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catena-Poly[μ-aqua-2:1′κ^2*O*:*O*-aqua-2κ*O*-(2-fluorobenzoato-1κ^2*O*,*O*′)(μ_2-2-fluorobenzoato-2′:1κ^2*O*:*O*′)bis(μ_3-2-fluorobenzoato)-2′:1:2κ^4*O*:*O*,*O*′:*O*′;-1:2:1′κ^5*F*,*O*:*O*,*O*′:*O*′-dilead(II)]

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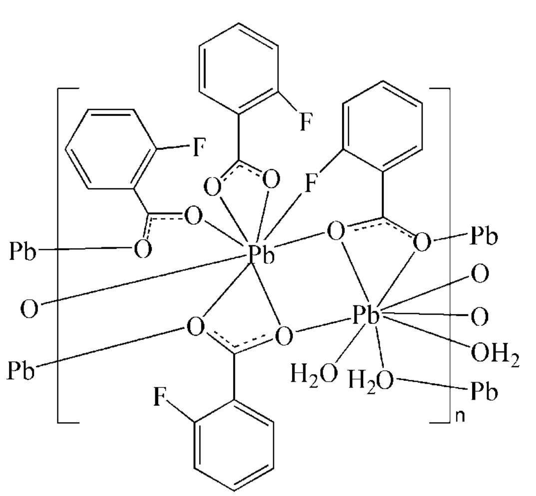
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.017 Å; R factor = 0.038; wR factor = 0.094; data-to-parameter ratio = 16.7.

In the title compound, $[Pb_2(C_7H_4FO_2)_4(H_2O)_2]_n$, one Pb^{II} atom is coordinated by seven O atoms and one F atom from five 2-fluorobenzoate ligands, and the other Pb^{II} atom is coordinated by five O atoms from four 2-fluorobenzoate ligands and three water molecules, resulting in distorted PbO_7F and PbO_8 polyhedra. The 2-fluorobenzoate ligands bridge Pb atoms, giving rise to a one-dimensional chain structure extending along the [100] direction. The polymeric chains are connected *via* C—H$\cdots$O hydrogen bonds and π–π interactions, with an interplanar distance of 3.46 (1) Å. An intramolecular O—H$\cdots$F interaction is also present.

Related literature

For related literature, see: Morsali & Mahjoub (2005); Xiao & Morsali (2007); Zhang (2004, 2005, 2006*a*,*b*,*c*); Zhang *et al.* (2005); Zhu *et al.* (1999).



Experimental

Crystal data

$[Pb_2(C_7H_4FO_2)_4(H_2O)_2]$
M_r = 1006.84
Triclinic, $P\overline{1}$
a = 7.1016 (14) Å
b = 14.794 (3) Å
c = 15.096 (3) Å
α = 111.56 (3)°
β = 95.32 (3)°
γ = 97.31 (3)°
V = 1446.2 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.71 mm^{-1}
T = 290 (2) K
0.44 × 0.19 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) T_{min} = 0.082, T_{max} = 0.223
14182 measured reflections
6646 independent reflections
5329 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.03
6646 reflections
397 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.74 e Å^{-3}
$\Delta\rho_{min}$ = −2.48 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pb1—O4	2.480 (6)	Pb2—O2	2.517 (5)
Pb1—O2	2.489 (5)	Pb2—O7	2.534 (6)
Pb1—O1	2.551 (6)	Pb2—O5	2.592 (6)
Pb1—O8	2.574 (5)	Pb2—O10	2.599 (6)
Pb1—O9	2.621 (6)	Pb2—O8	2.603 (5)
Pb1—O3	2.642 (6)	Pb2—O9^{ii}	2.670 (6)
Pb1—O6^{i}	2.766 (6)	Pb2—O7^{iii}	2.999 (6)
Pb1—F3^{ii}	2.856 (8)	Pb2—O1^{ii}	2.804 (5)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O7—H7$A\cdots$O6^{i}	0.82	2.15	2.881 (8)	148
O7—H7$B\cdots$O5^{iii}	0.82	2.66	3.360 (8)	144
O10—H10$A\cdots$O3^{ii}	0.82	2.07	2.892 (8)	174
O10—H10$B\cdots$O4	0.82	2.22	2.856 (8)	135
O10—H10$B\cdots$F2	0.82	2.44	3.161 (13)	147
C19—H19$\cdots$O3^{iv}	0.93	2.56	3.364 (13)	145

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2143).

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supplementary materials

Acta Cryst. (2008). E**64**, m1055-m1056 [**doi:10.1107/S1600536808022678**]

catena-Poly[μ-aqua-2:1'κ^2*O*:*O*-aqua-2κ*O*-(2-fluorobenzoato-1κ^2*O*,*O*')(μ_2-2-fluorobenzoato-2':1κ^2*O*:*O*')bis(μ_3-2-fluorobenzoato)-2':1:2κ^4*O*:*O*,*O*':*O*';1:2:1'κ^5*F*,*O*:*O*,*O*':*O*'-dilead(II)]

B.-S. Zhang

Comment

We have studied the metal complexes of halogen-substituted benzoic acid (*X*–C_6H_4COOH; *X* = F, Cl, Br and I) (Zhang, 2004, 2005; Zhang *et al.*, 2005; Zhang, 2006*a*,b,c). The related crystal structures can be found, such as $[Pb(phen)_n(NO_2)X]$ (phen = 1,10-phenanthroline; *X* = CH_3COO^-, NCS^- and ClO_4^-) (Morsali & Mahjoub, 2005), $[Pb_3(bpy)(H_2O)_5(sip)_2].0.5bpy.2H_2O$ (sip = 5-sulfoisophthalate; bpy = 2,2'-bipyridine) (Xiao & Morsali, 2007) and $PbI_2(L)$ (*L* = bpy, phen) (Zhu *et al.*, 1999). We report here the synthesis and structure of the title compound, a new one-dimensional Pb^{II} coordination polymer.

In the title compound, the Pb1 atom is coordinated by seven O atoms and one F atom from five 2-fluorobenzoate ligands to complete a significantly distorted PbO_7F polyhedron. The Pb1—O bond lengths are in the range of 2.480 (6) to 2.766 (6) Å and the Pb1—F bond length is 2.856 (8)Å (Table 1). The Pb2 atom is coordinated by five O atoms from four 2-fluorobenzoate ligands and three water molecules to complete a significantly distorted PbO_8 polyhedron. The Pb2—O bond lengths are in the range of 2.517 (5) to 2.999 (6)Å (Table 1). The 2-fluorobenzoate ligands bridge the Pb atoms, giving rise to a one-dimensional chain structure extending along the [100] direction (Fig. 2). There are intrachain O—H···O hydrogen bonds between the coordinated water molecules and the carboxylate O atoms of the 2-fluorobenzoate ligands (Table 2). The polymeric chains are connected *via* C—H···O hydrogen bonds and π–π stacking interactions between the benzene rings, with an interplanar distance of 3.46 (1) Å, into a two-dimensional supramolecular structure (Fig. 3).

Experimental

Freshly prepared $PbCO_3$ (0.140 g, 0.52 mmol), 2-fluorobenzoic acid (0.035 g, 0.25 mmol) in CH_3OH/H_2O (15 ml; 1:2 *v*/*v*) were mixed and stirred for *ca* 2 h. Subsequently, the resulting suspension was heated in a 23 ml Teflon-lined stainless steel autoclave at 423 K for 5 d. After the autoclave was cooled to room temperature, the solid was filtered off. The resulting colorless filtrate was allowed to stand at room temperature for one month, affording colorless block crystals suitable for X-ray analysis.

Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of water molecules were located on a difference Fourier map and fixed with O—H = 0.82Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The highest residual electron density was 0.78Å from atom Pb2 and the deepest hole 0.71Å from atom Pb2.

Figures

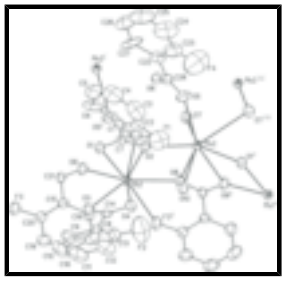

Fig. 1. The asymmetric unit of the title compound, together with symmetry-related atoms to complete the coordination units. Displacement ellipsoids are drawn at the 35% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) 1 - *x*, -*y*, -*z*; (ii) 1 + *x*, *y*, *z*; (iii) 2 - *x*, -*y*, -*z*.]

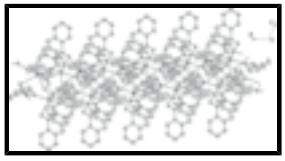

Fig. 2. View of one-dimensional chain structure extending along the [100] direction.

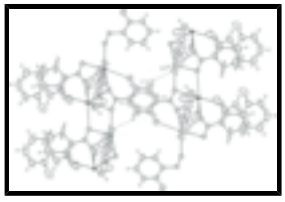

Fig. 3. The C—H···O hydrogen bonds (dashed lines) and the π–π stacking interactions in the title compound. [Symmetry code: (iv) -*x*, -*y*, 1 - *z*.]

catena-Poly[μ-aqua-2:1'κ^{2}O:O-aqua-2κO-(2-fluorobenzoato- 1κ^2*O*,*O*')(μ$_2$-2-fluorobenzoato-2':1κ^2*O*:*O*')bis(μ$_3$-2-fluorobenzoato)- 2':1:2κ^{4}O:O,O':O';1:2:1'κ^{5}F,O:O,O':O'-dilead(II)]

Crystal data

$[Pb_2(C_7H_4FO_2)_4(H_2O)_2]$	$Z = 2$
$M_r = 1006.84$	$F_{000} = 936$
Triclinic, $P\bar{1}$	$D_x = 2.312$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 7.1016$ (14) Å	Cell parameters from 14100 reflections
$b = 14.794$ (3) Å	θ = 3.0–27.5º
$c = 15.096$ (3) Å	μ = 11.71 mm^{-1}
α = 111.56 (3)º	$T = 290$ (2) K
β = 95.32 (3)º	Block, colorless
γ = 97.31 (3)º	0.44 × 0.19 × 0.13 mm
$V = 1446.2$ (6) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	6646 independent reflections
Radiation source: rotating anode	5329 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
Detector resolution: 10 pixels mm^{-1}	$\theta_{max} = 27.5$º

T = 290(2) K

ω scans

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

T_{min} = 0.082, T_{max} = 0.223

14182 measured reflections

θ_{min} = 3.0º

h = −8→9

k = −19→18

l = −19→19

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.038

$wR(F^2)$ = 0.094

S = 1.03

6646 reflections

397 parameters

3 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

$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 11.3431P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 3.74 e Å^{-3}

$\Delta\rho_{min}$ = −2.48 e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pb1	0.50250 (4)	0.06503 (2)	0.265288 (19)	0.02816 (8)
Pb2	0.99101 (4)	0.11234 (2)	0.13887 (2)	0.03456 (9)
F1	0.8986 (13)	0.3238 (6)	0.1926 (7)	0.106 (3)
F2	0.9276 (14)	0.3801 (7)	0.5078 (9)	0.145 (4)
F3	−0.3272 (8)	−0.0400 (6)	0.3676 (5)	0.0707 (19)
F4	1.0244 (18)	0.2764 (11)	−0.0872 (11)	0.180 (6)
O1	0.3833 (7)	0.1887 (4)	0.2019 (4)	0.0382 (12)
O2	0.6657 (7)	0.1535 (4)	0.1739 (4)	0.0343 (12)
O3	0.3924 (8)	0.2018 (4)	0.4107 (4)	0.0424 (13)
O4	0.6947 (8)	0.2189 (4)	0.3891 (4)	0.0417 (13)
O5	0.8814 (9)	0.1620 (5)	−0.0029 (5)	0.0533 (17)
O6	0.5976 (8)	0.0707 (4)	−0.0775 (4)	0.0377 (12)
O7	0.7609 (8)	−0.0319 (4)	0.0120 (4)	0.0425 (13)
H7A	0.6855	−0.0566	0.0382	0.064*
H7B	0.8141	−0.0784	−0.0152	0.064*
O8	0.8336 (8)	0.0170 (5)	0.2355 (4)	0.0442 (14)
O9	0.1307 (8)	0.0018 (5)	0.2258 (4)	0.0427 (14)
O10	1.0501 (8)	0.2362 (5)	0.3173 (4)	0.0490 (15)
H10A	1.1424	0.2256	0.3465	0.073*
H10B	0.9746	0.2651	0.3505	0.073*
C1	0.5762 (13)	0.2909 (6)	0.1437 (6)	0.0391 (18)
C2	0.7517 (15)	0.3433 (7)	0.1545 (8)	0.053 (2)
C3	0.790 (2)	0.4252 (8)	0.1307 (11)	0.086 (4)

H3	0.9146	0.4587	0.1389	0.103*
C4	0.635 (3)	0.4537 (10)	0.0945 (11)	0.097 (5)
H4	0.6530	0.5102	0.0807	0.117*
C5	0.455 (2)	0.4012 (10)	0.0783 (10)	0.082 (4)
H5	0.3580	0.4227	0.0496	0.098*
C6	0.396 (3)	0.3144 (9)	0.1011 (7)	0.105 (6)
H6	0.2716	0.2803	0.0912	0.126*
C7	0.5377 (11)	0.2061 (6)	0.1744 (5)	0.0306 (15)
C8	0.5995 (12)	0.3522 (6)	0.5128 (6)	0.0380 (17)
C9	0.4447 (16)	0.3912 (8)	0.5579 (7)	0.056 (2)
H9	0.3217	0.3540	0.5411	0.067*
C10	0.482 (2)	0.4869 (8)	0.6279 (8)	0.074 (4)
H10	0.3817	0.5141	0.6570	0.089*
C11	0.660 (2)	0.5406 (8)	0.6543 (9)	0.077 (4)
H11	0.6803	0.6037	0.7021	0.093*
C12	0.814 (2)	0.5043 (8)	0.6121 (8)	0.075 (4)
H12	0.9369	0.5418	0.6296	0.090*
C13	0.7761 (15)	0.4092 (8)	0.5425 (8)	0.058 (2)
C14	0.5595 (11)	0.2510 (6)	0.4324 (5)	0.0328 (16)
C15	−0.0168 (12)	−0.0643 (6)	0.3273 (6)	0.0349 (16)
C16	0.1421 (14)	−0.1041 (7)	0.3439 (8)	0.054 (2)
H16	0.2446	−0.0985	0.3111	0.064*
C17	0.1563 (18)	−0.1518 (9)	0.4069 (9)	0.073 (3)
H17	0.2674	−0.1756	0.4181	0.087*
C18	0.0000 (17)	−0.1632 (8)	0.4532 (8)	0.065 (3)
H18	0.0045	−0.1968	0.4945	0.078*
C19	−0.1581 (15)	−0.1259 (8)	0.4385 (7)	0.057 (3)
H19	−0.2618	−0.1333	0.4701	0.068*
C20	−0.1660 (12)	−0.0773 (7)	0.3773 (6)	0.0426 (19)
C21	−0.0202 (10)	−0.0121 (5)	0.2587 (5)	0.0292 (15)
C22	0.7003 (14)	0.2145 (6)	−0.1082 (6)	0.046 (2)
C23	0.849 (2)	0.2749 (9)	−0.1202 (9)	0.072 (3)
C24	0.828 (3)	0.3368 (10)	−0.1663 (12)	0.108 (6)
H24	0.9346	0.3763	−0.1729	0.129*
C25	0.650 (3)	0.3397 (10)	−0.2026 (11)	0.113 (7)
H25	0.6327	0.3816	−0.2348	0.136*
C26	0.491 (2)	0.2812 (9)	−0.1926 (9)	0.088 (4)
H26	0.3698	0.2864	−0.2180	0.105*
C27	0.501 (3)	0.2134 (9)	−0.1455 (8)	0.101 (6)
H27	0.3952	0.1736	−0.1392	0.121*
C28	0.7316 (12)	0.1442 (6)	−0.0584 (6)	0.0389 (18)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.02153 (14)	0.03441 (15)	0.03085 (15)	0.00615 (10)	0.00427 (10)	0.01469 (12)
Pb2	0.02253 (14)	0.05183 (19)	0.03065 (16)	0.00657 (12)	0.00338 (11)	0.01749 (14)
F1	0.098 (6)	0.095 (6)	0.116 (7)	−0.014 (5)	0.001 (5)	0.045 (5)

F2	0.087 (6)	0.111 (7)	0.172 (10)	−0.004 (5)	0.023 (7)	−0.014 (7)
F3	0.039 (3)	0.129 (6)	0.083 (4)	0.034 (3)	0.027 (3)	0.075 (4)
F4	0.120 (9)	0.226 (14)	0.235 (15)	−0.030 (9)	0.001 (10)	0.162 (13)
O1	0.025 (3)	0.051 (3)	0.044 (3)	0.008 (2)	0.009 (2)	0.023 (3)
O2	0.028 (3)	0.042 (3)	0.042 (3)	0.011 (2)	0.011 (2)	0.024 (3)
O3	0.031 (3)	0.049 (3)	0.038 (3)	0.002 (3)	0.006 (2)	0.008 (3)
O4	0.031 (3)	0.046 (3)	0.037 (3)	0.006 (2)	0.007 (2)	0.003 (3)
O5	0.042 (4)	0.074 (4)	0.047 (4)	−0.009 (3)	−0.009 (3)	0.037 (3)
O6	0.031 (3)	0.041 (3)	0.040 (3)	0.000 (2)	0.003 (2)	0.018 (3)
O7	0.036 (3)	0.041 (3)	0.046 (3)	0.006 (3)	0.008 (3)	0.013 (3)
O8	0.026 (3)	0.071 (4)	0.055 (4)	0.019 (3)	0.015 (3)	0.041 (3)
O9	0.028 (3)	0.055 (4)	0.055 (4)	0.010 (3)	0.011 (3)	0.031 (3)
O10	0.033 (3)	0.064 (4)	0.043 (3)	0.011 (3)	0.005 (3)	0.013 (3)
C1	0.053 (5)	0.034 (4)	0.036 (4)	0.019 (4)	0.018 (4)	0.014 (3)
C2	0.052 (6)	0.049 (5)	0.055 (6)	0.005 (4)	0.004 (5)	0.018 (5)
C3	0.111 (11)	0.047 (6)	0.111 (11)	0.003 (7)	0.049 (9)	0.039 (7)
C4	0.162 (16)	0.062 (8)	0.105 (11)	0.047 (10)	0.049 (11)	0.059 (8)
C5	0.125 (12)	0.069 (8)	0.077 (9)	0.052 (8)	0.024 (8)	0.044 (7)
C6	0.240 (19)	0.079 (8)	0.039 (6)	0.116 (11)	0.046 (8)	0.039 (6)
C7	0.031 (4)	0.038 (4)	0.022 (3)	0.006 (3)	0.004 (3)	0.010 (3)
C8	0.044 (5)	0.043 (4)	0.028 (4)	0.011 (4)	0.004 (3)	0.014 (3)
C9	0.063 (6)	0.059 (6)	0.045 (5)	0.016 (5)	0.016 (5)	0.014 (5)
C10	0.109 (10)	0.053 (6)	0.057 (7)	0.034 (7)	0.035 (7)	0.005 (5)
C11	0.126 (12)	0.041 (6)	0.053 (7)	0.011 (7)	0.020 (7)	0.004 (5)
C12	0.092 (9)	0.049 (6)	0.053 (7)	−0.018 (6)	0.006 (6)	−0.004 (5)
C13	0.054 (6)	0.063 (6)	0.055 (6)	0.014 (5)	0.016 (5)	0.018 (5)
C14	0.034 (4)	0.039 (4)	0.022 (3)	0.004 (3)	0.000 (3)	0.010 (3)
C15	0.039 (4)	0.038 (4)	0.030 (4)	0.010 (3)	0.003 (3)	0.015 (3)
C16	0.047 (5)	0.065 (6)	0.066 (6)	0.023 (5)	0.017 (5)	0.039 (5)
C17	0.074 (8)	0.090 (9)	0.083 (8)	0.038 (7)	0.009 (6)	0.059 (7)
C18	0.071 (7)	0.077 (7)	0.066 (7)	0.016 (6)	0.007 (6)	0.051 (6)
C19	0.054 (6)	0.074 (7)	0.054 (6)	0.004 (5)	0.007 (5)	0.039 (5)
C20	0.036 (4)	0.056 (5)	0.042 (5)	0.010 (4)	0.006 (4)	0.025 (4)
C21	0.025 (4)	0.031 (4)	0.034 (4)	0.005 (3)	0.006 (3)	0.015 (3)
C22	0.062 (6)	0.035 (4)	0.038 (5)	−0.005 (4)	0.006 (4)	0.015 (4)
C23	0.078 (9)	0.070 (7)	0.069 (8)	−0.010 (6)	−0.001 (6)	0.037 (6)
C24	0.141 (15)	0.075 (9)	0.111 (12)	−0.036 (9)	−0.004 (11)	0.065 (9)
C25	0.21 (2)	0.060 (8)	0.079 (10)	0.023 (11)	−0.002 (12)	0.043 (8)
C26	0.138 (13)	0.053 (7)	0.068 (8)	0.037 (8)	−0.017 (8)	0.019 (6)
C27	0.191 (15)	0.058 (7)	0.041 (6)	0.079 (9)	−0.037 (7)	0.000 (5)
C28	0.040 (4)	0.047 (5)	0.034 (4)	0.006 (4)	0.005 (3)	0.021 (4)

Geometric parameters (Å, °)

Pb1—O4	2.480 (6)	C4—C5	1.36 (2)
Pb1—O2	2.489 (5)	C4—H4	0.9300
Pb1—O1	2.551 (6)	C5—C6	1.469 (18)
Pb1—O8	2.574 (5)	C5—H5	0.9300
Pb1—O9	2.621 (6)	C6—H6	0.9300

Pb1—O3	2.642 (6)	C8—C13	1.354 (13)
Pb1—O6^{i}	2.766 (6)	C8—C9	1.420 (12)
Pb1—F3^{ii}	2.856 (8)	C8—C14	1.513 (11)
Pb2—O2	2.517 (5)	C9—C10	1.394 (14)
Pb2—O7	2.534 (6)	C9—H9	0.9300
Pb2—O5	2.592 (6)	C10—C11	1.344 (18)
Pb2—O10	2.599 (6)	C10—H10	0.9300
Pb2—O8	2.603 (5)	C11—C12	1.385 (18)
Pb2—O9^{ii}	2.670 (6)	C11—H11	0.9300
Pb2—O7^{iii}	2.999 (6)	C12—C13	1.386 (14)
Pb2—O1^{ii}	2.804 (5)	C12—H12	0.9300
F1—C2	1.261 (13)	C15—C16	1.381 (12)
F2—C13	1.294 (13)	C15—C20	1.389 (11)
F3—C20	1.351 (10)	C15—C21	1.502 (10)
F4—C23	1.290 (17)	C16—C17	1.381 (13)
O1—C7	1.239 (9)	C16—H16	0.9300
O2—C7	1.269 (9)	C17—C18	1.390 (16)
O3—C14	1.256 (9)	C17—H17	0.9300
O4—C14	1.256 (9)	C18—C19	1.347 (15)
O5—C28	1.227 (10)	C18—H18	0.9300
O6—C28	1.276 (10)	C19—C20	1.366 (12)
O7—H7A	0.8200	C19—H19	0.9300
O7—H7B	0.8200	C21—O8^{iv}	1.243 (9)
O8—C21^{ii}	1.243 (9)	C22—C23	1.366 (14)
O9—C21	1.247 (9)	C22—C27	1.467 (17)
O9—Pb2^{iv}	2.670 (6)	C22—C28	1.517 (11)
O10—H10A	0.8200	C23—C24	1.353 (17)
O10—H10B	0.8200	C24—C25	1.35 (2)
C1—C2	1.344 (13)	C24—H24	0.9300
C1—C7	1.491 (10)	C25—C26	1.39 (2)
C1—C6	1.515 (17)	C25—H25	0.9300
C2—C3	1.386 (14)	C26—C27	1.433 (16)
C3—C4	1.37 (2)	C26—H26	0.9300
C3—H3	0.9300	C27—H27	0.9300
O4—Pb1—O2	74.52 (19)	C1—C2—C3	125.1 (11)
O4—Pb1—O1	81.3 (2)	C4—C3—C2	116.2 (13)
O2—Pb1—O1	51.13 (16)	C4—C3—H3	121.9
O4—Pb1—O8	83.7 (2)	C2—C3—H3	121.9
O2—Pb1—O8	68.63 (17)	C5—C4—C3	121.3 (11)
O1—Pb1—O8	119.76 (17)	C5—C4—H4	119.3
O4—Pb1—O9	130.77 (18)	C3—C4—H4	119.3
O2—Pb1—O9	120.83 (18)	C4—C5—C6	127.4 (13)
O1—Pb1—O9	77.90 (17)	C4—C5—H5	116.3
O8—Pb1—O9	145.0 (2)	C6—C5—H5	116.3
O4—Pb1—O3	50.68 (17)	C5—C6—C1	107.1 (14)
O2—Pb1—O3	106.06 (18)	C5—C6—H6	126.4
O1—Pb1—O3	72.71 (19)	C1—C6—H6	126.4

O8—Pb1—O3	131.93 (19)	O1—C7—O2	120.4 (7)
O9—Pb1—O3	80.51 (19)	O1—C7—C1	120.1 (7)
O6^{i}—Pb1—F3^{ii}	104.7 (2)	O2—C7—C1	119.6 (6)
O1—Pb1—O6^{i}	85.90 (18)	C13—C8—C9	117.9 (9)
O2—Pb1—O6^{i}	77.99 (18)	C13—C8—C14	123.1 (8)
O9—Pb1—O6^{i}	69.51 (17)	C9—C8—C14	119.0 (8)
O8—Pb1—O6^{i}	81.25 (18)	C10—C9—C8	118.2 (11)
O3—Pb1—O6^{i}	146.29 (17)	C10—C9—H9	120.9
O4—Pb1—O6^{i}	151.93 (18)	C8—C9—H9	120.9
O4—Pb1—F3^{ii}	87.65 (20)	C11—C10—C9	121.4 (11)
O1—Pb1—F3^{ii}	168.83 (21)	C11—C10—H10	119.3
O3—Pb1—F3^{ii}	99.11 (19)	C9—C10—H10	119.3
O9—Pb1—F3^{ii}	108.72 (18)	C10—C11—C12	121.7 (10)
O2—Pb1—F3^{ii}	126.98 (22)	C10—C11—H11	119.2
O8—Pb1—F3^{ii}	59.89 (19)	C12—C11—H11	119.2
O2—Pb2—O7	76.62 (18)	C11—C12—C13	116.6 (11)
O2—Pb2—O5	78.46 (19)	C11—C12—H12	121.7
O7—Pb2—O5	71.2 (2)	C13—C12—H12	121.7
O2—Pb2—O10	75.17 (18)	F2—C13—C8	123.0 (10)
O7—Pb2—O10	144.72 (19)	F2—C13—C12	112.9 (11)
O5—Pb2—O10	122.4 (2)	C8—C13—C12	124.1 (10)
O2—Pb2—O8	67.75 (17)	O4—C14—O3	122.0 (7)
O7—Pb2—O8	75.8 (2)	O4—C14—C8	118.9 (7)
O5—Pb2—O8	137.09 (18)	O3—C14—C8	119.1 (7)
O10—Pb2—O8	74.2 (2)	C16—C15—C20	115.2 (7)
O2—Pb2—O9^{ii}	115.50 (16)	C16—C15—C21	120.1 (7)
O7—Pb2—O9^{ii}	93.94 (19)	C20—C15—C21	124.7 (7)
O5—Pb2—O9^{ii}	157.3 (2)	C17—C16—C15	123.2 (9)
O10—Pb2—O9^{ii}	79.6 (2)	C17—C16—H16	118.4
O8—Pb2—O9^{ii}	48.39 (16)	C15—C16—H16	118.4
O2—Pb2—O1^{ii}	141.13 (16)	C16—C17—C18	118.2 (10)
O5—Pb2—O1^{ii}	108.21 (19)	C16—C17—H17	120.9
O7—Pb2—O1^{ii}	142.21 (17)	C18—C17—H17	120.9
O8—Pb2—O1^{ii}	114.69 (18)	C19—C18—C17	120.3 (9)
O9—Pb2—O1^{ii}	150.98 (13)	C19—C18—H18	119.8
O10—Pb2—O1^{ii}	69.09 (17)	C17—C18—H18	119.8
O7^{iii}—Pb2—O1^{ii}	66.45 (15)	C18—C19—C20	120.0 (10)
O2—Pb2—O7^{iii}	146.84 (16)	C18—C19—H19	120.0
O5—Pb2—O7^{iii}	73.48 (19)	C20—C19—H19	120.0
O7—Pb2—O7^{iii}	77.86 (17)	F3—C20—C19	116.8 (8)
O8—Pb2—O7^{iii}	125.04 (17)	F3—C20—C15	120.2 (7)
O9—Pb2—O7^{iii}	138.80 (13)	C19—C20—C15	123.0 (8)
O10—Pb2—O7^{iii}	135.54 (17)	O8^{iv}—C21—O9	120.6 (7)

C7—O1—Pb1	92.7 (5)	O8^{iv}—C21—C15	121.9 (6)
C7—O2—Pb1	94.9 (4)	O9—C21—C15	117.5 (7)
C7—O2—Pb2	150.1 (5)	C23—C22—C27	121.0 (11)
Pb1—O2—Pb2	114.7 (2)	C23—C22—C28	122.1 (10)
C14—O3—Pb1	89.7 (4)	C27—C22—C28	116.9 (9)
C14—O4—Pb1	97.4 (5)	F4—C23—C24	114.8 (13)
C28—O5—Pb2	135.0 (5)	F4—C23—C22	121.2 (11)
Pb2—O7—H7A	109.5	C24—C23—C22	124.0 (14)
Pb2—O7—H7B	112.5	C25—C24—C23	118.3 (14)
H7A—O7—H7B	101.3	C25—C24—H24	120.8
C21—O8—Pb1^{ii}	171.78 (14)	C23—C24—H24	120.8
C21—O8—Pb2^{ii}	169.90 (14)	C24—C25—C26	121.1 (12)
Pb1—O8—Pb2	109.0 (2)	C24—C25—H25	119.4
C21—O9—Pb1	146.2 (5)	C26—C25—H25	119.4
C21^{iv}—O9—Pb2	161.84 (13)	C25—C26—C27	123.8 (15)
Pb1^{iv}—O9—Pb2	152.03 (16)	C25—C26—H26	118.1
Pb2—O10—H10A	109.5	C27—C26—H26	118.1
Pb2—O10—H10B	129.8	C26—C27—C22	111.7 (15)
H10A—O10—H10B	115.8	C26—C27—H27	124.1
C2—C1—C7	123.9 (8)	C22—C27—H27	124.1
C2—C1—C6	122.7 (10)	O5—C28—O6	125.0 (8)
C7—C1—C6	113.3 (9)	O5—C28—C22	118.3 (8)
F1—C2—C1	121.4 (9)	O6—C28—C22	116.7 (7)
F1—C2—C3	113.4 (11)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7A···O6^{i}	0.82	2.15	2.881 (8)	148
O7—H7B···O5^{iii}	0.82	2.66	3.360 (8)	144
O10—H10A···O3^{ii}	0.82	2.07	2.892 (8)	174
O10—H10B···O4	0.82	2.22	2.856 (8)	135
O10—H10B···F2	0.82	2.44	3.161 (13)	147
C19—H19···O3^{v}	0.93	2.56	3.364 (13)	145

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

Fig. 1

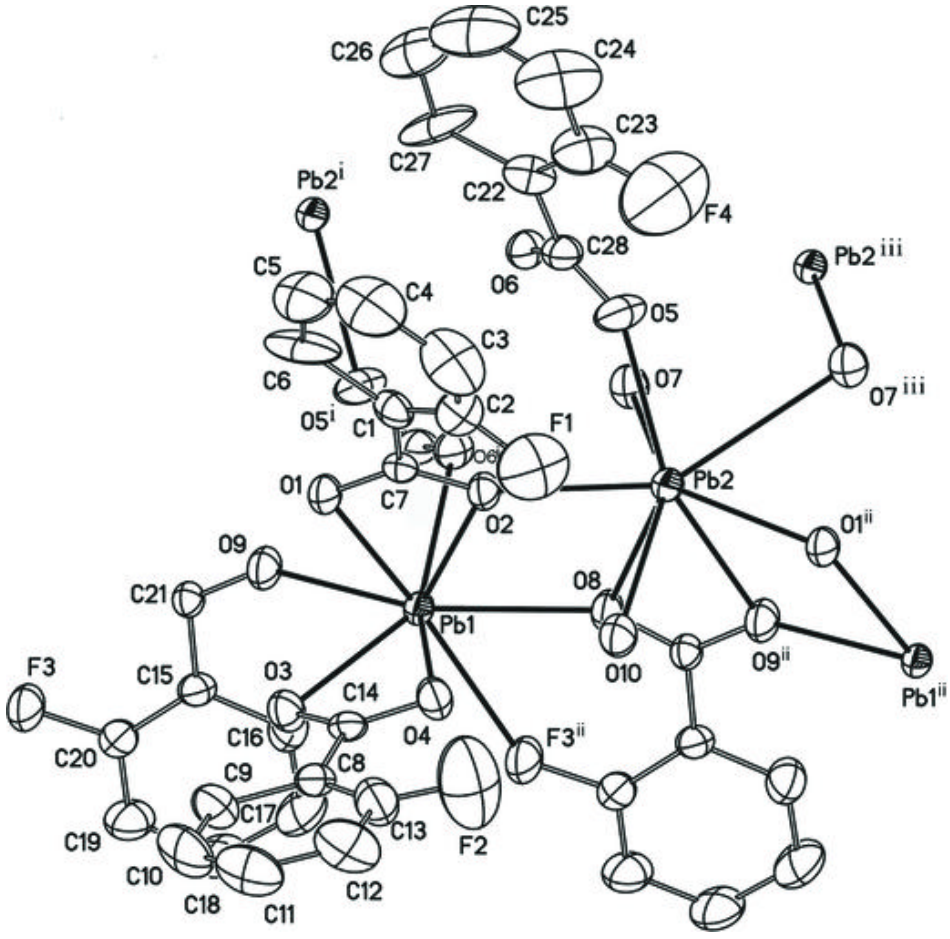
C25
C26
C24
C23
C27
C22
F4
Pb2i
C28
Pb2iii
C5
C4
O6
O5
C3
C6
O7
O7iii
O5i
C1
C2
F1
O6
O1
C7
O2
Pb2
O1ii
O9
C21
O8
Pb1
F3
C15
O3
C14
O10
O9ii
Pb1ii
C16
O4
F3ii
C20
C9
C8
C17
C13
F2
C19
C10
C12
C18
C11

Fig. 2

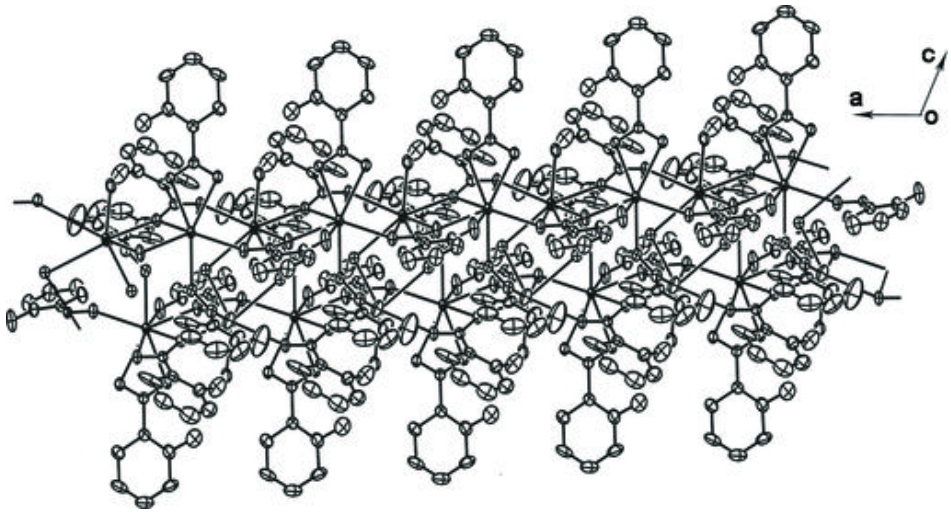

Fig. 3