

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# catena-Poly[[trimethyl(4-sulfanylphenyl)- azanium] [(chloridocadmate)-di- $\mu$ - chlorido]]

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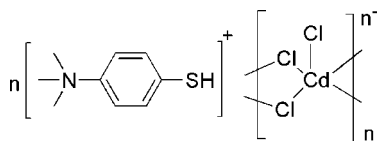
Received 29 September 2011; accepted 24 November 2011

Key indicators: single-crystal X-ray study;  $T = 223$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.026;  $wR$  factor = 0.069; data-to-parameter ratio = 18.2.

The title compound,  $\{(\text{C}_9\text{H}_{14}\text{NS})[\text{CdCl}_3]\}_n$ , consists of a linear  $[\text{CdCl}_3]_n^{n-}$  polyanion and a trimethyl(4-sulfanylphenyl)azanium cation. The  $\text{Cd}^{\text{II}}$  atom is pentacoordinated by four  $\mu_2$ -Cl atoms and one terminal Cl atom in a trigonal-bipyramidal geometry. The trigonal-bipyramidal units are linked by two opposite shared faces, giving rise to infinite  $[\text{CdCl}_3]_n$  chains parallel to the  $a$  axis. The cations surround the chain and are linked to them by  $\text{S}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\text{Cl}$  hydrogen bonds, forming a three-dimensional network.

## Related literature

For the synthesis of trimethylammoniumphenyl-4-thiol hexafluoridophosphate, see: DePamphilis *et al.* (1974).



## Experimental

## Crystal data

 $(\text{C}_9\text{H}_{14}\text{NS})[\text{CdCl}_3]$ 
 $M_r = 387.04$ 

Monoclinic,  $P2_1/c$   
 $a = 7.3207$  (15) Å  
 $b = 20.971$  (4) Å  
 $c = 9.1613$  (18) Å  
 $\beta = 103.96$  (3)°  
 $V = 1364.9$  (5) Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.31$  mm<sup>-1</sup>  
 $T = 223$  K  
 $0.50 \times 0.30 \times 0.20$  mm

## Data collection

Rigaku Mercury diffractometer  
 Absorption correction: multi-scan  
 (*CrystalClear*; Rigaku/MS, 2001)  
 $T_{\text{min}} = 0.442$ ,  $T_{\text{max}} = 0.635$

12984 measured reflections  
 2491 independent reflections  
 2424 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$   
 $wR(F^2) = 0.069$   
 $S = 1.11$   
 2491 reflections

137 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.56$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.79$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{S1}-\text{H1}\cdots\text{Cl1}^{\text{i}}$	1.20	2.55	3.746	180
$\text{C8}-\text{H8B}\cdots\text{Cl2}^{\text{ii}}$	0.97	2.72	3.640 (3)	158

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

Data collection: *CrystalClear* (Rigaku/MS, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Natural Science Foundation of the Education Commission of Jiangsu Province of China (No.11KJB150001) and a start-up grant from Changshu Institute of Technology (No. ky2009069).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5241).

## References

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 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supporting information

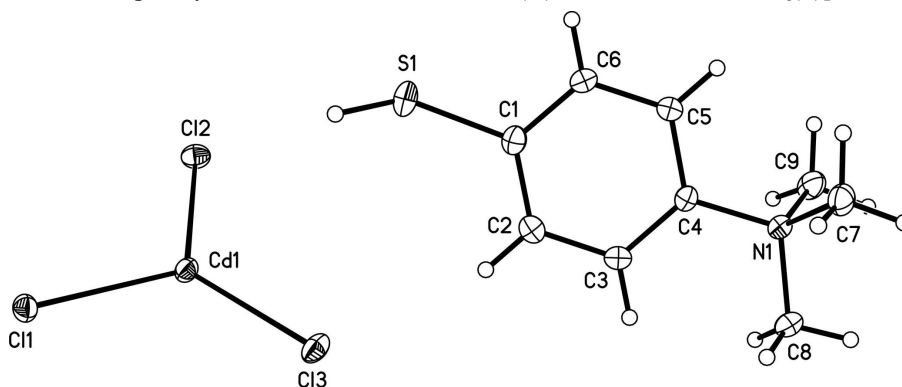
*Acta Cryst.* (2011). E67, m1883 [https://doi.org/10.1107/S1600536811050513]

**catena-Poly[[trimethyl(4-sulfanylphenyl)azanium] [(chloridocadmate)-di- $\mu$ -chlorido]]****Xiao-Yan Tang and Jian-Ping Lang****S1. Experimental**

The synthesis of trimethylammoniumphenyl-4-thiol hexafluorophosphate was according to the literature procedure (DePamphilis *et al.*, 1974). To a suspension containing TabHPF<sub>6</sub> (0.125 mg, 0.4 mmol) in MeOH (15 ml) was added Et<sub>3</sub>N (0.5 ml). The resulting colorless solution was then treated with a solution of CdCl<sub>2</sub>·2.5H<sub>2</sub>O (0.091 g, 0.4 mmol) in MeOH (10 ml). The mixture was stirred at room temperature for 1 h and treated with HCl to adjust the pH to 3, and then filtered. Diethyl ether (20 ml) was allowed to diffuse onto the filtrate. After standing it at ambient temperature for one week, colorless block crystals of (I) were formed. Yield: 0.100 g (65% based on Cd). The crystal used for the crystal structure determination was obtained directly from the above preparation. Analysis, found: C, 27.52; H, 3.31; N, 4.02%. calculated. for C<sub>9</sub>H<sub>14</sub>NSCdCl<sub>3</sub>: C, 27.93; H, 3.65; N, 3.62%.

**S2. Refinement**

Carbon-bond H atoms were positioned geometrically (C—H = 0.94 Å for methylene group and C—H = 0.97 Å for methyl group), and were included in the refinement in the riding mode approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for methylene group and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl group. The H atom attached to atom S1 was located in a difference Fourier map and refined isotropically without constraints with  $U_{\text{iso}}(\text{H})$  values fixed at  $1.2U_{\text{eq}}(\text{S})$ .

**Figure 1**

ORTEP plot of complex (I) at the 30% probability level. Hydrogen atoms are drawn as spheres of arbitrary radii.

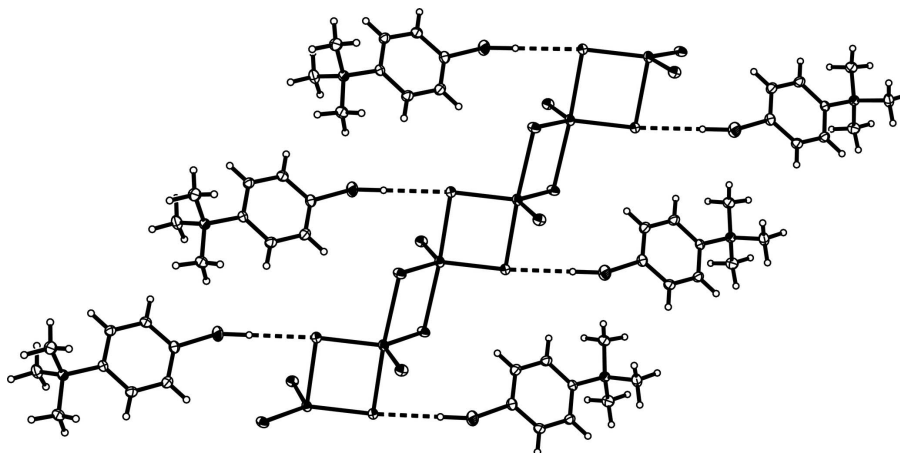


Figure 2

One dimensional structure formed by S—H...Cl interactions.

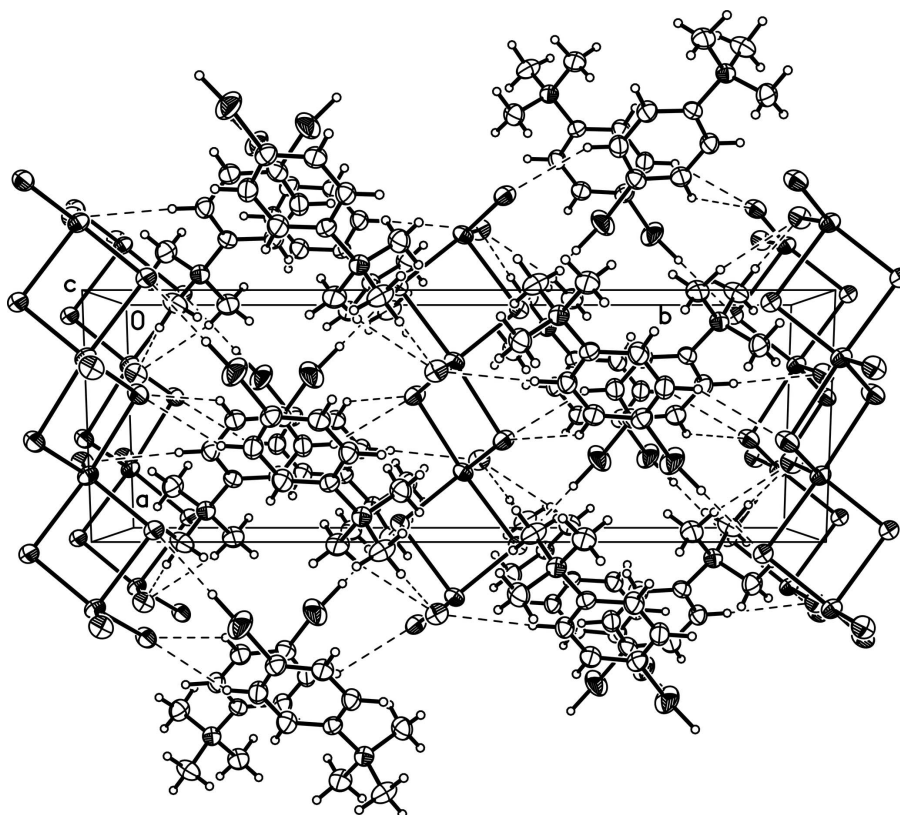


Figure 3

Three dimensional networks formed by S—H...Cl and C—H...Cl interactions.

*catena*-Poly[[[trimethyl(4-sulfanylphenyl)azanium] [(chloridocadmate)-di- $\mu$ -chlorido]]

*Crystal data*

(C<sub>9</sub>H<sub>14</sub>NS)[CdCl<sub>3</sub>]

$M_r = 387.04$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.3207(15) \text{ \AA}$

$b = 20.971(4) \text{ \AA}$

$c = 9.1613 (18) \text{ \AA}$   
 $\beta = 103.96 (3)^\circ$   
 $V = 1364.9 (5) \text{ \AA}^3$   
 $Z = 4$   
 $F(000) = 760$   
 $D_x = 1.883 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3007 reflections

$\theta = 3.0\text{--}25.4^\circ$   
 $\mu = 2.31 \text{ mm}^{-1}$   
 $T = 223 \text{ K}$   
 Block, colorless  
 $0.50 \times 0.30 \times 0.20 \text{ mm}$

*Data collection*

Rigaku Mercury  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (*CrystalClear*; Rigaku/MS2001)  
 $T_{\min} = 0.442$ ,  $T_{\max} = 0.635$

12984 measured reflections  
 2491 independent reflections  
 2424 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$   
 $\theta_{\max} = 25.4^\circ$ ,  $\theta_{\min} = 3.0^\circ$   
 $h = -8 \rightarrow 7$   
 $k = -22 \rightarrow 25$   
 $l = -11 \rightarrow 11$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.026$   
 $wR(F^2) = 0.069$   
 $S = 1.11$   
 2491 reflections  
 137 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods  
 Secondary atom site location: difference Fourier  
 map

Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.9902P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.56 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.79 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97* (Sheldrick,  
 2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0059 (5)

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.73386 (3)	0.993777 (10)	0.92593 (2)	0.02485 (11)
Cl1	0.95247 (10)	1.08537 (3)	0.99446 (8)	0.02873 (17)
Cl2	0.68785 (10)	0.96938 (3)	0.66114 (7)	0.03076 (18)
Cl3	0.59419 (8)	0.93630 (3)	1.11069 (7)	0.03094 (18)
S1	0.67638 (8)	0.79389 (3)	0.84461 (7)	0.0484 (2)
H1	0.7952	0.8326	0.8962	0.058*
C1	0.5039 (4)	0.74912 (14)	0.9045 (3)	0.0285 (6)
C2	0.3807 (4)	0.77654 (14)	0.9805 (3)	0.0319 (6)

H2	0.3876	0.8205	1.0016	0.038*
C3	0.2478 (4)	0.73917 (14)	1.0253 (3)	0.0303 (6)
H3	0.1638	0.7577	1.0760	0.036*
C4	0.2392 (4)	0.67468 (13)	0.9952 (3)	0.0238 (6)
C5	0.3603 (4)	0.64695 (14)	0.9182 (3)	0.0278 (6)
H5	0.3540	0.6030	0.8977	0.033*
C6	0.4898 (4)	0.68458 (14)	0.8721 (3)	0.0301 (6)
H6	0.5700	0.6662	0.8177	0.036*
C7	0.2022 (4)	0.58027 (15)	1.1450 (4)	0.0350 (7)
H7A	0.2689	0.5534	1.0889	0.053*
H7B	0.1119	0.5548	1.1813	0.053*
H7C	0.2914	0.5991	1.2297	0.053*
C8	-0.0195 (4)	0.66781 (15)	1.1295 (3)	0.0342 (7)
H8A	0.0607	0.6878	1.2174	0.051*
H8B	-0.1042	0.6381	1.1610	0.051*
H8C	-0.0922	0.7003	1.0654	0.051*
C9	-0.0285 (4)	0.60310 (16)	0.9076 (3)	0.0357 (7)
H9A	-0.0869	0.6365	0.8389	0.054*
H9B	-0.1251	0.5785	0.9381	0.054*
H9C	0.0436	0.5754	0.8578	0.054*
N1	0.1003 (3)	0.63245 (11)	1.0439 (2)	0.0250 (5)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.02433 (16)	0.02926 (16)	0.02258 (16)	-0.00438 (7)	0.00880 (10)	-0.00082 (7)
Cl1	0.0240 (3)	0.0261 (4)	0.0358 (4)	-0.0021 (3)	0.0065 (3)	-0.0020 (3)
Cl2	0.0328 (4)	0.0364 (4)	0.0230 (3)	0.0030 (3)	0.0066 (3)	-0.0025 (3)
Cl3	0.0280 (4)	0.0330 (4)	0.0359 (4)	0.0061 (3)	0.0157 (3)	0.0131 (3)
S1	0.0499 (5)	0.0405 (5)	0.0632 (6)	-0.0145 (4)	0.0301 (4)	0.0025 (4)
C1	0.0287 (15)	0.0301 (15)	0.0267 (14)	-0.0036 (11)	0.0066 (11)	0.0032 (11)
C2	0.0352 (16)	0.0247 (15)	0.0366 (16)	-0.0010 (12)	0.0105 (12)	-0.0012 (12)
C3	0.0336 (16)	0.0282 (16)	0.0322 (15)	0.0008 (12)	0.0141 (12)	-0.0046 (12)
C4	0.0220 (13)	0.0257 (14)	0.0240 (14)	-0.0025 (11)	0.0065 (10)	0.0012 (11)
C5	0.0310 (15)	0.0246 (15)	0.0297 (15)	-0.0001 (11)	0.0112 (12)	-0.0034 (11)
C6	0.0296 (15)	0.0310 (16)	0.0337 (16)	0.0005 (12)	0.0152 (12)	-0.0025 (12)
C7	0.0374 (17)	0.0319 (17)	0.0379 (17)	0.0022 (13)	0.0133 (13)	0.0094 (13)
C8	0.0333 (16)	0.0372 (17)	0.0377 (17)	-0.0009 (13)	0.0197 (13)	-0.0029 (13)
C9	0.0304 (16)	0.0440 (18)	0.0339 (16)	-0.0111 (13)	0.0101 (12)	-0.0082 (13)
N1	0.0265 (12)	0.0262 (12)	0.0245 (11)	-0.0007 (9)	0.0102 (9)	0.0000 (9)

*Geometric parameters (Å, °)*

Cd1—Cl2	2.4219 (8)	C4—N1	1.496 (3)
Cd1—Cl1	2.4819 (8)	C5—C6	1.375 (4)
Cd1—Cl3	2.4896 (7)	C5—H5	0.9400
Cd1—Cl3 <sup>i</sup>	2.7643 (7)	C6—H6	0.9400
Cd1—Cl1 <sup>ii</sup>	2.7842 (9)	C7—N1	1.509 (4)

C11—Cd1 <sup>ii</sup>	2.7842 (9)	C7—H7A	0.9700
C13—Cd1 <sup>i</sup>	2.7643 (7)	C7—H7B	0.9700
S1—C1	1.764 (3)	C7—H7C	0.9700
S1—H1	1.1999	C8—N1	1.505 (4)
C1—C6	1.384 (4)	C8—H8A	0.9700
C1—C2	1.390 (4)	C8—H8B	0.9700
C2—C3	1.386 (4)	C8—H8C	0.9700
C2—H2	0.9400	C9—N1	1.503 (4)
C3—C4	1.379 (4)	C9—H9A	0.9700
C3—H3	0.9400	C9—H9B	0.9700
C4—C5	1.387 (4)	C9—H9C	0.9700
C12—Cd1—C11	110.02 (3)	C5—C6—C1	121.1 (3)
C12—Cd1—C13	126.73 (3)	C5—C6—H6	119.4
C11—Cd1—C13	123.24 (3)	C1—C6—H6	119.4
C12—Cd1—C13 <sup>i</sup>	94.80 (3)	N1—C7—H7A	109.5
C11—Cd1—C13 <sup>i</sup>	96.23 (3)	N1—C7—H7B	109.5
C13—Cd1—C13 <sup>i</sup>	81.49 (3)	H7A—C7—H7B	109.5
C12—Cd1—C11 <sup>ii</sup>	92.47 (3)	N1—C7—H7C	109.5
C11—Cd1—C11 <sup>ii</sup>	87.38 (3)	H7A—C7—H7C	109.5
C13—Cd1—C11 <sup>ii</sup>	88.93 (3)	H7B—C7—H7C	109.5
C13 <sup>i</sup> —Cd1—C11 <sup>ii</sup>	170.23 (2)	N1—C8—H8A	109.5
Cd1—C11—Cd1 <sup>ii</sup>	92.62 (3)	N1—C8—H8B	109.5
Cd1—C13—Cd1 <sup>i</sup>	98.51 (3)	H8A—C8—H8B	109.5
C1—S1—H1	138.0	N1—C8—H8C	109.5
C6—C1—C2	119.2 (3)	H8A—C8—H8C	109.5
C6—C1—S1	118.4 (2)	H8B—C8—H8C	109.5
C2—C1—S1	122.4 (2)	N1—C9—H9A	109.5
C3—C2—C1	120.1 (3)	N1—C9—H9B	109.5
C3—C2—H2	120.0	H9A—C9—H9B	109.5
C1—C2—H2	120.0	N1—C9—H9C	109.5
C4—C3—C2	119.8 (3)	H9A—C9—H9C	109.5
C4—C3—H3	120.1	H9B—C9—H9C	109.5
C2—C3—H3	120.1	C4—N1—C9	109.2 (2)
C3—C4—C5	120.6 (3)	C4—N1—C8	112.8 (2)
C3—C4—N1	121.5 (2)	C9—N1—C8	107.9 (2)
C5—C4—N1	117.9 (2)	C4—N1—C7	109.9 (2)
C6—C5—C4	119.2 (3)	C9—N1—C7	109.3 (2)
C6—C5—H5	120.4	C8—N1—C7	107.6 (2)
C4—C5—H5	120.4		

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

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

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
S1—H1 $\cdots$ C11 <sup>ii</sup>	1.20	2.55	3.746	180

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C8—H8B $\cdots$ C12 <sup>iii</sup>	0.97	2.72	3.640 (3)	158
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Symmetry codes: (ii)  $-x+2, -y+2, -z+2$ ; (iii)  $x-1, -y+3/2, z+1/2$ .