Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Strontium disodium hexathiodiphosphate(IV) octahydrate

Claus Ehrhardt and Mimoza Gjikaj*

Institute of Inorganic and Analytical Chemistry, Clausthal University of Technology, Paul-Ernst-Strasse 4, 38678 Clausthal-Zellerfeld, Germany
Correspondence e-mail: mimoza.gjikaj@tu-clausthal.de

Received 11 June 2010; accepted 28 June 2010

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(P–P) = 0.001 Å; R factor = 0.036; wR factor = 0.087; data-to-parameter ratio = 21.0.

The crystal structure of $SrNa_2(P_2S_6)\cdot 8H_2O$ is isotypic with that of its calcium analogue. The asymmetric unit consists of one Sr^{2+} cation (2 symmetry), two Na^+ cations (2 and $\overline{1}$ symmetry, respectively), one-half of a centrosymmetric $(P_2S_6)^{4-}$ anion with a staggered confirmation and four water molecules. The crystal structure is built up from layers of cations and anions extending parallel to (101). Each SrO_8 polyhedron is connected *via* edge-sharing to two NaO_4S_2 octahedra and to one NaO_2S_4 octahedron. The NaO_4S_2 octaedra are, in turn, connected with two $(P_2S_6)^{4-}$ anions through common corners. Adjacent layers are held together by several O—H···S hydrogen-bonding interactions.

Related literature

For background to thiodiphosphates(IV), including their crystal structures, see: Jörgens *et al.* (2003); Klingen *et al.* (1973). For the synthesis of $Na_4(P_2S_6)\cdot 6H_2O$, see: Fincher *et al.* (1998). For the isotypic structure of $CaNa_2(P_2S_6)\cdot 8H_2O$, see: Ehrhardt &Gjikaj (2010).

Experimental

Crystal data

$SrNa_2(P_2S_6)\cdot 8H_2O$
M_r = 532.03
Monoclinic, $C2/c$
a = 14.9010 (19) Å
b = 9.3282 (7) Å
c = 14.1338 (19) Å
β = 114.918 (10)°
V = 1781.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.98 mm^{-1}
T = 223 K
0.28 × 0.26 × 0.25 mm

Data collection

Stoe IPDS 2 diffractometer
14472 measured reflections
2544 independent reflections
2302 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.087
S = 1.12
2544 reflections
121 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sr—O1	2.573 (2)	Na2—O2	2.570 (3)
Sr—O2	2.596 (2)	Na2—S1^{i}	2.9525 (15)
Sr—O3	2.631 (2)	Na2—S3	2.9924 (9)
Sr—O4	2.6459 (19)	P—S1	2.0162 (9)
Na1—O3	2.345 (2)	P—S2	2.0243 (9)
Na1—O4	2.372 (2)	P—S3	2.0248 (9)
Na1—S2^{i}	2.9741 (7)	P—P^{i}	2.2405 (12)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···S3^{ii}	0.76 (7)	2.66 (6)	3.324 (3)	146 (6)
O1—H1B···S2^{iii}	0.86 (6)	2.53 (6)	3.306 (3)	151 (5)
O2—H2A···S2^{ii}	0.82 (6)	2.51 (6)	3.334 (2)	176 (6)
O2—H2B···S2^{i}	0.79 (5)	2.43 (5)	3.214 (2)	176 (5)
O3—H3A···S1^{iv}	0.76 (7)	2.44 (7)	3.169 (2)	163 (5)
O3—H3B···S1^{ii}	0.88 (7)	2.40 (7)	3.222 (2)	157 (6)
O4—H4A···S3^{v}	0.95 (5)	2.29 (5)	3.245 (2)	175 (4)
O4—H4B···S3	0.91 (6)	2.30 (6)	3.199 (2)	171 (5)

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

Data collection: *X-AREA* (Stoe & Cie, 2008); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2365).

References

Brandenburg, K. (2004). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Ehrhardt, C. & Gjikaj, M. (2010). *Acta Cryst.* E**66**, i54.
Fincher, T., LeBret, G. & Cleary, D. A. (1998). *J. Solid State Chem.* **141**, 274–281.
Jörgens, S., Mewis, A., Hoffmann, R.-D., Pöttgen, R. & Mosel, B. D. (2003). *Z. Anorg. Allg. Chem.* **629**, 429–433.
Klingen, W., Ott, R. & Hahn, H. (1973). *Z. Anorg. Allg. Chem.* **396**, 271–278.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2008). *X-AREA*. Stoe & Cie, Darmstadt, Germany.

supporting information

Acta Cryst. (2010). E**66**, i55 [https://doi.org/10.1107/S1600536810025316]

Strontium disodium hexathiodiphosphate(IV) octahydrate

Claus Ehrhardt and Mimoza Gjikaj

S1. Comment

Alkaline earth hypothiodiphosphates were first reported by Klingen *et al.* (1973). The structure of the title compound, $SrNa_2(P_2S_6).8H_2O$, is isotypic with that of its calcium analogue, $CaNa_2(P_2S_6).8H_2O$ (Ehrhardt & Gjikaj, 2010). The asymmetric unit of $SrNa_2(P_2S_6).8H_2O$ contains one Sr^{2+} cation, two Na^+ cations, one half of a $(P_2S_6)^{4-}$ anion and four water molecules (Fig. 1)

Na(1) is octahedrally coordinated by four H_2O molecules and two sulfur atoms of two $(P_2S_6)^{4-}$ anions (Fig. 2). Na(2) is also octahedrally coordinated by two H_2O molecules and four sulfur atoms of two $(P_2S_6)^{4-}$ anions (Fig. 3). The strontium cation is eightfold coordinated by water O atoms with Sr—O distances from 2.573 (2) to 2.6459 (19) Å. The SrO_8 coordination polyhedron can be described as a bicapped trigonal prism.

The crystal structure is built up from layers of cations and anions extending parallel to (101). Within the layer each SrO_8 polyhedron is connected by edge-sharing to two $Na(1)O_4S_2$ octahedra and to one $Na(2)O_2S_4$ octaedron. Furthermore, the $Na(1)O_4S_2$ octaedra are connected through common corners with two $(P_2S_6)^{4-}$ anions.

The discrete ethane-like $(P_2S_6)^{4-}$ anion has a staggered conformation and is located on a centre of inversion associated with the midpoint of the P—P bond. The corresponding P—P distance is 2.2405 (12) Å; the P—S distances range from 2.0162 (9) to 2.0248 (9) Å. These values agree well with those reported previously for other hypothiodiphosphate structures (Jörgens *et al.*, 2003).

Neighbouring layers are held together by various O—H···S hydrogen bonding interactions. The donor—acceptor distances between O atoms of water molecules and S atoms of $(P_2S_6)^{4-}$ units range from 3.169 to 3.334 Å (Table 2).

With the exception of the *M*-O bond lengths (*M* = Ca, Sr), all other bond lengths and angles as well as the O—H···S hydrogen bonding scheme are very similar in the two isotypic $MNa_2(P_2S_6).8H_2O$ structures.

S2. Experimental

$Na_4(P_2S_6).6H_2O$ has been prepared according to Fincher *et al.* (1998). The title compound was obtained by adding a molar equivalent of strontium hydroxide to a solution of $Na_4(P_2S_6).6H_2O$ in 70 ml distilled water at 348 K. Slow cooling to room temperature yielded colorless crystals of the title compound within some days.

S3. Refinement

Hydrogen atoms were found from the difference Fourier map and were refined independently from their respective oxygen atoms with individual isotropic displacement parameters.

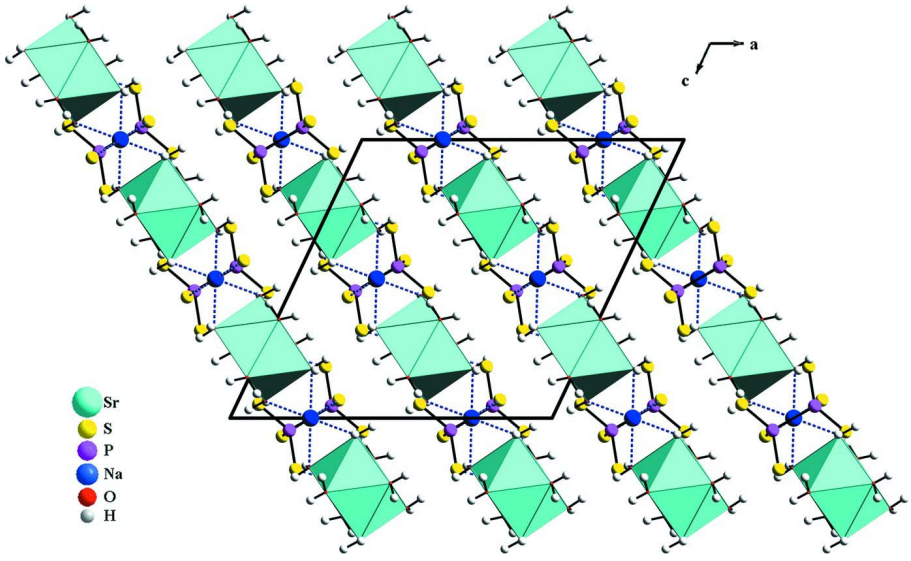

Figure 1

The crystal structure of $CaNa_2(P_2S_6).8H_2O$ in a projection along [010].

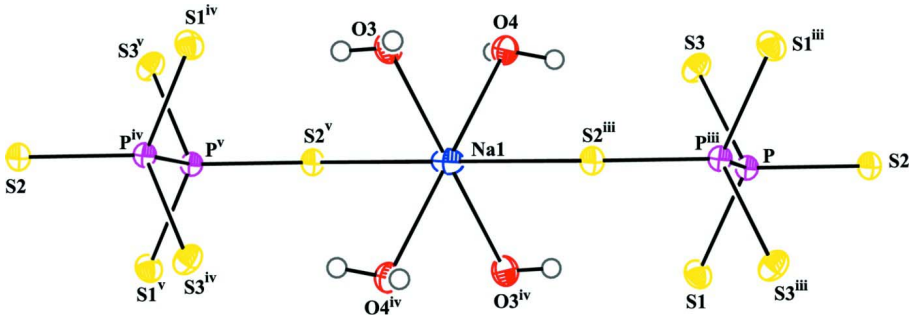

Figure 2

Coordination of Na1 with the atom labelling scheme. The displacement ellipsoids are drawn at the 50% probability level. Symmetry codes as in Table 1. H atoms are represented as spheres of arbirtary radius.

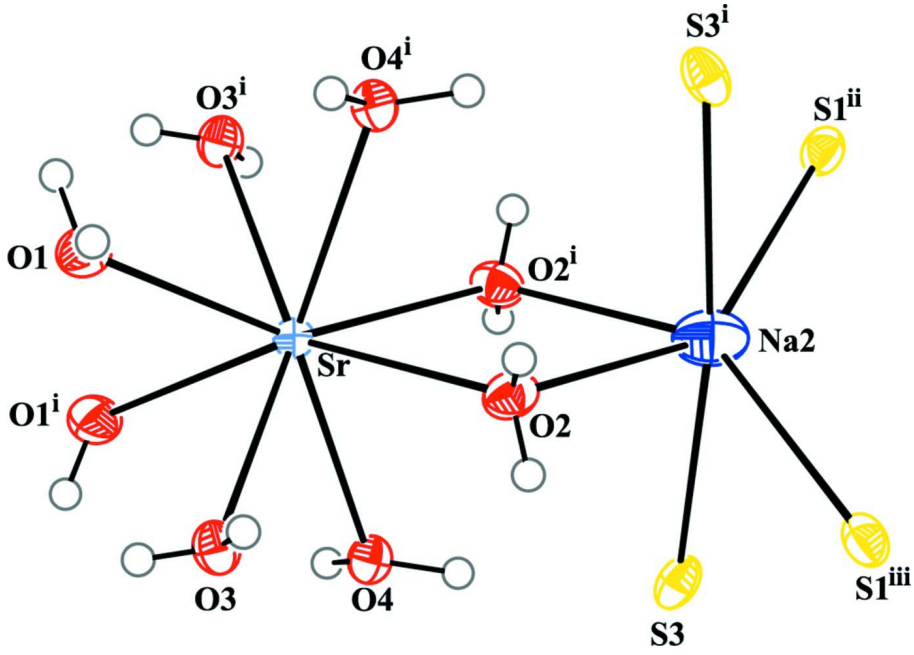

Figure 3

View of the edge-shared CaO_8 and $Na(2)O_2S_4$ polyhedra with the atom labelling scheme. The displacement ellipsoids are drawn at the 50% probability level. Symmetry codes as in Table 1. H atoms are represented as spheres of arbitrary radius.

Strontium disodium hexathiodiphosphate(IV) octahydrate

Crystal data

$SrNa_2(P_2S_6)\cdot 8H_2O$
$M_r = 532.03$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 14.9010\ (19)$ Å
$b = 9.3282\ (7)$ Å
$c = 14.1338\ (19)$ Å
$\beta = 114.918\ (10)°$
$V = 1781.7\ (4)$ Å^3
$Z = 4$
$F(000) = 1064$
$D_x = 1.983$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14971 reflections
$\theta = 1.0–29.8°$
$\mu = 3.98$ mm^{-1}
$T = 223$ K
Block, colorless
0.28 × 0.26 × 0.25 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–scans
14472 measured reflections
2544 independent reflections
2302 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 29.8°$, $\theta_{min} = 2.7°$
$h = -20\rightarrow20$
$k = -13\rightarrow11$
$l = -19\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.087$
$S = 1.12$
2544 reflections
121 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 5.0597P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
All H-atom parameters refined	$\Delta\rho_{max} = 1.14$ e Å^{-3}
	$\Delta\rho_{min} = -0.89$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr	0.5000	0.24637 (4)	0.2500	0.01746 (10)
Na1	0.2500	0.2500	0.0000	0.0260 (3)
Na2	0.5000	0.6875 (3)	0.2500	0.0440 (5)
P	0.20406 (5)	0.76351 (7)	0.04496 (5)	0.01570 (13)
S1	0.07286 (5)	0.67170 (8)	−0.04401 (6)	0.02445 (15)
S2	0.18992 (5)	0.97603 (7)	0.06433 (5)	0.01959 (14)
S3	0.28146 (5)	0.66742 (8)	0.18434 (5)	0.02452 (15)
O1	0.59794 (17)	0.0300 (3)	0.2305 (2)	0.0318 (5)
O2	0.50855 (17)	0.4687 (2)	0.14363 (17)	0.0259 (4)
O3	0.41245 (15)	0.1665 (2)	0.05340 (16)	0.0238 (4)
O4	0.31300 (14)	0.3293 (2)	0.17560 (15)	0.0220 (4)
H1A	0.627 (5)	0.042 (7)	0.197 (5)	0.08 (2)*
H1B	0.638 (4)	0.000 (6)	0.292 (5)	0.065 (17)*
H2A	0.555 (5)	0.473 (6)	0.127 (5)	0.070 (17)*
H2B	0.461 (4)	0.486 (5)	0.093 (4)	0.046 (13)*
H3A	0.404 (4)	0.086 (7)	0.048 (5)	0.067 (17)*
H3B	0.450 (5)	0.195 (8)	0.023 (5)	0.09 (2)*
H4A	0.282 (3)	0.283 (5)	0.214 (4)	0.037 (11)*
H4B	0.302 (4)	0.425 (7)	0.170 (4)	0.059 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr	0.01698 (15)	0.01714 (16)	0.01694 (15)	0.000	0.00585 (11)	0.000
Na1	0.0230 (7)	0.0303 (9)	0.0221 (7)	0.0003 (6)	0.0068 (6)	−0.0014 (6)
Na2	0.0384 (10)	0.0598 (15)	0.0284 (9)	0.000	0.0086 (8)	0.000
P	0.0192 (3)	0.0137 (3)	0.0171 (3)	−0.0002 (2)	0.0104 (2)	−0.0003 (2)
S1	0.0209 (3)	0.0200 (3)	0.0336 (3)	−0.0042 (2)	0.0127 (3)	−0.0043 (3)
S2	0.0232 (3)	0.0145 (3)	0.0219 (3)	0.0012 (2)	0.0103 (2)	−0.0008 (2)
S3	0.0343 (3)	0.0226 (3)	0.0197 (3)	0.0094 (3)	0.0144 (3)	0.0058 (2)
O1	0.0232 (10)	0.0306 (12)	0.0366 (12)	0.0049 (8)	0.0076 (9)	−0.0042 (10)
O2	0.0237 (9)	0.0299 (11)	0.0224 (9)	0.0016 (8)	0.0081 (8)	0.0062 (8)
O3	0.0277 (10)	0.0218 (10)	0.0236 (9)	−0.0005 (8)	0.0126 (8)	−0.0037 (8)
O4	0.0242 (9)	0.0205 (9)	0.0229 (9)	0.0013 (7)	0.0115 (7)	0.0007 (8)

Geometric parameters (Å, º)

Sr—O1	2.573 (2)	Na1—S2^{iv}	2.9741 (7)
Sr—O1^{i}	2.573 (2)	Na2—O2	2.570 (3)
Sr—O2^{i}	2.596 (2)	Na2—O2^{i}	2.570 (3)

Sr—O2	2.596 (2)	Na2—S1^{iv}	2.9525 (15)
Sr—O3	2.631 (2)	Na2—S1^{v}	2.9525 (15)
Sr—O3^{i}	2.631 (2)	Na2—S3	2.9924 (9)
Sr—O4	2.6459 (19)	Na2—S3^{i}	2.9925 (9)
Sr—O4^{i}	2.6459 (19)	P—S1	2.0162 (9)
Na1—O3^{ii}	2.344 (2)	P—S2	2.0243 (9)
Na1—O3	2.345 (2)	P—S3	2.0248 (9)
Na1—O4	2.372 (2)	P—P^{iv}	2.2405 (12)
Na1—O4^{ii}	2.372 (2)	S1—Na2^{iv}	2.9525 (15)
Na1—S2^{iii}	2.9741 (7)	S2—Na1^{vi}	2.9741 (7)
O1—Sr—O1^{i}	76.65 (12)	O3—Na1—S2^{iii}	91.09 (6)
O1—Sr—O2^{i}	149.01 (7)	O4—Na1—S2^{iii}	89.18 (5)
O1^{i}—Sr—O2^{i}	113.34 (9)	O4^{ii}—Na1—S2^{iii}	90.82 (5)
O1—Sr—O2	113.34 (9)	O3^{ii}—Na1—S2^{iv}	91.09 (6)
O1^{i}—Sr—O2	149.01 (7)	O3—Na1—S2^{iv}	88.91 (6)
O2^{i}—Sr—O2	73.96 (10)	O4—Na1—S2^{iv}	90.82 (5)
O1—Sr—O3	73.49 (8)	O4^{ii}—Na1—S2^{iv}	89.18 (5)
O1^{i}—Sr—O3	80.77 (8)	S2^{iii}—Na1—S2^{iv}	180.0
O2^{i}—Sr—O3	135.60 (7)	O2—Na2—O2^{i}	74.82 (12)
O2—Sr—O3	74.82 (7)	O2—Na2—S1^{iv}	82.23 (5)
O1—Sr—O3^{i}	80.78 (8)	O2^{i}—Na2—S1^{iv}	147.35 (8)
O1^{i}—Sr—O3^{i}	73.50 (8)	O2—Na2—S1^{v}	147.35 (8)
O2^{i}—Sr—O3^{i}	74.82 (7)	O2^{i}—Na2—S1^{v}	82.23 (5)
O2—Sr—O3^{i}	135.59 (7)	S1^{iv}—Na2—S1^{v}	127.17 (10)
O3—Sr—O3^{i}	147.09 (10)	O2—Na2—S3	94.85 (7)
O1—Sr—O4	137.47 (7)	O2^{i}—Na2—S3	79.40 (6)
O1^{i}—Sr—O4	73.86 (7)	S1^{iv}—Na2—S3	79.75 (3)
O2^{i}—Sr—O4	72.30 (7)	S1^{v}—Na2—S3	103.51 (3)
O2—Sr—O4	80.60 (7)	O2—Na2—S3^{i}	79.40 (6)
O3—Sr—O4	72.10 (6)	O2^{i}—Na2—S3^{i}	94.85 (7)
O3^{i}—Sr—O4	118.24 (6)	S1^{iv}—Na2—S3^{i}	103.51 (3)
O1—Sr—O4^{i}	73.86 (7)	S1^{v}—Na2—S3^{i}	79.75 (3)
O1^{i}—Sr—O4^{i}	137.47 (7)	S3—Na2—S3^{i}	172.83 (11)
O2^{i}—Sr—O4^{i}	80.60 (7)	S1—P—S2	111.81 (4)
O2—Sr—O4^{i}	72.30 (7)	S1—P—S3	115.08 (4)
O3—Sr—O4^{i}	118.23 (6)	S2—P—S3	110.55 (4)
O3^{i}—Sr—O4^{i}	72.10 (6)	S1—P—P^{iv}	105.20 (5)
O4—Sr—O4^{i}	145.98 (9)	S2—P—P^{iv}	108.07 (5)
O3^{ii}—Na1—O3	180.0	S3—P—P^{iv}	105.57 (5)
O3^{ii}—Na1—O4	97.64 (7)	P—S1—Na2^{iv}	106.45 (5)
O3—Na1—O4	82.36 (7)	P—S2—Na1^{vi}	137.58 (3)
O3^{ii}—Na1—O4^{ii}	82.36 (7)	P—S3—Na2	111.92 (4)
O3—Na1—O4^{ii}	97.64 (7)	Na2—O2—Sr	105.61 (9)
O4—Na1—O4^{ii}	180.0	Na1—O3—Sr	103.36 (8)
O3^{ii}—Na1—S2^{iii}	88.91 (6)	Na1—O4—Sr	102.17 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···S3^{vii}	0.76 (7)	2.66 (6)	3.324 (3)	146 (6)
O1—H1*B*···S2^{viii}	0.86 (6)	2.53 (6)	3.306 (3)	151 (5)
O2—H2*A*···S2^{vii}	0.82 (6)	2.51 (6)	3.334 (2)	176 (6)
O2—H2*B*···S2^{iv}	0.79 (5)	2.43 (5)	3.214 (2)	176 (5)
O3—H3*A*···S1^{ii}	0.76 (7)	2.44 (7)	3.169 (2)	163 (5)
O3—H3*B*···S1^{vii}	0.88 (7)	2.40 (7)	3.222 (2)	157 (6)
O4—H4*A*···S3^{ix}	0.95 (5)	2.29 (5)	3.245 (2)	175 (4)
O4—H4*B*···S3	0.91 (6)	2.30 (6)	3.199 (2)	171 (5)

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