

Technical University of Denmark



Polymeric strontium ranelate nonahydrate

Ståhl, Kenny; Frankær, Christian Grundahl; Raffalt, Anders Christer; Sørensen, Søren R.; Andersen, Jens Enevold Thaulov

Published in:

Acta Crystallographica. Section E: Structure Reports Online

Link to article, DOI:

[10.1107/S1600536811010099](https://doi.org/10.1107/S1600536811010099)

Publication date:

2011

Document Version

Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):

Ståhl, K., Frankær, C. G., Raffalt, A. C., Sørensen, S. R., & Andersen, J. E. T. (2011). Polymeric strontium ranelate nonahydrate. Acta Crystallographica. Section E: Structure Reports Online, 67, m471-m472. DOI: 10.1107/S1600536811010099

DTU Library

Technical Information Center of Denmark

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Polymeric strontium ranelate nonahydrate

Kenny Stahl,* Christian G. Frankaer, Anders C. Raffalt, Søren R. Sørensen and Jens E. T. Andersen

Department of Chemistry, Technical University of Denmark, DK-2800 Lyngby, Denmark

Correspondence e-mail: kenny@kemi.dtu.dk

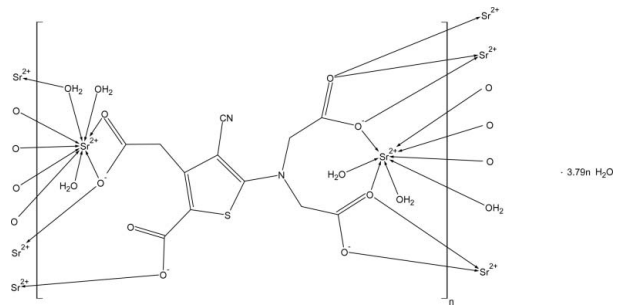
Received 9 March 2011; accepted 17 March 2011

Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; H-atom completeness 99%; disorder in main residue; R factor = 0.033; wR factor = 0.075; data-to-parameter ratio = 17.6.

The title compound, poly[[μ -aqua-tetraaqua $\{\mu$ -5-[bis-(carboxylatomethyl)amino]-3-carboxylatomethyl-4-cyanothiophene-2-carboxylato}distrontium(II)] tetrahydrate], $[\text{Sr}_2(\text{C}_{12}\text{H}_6\text{N}_2\text{O}_8\text{S})(\text{H}_2\text{O})_5] \cdot 3.79\text{H}_2\text{O}$, crystallizes with nine- and eight-coordinated Sr^{2+} cations. They are bound to seven of the eight ranelate O atoms and five of the water molecules. The SrO_8 and SrO_9 polyhedra are interconnected by edge-sharing, forming hollow layers parallel to (011). The layers are, in turn, interconnected by ranelate anions, forming a metal-organic framework (MOF) structure with channels along the a axis. The four water molecules not coordinated to strontium are located in these channels and hydrogen bonded to each other and to the ranelates. Part of the water H atoms are disordered. The compound dehydrates very easily and 0.210 (4) water molecules out of nine were lost during crystal mounting causing additional disorder in the water structure.

Related literature

For the effect of strontium on osteoporosis, see Schrooten *et al.* (2003). For a patent describing the synthesis and powder diffraction pattern of the title compound, see Horvath *et al.* (2008). For related strontium carboxylate structures, see, for example: Stahl *et al.* (2006).



Experimental

Crystal data

$[\text{Sr}_2(\text{C}_{12}\text{H}_6\text{N}_2\text{O}_8\text{S})(\text{H}_2\text{O})_5] \cdot 3.79\text{H}_2\text{O}$
 $M_r = 671.84$
 Triclinic, $P\bar{1}$
 $a = 8.3585$ (3) Å
 $b = 12.3865$ (5) Å
 $c = 12.6474$ (5) Å
 $\alpha = 109.880$ (1)°
 $\beta = 97.148$ (1)°

$\gamma = 105.321$ (1)°
 $V = 1154.00$ (8) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 4.80$ mm⁻¹
 $T = 120$ K
 $0.15 \times 0.10 \times 0.07$ mm

Data collection

Bruker SMART APEX
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.574$, $T_{\max} = 0.710$

17404 measured reflections
 6617 independent reflections
 5375 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.075$
 $S = 1.02$
 6617 reflections
 375 parameters
 21 restraints

H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{\max} = 1.48$ e Å⁻³
 $\Delta\rho_{\min} = -1.23$ e Å⁻³

Table 1

Selected bond lengths (Å).

Sr1—O8	2.4557 (18)	Sr2—O23	2.5921 (18)
Sr1—O3 ⁱ	2.4782 (19)	Sr2—O2 ^j	2.6222 (17)
Sr1—O5	2.5234 (16)	Sr2—O21	2.6445 (17)
Sr1—O7 ⁱⁱ	2.6149 (19)	Sr2—O6	2.6628 (16)
Sr1—O25	2.652 (2)	Sr2—O2 ^{iv}	2.6848 (16)
Sr1—O22	2.6560 (19)	Sr2—O1 ^{iv}	2.6944 (17)
Sr1—O27	2.657 (2)	Sr2—O22	2.7108 (18)
Sr1—O8 ⁱⁱ	2.7834 (17)	Sr2—O5	2.7228 (16)
Sr2—O6 ⁱⁱⁱ	2.5452 (16)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O21—H21A \cdots O25	0.81 (2)	1.98 (2)	2.781 (3)	169 (3)
O21—H21B \cdots O24 ⁱⁱⁱ	0.85 (2)	1.93 (2)	2.765 (3)	169 (3)
O22—H22A \cdots O2 ⁱ	0.81 (2)	2.16 (3)	2.761 (2)	131 (3)
O22—H22B \cdots O26 ^{iv}	0.82 (2)	1.94 (2)	2.755 (3)	173 (3)
O23—H23A \cdots O21 ⁱⁱⁱ	0.81 (2)	1.96 (2)	2.766 (3)	174 (4)
O23—H23B \cdots O26 ⁱ	0.80 (2)	2.11 (2)	2.867 (3)	159 (3)
O24—H24A \cdots O1 ^v	0.82 (2)	2.03 (2)	2.760 (3)	148 (3)
O24—H24B \cdots O4	0.84 (2)	1.93 (2)	2.756 (3)	172 (3)
O25—H25A \cdots N1 ⁱⁱ	0.82 (2)	2.15 (2)	2.898 (3)	152 (3)
O25—H25B \cdots O27 ⁱⁱ	0.80 (2)	1.93 (2)	2.648 (3)	150 (4)

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O26–H26A···O28 ^{vi}	0.85 (2)	1.90 (2)	2.731 (3)	164 (5)
O26–H26C···N1	0.85 (2)	2.37 (4)	3.108 (3)	146 (5)
O27–H27A···O4 ⁱ	0.83 (2)	1.79 (2)	2.615 (3)	172 (4)
O27–H27B···O29 ^{vii}	0.82 (2)	1.94 (2)	2.727 (4)	160 (4)
O28–H28A···O24 ^{iv}	0.80 (2)	1.97 (2)	2.756 (3)	167 (4)
O28–H28B···O28 ^{viii}	0.82 (2)	2.02 (2)	2.835 (4)	174 (8)
O28–H28C···O29	0.82 (2)	2.04 (3)	2.836 (4)	164 (7)
O29–H29A···O7	0.83 (2)	1.78 (2)	2.595 (3)	168 (7)
O29–H29B···O28	0.83 (2)	2.03 (3)	2.836 (4)	164 (7)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *ATOMS* (Dowty, 2000); software used to prepare material for publication: *SHELXL97*.

Ms L. Berring and Ms A. Schöneberg are gratefully acknowledged for the data collection and Dr Stephan Christgau for supplying the strontium ranelate.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2343).

References

- Bruker (1999). *SMART* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dowty, E. (2000). *ATOMS*. Shape Software, Kingsport, Tennessee, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Horvath, S., Demuyneck, I. & Damien, G. (2008). US Patent No. 7459568.
- Schrooten, I., Behets, G. J. S., Cabrera, W. E., Vercauteren, S. R., Lamberts, L. W., Verberckmoes, S. C., Bervoets, A. J., Dams, G., Goodman, W. G., De Broe, M. E. & D Haese, P. C. (2003). *Kidney Intl.* **63**, 927–935.
- Sheldrick, G. M. (2002). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Stahl, K., Andersen, J. E. T. & Christgau, S. (2006). *Acta Cryst.* **C62**, m144–m149.

supplementary materials

Acta Cryst. (2011). E67, m471-m472 [doi:10.1107/S1600536811010099]

Polymeric strontium ranelate nonahydrate

K. Stahl, C. G. Frankaer, A. C. Raffalt, S. R. Sørensen and J. E. T. Andersen

Comment

In recent years it has been found that Sr has a significant influence on the development and growth of bone and the effect of dose on bone structure has been investigated in great detail (Schrooten *et al.* 2003). Strontium ranelate (5-[bis(carboxymethyl) amino]-3-carboxymethyl-4-cyano-2-thiophenecarboxylate) is one promising pharmaceutical compound for treating osteoporosis marketed as Protelos^R by Servier (Horvath *et al.*, 2008). Strontium ranelate is known to form several hydrates with totally nine, eight, seven or four waters (Horvath *et al.*, 2008). The initial dehydration observed here results from an expulsion of O27 or O29 and migration of the remaining water to site O30. As a consequence Sr1 is partially seven-coordinated (c.f. Table 1). The water hydrogen sites connected to O26, O28 and O29 are disordered. In essence, the alternating hydrogen bonding scheme between O28 and O29 is transmitted to a partial O26 - O28 hydrogen bond, and leaves H26B and H29C without hydrogen bond acceptors (c.f. Table 2).

Experimental

Strontium ranelate nona hydrate of 97% purity (Clauson-Kaas A/S) was recrystallized at different temperatures. Recrystallization at temperatures above 353 K appeared to produce the crystals of better quality. Upon cooling to room temperature large crystals of millimeter dimensions were obtained in the saturated solution. However, when the crystals were removed from the solution they rapidly degraded into smaller units of micron dimension. The smaller crystals showed out to contain less crystal water, as compared to the large crystals, presumably seven or five water molecules per formula unit. Thus, wet crystals were quickly transferred to the goniometer for X-ray data collection at 120 K. Several crystal were tried before an acceptable structure refinement was achieved. For all cases of lower quality data the SOF of O30 was about 0.3, confirming its role in the initial dehydration of strontium ranelate and the deterioration of the crystals.

Refinement

The H atoms of the CH₂ groups were placed in calculated positions with C—H = 0.99, and refined as riding atoms. The H atoms of the water molecules were located in difference Fourier maps and refined with restrained O—H distances of 0.82 (2) Å. The H atoms of the partially occupied O30 (SOF=0.210 (4)) could not be located. The H displacement parameters were set to 1.2 (CH₂) or 1.5 (H₂O) times U_{eq} of the corresponding C or O atoms.

Figures

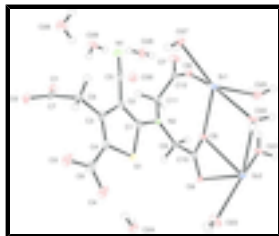


Fig. 1. The asymmetric unit of (I) showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen atoms are represented by circles of arbitrary size and shows one consistent set of water H atoms.

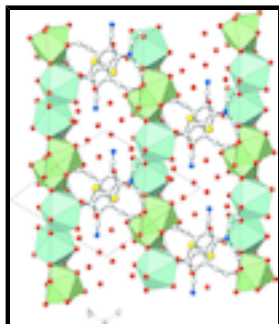


Fig. 2. The crystal packing of (I) viewed down the a-axis. Hydrogen atoms are omitted for clarity.

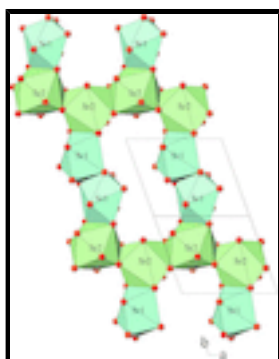


Fig. 3. The polyhedral layer of (I) viewed down the $(01\bar{1})$ direction.

Poly[[μ -aqua-tetraaqua{ μ -5-[bis(carboxylatomethyl)amino]-3- carboxylatomethyl-4-cyanothiophene-2-carboxylato}distrontium(II)] tetrahydrate]

Crystal data

$[\text{Sr}_2(\text{C}_{12}\text{H}_6\text{N}_2\text{O}_8\text{S})(\text{H}_2\text{O})_5] \cdot 3.79\text{H}_2\text{O}$

$M_r = 671.84$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.3585$ (3) Å

$b = 12.3865$ (5) Å

$c = 12.6474$ (5) Å

$\alpha = 109.880$ (1)°

$\beta = 97.148$ (1)°

$\gamma = 105.321$ (1)°

$V = 1154.00$ (8) Å³

$Z = 2$

$F(000) = 671.8$

$D_x = 1.933$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6752 reflections

$\theta = 2.6\text{--}30.6^\circ$

$\mu = 4.80$ mm⁻¹

$T = 120$ K

Tabular, colorless

$0.15 \times 0.10 \times 0.07$ mm

Data collection

Bruker SMART APEX diffractometer	6617 independent reflections
Radiation source: fine-focus sealed tube graphite	5375 reflections with $I > 2\sigma(I)$
ω scan, frame data integration	$R_{\text{int}} = 0.032$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$\theta_{\text{max}} = 30.9^\circ$, $\theta_{\text{min}} = 2.6^\circ$
$T_{\text{min}} = 0.574$, $T_{\text{max}} = 0.710$	$h = -12 \rightarrow 12$
17404 measured reflections	$k = -17 \rightarrow 17$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.033$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.075$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2]$
6617 reflections	where $P = (F_o^2 + 2F_c^2)/3$
375 parameters	$(\Delta/\sigma)_{\text{max}} = 0.002$
21 restraints	$\Delta\rho_{\text{max}} = 1.48 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -1.23 \text{ e } \text{\AA}^{-3}$

Special details

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

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sr1	0.52281 (3)	0.38668 (2)	0.836097 (18)	0.01665 (6)	
Sr2	0.26745 (3)	0.029136 (18)	0.557006 (17)	0.01072 (6)	
S1	0.13839 (8)	0.40229 (5)	0.50122 (5)	0.01584 (12)	
C1	0.1878 (3)	0.4919 (2)	0.6477 (2)	0.0160 (5)	
C2	0.3059 (3)	0.6056 (2)	0.6709 (2)	0.0183 (5)	
C3	0.3561 (3)	0.6182 (2)	0.5698 (2)	0.0168 (5)	

supplementary materials

C4	0.2738 (3)	0.5158 (2)	0.4721 (2)	0.0169 (5)	
C5	0.3781 (4)	0.7012 (2)	0.7831 (2)	0.0237 (6)	
N1	0.4382 (4)	0.7807 (2)	0.8712 (2)	0.0373 (7)	
C6	0.4862 (3)	0.7305 (2)	0.5736 (2)	0.0187 (5)	
H6A	0.5431	0.7077	0.5091	0.022*	
H6B	0.5745	0.7663	0.6470	0.022*	
C7	0.4063 (3)	0.8258 (2)	0.5642 (2)	0.0140 (4)	
O1	0.3026 (2)	0.85078 (16)	0.62454 (15)	0.0218 (4)	
O2	0.4503 (2)	0.87870 (15)	0.49792 (15)	0.0168 (3)	
C8	0.2835 (3)	0.4871 (2)	0.3498 (2)	0.0208 (5)	
O3	0.3592 (3)	0.57144 (17)	0.32159 (17)	0.0293 (4)	
O4	0.2095 (3)	0.37659 (16)	0.28052 (16)	0.0253 (4)	
N2	0.1127 (3)	0.44571 (17)	0.71912 (16)	0.0138 (4)	
C9	0.0097 (3)	0.3176 (2)	0.6705 (2)	0.0147 (4)	
H9A	-0.0850	0.3036	0.6067	0.018*	
H9B	-0.0415	0.2978	0.7309	0.018*	
C10	0.1092 (3)	0.2303 (2)	0.62385 (19)	0.0125 (4)	
O5	0.2644 (2)	0.25859 (14)	0.67064 (14)	0.0150 (3)	
O6	0.0259 (2)	0.13041 (14)	0.54187 (13)	0.0141 (3)	
C11	0.0937 (3)	0.5241 (2)	0.82968 (19)	0.0167 (5)	
H11A	-0.0207	0.4870	0.8398	0.020*	
H11B	0.0977	0.6033	0.8259	0.020*	
C12	0.2261 (3)	0.5475 (2)	0.9357 (2)	0.0177 (5)	
O7	0.2069 (3)	0.60995 (17)	1.03249 (15)	0.0266 (4)	
O8	0.3467 (2)	0.50536 (16)	0.92535 (15)	0.0213 (4)	
O21	0.1336 (2)	0.04188 (16)	0.73788 (14)	0.0177 (4)	
H21A	0.195 (3)	0.096 (2)	0.7968 (19)	0.027*	
H21B	0.111 (4)	-0.021 (2)	0.753 (3)	0.027*	
O22	0.5486 (2)	0.16837 (18)	0.73157 (15)	0.0218 (4)	
H22A	0.608 (4)	0.162 (3)	0.686 (2)	0.033*	
H22B	0.572 (4)	0.129 (3)	0.768 (3)	0.033*	
O23	0.2011 (2)	-0.02488 (19)	0.33592 (16)	0.0246 (4)	
H23A	0.102 (3)	-0.035 (3)	0.311 (3)	0.037*	
H23B	0.249 (4)	-0.006 (3)	0.291 (2)	0.037*	
O24	-0.0724 (3)	0.17943 (17)	0.24069 (16)	0.0233 (4)	
H24A	-0.138 (4)	0.198 (3)	0.282 (3)	0.035*	
H24B	0.015 (3)	0.240 (2)	0.260 (3)	0.035*	
O25	0.3787 (3)	0.23012 (19)	0.92443 (16)	0.0299 (5)	
H25A	0.430 (4)	0.204 (3)	0.965 (3)	0.045*	
H25B	0.316 (4)	0.259 (3)	0.958 (3)	0.045*	
O26	0.6112 (3)	1.0182 (2)	0.83803 (19)	0.0321 (5)	
H26A	0.686 (5)	1.030 (5)	0.897 (3)	0.048*	0.67
H26B	0.549 (6)	1.037 (5)	0.885 (4)	0.048*	0.67
H26C	0.532 (5)	0.952 (3)	0.823 (5)	0.048*	0.67
O27	0.7186 (3)	0.6180 (2)	0.91336 (19)	0.0194 (6)	0.790 (4)
H27A	0.740 (5)	0.626 (4)	0.854 (2)	0.029*	0.79
H27B	0.811 (4)	0.640 (4)	0.959 (3)	0.029*	0.79
O28	0.1058 (3)	0.92663 (19)	0.99457 (17)	0.0302 (5)	
H28A	0.111 (5)	0.896 (3)	0.9290 (18)	0.045*	

H28B	0.041 (8)	0.966 (6)	1.000 (7)	0.045*	0.50
H28C	0.059 (8)	0.873 (5)	1.015 (6)	0.045*	0.50
O29	0.0120 (4)	0.7429 (3)	1.0829 (2)	0.0287 (7)	0.790 (4)
H29A	0.073 (7)	0.701 (5)	1.058 (6)	0.043*	0.53
H29B	0.045 (9)	0.806 (4)	1.071 (6)	0.043*	0.53
H29C	-0.024 (10)	0.732 (8)	1.016 (3)	0.043*	0.53
O30	-0.0951 (12)	0.6963 (8)	0.9739 (8)	0.023 (2)*	0.210 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01489 (12)	0.02075 (12)	0.00915 (10)	0.00204 (9)	0.00133 (8)	0.00307 (9)
Sr2	0.01086 (11)	0.01068 (10)	0.00940 (10)	0.00340 (8)	0.00144 (7)	0.00290 (8)
S1	0.0195 (3)	0.0115 (3)	0.0149 (3)	0.0032 (2)	0.0029 (2)	0.0051 (2)
C1	0.0158 (12)	0.0144 (11)	0.0177 (11)	0.0064 (9)	-0.0008 (9)	0.0067 (9)
C2	0.0197 (12)	0.0133 (11)	0.0215 (12)	0.0061 (10)	-0.0004 (10)	0.0078 (10)
C3	0.0133 (11)	0.0122 (11)	0.0255 (12)	0.0049 (9)	0.0006 (9)	0.0087 (10)
C4	0.0164 (12)	0.0138 (11)	0.0241 (12)	0.0060 (9)	0.0057 (10)	0.0105 (10)
C5	0.0287 (15)	0.0139 (12)	0.0256 (13)	0.0010 (11)	-0.0027 (11)	0.0120 (11)
N1	0.0485 (17)	0.0204 (12)	0.0261 (13)	-0.0078 (11)	-0.0058 (12)	0.0083 (10)
C6	0.0129 (11)	0.0152 (12)	0.0301 (13)	0.0046 (9)	0.0032 (10)	0.0122 (10)
C7	0.0120 (11)	0.0104 (10)	0.0167 (11)	0.0015 (8)	0.0008 (9)	0.0042 (9)
O1	0.0269 (10)	0.0231 (9)	0.0262 (9)	0.0140 (8)	0.0147 (8)	0.0152 (8)
O2	0.0174 (9)	0.0160 (8)	0.0201 (8)	0.0055 (7)	0.0065 (7)	0.0101 (7)
C8	0.0220 (13)	0.0200 (13)	0.0260 (13)	0.0100 (11)	0.0119 (11)	0.0111 (11)
O3	0.0386 (12)	0.0209 (10)	0.0317 (11)	0.0058 (9)	0.0167 (9)	0.0141 (9)
O4	0.0348 (11)	0.0179 (9)	0.0252 (10)	0.0072 (8)	0.0152 (8)	0.0092 (8)
N2	0.0185 (10)	0.0084 (9)	0.0109 (9)	0.0030 (8)	0.0002 (7)	0.0016 (7)
C9	0.0142 (11)	0.0121 (11)	0.0150 (11)	0.0029 (9)	0.0014 (9)	0.0038 (9)
C10	0.0157 (11)	0.0109 (10)	0.0106 (10)	0.0022 (9)	0.0027 (8)	0.0056 (8)
O5	0.0125 (8)	0.0144 (8)	0.0140 (8)	0.0033 (6)	-0.0023 (6)	0.0032 (6)
O6	0.0140 (8)	0.0104 (8)	0.0127 (8)	0.0016 (6)	-0.0014 (6)	0.0016 (6)
C11	0.0195 (12)	0.0164 (11)	0.0125 (11)	0.0096 (10)	0.0008 (9)	0.0017 (9)
C12	0.0235 (13)	0.0113 (11)	0.0151 (11)	0.0023 (9)	0.0003 (9)	0.0055 (9)
O7	0.0378 (12)	0.0255 (10)	0.0124 (8)	0.0109 (9)	0.0040 (8)	0.0028 (7)
O8	0.0213 (9)	0.0194 (9)	0.0199 (9)	0.0077 (7)	-0.0036 (7)	0.0056 (7)
O21	0.0200 (9)	0.0184 (9)	0.0120 (8)	0.0043 (7)	0.0025 (7)	0.0046 (7)
O22	0.0186 (9)	0.0305 (10)	0.0139 (9)	0.0109 (8)	0.0024 (7)	0.0043 (8)
O23	0.0172 (9)	0.0421 (12)	0.0195 (9)	0.0106 (9)	0.0070 (8)	0.0164 (9)
O24	0.0270 (11)	0.0201 (9)	0.0198 (9)	0.0028 (8)	0.0098 (8)	0.0066 (8)
O25	0.0413 (13)	0.0248 (11)	0.0151 (9)	0.0009 (9)	0.0046 (9)	0.0060 (8)
O26	0.0299 (12)	0.0322 (12)	0.0283 (11)	0.0011 (10)	0.0029 (9)	0.0131 (10)
O27	0.0243 (13)	0.0161 (11)	0.0129 (11)	0.0003 (9)	0.0054 (9)	0.0042 (9)
O28	0.0422 (14)	0.0295 (12)	0.0163 (9)	0.0133 (10)	0.0022 (9)	0.0060 (9)
O29	0.0313 (15)	0.0330 (15)	0.0249 (14)	0.0161 (12)	0.0070 (11)	0.0107 (12)

Geometric parameters (\AA , $^\circ$)

Sr1—O8	2.4557 (18)	N2—C11	1.462 (3)
--------	-------------	--------	-----------

supplementary materials

Sr1—O3 ⁱ	2.4782 (19)	C9—C10	1.540 (3)
Sr1—O5	2.5234 (16)	C9—H9A	0.9900
Sr1—O7 ⁱⁱ	2.6149 (19)	C9—H9B	0.9900
Sr1—O25	2.652 (2)	C10—O5	1.258 (3)
Sr1—O22	2.6560 (19)	C10—O6	1.258 (3)
Sr1—O27	2.657 (2)	C11—C12	1.517 (3)
Sr1—O8 ⁱⁱ	2.7834 (17)	C11—H11A	0.9900
Sr2—O6 ⁱⁱⁱ	2.5452 (16)	C11—H11B	0.9900
Sr2—O23	2.5921 (18)	C12—O8	1.253 (3)
Sr2—O2 ⁱ	2.6222 (17)	C12—O7	1.262 (3)
Sr2—O21	2.6445 (17)	O21—H21A	0.809 (18)
Sr2—O6	2.6628 (16)	O21—H21B	0.845 (17)
Sr2—O2 ^{iv}	2.6848 (16)	O22—H22A	0.808 (18)
Sr2—O1 ^{iv}	2.6944 (17)	O22—H22B	0.819 (17)
Sr2—O22	2.7108 (18)	O23—H23A	0.807 (18)
Sr2—O5	2.7228 (16)	O23—H23B	0.798 (18)
S1—C1	1.733 (2)	O24—H24A	0.823 (18)
S1—C4	1.735 (2)	O24—H24B	0.837 (18)
C1—N2	1.358 (3)	O25—H25A	0.819 (18)
C1—C2	1.398 (3)	O25—H25B	0.796 (18)
C2—C5	1.431 (4)	O26—H26A	0.850 (19)
C2—C3	1.439 (4)	O26—H26B	0.849 (19)
C3—C4	1.368 (3)	O26—H26C	0.85 (2)
C3—C6	1.504 (3)	O27—H27A	0.827 (19)
C4—C8	1.482 (4)	O27—H27B	0.823 (19)
C5—N1	1.148 (3)	O28—H28A	0.799 (18)
C6—C7	1.532 (3)	O28—H28B	0.82 (2)
C6—H6A	0.9900	O28—H28C	0.82 (2)
C6—H6B	0.9900	O29—H29A	0.83 (2)
C7—O1	1.256 (3)	O29—H29B	0.83 (2)
C7—O2	1.261 (3)	O29—H29C	0.82 (2)
C8—O3	1.257 (3)	O27—O30 ^v	1.534 (10)
C8—O4	1.275 (3)	O29—O30	1.383 (10)
N2—C9	1.456 (3)		
O8—Sr1—O3 ⁱ	117.69 (6)	O22—Sr2—O5	67.10 (5)
O8—Sr1—O5	87.39 (5)	C1—S1—C4	92.44 (12)
O3 ⁱ —Sr1—O5	81.32 (6)	N2—C1—C2	130.8 (2)
O8—Sr1—O7 ⁱⁱ	118.97 (6)	N2—C1—S1	119.08 (17)
O3 ⁱ —Sr1—O7 ⁱⁱ	101.51 (7)	C2—C1—S1	110.09 (19)
O5—Sr1—O7 ⁱⁱ	146.34 (5)	C1—C2—C5	125.2 (2)
O8—Sr1—O25	85.98 (7)	C1—C2—C3	113.4 (2)
O3 ⁱ —Sr1—O25	150.13 (6)	C5—C2—C3	121.3 (2)
O5—Sr1—O25	81.94 (6)	C4—C3—C2	111.8 (2)
O7 ⁱⁱ —Sr1—O25	79.69 (7)	C4—C3—C6	124.9 (2)
O8—Sr1—O22	147.38 (6)	C2—C3—C6	123.3 (2)

O3 ⁱ —Sr1—O22	83.58 (6)	C3—C4—C8	131.1 (2)
O5—Sr1—O22	70.82 (5)	C3—C4—S1	112.22 (19)
O7 ⁱⁱ —Sr1—O22	76.14 (6)	C8—C4—S1	116.67 (18)
O25—Sr1—O22	67.59 (6)	N1—C5—C2	177.5 (3)
O8—Sr1—O27	74.49 (7)	C3—C6—C7	112.26 (19)
O3 ⁱ —Sr1—O27	70.14 (7)	C3—C6—H6A	109.2
O5—Sr1—O27	132.72 (6)	C7—C6—H6A	109.2
O7 ⁱⁱ —Sr1—O27	77.82 (7)	C3—C6—H6B	109.2
O25—Sr1—O27	137.67 (6)	C7—C6—H6B	109.2
O22—Sr1—O27	138.07 (7)	H6A—C6—H6B	107.9
O8—Sr1—O8 ⁱⁱ	70.87 (6)	O1—C7—O2	122.2 (2)
O3 ⁱ —Sr1—O8 ⁱⁱ	130.40 (6)	O1—C7—C6	119.1 (2)
O5—Sr1—O8 ⁱⁱ	147.09 (6)	O2—C7—C6	118.7 (2)
O7 ⁱⁱ —Sr1—O8 ⁱⁱ	48.19 (5)	O3—C8—O4	125.2 (2)
O25—Sr1—O8 ⁱⁱ	72.41 (6)	O3—C8—C4	118.9 (2)
O22—Sr1—O8 ⁱⁱ	115.58 (5)	O4—C8—C4	115.9 (2)
O27—Sr1—O8 ⁱⁱ	65.82 (6)	C1—N2—C9	117.63 (19)
O6 ⁱⁱⁱ —Sr2—O23	69.11 (6)	C1—N2—C11	121.82 (19)
O6 ⁱⁱⁱ —Sr2—O2 ⁱ	138.88 (5)	C9—N2—C11	118.5 (2)
O23—Sr2—O2 ⁱ	71.52 (6)	N2—C9—C10	114.24 (19)
O6 ⁱⁱⁱ —Sr2—O21	79.58 (5)	N2—C9—H9A	108.7
O23—Sr2—O21	145.03 (6)	C10—C9—H9A	108.7
O2 ⁱ —Sr2—O21	141.51 (5)	N2—C9—H9B	108.7
O6 ⁱⁱⁱ —Sr2—O6	68.34 (6)	C10—C9—H9B	108.7
O23—Sr2—O6	81.03 (5)	H9A—C9—H9B	107.6
O2 ⁱ —Sr2—O6	116.53 (5)	O5—C10—O6	123.3 (2)
O21—Sr2—O6	73.03 (5)	O5—C10—C9	119.92 (19)
O6 ⁱⁱⁱ —Sr2—O2 ^{iv}	96.94 (5)	O6—C10—C9	116.7 (2)
O23—Sr2—O2 ^{iv}	81.54 (6)	N2—C11—C12	115.7 (2)
O2 ⁱ —Sr2—O2 ^{iv}	65.68 (6)	N2—C11—H11A	108.3
O21—Sr2—O2 ^{iv}	118.40 (5)	C12—C11—H11A	108.3
O6—Sr2—O2 ^{iv}	160.37 (5)	N2—C11—H11B	108.3
O6 ⁱⁱⁱ —Sr2—O1 ^{iv}	79.58 (5)	C12—C11—H11B	108.3
O23—Sr2—O1 ^{iv}	116.26 (6)	H11A—C11—H11B	107.4
O2 ⁱ —Sr2—O1 ^{iv}	108.25 (5)	O8—C12—O7	122.9 (2)
O21—Sr2—O1 ^{iv}	71.00 (5)	O8—C12—C11	120.5 (2)
O6—Sr2—O1 ^{iv}	135.19 (5)	O7—C12—C11	116.7 (2)
O2 ^{iv} —Sr2—O1 ^{iv}	48.34 (5)	H21A—O21—H21B	106 (3)
O6 ⁱⁱⁱ —Sr2—O22	156.57 (6)	H22A—O22—H22B	104 (3)
O23—Sr2—O22	133.65 (6)	H23A—O23—H23B	104 (3)
O2 ⁱ —Sr2—O22	62.33 (5)	H24A—O24—H24B	108 (3)
O21—Sr2—O22	79.68 (6)	H25A—O25—H25B	109 (4)
O6—Sr2—O22	115.27 (5)	H26A—O26—H26B	87 (5)

supplementary materials

O2 ^{iv} —Sr2—O22	83.49 (5)	H26A—O26—H26C	108 (5)
O1 ^{iv} —Sr2—O22	83.47 (6)	H26B—O26—H26C	75 (5)
O6 ⁱⁱⁱ —Sr2—O5	114.87 (5)	H27A—O27—H27B	107 (4)
O23—Sr2—O5	109.66 (6)	H28A—O28—H28B	111 (6)
O2 ⁱ —Sr2—O5	89.11 (5)	H28A—O28—H28C	109 (6)
O21—Sr2—O5	69.47 (5)	H28B—O28—H28C	103 (7)
O6—Sr2—O5	48.56 (5)	H29A—O29—H29B	107 (7)
O2 ^{iv} —Sr2—O5	148.19 (5)	H29A—O29—H29C	87 (6)
O1 ^{iv} —Sr2—O5	133.93 (5)	H29B—O29—H29C	68 (6)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O21—H21A \cdots O25	0.81 (2)	1.98 (2)	2.781 (3)	169 (3)
O21—H21B \cdots O24 ⁱⁱⁱ	0.85 (2)	1.93 (2)	2.765 (3)	169 (3)
O22—H22A \cdots O2 ⁱ	0.81 (2)	2.16 (3)	2.761 (2)	131 (3)
O22—H22B \cdots O26 ^{iv}	0.82 (2)	1.94 (2)	2.755 (3)	173 (3)
O23—H23A \cdots O21 ⁱⁱⁱ	0.81 (2)	1.96 (2)	2.766 (3)	174 (4)
O23—H23B \cdots O26 ⁱ	0.80 (2)	2.11 (2)	2.867 (3)	159 (3)
O24—H24A \cdots O1 ^{vi}	0.82 (2)	2.03 (2)	2.760 (3)	148 (3)
O24—H24B \cdots O4	0.84 (2)	1.93 (2)	2.756 (3)	172 (3)
O25—H25A \cdots N1 ⁱⁱ	0.82 (2)	2.15 (2)	2.898 (3)	152 (3)
O25—H25B \cdots O27 ⁱⁱ	0.80 (2)	1.93 (2)	2.648 (3)	150 (4)
O26—H26A \cdots O28 ^{vii}	0.85 (2)	1.90 (2)	2.731 (3)	164 (5)
O26—H26C \cdots N1	0.85 (2)	2.37 (4)	3.108 (3)	146 (5)
O27—H27A \cdots O4 ⁱ	0.83 (2)	1.79 (2)	2.615 (3)	172 (4)
O27—H27B \cdots O29 ^v	0.82 (2)	1.94 (2)	2.727 (4)	160 (4)
O28—H28A \cdots O24 ^{vi}	0.80 (2)	1.97 (2)	2.756 (3)	167 (4)
O28—H28B \cdots O28 ^{viii}	0.82 (2)	2.02 (2)	2.835 (4)	174 (8)
O28—H28C \cdots O29	0.82 (2)	2.04 (3)	2.836 (4)	164 (7)
O29—H29A \cdots O7	0.83 (2)	1.78 (2)	2.595 (3)	168 (7)
O29—H29B \cdots O28	0.83 (2)	2.03 (3)	2.836 (4)	164 (7)

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

Fig. 1

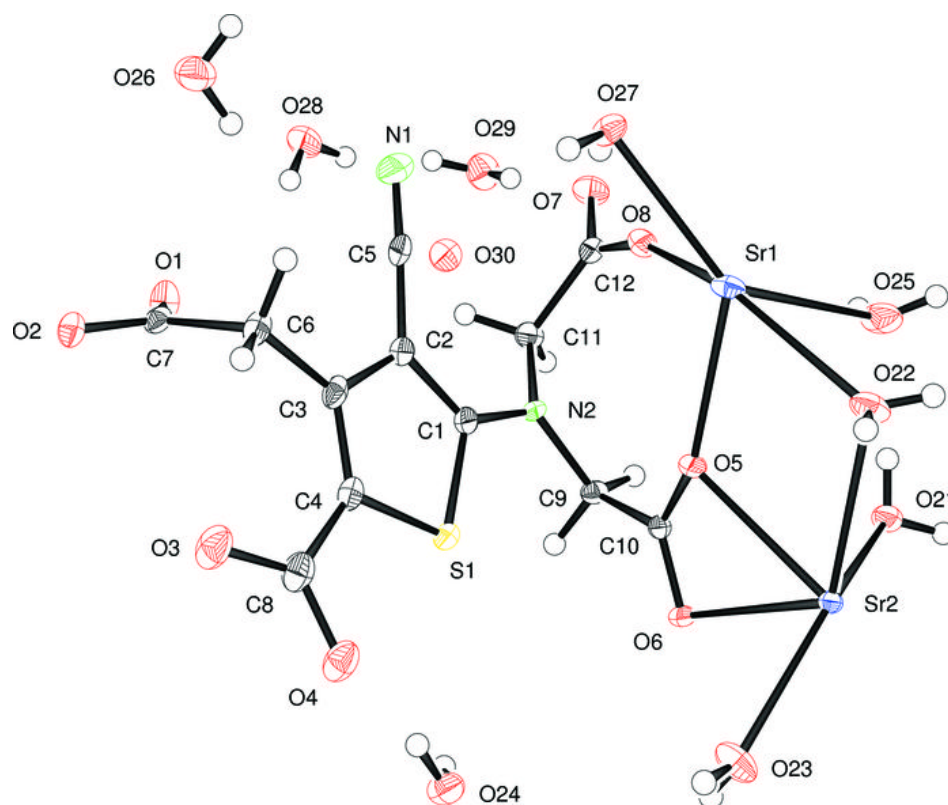


Fig. 2

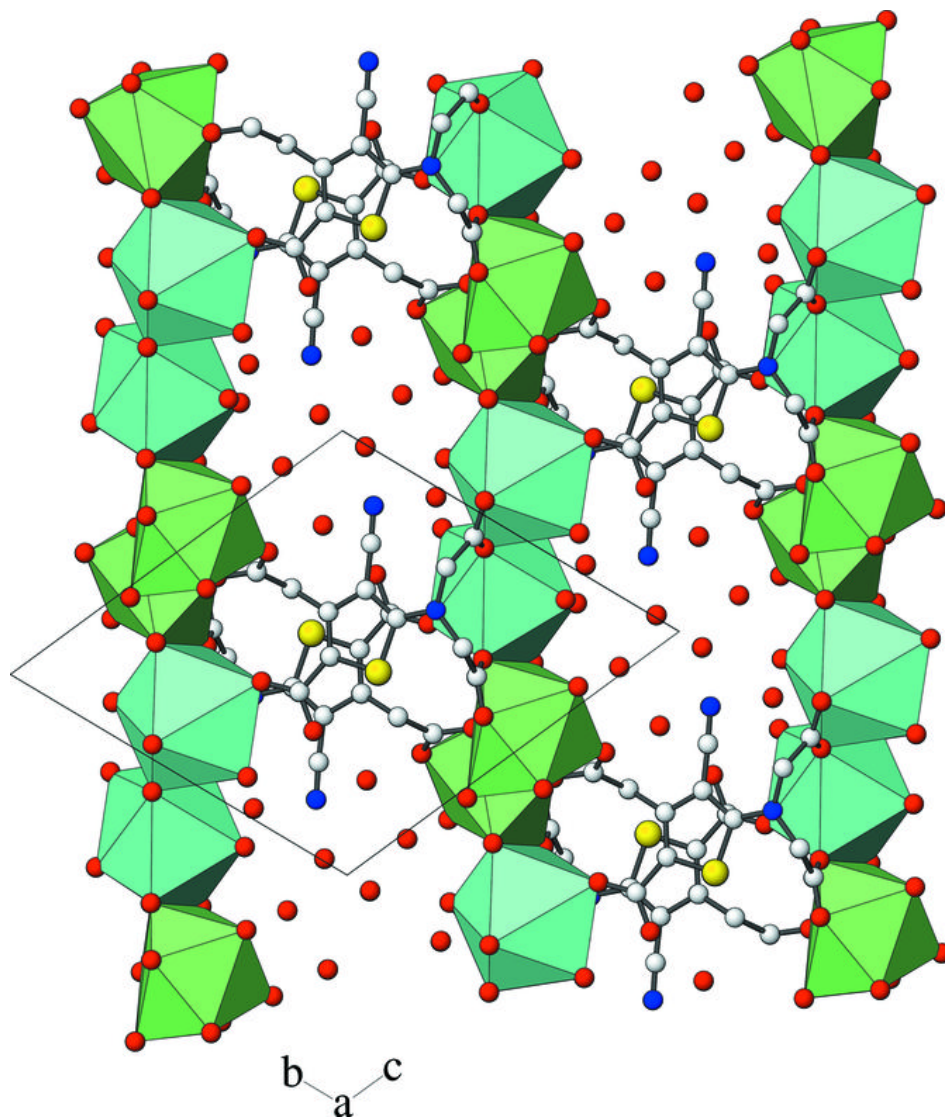


Fig. 3

