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The Crystal Structure of Phenylmercury(II) Acetate

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Phenylmercury(II) acetate crystallizes in the monoclinic system, the space group $P2_1/c$, with four molecules per unit cell. The unit cell dimensions are: $a=5.24\pm0.01$ Å, $b=24.20\pm0.04$ Å, $c=7.50\pm0.02$ Å, $\beta = 114.0\pm0.4°$, the measured and calculated densities are 2.54 and 2.57 g/cm^3, respectively. The structure has been solved using 551 independent reflections collected about c-axis on integrated equi-inclination Weissenberg photographs and refined by least-squares method to $R = 0.111$. The structure is built up of the discrete $C_6H_5HgOCOCH_3$ molecules. The mercury atom is covalently bound to the phenyl ring on one side and to one acetate-oxygen atom on the other to give the characteristic digonal co-ordination. The Hg—C and Hg—O bond lengths are 1.92± 0.06 and 2.11±0.04 Å, respectively. The C—Hg—O bond angle amounts to 170±2°.

Introduction

No crystal structure of any mercury acetate has been reported so far. Even the crystal structure of mercury(II) acetate is still unknown because the compound is sensitive to light and the crystals decompose under the X-ray radiation.[1] The crystal structure determination of phenylmercury(II) acetate has been undertaken to explain the way in which the acetate is bound to mercury. In molecules with the general formula RHgX, the mercury atom is bound in two different ways: covalently to the carbon atom, of the organic part of molecule, and with more or less ionic bond to the ion X^-.

It is well known that mercury does not show any tendency to form chelate structures, and such a structure was not expected also in the case of phenylmercury(II) acetate. The results of this investigation as well as the structures of tolylmercury(II) acetate, which is now in progress,[2] confirm this generally accepted consideration.

Experimental Section

The crystals of phenylmercury(II) acetate were prepared in the form of thin needles from benzene solution with commercially available chemicals. The crystals obtained were all twins with the basal pinacoid {001} as the twinning plane. It was impossible to separate the individual single crystal.

The lattice parameters were determined from oscillation and Weissenberg photographs at the room temperature and the standard deviations were estimated from several film measurements. The systematic absence of the reflections $h0l$ for l odd and $0k0$ for k odd uniquely determined the space group as $P2_1/c$. Crystal data are shown in Table I. Three-dimensional intensity data ($hk0 \rightarrow hk6$) were recorded on Nonius-Delft integrated multiple films equi-inclination Weissenberg photographs with CuK$_\alpha$ radiation and determined photometrically. A total of 551 independent reflections were strong enough to be observed. The intensities were corrected for Lorents and polarization factors but absorption and anomalous dispersion corrections were not applied. The brittle crystals could not be ground into spherical or cylindrical forms. The size of the crystal used was 0.16× 0.11×0.05 mm.

Table I. Crystallographic data for $C_6H_5HgOCOCH_3$.

M. W. = 333.74
Crystallographic system: monoclinic
Space group: $P2_1/c - C^5_{2h}$
Unit cell parameters: $a = 5.24\pm0.01$ Å
$b = 24.20\pm0.04$ Å
$c = 7.50\pm0.02$ Å
$\beta = 114.0\pm0.4°$
$V = 868.8$ Å^3
$Z = 4$
$d_{calc} = 2.57$ g cm^{-3}
$d_{obs} = 2.54$ g cm^{-3} (picnometrically)
μCuK$_\alpha$ = 348 cm^{-1}

The mercury atom was located from Patterson projections obtained by means of the von Eller photosommateur. A three-dimensional Fourier map was then calculated on the basis of the contribution of mercury atom which gave the R factor of 0.21. Although some spurious peaks were present on the Fourier map, particularly around the mercury atom, the locations of all light atoms were determined by computation of two successive Fourier and difference syntheses. The structure was than refined by several cycles of full-matrix least-squares refinement with isotropic thermal parameters for all except hydrogen atoms. At this stage of refinement the reliability index was $R=0.177$. Six cycles of the refinement

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(1) H. Puff, G. Lorbacher, and R. Skrabs, *Acta Cryst.*, *19*, 870 (1965).
(2) D. Grdenić, B. Kamenar, and M. Gjogić-Nöthig, to be published.

Table II. Observed and calculated structure factors (x 100).

h	k	l	F_o	F_c
0	4	0	14932	16345
	6		3446	3112
	8		9815	-9633
	10		17495	-17737
	12		20095	-21461
	14		17059	-17185
	16		10071	-9288
	20		4326	3826
	22		7020	7191
	24		7188	7980
	26		5150	5749
1	0	0	16839	15559
	1		10581	-8508
	2		21026	18675
	3		20328	-17978
	4		12939	11214
	5		23716	-22416
	6		4052	2497
	7		20311	-19347
	8		12150	-10436
	9		15757	-13829
	10		16335	-15127
	11		7410	-6606
	12		12863	-13148
	13		3663	2342
	14		11400	-11217
	15		7412	7477
	16		6498	-6293
	17		10677	10160
	19		7477	7663
	21		5248	4654
	22		4794	4196
	24		4138	4604
2	0	0	6025	-5164
	1		10132	-8068
	3		17929	-16313
	5		22518	-21202
	7		23077	-22317
	9		15637	-15261
	11		5171	-4712
	13		4138	3501
	15		9266	9472
	17		11007	11467
	19		9331	9532
	21		6389	7110
3	0	0	14061	-14474
	2		12535	-12092
	4		7371	-6603
	5		10716	-10307
	7		10247	-11069
	8		7625	7448
	9		6144	-6556
	10		11033	11176
	12		9864	10726
	14		7336	8674
	15		4273	3600
	16		5257	4999
	17		4283	5153
	19		5103	5708
4	0	0	12258	-13999
	2		10530	-12583
	4		5595	-7246
	8		4794	5679
	10		6779	9570
	12		7352	9627
	14		6525	7910
5	0	0	4017	-5820
	4		3954	-2949
	10		3984	3330
0	2	1	15777	-16499
	3		5648	4400
	4		16065	-16408
	5		3503	-2575
	6		20679	-22932
	8		16187	-17456
	10		10448	-10743
	14		7801	7500
	16		11304	12132
	18		10690	10535
	20		7827	7076
	22		4763	1417
1	1	1	17492	-15380
	2		13026	-10288
	3		10103	-9209
	4		19319	-12976
	5		2173	-2168
	6		15037	-13899
	7		6461	5482
	8		13098	-12493
	9		12524	11208
	10		3905	-4488
	11		11823	12180
	13		10999	11729
	15		8227	8341
	16		7181	7023
	17		4799	3030
	18		6624	6786
	20		3970	5067
	22		3240	2347
1	1	-1	19946	20238
	2		8812	7497
	3		7914	7654
	4		17299	16079
	5		6912	5617
	6		15495	15416
	7		3347	-4911
	8		12685	12741
	9		9745	-9638
	10		6766	6253
	11		16014	-15997
	13		13578	-13082
1	14	-1	4083	-3736
	15		8775	-8663
	16		8003	-6443
	18		7778	-7240
	20		5559	-4795
	26		2869	1643
2	1	1	20990	-21136
	2		5898	4746
	3		15876	-14932
	5		7217	-6239
	7		3479	3719
	9		11367	11202
	11		13157	14395
	13		11785	12151
	15		7605	8273
	21		5027	-4867
	23		4676	-5713
	25		4491	-4508
2	1	-1	29766	27891
	3		20543	17420
	4		3649	-2331
	5		9745	8340
	6		3602	-2619
	7		4036	-3239
	9		14461	-13447
	11		14512	-14385
	13		14393	-14144
	15		10802	-10663
	21		5629	5329
	23		3818	6439
	25		4472	5277
	27		1679	3130
3	3	1	5404	-7061
	4		10897	12127
	6		12276	14900
	8		11846	13197
	9		5374	6043
	10		3143	3130
	11		3901	5718
	13		5129	5306
	16		5607	-6488
	18		6256	-6953
	20		4606	-5307
3	1	-1	10609	10514
	2		11234	-10016
	3		10292	9883
	4		16331	-14661
	6		17803	-16507
	8		14118	-13554
	9		9398	-8535
	10		9174	-8481
	11		9855	-9008
	13		7914	-7653
	14		3877	4216
	15		6008	-5115
	16		7609	7626
	18		6899	7623
	20		5896	5833
	21		2160	3100
	22		2924	3388
	23		2763	3337
4	2	-1	7914	-7521
	4		12526	-13997
	6		13828	-16298
	8		12035	-14291
	10		4597	-6095
	14		3939	4538
	16		6586	7792
	18		6817	8421
	20		6126	6789
5	4	-1	4466	-5449
	6		4403	-5804
	8		4301	-4784
	10		5487	-5317
6	2	-1	4083	1546
	4		2990	2589
0	1	2	7586	6154
	2		26562	-27129
	3		6543	4137
	4		16743	-15971
	5		5521	3936
	6		3597	-1977
	8		10538	10254
	10		16933	16724
	12		17271	17956
	14		13719	14238
	16		7814	7920
	20		5503	-4576
	22		6300	-6310
	26		4489	-4979
1	0	2	17413	-15300
	1		10394	7468
	2		13750	-11645
	3		17821	14858
	4		8655	-7228
	5		21465	18352
	7		22234	20450
	8		6988	5272
	9		14945	13836
	10		10604	9570
	11		5616	5338
	12		9477	8965
	14		8053	7138
	15		7666	-7579
	17		8476	-9331
	19		7149	-7200
	21		5041	-5223
1	0	-2	18084	-24453
	1		10107	13100
	2		12483	-15900
1	3	-2	11879	14382
	4		6214	-7554
	5		12757	15329
	7		11574	14104
	8		8430	8830
	9		9776	10130
	10		13966	14085
	11		4942	4854
	12		15452	15700
	14		12784	12254
	15		8309	-7154
	16		7081	6954
	17		9386	-9184
	19		4936	-5262
	21		4394	-4017
	22		4380	-4296
	24		3426	-4961
	26		3082	-3756
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	2		5499	4393
	3		15454	13598
	5		18532	18450
	7		18354	18009
	9		12087	11923
	10		3197	-2441
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	15		6624	-6837
	17		8414	-9382
	19		7526	-8971
	21		5785	-5778
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	1		5705	5553
	3		16387	15822
	5		21208	20966
	7		20940	22163
	9		13801	13500
	11		4767	3499
	13		4238	-3560
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	17		12145	-11523
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	8		7497	-6629
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	12		7606	-8796
	14		7514	-8188
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	2		12724	11120
	3		9483	8516
	4		7697	6346
	5		13142	11416
	7		11580	10520
	8		7854	-7429
	9		8062	7974
	10		10841	-11483
	12		9891	-11260
	14		8451	-8483
	17		4390	-5067
	19		4353	-5185
	22		3257	3956
	24		2870	4032
4	0	-2	14467	15319
	2		13737	14212
	4		8570	8260
	8		6533	-6751
	10		8700	-10165
	12		8018	-9232
	14		7981	-8383
	16		4256	-4758
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	4		5606	5118
	10		5311	-4127
	14		2996	-3633
	18		2312	-250
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	4		18403	18945
	6		19981	20130
	8		16978	16882
	10		7599	8510
	14		5996	-5750
	16		10331	-10143
	18		10630	-10482
	20		7933	-7374
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	2		6350	5412
	3		10034	7111
	4		12485	10764
	6		13645	12354
	7		5088	-3747
	8		10299	10108
	9		9164	-8525
	10		6085	4882
	11		11899	-10865
	13		10448	-10123
	15		7545	-7270
	16		6076	-5653
	18		6779	-6081
	21		3760	2748
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	4		8755	-11397
	5		4235	-6036
	6		11426	-16157
	8		11795	-13239
	9		8670	9300
	10		8846	-9253
	11		12008	-12929
	13		10442	10839
	14		5220	3994
1	15	-3	7712	7810
	16		8013	7525
	18		7115	6149
	20		6183	4393
2	1	3	12142	14433
	3		13630	11820
	5		6968	5049
	9		10795	-11193
	11		10784	-11049
	13		9130	-9794
	15		7820	-6933
2	1	-3	22525	-23770
	3		17644	-18165
	5		7714	-7538
	7		4555	3317
	9		11294	11680
	11		15137	15789
	13		13753	14850
	15		10780	10200
	23		5168	-6132
	25		3253	-5600
3	1	-3	15031	-13708
	2		11170	9320
	3		10750	-9679
	4		15466	12889
	6		15581	14965
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	9		10494	9114
	10		7245	6057
	11		10238	10885
	13		9058	9714
	15		7191	7209
	16		7781	-7380
	18		8733	-7411
	20		6556	-5139
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	4		13855	14745
	6		17386	16979
	8		14423	14606
	10		8193	7177
	14		6163	-5058
	16		8067	-8266
	18		7636	-8816
	20		5174	-7178
5	4	-3	7284	7212
	6		6694	7828
	8		7135	6671
	10		5881	4192
	11		6332	-8446
	13		4543	-5268
	17		3498	-2110
0	2	4	17117	15844
	3		4556	-3309
	4		10861	8795
	5		5435	-3947
	7		5346	-3350
	8		8701	-7823
	10		13170	-13014
	12		13233	-13076
	14		10880	-10389
	16		5929	-4913
	24		4253	5087
	26		4010	3495
1	0	4	8840	7063
	2		8929	7892
	3		11754	-10066
	5		15576	-13648
	7		13527	-13389
	9		10584	-9720
	15		6326	5484
	20		2924	2126
1	2	-4	8763	11789
	3		5893	-8679
	4		5067	5984
	5		8089	-11560
	7		9240	-11039
	8		4939	-7103
	9		6213	-6782
	10		11099	-10562
	12		9069	-11996
	14		9792	-9767
	15		6083	5538
	16		6064	-5666
	17		7051	6378
	19		5457	5163
	24		2716	4034
	26		3196	3046
2	3	4	11121	-11701
	7		10757	-12229
	9		7701	-7921
	21		2892	3775
	23		1522	1221
2	1	-4	7085	-7780
	3		13192	-14625
	5		15234	-17585
	7		13449	-15941
	9		9674	-11629
	11		3663	-4720
	15		9512	8516
	17		9914	10232
	19		8951	7477
	21		4350	5169
3	0	-4	14172	-14381
	2		12797	-11860
	3		8087	-7073
	4		7513	-6527
	5		12409	-10339
	7		12096	-11655
	8		7032	6614
	10		8920	9927
3	12	-4	10312	9988
	14		9305	7995
	17		4477	4894
4	0	-4	16159	-16370
	2		15431	-13990
	4		9804	-8560
	8		6160	5800
	10		9924	10218
	12		10020	10559
	14		7706	8295
5	0	-4	6326	-6280
	3		7737	7636
	5		10892	10101
	7		8807	10371
	9		10131	6656
	11		2957	2064
	17		5105	-5499
6	10	-4	2957	-2087
0	2	5	10387	-9697
	4		14613	-13701
	6		16053	-15433
	8		13491	-13070
	10		8157	-7422
	16		8781	7900
	18		8337	7831
	20		5154	6113
1	1	5	13287	-11310
	3		11192	-8540
	4		9228	-6923
	6		7716	-8213
	8		8853	-7283
	9		6931	7233
	11		8134	8613
	13		7049	7688
	15		5640	5754
1	1	-5	10287	12060
	2		6061	7273
	3		7367	8688
	4		9557	11714
	6		11109	13770
	8		9522	11346
	9		6387	-6249
	10		6725	7070
	11		6107	-7301
	13		7607	-7172
	15		6931	-4854
	16		5743	-6233
	18		5743	-6535
2	1	-5	14856	19327
	3		10573	11645
	5		5586	5977
	9		8558	-9339
	11		12824	-13468
	13		12093	-12140
	15		8970	-8409
3	1	-5	11123	12109
	2		7962	-6467
	3		9697	9216
	4		9933	-9240
	6		9419	-9865
	8		9385	-8070
	9		8956	-8488
	10		6513	-4998
	11		8624	-9104
	13		8970	-8950
	15		5763	-6978
	20		5199	3515
4	2	-5	10089	-7627
	4		14461	-12447
	6		16706	-14273
	8		13516	-11780
	10		7049	-6046
	16		6628	7297
	18		6115	7611
5	4	-5	8085	-6915
	6		9809	-8140
	8		6823	-7173
	9		6725	6226
	10		5594	-5666
	11		6471	7303
	13		4965	6249
	15		3204	4043
0	2	6	11044	-9959
	4		7244	-5915
	8		5864	5595
	10		7318	8762
	12		7666	8633
1	0	-6	10043	-11831
	15		6994	-4073
2	0	-6	1728	-2232
	7		10768	13243
	9		8531	9080
	15		4945	-6345
3	0	-6	12662	13494
	2		9150	9760
	3		7654	7130
	5		9980	9440
	7		9754	9460
	9		8014	6796
	10		8210	-7133
	12		8493	-8572
4	0	-6	14862	14070
	2		14937	12263
	4		10411	7658
	10		8570	-9649
	12		8466	-9689
	14		8186	-8087
5	3	-6	6890	-6587
	5		6827	-8798
	7		6697	-8543

Table III. Atomic and thermal parameters[a] with their estimated standard deviations (in parentheses).

Atom	x/a	y/b	z/c	B(Å^2)
Hg	0.1347(6)	0.0410(1)	0.2559(5)	—
C(1)	0.280(13)	0.115(3)	0.303(11)	1.76(1.6)
C(2)	0.581(16)	0.122(3)	0.460(13)	4.01(1.5)
C(3)	0.708(23)	0.171(5)	0.470(18)	7.70(1.9)
C(4)	0.560(22)	0.223(4)	0.424(17)	6.58(2.0)
C(5)	0.270(19)	0.217(4)	0.303(16)	5.76(2.4)
C(6)	0.164(18)	0.167(3)	0.262(16)	4.60(2.1)
C(7)	—0.438(18)	—0.097(4)	0.132(16)	5.45(2.0)
C(8)	—0.257(13)	—0.044(3)	0.207(11)	2.60(1.5)
O(1)	—0.053(7)	—0.037(2)	0.156(6)	1.27(0.75)
O(2)	—0.326(10)	—0.008(2)	0.308(8)	3.75(1.14)

Hg	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
	0.0185(10)	0.0018(5)	0.0114(7)	0.0002(3)	0.0075(7)	—0.0003(3)

[a] The anisotropic temperature factors for the Hg atom are in the form: $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+\beta_{23}kl)]$.

Table IV. Intramolecular and intermolecular distances (in Å) and angles[a] (in deg.) with their estimated standard deviations[6] in parentheses).

Hg-O(1)	2.11(4)	O(1)-Hg-C(1)	170(2)
Hg-C(1)	1.92(6)	O(1)-Hg-O(2)	52(2)
C(1)-C(2)	1.55(11)	O(1)-Hg-O(2)^{iii}	89(2)
C(2)-C(3)	1.35(14)	C(1)-Hg-O(2)^{iii}	93(2)
C(3)-C(4)	1.44(15)	C(1)-Hg-O(2)	131(2)
C(4)-C(5)	1.43(15)	C(6)-C(1)-C(2)	107(6)
C(5)-C(6)	1.33(13)	C(1)-C(2)-C(3)	118(8)
C(6)-C(1)	1.37(11)	C(2)-C(3)-C(4)	123(7)
C(7)-C(8)	1.54(12)	C(3)-C(4)-C(5)	114(9)
C(8)-O(1)	1.29(8)	C(4)-C(5)-C(6)	119(8)
C(8)-O(2)	1.31(9)	C(5)-C(6)-C(1)	133(8)
Hg-O(2)	2.85(5)	C(7)-C(8)-O(1)	118(6)
Hg-O(2)^{i}	3.11(5)	C(7)-C(8)-O(2)	120(6)
Hg-O(1)^{ii}	2.95(4)	O(1)-C(8)-O(2)	122(6)
Hg-O(2)^{iii}	2.94(5)		
C(3)-C(6)^{iii}	3.35(15)		
C(2)-C(7)^{i}	3.50(15)		
C(1)^{iv}-C(7)^{i}	3.71(14)		
C(4)-C(4)^{v}	3.97(14)		

[a] The positions are denoted as follows: no label x, y, z; (i) —x, —y, 1—z; (ii) —x, —y, —z; (iii) 1+x, y, z; (iv) x, y, 1+z; (v) x, 1/2—y, 1/2+z.

process were then computed using anisotropic thermal parameters for the mercury atom only. The weighting scheme adopted was $w=1$ for all reflections whose intensities were determined with an optical densitometer, and $w=0.25$ for reflections which were estimated visually (slightly above film background). The final reliability index R for the observed reflections was 0.111. Table II lists the observed structure amplitudes and calculated structure factors based on the final atomic parameters given in Table III. Atomic scattering factors used were taken from International Tables for X-ray Crystallography.[3]

Structure factors and Fourier syuthesis were calculated on the Science Research Coucil Atlas computer at Didcot, England, while the difference syntheses[4] and least-squares refinement[5,6] were carried out on the University Institute of Mathematics CAE 90.40 computer in Zagreb.

Results and discussion

The structure is shown in Figure 1 and the intramolecular and intermolecular distances and interbond angles are given in Table IV.

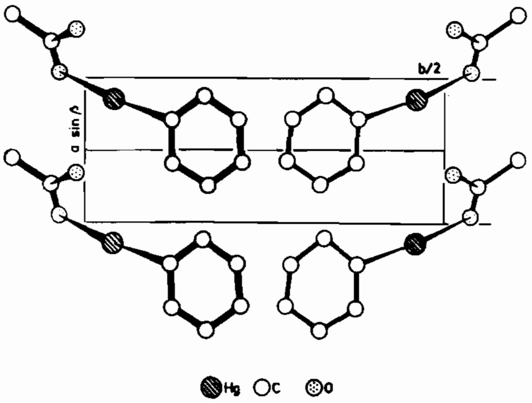

Figure 1. The structure of phenylmercury(II) acetate projected down the *c*-axis.

The crystal structure is built up from isolated phenylmercury(II) acetate molecules. The mercury atom, which is in general position in the unit cell, is on one side covalently bound to the phenyl ring and on the other side to one oxygen atom from the acetate ion so that the mercury has the charasteristic digonal co-ordination with two almost collinear bonds. The phenyl-carbon to mercury bond lenght of 1.92 Å is relatively short but similar to that of 1.97 Å found in mercury(II) oxycyanide.[7] The mercury-oxygen (from the acetate ion) bond length 2.11 Å, is very close to the values found in mercury(II) sulphate monohydrate[8] as well as in basic mercury(II)

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(3) « International Tables for X-ray Crystallography », Vol. III, Kynoch Press, Birmingham, 1962, p. 220.

(4) B. Zelenko, (1968). Private communication.

(5) S. Polić, (1968). A local version of the program by W.R. Busing, K.O. Martin, and H.A. Levy, ORFFE, A Fortran Crystallographic Function nad Error Program, U.S. Atomic Energy Commision Report ORHL-TM-305 (1962).

(6) «International Tables for X-ray Crystallography», Vol. II, Kynoch Press, Birmingham, 1959, p. 331

(7) (a) S. Šćavničar, *Acta Cryst.*, *13*, A57 (1960); (b) S. Šćavničar, *Z. Krist.*, *118*, 248 (1963).

(8) A. Bonefačić, *Acta Cryst.*, *14*, 116 (1961).

suphate dihydrate[9] (2.10 and 2.12 Å respectively). The second oxygen atom of the same acetate ion is 2.85 Å from mercury showing clearly that the phenylmercury(II) acetate does not have a chelate structure. This oxygen is approximately half way between two mercury atoms related by translation along the *a*-axis direction: the mercury-to-oxygen contact from the next nearest acetate along *a*-axis is 2.94 Å. The oxygen of the acetates of the upper and lower neighbouring molecules are 3.11 and 2.95 Å from mercury (Figure 2). All these values are the same or close to the sum of the van der Waals radii of mercury and oxygen (1.50+1.40).[10] The O–Hg–C bond angle deviates 10° from linearity what is very known in the stereochemistry of mercury.[10]

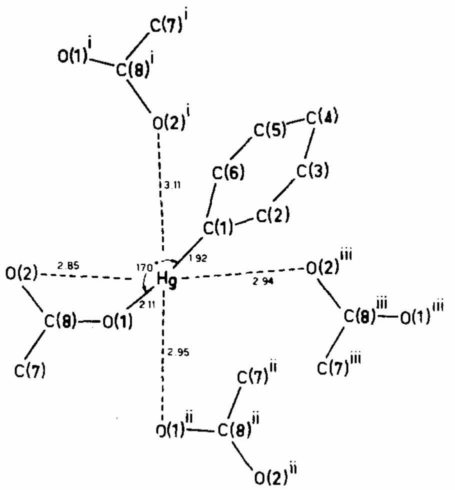

Figure 2. The arrangement of the acetate around mercury with atom designations.

The rather high standard deviations of the positional parameters of light atoms are explained by the presence of heavy mercury atom and the absence of an absorption correction. Nevertheless, the bond distances and angles within acetato ion and phenyl ring are consisten with the expected values.

The contacts between molecules are those expected for van der Waals interactions. The molecules are arranged in such a way that the planes of the phenyl rings are approximately parallel to the (110) plane of the crystal. The methyl groups of acetate ions are located between these phenyl rings planes so that there are two methyl-to-phenyl contacts ($C(2)...C(7)^{i}$ and $C(1)^{iv}...C(7)^{i}$) of 3.50 and 3.71 Å respectively. Along the *b*-axis direction the nearest intermolecular contact ($C(4)...C(4)^{v}$) of 3.97 Å is between two phenyl rings symmetrically related by the glide plane. Two phenyl rings symmetrically related by translation along the *a*-axis come close together making the distance between $C(3)...C(6)^{iii}$ atoms relatively short, 3.35 Å.

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(9) (a) A. Bonefačić, *Acta Cryst.*, *16*, A30 (1963); (b) A. Bonefacic, Thesis, University of Zagreb, 1963.

(10) D. Grdenić, *Quart. Rev. Chem. Soc., Lond.*, *19*, 303 (1965).