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Crystal structure of strontium and barium acesulafame (6-methyl-4-oxo-4*H*-1,2,3-oxathiazin-3-ide 2,2-dioxide)

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CCDC references: 1838460; 1838459

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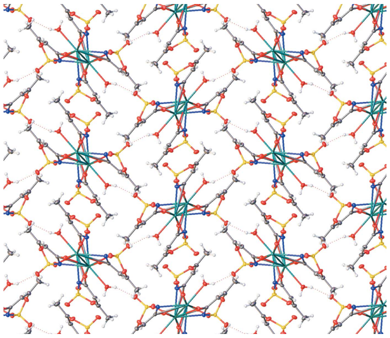
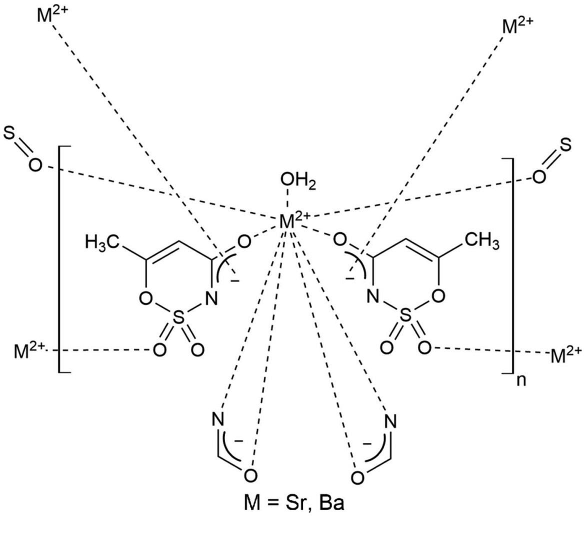
Both strontium and barium acesulfames, namely poly[aquabis(μ_3-6-methyl-2,2-dioxo-1,2λ^6,3-oxathiazin-4-olato)strontium(II)], $[Sr(C_4H_4NO_4S)_2(H_2O)]_n$, and the barium(II) analogue, $[Ba(C_4H_4NO_4S)_2(H_2O)]_n$, crystallize in nearly identical isotypic forms, with barium–oxygen interatomic distances being longer due to the larger ionic radius of the barium(II) ion. The coordination number of the metal ion is 9; the coordination polyhedra can be described as distorted capped square antiprisms [Johnson solid **J10**; Johnson (1966). *Can. J. Math.* **18**, 169–200]. The conformation of the acesulafame ions is a distorted envelope with an out-of-plane S atom. Metal and acesulfame ions are assembled into infinitive chains along the [100] axis. These chains are connected *via* hydrogen bonds into a three-dimensional network.



1. Chemical context

Acesulfame is one of the most common sweeteners; usually it is used in the form of a potassium salt. Salts with all alkali metals, ammonium, magnesium, and calcium ions, as well as its protonated molecular form, are also known. The almost identical crystal structures of the strontium and barium salts are reported here.



2. Structural commentary

Both the strontium and barium compounds crystallize in nearly identical isotypic forms (Fig. 1), with the barium–oxygen interatomic distances being longer due to the larger ionic radius of the barium(II) ion (Tables 1 and 2). Because of

Table 1
Selected bond lengths (Å) for Sr.

Sr1—O1	2.6000 (14)	Sr1—O6^{iii}	2.8070 (13)
Sr1—O2^{i}	2.9039 (14)	Sr1—O9^{iv}	2.5782 (12)
Sr1—O2	2.5026 (12)	Sr1—N1^{i}	2.7553 (15)
Sr1—O5^{ii}	2.5790 (13)	Sr1—N2^{iii}	2.7447 (14)
Sr1—O6	2.5116 (12)		

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

Table 2
Selected bond lengths (Å) for Ba.

Ba1—O1	2.732 (2)	Ba1—O6^{iii}	2.9192 (18)
Ba1—O2^{i}	2.9714 (19)	Ba1—O9^{iv}	2.7478 (18)
Ba1—O2	2.6812 (17)	Ba1—N1^{i}	2.921 (2)
Ba1—O5^{ii}	2.7560 (18)	Ba1—N2^{iii}	2.9077 (19)
Ba1—O6	2.6788 (16)		

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

the similarity of the structures, representations would be visually identical, and all figures are shown for the strontium salt only. In both cases, the coordination sphere of the metal ion contains a water molecule, two O atoms from carbonyl groups, two O atoms from sulfonyl fragments, and two bidentate amide groups coordinated through both their carbonyl group and the adjacent deprotonated N atom (Fig. 2). The total coordination number is nine. This coordination polyhedron can be described as a distorted capped square antiprism. The corresponding ideal polyhedron is a gyro-elongated square pyramid, a Johnson solid **J10** (Johnson, 1966). In this case, the base of the polyhedron is not a square but a rectangle formed by two N and two O atoms from two bidentate amide groups. Nitrogen–oxygen distances within each of the groups are practically the same: N1$^{i}\cdots$O2^{i} = 2.232 (2) Å and N2$^{iii}\cdots$O6^{iii} = 2.233 (2) Å (Sr); and N1$^{i}\cdots$O2^{i} = 2.233 (3) Å and N2$^{iii}\cdots$O6^{iii} = 2.239 (2) Å (Ba). The inter-atomic separations between these groups are much longer: N1$^{i}\cdots$O6^{iii} = 3.0609 (19) (Sr) and 3.174 (3) Å (Ba), and N2$^{iii}\cdots$O2^{i} = 3.0787 (18) (Sr) and 3.184 (3) Å (Ba) [symmetry codes: (i) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y+1, -z+1$.]

Deviations from exact right angles are around 5° for the Sr and 1.5° for the Ba structure. The upper square of the coordination polyhedron is less distorted, with angles very close (mostly within 1°) to 90°. The two average planes of the base rectangle and upper square are nearly coplanar, with the angles between them being 1.17 (4) (Sr) and 0.99 (6)° (Ba). The line between the metal ions and the capping oxygen of the water molecules are nearly perpendicular to these planes: the angles between the upper plane normal and the connecting line are 4.90 (4) (Sr) and 5.58 (6)° (Ba).

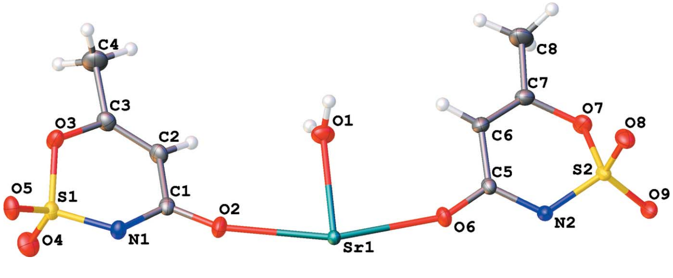


Figure 1
The numbering scheme of strontium acesulfame monohydrate, shown with 50% probability displacement ellipsoids.

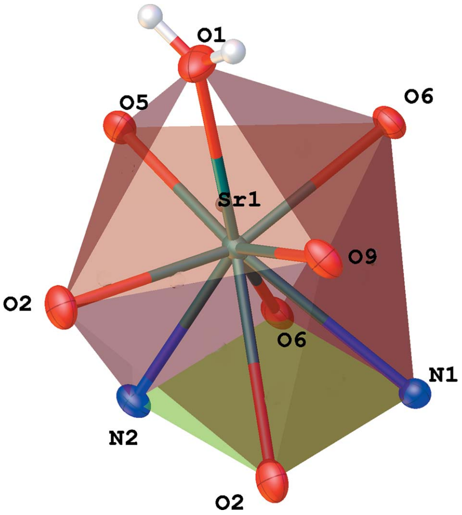


Figure 2
The coordination polyhedron of the Sr metal ion. Symmetry codes for the base rectangle atoms are: N1 and O2 at ($-x+1, -y+1, -z+1$), N2 and O6 at ($-x+2, -y+1, -z+1$). For the upper rectangle: O9 is at ($x-1, y, z$) and O5 is at ($x+1, y, z$).

The geometries of the two acesulfame anions in each structure are very similar to each other (Fig. 3), as well as to

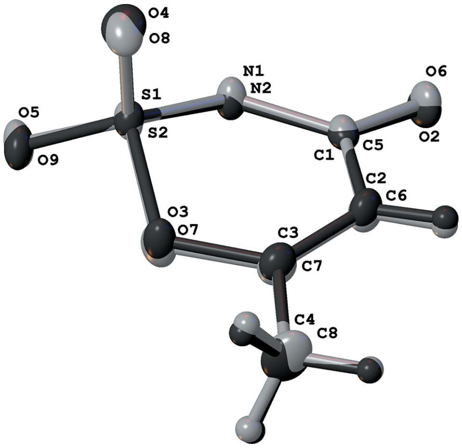


Figure 3
Overlay of the two acesulafame ions in the Sr structure.

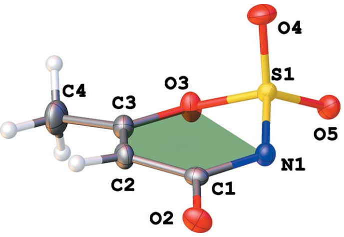


Figure 4
View of the acesulafame anion in the Sr structure. Deviations from the average plane of five atoms in six-membered ring are 0.031 (N1), −0.010 (O3), −0.011 (C3), +0.042 (C2), −0.052 (C1) and 0.5377 (15) Å (S1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O4$^{\rm v}$	0.79 (3)	2.18 (3)	2.899 (2)	151 (3)
O1—H1*B*···O8$^{\rm vi}$	0.83 (3)	2.22 (3)	2.9850 (19)	152 (3)
C4—H4*B*···O5$^{\rm v}$	0.98	2.37	3.273 (3)	153
C6—H6···O8$^{\rm vi}$	0.95	2.47	3.318 (2)	148

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O4$^{\rm v}$	0.74 (4)	2.12 (4)	2.829 (3)	162 (4)
O1—H1*B*···O8$^{\rm vi}$	0.74 (4)	2.20 (4)	2.889 (3)	156 (4)
C4—H4*B*···O5$^{\rm v}$	0.98	2.44	3.361 (4)	155
C6—H6···O8$^{\rm vi}$	0.95	2.52	3.357 (3)	147

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

those of previously reported compounds. The six-membered rings have only one atom with a tetrahedral environment (S). The other five atoms deviate only slightly from their average planes (Fig. 4). This conformation can be described as an envelope, slightly distorted toward a boat.

3. Supramolecular features

Each acesulfame anion is connected to three strontium (or barium) ions *via* a bridging O atom of the amide carbonyl group, an N atom of this group, and one of the O atoms of a sulfonyl group. Each metal ion is directly connected to six acesulfame anions. As a result, metal ions and acesulfame anions form infinite chains along the [100] axis (Fig. 5). The O atoms of the two sulfonyl groups that are not connected to metal ions form, instead, strong hydrogen bonds with both H atoms of the water molecule. These hydrogen bonds (Tables 3 and 4) connect each chain to four neighboring parellel chains, thus creating a three-dimensional assembly (Fig. 6). There are also two short C—H···O contacts (Tables 3 and 4) which may additionally stabilize the crystal structures.

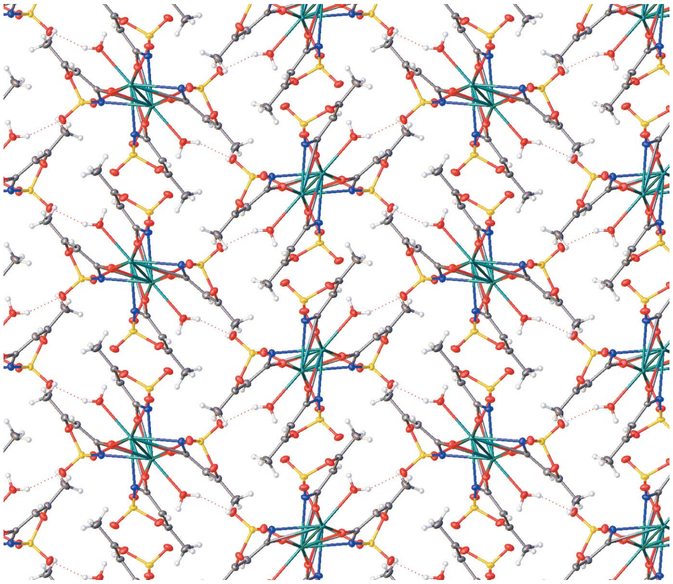


Figure 6
The packing of Sr acesulafame, viewed along the [100] axis.

4. Database survey

There are over 40 acesulfame structures deposited in the Cambridge Structural Database (CSD; Groom *et al.*, 2016; Version 5.38). Of these structures, alkali metal, ammonium, and thallium salts FEQPUP (Piro *et al.*, 2017), KMTOZD (Paulus, 1975), SUQTOP, SURCIT and SURCOZ (Piro *et al.*, 2015), TOFPEL (Echeverría *et al.*, 2014), OCAHUY (Baran *et al.*, 2015), magnesium salt XAGVAF (Piro *et al.*, 2016), calcium salt EXUCOR (Demirtas *et al.*, 2012), and protonated forms WURMOM and WURMOM01 (Velaga *et al.*, 2010) are closely related to the structures of the title compounds. Several other structures describe coordination compounds

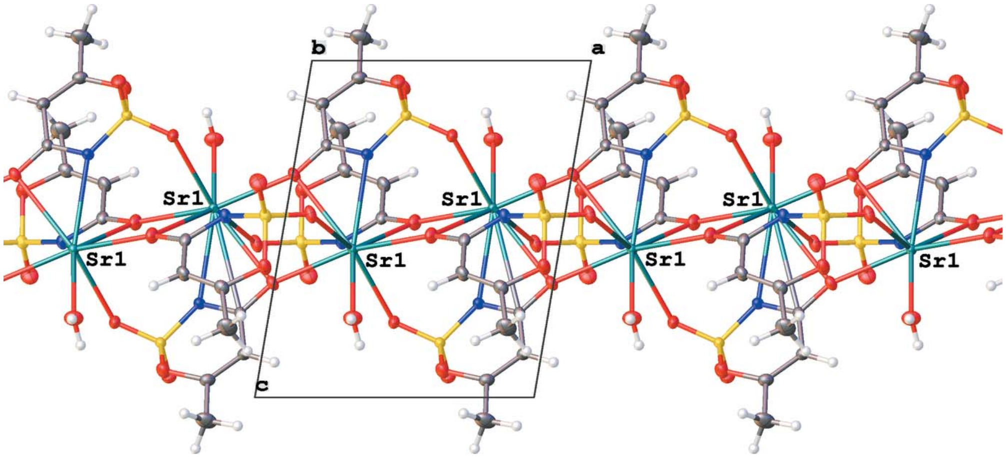


Figure 5
The infinite chain of metal ions and acesulafame anions along the [100] axis. The view is along the [010] vector.

Table 5
Experimental details.

	Sr complex	Ba complex
Crystal data		
Chemical formula	$[Sr(C_4H_4NO_4S)_2(H_2O)]$	$[Ba(C_4H_4NO_4S)_2(H_2O)]$
M_r	429.92	479.64
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
Temperature (K)	173	173
a, b, c (Å)	7.9695 (3), 18.5217 (8), 9.7310 (4)	8.2086 (5), 18.8899 (11), 9.8999 (6)
β (°)	99.651 (1)	99.5197 (10)
V (Å^3)	1416.05 (10)	1513.93 (16)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	4.15	2.94
Crystal size (mm)	0.55 × 0.13 × 0.07	0.52 × 0.21 × 0.20
Data collection		
Diffractometer	Bruker PHOTON-100 CMOS	Bruker PHOTON-100 CMOS
Absorption correction	Numerical (*SADABS*; Krause *et al.*, 2015)	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.228, 0.797	0.309, 0.635
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	54583, 5414, 4548	41654, 6324, 5218
R_{int}	0.043	0.048
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.771	0.794
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.062, 1.04	0.032, 0.059, 1.09
No. of reflections	5414	6324
No. of parameters	209	209
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.73, −0.46	1.02, −0.61

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

with transition-metal ions and various salts of bulky organic cations.

5. Synthesis and crystallization

The protonated form of acesulfame, 6-methyl-1,2,3-oxathiazin-4(3*H*)-one 2,2-dioxide, was synthesized following a published procedure (Velaga *et al.*, 2010). The starting compound, potassium acesulfame, was obtained at a stated purity of 99% and no attempt was made at further purification. 2 g (0.01 mol) of it were dissolved in water (10 ml), acidified with 10 ml of 6 *M* HCl, and extracted with several portions of methylene chloride (15 ml each). Evaporation of the methylene chloride extract resulted in crystals of protonated acesulfame (identified by X-ray diffraction; CSD refcode WURMOM). Both strontium oxide (100 mg, 0.001 mol) and barium oxide (150 mg, 0.001 mol) were treated with a small amount of water (*ca* 10 ml), forming the corresponding hydroxides. Stoichiometric amounts (0.002 mol, 320 mg) of 6-methyl-1,2,3-oxathiazin-4(3*H*)-one 2,2-dioxide were added under gentle heating to neutralize the alkaline solutions. Slow evaporation of the filtrated solutions resulted in colorless crystals (around 100 mg), some of which were suitable for X-ray investigation. No attempts to optimize the reaction conditions or to recover more material were made. Several crystals were tested; the best results obtained are reported here. FT-IR-ATR, Sr–acesulfame (cm^{-1}): 3620, 3550 (H_2O), 1641 (amide), 1555, 1173 (SO_2), 938.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. All H atoms of water molecules are refined in isotropic approximation. All other H atoms are refined with riding coordinates; methyl H atoms are refined as rotating idealized methyl groups and with $U_{iso}(H) = 1.5U_{iso}(C)$.

Acknowledgements

Financial support from the State University of New York for acquisition and maintenance of the X-ray diffractometer is gratefully acknowledged.

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supporting information

Acta Cryst. (2018). E**74**, 698-702 [https://doi.org/10.1107/S2056989018006059]

Crystal structure of strontium and barium acesulafame (6-methyl-4-oxo-4*H*-1,2,3-oxathiazin-3-ide 2,2-dioxide)

Alexander Y. Nazarenko

Computing details

For both structures, data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013). Program(s) used to solve structure: SHELXT (Sheldrick, 2015a) for Sr. Program(s) used to refine structure: SHELXLL2016 (Sheldrick, 2015b) for Sr; *SHELXL97* (Sheldrick, 2008) for Ba. For both structures, molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Poly[aquabis(μ_3-6-methyl-2,2-dioxo-1,2λ^6,3-oxathiazin-4-olato)strontium(II)] (Sr)

Crystal data

$[Sr(C_4H_4NO_4S)_2(H_2O)]$
$M_r = 429.92$
Monoclinic, $P2_1/n$
$a = 7.9695$ (3) Å
$b = 18.5217$ (8) Å
$c = 9.7310$ (4) Å
$\beta = 99.651$ (1)°
$V = 1416.05$ (10) Å^3
$Z = 4$
$F(000) = 856$
$D_x = 2.017$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9082 reflections
$\theta = 3.1–33.3$°
$\mu = 4.15$ mm^{-1}
$T = 173$ K
Needle, colourless
0.55 × 0.13 × 0.07 mm

Data collection

Bruker PHOTON-100 CMOS diffractometer
φ and ω scans
Absorption correction: numerical (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.228$, $T_{max} = 0.797$
54583 measured reflections
5414 independent reflections
4548 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 33.2°$, $\theta_{min} = 3.1°$
$h = -12 \rightarrow 12$
$k = -28 \rightarrow 28$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.062$
$S = 1.04$
5414 reflections
209 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 1.3759P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
Sr1	0.73894 (2)	0.46960 (2)	0.43922 (2)	0.01161 (4)
S1	0.07248 (5)	0.32528 (2)	0.53917 (4)	0.01432 (7)
S2	1.37055 (5)	0.52355 (2)	0.16245 (4)	0.01457 (8)
O1	0.69696 (19)	0.37734 (8)	0.23495 (15)	0.0236 (3)
H1A	0.703 (4)	0.3346 (16)	0.232 (3)	0.038 (8)*
H1B	0.656 (4)	0.3914 (17)	0.155 (3)	0.049 (9)*
O2	0.46642 (16)	0.41317 (7)	0.48048 (14)	0.0216 (3)
O3	0.04339 (16)	0.28794 (7)	0.38723 (14)	0.0207 (3)
O4	0.11859 (18)	0.26877 (7)	0.63821 (14)	0.0247 (3)
O5	−0.08823 (16)	0.35905 (7)	0.54351 (14)	0.0200 (2)
O6	1.00611 (16)	0.48946 (7)	0.33932 (13)	0.0185 (2)
O7	1.34454 (16)	0.44775 (8)	0.07948 (14)	0.0218 (3)
O8	1.31994 (17)	0.57900 (8)	0.06234 (13)	0.0223 (3)
O9	1.54716 (15)	0.52276 (7)	0.22320 (13)	0.0197 (2)
N1	0.21644 (18)	0.38308 (8)	0.53881 (15)	0.0159 (3)
N2	1.25495 (18)	0.51967 (8)	0.27867 (14)	0.0162 (3)
C1	0.3450 (2)	0.36951 (9)	0.46730 (17)	0.0149 (3)
C2	0.3318 (2)	0.30990 (10)	0.36758 (18)	0.0191 (3)
H2	0.4300	0.2956	0.3311	0.023*
C3	0.1853 (2)	0.27495 (10)	0.32641 (18)	0.0188 (3)
C4	0.1419 (3)	0.22384 (12)	0.2083 (2)	0.0310 (4)
H4A	0.0983	0.1789	0.2419	0.046*
H4B	0.2441	0.2135	0.1680	0.046*
H4C	0.0548	0.2454	0.1370	0.046*
C5	1.1042 (2)	0.48462 (9)	0.25133 (17)	0.0142 (3)
C6	1.0638 (2)	0.43825 (10)	0.12897 (17)	0.0175 (3)
H6	0.9511	0.4203	0.1040	0.021*
C7	1.1800 (2)	0.42032 (10)	0.05129 (17)	0.0186 (3)
C8	1.1604 (3)	0.36965 (12)	−0.0686 (2)	0.0312 (4)
H8A	1.1812	0.3954	−0.1521	0.047*
H8B	1.0446	0.3500	−0.0848	0.047*
H8C	1.2424	0.3301	−0.0480	0.047*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01046 (6)	0.01363 (7)	0.01116 (6)	−0.00146 (5)	0.00300 (4)	−0.00080 (5)
S1	0.01438 (17)	0.01221 (16)	0.01734 (18)	−0.00014 (13)	0.00547 (13)	−0.00002 (13)
S2	0.01118 (16)	0.0224 (2)	0.01036 (16)	−0.00041 (14)	0.00245 (12)	−0.00008 (14)

O1	0.0324 (7)	0.0183 (6)	0.0196 (6)	−0.0036 (5)	0.0034 (5)	−0.0044 (5)
O2	0.0156 (6)	0.0261 (7)	0.0230 (6)	−0.0074 (5)	0.0032 (5)	0.0018 (5)
O3	0.0161 (6)	0.0236 (6)	0.0235 (6)	−0.0044 (5)	0.0061 (5)	−0.0086 (5)
O4	0.0291 (7)	0.0179 (6)	0.0278 (7)	0.0027 (5)	0.0068 (5)	0.0079 (5)
O5	0.0156 (5)	0.0187 (6)	0.0280 (7)	0.0015 (5)	0.0101 (5)	0.0016 (5)
O6	0.0160 (5)	0.0223 (6)	0.0189 (6)	−0.0016 (5)	0.0085 (5)	−0.0008 (5)
O7	0.0185 (6)	0.0283 (7)	0.0202 (6)	−0.0013 (5)	0.0077 (5)	−0.0082 (5)
O8	0.0196 (6)	0.0301 (7)	0.0168 (6)	0.0013 (5)	0.0020 (5)	0.0068 (5)
O9	0.0113 (5)	0.0322 (7)	0.0153 (5)	−0.0004 (5)	0.0016 (4)	0.0019 (5)
N1	0.0139 (6)	0.0156 (6)	0.0190 (6)	−0.0005 (5)	0.0049 (5)	−0.0018 (5)
N2	0.0132 (6)	0.0233 (7)	0.0124 (6)	−0.0028 (5)	0.0029 (5)	−0.0021 (5)
C1	0.0129 (6)	0.0160 (7)	0.0155 (7)	0.0003 (5)	0.0014 (5)	0.0042 (5)
C2	0.0178 (7)	0.0211 (8)	0.0201 (8)	0.0020 (6)	0.0077 (6)	−0.0022 (6)
C3	0.0213 (8)	0.0174 (8)	0.0190 (8)	0.0012 (6)	0.0066 (6)	−0.0017 (6)
C4	0.0377 (11)	0.0292 (10)	0.0274 (10)	−0.0034 (9)	0.0092 (8)	−0.0135 (8)
C5	0.0120 (6)	0.0177 (7)	0.0130 (7)	0.0006 (5)	0.0024 (5)	0.0028 (5)
C6	0.0162 (7)	0.0220 (8)	0.0138 (7)	−0.0033 (6)	0.0008 (6)	−0.0008 (6)
C7	0.0217 (8)	0.0199 (8)	0.0137 (7)	−0.0022 (6)	0.0016 (6)	−0.0014 (6)
C8	0.0420 (12)	0.0308 (10)	0.0223 (9)	−0.0102 (9)	0.0099 (8)	−0.0113 (8)

Geometric parameters (Å, º)

Sr1—Sr1$^{\rm i}$	4.2816 (3)	O5—Sr1$^{\rm iv}$	2.5789 (13)
Sr1—O1	2.6000 (14)	O6—Sr1$^{\rm i}$	2.8070 (13)
Sr1—O2$^{\rm ii}$	2.9039 (14)	O6—C5	1.2556 (19)
Sr1—O2	2.5026 (12)	O7—C7	1.390 (2)
Sr1—O5$^{\rm iii}$	2.5790 (13)	O9—Sr1$^{\rm iii}$	2.5782 (12)
Sr1—O6	2.5116 (12)	N1—Sr1$^{\rm ii}$	2.7553 (15)
Sr1—O6$^{\rm i}$	2.8070 (13)	N1—C1	1.355 (2)
Sr1—O9$^{\rm iv}$	2.5782 (12)	N2—Sr1$^{\rm i}$	2.7448 (14)
Sr1—N1$^{\rm ii}$	2.7553 (15)	N2—C5	1.352 (2)
Sr1—N2$^{\rm i}$	2.7447 (14)	C1—Sr1$^{\rm ii}$	3.2186 (17)
Sr1—C1$^{\rm ii}$	3.2186 (17)	C1—C2	1.462 (2)
Sr1—C5$^{\rm i}$	3.1761 (16)	C2—H2	0.9500
S1—O3	1.6134 (13)	C2—C3	1.336 (2)
S1—O4	1.4285 (13)	C3—C4	1.484 (3)
S1—O5	1.4323 (13)	C4—H4A	0.9800
S1—N1	1.5697 (15)	C4—H4B	0.9800
S2—O7	1.6156 (14)	C4—H4C	0.9800
S2—O8	1.4264 (13)	C5—Sr1$^{\rm i}$	3.1762 (16)
S2—O9	1.4324 (13)	C5—C6	1.460 (2)
S2—N2	1.5755 (14)	C6—H6	0.9500
O1—H1A	0.79 (3)	C6—C7	1.332 (2)
O1—H1B	0.84 (3)	C7—C8	1.485 (3)
O2—Sr1$^{\rm ii}$	2.9040 (14)	C8—H8A	0.9800
O2—C1	1.251 (2)	C8—H8B	0.9800
O3—C3	1.383 (2)	C8—H8C	0.9800

O1—Sr1—Sr1^{i}	112.25 (3)	O4—S1—O5	115.48 (8)
O1—Sr1—O2^{ii}	133.71 (4)	O4—S1—N1	113.32 (8)
O1—Sr1—O6^{i}	138.44 (4)	O5—S1—O3	102.85 (7)
O1—Sr1—N1^{ii}	135.12 (5)	O5—S1—N1	111.08 (8)
O1—Sr1—N2^{i}	142.25 (5)	N1—S1—O3	106.45 (7)
O1—Sr1—C1^{ii}	144.92 (5)	O8—S2—O7	106.65 (8)
O1—Sr1—C5^{i}	151.65 (5)	O8—S2—O9	115.79 (8)
O2—Sr1—Sr1^{i}	153.49 (3)	O8—S2—N2	113.00 (8)
O2^{ii}—Sr1—Sr1^{i}	107.12 (3)	O9—S2—O7	103.43 (8)
O2—Sr1—O1	81.04 (5)	O9—S2—N2	110.83 (8)
O2—Sr1—O2^{ii}	74.08 (5)	N2—S2—O7	106.12 (7)
O2—Sr1—O5^{iii}	91.48 (4)	Sr1—O1—H1A	133 (2)
O2—Sr1—O6	159.74 (4)	Sr1—O1—H1B	119 (2)
O2—Sr1—O6^{i}	121.71 (4)	H1A—O1—H1B	107 (3)
O2—Sr1—O9^{iv}	83.02 (4)	Sr1—O2—Sr1^{ii}	105.92 (5)
O2—Sr1—N1^{ii}	120.35 (4)	C1—O2—Sr1	158.55 (12)
O2—Sr1—N2^{i}	74.94 (4)	C1—O2—Sr1^{ii}	92.84 (10)
O2^{ii}—Sr1—C1^{ii}	22.85 (4)	C3—O3—S1	117.69 (11)
O2—Sr1—C1^{ii}	96.57 (4)	S1—O5—Sr1^{iv}	139.14 (7)
O2^{ii}—Sr1—C5^{i}	72.26 (4)	Sr1—O6—Sr1^{i}	107.09 (4)
O2—Sr1—C5^{i}	100.00 (4)	C5—O6—Sr1^{i}	95.14 (10)
O5^{iii}—Sr1—Sr1^{i}	70.73 (3)	C5—O6—Sr1	156.71 (12)
O5^{iii}—Sr1—O1	76.75 (5)	C7—O7—S2	117.00 (11)
O5^{iii}—Sr1—O2^{ii}	140.87 (4)	S2—O9—Sr1^{iii}	138.38 (8)
O5^{iii}—Sr1—O6^{i}	69.04 (4)	S1—N1—Sr1^{ii}	139.48 (8)
O5^{iii}—Sr1—N1^{ii}	134.61 (4)	C1—N1—Sr1^{ii}	97.17 (10)
O5^{iii}—Sr1—N2^{i}	75.24 (4)	C1—N1—S1	119.36 (12)
O5^{iii}—Sr1—C1^{ii}	138.28 (4)	S2—N2—Sr1^{i}	143.15 (8)
O5^{iii}—Sr1—C5^{i}	74.90 (4)	C5—N2—Sr1^{i}	95.61 (9)
O6^{i}—Sr1—Sr1^{i}	34.10 (2)	C5—N2—S2	119.20 (12)
O6—Sr1—Sr1^{i}	38.80 (3)	O2—C1—Sr1^{ii}	64.31 (9)
O6—Sr1—O1	79.00 (4)	O2—C1—N1	117.77 (16)
O6^{i}—Sr1—O2^{ii}	87.68 (4)	O2—C1—C2	121.63 (15)
O6—Sr1—O2^{ii}	123.18 (4)	N1—C1—Sr1^{ii}	58.14 (9)
O6—Sr1—O5^{iii}	80.62 (4)	N1—C1—C2	120.30 (15)
O6—Sr1—O6^{i}	72.91 (4)	C2—C1—Sr1^{ii}	153.07 (11)
O6—Sr1—O9^{iv}	93.08 (4)	C1—C2—H2	119.1
O6—Sr1—N1^{ii}	77.19 (4)	C3—C2—C1	121.80 (15)
O6—Sr1—N2^{i}	120.16 (4)	C3—C2—H2	119.1
O6^{i}—Sr1—C1^{ii}	71.99 (4)	O3—C3—C4	109.98 (16)
O6—Sr1—C1^{ii}	101.74 (4)	C2—C3—O3	121.56 (16)
O6—Sr1—C5^{i}	95.93 (4)	C2—C3—C4	128.27 (17)
O6^{i}—Sr1—C5^{i}	23.19 (4)	C3—C4—H4A	109.5
O9^{iv}—Sr1—Sr1^{i}	122.73 (3)	C3—C4—H4B	109.5
O9^{iv}—Sr1—O1	69.20 (5)	C3—C4—H4C	109.5
O9^{iv}—Sr1—O2^{ii}	69.51 (4)	H4A—C4—H4B	109.5
O9^{iv}—Sr1—O5^{iii}	145.95 (4)	H4A—C4—H4C	109.5
O9^{iv}—Sr1—O6^{i}	140.95 (4)	H4B—C4—H4C	109.5

O9^{iv}—Sr1—N1^{ii}	74.71 (4)	O6—C5—Sr1^{i}	61.67 (9)
O9^{iv}—Sr1—N2^{i}	134.15 (4)	O6—C5—N2	117.76 (15)
O9^{iv}—Sr1—C1^{ii}	75.76 (4)	O6—C5—C6	121.39 (15)
O9^{iv}—Sr1—C5^{i}	139.15 (4)	N2—C5—Sr1^{i}	59.32 (8)
N1^{ii}—Sr1—Sr1^{i}	67.12 (3)	N2—C5—C6	120.67 (14)
N1^{ii}—Sr1—O2^{ii}	46.36 (4)	C6—C5—Sr1^{i}	158.19 (11)
N1^{ii}—Sr1—O6^{i}	66.77 (4)	C5—C6—H6	119.0
N1^{ii}—Sr1—C1^{ii}	24.69 (4)	C7—C6—C5	122.03 (16)
N1^{ii}—Sr1—C5^{i}	68.71 (4)	C7—C6—H6	119.0
N2^{i}—Sr1—Sr1^{i}	81.44 (3)	O7—C7—C8	110.95 (16)
N2^{i}—Sr1—O2^{ii}	65.98 (4)	C6—C7—O7	121.31 (15)
N2^{i}—Sr1—O6^{i}	47.42 (4)	C6—C7—C8	127.71 (17)
N2^{i}—Sr1—N1^{ii}	82.54 (4)	C7—C8—H8A	109.5
N2^{i}—Sr1—C1^{ii}	67.66 (4)	C7—C8—H8B	109.5
N2^{i}—Sr1—C5^{i}	25.07 (4)	C7—C8—H8C	109.5
C1^{ii}—Sr1—Sr1^{i}	85.22 (3)	H8A—C8—H8B	109.5
C5^{i}—Sr1—Sr1^{i}	57.18 (3)	H8A—C8—H8C	109.5
C5^{i}—Sr1—C1^{ii}	63.40 (4)	H8B—C8—H8C	109.5
O4—S1—O3	106.58 (8)		

Sr1—O2—C1—Sr1^{ii}	−151.3 (3)	O3—S1—N1—C1	−35.06 (15)
Sr1—O2—C1—N1	−175.1 (2)	O4—S1—O3—C3	−82.71 (14)
Sr1^{ii}—O2—C1—N1	−23.76 (15)	O4—S1—O5—Sr1^{iv}	170.15 (11)
Sr1—O2—C1—C2	−1.4 (4)	O4—S1—N1—Sr1^{ii}	−126.76 (12)
Sr1^{ii}—O2—C1—C2	149.95 (14)	O4—S1—N1—C1	81.76 (15)
Sr1—O6—C5—Sr1^{i}	−162.9 (3)	O5—S1—O3—C3	155.40 (13)
Sr1^{i}—O6—C5—N2	−20.16 (16)	O5—S1—N1—Sr1^{ii}	5.17 (15)
Sr1—O6—C5—N2	177.0 (2)	O5—S1—N1—C1	−146.30 (13)
Sr1—O6—C5—C6	−7.8 (4)	O6—C5—C6—C7	−165.34 (17)
Sr1^{i}—O6—C5—C6	155.04 (14)	O7—S2—O9—Sr1^{iii}	−82.06 (12)
Sr1^{ii}—N1—C1—O2	25.31 (16)	O7—S2—N2—Sr1^{i}	123.73 (13)
Sr1^{ii}—N1—C1—C2	−148.50 (13)	O7—S2—N2—C5	−35.08 (15)
Sr1^{i}—N2—C5—O6	20.65 (16)	O8—S2—O7—C7	−79.80 (14)
Sr1^{i}—N2—C5—C6	−154.58 (13)	O8—S2—O9—Sr1^{iii}	161.68 (10)
Sr1^{ii}—C1—C2—C3	−67.2 (3)	O8—S2—N2—Sr1^{i}	−119.74 (13)
Sr1^{i}—C5—C6—C7	−73.7 (4)	O8—S2—N2—C5	81.44 (15)
S1—O3—C3—C2	−19.8 (2)	O9—S2—O7—C7	157.64 (12)
S1—O3—C3—C4	164.84 (13)	O9—S2—N2—Sr1^{i}	12.10 (16)
S1—N1—C1—Sr1^{ii}	161.78 (14)	O9—S2—N2—C5	−146.71 (13)
S1—N1—C1—O2	−172.91 (13)	N1—S1—O3—C3	38.52 (15)
S1—N1—C1—C2	13.3 (2)	N1—S1—O5—Sr1^{iv}	39.33 (14)
S2—O7—C7—C6	−24.5 (2)	N1—C1—C2—C3	11.3 (3)
S2—O7—C7—C8	157.25 (14)	N2—S2—O7—C7	40.92 (14)
S2—N2—C5—Sr1^{i}	167.42 (14)	N2—S2—O9—Sr1^{iii}	31.28 (14)
S2—N2—C5—O6	−171.93 (13)	N2—C5—C6—C7	9.7 (3)
S2—N2—C5—C6	12.8 (2)	C1—C2—C3—O3	−7.2 (3)
O2—C1—C2—C3	−162.30 (17)	C1—C2—C3—C4	167.20 (19)

O3—S1—O5—Sr1^{iv}	−74.19 (13)	C5—C6—C7—O7	−3.0 (3)
O3—S1—N1—Sr1^{ii}	116.42 (12)	C5—C6—C7—C8	175.01 (18)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O4^{v}	0.79 (3)	2.18 (3)	2.899 (2)	151 (3)
O1—H1*B*···O8^{vi}	0.83 (3)	2.22 (3)	2.9850 (19)	152 (3)
C4—H4*B*···O5^{v}	0.98	2.37	3.273 (3)	153
C6—H6···O8^{vi}	0.95	2.47	3.318 (2)	148

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

Aquabis(μ_3-6-methyl-2,2-dioxo-1,2λ^6,3-oxathiazin-4-olato)barium(II) (Ba)

Crystal data

$[Ba(C_4H_4NO_4S)_2(H_2O)]$
$M_r = 479.64$
Monoclinic, $P2_1/n$
$a = 8.2086$ (5) Å
$b = 18.8899$ (11) Å
$c = 9.8999$ (6) Å
$\beta = 99.5197$ (10)°
$V = 1513.93$ (16) Å^3
$Z = 4$
$F(000) = 928$
$D_x = 2.104$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 9794 reflections
$\theta = 3.0$–36.3°
$\mu = 2.94$ mm^{-1}
$T = 173$ K
Block, colourless
0.52 × 0.21 × 0.20 mm

Data collection

Bruker PHOTON-100 CMOS diffractometer
Radiation source: sealedtube
φ and *ω* scans
Absorption correction: numerical (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.309$, $T_{max} = 0.635$
41654 measured reflections
6324 independent reflections
5218 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 34.3°$, $\theta_{min} = 3.0°$
$h = -13 \rightarrow 13$
$k = -29 \rightarrow 29$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.059$
$S = 1.09$
6324 reflections
209 parameters
0 restraints
Primary atom site location: isomorphous structure methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0158P)^2 + 2.2204P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.02$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ba1	0.73689 (2)	0.46819 (2)	0.43614 (2)	0.01376 (3)
S1	0.07538 (7)	0.32148 (3)	0.54490 (6)	0.01768 (10)
S2	1.36455 (6)	0.52303 (3)	0.15371 (6)	0.01847 (11)
O1	0.6927 (3)	0.37493 (12)	0.2222 (2)	0.0313 (4)
H1A	0.692 (5)	0.336 (2)	0.213 (4)	0.047 (12)*
H1B	0.664 (5)	0.389 (2)	0.153 (4)	0.041 (11)*
O2	0.4531 (2)	0.40981 (10)	0.48151 (19)	0.0255 (4)
O3	0.0469 (2)	0.28363 (10)	0.39659 (19)	0.0259 (4)
O4	0.1222 (3)	0.26718 (10)	0.6433 (2)	0.0314 (4)
O5	−0.0809 (2)	0.35404 (9)	0.5498 (2)	0.0260 (4)
O6	1.0152 (2)	0.48791 (10)	0.33283 (18)	0.0227 (4)
O7	1.3411 (2)	0.44828 (10)	0.07381 (19)	0.0270 (4)
O8	1.3107 (2)	0.57651 (11)	0.05494 (18)	0.0270 (4)
O9	1.5363 (2)	0.52380 (11)	0.21146 (18)	0.0257 (4)
N1	0.2129 (2)	0.37885 (10)	0.5425 (2)	0.0190 (4)
N2	1.2552 (2)	0.51888 (11)	0.27018 (19)	0.0190 (4)
C1	0.3361 (3)	0.36655 (12)	0.4691 (2)	0.0185 (4)
C2	0.3227 (3)	0.30894 (13)	0.3700 (3)	0.0240 (5)
H2	0.416716	0.296609	0.330515	0.029*
C3	0.1826 (3)	0.27297 (13)	0.3330 (3)	0.0233 (5)
C4	0.1416 (4)	0.22233 (17)	0.2179 (3)	0.0381 (7)
H4A	0.104320	0.177552	0.252407	0.057*
H4B	0.239932	0.213846	0.175937	0.057*
H4C	0.053596	0.242128	0.149386	0.057*
C5	1.1101 (3)	0.48350 (12)	0.2459 (2)	0.0169 (4)
C6	1.0711 (3)	0.43709 (13)	0.1272 (2)	0.0213 (4)
H6	0.962455	0.418511	0.104690	0.026*
C7	1.1828 (3)	0.41992 (14)	0.0493 (2)	0.0237 (5)
C8	1.1637 (5)	0.36907 (18)	−0.0670 (3)	0.0422 (8)
H8A	1.184568	0.393477	−0.149831	0.063*
H8B	1.051152	0.350013	−0.082391	0.063*
H8C	1.242929	0.330240	−0.045421	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01155 (5)	0.01638 (6)	0.01386 (6)	−0.00196 (5)	0.00359 (4)	−0.00155 (5)
S1	0.0171 (2)	0.0136 (2)	0.0238 (3)	0.00023 (19)	0.0076 (2)	0.0012 (2)
S2	0.0133 (2)	0.0298 (3)	0.0126 (2)	−0.0002 (2)	0.00297 (18)	0.0006 (2)

O1	0.0517 (13)	0.0203 (10)	0.0211 (10)	−0.0050 (9)	0.0039 (9)	−0.0042 (8)
O2	0.0182 (8)	0.0281 (9)	0.0304 (10)	−0.0065 (7)	0.0049 (7)	0.0006 (8)
O3	0.0212 (8)	0.0291 (9)	0.0286 (9)	−0.0067 (7)	0.0076 (7)	−0.0093 (8)
O4	0.0402 (11)	0.0195 (9)	0.0348 (11)	0.0034 (8)	0.0072 (9)	0.0098 (8)
O5	0.0188 (8)	0.0224 (8)	0.0397 (11)	0.0023 (7)	0.0135 (7)	0.0028 (8)
O6	0.0171 (7)	0.0319 (9)	0.0211 (8)	−0.0024 (7)	0.0093 (6)	−0.0025 (7)
O7	0.0230 (8)	0.0367 (10)	0.0232 (9)	0.0001 (7)	0.0098 (7)	−0.0092 (8)
O8	0.0237 (8)	0.0377 (11)	0.0195 (9)	0.0005 (8)	0.0026 (7)	0.0089 (8)
O9	0.0139 (7)	0.0438 (11)	0.0193 (8)	−0.0010 (7)	0.0023 (6)	0.0032 (8)
N1	0.0163 (8)	0.0172 (9)	0.0244 (10)	−0.0023 (7)	0.0065 (7)	−0.0016 (7)
N2	0.0154 (8)	0.0290 (11)	0.0131 (8)	−0.0037 (7)	0.0045 (7)	−0.0021 (7)
C1	0.0146 (9)	0.0190 (10)	0.0217 (11)	0.0016 (8)	0.0021 (8)	0.0032 (8)
C2	0.0227 (11)	0.0232 (12)	0.0282 (13)	0.0035 (9)	0.0109 (10)	−0.0014 (10)
C3	0.0263 (12)	0.0225 (11)	0.0220 (11)	0.0014 (9)	0.0072 (9)	−0.0030 (9)
C4	0.0475 (18)	0.0343 (15)	0.0342 (16)	−0.0044 (13)	0.0123 (14)	−0.0140 (13)
C5	0.0154 (9)	0.0202 (10)	0.0153 (10)	0.0007 (8)	0.0028 (8)	0.0020 (8)
C6	0.0197 (10)	0.0264 (12)	0.0172 (11)	−0.0047 (9)	0.0014 (8)	−0.0023 (9)
C7	0.0283 (12)	0.0256 (12)	0.0171 (11)	−0.0021 (10)	0.0036 (9)	−0.0017 (9)
C8	0.058 (2)	0.0421 (18)	0.0293 (15)	−0.0127 (15)	0.0151 (14)	−0.0172 (13)

Geometric parameters (Å, º)

Ba1—Ba1^{i}	4.4491 (3)	O1—H1B	0.74 (4)
Ba1—O1	2.732 (2)	O2—C1	1.252 (3)
Ba1—O2^{i}	2.9714 (19)	O3—C3	1.382 (3)
Ba1—O2	2.6812 (17)	O6—C5	1.256 (3)
Ba1—O5^{ii}	2.7560 (18)	O7—C7	1.389 (3)
Ba1—O6	2.6788 (16)	N1—C1	1.359 (3)
Ba1—O6^{iii}	2.9192 (18)	N2—C5	1.352 (3)
Ba1—O9^{iv}	2.7478 (18)	C1—C2	1.457 (3)
Ba1—N1^{i}	2.921 (2)	C2—H2	0.9500
Ba1—N2^{iii}	2.9077 (19)	C2—C3	1.334 (4)
Ba1—C1^{i}	3.342 (2)	C3—C4	1.483 (4)
Ba1—C5^{iii}	3.318 (2)	C4—H4A	0.9800
S1—O3	1.6149 (19)	C4—H4B	0.9800
S1—O4	1.4232 (19)	C4—H4C	0.9800
S1—O5	1.4309 (17)	C5—C6	1.459 (3)
S1—N1	1.568 (2)	C6—H6	0.9500
S2—O7	1.6143 (19)	C6—C7	1.332 (3)
S2—O8	1.4245 (19)	C7—C8	1.488 (4)
S2—O9	1.4313 (17)	C8—H8A	0.9800
S2—N2	1.5758 (19)	C8—H8B	0.9800
O1—H1A	0.75 (4)	C8—H8C	0.9800
O1—Ba1—Ba1^{i}	112.59 (5)	O4—S1—O5	115.39 (12)
O1—Ba1—O2^{i}	134.76 (6)	O4—S1—N1	113.25 (12)
O1—Ba1—O5^{ii}	78.79 (7)	O5—S1—O3	103.03 (11)
O1—Ba1—O6^{iii}	140.94 (6)	O5—S1—N1	110.81 (11)

O1—Ba1—O9^{iv}	68.53 (7)	N1—S1—O3	106.77 (10)
O1—Ba1—N1^{i}	133.85 (6)	O8—S2—O7	106.60 (11)
O1—Ba1—N2^{iii}	143.83 (6)	O8—S2—O9	116.14 (11)
O1—Ba1—C1^{i}	144.37 (7)	O8—S2—N2	112.82 (11)
O1—Ba1—C5^{iii}	153.32 (7)	O9—S2—O7	103.55 (11)
O2^{i}—Ba1—Ba1^{i}	35.84 (3)	O9—S2—N2	110.54 (10)
O2—Ba1—Ba1^{i}	40.45 (4)	N2—S2—O7	106.20 (10)
O2—Ba1—O1	81.78 (6)	Ba1—O1—H1A	137 (3)
O2—Ba1—O2^{i}	76.29 (6)	Ba1—O1—H1B	118 (3)
O2—Ba1—O5^{ii}	92.16 (5)	H1A—O1—H1B	105 (4)
O2—Ba1—O6^{iii}	119.87 (5)	Ba1—O2—Ba1^{i}	103.71 (6)
O2—Ba1—O9^{iv}	82.65 (5)	C1—O2—Ba1	157.81 (16)
O2—Ba1—N1^{i}	120.71 (5)	C1—O2—Ba1^{i}	95.98 (14)
O2—Ba1—N2^{iii}	75.13 (5)	C3—O3—S1	118.19 (16)
O2^{i}—Ba1—C1^{i}	21.87 (5)	S1—O5—Ba1^{iv}	138.72 (10)
O2—Ba1—C1^{i}	97.82 (6)	Ba1—O6—Ba1^{iii}	105.57 (5)
O2—Ba1—C5^{iii}	99.04 (5)	C5—O6—Ba1^{iii}	97.13 (14)
O2^{i}—Ba1—C5^{iii}	70.11 (5)	C5—O6—Ba1	156.59 (16)
O5^{ii}—Ba1—Ba1^{i}	122.42 (4)	C7—O7—S2	117.07 (15)
O5^{ii}—Ba1—O2^{i}	140.25 (5)	S2—O9—Ba1^{ii}	137.59 (10)
O5^{ii}—Ba1—O6^{iii}	68.99 (5)	S1—N1—Ba1^{i}	140.88 (10)
O5^{ii}—Ba1—N1^{i}	133.14 (6)	C1—N1—Ba1^{i}	95.70 (13)
O5^{ii}—Ba1—N2^{iii}	74.73 (6)	C1—N1—S1	119.41 (17)
O5^{ii}—Ba1—C1^{i}	136.60 (6)	S2—N2—Ba1^{iii}	143.73 (10)
O5^{ii}—Ba1—C5^{iii}	74.53 (6)	C5—N2—Ba1^{iii}	95.30 (13)
O6—Ba1—Ba1^{i}	155.73 (4)	C5—N2—S2	119.09 (16)
O6^{iii}—Ba1—Ba1^{i}	103.27 (3)	O2—C1—Ba1^{i}	62.15 (13)
O6—Ba1—O1	78.82 (6)	O2—C1—N1	117.5 (2)
O6^{iii}—Ba1—O2^{i}	83.93 (5)	O2—C1—C2	121.7 (2)
O6—Ba1—O2	160.13 (6)	N1—C1—Ba1^{i}	60.43 (12)
O6—Ba1—O2^{i}	121.09 (5)	N1—C1—C2	120.5 (2)
O6—Ba1—O5^{ii}	79.94 (5)	C2—C1—Ba1^{i}	152.82 (16)
O6—Ba1—O6^{iii}	74.43 (5)	C1—C2—H2	119.0
O6—Ba1—O9^{iv}	94.15 (5)	C3—C2—C1	122.1 (2)
O6^{iii}—Ba1—N1^{i}	65.83 (5)	C3—C2—H2	119.0
O6—Ba1—N1^{i}	76.77 (5)	O3—C3—C4	110.3 (2)
O6—Ba1—N2^{iii}	119.39 (5)	C2—C3—O3	121.6 (2)
O6^{iii}—Ba1—C1^{i}	69.44 (5)	C2—C3—C4	128.0 (2)
O6—Ba1—C1^{i}	100.43 (5)	C3—C4—H4A	109.5
O6—Ba1—C5^{iii}	96.38 (5)	C3—C4—H4B	109.5
O6^{iii}—Ba1—C5^{iii}	22.06 (5)	C3—C4—H4C	109.5
O9^{iv}—Ba1—Ba1^{i}	72.06 (4)	H4A—C4—H4B	109.5
O9^{iv}—Ba1—O2^{i}	69.77 (5)	H4A—C4—H4C	109.5
O9^{iv}—Ba1—O5^{ii}	147.31 (6)	H4B—C4—H4C	109.5
O9^{iv}—Ba1—O6^{iii}	140.57 (6)	O6—C5—Ba1^{iii}	60.81 (12)
O9^{iv}—Ba1—N1^{i}	74.86 (6)	O6—C5—N2	118.3 (2)
O9^{iv}—Ba1—N2^{iii}	133.52 (6)	O6—C5—C6	120.9 (2)
O9^{iv}—Ba1—C1^{i}	76.05 (6)	N2—C5—Ba1^{iii}	60.77 (11)

O9$^{\text{iv}}$—Ba1—C5$^{\text{iii}}$	138.14 (6)	N2—C5—C6	120.65 (19)
N1$^{\text{i}}$—Ba1—Ba1$^{\text{i}}$	80.31 (4)	C6—C5—Ba1$^{\text{iii}}$	158.10 (16)
N1$^{\text{i}}$—Ba1—O2$^{\text{i}}$	44.54 (5)	C5—C6—H6	118.9
N1$^{\text{i}}$—Ba1—C1$^{\text{i}}$	23.87 (5)	C7—C6—C5	122.1 (2)
N1$^{\text{i}}$—Ba1—C5$^{\text{iii}}$	68.44 (6)	C7—C6—H6	118.9
N2$^{\text{iii}}$—Ba1—Ba1$^{\text{i}}$	64.48 (4)	O7—C7—C8	111.1 (2)
N2$^{\text{iii}}$—Ba1—O2$^{\text{i}}$	65.57 (5)	C6—C7—O7	121.2 (2)
N2$^{\text{iii}}$—Ba1—O6$^{\text{iii}}$	45.20 (5)	C6—C7—C8	127.6 (3)
N2$^{\text{iii}}$—Ba1—N1$^{\text{i}}$	82.24 (6)	C7—C8—H8A	109.5
N2$^{\text{iii}}$—Ba1—C1$^{\text{i}}$	67.43 (6)	C7—C8—H8B	109.5
N2$^{\text{iii}}$—Ba1—C5$^{\text{iii}}$	23.94 (5)	C7—C8—H8C	109.5
C1$^{\text{i}}$—Ba1—Ba1$^{\text{i}}$	57.47 (4)	H8A—C8—H8B	109.5
C5$^{\text{iii}}$—Ba1—Ba1$^{\text{i}}$	82.39 (4)	H8A—C8—H8C	109.5
C5$^{\text{iii}}$—Ba1—C1$^{\text{i}}$	62.23 (6)	H8B—C8—H8C	109.5
O4—S1—O3	106.60 (11)		

Ba1—O2—C1—Ba1$^{\text{i}}$	−152.6 (4)	O3—S1—N1—C1	−33.6 (2)
Ba1—O2—C1—N1	−177.7 (3)	O4—S1—O3—C3	−84.9 (2)
Ba1$^{\text{i}}$—O2—C1—N1	−25.2 (2)	O4—S1—O5—Ba1$^{\text{iv}}$	170.65 (15)
Ba1—O2—C1—C2	−3.7 (6)	O4—S1—N1—Ba1$^{\text{i}}$	−125.67 (17)
Ba1$^{\text{i}}$—O2—C1—C2	148.9 (2)	O4—S1—N1—C1	83.4 (2)
Ba1—O6—C5—Ba1$^{\text{iii}}$	−165.9 (4)	O5—S1—O3—C3	153.20 (18)
Ba1$^{\text{iii}}$—O6—C5—N2	−20.6 (2)	O5—S1—N1—Ba1$^{\text{i}}$	5.8 (2)
Ba1—O6—C5—N2	173.5 (3)	O5—S1—N1—C1	−145.06 (19)
Ba1—O6—C5—C6	−11.1 (5)	O6—C5—C6—C7	−165.8 (2)
Ba1$^{\text{iii}}$—O6—C5—C6	154.73 (19)	O7—S2—O9—Ba1$^{\text{ii}}$	−80.89 (17)
Ba1$^{\text{i}}$—N1—C1—O2	25.6 (2)	O7—S2—N2—Ba1$^{\text{iii}}$	124.24 (18)
Ba1$^{\text{i}}$—N1—C1—C2	−148.52 (19)	O7—S2—N2—C5	−35.3 (2)
Ba1$^{\text{iii}}$—N2—C5—O6	20.6 (2)	O8—S2—O7—C7	−79.77 (19)
Ba1$^{\text{iii}}$—N2—C5—C6	−154.73 (19)	O8—S2—O9—Ba1$^{\text{ii}}$	162.65 (14)
Ba1$^{\text{i}}$—C1—C2—C3	−74.1 (4)	O8—S2—N2—Ba1$^{\text{iii}}$	−119.34 (18)
Ba1$^{\text{iii}}$—C5—C6—C7	−77.8 (5)	O8—S2—N2—C5	81.1 (2)
S1—O3—C3—C2	−18.7 (3)	O9—S2—O7—C7	157.23 (18)
S1—O3—C3—C4	165.55 (19)	O9—S2—N2—Ba1$^{\text{iii}}$	12.6 (2)
S1—N1—C1—Ba1$^{\text{i}}$	162.0 (2)	O9—S2—N2—C5	−146.95 (19)
S1—N1—C1—O2	−172.35 (18)	N1—S1—O3—C3	36.4 (2)
S1—N1—C1—C2	13.5 (3)	N1—S1—O5—Ba1$^{\text{iv}}$	40.3 (2)
S2—O7—C7—C6	−24.1 (3)	N1—C1—C2—C3	9.8 (4)
S2—O7—C7—C8	157.7 (2)	N2—S2—O7—C7	40.8 (2)
S2—N2—C5—Ba1$^{\text{iii}}$	168.0 (2)	N2—S2—O9—Ba1$^{\text{ii}}$	32.5 (2)
S2—N2—C5—O6	−171.40 (18)	N2—C5—C6—C7	9.4 (4)
S2—N2—C5—C6	13.3 (3)	C1—C2—C3—O3	−6.5 (4)
O2—C1—C2—C3	−164.1 (2)	C1—C2—C3—C4	168.5 (3)
O3—S1—O5—Ba1$^{\text{iv}}$	−73.61 (18)	C5—C6—C7—O7	−3.1 (4)
O3—S1—N1—Ba1$^{\text{i}}$	117.32 (17)	C5—C6—C7—C8	174.7 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O4^{v}	0.74 (4)	2.12 (4)	2.829 (3)	162 (4)
O1—H1*B*···O8^{vi}	0.74 (4)	2.20 (4)	2.889 (3)	156 (4)
C4—H4*B*···O5^{v}	0.98	2.44	3.361 (4)	155
C6—H6···O8^{vi}	0.95	2.52	3.357 (3)	147

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