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catena-Poly[1,10-phenanthroline-1,10-diium [[dichloridobismuthate(III)]-di-μ-chlorido]]

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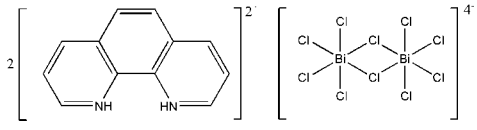
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.015 Å; disorder in main residue; R factor = 0.037; wR factor = 0.105; data-to-parameter ratio = 14.6.

The asymmetric unit of the title compound, $\{(C_{12}H_{10}N_2)[BiCl_4]\}_n$, comprises one 1,10-phenanthrolinium dication and one Bi atom with two terminal and two bridging chloride anions. The Bi atoms adopt a distorted octahedral configuration and are each bridged to two other Bi atoms by four chloride ligands to generate a one-dimensional polymer chain running along a. C—H···Cl hydrogen bonds link the phenanthrolinium dications to these chlorobismuthate chains.

Related literature

For a general background to bismuth coordination chemistry see Summers *et al.* (1994), and for applications in medicine see Sun *et al.* (1997) and Baxter (1992). For related structures, see: Bowmaker *et al.* (1998); Benetollo *et al.* (1998); Blažič & Lazarini (1985).



Experimental

Crystal data

$(C_{12}H_{10}N_2)[BiCl_4]$
M_r = 533.00
Triclinic, $P\overline{1}$
a = 7.2569 (14) Å
b = 10.1924 (19) Å
c = 12.139 (2) Å
α = 77.944 (3)°
β = 75.044 (2)°
γ = 69.313 (2)°
V = 804.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.61 mm^{-1}
T = 298 (2) K
0.22 × 0.21 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.088, T_{max} = 0.098
4232 measured reflections
2804 independent reflections
2469 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.105
S = 1.00
2804 reflections
192 parameters
13 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.70 e Å^{-3}
$\Delta\rho_{min}$ = −1.53 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···Cl2^{i}	0.93	3.10	3.951 (17)	153
C12′—H12′···Cl2^{ii}	0.93	2.90	3.77 (2)	155

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2292).

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supplementary materials

Acta Cryst. (2007). E**63**, m1746 [**doi:10.1107/S1600536807023318**]

catena-Poly[1,10-phenanthroline-1,10-diium [[dichloridobismuthate(III)]-di-μ-chlorido]]

F. Li, H. Yin and J. Simpson

Comment

The coordination chemistry of bismuth(III) is not widely investigated, although a number of adducts formed by nitrogen-containing ligands with bismuth(III) salts have been reported (Summers *et al.*, 1994). More recently however, bismuth(III) coordination chemistry has gained more prominence, particularly in the light of the role of bismuth compounds in ^{212}Bi isotope therapy in cancer research (Sun *et al.*, 1997) and the use of bismuth complexes in the treatment of peptic ulcers (Sun *et al.*, 1997; Baxter, 1992). In a continuation of our studies of metal complexes with nitrogen ligands and salts of protonated nitrogen ligands with metal containing anions, we report here the synthesis and structure of the title compound, $(phenH_2^{2+})_2(Bi_2Cl_8^{4-})$.

The asymmetric unit of the title compound, $C_{12}H_{10}BiCl_4N_2$, comprises one 1,10-phenanthrolinium dication and one half of an octachlorodibismuthate tetraanion which lies about an inversion centre and forms the tetranion *via* Bi1—Cl1—Bi1^{i} and Bi1—Cl1^{i}—Bi1^{i} bridges [i = − *x* + 1, − *y* + 1, − *z* + 1] to build the complex $(phenH_2^{2+})_2(Bi_2Cl_8^{4-})$. A view of the formula unit made up of two cations and anion is shown in Fig. 1. The dications are disordered with the two disorder components related in a head to tail fashion Fig 3.

The dimeric $[Bi_2Cl_8]^{4-}$ tetraanions are made up from two octahedra sharing a common edge. The coordination geometry about Bi is distorted octahedral with Cl—Bi—Cl angles varying from 82.85 (7) − 94.43 (7)° for *cis* and 71.16 (8) −175.56 (6)° for *trans* arrangements. The Bi—Cl bond distances also vary with the role they play in the structure. The terminal Bi—Cl3 [2.508 (2) Å] and Bi—Cl4 [2.560 (2) Å] bonds are significantly shorter than those involving Cl bridges which range from 2.699 (2) to 2.985 (2) Å.

In the crystal tetraanions are further linked by Bi1—Cl2^{ii}—Bi1 bridges [ii = − *x* + 2, − *y* + 1, − *z* + 1] to generate a one-dimensional polymer chain running along *c* axis. Cations and anions are linked by C—H···Cl hydrogen bonds (Fig. 2).

Experimental

Bismuth trichloride (0.5 mmol) was dissolved in 20 ml of dicholoromethane, and 0.5 mmol of 1,10-phenanthroline were added under stirring at room temperature. Pale yellow crystals precipitated after a few days and were filtered, washed with acetone and dried under vacuum. Yield 81%. m.p.: 421 K. Analysis calculated for $C_{12}H_{10}BiCl_4N_2$: C 27.04, H 1.89, N 5.26%. Found: C 27.32, H 1.73, N 5.45%.

Refinement

All H atoms were placed geometrically (C—H = 0.93 Å, N—H = 0.88 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier). Atoms N1, N2, C4, C7, C11 and C12 of the 1,10-phenanthrolinium cations are disordered over two positions with occu-

pancies that were fixed at at 0.58 (1) and 0.42 (1) for all five atoms in the final stages of the refinement. Atoms C1—C3, C5, C7 and C8—C10 were common to both disorder components, while the atom pairs C4, N1'; C7 N2'; N1, C4' and N2, C7' shared identical coordinates.

Figures

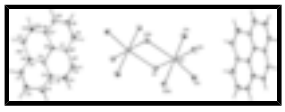

Fig. 1. The structure of (I) with 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabeled atoms are related to the corresponding labeled atoms by the symmetry code −*x* + 1,-*y* + 1,-*z* + 1 with Cl2 related to Cl2A by the symmetry code −*x* + 2,-*y* + 1,-*z* + 1.

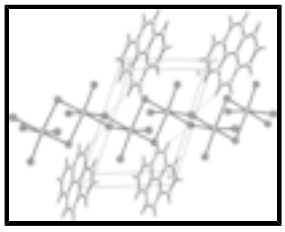

Fig. 2. The crystal packing of (I) viewed down the *c* axis. Polymeric chains of chloride bridged octachlorodibismuthate tetraanions are linked to the cations by intermolecular C—H···Cl hydrogen bonds drawn as dashed lines.

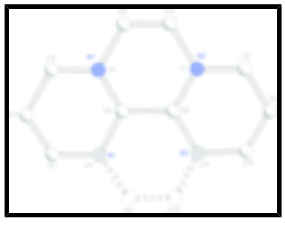

Fig. 3. A representation of the disorder in the phenathrolinium cations of (I). Atoms of the minor component are linked by double dashed lines and atoms sharing common coordinates are displayed as filled spheres.

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Crystal data

$(C_{12}H_{10}N_2)[BiCl_4]$	$Z = 2$
$M_r = 533.00$	$F_{000} = 494$
Triclinic, $P\overline{1}$	$D_x = 2.200$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.2569$ (14) Å	Cell parameters from 2619 reflections
$b = 10.1924$ (19) Å	$\theta = 2.2$–26.6º
$c = 12.139$ (2) Å	$\mu = 11.61$ mm^{-1}
$\alpha = 77.944$ (3)º	$T = 298$ (2) K
$\beta = 75.044$ (2)º	Block, yellow
$\gamma = 69.313$ (2)º	0.22 × 0.21 × 0.20 mm
$V = 804.6$ (3) Å^3	

Data collection

CCD area detector diffractometer	2804 independent reflections
Radiation source: fine-focus sealed tube	2469 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$

T = 298(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.088, T_{max} = 0.098

4232 measured reflections

θ_{max} = 25.0º

θ_{min} = 1.8º

h = −8→8

k = −11→12

l = −14→13

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.037

$wR(F^2)$ = 0.105

S = 1.00

2804 reflections

192 parameters

13 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

$w = 1/[\sigma^2(F_o^2) + (0.0769P)^2 + 0.0334P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 3.70 e Å^{-3}

$\Delta\rho_{min}$ = −1.53 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 $F^2 > \sigma(F^2)$ 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}	Occ. (<1)
Bi1	0.68159 (4)	0.57991 (3)	0.56389 (2)	0.03303 (15)	
Cl1	0.3605 (3)	0.6925 (2)	0.4619 (2)	0.0430 (5)	
Cl2	1.0241 (4)	0.4526 (3)	0.6542 (2)	0.0473 (5)	
Cl3	0.6950 (4)	0.8238 (3)	0.5580 (2)	0.0544 (6)	
Cl4	0.4662 (4)	0.5734 (3)	0.7672 (2)	0.0570 (7)	
N1	0.3086 (11)	−0.0610 (8)	−0.0603 (7)	0.041 (2)	0.580 (11)
H1A	0.2899	−0.1385	−0.0233	0.049*	0.580 (11)
N2	0.1154 (12)	−0.0722 (9)	0.1714 (7)	0.0421 (19)	0.580 (11)
H2A	0.1572	−0.1471	0.1381	0.050*	0.580 (11)
C4	0.2683 (12)	0.1853 (9)	−0.0634 (7)	0.0399 (18)	0.580 (11)
C7	0.0775 (12)	0.1708 (9)	0.1679 (7)	0.0407 (19)	0.580 (11)

C4'	0.3086 (11)	−0.0610 (8)	−0.0603 (7)	0.041 (2)	0.420 (11)
C7'	0.1154 (12)	−0.0722 (9)	0.1714 (7)	0.0421 (19)	0.420 (11)
N1'	0.2683 (12)	0.1853 (9)	−0.0634 (7)	0.0399 (18)	0.420 (11)
H1'	0.2268	0.2581	−0.0276	0.048*	0.420 (11)
N2'	0.0775 (12)	0.1708 (9)	0.1679 (7)	0.0407 (19)	0.420 (11)
H2'	0.0972	0.2486	0.1325	0.049*	0.420 (11)
C1	0.4030 (14)	−0.0518 (10)	−0.1717 (8)	0.044 (2)	
H1	0.4517	−0.1329	−0.2078	0.053*	
C2	0.4303 (16)	0.0681 (11)	−0.2330 (9)	0.052 (3)	
H2	0.4927	0.0715	−0.3103	0.063*	
C3	0.3575 (16)	0.1941 (13)	−0.1730 (10)	0.060 (3)	
H3	0.3743	0.2792	−0.2120	0.072*	
C5	0.2425 (12)	0.0623 (9)	−0.0078 (7)	0.0339 (18)	
C6	0.1431 (13)	0.0550 (9)	0.1109 (8)	0.0363 (19)	
C8	−0.0172 (15)	0.1638 (12)	0.2782 (9)	0.054 (3)	
H8	−0.0625	0.2437	0.3156	0.065*	
C9	−0.0488 (18)	0.0387 (13)	0.3378 (10)	0.060 (3)	
H9	−0.1176	0.0348	0.4139	0.072*	
C10	0.0207 (14)	−0.0742 (11)	0.2841 (9)	0.049 (2)	
H10	0.0045	−0.1588	0.3249	0.059*	
C11	0.203 (3)	0.311 (2)	−0.0032 (15)	0.051 (4)	0.580 (11)
H11	0.2299	0.3932	−0.0413	0.061*	0.580 (11)
C12	0.107 (2)	0.3055 (17)	0.1029 (14)	0.044 (4)	0.580 (11)
H12	0.0569	0.3867	0.1389	0.053*	0.580 (11)
C11'	0.278 (3)	−0.195 (2)	0.011 (2)	0.043 (6)	0.420 (11)
H11'	0.3238	−0.2774	−0.0236	0.051*	0.420 (11)
C12'	0.189 (3)	−0.1999 (19)	0.1209 (18)	0.040 (5)	0.420 (11)
H12'	0.1748	−0.2839	0.1639	0.047*	0.420 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.0318 (2)	0.0319 (2)	0.0345 (2)	−0.00910 (14)	−0.00571 (13)	−0.00526 (13)
Cl1	0.0442 (12)	0.0359 (11)	0.0463 (13)	−0.0084 (9)	−0.0142 (10)	−0.0009 (9)
Cl2	0.0451 (13)	0.0528 (14)	0.0400 (12)	−0.0084 (10)	−0.0132 (10)	−0.0042 (10)
Cl3	0.0726 (17)	0.0413 (13)	0.0529 (14)	−0.0248 (12)	−0.0050 (12)	−0.0112 (10)
Cl4	0.0592 (16)	0.0574 (15)	0.0435 (14)	−0.0164 (12)	0.0023 (11)	−0.0027 (11)
N1	0.043 (5)	0.044 (5)	0.040 (5)	−0.014 (4)	−0.013 (4)	−0.007 (4)
N2	0.035 (4)	0.043 (5)	0.049 (5)	−0.010 (4)	−0.015 (4)	−0.003 (4)
C4	0.041 (4)	0.040 (5)	0.036 (4)	−0.009 (4)	−0.009 (4)	−0.004 (3)
C7	0.038 (4)	0.042 (5)	0.039 (5)	−0.008 (4)	−0.009 (4)	−0.007 (4)
C4'	0.043 (5)	0.044 (5)	0.040 (5)	−0.014 (4)	−0.013 (4)	−0.007 (4)
C7'	0.035 (4)	0.043 (5)	0.049 (5)	−0.010 (4)	−0.015 (4)	−0.003 (4)
N1'	0.041 (4)	0.040 (5)	0.036 (4)	−0.009 (4)	−0.009 (4)	−0.004 (3)
N2'	0.038 (4)	0.042 (5)	0.039 (5)	−0.008 (4)	−0.009 (4)	−0.007 (4)
C1	0.046 (5)	0.045 (5)	0.046 (6)	−0.017 (4)	−0.010 (4)	−0.010 (4)
C2	0.049 (6)	0.060 (7)	0.046 (6)	−0.012 (5)	−0.003 (5)	−0.018 (5)
C3	0.055 (6)	0.067 (7)	0.056 (7)	−0.010 (5)	−0.022 (5)	−0.007 (5)

C5	0.028 (4)	0.036 (5)	0.038 (5)	−0.006 (3)	−0.010 (4)	−0.006 (4)
C6	0.041 (5)	0.036 (5)	0.037 (5)	−0.015 (4)	−0.014 (4)	0.000 (4)
C8	0.043 (5)	0.062 (7)	0.058 (7)	−0.011 (5)	−0.008 (5)	−0.026 (5)
C9	0.064 (7)	0.073 (8)	0.043 (6)	−0.025 (6)	−0.016 (5)	0.001 (5)
C10	0.038 (5)	0.047 (6)	0.053 (6)	−0.016 (4)	−0.008 (4)	0.017 (5)
C11	0.044 (9)	0.055 (11)	0.051 (10)	−0.021 (8)	0.003 (8)	−0.009 (8)
C12	0.043 (7)	0.042 (7)	0.045 (7)	−0.011 (6)	−0.009 (6)	−0.005 (6)
C11'	0.038 (12)	0.031 (11)	0.059 (14)	−0.018 (9)	0.000 (10)	−0.003 (10)
C12'	0.039 (8)	0.045 (9)	0.036 (8)	−0.015 (7)	−0.010 (7)	−0.003 (7)

Geometric parameters (Å, °)

Bi1—Cl3	2.508 (2)	C7—C12	1.492 (18)
Bi1—Cl4	2.560 (2)	C1—C2	1.343 (14)
Bi1—Cl1	2.699 (2)	C1—H1	0.9300
Bi1—Cl2	2.756 (2)	C2—C3	1.474 (15)
Bi1—Cl2^{i}	2.937 (2)	C2—H2	0.9300
Bi1—Cl1^{ii}	2.985 (2)	C3—H3	0.9300
Cl1—Bi1^{ii}	2.985 (2)	C5—C6	1.435 (13)
Cl2—Bi1^{i}	2.937 (2)	C8—C9	1.393 (16)
N1—C1	1.349 (12)	C8—H8	0.9300
N1—C5	1.403 (11)	C9—C10	1.317 (16)
N1—H1A	0.8600	C9—H9	0.9300
N2—C10	1.363 (13)	C10—H10	0.9300
N2—C6	1.405 (12)	C11—C12	1.30 (2)
N2—H2A	0.8600	C11—H11	0.9300
C4—C3	1.321 (14)	C12—H12	0.9300
C4—C5	1.345 (12)	C11'—C12'	1.32 (3)
C4—C11	1.475 (19)	C11'—H11'	0.9300
C7—C8	1.338 (13)	C12'—H12'	0.9300
C7—C6	1.367 (12)		
Cl3—Bi1—Cl4	94.42 (9)	N1—C1—H1	118.3
Cl3—Bi1—Cl1	89.50 (9)	C1—C2—C3	117.3 (10)
Cl4—Bi1—Cl1	93.70 (8)	C1—C2—H2	121.3
Cl3—Bi1—Cl2	92.93 (9)	C3—C2—H2	121.3
Cl4—Bi1—Cl2	89.82 (9)	C4—C3—C2	119.6 (11)
Cl1—Bi1—Cl2	175.56 (6)	C4—C3—H3	120.2
Cl3—Bi1—Cl2^{i}	90.29 (8)	C2—C3—H3	120.2
Cl4—Bi1—Cl2^{i}	170.84 (8)	C4—C5—N1	123.1 (8)
Cl1—Bi1—Cl2^{i}	94.19 (7)	C4—C5—C6	119.2 (7)
Cl2—Bi1—Cl2^{i}	82.09 (7)	N1—C5—C6	117.7 (8)
Cl3—Bi1—Cl1^{ii}	171.16 (8)	C7—C6—N2	118.8 (8)
Cl4—Bi1—Cl1^{ii}	90.50 (8)	C7—C6—C5	120.7 (8)
Cl1—Bi1—Cl1^{ii}	82.85 (7)	N2—C6—C5	120.5 (8)
Cl2—Bi1—Cl1^{ii}	94.43 (7)	C7—C8—C9	120.9 (10)
Cl2^{i}—Bi1—Cl1^{ii}	85.88 (7)	C7—C8—H8	119.6

Bi1—Cl1—Bi1^{ii}	97.15 (7)	C9—C8—H8	119.6
Bi1—Cl2—Bi1^{i}	97.91 (7)	C10—C9—C8	118.6 (10)
C1—N1—C5	116.6 (8)	C10—C9—H9	120.7
C1—N1—H1A	121.7	C8—C9—H9	120.7
C5—N1—H1A	121.7	C9—C10—N2	122.7 (9)
C10—N2—C6	118.4 (8)	C9—C10—H10	118.6
C10—N2—H2A	120.8	N2—C10—H10	118.6
C6—N2—H2A	120.8	C12—C11—C4	119.6 (15)
C3—C4—C5	119.9 (9)	C12—C11—H11	120.2
C3—C4—C11	119.0 (10)	C4—C11—H11	120.2
C5—C4—C11	121.1 (10)	C11—C12—C7	120.8 (15)
C8—C7—C6	120.5 (9)	C11—C12—H12	119.6
C8—C7—C12	121.1 (10)	C7—C12—H12	119.6
C6—C7—C12	118.4 (9)	C12'—C11'—H11'	118.9
C2—C1—N1	123.5 (9)	C11'—C12'—H12'	121.0
C2—C1—H1	118.3		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···Cl2^{ii}	0.93	3.10	3.951 (17)	153
C12'—H12'···Cl2^{iii}	0.93	2.90	3.77 (2)	155

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

Fig. 1

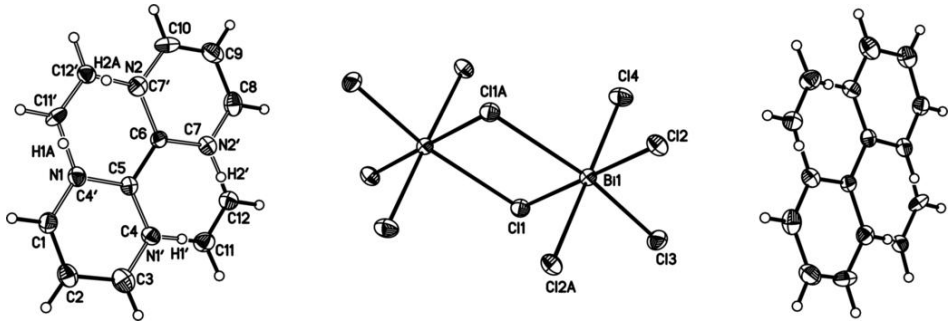
C10
C9
H2A
N2
C12'
C7'
C8
C11'
C6
C7
N2'
H1A
C5
H2'
N1
C4'
C12
C1
C4
N1'
H1'
C11
C3
C2
Cl1A
Cl4
Cl2
Bi1
Cl1
Cl3
Cl2A

Fig. 2

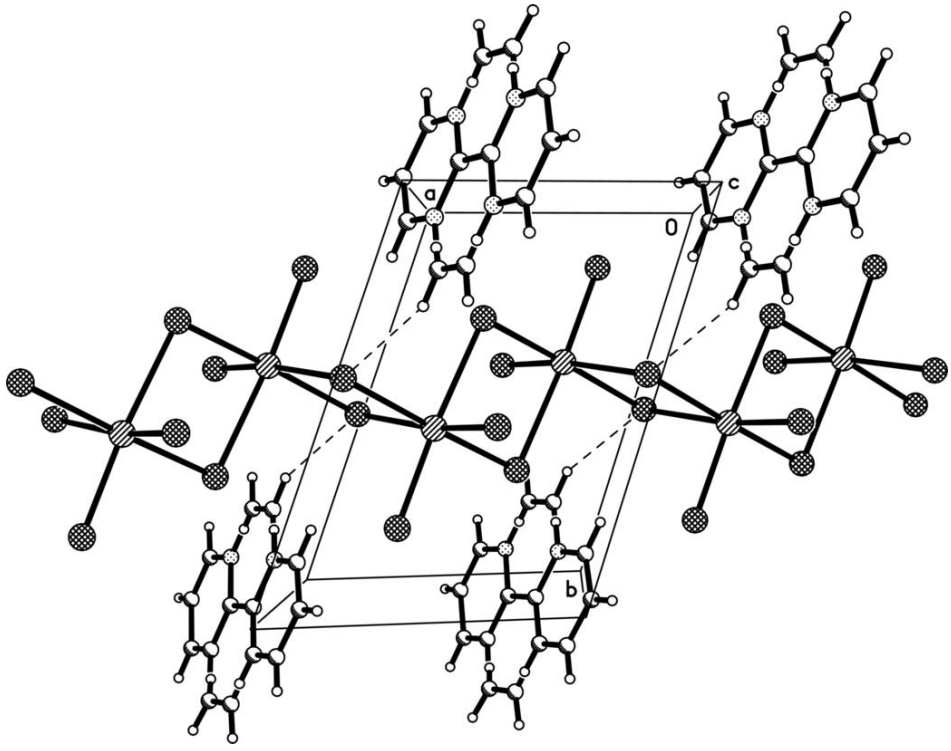

Fig. 3