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

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Two structurally different metal–organic frameworks based on Sr$^{2+}$ 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'',$^iv$-(benzene-1,2,4,5-tetrayl)tetrabenzoato][dimethylformamide]]distrionium(II)], [Sr$_2$(C$_{34}$H$_{18}$O$_8$)-(C$_7$H$_7$NO)$_2$]$_n$, and poly[tetraaqua[[μ$_{12}$-4,4'-[4,5-bis(4-carboxyphenyl)benzene-1,2-diyl]dibenzoato]tristrionium(II)]], [Sr$_3$(C$_{34}$H$_{20}$O$_8$).H$_2$O]. 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[[\mu_2\cdot4,4',4''\cdot4''\cdot(\text{benzene}-1,2,4,5-tetrayl)tetrabenzoato] \text{dimethylformamide} \text{distronium} \text{(II)}] and poly[[\text{tetraqua}\cdot\mu_2\cdot4,5\cdot\text{bis}-(\text{carboxyphenyl})\cdot4,4'\cdot(\text{benzene}-1,2-diyl)dibenzoato] \text{tristrontium} \text{(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 O7 coordination set is present; however, in MOF2 the asymmetric unit contains two Sr atoms, one seven- and the other eight-coordinated. In MOF1, the O7 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.

### Table 1

| Sr1–O4 | 2.5094 (15) | Sr1–O1vv | 2.5792 (16) |
| Sr1–O2v | 2.5170 (16) | Sr1–O3v | 2.5848 (16) |
| Sr1–O3 | 2.5180 (15) | Sr1–O1v | 2.6176 (16) |
| Sr1–O5 | 2.5780 (18) | |

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

### Table 2

| Sr1–O7 | 2.4788 (14) | Sr2–O9w | 2.5646 (13) |
| Sr1–O6v | 2.5935 (14) | Sr2–O7w | 2.6392 (14) |
| Sr1–O8 | 2.5938 (14) | Sr2–O4w | 2.6598 (14) |
| Sr1–O5 | 2.7767 (15) | Sr2–O8w | 2.6849 (15) |
| Sr2–O5 | 2.5510 (16) | Sr2–O9w | 2.8510 (14) |

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

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⋯A  | D—H | H⋯A | D⋯A  | D—H⋯A  |
|--------|------|-----|------|--------|
| O1—H1⋯O4' | 0.84 | 1.79 | 2.6051 (18) | 164 |
| O10—H10⋯O2" | 0.84 (3) | 1.97 (3) | 2.795 (2) | 168 (3) |
| O10—H10B⋯O6" | 0.78 (3) | 2.01 (3) | 2.787 (2) | 173 (3) |
| O8—H8B⋯O3" | 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.

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-T, with some exceptions (see Table 4).

(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⋯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.
The dihedral angles between the phenyl rings and the central benzene moiety in the ligand are nearly equal: two pairs of 52.66 (18)°/C14 and two pairs of 51.05 (18)°/C14. 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
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 \( a = 9.274 (1), b = 11.391 (1), c = 19.274 (3) \text{Å}, \alpha = 80.38 (1), \beta = 82.04 (1), \gamma = 86.11 (1)°\), \( V = 1986.3 \text{Å}^3\). 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, \( U_{eq}(C) = 1.2 U_{eq}(C) \). All O-bound H atoms were 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-carboxy-phenyl)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''''-(benzene-1,2,4,5-tetrayl)tetrabenzoato](dimethylformamide)distrontium(II)] (MOF1)

Crystal data

$[\text{Sr}_2(\text{C}_{34}\text{H}_{18}\text{O}_8)(\text{C}_3\text{H}_7\text{NO})_2]$  
$M_r = 875.92$
Monoclinic, $P2_1/c$
$a = 5.9350$ (2) Å
$b = 18.6130$ (8) Å
$c = 16.1256$ (7) Å
$\beta = 91.853$ (2)$^\circ$
$V = 1780.43$ (12) Å$^3$
$Z = 2$

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: microfocus sealed tube, sealed tube
Multilayer mirror monochromator
Detector resolution: 10.4167 pixels mm$^{-1}$
$\omega$ and $\phi$ scans, narrow frame width, shutterless
Absorption correction: multi-scan (SADABS; Krause et al., 2015)

$T_{\text{min}} = 0.63$, $T_{\text{max}} = 0.75$
91152 measured reflections
5387 independent reflections
4453 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.092$
$\theta_{\text{max}} = 30.4^\circ$, $\theta_{\text{min}} = 2.5^\circ$
h $=$ $-8$$\rightarrow$ $8$
k $=$ $-26$$\rightarrow$ $26$
l $=$ $-22$$\rightarrow$ $22$

Refinement

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.113$
$S = 0.87$
5387 reflections
246 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$F(000) = 884$
$D_x = 1.634$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9912 reflections
$\theta = 2.5$$\rightarrow$$30.3^\circ$
$\mu = 3.06$ mm$^{-1}$
$T = 173$ K
Needle, colourless
0.41 × 0.12 × 0.10 mm
$$w = 1/ [\sigma^2(F_o^2) + (0.1P)^2]$$

where

$$P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} = 0.002$$

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

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

**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 Å 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      | Ueq    |
| 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 (4) | 0.633313 (14) | 0.205003 (14) | 0.012 (4) |
| C4   | 0.2716 (3)   | 0.57343 (12) | 0.29489 (14) | 0.0104 (4)  |
| C5   | 0.412954 (4) | 0.597216 (15) | 0.300185 (15) | 0.013 (4) |
| C6   | 0.5993 (4)   | 0.53065 (11) | 0.35938 (14) | 0.0094 (4)  |
| C7   | −0.0111 (4)  | 0.49740 (14) | 0.35140 (14) | 0.0131 (4)  |
| H6   | −0.06246 (4) | 0.468151 (15) | 0.395216 (15) | 0.016 (4) |
| C8   | −0.1471 (4)  | 0.50652 (13) | 0.27989 (15) | 0.0127 (4)  |
| C9   | −0.29139 (4) | 0.484462 (15) | 0.275591 (15) | 0.015 (4) |
| C10  | 0.3496 (4)   | 0.51761 (11) | 0.43368 (14) | 0.0094 (4)  |
| C11  | 0.4097 (4)   | 0.44680 (12) | 0.45112 (14) | 0.0106 (4)  |
| H12  | 0.34665 (4)  | 0.409848 (14) | 0.417002 (14) | 0.013 (4) |
| C13  | 0.5582 (3)   | 0.42735 (11) | 0.51635 (13) | 0.0097 (4)  |
| C14  | 0.6141 (4)   | 0.35008 (11) | 0.52796 (13) | 0.0096 (4)  |
| C15  | 0.8328 (4)   | 0.32679 (12) | 0.54984 (15) | 0.0123 (4)  |
| H12  | 0.950402 (4) | 0.361023 (15) | 0.557342 (15) | 0.015 (4) |
| C13  | 0.8791 (3)   | 0.25430 (12) | 0.56065 (15) | 0.0119 (4)  |
### 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) | -0.00012 (7) |
| O1    | 0.0118 (7) | 0.0121 (8) | 0.0096 (7) | -0.00008 (6) | 0.00000 (6) | -0.00014 (6) |
| O2    | 0.0084 (7) | 0.0193 (9) | 0.0128 (8) | 0.00002 (6) | -0.00036 (6) | -0.00017 (6) |
| O3    | 0.0109 (7) | 0.0073 (7) | 0.0142 (8) | -0.0020 (6) | -0.00014 (6) | -0.00011 (6) |
| O4    | 0.0104 (7) | 0.0106 (8) | 0.0188 (8) | 0.0039 (6) | -0.00041 (6) | -0.00012 (6) |
| O5    | 0.0218 (9) | 0.0208 (10) | 0.0232 (10) | 0.0048 (7) | -0.00053 (7) | -0.00092 (7) |
| N1    | 0.0247 (11) | 0.0178 (11) | 0.0283 (12) | 0.0004 (9) | -0.00026 (9) | -0.00089 (9) |
| C1    | 0.0104 (9) | 0.0064 (10) | 0.0092 (9) | -0.0007 (7) | -0.00022 (7) | -0.00014 (7) |
| C2    | 0.0094 (9) | 0.0091 (10) | 0.0088 (9) | 0.0023 (8) | -0.00018 (7) | -0.00026 (8) |
| C3    | 0.0099 (9) | 0.0086 (9) | 0.0115 (10) | 0.0006 (7) | -0.00021 (8) | -0.00002 (8) |
| C4    | 0.0080 (9) | 0.0099 (10) | 0.0131 (10) | -0.0008 (7) | -0.00038 (7) | -0.00013 (8) |
| C5    | 0.0111 (10) | 0.0072 (10) | 0.0096 (10) | 0.0017 (7) | -0.00038 (8) | -0.00007 (7) |
| C6    | 0.0143 (10) | 0.0132 (10) | 0.0118 (11) | -0.0032 (9) | -0.00015 (8) | -0.00030 (9) |
| C7    | 0.0094 (9) | 0.0141 (11) | 0.0146 (11) | -0.0023 (8) | -0.00010 (8) | -0.00003 (9) |
| C8    | 0.0094 (9) | 0.0090 (10) | 0.0095 (10) | 0.0017 (7) | -0.00030 (8) | 0.00020 (7) |
| C9    | 0.0134 (9) | 0.0083 (10) | 0.0098 (10) | 0.0002 (8) | -0.00048 (8) | -0.00007 (8) |
| C10   | 0.0114 (9) | 0.0083 (10) | 0.0093 (10) | 0.0000 (7) | -0.00017 (7) | 0.00001 (7) |
| C11   | 0.0121 (9) | 0.0053 (9) | 0.0112 (10) | 0.0017 (7) | -0.00031 (7) | 0.00004 (7) |
| C12   | 0.0113 (10) | 0.0063 (10) | 0.0193 (11) | -0.0017 (8) | -0.00015 (8) | 0.00009 (8) |
| C13   | 0.0071 (9) | 0.0090 (10) | 0.0195 (11) | 0.0022 (7) | -0.00032 (8) | -0.00004 (8) |
| C14   | 0.0095 (9) | 0.0074 (9) | 0.0122 (10) | 0.0015 (7) | -0.00011 (8) | 0.00001 (8) |
| C15   | 0.0110 (10) | 0.0090 (10) | 0.0246 (12) | -0.0023 (8) | -0.00047 (9) | 0.00012 (9) |
| C16   | 0.0091 (9) | 0.0083 (10) | 0.0249 (12) | -0.0004 (7) | -0.00045 (8) | 0.00020 (9) |
| C17   | 0.0115 (9) | 0.0085 (10) | 0.0067 (9) | -0.0005 (7) | 0.00007 (7) | -0.00009 (7) |
| C18   | 0.0186 (11) | 0.0243 (13) | 0.0172 (12) | 0.0013 (10) | -0.00056 (9) | -0.00056 (10) |
| C19   | 0.0467 (19) | 0.0247 (16) | 0.056 (2) | 0.0092 (14) | -0.00039 (16) | -0.0189 (16) |
| C20   | 0.0273 (15) | 0.0388 (19) | 0.053 (2) | -0.0104 (13) | -0.00019 (14) | -0.0190 (16) |

*supporting information*
supporting information

| Geometric parameters (Å, º) |
|-----------------------------|
| Sr1—O4                     | 2.5094 (15) |
| Sr1—O2i                    | 2.5170 (16) |
| Sr1—O3ii                   | 2.5180 (15) |
| Sr1—O5                     | 2.5780 (18) |
| Sr1—O1iii                  | 2.5792 (16) |
| Sr1—O3iv                   | 2.5848 (16) |
| Sr1—O1v                    | 2.6176 (16) |
| Sr1—C3v                    | 3.193 (2)   |
| Sr1—C1                     | 1.274 (3)   |
| Sr1—C4                     | 1.391 (3)   |
| Sr1—C3                     | 1.399 (3)   |
| C5—C8                      | 1.490 (3)   |
| C6—C7                      | 1.396 (3)   |
| C6—H6                      | 0.95        |
| C7—H7                      | 0.95        |
| C8—C9                      | 1.392 (3)   |
| C8—C10i                    | 1.403 (3)   |
| C9—C10                     | 1.398 (3)   |
| C9—H9                      | 0.95        |
| C10                   | 1.487 (3)   |
| C11                   | 1.392 (3)   |
| C12                   | 1.402 (3)   |
| C13                   | 1.387 (3)   |
| C12                     | 1.39 (3)    |
| C12—H12                  | 0.95        |
| C13—C14                  | 1.389 (3)   |
| C13—H13                  | 0.95        |
| C14—C15                  | 1.398 (3)   |
| C14—C17                  | 1.508 (3)   |
| C15—C16                  | 1.392 (3)   |
| C15—H15                  | 0.95        |
| C16—H16                  | 0.95        |
| C18—H18                  | 0.95        |
| C19—H19A                | 0.98        |
| C19—H19B                | 0.98        |
| C19—H19C                | 0.98        |
| C20—H20A                | 0.98        |
| C20—H20B                | 0.98        |
| C20—H20C                | 0.98        |
| C1—C2                    | 1.505 (3)   |
| C1—O1                   | 1.243 (2)   |
| C1—O2                   | 1.243 (2)   |
| C1—C13                  | 1.274 (3)   |
| C1—C14                  | 1.391 (3)   |
| C1—C15                  | 1.399 (3)   |
| C1—C16                  | 1.397 (3)   |
| C1—C17                  | 1.391 (3)   |
| C1—C18                  | 1.399 (3)   |
| C2—C1                   | 1.505 (3)   |
| C2—C3                   | 1.399 (3)   |
| C2—C4                   | 1.387 (3)   |
| C2—H3                   | 1.0         |
| C3—C4                   | 1.387 (3)   |
| C3—H3                   | 1.0         |
| C4—C5                   | 1.389 (3)   |
| C4—H4                   | 0.95        |
| C5—C6                   | 1.396 (3)   |
| C6—C7                   | 1.389 (3)   |
| C6—C7                   | 1.391 (3)   |
| C6—H6                   | 0.95        |
| C7—C2                   | 1.397 (3)   |
| C7—O4                   | 1.4734 (5)  |
| C7—O2i                  | 1.1395 (5)  |
| C7—O3ii                 | 0.7387 (5)  |
| C7—O5                   | 0.7358 (5)  |
| C8—C10i                 | 0.7782 (6)  |
| C8—C10                  | 0.7734 (6)  |
| C9—C10                  | 0.7083 (5)  |
| C9—O1i                  | 0.14162 (5) |
| C9—O1v                 | 0.8667 (5)  |
| C9—O3i                  | 0.13036 (5) |
| C9—O3iv                | 0.13890 (5) |
| C9—O1vi                 | 0.7132 (5)  |
| C9—O3v                 | 0.8436 (5)  |
| C10—C1                 | 1.14747 (5) |
| C10—C3v                | 0.7415 (5)  |
| C10—O1v                | 0.7582 (5)  |
| C10—O1i                | 0.10802 (5) |
| C11—C1                | 1.2243 (2)  |
| C12—C3v               | 1.1391 (3)  |
| C13—C3v              | 1.1399 (3)  |
| C14—C3v              | 1.1387 (3)  |
| C15—C3v             | 1.0         |
| C16—C3v            | 1.0         |
| C17—C3v           | 1.0         |
| C18—C3v          | 1.0         |
| C19—C3v         | 1.0         |
| C20—C3v        | 1.0         |
| C2—C1v         | 1.1170 (2)  |
| C2—C1vv     | 1.1255 (2)  |
| C2—C1vvi    | 1.1178 (19) |
| C2—C1viii   | 1.1162 (18) |
| C3—C1v      | 1.1485 (15) |
| C3—C1vvi   | 1.1468 (10) |
| C3—C1viii  | 0.7798 (11) |
| C3—C1vii  | 0.1197 (2)  |
| C4—C1v     | 0.1200 (19) |
| C4—C1vii  | 0.1200 (19) |
| C4—C1viii | 0.1200 (19) |
| C4—C1v    | 0.1200 (19) |
| C4—C1v    | 0.1200 (19) |
| C5—C1v     | 0.1200 (19) |
| C5—C1vii  | 0.1200 (19) |
| C5—C1viii | 0.1200 (19) |
| C5—C1v   | 0.1200 (19) |
| C5—C1v    | 0.1200 (19) |

*Acta Cryst. (2021). E77, 1243-1248*
O3\textsuperscript{ii}—Sr1—O1\textsuperscript{v} 159.75 (5)  
O5—Sr1—O1\textsuperscript{v} 122.91 (6)  
O1\textsuperscript{iv}—Sr1—O1\textsuperscript{v} 79.85 (5)  
O3\textsuperscript{ii}—Sr1—O1\textsuperscript{v} 77.49 (5)  
O4—Sr1—C3\textsuperscript{v} 95.21 (6)  
O2—Sr1—C3\textsuperscript{v} 63.58 (5)  
O3\textsuperscript{ii}—Sr1—C3\textsuperscript{v} 134.51 (5)  
O5—Sr1—C3\textsuperscript{v} 78.67 (6)  
O1\textsuperscript{iv}—Sr1—C3\textsuperscript{v} 137.38 (5)  
O3\textsuperscript{ii}—Sr1—C3\textsuperscript{v} 96.19 (5)  
O1—Sr1—C3\textsuperscript{v} 57.55 (5)  
O4—Sr1—C1\textsuperscript{v} 65.57 (5)  
O2—Sr1—C1\textsuperscript{v} 106.31 (5)  
O3\textsuperscript{ii}—Sr1—C1\textsuperscript{v} 179.38 (5)  
O5—Sr1—C1\textsuperscript{v} 102.11 (6)  
O1\textsuperscript{iv}—Sr1—C1\textsuperscript{v} 93.50 (5)  
O3\textsuperscript{ii}—Sr1—C1\textsuperscript{v} 96.26 (5)  
O1—Sr1—C1\textsuperscript{v} 20.81 (5)  
C3\textsuperscript{v}—Sr1—C1\textsuperscript{v} 45.45 (5)  
O4—Sr1—C2\textsuperscript{v} 72.01 (5)  
O2—Sr1—C2\textsuperscript{v} 88.00 (5)  
O3\textsuperscript{ii}—Sr1—C2\textsuperscript{v} 153.58 (5)  
O5—Sr1—C2\textsuperscript{v} 80.19 (6)  
O1\textsuperscript{iv}—Sr1—C2\textsuperscript{v} 118.76 (5)  
O3\textsuperscript{ii}—Sr1—C2\textsuperscript{v} 108.25 (5)  
O1—Sr1—C2\textsuperscript{v} 44.66 (5)  
C3\textsuperscript{v}—Sr1—C2\textsuperscript{v} 24.57 (5)  
C1\textsuperscript{v}—Sr1—C2\textsuperscript{v} 26.10 (5)  
O4—Sr1—Sr1\textsuperscript{vi} 141.76 (4)  
O2—Sr1—Sr1\textsuperscript{vi} 66.18 (4)  
O3\textsuperscript{ii}—Sr1—Sr1\textsuperscript{vi} 42.86 (4)  
O5—Sr1—Sr1\textsuperscript{vi} 115.48 (4)  
O1\textsuperscript{iv}—Sr1—Sr1\textsuperscript{vi} 76.98 (3)  
O3\textsuperscript{ii}—Sr1—Sr1\textsuperscript{vi} 41.50 (3)  
O1—Sr1—Sr1\textsuperscript{vi} 118.46 (4)  
C3\textsuperscript{v}—Sr1—Sr1\textsuperscript{vi} 122.72 (4)  
C1\textsuperscript{v}—Sr1—Sr1\textsuperscript{vi} 137.76 (4)  
C2\textsuperscript{v}—Sr1—Sr1\textsuperscript{vi} 144.14 (4)  
O4—Sr1—Sr1\textsuperscript{iv} 68.07 (4)  
O2—Sr1—Sr1\textsuperscript{iv} 135.27 (4)  
O3\textsuperscript{ii}—Sr1—Sr1\textsuperscript{iv} 125.35 (4)  
O5—Sr1—Sr1\textsuperscript{iv} 140.89 (4)  
O1\textsuperscript{iv}—Sr1—Sr1\textsuperscript{iv} 40.28 (4)  
O3\textsuperscript{ii}—Sr1—Sr1\textsuperscript{iv} 71.39 (4)  
O1—Sr1—Sr1\textsuperscript{iv} 39.57 (3)  
C3\textsuperscript{v}—Sr1—Sr1\textsuperscript{iv} 97.11 (4)  
C1\textsuperscript{v}—Sr1—Sr1\textsuperscript{iv} 54.94 (4)  
C2\textsuperscript{v}—Sr1—Sr1\textsuperscript{iv} 81.03 (4)  

Acta Cryst. (2021). E77, 1243-1248
Poly[tetraaquap(μ₂-4,4'-[4,5-bis(4-carboxyphenyl)benzene-1,2-diyl]dibenzoato)tristrontium(II)] (MOF2)

Crystal data

\[
\begin{align*}
\text{Sr}_{3}[(\text{C}_{34}\text{H}_{20}\text{O}_{8})_{2}](\text{H}_{2}\text{O})_{4}] & \quad Z = 1 \\
M_r &= 1445.91 \\
\text{Triclinic, } P\bar{1} & \quad F(000) = 728 \\
a &= 9.240 (3) \text{ Å} & \quad D_x = 1.213 \text{ Mg m}^{-3} \\
b &= 11.330 (4) \text{ Å} \quad \text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ Å} \\
c &= 19.414 (7) \text{ Å} \quad \text{Cell parameters from 6851 reflections} \\
\alpha &= 80.147 (6)° & \quad \theta = 2.2–29.5° \\
\beta &= 81.815 (7)° & \quad \mu = 2.08 \text{ mm}^{-1} \\
\gamma &= 85.494 (7)° & \quad T = 100 \text{ K} \\
V &= 1979.1 (12) \text{ Å}^3 & \quad \text{Block, colourless} \\
\hline
\end{align*}
\]

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause et al., 2015)

\[\begin{align*}
T_{\text{min}} &= 0.636, T_{\text{max}} = 0.746 \\
10986 \text{ independent reflections} & \quad 33795 \text{ measured reflections} \\
9468 \text{ reflections with } I > 2\sigma(I) & \quad 10986 \text{ independent reflections} \\
R_{\text{int}} = 0.027 & \quad 9468 \text{ reflections with } I > 2\sigma(I) \\
\theta_{\text{max}} = 29.6°, \theta_{\text{min}} = 1.1° & \quad R_{\text{int}} = 0.027 \\
h = -12\rightarrow12 & \quad \theta_{\text{max}} = 29.6°, \theta_{\text{min}} = 1.1° \\
k = -15\rightarrow15 & \quad \theta_{\text{max}} = 29.6°, \theta_{\text{min}} = 1.1° \\
l = -26\rightarrow26 & \quad \theta_{\text{max}} = 29.6°, \theta_{\text{min}} = 1.1° \\
\end{align*}\]

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\[
\begin{align*}
R[F^2 > 2\sigma(F^2)] &= 0.030 \\
wR(F^2) &= 0.085 \\
S &= 1.08 \\
10986 \text{ reflections} & \quad \text{Hydrogen site location: mixed} \\
429 \text{ parameters} & \quad \text{H atoms treated by a mixture of independent} \\
0 \text{ restraints} & \quad \text{and constrained refinement} \\
\end{align*}
\]

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

\[
\begin{align*}
w &= \frac{1}{\sigma(F_c^2) + (0.0478P)^2 + 0.5586P} \\
\text{where } P &= (F_c^2 + 2F_s^2)/3 \\
(\Delta\sigma)_{\text{max}} &= 0.003 \\
\Delta\rho_{\text{max}} &= 0.58 \text{ e Å}^{-3} \\
\Delta\rho_{\text{min}} &= -0.40 \text{ e Å}^{-3} \\
\end{align*}
\]
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)

| Atom | x           | y           | z           | Uiso* / Ueq |
|------|-------------|-------------|-------------|-------------|
| 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    | 0.76753     | 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)  |
| Atom | x     | y     | z     | U11  | U22  | U33  | U12  | U13  | U23  |
|------|-------|-------|-------|------|------|------|------|------|------|
| H29  | 0.99799 | 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) |
| H17  | 0.666923 | 0.709008 | 0.579356 | 0.017* |
| C12  | 0.62918 (19) | 0.60830 (16) | 0.41139 (9) | 0.0162 (3) |
| C11  | 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) |
| C12  | 0.62771 (19) | 0.67390 (16) | 0.34409 (9) | 0.0156 (3) |
| 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 (7) | −0.0003 (6) | 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, °)**

| Bond or Angle | Value (Å) | Value (°) |
|---------------|-----------|-----------|
| Sr1—Sr2i      | 3.9099 (11) | 1.401 (2) |
| Sr1—Sr2ii     | 3.9099 (11) | 1.415 (2) |
| Sr1—O7        | 2.4788 (14) | 1.494 (2) |
| Sr1—O7iii     | 2.4787 (14) | 1.397 (2) |
| Sr1—O6'       | 2.5935 (14) | 1.393 (2) |
| Sr1—O8        | 2.5938 (14) | 1.397 (2) |
| Sr1—O8iii     | 2.5938 (13) | 0.9500 |
| Sr1—O5'       | 2.7767 (15) | 1.385 (2) |
| Sr1—O5ii      | 2.7767 (15) | 1.397 (2) |
| Sr1—O6ii      | 2.5935 (14) | 1.220 (2) |
| Sr1—C23i      | 3.0535 (18) | 0.9500 |
| Sr1—C23ii     | 3.0535 (18) | 1.402 (2) |
| Sr2—Sr2iv     | 4.4117 (11) | 0.9500 |
| Bond (distance) | Value      | Bond (distance) | Value      |
|----------------|------------|----------------|------------|
| 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)  |
| O7ii—Sr1—Sr2ii | 41.73 (3)  | H8A—O8—H8B     | 103 (2)    |
| O7ii—Sr1—Sr2ii | 138.27 (3) | C1—O1—H1       | 109.5      |
| O7ii—Sr1—O7    | 180.0      | Sr2—O5—Sr1 vii | 94.33 (4)  |
| O7ii—Sr1—O8ii  | 77.85 (5)  | C23—O5—Sr1 vii | 90.30 (10) |
| O7ii—Sr1—O8ii  | 102.15 (5) | C23—O5—sr2     | 164.35 (13)|
| O7—Sr1—O8     | 77.85 (5)  | C23—O6—Sr1 vii | 98.52 (10) |
| O7—Sr1—O8     | 102.15 (5) | Sr2—O10—H10A   | 114 (2)    |
| O7ii—Sr1—O5i  | 66.62 (4)  | Sr2—O10—H10B   | 131 (2)    |
| O7ii—Sr1—O5ii | 113.38 (4) | H10A—O10—H10B  | 108 (3)    |
| O7—Sr1—O5i    | 66.62 (4)  | C22—C24—H24    | 119.8      |
| O7—Sr1—O5i    | 113.38 (4) | C25—C24—H24    | 119.8      |
| O7ii—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)
O7—Sr1—O6iii 81.38 (5) O7—C32—Sr2ii 56.97 (8)
O7—Sr1—C23i 98.92 (5) O7—C32—C31 117.79 (14)
O7—Sr1—C23ii 81.08 (5) C31—C32—Sr2ii 167.23 (10)
O7—Sr1—C23iii 98.92 (5) C29—C28—C26 119.86 (15)
O8—Sr1—Sr2i 43.11 (3) C34—C28—C26 121.10 (15)
O8—Sr1—Sr2ii 136.89 (3) C34—C28—C29 119.01 (15)
O8—Sr1—Sr2iii 180.0 C32—C31—C32 120.60 (15)
O8—Sr1—O5i 113.92 (4) C2—C3—H3 120.2
O8—Sr1—O5ii 66.08 (4) C2—C3—C4 119.53 (17)
O8—Sr1—Sr2i 136.89 (3) C4—C3—H3 120.2
O8—Sr1—Sr2ii 180.0 C24—C25—H25 119.5
O8—Sr1—Sr2iii 66.08 (4) C24—C25—C19 120.94 (15)
O9—C32—Sr2ii 180.0 O6—C23—Sr1vii 57.14 (8)
O9—C32—C31 119.81 (15) O6—C23—Sr1vii 57.14 (8)
O9—C32—Sr2ii 180.0 O6—C23—Sr1vii 57.14 (8)
O7—C32—Sr2ii 56.97 (8) O6—C23—Sr1vii 57.14 (8)
O7—C32—C31 117.79 (14) O6—C23—Sr1vii 57.14 (8)
O7—C32—Sr2ii 180.0 C2—C3—C7 118.9
O7—C32—C31 119.81 (15) C2—C3—C7 118.9
O7—C32—Sr2ii 56.97 (8) C7—C2—C1 119.46 (16)
O7—C32—C31 117.79 (14) C7—C2—C1 119.46 (16)
O7—C32—Sr2ii 180.0 C2—C3—C7 118.9
O7—C32—C31 119.81 (15) C7—C2—C1 119.46 (16)

Acta Cryst. (2021). E77, 1243-1248

sup-11
| Bond                | Angle (°) | Standard Deviation |
|---------------------|-----------|--------------------|
| C23i—Sr1—Sr2ii      | 115.71    | 4                   |
| C23ii—Sr1—Sr2ii     | 64.29     | 3                   |
| C23ii—Sr1—C23i      | 180.0     |                     |
| Sr1iii—Sr2—Sr2iv    | 93.96     | 3                   |
| O4vi—Sr2—Sr1ii      | 106.35    | 3                   |
| O4vi—Sr2—Sr2iv      | 137.39    | 3                   |
| O4vi—Sr2—O9ii       | 168.98    | 4                   |
| O4vi—Sr2—O8ii       | 83.07     | 4                   |
| O4vi—Sr2—C32ii      | 166.58    | 4                   |
| O9ii—Sr2—Sr1ii      | 105.08    | 3                   |
| O9ii—Sr2—Sr2iv      | 33.35     | 3                   |
| O9ii—Sr2—Sr2v       | 37.67     | 3                   |
| O9ii—Sr2—O4vi       | 100.08    | 4                   |
| O9ii—Sr2—O9ii       | 71.01     | 4                   |
| O9ii—Sr2—O7ii       | 101.82    | 4                   |
| O9ii—Sr2—O8ii       | 76.22     | 5                   |
| O9ii—Sr2—C32ii      | 24.19     | 4                   |
| O9ii—Sr2—C32ii      | 88.37     | 4                   |
| O7ii—Sr2—Sr1ii      | 38.69     | 3                   |
| O7ii—Sr2—Sr2iv      | 71.57     | 4                   |
| O7ii—Sr2—Sr2v       | 142.86    | 4                   |
| O7ii—Sr2—O9ii       | 47.66     | 4                   |
| O7ii—Sr2—O8ii       | 73.57     | 4                   |
| O7ii—Sr2—C32ii      | 23.75     | 4                   |
| O8ii—Sr2—Sr1ii      | 41.32     | 3                   |
| O8ii—Sr2—Sr2iv      | 88.84     | 4                   |
| O8ii—Sr2—O9ii       | 100.54    | 4                   |
| O8ii—Sr2—C32ii      | 88.92     | 4                   |
| O5—Sr2—Sr1iv        | 45.08     | 3                   |
| O5—Sr2—Sr2iv        | 137.42    | 3                   |
| O5—Sr2—O4vi         | 76.87     | 4                   |
| O5—Sr2—O9ii         | 114.15    | 4                   |
| O5—Sr2—O9v          | 144.28    | 4                   |
| O5—Sr2—O7ii         | 67.83     | 4                   |
| O5—Sr2—O8ii         | 68.06     | 5                   |
| O5—Sr2—C32ii        | 90.17     | 4                   |
| O10—Sr2—Sr1iv       | 178.20    | 4                   |
| O10—Sr2—Sr2ii       | 85.99     | 4                   |
| O10—Sr2—O4vi        | 74.80     | 5                   |
| O10—Sr2—O9v         | 75.95     | 5                   |
| O10—Sr2—O9ii        | 96.32     | 5                   |
| O10—Sr2—O7ii        | 139.82    | 5                   |
| O10—Sr2—O8ii        | 140.46    | 5                   |
| O10—Sr2—O5          | 134.53    | 5                   |
| O10—Sr2—C32ii       | 117.68    | 5                   |
| C32ii—Sr2—Sr1iv     | 61.05     | 3                   |
| C32ii—Sr2—Sr2iv     | 52.70     | 3                   |

**Acta Cryst. (2021). E77, 1243-1248**
| Bond                  | Distance (Å)  | Bond                  | Distance (Å)  | Bond                  | Distance (Å)  |
|----------------------|---------------|----------------------|---------------|----------------------|---------------|
| C14—O4—Sr2<sup>ii</sup> | 122.70 (10)   | C19—C20—H20         | 119.6         |
| Sr2<sup>iii</sup>—O9—Sr2<sup>ii</sup> | 108.99 (4)    | C21—C20—C19         | 120.87 (16)   |
| C32—O9—Sr2<sup>ii</sup> | 131.25 (11)   | C21—Sr2—H20         | 119.6         |
| C32—O9—Sr2<sup>ii</sup> | 89.23 (10)    | C5—C6—H6            | 120.2         |
| Sr1—O7—Sr2<sup>ii</sup> | 99.58 (4)     | C5—C6—C7            | 119.68 (18)   |
| C32—O9—Sr2<sup>ii</sup> | 149.74 (11)   | C7—C6—H6            | 120.2         |
| Sr1—O8—Sr2<sup>ii</sup> | 99.28 (10)    | C2—C7—C6            | 121.07 (18)   |
| Sr1—O8—H8A          | 95.57 (5)     | C2—C7—H7            | 119.5         |
| Sr1—O8—H8A          | 120.0 (17)    | C6—C7—H7            | 119.5         |
| Sr1—O7—C32—Sr2<sup>ii</sup> | −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)      |
| Sr1<sup>ii</sup>—O5—C23—O6 | −6.63 (18)   | C3—C4—C5—C8         | 179.25 (16)   |
| Sr1<sup>ii</sup>—O5—C23—C22 | 173.24 (14) | C3—C4—C5—C6         | −0.8 (3)      |
| Sr1<sup>ii</sup>—O6—C23—C23—O5 | 7.2 (2)     | C25—C24—C22—C23     | −178.49 (16)  |
| Sr1<sup>ii</sup>—O6—C23—C22 | −172.70 (13) | C25—C24—C22—C21     | 0.5 (3)       |
| Sr2<sup>ii</sup>—O4—C14—O3 | −11.3 (2)    | C25—C19—C18—C26     | 47.3 (3)      |
| Sr2<sup>ii</sup>—O4—C14—C13 | 166.13 (10)  | C25—C19—C18—C17     | −131.15 (18)  |
| Sr2<sup>ii</sup>—O9—C32—Sr2<sup>ii</sup> | 114.91 (12)  | C25—C19—C20—C21     | 0.5 (3)       |
| Sr2<sup>ii</sup>—O9—C32—O7 | −11.91 (16)   | C23—C22—C21—C20     | 177.01 (19)   |
| Sr2<sup>ii</sup>—O9—C32—Sr2<sup>ii</sup> | 102.99 (17)  | C27—C8—C9—C10       | 175.15 (16)   |
| Sr2<sup>ii</sup>—O9—C32—C31 | −77.48 (19)  | C27—C8—C9—C17       | −4.1 (2)      |
| Sr2<sup>ii</sup>—O9—C32—C31 | 167.61 (13)  | C27—C8—C5—C4        | 59.6 (2)      |
| Sr2<sup>ii</sup>—O7—C32—Sr2<sup>ii</sup> | 13.06 (17)   | C27—C8—C5—C6        | −120.3 (2)    |
| Sr2<sup>ii</sup>—O7—C32—C31 | −166.47 (12) | C27—C26—C18—C19     | 177.53 (16)   |
| Sr2<sup>ii</sup>—O5—C23—Sr1<sup>ii</sup> | −107.4 (4)   | C27—C26—C18—C17     | −4.0 (2)      |
| Sr2<sup>ii</sup>—O5—C23—O6 | −114.0 (4)    | C19—C18—C17—C9      | −178.88 (16)  |
| Sr2<sup>ii</sup>—O5—C23—C22 | 65.9 (5)     | C10—C9—C17—C18      | −177.77 (16)  |
| Sr2<sup>ii</sup>—C32—C31—C30 | 122.0 (5)    | C2—C3—C4—C5         | 0.3 (3)       |
| Sr2<sup>ii</sup>—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)       |
| O4—C14—C13—C12 | 166.39 (15)   | C4—C5—C6—C7         | 0.3 (3)       |
| O9—C32—C31—C30 | 5.0 (2)       | C14—C13—C12—C11     | 176.26 (15)   |
| O9—C32—C31—C33 | −175.99 (16)  | C5—C8—C9—C10        | −5.7 (3)      |
| O7—C32—C31—C30 | −175.50 (16)  | C5—C8—C9—C17        | 175.09 (16)   |
| O7—C32—C31—C33 | 3.6 (2)       | C5—C8—C27—C26       | −176.56 (15)  |
| O3—C14—C13—C15 | 160.52 (16)   | C5—C6—C7—C2         | 0.7 (4)       |
| O3—C14—C13—C12 | −16.0 (2)     | C29—C28—C26—C27     | 69.2 (2)      |
| C24—C22—C23—O5         | −169.00 (17) | C29—C28—C26—C18     | −111.8 (2)    |
| C24—C22—C23—C6         | 10.9 (3)     | C29—C28—C34—C33     | −2.1 (3)      |
| C24—C22—C21—C20        | −2.0 (3)     | C15—C13—C12—C11     | −0.4 (3)      |
| C24—C25—C19—C18        | 175.55 (16)  | C13—C15—C16—C10     | 1.1 (3)       |
| C24—C25—C19—C20        | −2.0 (3)     | C13—C12—C11—C10     | 0.0 (3)       |
| C32—C31—C30—C29        | 176.78 (16)  | C18—C26—C27—C8      | 1.5 (3)       |
| C32—C31—C33—C34        | −178.78 (16) | C18—C19—C20—C21     | −177.09 (19)  |
| C28—C26—C27—C8         | −179.53 (15) | C16—C10—C11—C12     | 0.9 (2)       |
| C28—C26—C18—C19        | −1.4 (3)     | 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)
C26—C18—C17—C8 2.7 (3) C1—C2—C7—C6 179.1 (2)
C9—C8—C27—C26 −119.61 (19) C20—C19—C18—C17 46.4 (3)
C9—C8—C27—C26 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—C16—C15 −178.55 (16) C7—C2—C1—O2 4.6 (3)

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

| D—H···A | D—H | H···A | D···A  | D—H···A |
|---------|-----|------|-------|---------|
| O1—H1···O4i | 0.84 (3) | 1.79 | 2.6051 (18) | 164 |
| O10—H10A···O2ix | 0.84 (3) | 1.97 (3) | 2.795 (2) | 168 (3) |
| O10—H10B···O6x | 0.78 (3) | 2.01 (3) | 2.787 (2) | 173 (3) |
| O8—H8B···O3xi | 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.