 (8)	0.00779 (7)	0.00083 (5)	−0.00211 (5)	−0.00080 (5)
O4	0.0191 (6)	0.0167 (6)	0.0094 (5)	−0.0026 (5)	−0.0017 (4)	−0.0003 (5)
O9	0.0140 (6)	0.0154 (6)	0.0135 (6)	0.0022 (5)	−0.0041 (4)	0.0009 (5)
O7	0.0164 (6)	0.0202 (6)	0.0104 (5)	−0.0057 (5)	−0.0031 (5)	0.0032 (5)
O8	0.0196 (6)	0.0158 (6)	0.0113 (6)	0.0006 (5)	−0.0017 (5)	0.0023 (5)
O1	0.0250 (7)	0.0169 (6)	0.0146 (6)	−0.0032 (5)	−0.0023 (5)	−0.0074 (5)
O3	0.0294 (7)	0.0219 (6)	0.0099 (6)	−0.0098 (5)	−0.0066 (5)	0.0007 (5)
O5	0.0202 (6)	0.0334 (8)	0.0147 (6)	0.0106 (6)	−0.0026 (5)	−0.0097 (5)
O6	0.0170 (6)	0.0361 (8)	0.0216 (7)	−0.0007 (6)	−0.0016 (5)	−0.0184 (6)
O10	0.0168 (7)	0.0388 (8)	0.0207 (7)	−0.0069 (6)	−0.0011 (6)	−0.0146 (6)
C24	0.0146 (7)	0.0166 (8)	0.0105 (7)	−0.0002 (6)	−0.0029 (6)	−0.0037 (6)
C32	0.0174 (8)	0.0080 (7)	0.0085 (7)	−0.0005 (6)	−0.0037 (6)	−0.0008 (6)
C28	0.0176 (8)	0.0104 (7)	0.0057 (7)	−0.0017 (6)	−0.0023 (6)	0.0002 (6)

C8	0.0138 (7)	0.0146 (8)	0.0077 (7)	−0.0028 (6)	−0.0004 (6)	−0.0029 (6)
C22	0.0143 (7)	0.0184 (8)	0.0100 (7)	0.0012 (6)	−0.0003 (6)	−0.0054 (6)
C26	0.0144 (7)	0.0148 (8)	0.0068 (7)	−0.0014 (6)	−0.0020 (6)	0.0002 (6)
C9	0.0160 (8)	0.0148 (8)	0.0065 (7)	−0.0011 (6)	−0.0023 (6)	0.0002 (6)
C31	0.0152 (7)	0.0099 (7)	0.0080 (7)	−0.0003 (6)	−0.0026 (6)	−0.0001 (6)
C3	0.0218 (9)	0.0143 (8)	0.0158 (8)	−0.0054 (7)	0.0014 (7)	−0.0040 (6)
O2	0.0733 (14)	0.0800 (14)	0.0415 (11)	−0.0564 (12)	0.0388 (10)	−0.0477 (11)
C25	0.0132 (7)	0.0147 (8)	0.0125 (7)	0.0013 (6)	−0.0018 (6)	−0.0024 (6)
C23	0.0157 (8)	0.0170 (8)	0.0089 (7)	−0.0005 (6)	0.0022 (6)	−0.0035 (6)
C27	0.0160 (7)	0.0109 (7)	0.0093 (7)	−0.0014 (6)	−0.0018 (6)	0.0002 (6)
C19	0.0178 (8)	0.0155 (8)	0.0074 (7)	0.0015 (6)	−0.0016 (6)	−0.0021 (6)
C10	0.0183 (8)	0.0135 (7)	0.0068 (7)	0.0030 (6)	−0.0011 (6)	−0.0014 (6)
C2	0.0191 (8)	0.0215 (9)	0.0112 (8)	−0.0047 (7)	−0.0007 (6)	−0.0073 (7)
C4	0.0248 (9)	0.0141 (8)	0.0132 (8)	−0.0053 (7)	0.0053 (7)	−0.0032 (6)
C14	0.0152 (7)	0.0150 (8)	0.0081 (7)	0.0009 (6)	−0.0016 (6)	0.0008 (6)
C5	0.0154 (7)	0.0135 (7)	0.0079 (7)	0.0010 (6)	−0.0028 (6)	−0.0013 (6)
C29	0.0165 (8)	0.0192 (8)	0.0121 (8)	0.0032 (7)	0.0019 (6)	0.0036 (6)
C15	0.0201 (8)	0.0136 (8)	0.0113 (7)	−0.0024 (6)	−0.0035 (6)	0.0004 (6)
C13	0.0142 (7)	0.0147 (7)	0.0074 (7)	0.0010 (6)	−0.0014 (6)	−0.0009 (6)
C18	0.0161 (7)	0.0157 (8)	0.0091 (7)	0.0017 (6)	−0.0026 (6)	−0.0042 (6)
C16	0.0228 (8)	0.0151 (8)	0.0097 (7)	−0.0015 (7)	−0.0064 (6)	−0.0020 (6)
C30	0.0120 (7)	0.0218 (9)	0.0142 (8)	0.0043 (6)	−0.0007 (6)	0.0036 (7)
C34	0.0137 (8)	0.0282 (9)	0.0122 (8)	−0.0020 (7)	−0.0061 (6)	0.0045 (7)
C12	0.0164 (8)	0.0214 (9)	0.0091 (7)	−0.0042 (7)	−0.0041 (6)	0.0013 (6)
C17	0.0199 (8)	0.0128 (7)	0.0099 (7)	0.0013 (6)	−0.0030 (6)	−0.0010 (6)
C11	0.0183 (8)	0.0200 (8)	0.0094 (7)	−0.0044 (7)	−0.0022 (6)	0.0018 (6)
C33	0.0135 (8)	0.0272 (9)	0.0105 (8)	−0.0048 (7)	−0.0013 (6)	0.0049 (7)
C21	0.0218 (9)	0.0350 (11)	0.0211 (9)	0.0145 (8)	−0.0103 (7)	−0.0165 (8)
C1	0.0270 (10)	0.0293 (10)	0.0146 (8)	−0.0101 (8)	0.0014 (7)	−0.0111 (7)
C20	0.0263 (10)	0.0357 (11)	0.0174 (9)	0.0144 (8)	−0.0133 (7)	−0.0144 (8)
C6	0.0261 (10)	0.0342 (11)	0.0182 (9)	−0.0179 (8)	0.0082 (7)	−0.0162 (8)
C7	0.0312 (11)	0.0487 (13)	0.0207 (10)	−0.0255 (10)	0.0153 (8)	−0.0223 (10)

Geometric parameters (Å, º)

Sr1—Sr2[i]	3.9099 (11)	C26—C27	1.401 (2)
Sr1—Sr2[ii]	3.9099 (11)	C26—C18	1.415 (2)
Sr1—O7	2.4788 (14)	C9—C10	1.494 (2)
Sr1—O7[iii]	2.4787 (14)	C9—C17	1.397 (2)
Sr1—O6[i]	2.5935 (14)	C31—C30	1.393 (2)
Sr1—O8	2.5938 (14)	C31—C33	1.397 (2)
Sr1—O8[iii]	2.5938 (13)	C3—H3	0.9500
Sr1—O5[i]	2.7767 (15)	C3—C2	1.385 (2)
Sr1—O5[ii]	2.7767 (15)	C3—C4	1.397 (2)
Sr1—O6[ii]	2.5935 (14)	O2—C1	1.220 (2)
Sr1—C23[i]	3.0535 (18)	C25—H25	0.9500
Sr1—C23[ii]	3.0535 (18)	C25—C19	1.402 (2)
Sr2—Sr2[iv]	4.4117 (11)	C27—H27	0.9500

Sr2—O5	2.5510 (16)	C19—C18	1.491 (2)
Sr2—O9ᵛ	2.5646 (13)	C19—C20	1.404 (2)
Sr2—O7ⁱⁱ	2.6392 (14)	C10—C16	1.398 (3)
Sr2—O4ᵛⁱ	2.6598 (14)	C10—C11	1.403 (2)
Sr2—O8ⁱⁱ	2.6849 (15)	C2—C1	1.501 (2)
Sr2—O9ⁱⁱ	2.8510 (14)	C2—C7	1.391 (3)
Sr2—O10	2.5392 (16)	C4—H4	0.9500
Sr2—C32ⁱⁱ	3.1066 (18)	C4—C5	1.396 (3)
O4—C14	1.286 (2)	C14—C13	1.509 (2)
O9—C32	1.273 (2)	C5—C6	1.394 (2)
O7—C32	1.268 (2)	C29—H29	0.9500
O8—H8A	0.85 (3)	C29—C30	1.394 (2)
O8—H8B	0.83 (3)	C15—H15	0.9500
O1—H1	0.8400	C15—C13	1.399 (2)
O1—C1	1.308 (2)	C15—C16	1.397 (2)
O3—C14	1.255 (2)	C13—C12	1.399 (3)
O5—C23	1.256 (2)	C18—C17	1.404 (2)
O6—C23	1.273 (2)	C16—H16	0.9500
O10—H10A	0.84 (3)	C30—H30	0.9500
O10—H10B	0.78 (3)	C34—H34	0.9500
C24—H24	0.9500	C34—C33	1.395 (2)
C24—C22	1.398 (2)	C12—H12	0.9500
C24—C25	1.390 (2)	C12—C11	1.390 (2)
C32—C31	1.502 (2)	C17—H17	0.9500
C28—C26	1.498 (2)	C11—H11	0.9500
C28—C29	1.402 (2)	C33—H33	0.9500
C28—C34	1.391 (2)	C21—H21	0.9500
C8—C9	1.412 (2)	C21—C20	1.392 (2)
C8—C27	1.399 (2)	C20—H20	0.9500
C8—C5	1.495 (2)	C6—H6	0.9500
C22—C23	1.507 (2)	C6—C7	1.394 (3)
C22—C21	1.394 (2)	C7—H7	0.9500
Sr2ⁱⁱ—Sr1—Sr2ⁱ	180.0	Sr1—O8—H8B	128.5 (18)
O7—Sr1—Sr2ⁱ	138.27 (3)	Sr2ⁱⁱ—O8—H8A	111.1 (17)
O7—Sr1—Sr2ⁱⁱ	41.73 (3)	Sr2ⁱⁱ—O8—H8B	93.8 (18)
O7ⁱⁱⁱ—Sr1—Sr2ⁱ	41.73 (3)	H8A—O8—H8B	103 (2)
O7ⁱⁱⁱ—Sr1—Sr2ⁱⁱ	138.27 (3)	C1—O1—H1	109.5
O7ⁱⁱⁱ—Sr1—O7	180.0	Sr2—O5—Sr1ᵛⁱⁱ	94.33 (4)
O7ⁱⁱⁱ—Sr1—O8ⁱⁱⁱ	77.85 (5)	C23—O5—Sr1ᵛⁱⁱ	90.30 (10)
O7ⁱⁱⁱ—Sr1—O8	102.15 (5)	C23—O5—Sr2	164.35 (13)
O7—Sr1—O8	77.85 (5)	C23—O6—Sr1ᵛⁱⁱ	98.52 (10)
O7—Sr1—O8ⁱⁱⁱ	102.15 (5)	Sr2—O10—H10A	114 (2)
O7ⁱⁱⁱ—Sr1—O5ⁱ	66.62 (4)	Sr2—O10—H10B	131 (2)
O7ⁱⁱⁱ—Sr1—O5ⁱⁱ	113.38 (4)	H10A—O10—H10B	108 (3)
O7—Sr1—O5ⁱⁱ	66.62 (4)	C22—C24—H24	119.8
O7—Sr1—O5ⁱ	113.38 (4)	C25—C24—H24	119.8
O7ⁱⁱⁱ—Sr1—O6ⁱ	98.62 (5)	C25—C24—C22	120.34 (15)

O7—Sr1—O6ⁱ	81.38 (5)	O9—C32—Sr2ⁱⁱ	66.58 (9)
O7—Sr1—O6ⁱⁱ	98.62 (5)	O9—C32—C31	119.81 (15)
O7ⁱⁱⁱ—Sr1—O6ⁱⁱ	81.38 (5)	O7—C32—Sr2ⁱⁱ	56.97 (8)
O7ⁱⁱⁱ—Sr1—C23ⁱ	81.08 (5)	O7—C32—O9	122.40 (15)
O7—Sr1—C23ⁱ	98.92 (5)	O7—C32—C31	117.79 (14)
O7—Sr1—C23ⁱⁱ	81.08 (5)	C31—C32—Sr2ⁱⁱ	167.23 (10)
O7ⁱⁱⁱ—Sr1—C23ⁱⁱ	98.92 (5)	C29—C28—C26	119.86 (15)
O8ⁱⁱⁱ—Sr1—Sr2ⁱ	43.11 (3)	C34—C28—C26	121.10 (15)
O8ⁱⁱⁱ—Sr1—Sr2ⁱⁱ	136.89 (3)	C34—C28—C29	119.01 (15)
O8—Sr1—Sr2ⁱⁱ	43.11 (3)	C9—C8—C5	123.17 (14)
O8—Sr1—Sr2ⁱ	136.89 (3)	C27—C8—C9	118.73 (14)
O8—Sr1—O8ⁱⁱⁱ	180.0	C27—C8—C5	118.10 (14)
O8ⁱⁱⁱ—Sr1—O5ⁱⁱ	113.92 (4)	C24—C22—C23	120.60 (15)
O8ⁱⁱⁱ—Sr1—O5ⁱ	66.08 (4)	C21—C22—C24	119.23 (15)
O8—Sr1—O5ⁱ	113.92 (4)	C21—C22—C23	120.16 (15)
O8—Sr1—O5ⁱⁱ	66.08 (4)	C27—C26—C28	117.55 (14)
O8—Sr1—C23ⁱⁱ	87.51 (5)	C27—C26—C18	119.17 (14)
O8—Sr1—C23ⁱ	92.49 (5)	C18—C26—C28	123.26 (14)
O8ⁱⁱⁱ—Sr1—C23ⁱⁱ	92.49 (5)	C8—C9—C10	122.08 (14)
O8ⁱⁱⁱ—Sr1—C23ⁱ	87.51 (5)	C17—C9—C8	118.99 (14)
O5ⁱⁱ—Sr1—Sr2ⁱ	139.41 (3)	C17—C9—C10	118.92 (15)
O5ⁱ—Sr1—Sr2ⁱⁱ	139.41 (3)	C30—C31—C32	120.86 (14)
O5ⁱⁱ—Sr1—Sr2ⁱⁱ	40.59 (3)	C30—C31—C33	119.19 (15)
O5ⁱ—Sr1—Sr2ⁱ	40.59 (3)	C33—C31—C32	119.94 (15)
O5ⁱⁱ—Sr1—O5ⁱ	180.0	C2—C3—H3	120.2
O5ⁱⁱ—Sr1—C23ⁱ	155.72 (4)	C2—C3—C4	119.53 (17)
O5ⁱ—Sr1—C23ⁱⁱ	155.72 (4)	C4—C3—H3	120.2
O5ⁱⁱ—Sr1—C23ⁱⁱ	24.28 (4)	C24—C25—H25	119.5
O5ⁱ—Sr1—C23ⁱ	24.28 (4)	C24—C25—C19	120.94 (15)
O6ⁱ—Sr1—Sr2ⁱ	88.58 (4)	C19—C25—H25	119.5
O6ⁱⁱ—Sr1—Sr2ⁱ	91.42 (4)	O5—C23—Sr1^{vii}	65.42 (9)
O6ⁱⁱ—Sr1—Sr2ⁱⁱ	88.58 (4)	O5—C23—O6	122.20 (15)
O6ⁱ—Sr1—Sr2ⁱⁱ	91.42 (4)	O5—C23—C22	119.59 (15)
O6ⁱ—Sr1—O8ⁱⁱⁱ	107.63 (5)	O6—C23—Sr1^{vii}	57.14 (8)
O6ⁱⁱ—Sr1—O8	107.63 (5)	O6—C23—C22	118.21 (14)
O6ⁱ—Sr1—O8	72.37 (5)	C22—C23—Sr1^{vii}	172.18 (11)
O6ⁱⁱ—Sr1—O8ⁱⁱⁱ	72.37 (5)	C8—C27—C26	122.21 (15)
O6ⁱ—Sr1—O5ⁱ	48.54 (4)	C8—C27—H27	118.9
O6ⁱ—Sr1—O5ⁱⁱ	131.46 (4)	C26—C27—H27	118.9
O6ⁱⁱ—Sr1—O5ⁱ	131.46 (4)	C25—C19—C18	121.83 (14)
O6ⁱⁱ—Sr1—O5ⁱⁱ	48.54 (4)	C25—C19—C20	118.21 (15)
O6ⁱⁱ—Sr1—O6ⁱ	180.0	C20—C19—C18	119.91 (15)
O6ⁱ—Sr1—C23ⁱ	24.34 (4)	C16—C10—C9	119.67 (15)
O6ⁱ—Sr1—C23ⁱⁱ	155.66 (4)	C16—C10—C11	118.95 (15)
O6ⁱⁱ—Sr1—C23ⁱⁱ	24.34 (4)	C11—C10—C9	121.38 (16)
O6ⁱⁱ—Sr1—C23ⁱ	155.66 (4)	C3—C2—C1	120.94 (17)
C23ⁱ—Sr1—Sr2ⁱ	64.29 (4)	C3—C2—C7	119.59 (16)
C23ⁱⁱ—Sr1—Sr2ⁱ	115.71 (4)	C7—C2—C1	119.46 (16)

C23ⁱ—Sr1—Sr2ⁱⁱ	115.71 (4)	C3—C4—H4	119.4
C23ⁱⁱ—Sr1—Sr2ⁱⁱ	64.29 (4)	C5—C4—C3	121.16 (16)
C23ⁱⁱ—Sr1—C23ⁱ	180.0	C5—C4—H4	119.4
Sr1^{vii}—Sr2—Sr2^{iv}	93.96 (3)	O4—C14—C13	119.38 (15)
O4^{vi}—Sr2—Sr1^{vii}	106.35 (3)	O3—C14—O4	123.88 (15)
O4^{vi}—Sr2—Sr2^{iv}	137.39 (3)	O3—C14—C13	116.68 (15)
O4^{vi}—Sr2—O9ⁱⁱ	168.98 (4)	C4—C5—C8	119.14 (15)
O4^{vi}—Sr2—O8ⁱⁱ	83.07 (4)	C6—C5—C8	121.91 (16)
O4^{vi}—Sr2—C32ⁱⁱ	166.58 (4)	C6—C5—C4	118.95 (16)
O9^v—Sr2—Sr1^{vii}	105.08 (3)	C28—C29—H29	119.7
O9ⁱⁱ—Sr2—Sr1^{vii}	82.69 (3)	C30—C29—C28	120.56 (16)
O9ⁱⁱ—Sr2—Sr2^{iv}	33.35 (3)	C30—C29—H29	119.7
O9^v—Sr2—Sr2^{iv}	37.67 (3)	C13—C15—H15	120.0
O9^v—Sr2—O4^{vi}	100.08 (4)	C16—C15—H15	120.0
O9^v—Sr2—O9ⁱⁱ	71.01 (4)	C16—C15—C13	120.00 (17)
O9^v—Sr2—O7ⁱⁱ	101.82 (4)	C15—C13—C14	121.99 (16)
O9^v—Sr2—O8ⁱⁱ	76.22 (5)	C12—C13—C14	118.85 (15)
O9ⁱⁱ—Sr2—C32ⁱⁱ	24.19 (4)	C12—C13—C15	119.08 (15)
O9^v—Sr2—C32ⁱⁱ	88.37 (4)	C26—C18—C19	123.52 (14)
O7ⁱⁱ—Sr2—Sr1^{vii}	38.69 (3)	C17—C18—C26	118.15 (14)
O7ⁱⁱ—Sr2—Sr2^{iv}	71.57 (4)	C17—C18—C19	118.32 (15)
O7ⁱⁱ—Sr2—O4^{vi}	142.86 (4)	C10—C16—H16	119.6
O7ⁱⁱ—Sr2—O9ⁱⁱ	47.66 (4)	C15—C16—C10	120.86 (16)
O7ⁱⁱ—Sr2—O8ⁱⁱ	73.57 (4)	C15—C16—H16	119.6
O7ⁱⁱ—Sr2—C32ⁱⁱ	23.75 (4)	C31—C30—C29	120.23 (15)
O8ⁱⁱ—Sr2—Sr1^{vii}	41.32 (3)	C31—C30—H30	119.9
O8ⁱⁱ—Sr2—Sr2^{iv}	88.84 (4)	C29—C30—H30	119.9
O8ⁱⁱ—Sr2—O9ⁱⁱ	100.54 (4)	C28—C34—H34	119.8
O8ⁱⁱ—Sr2—C32ⁱⁱ	88.92 (4)	C28—C34—C33	120.36 (16)
O5—Sr2—Sr1^{vii}	45.08 (3)	C33—C34—H34	119.8
O5—Sr2—Sr2^{iv}	137.42 (3)	C13—C12—H12	119.5
O5—Sr2—O4^{vi}	76.87 (4)	C11—C12—C13	120.96 (16)
O5—Sr2—O9ⁱⁱ	114.15 (4)	C11—C12—H12	119.5
O5—Sr2—O9^v	144.28 (4)	C9—C17—C18	122.55 (15)
O5—Sr2—O7ⁱⁱ	67.83 (4)	C9—C17—H17	118.7
O5—Sr2—O8ⁱⁱ	68.06 (5)	C18—C17—H17	118.7
O5—Sr2—C32ⁱⁱ	90.17 (4)	C10—C11—H11	119.9
O10—Sr2—Sr1^{vii}	178.20 (4)	C12—C11—C10	120.14 (17)
O10—Sr2—Sr2^{iv}	85.99 (4)	C12—C11—H11	119.9
O10—Sr2—O4^{vi}	74.80 (5)	C31—C33—H33	119.7
O10—Sr2—O9^v	75.95 (5)	C34—C33—C31	120.58 (16)
O10—Sr2—O9ⁱⁱ	96.32 (5)	C34—C33—H33	119.7
O10—Sr2—O7ⁱⁱ	139.82 (5)	C22—C21—H21	119.8
O10—Sr2—O8ⁱⁱ	140.46 (5)	C20—C21—C22	120.36 (16)
O10—Sr2—O5	134.53 (5)	C20—C21—H21	119.8
O10—Sr2—C32ⁱⁱ	117.68 (5)	O1—C1—C2	114.09 (16)
C32ⁱⁱ—Sr2—Sr1^{vii}	61.05 (3)	O2—C1—O1	123.89 (18)
C32ⁱⁱ—Sr2—Sr2^{iv}	52.70 (3)	O2—C1—C2	122.01 (18)

C14—O4—Sr2ⁿᵛⁱ	122.70 (10)	C19—C20—H20	119.6
Sr2ᵛⁱⁱⁱ—O9—Sr2ⁿⁱⁱ	108.99 (4)	C21—C20—C19	120.87 (16)
C32—O9—Sr2ᵛⁱⁱⁱ	131.25 (11)	C21—C20—H20	119.6
C32—O9—Sr2ⁿⁱⁱ	89.23 (10)	C5—C6—H6	120.2
Sr1—O7—Sr2ⁿⁱⁱ	99.58 (4)	C5—C6—C7	119.68 (18)
C32—O7—Sr1	149.74 (11)	C7—C6—H6	120.2
C32—O7—Sr2ⁿⁱⁱ	99.28 (10)	C2—C7—C6	121.07 (18)
Sr1—O8—Sr2ⁿⁱⁱ	95.57 (5)	C2—C7—H7	119.5
Sr1—O8—H8A	120.0 (17)	C6—C7—H7	119.5
Sr1—O7—C32—Sr2ⁿⁱⁱ	−127.9 (2)	C3—C2—C1—O1	4.7 (3)
Sr1—O7—C32—O9	−114.9 (2)	C3—C2—C1—O2	−175.1 (2)
Sr1—O7—C32—C31	65.6 (3)	C3—C2—C7—C6	−1.2 (3)
Sr1ᵛⁱⁱ—O5—C23—O6	−6.63 (18)	C3—C4—C5—C8	179.25 (16)
Sr1ᵛⁱⁱ—O5—C23—C22	173.24 (14)	C3—C4—C5—C6	−0.8 (3)
Sr1ᵛⁱⁱ—O6—C23—O5	7.2 (2)	C25—C24—C22—C23	−178.49 (16)
Sr1ᵛⁱⁱ—O6—C23—C22	−172.70 (13)	C25—C24—C22—C21	0.5 (3)
Sr2ⁿᵛⁱ—O4—C14—O3	−11.3 (2)	C25—C19—C18—C26	47.3 (3)
Sr2ⁿᵛⁱ—O4—C14—C13	166.13 (10)	C25—C19—C18—C17	−131.15 (18)
Sr2ᵛⁱⁱⁱ—O9—C32—Sr2ⁿⁱⁱ	114.91 (12)	C25—C19—C20—C21	0.5 (3)
Sr2ⁿⁱⁱ—O9—C32—O7	−11.91 (16)	C23—C22—C21—C20	177.01 (19)
Sr2ᵛⁱⁱⁱ—O9—C32—O7	102.99 (17)	C27—C8—C9—C10	175.15 (16)
Sr2ᵛⁱⁱⁱ—O9—C32—C31	−77.48 (19)	C27—C8—C9—C17	−4.1 (2)
Sr2ⁿⁱⁱ—O9—C32—C31	167.61 (13)	C27—C8—C5—C4	59.6 (2)
Sr2ⁿⁱⁱ—O7—C32—O9	13.06 (17)	C27—C8—C5—C6	−120.3 (2)
Sr2ⁿⁱⁱ—O7—C32—C31	−166.47 (12)	C27—C26—C18—C19	177.53 (16)
Sr2—O5—C23—Sr1ᵛⁱⁱ	−107.4 (4)	C27—C26—C18—C17	−4.0 (2)
Sr2—O5—C23—O6	−114.0 (4)	C19—C18—C17—C9	−178.88 (16)
Sr2—O5—C23—C22	65.9 (5)	C10—C9—C17—C18	−177.77 (16)
Sr2ⁿⁱⁱ—C32—C31—C30	122.0 (5)	C2—C3—C4—C5	0.3 (3)
Sr2ⁿⁱⁱ—C32—C31—C33	−58.9 (6)	C4—C3—C2—C1	−179.59 (17)
O4—C14—C13—C15	−17.0 (2)	C4—C3—C2—C7	0.7 (3)
O9—C32—C31—C30	5.0 (2)	C4—C5—C6—C7	0.3 (3)
O9—C32—C31—C33	−175.99 (16)	C14—C13—C12—C11	176.26 (15)
O7—C32—C31—C30	−175.50 (16)	C5—C8—C9—C10	−5.7 (3)
O7—C32—C31—C33	3.6 (2)	C5—C8—C9—C17	175.09 (16)
O3—C14—C13—C15	160.52 (16)	C5—C8—C27—C26	−176.56 (15)
O3—C14—C13—C12	−16.0 (2)	C5—C6—C7—C2	0.7 (4)
C24—C22—C23—O5	−169.00 (17)	C29—C28—C26—C27	69.2 (2)
C24—C22—C23—O6	10.9 (3)	C29—C28—C26—C18	−111.8 (2)
C24—C22—C21—C20	−2.0 (3)	C29—C28—C34—C33	−2.1 (3)
C24—C25—C19—C18	175.55 (16)	C15—C13—C12—C11	−0.4 (3)
C24—C25—C19—C20	−2.0 (3)	C13—C15—C16—C10	1.1 (3)
C32—C31—C30—C29	176.78 (16)	C13—C12—C11—C10	0.0 (3)
C32—C31—C33—C34	−178.78 (16)	C18—C26—C27—C8	1.5 (3)
C28—C26—C27—C8	−179.53 (15)	C18—C19—C20—C21	−177.09 (19)
C28—C26—C18—C19	−1.4 (3)	C16—C10—C11—C12	0.9 (2)
		C16—C15—C13—C14	−176.71 (15)

C28—C26—C18—C17	177.02 (16)	C16—C15—C13—C12	−0.2 (2)
C28—C29—C30—C31	2.1 (3)	C30—C31—C33—C34	0.3 (3)
C28—C34—C33—C31	1.9 (3)	C34—C28—C26—C27	−108.97 (19)
C8—C9—C10—C16	−120.06 (19)	C34—C28—C26—C18	70.0 (2)
C8—C9—C10—C11	59.4 (2)	C34—C28—C29—C30	0.1 (3)
C8—C9—C17—C18	1.5 (3)	C17—C9—C10—C16	59.2 (2)
C8—C5—C6—C7	−179.76 (19)	C17—C9—C10—C11	−121.37 (19)
C22—C24—C25—C19	1.5 (3)	C11—C10—C16—C15	−1.5 (2)
C22—C21—C20—C19	1.5 (3)	C33—C31—C30—C29	−2.3 (3)
C26—C28—C29—C30	−178.16 (16)	C21—C22—C23—O5	12.0 (3)
C26—C28—C34—C33	176.15 (17)	C21—C22—C23—O6	−168.11 (18)
C26—C18—C17—C9	2.6 (3)	C1—C2—C7—C6	179.1 (2)
C9—C8—C27—C26	2.7 (3)	C20—C19—C18—C26	−135.20 (19)
C9—C8—C5—C4	−119.61 (19)	C20—C19—C18—C17	46.4 (3)
C9—C8—C5—C6	60.5 (2)	C7—C2—C1—O1	−175.59 (19)
C9—C10—C16—C15	177.99 (15)	C7—C2—C1—O2	4.6 (3)
C9—C10—C11—C12	−178.55 (16)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O4[i]	0.84	1.79	2.6051 (18)	164
O10—H10*A*···O2[ix]	0.84 (3)	1.97 (3)	2.795 (2)	168 (3)
O10—H10*B*···O6[x]	0.78 (3)	2.01 (3)	2.787 (2)	173 (3)
O8—H8*B*···O3[xi]	0.83 (3)	1.77 (3)	2.5948 (19)	170 (3)

Symmetry codes: (i) *x*, *y*−1, *z*; (ix) −*x*+1, −*y*+1, −*z*+1; (x) *x*−1, *y*, *z*; (xi) *x*, *y*−1, *z*+1.