

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

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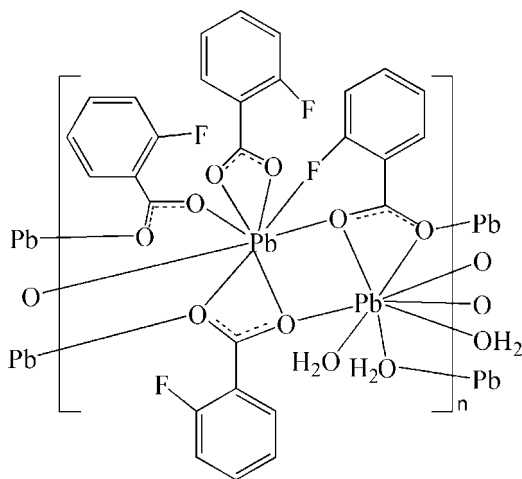
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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.017$ Å; R factor = 0.038; wR factor = 0.094; data-to-parameter ratio = 16.7.

In the title compound, $[\text{Pb}_2(\text{C}_7\text{H}_4\text{FO}_2)_4(\text{H}_2\text{O})_2]_n$, 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* $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and $\pi-\pi$ interactions, with an interplanar distance of 3.46 (1) Å. An intramolecular $\text{O}-\text{H}\cdots\text{F}$ 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

$[\text{Pb}_2(\text{C}_7\text{H}_4\text{FO}_2)_4(\text{H}_2\text{O})_2]$	$\gamma = 97.31$ (3) $^\circ$
$M_r = 1006.84$	$V = 1446.2$ (6) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.1016$ (14) Å	Mo $K\alpha$ radiation
$b = 14.794$ (3) Å	$\mu = 11.71$ mm ⁻¹
$c = 15.096$ (3) Å	$T = 290$ (2) K
$\alpha = 111.56$ (3) $^\circ$	$0.44 \times 0.19 \times 0.13$ mm
$\beta = 95.32$ (3) $^\circ$	

Data collection

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

Refinement

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

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, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O7—H7A \cdots O6 ⁱ	0.82	2.15	2.881 (8)	148
O7—H7B \cdots O5 ⁱⁱⁱ	0.82	2.66	3.360 (8)	144
O10—H10A \cdots O3 ⁱⁱ	0.82	2.07	2.892 (8)	174
O10—H10B \cdots O4	0.82	2.22	2.856 (8)	135
O10—H10B \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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supporting information

Acta Cryst. (2008). E64, m1055–m1056 [doi:10.1107/S1600536808022678]

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

Bi-Song Zhang

S1. Comment

We have studied the metal complexes of halogen-substituted benzoic acid (X -C₆H₄COOH; X = F, Cl, Br and I) (Zhang, 2004, 2005; Zhang *et al.*, 2005; Zhang, 2006a,b,c). The related crystal structures can be found, such as [Pb(phen)_n(NO₂)_nX] (phen = 1,10-phenanthroline; X = CH₃COO⁻, NCS⁻ and ClO₄⁻) (Morsali & Mahjoub, 2005), [Pb₃(bpy)(H₂O)₅(sip)₂].0.5bpy.2H₂O (sip = 5-sulfoisophthalate; bpy = 2,2'-bipyridine) (Xiao & Morsali, 2007) and PbI₂(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 PbO₇F 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 PbO₈ 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 \cdots 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 \cdots 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).

S2. Experimental

Freshly prepared PbCO₃ (0.140 g, 0.52 mmol), 2-fluorobenzoic acid (0.035 g, 0.25 mmol) in CH₃OH/H₂O (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.

S3. Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of water molecules were located on a difference Fourier map and fixed with O—H = 0.82 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The highest residual electron density was 0.78 Å⁻³ from atom Pb2 and the deepest hole 0.71 Å⁻³ from atom Pb2.

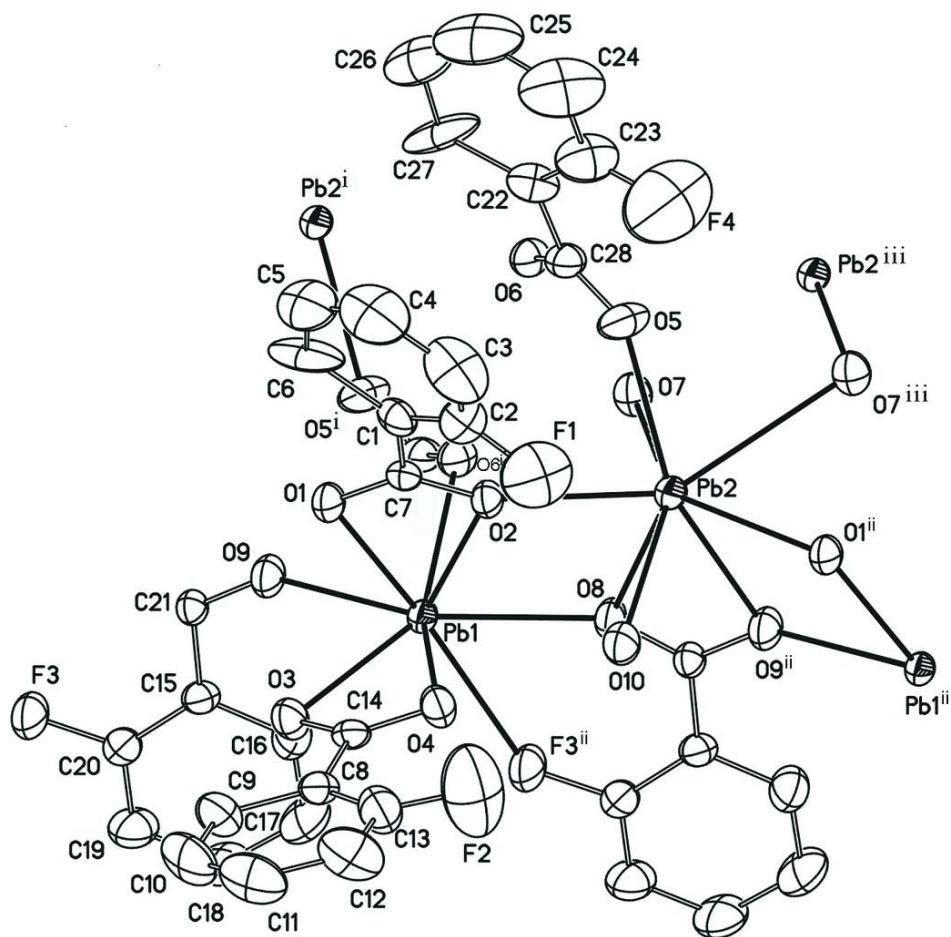
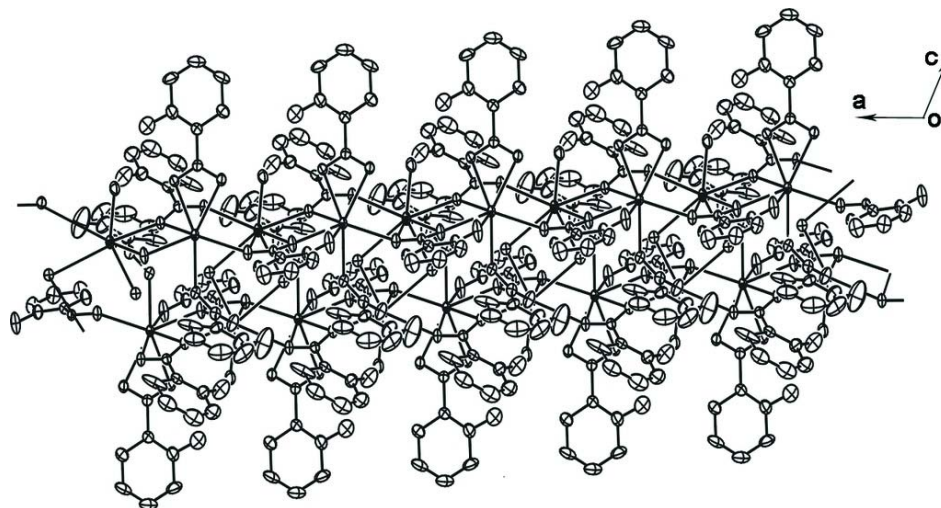


Figure 1

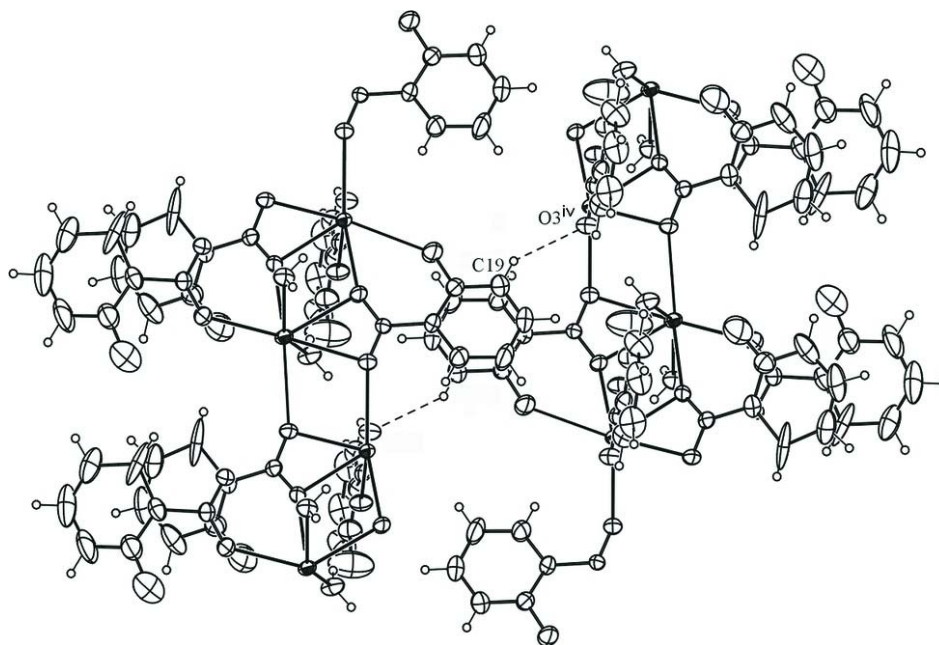
The asymmetric unit of the title compound, together with symmetry-related atoms to complete the coordination units.

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) $2 - x, -y, -z$.]


Figure 2

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


Figure 3

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

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Crystal data

[Pb₂(C₇H₄FO₂)₄(H₂O)₂]

$M_r = 1006.84$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.1016 (14) \text{ \AA}$

$b = 14.794 (3) \text{ \AA}$

$c = 15.096 (3) \text{ \AA}$

$\alpha = 111.56 (3)^\circ$

$\beta = 95.32 (3)^\circ$
 $\gamma = 97.31 (3)^\circ$
 $V = 1446.2 (6) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 936$
 $D_x = 2.312 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 14100 reflections
 $\theta = 3.0\text{--}27.5^\circ$
 $\mu = 11.71 \text{ mm}^{-1}$
 $T = 290 \text{ K}$
 Block, colorless
 $0.44 \times 0.19 \times 0.13 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID
 diffractometer
 Radiation source: rotating anode
 Graphite monochromator
 Detector resolution: $10 \text{ pixels mm}^{-1}$
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.082$, $T_{\max} = 0.223$

14182 measured reflections
 6646 independent reflections
 5329 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.0^\circ$
 $h = -8 \rightarrow 9$
 $k = -19 \rightarrow 18$
 $l = -19 \rightarrow 19$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 3.74 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -2.48 \text{ e \AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^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	87.7 (2)	C11—C10—C9	121.4 (11)
O1—Pb1—F3 ⁱⁱ	168.8 (2)	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	127.0 (2)	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, °)

<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>
O7—H7A \cdots O6 ⁱ	0.82	2.15	2.881 (8)	148
O7—H7B \cdots O5 ⁱⁱⁱ	0.82	2.66	3.360 (8)	144
O10—H10A \cdots O3 ⁱⁱ	0.82	2.07	2.892 (8)	174
O10—H10B \cdots O4	0.82	2.22	2.856 (8)	135
O10—H10B \cdots F2	0.82	2.44	3.161 (13)	147
C19—H19 \cdots O3 ^v	0.93	2.56	3.364 (13)	145

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