Table 3. *Comparison of distances and angles in* $Mo_2O_5^{2+}$ *complexes*

O*t* = terminal oxygen; O*b* = bridging oxygen.

	Mo—O—Mo (°)	Mo—O*b* (Å)	Mo—O*t* (Å)	Reference
$Mo_2O_5(C_2O_4)_2(H_2O)_2$	180	1·876	1·68, 1·70	(*a*)
$[Mo_2O_5(O_2)_4(H_2O)_2]K_2(H_2O)_2$	136·1	1·93	1·66	(*b*)
$Mo_2O_5(DMF)_4Cl_2$	171	1·90	1·68	(*c*)
$Mo_2O_5(phen)_2(NCS)_2$	162·7	1·865, 1·885	1·685, 1·688 1·691, 1·694	(*d*)
$Mo_2O_5(Hnta)_2$*	180	1·88	1·68, 1·71	(*e*)
$Mo_2O_5[(CH_3)_2NCH_2CH_2NHCH_2C(CH_3)_2S]_2$	143·8	1·929, 1·917	1·715, 1·715 1·714, 1·709	(*f*)
$Mo_2O_5(NCS)_2(Me_2SO)_4$	180	1·864	1·691, 1·686	(*g*)
$Mo_2O_5[HB(Me_2pz)_3]_2$	167·1	1·889	1·701, 1·696	(*h*)

References: (*a*) Cotton *et al.* (1964); (*b*) Stomberg (1968); (*c*) Atovmyan, Sokovova & Thachey (1970); (*d*) Viossat & Rodier (1981); (*e*) Knobler, Robinson, Wilkins & Wilson (1983); (*f*) Marabella *et al.* (1983); (*g*) Shibahara, Kuroya, Ooi & Mori (1983); (*h*) this work.

* Hnta = nitrilotriacetate(2−).

an Mo—O—Mo angle of 167·1°. Both the bridging Mo—O distance of 1·889 Å and the terminal Mo—O distances of 1·701 Å and 1·696 Å are within the range of comparable distances found in the other complexes.

The remaining *fac* positions are occupied by coordination through the chemically identical N atoms of the pyrazolylborate ligand, $HB(Me_2pz)_3^-$. Significant differences are found for the Mo—N bond distances. The Mo—N distances for the N atoms *trans* to the terminal oxygens are 2·318 and 2·314 Å, while the Mo—N distance for the N atom *trans* to the bridging oxygen is significantly shorter, at 2·208 Å. These differences in the Mo—N bond distances are similar to the differences found for the binuclear Mo^{II} compound of this trispyrazolylborate ligand, $[HB(Me_2pz)_3Mo(CO)_2]_2S$, which has sulfur as its bridging atom. There the Mo—N distances *trans* to terminal carbonyl groups are 2·247 and 2·260 Å, and the Mo—N *trans* to bridging S is 2·188 Å (Enemark, unpublished results).

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The Structure of the Monobasic Lead Salt of 2,4,6-Trinitro-1,3-benzenediol (β Polymorph), $Pb_2(OH)_2^{2+}.C_6HN_3O_8^{2-}$

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Abstract. $M_r = 691·5$, monoclinic, $P2/c$, $a = 16·606\ (4)$, $b = 16·635\ (8)$, $c = 20·462\ (7)$ Å, $\beta = 127·5\ (14)°$, $U = 4484·4$ Å^3, $Z = 16$, $D_x = 4·10$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 30·24$ mm^{-1}, $F(000) = 4864$, room temperature, final $R = 0·076$ for 4479 reflections. The Pb atoms are clustered into two independent $[Pb_4(OH)_4]^{4+}$ units each with Pb atoms at the vertices of a tetrahedron and

hydroxyl O atoms capping the faces. Pb coordination varies from four to eight. The light atoms are not well defined, but the styphnate ions all show some distortion, with long C—C bonds, short C—O bonds and rotation of the nitro groups.

Introduction. This work is part of a programme of research into the structural properties of primary explosives. The title compound (henceforth β-monobasic lead styphnate) is less electrostatically sensitive than the 'normal' lead styphnates [the structures of which have been reported (Pierce-Butler, 1982*b*, 1984)] and hence finds use in different applications. No crystal structures of basic lead salts of nitrophenols have previously been reported.

Experimental. Some difficulty was experienced in obtaining a suitable single crystal, as synthesis produced very small multiple crystals and the material is almost insoluble. An adequate crystal (approximate dimensions 0·11 × 0·12 × 0·12 mm) was finally selected from material which had grown in β-normal lead styphnate stored under water for about 20 y. Intensity data measured on Hilger and Watts Y290 four-circle automatic diffractometer, niobium-filtered Mo $K\alpha$ radiation, θ–2θ scans, scan rate 0·002° s^{-1}, scan ranges from 0·6 (low θ) to 0·7° (high θ), backgrounds measured on both sides of the peak for half the peak scan time, $2\theta_{\max} = 50°$ ($h = 0\rightarrow19$, $k = 0\rightarrow19$, $l = -24\rightarrow19$), 7419 unique reflections, 4202 considered observed [$I/\sigma(I) > 2$]. Three standard reflections monitored every 50 showed no significant deterioration. Intensities corrected for Lorentz and polarization effects and absorption using method of Alcock (1970) (transmission factors from 0·16 to 0·37). Lattice parameters obtained by least-squares fit to the reflecting angles of 12 reflections ($2\theta > 43°$). Lattice extinctions ($h0l$; $l = 2n + 1$) indicated space group Pc or $P2/c$. Centrosymmetric group chosen on the basis of intensity statistics and this was subsequently confirmed by refinement. The eight independent Pb atoms located by direct methods using *MULTAN* (Germain, Main & Woolfson, 1971), remaining non-hydrogen atoms by successive difference syntheses; least-squares refinement (using F), anisotropic temperature factors for Pb atoms. In final cycle max. Δ/σ 1·9, residual electron density in final difference map within ±3 e Å^{-3}. Reflections contributing to refinement were all observed reflections above $2\theta = 5°$ together with those unobserved reflections with $F_c > F_o$; $w = 1{\cdot}0/(A + DF_o + EF_o^2 + GF_o^H)$adjusted to make average $w\Delta^2$ independent of F_o ($A = 1340{\cdot}0$, $D = -6{\cdot}31$, $E = 0{\cdot}011$, $G = 0{\cdot}00004$, $H = 3$). Final $R = 0{\cdot}076$ (4479 reflections), $wR = 0{\cdot}079$. Atomic scattering factors (metal atoms assumed ionic) and anomalous-dispersion coefficients from *International Tables for X-ray Crystallography* (1974). Calculations performed at Rutherford and Appleton Computer Laboratory using *XRAY74* (Stewart, Kruger, Ammon Dickinson & Hall, 1972).

Discussion. Table 1* lists the atomic coordinates. Fig. 1 shows the four styphnate anions, indicating the atomic numbering scheme and important bond distances and angles. The e.s.d.'s for the light atoms are high and so little significance can be attached to individual values. However, averaged bond lengths and angles* are consistent and follow the trends observed previously in other styphnate ions (Pierce-Butler, 1982*b*, 1984), the distortions being predictable on consideration of the electronic properties of the substituents and their interaction. Thus, on average, C—C bonds are long; C—O bonds are short; internal ring angles at $-NO_2$ positions are large; those at —O positions are small. Least-squares planes were calculated* for the rings, including all six C atoms. There is no significant deviation from planarity [$\Delta_{\max} = 0{\cdot}08\,(5)$ (ring 1); 0·06 (4) (ring 2); 0·05 (3) (ring 3); 0·06 (4) Å (ring 4)], although in each ring one of the —O substituents is bent significantly out of the plane, O(11) by 0·29 (5), O(22) by 0·18 (4), O(31) by 0·19 (3), O(42) by 0·23 (4) Å. The nitro groups are all rotated with respect to the ring planes, this rotation being largest for the $-NO_2$ group *ortho* to both hydroxyl O atoms [61 (4), 80 (5), 59 (6), 55 (4)°, for rings 1 to 4, respectively]. The remaining $-NO_2$ group rotations range from 15 (4) to 33 (5)°.

There are two independent $[Pb_4(OH)_4]^{4+}$ units. In each of these the Pb atoms are found at the vertices of a distorted tetrahedron, with hydroxide O atoms capping the faces (see Fig. 2). All these hydroxide O atoms are 1·0 (4) Å from the plane described by the nearest three Pb atoms. Thus each Pb atom is coordinated to three hydroxide O atoms and each hydroxide O atom is coordinated to three Pb atoms. This situation is very similar to the $[Pb_4(OH)_4]^{4+}$ units described in basic lead perchlorates (Hong & Olin, 1973, 1974).

The Pb atoms are also involved in coordination with the O atoms from the styphnate ions. The coordination number of Pb varies from four to eight. Table 2 lists Pb—O distances less than 3·0 Å. As expected, on consideration of ionic radii, the Pb—O distances involving hydroxides are a little shorter than the others, ranging from 2·29 (3) to 2·65 (4) Å (average 2·41 Å) [*cf.* 2·32 to 2·63 Å from addition of ionic radii (Shannon, 1976), and 2·34 to 2·52 Å found in basic lead azotetrazole (Pierce-Butler, 1982*a*)]. The next-nearest interactions range from 2·53 (4) to 2·77 (6) Å (average 2·64 Å).

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* Lists of structure factors, anisotropic thermal parameters, averaged bond lengths and angles for the styphnate ions and the results of least-squares plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39447 (52 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Positional parameters* (×10⁴ *for* Pb; ×10³ *for other atoms*) *with e.s.d.'s in parentheses and equivalent isotropic* (Pb) *and isotropic temperature factors* (*other atoms*)

	x	*y*	*z*	U_{eq}/U(Å² × 10²)*
Pb(1)	1287 (2)	8597 (1)	502 (1)	3·3 (1)
Pb(2)	4177 (2)	6367 (1)	−89 (1)	3·7 (1)
Pb(3)	4102 (2)	8659 (1)	−494 (1)	3·5 (1)
Pb(4)	904 (1)	6358 (1)	839 (1)	3·2 (1)
Pb(5)	−1147 (1)	7749 (1)	177 (1)	3·3 (1)
Pb(6)	5642 (1)	7410 (1)	−765 (1)	3·3 (1)
Pb(7)	6402 (1)	7578 (1)	1450 (1)	2·8 (1)
Pb(8)	−476 (1)	7400 (1)	−1294 (1)	3·0 (1)
O(1)	45 (2)	163 (2)	48 (2)	2·5 (7)
O(2)	422 (2)	160 (2)	−11 (2)	1·6 (6)
O(3)	122 (2)	268 (2)	504 (2)	2·7 (7)
O(4)	406 (2)	260 (2)	399 (2)	2·6 (7)
O(5)	416 (2)	663 (2)	464 (2)	2·2 (7)
O(6)	71 (2)	329 (2)	39 (2)	2·4 (7)
O(7)	460 (2)	764 (2)	54 (2)	2·2 (6)
O(8)	68 (2)	771 (2)	109 (2)	3·8 (8)
O(11)	445 (2)	127 (2)	342 (2)	3·0 (8)
O(12)	303 (2)	146 (2)	61 (2)	2·5 (7)
O(21)	197 (3)	156 (2)	248 (2)	4·5 (9)
O(22)	79 (2)	130 (2)	406 (2)	2·6 (7)
O(31)	56 (2)	648 (2)	393 (2)	2·2 (6)
O(32)	199 (2)	634 (2)	251 (2)	3·6 (8)
O(41)	302 (3)	626 (2)	47 (2)	4·9 (10)
O(42)	433 (2)	648 (2)	326 (2)	3·5 (8)
O(111)	328 (3)	17 (2)	3 (2)	3·9 (9)
O(112)	309 (3)	−93 (2)	43 (2)	4·6 (10)
O(121)	254 (3)	248 (2)	151 (2)	4·6 (9)
O(122)	413 (3)	258 (3)	249 (3)	7·1 (12)
O(131)	441 (3)	−25 (3)	387 (2)	5·6 (11)
O(132)	453 (2)	−114 (2)	323 (2)	3·4 (8)
O(211)	241 (3)	240 (3)	415 (3)	6·3 (11)
O(212)	97 (5)	266 (4)	300 (4)	10·9 (19)
O(221)	157 (3)	20 (2)	158 (2)	4·0 (9)
O(222)	206 (3)	−84 (2)	235 (2)	3·9 (9)
O(231)	96 (3)	−20 (3)	459 (2)	6·2 (11)
O(232)	47 (3)	−107 (2)	365 (2)	3·7 (8)
O(311)	46 (3)	404 (2)	395 (2)	4·1 (9)
O(312)	69 (3)	506 (2)	466 (2)	4·2 (9)
O(321)	97 (3)	765 (3)	264 (3)	6·8 (12)
O(322)	199 (2)	760 (2)	397 (2)	2·8 (7)
O(331)	170 (3)	484 (2)	185 (2)	4·8 (9)
O(332)	228 (3)	392 (2)	283 (2)	4·9 (10)
O(411)	296 (3)	384 (2)	62 (2)	4·7 (10)
O(412)	331 (3)	478 (2)	12 (2)	4·0 (9)
O(421)	389 (3)	760 (3)	153 (3)	7·7 (12)
O(422)	291 (2)	759 (2)	187 (2)	3·0 (7)
O(431)	425 (3)	510 (2)	391 (2)	4·1 (9)
O(432)	461 (3)	411 (2)	347 (2)	3·8 (8)
N(11)	322 (3)	−21 (3)	48 (3)	3·6 (10)
N(12)	341 (3)	218 (2)	198 (2)	3·3 (9)
N(13)	426 (3)	−48 (3)	322 (2)	3·7 (10)
N(21)	160 (3)	226 (2)	351 (2)	1·5 (7)
N(22)	170 (3)	−17 (2)	218 (2)	2·6 (8)
N(23)	80 (2)	−43 (2)	396 (2)	1·2 (7)
N(31)	66 (3)	477 (2)	411 (2)	3·1 (10)
N(32)	144 (3)	726 (3)	329 (2)	3·1 (10)
N(33)	184 (3)	454 (2)	248 (2)	2·9 (9)
N(41)	319 (3)	455 (3)	60 (3)	3·6 (10)
N(42)	351 (3)	722 (3)	178 (2)	2·9 (10)
N(43)	429 (3)	480 (2)	338 (2)	2·7 (10)
C(11)	342 (3)	23 (2)	121 (2)	2·0 (9)
C(12)	336 (3)	105 (3)	120 (3)	2·6 (10)
C(13)	360 (4)	137 (3)	199 (3)	3·4 (12)
C(14)	404 (4)	89 (3)	272 (3)	3·3 (11)
C(15)	402 (4)	8 (3)	263 (3)	1·9 (11)
C(16)	373 (3)	−31 (3)	186 (3)	2·9 (11)
C(21)	107 (3)	11 (2)	355 (2)	1·8 (9)
C(22)	109 (4)	95 (3)	368 (3)	2·3 (11)
C(23)	145 (3)	137 (3)	329 (2)	1·9 (9)
C(24)	160 (3)	107 (3)	275 (3)	2·5 (9)
C(25)	155 (3)	26 (2)	271 (2)	1·2 (8)
C(26)	130 (3)	−23 (2)	311 (2)	1·6 (8)
C(31)	99 (3)	522 (2)	371 (2)	1·3 (9)
C(32)	93 (2)	610 (2)	368 (2)	0·8 (7)
C(33)	133 (3)	646 (3)	327 (2)	1·9 (9)
C(34)	162 (4)	599 (3)	284 (3)	4·3 (13)
C(35)	154 (3)	514 (3)	291 (3)	2·6 (10)
C(36)	128 (3)	471 (3)	334 (3)	2·0 (9)
C(41)	397 (3)	517 (3)	267 (3)	2·2 (10)
C(42)	395 (3)	610 (2)	263 (2)	1·9 (9)
C(43)	366 (3)	636 (3)	186 (3)	2·0 (10)
C(44)	332 (4)	593 (3)	112 (3)	3·9 (12)
C(45)	347 (4)	507 (3)	129 (3)	2·1 (10)
C(46)	373 (4)	479 (3)	202 (3)	2·5 (11)

* $U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

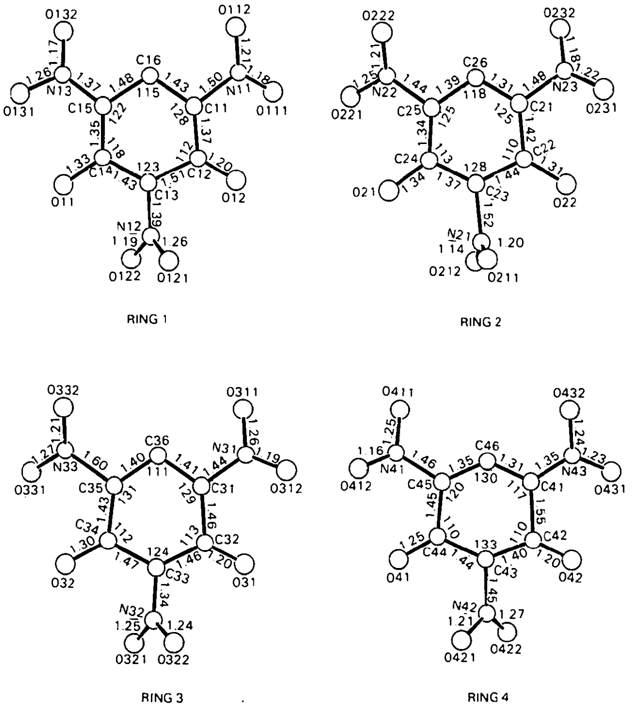

Fig. 1. The four independent styphnate ions, showing the atom numbering scheme and important bond lengths (Å) and angles (°). E.s.d.'s range from 0·05 to 0·10 Å and from 3 to 6°.

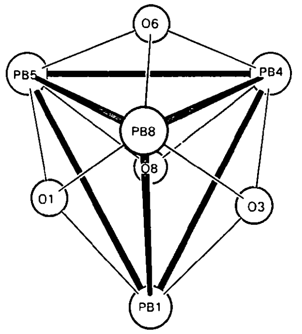

Fig. 2. A $[Pb_4(OH)_4]^{4+}$ unit.

Despite some delocalization of charge onto the ring, the hydroxyl O atoms of the styphnates may be expected to retain some negative charge and thus be most likely to be involved in coordination with lead. This is consistent with the results, as these O atoms in general are closer to the lead than the nitro O atoms.

Table 2. *Metal–metal and metal–oxygen distances* (Å) *with e.s.d.'s in parentheses*

Pb(1)–Pb(4)	3·910 (3)	Pb(2)–Pb(3)	3·887 (4)
Pb(1)–Pb(5)	3·936 (4)	Pb(2)–Pb(6)	3·865 (4)
Pb(1)–Pb(8)	3·598 (3)	Pb(2)–Pb(7)	3·668 (3)
Pb(4)–Pb(5)	3·628 (3)	Pb(3)–Pb(6)	3·591 (4)
Pb(4)–Pb(8)	3·888 (3)	Pb(3)–Pb(7)	3·892 (3)
Pb(5)–Pb(8)	3·836 (4)	Pb(6)–Pb(7)	3·906 (4)
Pb(1)–O(8)	2·48 (5)	Pb(2)–O(7)	2·35 (3)
Pb(1)–O($1^{\rm i}$)	2·33 (6)	Pb(2)–O($4^{\rm ii}$)	2·48 (4)
Pb(1)–O($3^{\rm ii}$)	2·29 (3)	Pb(2)–O($5^{\rm iii}$)	2·36 (4)
Pb(1)–O($22^{\rm ii}$)	2·53 (4)	Pb(2)–O(41)	2·77 (6)
Pb(1)–O(422)	2·96 (6)	Pb(2)–O($42^{\rm iii}$)	2·98 (7)
Pb(3)–O(7)	2·44 (3)	Pb(4)–O(8)	2·38 (4)
Pb(3)–O($2^{\rm iv}$)	2·30 (4)	Pb(4)–O($6^{\rm i}$)	2·37 (6)
Pb(3)–O($4^{\rm ii}$)	2·33 (3)	Pb(4)–O($3^{\rm ii}$)	2·55 (4)
Pb(3)–O($11^{\rm ii}$)	2·61 (5)	Pb(4)–O(32)	2·72 (6)
Pb(5)–O(8)	2·41 (6)	Pb(4)–O($31^{\rm v}$)	2·74 (4)
Pb(5)–O($1^{\rm i}$)	2·47 (5)	Pb(6)–O($2^{\rm iv}$)	2·34 (3)
Pb(5)–O($6^{\rm i}$)	2·43 (4)	Pb(6)–O($4^{\rm ii}$)	2·36 (4)
Pb(5)–O($31^{\rm v}$)	2·56 (3)	Pb(6)–O($5^{\rm iii}$)	2·49 (4)
Pb(5)–O($121^{\rm i}$)	2·77 (7)	Pb(6)–O($11^{\rm ii}$)	2·73 (4)
Pb(5)–O($12^{\rm i}$)	2·82 (5)	Pb(6)–O($12^{\rm iv}$)	2·77 (4)
Pb(5)–O($232^{\rm vi}$)	2·76 (4)	Pb(6)–O($122^{\rm ii}$)	2·85 (7)
Pb(5)–O($322^{\rm v}$)	2·83 (5)	Pb(6)–O($432^{\rm ii}$)	2·91 (4)
Pb(7)–O(7)	2·37 (5)	Pb(8)–O($1^{\rm i}$)	2·30 (4)
Pb(7)–O($2^{\rm iv}$)	2·65 (4)	Pb(8)–O($6^{\rm i}$)	2·39 (4)
Pb(7)–O($5^{\rm iii}$)	2·40 (4)	Pb(8)–O($3^{\rm ii}$)	2·46 (7)
Pb(7)–O($42^{\rm iii}$)	2·46 (4)	Pb(8)–O($21^{\rm i}$)	2·77 (5)
Pb(7)–O($422^{\rm iii}$)	2·88 (4)	Pb(8)–O($29^{\rm ii}$)	2·78 (3)
Pb(7)–O($132^{\rm vii}$)	2·92 (4)	Pb(8)–O($311^{\rm ii}$)	2·73 (4)

Symmetry code: (i) $-x, 1-y, -z$; (ii) $x, 1-y, z-\frac{1}{2}$; (iii) $1-x, y, \frac{1}{2}-z$; (iv) $1-x, 1-y, -z$; (v) $-x, 1-y, -z$; (vi) $-x, 1+y, \frac{1}{2}-z$; (vii) $1-x, 1+y, \frac{1}{2}-z$.

Pb–Pb distances range from 3·591 (4) to 3·936 (4) Å (average 3·80 Å) and are similar to those found in the basic lead perchlorates. Metallic lead has Pb–Pb = 3·50 Å (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1958).

Fig. 3 illustrates the packing arrangement within half a unit cell ($b/2$). The Pb tetrahedra form sheets linked by styphnate ions. Each styphnate ion is linked to two or more Pb clusters. In other styphnate structures studied there has been a tendency for the anions to lie in parallel planes. This is not observed in this compound.

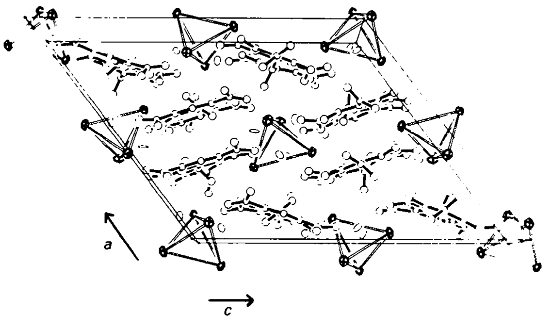

Fig. 3. The packing arrangement within half a unit cell ($a \times b/2 \times c$), viewed along **b**.

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Structure of 2-Hydroxyethanethiolatolead(II) Nitrate, $Pb(SCH_2CH_2OH)(NO_3)$, a Sheet Polymer

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Abstract. $M_r = 346·32$, orthorhombic, $Pbca$, $a = 17·969\ (5)$, $b = 11·860\ (3)$, $c = 6·043\ (2)$ Å, $U = 1287·8$ Å^3, $Z = 8$, $D_x = 3·572$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 26·7$ mm^{-1}, $F(000) = 1232$, $T = 291$ K, $R = 0·038$ for 935 observed reflections. The structure consists of polymeric sheets. Pb has an

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