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The Crystal Structure of the Molecular Compound Lead Isopropylxanthate–Pyridine

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Lead isopropylxanthate crystallizes by accommodation of pyridine molecules into a molecular compound, lead isopropylxanthate–pyridine, $Pb(SSCOC_3H_7)_2.C_5H_5N$. The crystal is monoclinic with $a=17{\cdot}80\pm0{\cdot}03$, $b=11{\cdot}18\pm0{\cdot}02$, $c=10{\cdot}61\pm0{\cdot}02$ Å; $\beta=107{\cdot}8\pm0{\cdot}2°$, and space group $P2_1/c$. The unit cell contains four formula units. A three-dimensional X-ray structure analysis has shown that the crystal is like a sandwich consisting of alternate layers of lead isopropylxanthate molecules and pyridine molecules piled up by van der Waals contact in the *a* axis direction. In the atmosphere the crystal loses pyridine and decomposes into a polycrystalline aggregate of lead isopropylxanthate. The lead atom is bonded to one xanthate group with Pb–S distances of $2{\cdot}833\pm0{\cdot}018$ and $2{\cdot}896\pm0{\cdot}013$ Å and to the other with $2{\cdot}722\pm0{\cdot}019$ and $3{\cdot}057\pm0{\cdot}016$ Å. The last value is the same as the sum of the ionic radii of $Pb^{2+}$and S^{2-}, 3·04 Å. The shortest Pb–S bond and sulphur atoms of the other xanthate group make S–Pb–S bonds with bond angles of $95{\cdot}0\pm0{\cdot}6°$ and $87{\cdot}5\pm0{\cdot}5°$.

Introduction

The structure analysis of the lead isopropylxanthate crystal was undertaken in connexion with the analyses of lead ethylxanthate crystals (Hagihara & Yamashita, 1966) and the disordered crystals of lead n-butylxanthate (Hagihara, Watanabe & Yamashita, 1968), which were carried out in order to elucidate the action of alkyl xanthate on galena surfaces during a flotation process (Hagihara, Uchikoshi & Yamashita, 1957; Hagihara, Sakurai & Ikeda, 1967).

Thin needle-like crystals of Pb isoP X† were obtained in two forms from an acetone solution of the powder. The crystal condensed from the vapour phase had a fibre structure corresponding to the complete rotation of a hexagonal crystal with $a=9{\cdot}48$ and $c=9{\cdot}31$ Å around the *c* axis. Although single crystals precipitated from the liquid phase were stable, they always showed a hexagonal superlattice structure with $a=56{\cdot}88$ ($9{\cdot}48\times6$) and $c=9{\cdot}31$ Å, the cell dimensions of which were too large to allow the immediate determination of the crystal structure.

Crystals used in the present X-ray study were those obtained from pyridine solutions. Large transparent crystals with well developed crystal faces were obtained and had the appearance of a molecular compound between Pb isoP X and pyridine. In the atmosphere they lost pyridine slowly from the surface and decomposed into a white polycrystalline aggregate of Pb isoP X, although the external shape of the crystals was retained. The aggregate, when dissolved in pyridine, crystallized again into crystals of the above molecular compound. The ease with which this crystal was grown to a reasonable size and also the appropriateness of its cell dimensions favoured the X-ray analysis of this molecular compound.

Experimental

Pb isoP X powder was obtained by mixing aqueous solutions of purified lead acetate and potassium isopropylxanthate. The dried powder was dissolved in pyridine and single crystals were obtained by slow evaporation of the solvent. The crystals were preferentially elongated along the *c* axis. A needle-shaped crystal with cross section approximately 0·1 × 0·1 mm, sealed in a glass capillary tube, was used for X-ray diffraction work about the *c* axis. Another crystal, cut parallel to the *b* axis with cross section approximately 0·3 × 0·2 mm, was used for the diffraction work about the *b* axis.

Lead isopropylxanthate–pyridine, $Pb(SSCOC_3H_7)_2$ C_5H_5N, is monoclinic, with space group $P2_1/c$. $a=17{\cdot}80\pm0{\cdot}03$ Å, $b=11{\cdot}18\pm0{\cdot}02$, $c=10{\cdot}61\pm0{\cdot}02$; $\beta=107{\cdot}8\pm0{\cdot}2°$. $D_m=1{\cdot}72$–$1{\cdot}78$ g.cm^{-3} (flotation), $D_c=1{\cdot}82$ g.cm^{-3}, $Z=4$.

The linear absorption coefficient for Cu radiation was 200 cm^{-1}.

A series of Weissenberg photographs of $L=0$ to 9 layers with a *c*-axis oriented crystal and another series of $K=0$ to 4 layers with a *b*-axis oriented crystal were taken with filtered Cu $K\alpha$ radiation at room temperature. A total of 2763 independent reflexions are to be observed within $L=0$ to 9 and $\sin\theta<0{\cdot}88$, but only 1797 reflexions (65·6%) of these gave measurable intensities. Another 142 reflexions within $L=0$ to 9 with $\sin\theta>0{\cdot}88$ and 60 reflexions with the index $L=10$, obtained from the *b*-axis oriented crystal, gave measurable intensities. The intensities of the total 1999 observed reflexions were measured visually. They were corrected for Lorentz and polarization factors. No absorption correction was made.

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[†] Hereafter, lead ethylxanthate, lead n-butylxanthate and lead isopropylxanthate will be written as Pb E X, Pb nB X and Pb isoP X, respectively.

Table 1. *Atomic parameters of lead isopropylxanthate–pyridine*

The β_{ij} values (with e.s.d.'s) as given here are defined by:

$$T=\exp\{-10^{-4}(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)\}\,.$$

	x_i	x_i/a_i	$\sigma(x_i)$	B	$\sigma(B)$	$\lvert\Delta x_i\rvert/\sigma(x_i)$	$\lvert\Delta B\rvert/\sigma(B)$
Pb	x	0·25531	0·0019 Å	2·64 Å^2	0·07	0·02	
	y	0·29320	0·0022			0·01	
	z	0·48288	0·0020			0·01	
S(1)	x	0·1266	0·015	4·3	0·5	0·02	
	y	0·4188	0·022			0·06	
	z	0·5243	0·015			0·04	
S(2)	x	0·2725	0·011	2·3	0·3	0·01	
	y	0·3874	0·015			0·01	
	z	0·7445	0·012			0·01	
S(3)	x	0·3309	0·016	4·4	0·5	0·00	
	y	0·4929	0·019			0·00	
	z	0·4382	0·016			0·01	
S(4)	x	0·1880	0·015	3·7	0·5	0·03	
	y	0·4204	0·017			0·08	
	z	0·2171	0·015			0·04	
O(1)	x	0·142	0·032	3·0	1·2	0·01	
	y	0·422	0·039			0·00	
	z	0·787	0·034			0·02	
O(2)	x	0·281	0·040	4·8	1·2	0·05	
	y	0·600	0·051			0·03	
	z	0·225	0·040			0·03	
C(1)	x	0·172	0·044	2·5	1·5	0·11	
	y	0·414	0·046			0·21	
	z	0·677	0·055			0·05	
C(2)	x	0·257	0·053	3·4	2·0	0·04	
	y	0·512	0·058			0·12	
	z	0·291	0·059			0·14	
C(3)	x	0·056	0·14	6·6	3·2	0·07	0·19
	y	0·460	0·14			0·12	
	z	0·751	0·14			0·11	
C(4)	x	0·015	0·13	6·3	3·0	0·27	0·26
	y	0·329	0·14			0·05	
	z	0·704	0·13			0·03	
C(5)	x	0·045	0·15	6·4	3·7	0·00	0·13
	y	0·549	0·16			0·14	
	z	0·854	0·15			0·00	
C(6)	x	0·223	0·13	6·7	3·0	0·65	0·32
	y	0·625	0·14			0·29	
	z	0·103	0·13			1·36	
C(7)	x	0·190	0·18	6·7	4·9	0·12	0·46
	y	0·752	0·19			0·21	
	z	0·114	0·18			0·55	
C(8)	x	0·279	0·13	10·0	3·0	1·45	1·47
	y	0·638	0·13			0·72	
	z	−0·005	0·13			0·75	
N	x	0·397	0·045	3·7	1·7	0·19	
	y	0·222	0·051			0·21	
	z	0·590	0·064			0·30	
C(9)	x	0·457	0·18	11·4	4·9	0·39	0·53
	y	0·243	0·19			0·13	
	z	0·568	0·18			0·27	
C(10)	x	0·551	0·18	8·2	4·7	0·25	0·16
	y	0·224	0·19			0·16	
	z	0·636	0·18			0·37	
C(11)	x	0·559	0·17	8·2	4·5	0·50	0·04
	y	0·129	0·19			0·17	
	z	0·681	0·17			0·72	
C(12)	x	0·501	0·21	12·4	5·6	0·04	0·39
	y	0·066	0·21			0·26	
	z	0·708	0·19			0·12	
C(13)	x	0·410	0·16	6·9	4·1	0·22	0·19
	y	0·128	0·17			0·02	
	z	0·650	0·16			0·47	

Table 1 (*cont.*)

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	$\lvert\Delta\beta_{ij}\rvert/\sigma(\beta_{ij})$*
Pb	27 (1)	89 (2)	86 (2)	−3 (1)	14 (1)	4 (2)	0·05
S(1)	33 (5)	221 (28)	80 (15)	−35 (11)	5 (7)	1 (16)	0·06
S(2)	17 (4)	126 (16)	55 (12)	15 (7)	11 (5)	20 (11)	0·18
S(3)	43 (6)	120 (19)	128 (18)	−34 (10)	−7 (9)	34 (16)	0·05
S(4)	38 (6)	113 (18)	104 (16)	4 (8)	16 (8)	29 (14)	0·10
O(1)	28 (13)	135 (47)	99 (40)	−7 (20)	27 (19)	41 (35)	0·05
O(2)	39 (16)	173 (61)	122 (48)	−24 (27)	−13 (22)	42 (45)	0·15
C(1)	15 (15)	41 (43)	154 (66)	18 (21)	−14 (26)	2 (43)	0·45
C(2)	31 (20)	78 (57)	133 (72)	15 (30)	13 (31)	−20 (53)	0·17
N	36 (17)	87 (54)	376 (102)	−17 (27)	54 (36)	−144 (66)	0·68

* Six $\lvert\Delta\beta_{ij}\rvert/\sigma(\beta_{ij})$ values for each atom are smaller than the value listed in this column.

Determination of the structure

The coordinates of the lead atom were determined from Patterson functions. The coordinates of the sulphur, oxygen, carbon and nitrogen atoms were determined and refined successively by the usual procedures of the heavy atom method, from Fourier and difference Fourier syntheses. After three cycles of the least-squares refinement with isotropic temperature factors for all atoms, the R value for the 1999 observed reflexions with equal weight fell from 0·43 to 0·18. The B values obtained after this refinement are shown in Table 1. Further refinements were carried out by assuming anisotropic temperature factors, first for the lead and four sulphur atoms and finally for the lead atom and the sulphur, oxygen and carbon atoms of the xanthate groups, and for the nitrogen atom of the pyridine molecule. After three cycles of the refinement the R value was reduced to 0·149.

The atomic coordinates, temperature factors, their standard deviations and parameter shifts, as fractions of the standard deviation obtained by the final cycle of refinement, are tabulated in Table 1.

The observed and calculated structure factors (FO and FC, respectively) are shown in Table 2. FC values for the unobserved reflexions which are marked with asterisks are those calculated with parameters obtained after the refinement with anisotropic temperature factors for the lead and four sulphur atoms only.

The configuration of atoms in the structure is shown in Fig. 1. Atomic distances and bond angles are shown in Fig. 2 and with standard deviations in Table 3.

The computations were carried out by the program system *UNICS* (Sakurai *et al.*, 1967) on the HITAC 5020 computer of Tokyo University and the OKITAC 5090 H computer of this Institute. The atomic scattering factors used were those tabulated in *International Tables for X-ray Crystallography* (1962).

Discussion

Description of the structure

As shown in Fig. 1 the crystal is like a sandwich consisting of alternate layers of Pb isoP X molecules and pyridine molecules. In the c-axis direction Pb isoP X molecules are in van der Waals contact; the S(2)–S(4.G) and S(4)–S(2.$G,-c$) separations are both 3·73 ± 0·02 Å and the C(5)–C(6, $+c$) and C(5)–C(7, c) separations are 3·6 ± 0·3 and 3·9 ± 0·3 Å respectively. The molecules are piled up in the b-axis direction parallel to the two-fold screw axes, with van der Waals contacts at the methyl ends; the distances C(5)–C(4′.$G,-a$) and C(4)–C(5′.$G,-a,-b$) are both 3·3 ± 0·3 Å.

The crystalllization proceeds in the a-axis direction by the inclusion of pyridine molecules. The Pb–N distance, 2·55 ± 0·04 Å, is nearly equal to the sum of the radii of the Pb^{2+} ion and the van der Waals radius of the nitrogen atom, *i.e.* 1·2 + 1·5 = 2·7 Å, whereas it is longer by 0·27 Å than the sum of the single-bond radii of lead and nitrogen atoms (1·54 + 0·74 = 2·28 Å) (Pauling, 1960). It is interesting to compare this result with the Zn–N distance in the crystal of bis-(N,N-dimethyldithiocarbamato)pyridinezinc (Fraser & Harding, 1967). In this compound each pyridine molecule is bonded to a zinc dimethyldithiocarbamate group through a Zn–N bond of length 2·08 ± 0·01 Å. This value is longer by 0·09 Å than the sum of the single-bond radii of zinc and nitrogen atoms. The present result, that the Pb–N distance is longer by 0·27 Å than the sum of the single-bond radii of lead and nitrogen atoms, suggests that the bonding between the Pb isoP X molecule and the pyridine molecule must be a loose one. This interpretation is also supported by the fact that pyridine molecules are not accommodated at all in the crystal when Pb E X is crystallized from its pyridine solution; the crystal obtained is the same as that crystallized from its acetone or alcohol solution (Hagihara & Yamashita, 1966).

The pyridine molecule is in van der Waals contact with the surrounding four Pb isoP X molecules at C–S distances of 3·6 ± 0·2 to 4·00 ± 0·2 Å; the van der Waals approach distance between the CH group and the sulphur atom is 2·00 + 1·85 = 3·85 Å. The nearest distances of approach of the CH groups between two pyridine molecules [C(9)–C(12′.G) and C(10)–C(12′.G)] are 4·3 ± 0·3 and 4·4 ± 0·3 Å respectively.

Molecular structure of Pb *iso*P X (*Figs. 2 and* 3)

The two sulphur atoms belonging to a xanthate group [S(1) and S(2)] are bonded to the lead atom at

Table 2. *Observed* (FO) *and calculated* (FC) *structure factors*

Asterisks denote unobserved reflexions.

H	K	FO	FC
L=0			
1	0*	-	-16
2	0	427	-429
3	0	35	-28
4	0	337	318
5	0	82	-60
6	0	245	-230
7	0	155	141
8	0	241	203
9	0	130	-94
10	0	199	-186
11	0	87	78
12	0	147	130
13	0	119	-116
14	0	123	-119
15	0	125	106
16	0	101	91
17	0	43	-55
18	0	49	-48
19	0	25	29
20	0	21	25
21	0	13	-31
1	1	397	-364
2	1*	-	-9
3	1	206	232
4	1	21	-23
5	1	205	-213
6	1	59	54
7	1	272	244
8	1	131	-97
9	1	241	-198
10	1	58	65
11	1	152	139
12	1	93	-66
13	1	138	-129
14	1	101	79
15	1	125	94
16	1	56	-59
17	1	86	-70
18	1	28	35
19	1	25	43
20	1	20	-35
21	1	18	-29
0	2	130	-131
1	2	86	79
2	2	190	165
3	2*	-	-11
4	2	228	-249
5	2	40	-31
6	2	253	254
7	2	67	-51
8	2	204	-175
9	2	50	45
10	2	118	114
11	2	89	-70
12	2	133	-104
13	2	31	22
14	2	124	86
15	2	32	-23
16	2	71	-60
17	2	30	32
18	2	62	53
19	2	24	-34
20	2	28	-46
21	2	14	31
1	3	48	71
2	3	140	-136
3	3	148	-179
4	3	69	80
5	3	235	236
6	3*	-	-6
7	3	140	-159
8	3*	-	12
9	3	114	110
10	3*	-	-19
11	3	112	-95
12	3*	-	4
13	3	100	85
14	3*	-	7
15	3	65	-50
16	3*	-	16
17	3	42	36
18	3	27	-34
19	3	33	-45
20	3	18	25
0	4	68	70
1	4	50	-38
2	4	70	-59
3	4	60	49
4	4	77	72
5	4*	-	-9
6	4	71	-56
7	4	24	-39
8	4	70	52
9	4*	-	18
10	4	89	-86
11	4*	-	-16
12	4	98	80
13	4*	-	6
14	4	80	-65
15	4*	-	16
16	4	31	39
17	4	28	-22
18	4	26	-35
19	4	21	14
20	4	15	35
1	5	119	-83
2	5	29	-23
3	5	43	25
4	5	38	29
5	5*	-	2
6	5*	-	4
7	5*	-	19
8	5*	-	5
9	5	40	-38
10	5*	-	-1
11	5	31	36
12	5*	-	3
13	5*	-	-17
14	5*	-	12
15	5*	-	22
16	5*	-	-6
17	5*	-	-20
0	6	72	-54
1	6	40	-26
2	6	23	10
3	6	105	88
4	6	24	25
5	6	25	-21
6	6*	-	-14
7	6*	-	-16
8	6*	-	5
9	6*	-	25
10	6*	-	-16
11	6*	-	-13
12	6*	-	25
13	6*	-	9
14	6*	-	-8
15	6*	-	-0
16	6*	-	-7
17	6*	-	-12
1	7	26	-31
2	7*	-	15
3	7	37	40
4	7*	-	-17
5	7	50	-36
6	7*	-	-5
7	7*	-	26
8	7*	-	6
9	7	44	-35
10	7*	-	-2
11	7	46	36
12	7*	-	-2
13	7*	-	-22
14	7*	-	3
15	7*	-	11
16	7*	-	-9
0	8	63	-62
1	8	28	-29
2	8	57	53
3	8	29	21
4	8	58	-50
5	8*	-	-8
6	8	43	42
7	8*	-	-13
8	8	45	-56
9	8*	-	25
10	8	33	44
11	8*	-	-16
12	8*	-	-31
13	8*	-	12
14	8*	-	28
15	8*	-	-10
1	9	117	103
2	9	31	24
3	9	97	-84
4	9*	-	-16
5	9	88	63
6	9*	-	-13
7	9	65	-57
8	9*	-	26
9	9	32	53
10	9*	-	-23
11	9	31	-42
12	9	29	25
13	9	28	41
15	9	40	-43
0	10	110	94
1	10*	-	-6
2	10	110	-95
3	10*	-	13
4	10	91	71
5	10*	-	-18
6	10	65	-61
7	10*	-	20
8	10	56	58
9	10*	-	-17
10	10	43	-49
11	10	29	24
12	10	27	49
1	11	73	-64
2	11*	-	20
3	11	72	62
4	11*	-	-23
5	11	55	-61
6	11*	-	15
7	11	54	57
8	11*	-	-12
9	11	41	-47
11	11	26	40
13	11	20	-32
0	12	44	-40
1	12*	-	7
2	12	44	42
3	12*	-	-12
4	12	53	-51
5	12*	-	10
6	12	50	58
7	12*	-	-9
8	12	38	-45
10	12	22	34
1	13	28	33
3	13	27	-35
5	13	25	35
7	13	22	-35
L=1			
-19	1*	-	19
-18	1*	-	-20
-17	1*	-	-28
-16	1*	-	38
-15	1	50	52
-14	1*	-	-37
-13	1	50	-55
-12	1*	-	38
-11	1*	-	-11
-10	1	80	-64
-9	1	89	71
-8	1	151	119
-7	1	28	22
-6	1	56	-56
-5	1	50	-47
-4	1	44	42
-3	1	107	106
-2	1	55	-60
-1	1*	-	-21
0	1	119	121
1	1	39	49
2	1	166	-156
3	1	54	-43
4	1	45	-30
5	1	88	-84
6	1*	-	13
7	1	30	30
8	1	33	30
9	1*	-	-12
10	1	54	-54
11	1*	-	-1
12	1	61	49
13	1*	-	-5
14	1	42	-38
15	1*	-	14
16	1*	-	23
17	1*	-	-1
18	1*	-	-4
-19	2*	-	-27
-18	2	41	-38
-17	2	54	48
-16	2	72	51
-15	2	73	-66
-14	2	100	-70
-13	2	62	50
-12	2	59	56
-11	2	86	-84
-10	2*	-	3
-9	2	168	154
-8	2	29	-21
-7	2	181	-192
-6	2	72	-51
-5	2	169	204
-4	2*	-	14
-3	2	235	-201
-2	2	113	105
-1	2	169	147
0	2	38	-36
1	2	283	-270
2	2	44	36
3	2	69	87
4	2	66	-64
5	2	53	-59
6	2	85	74
7	2	63	54
8	2	53	-64
9	2	88	-83
10	2	36	23
11	2	72	53
12	2*	-	-17
13	2	55	-41
14	2*	-	12
15	2	42	37
16	2*	-	-0
17	2*	-	-25
18	2*	-	-5
-19	3	40	-45
-18	3	50	47
-17	3*	-	38
-16	3	70	-70
-15	3*	-	-33
-14	3	70	74
-13	3	40	44
-12	3	115	-103
-11	3	89	-63
-10	3	102	109
-9	3	79	62
-8	3	126	-146
-7	3	48	-58
-6	3	179	199
-5	3	25	27
-4	3	189	-203
-3	3	36	31
-2	3	187	176
-1	3	47	-63
0	3	132	-110
1	3	22	-30
2	3	144	120
3	3*	-	-5
4	3	203	-178
5	3*	-	8
6	3	152	139
7	3*	-	-11
8	3	175	-144
9	3	50	50
10	3	89	97
11	3	39	-47
12	3	54	-53
13	3	40	37
14	3	56	59
15	3*	-	-13
16	3	40	-47
17	3*	-	13
18	3	40	42
-18	4*	-	42
-17	4	50	-47
-16	4*	-	-37
-15	4	70	63
-14	4*	-	28
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-1	1	40	5
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4	1*	-	13
5	1*	-	5
6	1*	-	-16
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8	1*	-	20
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-17	2*	-	-4
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3	2	29	35
4	2	30	13
5	2*	-	-23
6	2*	-	-2
7	2*	-	19
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-17	3	28	51
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-15	3	49	-56
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-9	3	70	62
-8	3	37	-21
-7	3	57	-59
-6	3*	-	27
-5	3	65	62
-4	3	29	-26
-3	3	49	-59
-2	3	45	39
-1	3	56	58
0	3	56	-49
1	3	61	-43
2	3	65	41
3	3	29	27
4	3	49	-33
5	3	31	-28
6	3*	-	24
7	3*	-	23
8	3	35	-23
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7	7	22	25
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1	8	24	26
2	8	28	22
3	8	28	-27
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-4	9	30	15
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1	9	28	17
	L=10		
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-11	2	53	-60
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3	2	32	39
4	2	27	-33
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-10	3	52	55
-9	3*	-	-22
-8	3	58	-64
-7	3*	-	29
-6	3	58	60
-5	3	27	-33
-4	3	58	-59
-3	3	26	40
-2	3	47	71
-1	3*	-	-37
0	3	47	-65
1	3*	-	23
2	3*	-	39
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4	3*	-	-18
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-8	4*	-	15
-7	4	48	55
-6	4*	-	-21
-5	4	44	-49
-4	4*	-	26
-3	4	33	39
-2	4*	-	-31
-1	4	38	-40
0	4*	-	21
1	4*	-	31

distances of 2·833 ± 0·018 and 2·896 ± 0·013 Å respectively. The difference, 0·063 ± 0·022 Å, between them is significant (see *e.g.* Lipson & Cochran, 1966). The atoms S(1), S(2), O(1) and C(1) are coplanar, and the deviation of the C(1) atom from the plane defined by the S(1), S(2) and O(1) atoms is only 0·04 ± 0·06 Å. On the other hand, the lead atom is not coplanar with this plane, and the plane defined by the Pb, S(1) and S(2) atoms makes an angle of 24·5 ± 2·5° with the plane of the xanthate group.

The S(3) atom is bonded to the lead atom at a distance of 2·722 ± 0·019 Å. The Pb–S(3) distance is the shortest of the four Pb–S distances and nearest to the sum of the single-bond radii of lead and sulphur atoms, 1·54 + 1·04 = 2·58 Å. The Pb–S(4) distance, 3·057 ± 0·016 Å, is the same as the sum of the ionic radii of Pb^{2+} and S^{2-} (3·04 Å) (Pauling, 1960). The S(3), S(4), O(2) and C(2) atoms are almost coplanar; the C(2) atom is displaced from the plane, defined by the S(3), S(4) and O(2) atoms, by a distance of 0·16 ± 0·07 Å.

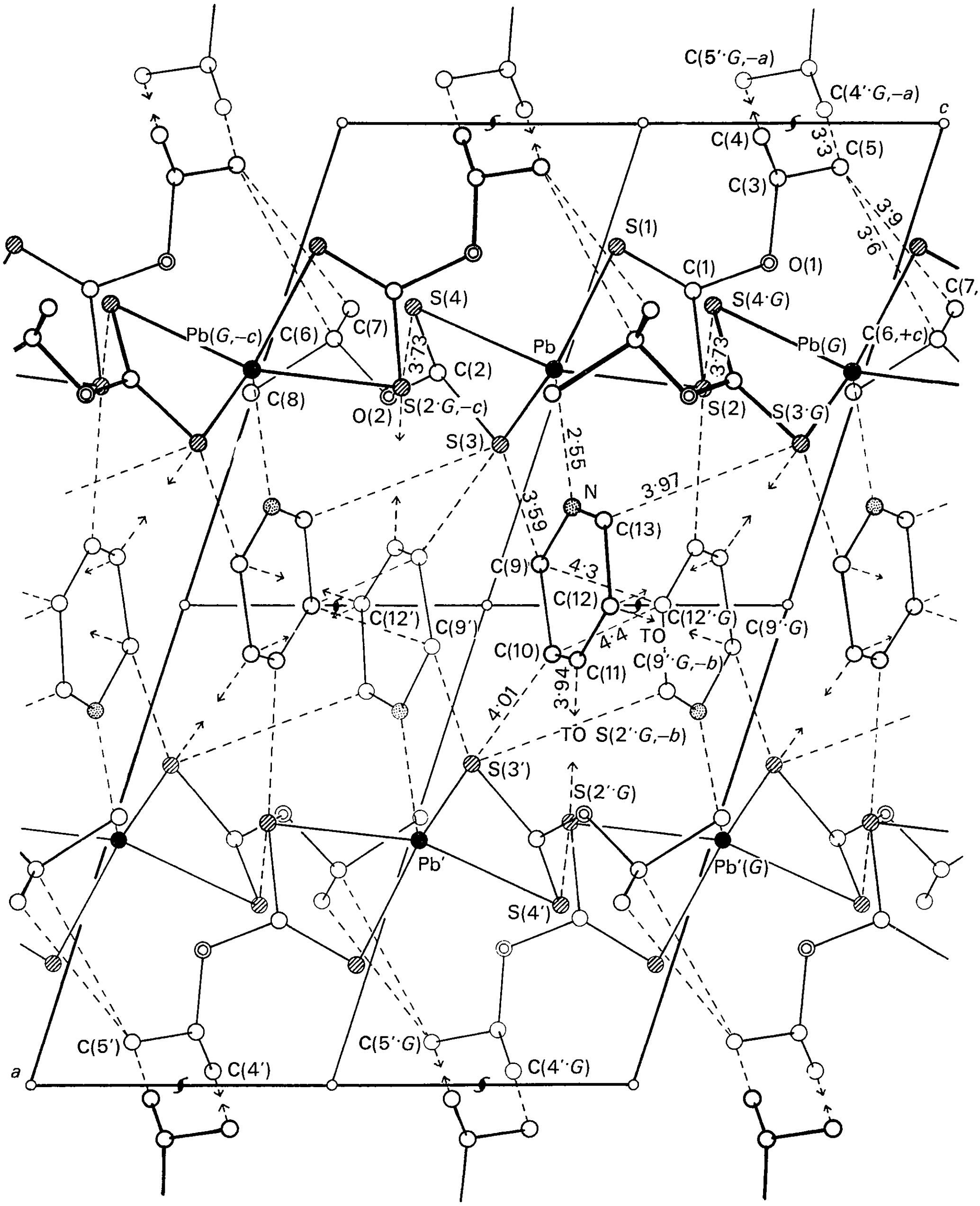
C(5'·G,−a)
C(4'·G,−a)
c
C(4)
3·3
C(5)
C(3)
3·9
3·6
S(1)
C(1)
O(1)
C(7,+c)
S(4·G)
Pb(G)
C(6,+c)
S(4)
C(7)
C(6)
Pb(G,−c)
3·73
C(2)
Pb
3·73
S(2)
S(3·G)
C(8)
O(2)
S(2·G,−c)
S(3)
2·55
N
3·97
3·59
C(13)
C(9)
4·3
C(12)
C(12'·G)
C(9'·G)
C(12')
C(9')
TO
4·4
C(10)
C(11)
C(9'·G,−b)
4·01
3·94
TO S(2'·G,−b)
S(3')
S(2'·G)
Pb'
Pb'(G)
S(4')
C(5')
C(4')
C(5'·G)
C(4'·G)
a

Fig. 1. Configuration of atoms in the molecular compound, lead isopropylxanthate–pyridine, $Pb(SSCOC_3H_7)_2 . C_5H_5N$, viewed along the *b* axis. The dotted lines and figures show van der Waals contact approach distances.

The lead atom is coplanar with the plane of this xanthate group; the distance between the lead atom and the plane is 0·03 ± 0·12 Å.

The bond angles S(3)–Pb–S(1) and S(3)–Pb–S(2) are 95·0 ± 0·6° and 87·5 ± 0·5° respectively. These angles and the Pb–S distances, together with the condition that S(1) and S(2) atoms belonging to a xanthate group are at a distance of 2·94 ± 0·02 Å, determine the arrangement of the Pb, S(1), S(2) and S(3) atoms. The bond angle S(3)–C(2)–S(4) (128 ± 4°) is the largest of any S–C–S bond angles found in Pb E X and Pb nB X, which are mostly in the range 118° to 124°. It is comparable with the S–C–S bond angles in arsenious xanthate (129·5 ± 3°) (Carrai & Gottardi, 1960), and antimonious xanthate (130·5 ± 2°) (Gottardi, 1961). In these compounds one sulphur atom is bound to the metal atom, while the other is not, as was the case with the S(3) and S(4) atoms in relation to the lead atom in the present example. The S(4) atom is so situated that it comes into van der Waals contact with the S(1) atom at a distance of 3·74 ± 0·02 Å.

When the bond numbers are calculated for the four Pb–S distances, by Pauling's equation, with 2·58 Å as the Pb–S single-bond distance (Pauling, 1960), the following values are obtained: Pb–S(1), 0·38 ± 0·03; Pb–S(2), 0·30 ± 0·02; Pb–S(3), 0·58 ± 0·04; Pb–S(4), 0·16 ± 0·01. The idealized picture of the fractional bonds is shown in Fig. 3, where the Pb–S(3) bond is drawn with a continuous thick line and the Pb–S(1) and Pb–S(2) bonds are drawn with thick broken lines.

A comparison of the configuration of four dithiocarbonic sulphur atoms around the lead atom with that in the case of Pb nB X

The configuration of the Pb, S(1), S(2) and S(3) atoms is similar in both Pb isoP X and Pb nB X. As is clear from Fig. 3, all the differences in the corresponding Pb–S and S–S distances in the two cases (values for Pb nB X are written in parentheses) are not significant, except for the difference in Pb–S(2). The deviations of the lead atoms from the plane defined by the S(1), S(2) and S(3) atoms (1·79 ± 0·02 and 1·75 ± 0·09 Å, for Pb isoP X and Pb nB X, respectively) are the same within the limit of error. The Pb–S(4) distances (3·06 ± 0·02 and 3·03 ± 0·08 Å, for Pb isoP X and Pb nB X, respectively) are also the same. However, the distances of the S(4) atoms from the above planes are 1·12 ± 0·03 Å for Pb isoP X and 1·74 ± 0·14 Å for Pb nB X. The difference, 0·62 ± 0·15 Å, is definitely significant. This difference is interpreted as being caused by the rotation of the xanthate group S(3)S(4)C(2)O(2) around the Pb–S(3) bond so as to satisfy the conditions of the closest packing of molecules.

The bonding of the lead atom to the dithiocarbonic sulphur atoms is summarized as follows: the lead atom is bonded to one xanthate group by a Pb–S single bond

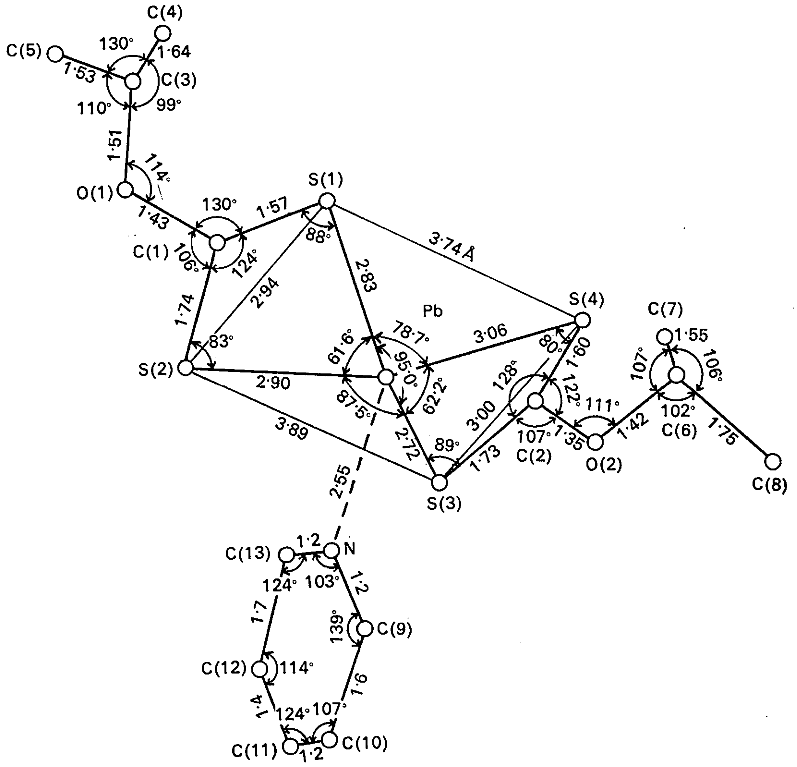

Fig. 2. Interatomic distances and bond angles in lead isopropylxanthate and pyridine in the molecular compound, $Pb(SSCOC_3H_7)_2.C_5H_5N$.

Table 3. *Interatomic distances, bond angles and their standard deviations*

Interatomic distances	
Pb isoP X	
Pb —S(1)	2·833±0·018 Å
Pb —S(2)	2·896±0·013
Pb —S(3)	2·722±0·019
Pb —S(4)	3·057±0·016
S(1) -S(2)	2·94±0·02
S(3) -S(4)	3·00±0·02
S(2) -S(3)	3·89±0·02
S(4) -S(1)	3·74±0·02
C(1)-S(1)	1·57±0·05
C(1)-S(2)	1·74±0·04
C(2)-S(3)	1·73±0·05
C(2)-S(4)	1·60±0·05
C(1)-O(1)	1·43±0·07
C(2)-O(2)	1·35±0·08
O(1)-C(3)	1·51±0·14
C(3)-C(4)	1·64±0·20
C(3)-C(5)	1·53±0·22
O(2)-C(6)	1·42±0·12
C(6)-C(7)	1·55±0·25
C(6)-C(8)	1·75±0·21
Pyridine	
N——C(9)	1·19±0·20
N——C(13)	1·22±0·18
C(9)—C(10)	1·61±0·23
C(10)-C(11)	1·15±0·28
C(11)-C(12)	1·36±0·29
C(12)-C(13)	1·69±0·25
Pb isoP X - Pb isoP X	
S(2) -S(4.G)	3·73±0·02
C(5)-C(6, +c)	3·6±0·3
C(5)-C(7, +c)	3·9±0·3
C(5)-C(4′.G, −a)	3·3±0·3
Pb isoP X - pyridine	
Pb-N	2·55±0·04
S(3)-C(9)	3·59±0·18
S(3′)-C(10)	4·01±0·15
S(2′.G, −b)-C(11)	3·94±0·15
S(3.G)-C(13)	3·97±0·15
Pyridine - pyridine	
C(9)—C(12′.G)	4·3±0·3
C(10)-C(12′.G)	4·4±0·3

Bond angles	
Pb isoP X	
S(1)-Pb-S(3)	95·0±0·6°
S(2)-Pb-S(3)	87·5±0·5
S(1)-Pb-S(4)	78·7±0·5
S(2)-Pb-S(4)	127·7±0·5
S(1)-Pb-S(2)	61·6±0·4
S(3)-Pb-S(4)	62·2±0·4
Pb-S(1)-C(1)	87·7±1·9
Pb-S(2)-C(1)	82·8±1·9
Pb-S(3)-C(2)	88·8±2·1
Pb-S(4)-C(2)	79·8±2·1
S(1)-C(1)-S(2)	124·4±3·6
S(3)-C(2)-S(4)	128·3±3·7
S(1)-C(1)-O(1)	129·8±3·2
S(2)-C(1)-O(1)	105·7±3·0
S(3)-C(2)-O(2)	106·5±3·4
S(4)-C(2)-O(2)	122·2±4·0
C(1)-O(1)-C(3)	114± 6
O(1)-C(3)-C(4)	99±10
O(1)-C(3)-C(5)	110± 9
C(4)-C(3)-C(5)	130±13
C(2)-O(2)-C(6)	111± 7
O(2)-C(6)-C(7)	107±10
O(2)-C(6)-C(8)	102± 9
C(7)-C(6)-C(8)	106±12
Pyridine	
C(13)-N—C(9)	103±12
N——C(9)—C(10)	139±16
C(9)—C(10)-C(11)	107±17
C(10)-C(11)-C(12)	124±19
C(11)-C(12)-C(13)	114±16
C(12)-C(13)-N	124±15
Pb isoP X - pyridine	
S(2)-Pb-N	83·5±1·4
S(3)-Pb-N	81·9±1·2
Pb—N -C(9)	133±9
Pb—N -C(13)	121±8

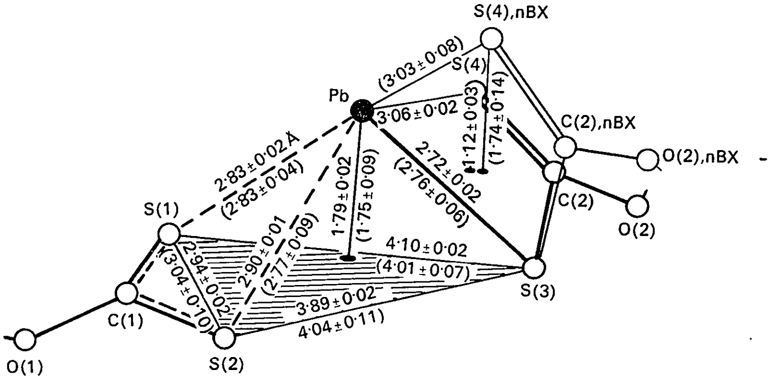

Fig. 3. Configuration of two xanthate groups about the lead atom in lead isopropylxanthate in the molecular compound, $Pb(SSCOC_3H_7)_2.C_5H_5N$. For comparison S(4), C(2) and O(2) atoms of a molecule of lead n-butylxanthate in the disordered crystal are shown by thin circles. The atomic distances for lead n-butylxanthate are written in parentheses.

and to the other xanthate group by two Pb–S bonds, each of which is intermediate in length between a single bond and an ionic bond and makes an angle of approximately 90° with the Pb–S single bond. In order to collect further relevant experimental data the structure analyses of the ordered crystal of Pb nB X and the Pb isoP X crystals obtained from the acetone solution are now in progress.

References

CARRAI, G. & GOTTARDI, G. (1960). *Z. Kristallogr.* **113**, 373.

FRASER, K. A. & HARDING, M. M. (1967). *Acta Cryst.* **22**, 75.

GOTTARDI, G. (1961). *Z. Kristallogr.* **115**, 451.

HAGIHARA, H., UCHIKOSHI, H. & YAMASHITA, S. (1957). Proc. 2nd Intern. Conference on Surface Activity. Vol. 3, pp. 343–348. London: Butterworths.

HAGIHARA, H., SAKURAI, T. & IKEDA, T. (1967). *Chemistry, Physics and Application of Surface Active Substances* (Proc. 4th Intern. Congr. on Surface Active Substances, Brussels, 1964), Vol. 2, pp. 361–373. New York: Gordon & Breach.

HAGIHARA, H. & YAMASHITA, S. (1966). *Acta Cryst.* **21**, 350.

HAGIHARA, H., WATANABE, Y. & YAMASHITA, S. (1968). *Acta Cryst.* B**24**, 960.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

LIPSON, H. & COCHRAN, W. (1966). *The Determination of Crystal Structures.* 3rd ed. p. 356. London: Bell.

PAULING, L. (1960). The Nature of the Chemical Bond. 3rd ed. Pp. 221–264. Ithaca: Cornell Univ. Press.

SAKURAI, T. *et al.* (1967). *Universal Crystallographic Computation Program System.* Ed. T. SAKURAI. Crystallographic Society of Japan.

Acta Cryst. (1969). B**25**, 1784

On the Water Molecules in $FeSO_4.7H_2O$. A Nuclear Magnetic Resonance Study*

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The angular dependence of the nuclear magnetic resonance spectrum of single crystals of monoclinic $FeSO_4.7H_2O$ has been studied in nine planes of rotation with a view to establishing the proton–proton vectors. The experimentally determined vectors were employed to confirm the hydrogen-bonding scheme suggested by Baur, (*Acta Cryst.* (1964) **17**, 1167) and to determine the coordinates of the hydrogen atoms.

The crystal structure of monoclinic $FeSO_4.7H_2O$ was first studied by Leonhardt & Ness (1947) who gave the cell constants, space group and essentially correct positional parameters for iron and sulfur. More recently, Baur (1964) reported a complete determination of the structure of this compound. The X-ray studies reveal that the space group is $P2_1/c$ with $a=14{\cdot}072$, $b=6{\cdot}503$, $c=11{\cdot}041$ Å, $\beta=105°34'$, $Z=4$. The iron ions occupy special positions and are surrounded by six water molecules which form hydrogen bonds to SO_4^{2-} and to the seventh water molecule which is not coordinated to Fe^{2+}. The hydrogen-bonding scheme suggested by Baur (1964) is, in his atomic designation, as follows:

O(1)...H(11)–O(*w*1)–H(12)...O(2)
O(2)...H(22)–O(*w*2)–H(24)...O(4)
O(1)...H(31)–O(*w*3)–H(32)...O(2)
O(3)...H(43)–O(*w*4)–H(47)...O(*w*7)
O(4)...H(54)–O(*w*5)–H(57)...O(*w*7)
O(1)...H(61)–O(*w*6)–H(63)...O(3)
O(4)...H(74)–O(*w*7)–H(76)...O(*w*6) .

According to this scheme, the iron-coordinated water molecule O(*w*6) receives an 'outward' hydrogen bond from O(*w*7) which may account for the fact that Fe–O(*w*6) is significantly longer than the mean Fe–O(*w*). The alternative arrangement O(3)...H–O(*w*7)...O(4) which is geometrically feasible is ruled out by Baur.

In the present study, nuclear magnetic resonance (n.m.r.) has been employed to determine the orientations of the water molecules in $FeSO_4.7H_2O$. The equipment and method employed have been described in detail by the author (El Saffar, 1969). The magnetic field strength of 960 gauss employed in this study is considered low enough to render negligible any possible anisotropic shift of the resonance lines resulting from crystal paramagnetism. The measurements were made at room temperature on nine single crystals each of about 1 cm³ in volume. Each of these crystals was mounted in a Teflon holder which was in turn attached to an indexed head that allowed rotation of the crystal about an axis normal to the external magnetic field. The axes of rotation were determined to within 1° with the aid of the crystal morphology as quoted by Groth (1908), and a precision optical goniometer. The n.m.r. spectra were recorded for each crystal over a range of 180° in steps of 5°. Readings on the oscilloscope were

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* The experimental part of this work was carried out at the Department of Chemistry, Johns Hopkins University, Baltimore, Maryland, U.S.A.