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2,3-Dimethylquinoxalinediium hexabromidostannate(IV) trihydrate

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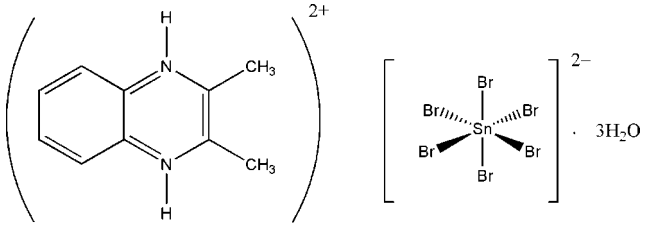
Key indicators: single-crystal X-ray study; T = 84 K; mean σ(C–C) = 0.013 Å; R factor = 0.062; wR factor = 0.132; data-to-parameter ratio = 23.0.

In the title compound, $(C_{10}H_{12}N_2)[SnBr_6]\cdot 3H_2O$, the asymmetric unit contains one cation, one anion and three water molecules, and the Sn atom has a distorted octahedral environment. In the crystal structure, intra- and intermolecular hydrogen bonds and Br···Br interactions [Br···Br = 3.6726 (19), 3.6913 (18) and 3.6517 (21) Å] lead to the formation of a supramolecular architecture.

Related literature

For related literature, see: Desiraju (1997); Ali *et al.* (2007); Ali & Al-Far (2007); Al-Far & Ali (2007*a*,*b*); Al-Far *et al.* (2007); Tudela & Khan (1991); Willey *et al.* (1998). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$(C_{10}H_{12}N_2)[SnBr_6]\cdot 3H_2O$
M_r = 812.37
Monoclinic, $P2_1/c$
a = 9.898 (3) Å
b = 13.620 (5) Å
c = 16.098 (6) Å
β = 103.599 (6)°
V = 2109.3 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 12.59 mm^{-1}
T = 84 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.055, T_{max} = 0.277
27021 measured reflections
4633 independent reflections
4210 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.132
S = 1.20
4633 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.41 e Å^{-3}
$\Delta\rho_{min}$ = −1.11 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—Br1	2.4405 (12)	Sn1—Br6	2.6570 (12)
Sn1—Br3	2.4603 (12)	Sn1—Br5	2.7026 (12)
Sn1—Br4	2.6534 (11)	Sn1—Br2	2.7114 (11)
Br1—Sn1—Br3	177.29 (4)	Br4—Sn1—Br5	85.87 (4)
Br1—Sn1—Br4	93.48 (4)	Br6—Sn1—Br5	178.17 (3)
Br3—Sn1—Br4	88.41 (4)	Br1—Sn1—Br2	87.41 (4)
Br1—Sn1—Br6	86.37 (4)	Br3—Sn1—Br2	90.69 (4)
Br3—Sn1—Br6	95.38 (4)	Br4—Sn1—Br2	179.08 (4)
Br4—Sn1—Br6	95.87 (4)	Br6—Sn1—Br2	84.41 (4)
Br1—Sn1—Br5	92.93 (3)	Br5—Sn1—Br2	93.86 (4)
Br3—Sn1—Br5	85.26 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O2W	0.86	1.78	2.640 (14)	170.00
O1W—H1W2···Br3^{i}	0.87	2.79	3.348 (9)	123.1 (5)
O2W—H2W1···Br2^{ii}	0.84	2.57	3.401 (12)	167.4 (7)
O2W—H2W2···Br3^{ii}	0.87	2.83	3.482 (11)	132.9 (7)
O3W—H3W2···Br1	0.86	2.83	3.349 (11)	120.00
N1—H1N···O1W	0.86	1.82	2.672 (10)	172
N2—H2N···O3W^{iii}	0.86	1.81	2.660 (11)	172

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Al al-Bayt University and Al-Balqa'a Applied University are thanked for their support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2278).

References

Al-Far, R. & Ali, B. F. (2007*a*). *Acta Cryst.* C**63**, m137–m139.
Al-Far, R. & Ali, B. F. (2007*b*). *Acta Cryst.* E**63**, o2530–o2532.
Al-Far, R., Ali, B. F. & Al-Sou'od, K. (2007). *J. Chem. Cryst.* **37**, 265–273.
Ali, B. F. & Al-Far, R. (2007). *Acta Cryst.* E**63**, m892–m894.
Ali, B. F., Al-Far, R. & Haddad, S. (2007). *Acta Cryst.* E**63**, m1569.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Desiraju, G. R. (1997). *Chem. Commun.* pp. 1475–1482.
Rigaku (2000). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.

  doi:10.1107/S1600536807032771

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Tudela, D. & Khan, M. A. (1991). *J. Chem. Soc. Dalton Trans.* pp. 1003–1006.
Willey, G. R., Woodman, T. J., Somasundaram, U., Aris, D. R. & Errington, W. (1998). *J. Chem. Soc. Dalton Trans.* pp. 2573–2576.

supplementary materials

Acta Cryst. (2007). E**63**, m2102-m2103 [**doi:10.1107/S1600536807032771**]

2,3-Dimethylquinoxalinediium hexabromidostannate(IV) trihydrate

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Comment

Noncovalent interactions play an important role in organizing structural units in both natural and artificial systems (Desiraju, 1997). In connection with ongoing studies (Ali *et al.*, 2007; Ali & Al-Far, 2007; Al-Far & Ali, 2007*a*,b) of the structural aspects of bromo metal anions salts, we herein report the crystal structure of the title compound, (I).

The asymmetric unit of the title compound, (I), contains one cation, one anion and three water molecules, where the Sn atom has a distorted octahedral environment (Fig. 1, Table 1). The bond lengths and angles (Table 1) are generally within normal ranges (Allen *et al.*, 1987). In the anion, the Sn1—Br1 [2.4406 (12) Å] and Sn1—Br3 [2.4605 (12) Å] bonds are shorter than the other Sn—Br bonds, in which they are within the range of Sn—Br bonds reported previously for compounds containing $[SnBr_6]^{2-}$ anions (Ali & Al-Far, 2007; Al-Far & Ali, 2007*a*,b; Al-Far *et al.*, 2007; Tudela & Khan, 1991; Willey *et al.*, 1998). In the cation, the bond lengths and angles are in accordance with the corresponding values (Al-Far & Ali, 2007*a*,b; Ali *et al.*, 2007). The cation is, of course, planar, in which C1 and C10 atoms are also coplanar.

The packing of the structure can be regarded as alternating layers of anions and cations (Fig. 2). The anions within each layer (Fig. 3) interact *via* Br1···Br3^{iv} = 3.6726 (19) Å [symmetry code: (iv) x, 3/2 + y, 1/2 + z] interactions parallel to c axis. Each anionic layer further interacts *via* Br2···Br6^{v} = 3.6913 (18) Å [symmetry code: (v) −x + 3, 1/2 + y, 1/2 − z] and Br4···Br4^{vi} = 3.6517 (21) Å [symmetry code: (vi) −x + 2, −y + 1, −z] interactions to form a two-dimensional anionic network parallel to *ac* plane (Fig. 3).

The crystal supramolecularity is represented in the significantly short hydrogen bonds (Table 2, Fig. 4) along with Br···Br interactions that allow the formation of supramolecular assembly of the anion, cation and water molecules in three-dimensional structure, in which they may be effective in the stabilization of the crystal structure.

Experimental

For the preparation of (I), tin metal (0.119 mg, 1 mmol) dissolved in absolute ethanol (10 ml), HBr (60%, 5 ml) and liquid Br_2 (60%, 2 ml), was added dropwise to a stirred hot solution of 2,3-dimethylquinoxalinium (0.158 mg, 1 mmol) dissolved in ethanol (10 ml) and HBr (60%, 2 ml). After refluxing for 1 h, the mixture was filtered off, and then allowed to stand undisturbed at room temperature. The salt crystallized over 1 d as yellow crystals. Crystals were filtered off, washed with diethylether and dried under vacuum (yield; 0.750 mg; 92.4%).

Refinement

H atoms were positioned geometrically, with O—H = 0.84–0.90 Å (for H_2O), N—H = 0.86 Å (for NH) and C—H = 0.95 and 0.98 Å, for aromatic and methylene H atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*O*,*N*), where x = 1.2 for NH and aromatic H atoms, and x = 1.5 for all other H atoms.

Figures

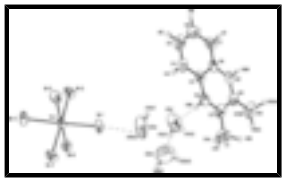

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

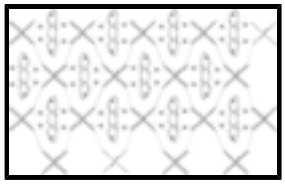

Fig. 2. A partial packing diagram of (I). Hydrogen bonds and Br···Br interactions are shown as dashed lines. Viewed down *c* axis, where a and b axes are horizontal and vertical, respectively.

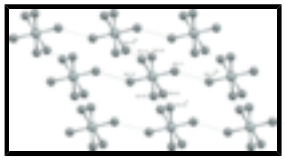

Fig. 3. Anion network of Br···Br interactions. Viewed down *b* axis, where c and a axes are horizontal and vertical, respectively [Symmetry codes: (iv) *x*, 3/2 + *y*, 1/2 + *z*; (v) −*x* + 3, 1/2 + *y*, 1/2 − *z*; (vi) −*x* + 2, −*y* + 1, −*z*].

Fig. 4. Anion, cation and water molecules intermolecular interactions. Sn—Br···H—O, H_2O···H—OH, H_2O···H—N and Br···Br (parallel to *c* axis) intermolecular interactions are shown as dashed lines. Viewed down *b* axis, where c and a axes are horizontal and vertical, respectively. H atoms are omitted for clarity. Oxygen atoms of water molecules shown as balls.

'2,3-Dimethylquinoxalinediium hexabromostannate(IV) trihydrate'

Crystal data

$(C_{10}H_{12}N_2)[SnBr_6]\cdot 3H_2O$	F_{000} = 1504
M_r = 812.37	D_x = 2.558 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: -P 2ybc	Cell parameters from 4210 reflections
a = 9.898 (3) Å	θ = 1.3–27.9º
b = 13.620 (5) Å	μ = 12.59 mm^{-1}
c = 16.098 (6) Å	*T* = 84 (2) K
β = 103.599 (6)º	Needle, yellow
V = 2109.3 (13) Å^3	0.30 × 0.20 × 0.10 mm
Z = 4	

Data collection

Rigaku Mercury CCD diffractometer	4633 independent reflections
Radiation source: fine-focus sealed tube	4210 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
Detector resolution: 14.6306 pixels mm^{-1}	θ_{max} = 27.5º
T = 84(2) K	θ_{min} = 2.1º

dtintegrate.ref scans
Absorption correction: multi-scan
Shape Tracing Software
T_{min} = 0.055, T_{max} = 0.277
27021 measured reflections

$h = -12 \rightarrow 11$
$k = -17 \rightarrow 17$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.132$
$S = 1.20$
4633 reflections
201 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 7.030P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.41$ e Å^{-3}
$\Delta\rho_{min} = -1.11$ e Å^{-3}
Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	1.23031 (5)	0.73783 (4)	0.15141 (3)	0.03598 (16)
Br1	1.17497 (9)	0.68693 (8)	0.28495 (5)	0.0562 (3)
Br2	1.41637 (10)	0.86480 (7)	0.24513 (6)	0.0600 (3)
Br3	1.28560 (9)	0.79729 (8)	0.01892 (5)	0.0594 (3)
Br4	1.04854 (9)	0.61509 (7)	0.05744 (6)	0.0573 (3)
Br5	1.02270 (9)	0.87143 (7)	0.11762 (6)	0.0538 (2)
Br6	1.43853 (9)	0.60996 (7)	0.18886 (6)	0.0529 (2)
O1W	0.5390 (9)	0.6748 (7)	0.4150 (5)	0.099 (3)
H1W1	0.5917	0.6271	0.4063	0.149*
H1W2	0.4568	0.6502	0.4107	0.149*
O2W	0.7208 (12)	0.5361 (8)	0.4048 (8)	0.150 (5)
H2W1	0.6941	0.4985	0.3624	0.226*
H2W2	0.7408	0.5002	0.4510	0.226*

O3W	0.9249 (12)	0.6547 (9)	0.3909 (5)	0.134 (4)
H3W1	0.9395	0.7059	0.4277	0.201*
H3W2	1.0060	0.6290	0.3961	0.201*
N1	0.6611 (6)	0.7296 (5)	0.5744 (4)	0.0432 (15)
H1N	0.6144	0.7109	0.5249	0.052*
N2	0.8084 (7)	0.7870 (5)	0.7326 (4)	0.0457 (16)
H2N	0.8534	0.8050	0.7827	0.055*
C1	0.6530 (10)	0.5601 (7)	0.6141 (7)	0.067 (3)
H1A	0.5879	0.5584	0.5579	0.101*
H1B	0.6076	0.5337	0.6572	0.101*
H1C	0.7349	0.5202	0.6126	0.101*
C2	0.6965 (8)	0.6629 (7)	0.6361 (6)	0.049 (2)
C3	0.6962 (7)	0.8271 (6)	0.5865 (5)	0.0399 (17)
C4	0.6556 (9)	0.8934 (7)	0.5197 (5)	0.050 (2)
H4	0.6045	0.8736	0.4646	0.060*
C5	0.6936 (10)	0.9891 (8)	0.5380 (7)	0.063 (3)
H5	0.6690	1.0367	0.4939	0.075*
C6	0.7682 (10)	1.0201 (7)	0.6201 (8)	0.067 (3)
H6	0.7899	1.0878	0.6289	0.080*
C8	0.7744 (7)	0.8569 (6)	0.6704 (5)	0.0399 (17)
C7	0.8110 (9)	0.9554 (7)	0.6884 (6)	0.055 (2)
H7	0.8613	0.9766	0.7432	0.066*
C9	0.7761 (8)	0.6942 (6)	0.7202 (5)	0.0453 (19)
C10	0.8231 (11)	0.6235 (8)	0.7927 (6)	0.073 (3)
H10A	0.7928	0.6469	0.8429	0.109*
H10B	0.9248	0.6186	0.8064	0.109*
H10C	0.7826	0.5587	0.7761	0.109*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0316 (3)	0.0490 (3)	0.0301 (3)	−0.0024 (2)	0.0128 (2)	−0.0062 (2)
Br1	0.0512 (5)	0.0851 (7)	0.0392 (4)	0.0018 (4)	0.0247 (4)	0.0052 (4)
Br2	0.0516 (5)	0.0684 (6)	0.0626 (6)	−0.0193 (4)	0.0188 (4)	−0.0240 (5)
Br3	0.0540 (5)	0.0901 (7)	0.0412 (4)	−0.0031 (5)	0.0252 (4)	0.0099 (4)
Br4	0.0517 (5)	0.0687 (6)	0.0546 (5)	−0.0196 (4)	0.0184 (4)	−0.0223 (4)
Br5	0.0447 (5)	0.0622 (5)	0.0588 (5)	0.0063 (4)	0.0210 (4)	−0.0041 (4)
Br6	0.0473 (5)	0.0622 (5)	0.0540 (5)	0.0130 (4)	0.0217 (4)	0.0009 (4)
O1W	0.106 (6)	0.134 (7)	0.054 (4)	0.010 (6)	0.013 (4)	−0.019 (5)
O2W	0.175 (11)	0.107 (8)	0.209 (13)	−0.005 (7)	0.123 (10)	−0.016 (8)
O3W	0.151 (9)	0.206 (11)	0.043 (4)	0.017 (8)	0.016 (5)	0.017 (6)
N1	0.035 (3)	0.056 (4)	0.040 (3)	0.003 (3)	0.011 (3)	−0.004 (3)
N2	0.038 (4)	0.070 (5)	0.032 (3)	0.001 (3)	0.013 (3)	0.000 (3)
C1	0.059 (6)	0.056 (6)	0.094 (8)	−0.003 (5)	0.030 (5)	−0.005 (5)
C2	0.031 (4)	0.059 (5)	0.059 (5)	−0.001 (4)	0.016 (4)	0.011 (4)
C3	0.032 (4)	0.049 (4)	0.045 (4)	0.004 (3)	0.021 (3)	0.002 (4)
C4	0.046 (5)	0.065 (6)	0.042 (4)	0.007 (4)	0.017 (4)	0.012 (4)
C5	0.054 (6)	0.071 (7)	0.070 (6)	0.013 (5)	0.030 (5)	0.023 (5)

C6	0.065 (6)	0.047 (5)	0.103 (8)	0.003 (4)	0.049 (6)	0.001 (5)
C8	0.027 (4)	0.061 (5)	0.036 (4)	0.002 (3)	0.015 (3)	0.001 (3)
C7	0.049 (5)	0.061 (5)	0.065 (6)	−0.005 (4)	0.032 (4)	−0.015 (5)
C9	0.036 (4)	0.060 (5)	0.043 (4)	−0.001 (4)	0.017 (3)	0.007 (4)
C10	0.063 (6)	0.099 (8)	0.060 (6)	0.009 (6)	0.023 (5)	0.037 (6)

Geometric parameters (Å, °)

Sn1—Br1	2.4405 (12)	C1—H1A	0.9800
Sn1—Br3	2.4603 (12)	C1—H1B	0.9800
Sn1—Br4	2.6534 (11)	C1—H1C	0.9800
Sn1—Br6	2.6570 (12)	C2—C9	1.461 (12)
Sn1—Br5	2.7026 (12)	C3—C4	1.391 (11)
Sn1—Br2	2.7114 (11)	C3—C8	1.447 (11)
O1W—H1W1	0.86000	C4—C5	1.368 (13)
O1W—H1W2	0.87000	C4—H4	0.9500
O2W—H2W1	0.84000	C5—C6	1.418 (14)
O2W—H2W2	0.87000	C5—H5	0.9500
O3W—H3W1	0.90000	C6—C7	1.395 (14)
O3W—H3W2	0.86000	C6—H6	0.9500
N1—C2	1.330 (10)	C8—C7	1.403 (12)
N1—C3	1.375 (10)	C7—H7	0.9500
N1—H1N	0.8600	C9—C10	1.500 (11)
N2—C9	1.308 (11)	C10—H10A	0.9800
N2—C8	1.365 (10)	C10—H10B	0.9800
N2—H2N	0.8600	C10—H10C	0.9800
C1—C2	1.483 (13)		
Br1—Sn1—Br3	177.29 (4)	N1—C2—C9	118.9 (8)
Br1—Sn1—Br4	93.48 (4)	N1—C2—C1	117.1 (8)
Br3—Sn1—Br4	88.41 (4)	C9—C2—C1	124.0 (8)
Br1—Sn1—Br6	86.37 (4)	N1—C3—C4	120.0 (8)
Br3—Sn1—Br6	95.38 (4)	N1—C3—C8	117.8 (7)
Br4—Sn1—Br6	95.87 (4)	C4—C3—C8	122.2 (7)
Br1—Sn1—Br5	92.93 (3)	C5—C4—C3	115.9 (8)
Br3—Sn1—Br5	85.26 (4)	C5—C4—H4	122.0
Br4—Sn1—Br5	85.87 (4)	C3—C4—H4	122.0
Br6—Sn1—Br5	178.17 (3)	C4—C5—C6	122.7 (9)
Br1—Sn1—Br2	87.41 (4)	C4—C5—H5	118.6
Br3—Sn1—Br2	90.69 (4)	C6—C5—H5	118.6
Br4—Sn1—Br2	179.08 (4)	C7—C6—C5	122.8 (9)
Br6—Sn1—Br2	84.41 (4)	C7—C6—H6	118.6
Br5—Sn1—Br2	93.86 (4)	C5—C6—H6	118.6
H1W1—O1W—H1W2	106.70	N2—C8—C7	120.5 (8)
H2W1—O2W—H2W2	108.30	N2—C8—C3	118.3 (7)
H3W1—O3W—H3W2	104.40	C7—C8—C3	121.1 (8)
C2—N1—C3	122.6 (7)	C6—C7—C8	115.2 (9)
C2—N1—H1N	118.7	C6—C7—H7	122.4
C3—N1—H1N	118.7	C8—C7—H7	122.4
C9—N2—C8	123.5 (7)	N2—C9—C2	118.9 (7)

C9—N2—H2N	118.2	N2—C9—C10	118.8 (8)
C8—N2—H2N	118.2	C2—C9—C10	122.4 (8)
C2—C1—H1A	109.5	C9—C10—H10A	109.5
C2—C1—H1B	109.5	C9—C10—H10B	109.5
H1A—C1—H1B	109.5	H10A—C10—H10B	109.5
C2—C1—H1C	109.5	C9—C10—H10C	109.5
H1A—C1—H1C	109.5	H10A—C10—H10C	109.5
H1B—C1—H1C	109.5	H10B—C10—H10C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2W	0.86	1.78	2.640 (14)	170.00
O1W—H1W2···Br3^{i}	0.87	2.79	3.348 (9)	123.1 (5)
O2W—H2W1···Br2^{ii}	0.84	2.57	3.401 (12)	167.4 (7)
O2W—H2W2···Br3^{ii}	0.87	2.83	3.482 (11)	132.9 (7)
O3W—H3W2···Br1	0.86	2.83	3.349 (11)	120.00
N1—H1N···O1W	0.86	1.82	2.672 (10)	172
N2—H2N···O3W^{iii}	0.86	1.81	2.660 (11)	172

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

Fig. 1

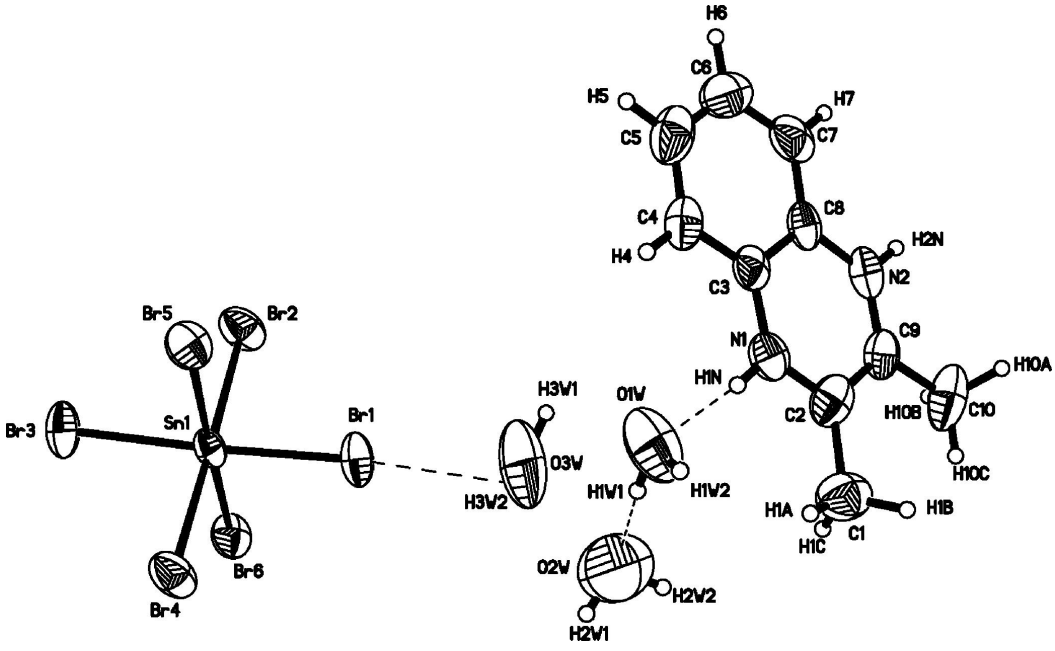
H6
C6
H5
H7
C5
C7
C4
C8
H4
H2N
N2
C3
N1
C9
H10A
H1N
O1W
H3W1
C2
H10B
C10
Br5
Br2
Br3
Sn1
Br1
O3W
H3W2
H1W1
H1W2
H1C
C1
H1A
H1B
H10C
O2W
H2W2
H2W1
Br6
Br4

Fig. 2

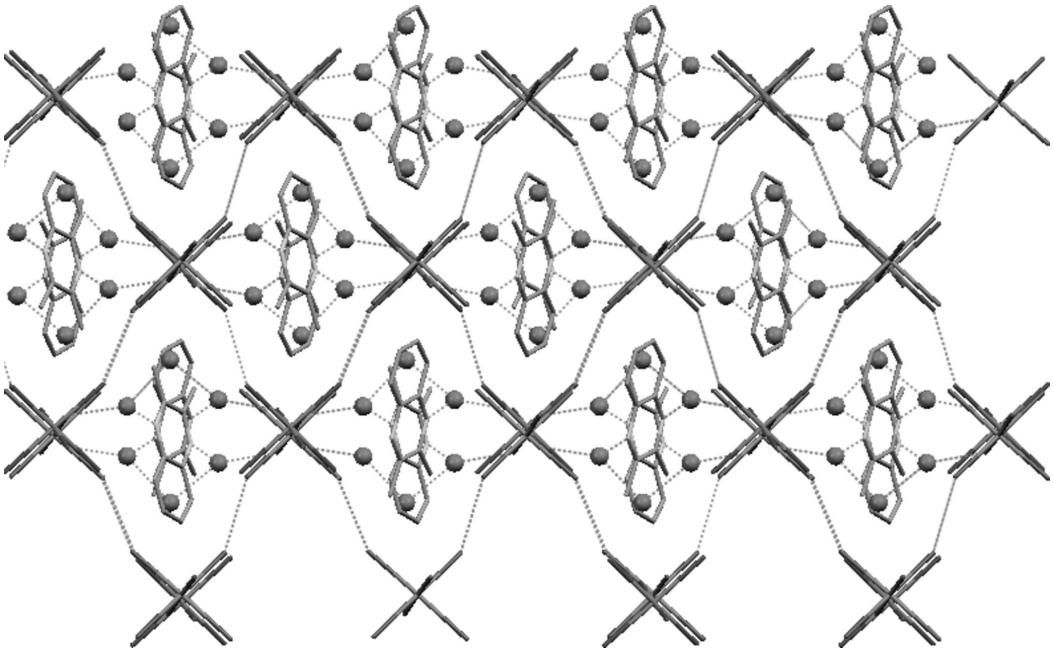

Fig. 3

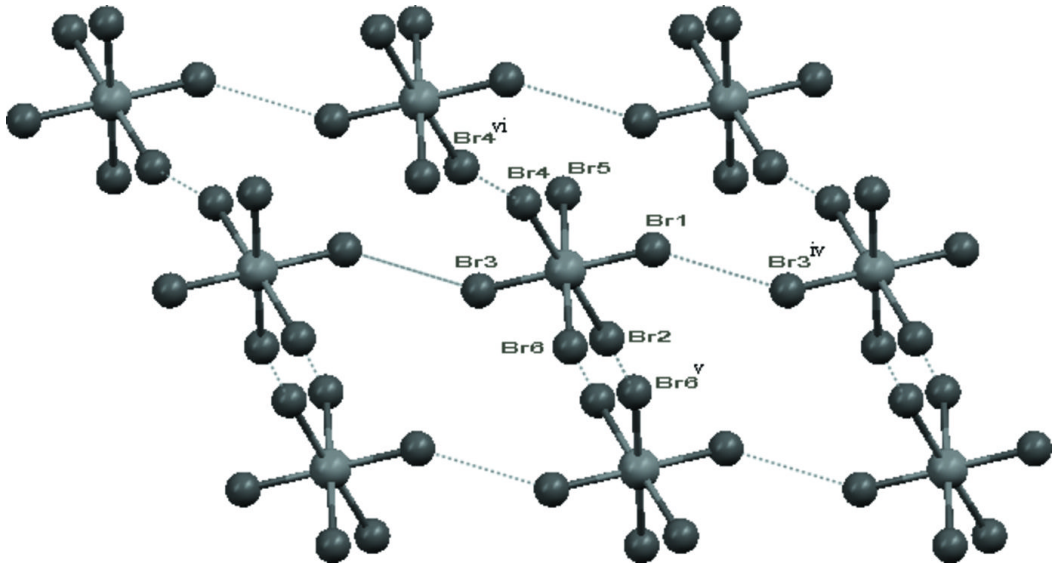

Fig. 4