Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[cadmium(II)-(μ-3-ammonio-3-phenylpropanoato-κ²*O*:*O*′)-di-μ-chlorido]

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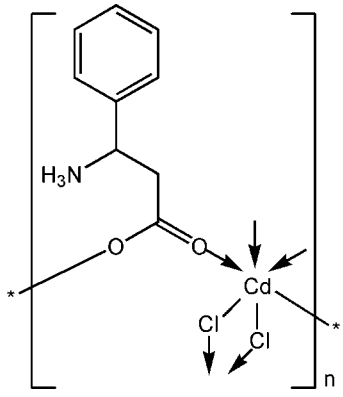
Received 22 July 2008; accepted 23 July 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.018; wR factor = 0.041; data-to-parameter ratio = 16.3.

The title compound, $[CdCl_2(C_9H_{11}NO_2)]_n$, is a coordination polymer prepared by the hydrothermal reaction of cadmium(II) chloride and 3-amino-3-phenylpropanoic acid. Geometric parameters are in the usual ranges. The cadmium cation is octahedrally coordinated by four Cl atoms at equatorial sites and two O atoms from two ligands at the axial sites. The material is composed of one-dimensional extended polymeric chains in which two Cl atoms bridge Cd atoms. The crystal structure is stabilized by an intramolecular N—H···O hydrogen bond.

Related literature

For related literature, see: Arki *et al.* (2004); Cohen *et al.* (2002); Zeller *et al.* (1965); Zhao (2007); Qu *et al.* (2004).



Experimental

Crystal data

$[CdCl_2(C_9H_{11}NO_2)]$
M_r = 348.49
Monoclinic, $P2_1/c$
a = 11.879 (2) Å
b = 6.9364 (14) Å
c = 14.072 (3) Å
β = 110.26 (3)°
V = 1087.7 (4) Å³
Z = 4
Mo $K\alpha$ radiation
μ = 2.48 mm⁻¹
T = 293 (2) K
0.25 × 0.18 × 0.15 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.592, T_{max} = 0.690
9829 measured reflections
2148 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.041
S = 0.92
2148 reflections
132 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å⁻³
$\Delta\rho_{min}$ = −0.31 e Å⁻³

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*C*···O1	0.89	2.08	2.735 (3)	130

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *PRPKAPPA* (Ferguson, 1999).

This work was supported by a Start-up Grant from Southeast University to ZRQ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2165).

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supplementary materials

Acta Cryst. (2008). E**64**, m1085 [**doi:10.1107/S1600536808023179**]

catena-Poly[cadmium(II)-(μ-3-ammonio-3-phenylpropanoato-κ^2O:O')-di-μ-chlorido]

Z.-R. Qu and X.-Z. Li

Comment

Coordination frameworks have received much attention over the past decade because of their potential applications. β-amino acids are important molecules due to their pharmacological properties. Recently, there is an increased interest in the enantiomeric preparation of β-amino acids as precursors for the synthesis of novel biologically active compounds (Arki *et al.*, 2004; Cohen *et al.*, 2002; Zeller *et al.*, 1965). We report here the crystal structure of the title compound, which was obtained by the hydrothermal reaction of cadmium chloride and 3-amino-3-phenylpropanoic acid. In the structure of the title compoud, The geometric parameters are in the usual ranges (Zhao, 2007; Qu *et al.*, 2004). The cadmium cation is octahedrally coordinated by four Cl atoms at equatorial sites and two O atoms from two ligands at at axial sites (Fig. 1). The material is composed of one-dimensional extended polymeric chains in which two Cl atoms bridges Cd atoms (Fig. 2). The crystal structure is stabilized by an intramolecular hydrogen bond, (Table 1).

Experimental

A mixture of $CdCl_2$ (0.2 mmol, 0.037 g) and 3-amino-3-phenylpropanoic acid (0.2 mmol, 0.033 g) in H_2O (4 ml) was heated in Pyrex tube at 100°C for two days. After slowly cooling down to room temperature over a period of 12 h, colorless crystals of the title compound suitable for diffraction were isolated.

Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C, N atoms to which they are bonded. C—H = 0.97–0.98 Å, with $1.5U_{eq}$(methyl), C—H = 0.93 Å with U_{iso}(H) = $1.2U_{eq}$(Caromatic) and N—H = 0.89 Å with U_{iso}(H) = $1.5U_{eq}$(N).

Figures

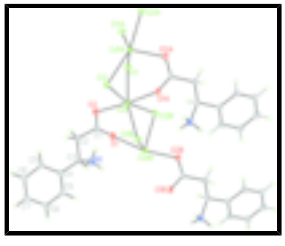


Fig. 1. A partial packing diagram of the title compound, with the displacement ellipsoids were drawn at the 30% probability level. [Symmetry codes: (A) -*x*+1, *y* - 1/2, -*z* + 3/2; (B) -*x* + 1, *y* + 1/2, *z* + 3/2.]

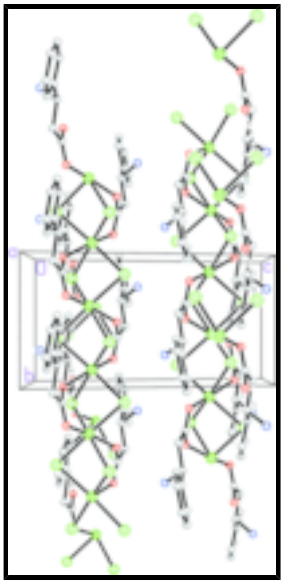


Fig. 2. Packing diagram of the title compound, showing the structure along the *b* axis. H atoms have been omitted for clarity.

catena-Poly[cadmium(II)-(μ-3-ammonio-3-phenylpropanoato- κ^2O:O^1)-di-μ-chlorido]

Crystal data

$[CdCl_2(C_9H_{11}NO_2)]$	F_{000} = 680
M_r = 348.49	D_x = 2.128 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -p 2ybc	Cell parameters from 1979 reflections
a = 11.879 (2) Å	θ = 3.1–27.5º
b = 6.9364 (14) Å	μ = 2.48 mm^{-1}
c = 14.072 (3) Å	T = 293 (2) K
β = 110.26 (3)º	Prism, colourless
V = 1087.7 (4) Å^3	0.25 × 0.18 × 0.15 mm
Z = 4	

Data collection

Rigaku SCXmini diffractometer	2148 independent reflections
Radiation source: fine-focus sealed tube	1963 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 3.1º
CCD Profile fitting scans	h = −14→14
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −8→8
T_{min} = 0.592, T_{max} = 0.690	l = −17→17
9829 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.018$	$w = 1/[\sigma^2(F_o^2) + (0.0175P)^2 + 1.2054P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.041$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.92$	$\Delta\rho_{max} = 0.29$ e Å^{-3}
2148 reflections	$\Delta\rho_{min} = -0.31$ e Å^{-3}
132 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0014 (2)
Secondary atom site location: difference Fourier map	

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}
Cd1	0.523335 (14)	0.11166 (2)	0.744199 (12)	0.02328 (7)
Cl1	0.40439 (5)	−0.13994 (8)	0.60907 (4)	0.02792 (13)
Cl2	0.67267 (5)	−0.16544 (8)	0.83106 (4)	0.02717 (13)
O1	0.57035 (16)	0.4852 (3)	0.64381 (14)	0.0390 (4)
O2	0.64928 (15)	0.1924 (2)	0.65962 (13)	0.0336 (4)
N1	0.66195 (17)	0.7705 (3)	0.55775 (16)	0.0339 (5)
H1A	0.6566	0.7490	0.4940	0.051*
H1B	0.6696	0.8964	0.5705	0.051*
H1C	0.5959	0.7275	0.5670	0.051*
C1	0.6496 (2)	0.3701 (3)	0.64067 (17)	0.0248 (5)
C2	0.7528 (2)	0.4489 (3)	0.61134 (18)	0.0261 (5)
H2A	0.7376	0.4211	0.5404	0.031*
H2B	0.8263	0.3834	0.6508	0.031*
C3	0.76996 (19)	0.6662 (3)	0.62857 (17)	0.0238 (5)
H3	0.7715	0.6913	0.6975	0.029*
C4	0.8836 (2)	0.7527 (3)	0.62093 (17)	0.0243 (5)

C5	0.9706 (2)	0.6450 (3)	0.6001 (2)	0.0315 (5)
H5	0.9576	0.5147	0.5847	0.038*
C6	1.0771 (2)	0.7308 (4)	0.6019 (2)	0.0373 (6)
H6	1.1362	0.6563	0.5903	0.045*
C7	1.0959 (2)	0.9252 (4)	0.62066 (19)	0.0359 (6)
H7	1.1661	0.9831	0.6198	0.043*
C8	1.0096 (2)	1.0326 (4)	0.6407 (2)	0.0355 (6)
H8	1.0217	1.1640	0.6533	0.043*
C9	0.9049 (2)	0.9479 (4)	0.64233 (19)	0.0318 (5)
H9	0.8483	1.0219	0.6578	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02816 (10)	0.01635 (9)	0.02832 (10)	−0.00091 (7)	0.01356 (7)	−0.00123 (6)
Cl1	0.0328 (3)	0.0208 (3)	0.0266 (3)	0.0000 (2)	0.0057 (2)	0.0004 (2)
Cl2	0.0264 (3)	0.0230 (3)	0.0326 (3)	0.0018 (2)	0.0108 (2)	0.0014 (2)
O1	0.0391 (10)	0.0336 (10)	0.0582 (12)	0.0027 (8)	0.0345 (9)	0.0042 (9)
O2	0.0390 (10)	0.0263 (9)	0.0436 (10)	−0.0021 (8)	0.0244 (8)	0.0053 (8)
N1	0.0275 (10)	0.0356 (12)	0.0424 (12)	0.0052 (9)	0.0169 (9)	0.0133 (10)
C1	0.0291 (12)	0.0263 (12)	0.0220 (11)	−0.0050 (10)	0.0127 (9)	−0.0003 (9)
C2	0.0280 (12)	0.0224 (11)	0.0337 (13)	−0.0031 (9)	0.0182 (10)	−0.0014 (10)
C3	0.0250 (11)	0.0238 (11)	0.0255 (11)	0.0017 (9)	0.0127 (9)	0.0026 (9)
C4	0.0251 (11)	0.0251 (12)	0.0246 (11)	−0.0017 (9)	0.0110 (9)	0.0022 (9)
C5	0.0333 (13)	0.0250 (12)	0.0421 (14)	−0.0014 (10)	0.0205 (11)	−0.0035 (11)
C6	0.0284 (13)	0.0446 (16)	0.0444 (15)	0.0016 (12)	0.0195 (11)	−0.0013 (13)
C7	0.0278 (12)	0.0443 (16)	0.0344 (14)	−0.0108 (11)	0.0095 (11)	0.0023 (12)
C8	0.0366 (14)	0.0259 (12)	0.0401 (15)	−0.0078 (11)	0.0081 (11)	−0.0009 (11)
C9	0.0311 (13)	0.0267 (12)	0.0378 (14)	0.0016 (10)	0.0123 (11)	−0.0028 (11)

Geometric parameters (Å, °)

Cd1—O2	2.2807 (17)	C2—C3	1.529 (3)
Cd1—O1^{i}	2.3888 (18)	C2—H2A	0.9700
Cd1—Cl1^{ii}	2.5965 (8)	C2—H2B	0.9700
Cd1—Cl1	2.6072 (8)	C3—C4	1.515 (3)
Cd1—Cl2	2.6141 (8)	C3—H3	0.9800
Cd1—Cl2^{ii}	2.6880 (8)	C4—C5	1.386 (3)
Cl1—Cd1^{i}	2.5965 (8)	C4—C9	1.391 (3)
Cl2—Cd1^{i}	2.6880 (8)	C5—C6	1.391 (3)
O1—C1	1.246 (3)	C5—H5	0.9300
O1—Cd1^{ii}	2.3888 (18)	C6—C7	1.377 (4)
O2—C1	1.261 (3)	C6—H6	0.9300
N1—C3	1.509 (3)	C7—C8	1.373 (4)
N1—H1A	0.8900	C7—H7	0.9300
N1—H1B	0.8900	C8—C9	1.383 (3)
N1—H1C	0.8900	C8—H8	0.9300

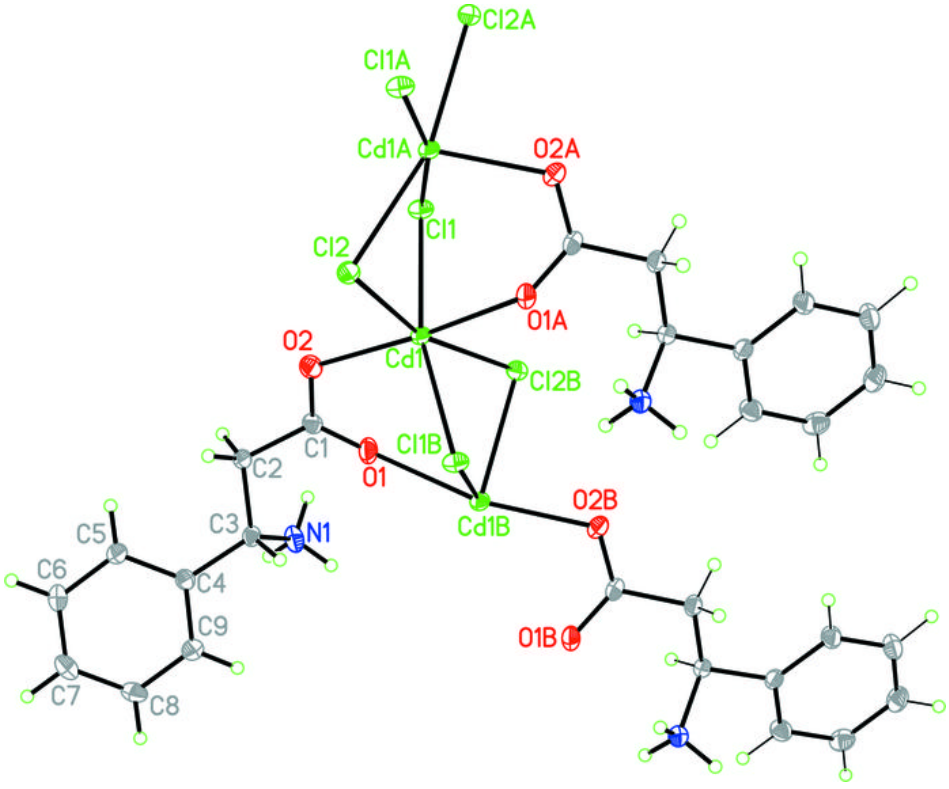
C1—C2	1.524 (3)	C9—H9	0.9300
O2—Cd1—O1^{i}	166.93 (6)	C1—C2—H2A	109.0
O2—Cd1—Cl1^{ii}	98.98 (5)	C3—C2—H2A	109.0
O1^{i}—Cd1—Cl1^{ii}	79.65 (5)	C1—C2—H2B	109.0
O2—Cd1—Cl1	94.10 (5)	C3—C2—H2B	109.0
O1^{i}—Cd1—Cl1	88.67 (5)	H2A—C2—H2B	107.8
Cl1^{ii}—Cd1—Cl1	166.089 (9)	N1—C3—C4	109.76 (18)
O2—Cd1—Cl2	87.88 (5)	N1—C3—C2	109.37 (19)
O1^{i}—Cd1—Cl2	79.47 (5)	C4—C3—C2	116.91 (19)
Cl1^{ii}—Cd1—Cl2	97.59 (3)	N1—C3—H3	106.8
Cl1—Cd1—Cl2	87.56 (3)	C4—C3—H3	106.8
O2—Cd1—Cl2^{ii}	106.76 (5)	C2—C3—H3	106.8
O1^{i}—Cd1—Cl2^{ii}	86.18 (5)	C5—C4—C9	118.5 (2)
Cl1^{ii}—Cd1—Cl2^{ii}	86.24 (3)	C5—C4—C3	123.3 (2)
Cl1—Cd1—Cl2^{ii}	85.47 (3)	C9—C4—C3	118.0 (2)
Cl2—Cd1—Cl2^{ii}	164.176 (16)	C4—C5—C6	120.4 (2)
Cd1^{i}—Cl1—Cd1	85.28 (3)	C4—C5—H5	119.8
Cd1—Cl2—Cd1^{i}	83.32 (3)	C6—C5—H5	119.8
C1—O1—Cd1^{ii}	142.04 (16)	C7—C6—C5	120.5 (2)
C1—O2—Cd1	113.60 (14)	C7—C6—H6	119.7
C3—N1—H1A	109.5	C5—C6—H6	119.7
C3—N1—H1B	109.5	C8—C7—C6	119.2 (2)
H1A—N1—H1B	109.5	C8—C7—H7	120.4
C3—N1—H1C	109.5	C6—C7—H7	120.4
H1A—N1—H1C	109.5	C7—C8—C9	120.8 (2)
H1B—N1—H1C	109.5	C7—C8—H8	119.6
O1—C1—O2	124.1 (2)	C9—C8—H8	119.6
O1—C1—C2	117.9 (2)	C8—C9—C4	120.5 (2)
O2—C1—C2	118.0 (2)	C8—C9—H9	119.8
C1—C2—C3	112.72 (19)	C4—C9—H9	119.8

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) −*x*+1, *y*+1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1C···O1	0.89	2.08	2.735 (3)	130

Fig. 1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Cl1A
Cd1A
O2A
Cl1
Cl2
O1A
O2
Cd1
Cl2B
C1
Cl1B
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C7
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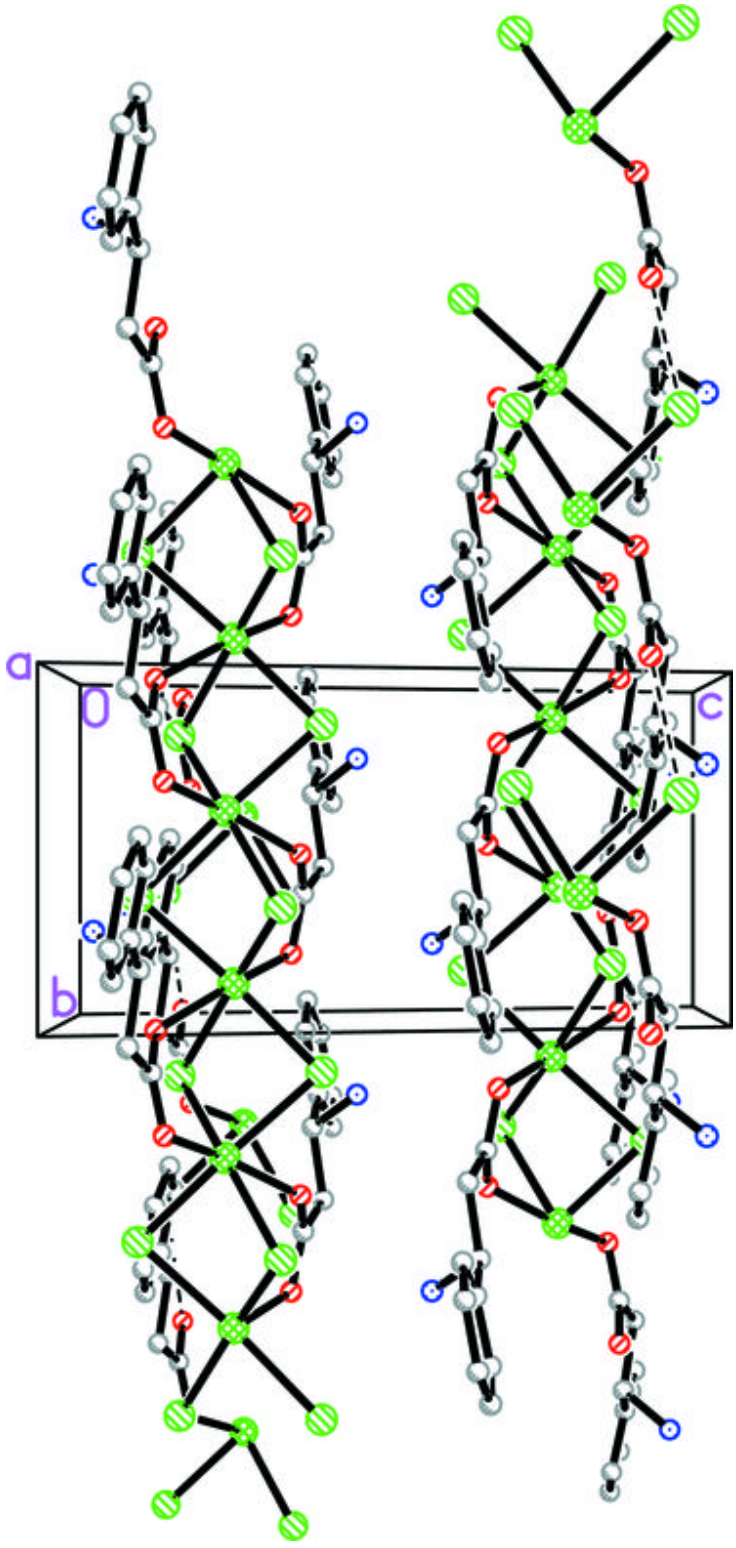
Fig. 2