718. An X-Ray Diffraction Determination of the Crystal and Molecular Structure of Pentaphenylantimony.

By P. J. WHEATLEY.

A two-dimensional X-ray diffraction analysis of pentaphenylantimony, $Sb(C_6H_5)_5$, confirms that the molecule, unlike the phosphorus and arsenic homologues, approximates to a square pyramidal structure. The Sb-C bond lengths vary from 2.05 to 2.23 Å, with a standard deviation of 0.07 Å. The mean value of the length is 2.14 Å. There is no evidence that the axial Sb-C bond has a length different from the other four.

A RECENT communication ¹ listed the crystallographic constants and some of the physical properties of the pentaphenyls of phosphorus, arsenic, and antimony. It was stated that pentaphenyl antimony has a square pyramidal structure, and it was concluded, from the trend in the dipole moments, that the lower homologues would have similar structures. It has now been confirmed that the structure proposed for the antimony compound is correct, but a parallel three-dimensional analysis of the phosphorus compound has demonstrated that the two lower homologues, which are isomorphous, adopt trigonal bipyramidal configurations.

EXPERIMENTAL

 $C_{30}H_{25}Sb. M = 507.3.$ Triclinic. $a = 10.27_7 \pm 0.05, b = 10.57_4 \pm 0.05, c = 13.59_4 \pm 0.07 \text{ Å}, a = 79^{\circ} 00' \pm 30', \beta = 79^{\circ} 34' \pm 30', \gamma = 119^{\circ} 37' \pm 30'. U = 1139.4 \text{ Å}^3. D_m = 1.42. Z = 2. D_c = 1.412. F(000) = 512.$ Space group PI (C^1_i , No. 2). Cu- K_{α} radiation ($\lambda = 1.542$ Å), single crystal rotation and Weissenberg photographs.

The crystals (m. p. $171-172^{\circ}$) are white and beautifully formed. Each crystal exhibits many faces, and no two crystals appear alike under the microscope. Multiple-film Weissenberg

¹ Wheatley and Wittig, Proc. Chem. Soc., 1962, 251.



FIG. 1. Fourier projection down [b] calculated with antimony phases only. Contours are in steps of $2 \cdot 5 \text{ e}/\text{Å}^2$, starting at $5 \cdot 0 \text{ e}/\text{Å}^2$, except in the antimony peak where the contours are in steps of $10 \cdot 0 \text{ e}/\text{Å}^2$, starting at $10 \text{ e}/\text{Å}^2$.

ТΑ	BLE	1.

Atomic co-ordinates and orthogonal atomic co-ordinates in Å.

Atom	X	Y	Ζ	X'	Y'	Z'
Sb	1.6865	0.4090	3.4364	2.5548	0.2312	3·1928
C(1)	2.380	2.081	4.730	3.568	1.807	4.395
Č(2)	2.573	1.660	6.034	4.148	1.540	5.606
C(3)	3.068	2.769	6.744	4.803	2.540	6.266
C(4)	3.333	4.301	6.237	4.873	3.844	5.795
Č(5)	2.951	4.643	4.931	4.128	4.125	4.582
C(6)	2.543	3.636	4.225	3.549	3.185	3.925
C(7)	$2 \cdot 306$	-0.997	4.740	3.506	-1.232	4.404
C(8)	1.253	-2.269	5.967	2.980	-1.749	5.544
C(9)	1.721	-3.184	6.851	3.667	-2.727	6.366
C(10)	3.419	-2.507	6.579	5.057	-2.942	6.113
C(11)	4.394	-1.163	5.436	5.542	-2.297	5.051
C(12)	3.951	-0.552	4.660	4.911	-1.612	4.330
C(13)	-0.184	-1.840	3.256	0.871	-1.127	3.025
C(14)	-1.675	-2.196	3.133	-0.461	-0.771	2.911
C(15)	-2.685	-3.651	3.057	-1.366	-1.740	2.840
C(16)	-2.461	-4.872	3.064	-1.169	-3.071	2.847
C(17)	-1.061	-4.445	3.146	0.075	-3.321	2.923
C(18)	0.069	-2.906	3.254	1.091	-2.319	3.023
C(19)	3.723	1.677	1.526	3.720	0.129	1.418
C(20)	3.756	0.991	0.528	3.433	-0.765	0.491
C(21)	4.947	1.807	-0.880	4.022	-0.806	-0.812
C(22)	6.258	3.303	-1.032	5.112	0.013	-0.962
C(23)	6.281	4.009	-0.138	5.417	0.879	-0.128
C(24)	4.940	3.121	1.302	4.707	0.958	1.209
C(25)	0.437	1.325	2.655	1.221	1.616	2.467
C(26)	-0.632	1.306	3.449	0.539	2.278	3.204
C(27)	-1.777	1.954	3.005	-0.594	3.402	2.789
C(28)	-1.628	$2 \cdot 292$	1.665	-0.888	3.412	1.547
C(29)	-0.620	1.389	0.746	-0.346	2.862	0.693
C(30)	0.502	1.708	1.211	0.822	1.689	1.125

TABLE 2.

Observed and calculated structure factors on absolute scale $\times~10^2.$

	~	,	F		n n		~			n 7			~				
n	0	ı	F ₀	F _c I	$F_0 - F_c$	n	0	l	F ₀	F _c F	$r_0 \rightarrow F_c$	n	0	ı	F ₀	F _c f	$r_0 - F_c$
0	0	1	-865	- 560	305			10	4286	3439	847			$^{-1}$	1400	1493	- 93
*		2	9883	-9327	-556			-10	2600	2658	- 58			2	-3226	-3018	-208
		3	-856	-1093	237			11	-952	-801	-151			-2	-1478	-1853	375
*		4	12,891	11,619	1272			12	-3298	-2985	-313			3	3208	3050	158
		5	-1482	-1411	-71			-12	-1730	-1808	78			-3	-2450	-3022	572
*		6	-7624	8547	923			-13	611	569	42			4	3579	3277	302
		7	3068	-3592	524			14	1975	1706	269			-4	1362	1451	-89
		8	5334	6122	788			-14	983	1181	-198			5	-3233	-2702	-531
		9	1230	1168	62			15	-626	- 656	30			-5	1864	2129	-265
		10	-4237	-4256	19			16	-1850	-1694	156			6	-2232	-1943	-289
		12	2856	3061	205	4	0	10	-2522	- 2988	466			-6	-1177	-1482	305
		12	596	412	172	Ŧ	0	ň	4919	4956	- 44				4350	2673	677
		10	1025	1704	-175			1	5012	5590	567			-	1159	1974	000
		14	1835	-1704	-131			-1	- 3013	- 5580	567			-!	- 1152	-13/4	170
*1	~	10	1407	1338	49			4	/0/	-014				8	2001	24/0	1/8
. <u>*</u> 1	0	0	7276	6785	491			-2	2354	2142	212			-8	963	1266	- 303
*		1	-9287	-9928	641			3	-5178	-5531	353			9	3385	-2574	
*		-1	8926	8589	337			3	4549	4845	-296			-9	633	932	
*		2	-4839	- 5419	580			4	-1788	-1673	-115			10	-689	600	- 89
*		-2	20,605	-17,646	-2959			-4	3851	-3970	119			11	1572	1394	178
		3	-2803	3884	1081			5	5394	5261	133			12	1050	1129	- 79
		3	-2905	-2491	-414			- 5	-2642	-3271	629			13	-2441	-1831	-610
		4	4187	4796	609			6	2997	2838	159			14	-769	-622	-147
*		-4	10.179	9652	527			6	1944	1849	95			15	1291	1198	93
		5	-2401	-2895	494	*		7	-7593	-6648	-945			16	744	657	87
		5	5117	5004	113			-7	1514	2308	-794	8	0	0	- 535	- 565	30
		ĕ	-2977	- 2873	-104			8	-1422	-1317	-105	5	,	ĩ	-2395	-2197	-198
		ĕ	-6079	- 6494	352			_ă	-2290	-2799	509			_î	2553	2582	- 29
		7	1714	2198	-484			ğ	4283	4125	158			2	1382	970	412
			-2388	-2469	81			_ 9	-1431	-1814	383			$-\overline{2}$	599	649	50
		8	2544	2815	_ 271			10	1360	1352	17			3	4129	3272	857
			2200	3080	_ 683			10	1996	1857	-121			_ ?	-1755	-1748	7
		-0	_ 2411	2720	200			11	_4277	_ 3954	592				-1690	_1695	_ 85
		9	- 3411	3139	040 040			11	- 40//	1709				_4		- 1020	- 00
			-1407	0/92 100F	- 202			19	1029	1139	-1404				- 3295		- 04
		10	-1407		182			14	-1070	902	-108			5	- 3380	- 2000	- / 52
		-10	2720	- 3035	808			-12	- 902	1121	109			-3	1509	1000	491
		11	3233	2944	291			10	2883	2967	- 84			2	1070	104	842
		-11	-2395	-2723	328			-13	- 697	903	206			-	2220	2602	185
		-12	2156	2566	-410			14	809	760	49			-1	- 920	-1317	397
		13	-2522	-2480	-42			15	-2352	- 2076	-276			8	-2441	-2003	-438
		-13	1342	1722	-380			16	- 595	396	-199			.9	-1007	-883	-124
		14	- 787	-514	-273	-	-	17	1371	1233	138			10	1514	1290	224
		-14	-1081	-1406	325	5	0	0	2954	3000	-46			11	2399	1996	403
		15	1714	1450	264			1	5474	5122	352			12	-1436	-1084	-352
		-15	-1179	-1218	39			-1	-2731	- 3366	635			13	-1728	-1252	-476
		16	410	463	-53			2	-3581	-3103	-478			14	934	937	-3
*2	0	0	-6299	-6419	120			-2	3324	-3435	111			15	1304	883	421
*		1	5133	5101	32			3	-4370	- 3954	-416	9	0	0	-2332	-2582	250
*		-1	8032	8737	705			- 3	4482	5045	-563			1	-1297	-1073	-224
*		2	4821	6216	-1395			4	3385	2785	600			2	2287	2167	120
		-2	1659	1800	-141			-4	1215	1268	- 53			-2	1710	1827	-117
*		3	7343	8791	-1448	*		5	8536	7556	980			4	3280	-2693	-587
*		-3	-6656	-7171	515			5	-3452	-4000	548			-4	-1097	-1413	316
		4	-2881	- 3417	536			6	-2907	-2145	-762			-5	472	410	62
		$-\bar{4}$	-3757	3723	- 34			6	- 686	-1056	370			6	3443	2735	708
		5	-3507	-3340	-167			7	-4963	-3796	-1167			8	-2658	-2285	-373
		- 5	4638	4215	423			7	2073	2557	-484			10	2067	1585	482
		ĕ	633	935	- 302			8	3964	3392	572			12	-2629	-2112	- 517
		-6	- 967	-1089	122			, ğ	5659	4783	876			14	1431	1172	259
		7	4442	4668	-226			-9	-1679	-2179	500	10	0	-0	1070	-1277	207
		-7	-3523	- 3569	46			10	-2439	-2110	- 329		, v	ĭ	822	1128	- 306
		ġ	-4874	-4646	228			îĭ	- 3641	- 3055	586			$-\overline{1}$	- 802	-1053	251
		-8	-1235	-1197	38			-11	1054	1536	-482			2	1534	1384	150
		ğ	- 3380	- 3388				12	2020	1705	315			$-\overline{2}$	695	892	-197
		-9	2140	1728	412			13	2319	1896	423			3	985	-1376	391
		JÕ	3186	3272	-86			14	-2031	-1516	-515			4	-729	-808	79
		-10	927	755	172			15	-1761	-1384	-377			5	1346	1444	- 98
		îĭ	3596	3608	-12			16	1103	785	318			Ř	1233	1117	116
		-11	-2363	-2589	226	6	0	ĨÕ	5180	4373	807			7	-1634	-1790	156
		19	-2370	_1000	- 371	v	•	ň	-760	-87	673			ġ	691	- 655	36
		าร์		_1519	71			2	_5171	4919	- 259			ă	1041	1817	- 276
		-1º	1800	1765	75				- 2760	-2763	3			10	782	744	38
		14	1050	015	- 13					- 2103	- 246			îĭ	-1150		
		15	1700	1600	101			2	500		-198			12	_608	- 946	- 362
		10	_1447		_ 901			0	5210	1269	048	11	Δ	- 5	_ 503	- 789	100
±9	0	10	5541	- 1100	- 291			4	9790	4200	_ 529	11	0	2	- 050	-1224	250
-9	0	1	0041	0/19	200				3139	4344	- 203			0 4	- 309		05
		1	- 595	- 307	- 288			9	- /02	- 407	- 000			4	1070	1410	20
*		-1	474	91	383			- 2	-8/4		402			0	10/0	1410	340
-		Z	0891	0803	38			0	- 3822	-4994	- 020			2	- 821	- 898	11
*		z	10,019	9991	68			-6	-2305	- 2520	10			1	- 880	-1170	290
		3	- 593	- 929	336			7	- 695	-625	-70			8	954	1018	64
		4	-4234	-4228	-6			8	6843	5227	1616			9	898	1097	- 199
		-4	- 5307	-5474	167			-8	1672	2129	-457						
		5	802	-610	-192			-9	-535	-581	46	0	k	1	F_{0}	Fe	$F_0 - F_2$
		5	1346	1016	330			10	3556	3188	- 368	_					
*		6	6587	6219	368			-10	-970	-1271	301	_0	0	ř	-763	- 560	- 203
		-6	5015	5436	-421			12	2682	2281	401	*		2	- 9624	- 9281	- 343
		7	394	222	172			13	-706	-516	- 190			3	694	-1081	387
		-7	-1273	-1279	6			14	-2343	- 1934	-409			4	10,901	11,391	- 490
		8	-4906	-4700	-206		-	16	1915	1458	457			5	-1817	-1368	-449
		8	- 3434	-3330	-104	7	0	0	1904	1809	95			6	-8112	-8176	64
		9	1694	1258	436			1	-3628	3509	-119			7	-3404	-3382	-22

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TABLE 2. (Continued.)

0	ŀ	1	Fa	E _o E	$a - F_{c}$	0	k l	Fo	F _c F	$F_0 - F_0$	0	k	1 1	F.0.	Fc F	$a - F_{c}$
0	'n	v	10	• 0 •	0 - 0	0		- 0		0 -0	•		•	U	- 0 -	0 - C
		8	6084	5655	429			-1058	-978	80		1	15]	135	1307	-172
		ā	998	1056	58		12	1682	1799	-117	0	7	1	1575	- 3398	-177
		30	000	1000	-00		10	1500	1,00		0	'		0000	- 0000	970
		10	-3746	3761	15		-12	1980	1562	18			·1 8	1307	2931	376
		12	2936	2561	375		13	-1568	-1592	24			2 1	175	1278	-103
		19	E 9.4	0.05	100		10	2000	661	20			2 6	010	2270	51
		13	534	- 339	-199		-13	690	001	29			9	219	2210	
		14	-1491	-1337	-154		14	-1173	-1186	13			-33	3076 -	-2763	- 313
		1.0	1008	080	10		14	- 798	777	40			A _	594	- 517	-7
		10	1008	989	19		-14	- 128	- 111	49			* -	524	517	
*0	1	0	12.839	11.980	859		15	1478	1515	- 37			5	2947	-2873	-74
		i	2007	9529	375		16	544	502	_48			.5 1	684	1464	220
		1	- 2007	- 2052	515		10	044	1002	- 40		-			1101	100
		-1	2641	3150	509		17	-852	-1065	213			-6	565	403	-162
*		9			- 374	0	4 0	2005	1830	175			7 5	2914	3008	- 94
		4	-11,010			0	- U	2000	1000	100			+ 2	100	1//00	400
*		-2	-7325	-6394	971		1	- 5268	5390	122		_	·7 —2	132	- 1723	-409
		3	- 900		-747		-1	2575	3010	-435			9 -2	2450	-2772	322
			9100	0500	0.00		ā	2401	9700	070			ň i	000	005	090
		3	3128	2762	900		2	3421	3700	279			. 9	225	999	235
		4	2410	2866	-456		-2	-1811	-1860	49		1	10 1	123	922	201
*			7071	2000	771			9900	2000	0804		1	11 6	0.91	0120	0.9
		4	1011	6900	(11		5	0090	6202	2094			4	231	2139	54
		5	-1241	-155	-1086		-3	-7257	-6545	-712		1	2 -	759	-672	87
		É.	.1125	044	101		4	5994	4066	1158		1	19 _ 1	508	-1670	162
			-11.50	- 344	131		.	0224	4000	1100					-1010	102
		6	4051	-4511	460			2708	2642	66		1	lə	832	873	-41
		-6	-7891	-7534	-357		5	-8080	- 8893	813	0	8	0 -1	589	-1336	-253
		· ě	1505	1100	970		Ĕ	4105	9475	790		-	ň í	500	0020	190
			1909	1199	314		5	4190	3410	120			1	000	2038	150
		8	4010	4115	-105		6	-2084	-1906	-178			-1 :	2670 -	2205	465
		è	4916	3786	430		_6	- 2210	2063	-156			9 1	370	1575	205
			1210	11100	100		- 0	0100	- 2000	- 100			ã - 1	101	1010	
		9		-1516	- 21		7	3126	3639	- 913		_	·2 1	.104	778	326
		10	-3735	- 3505	-230		-7	-2999	-2663	-336			3 1	832	1999	-167
		10	4047	2510	595		ò	1011	1579	022			ğ i	077	1792	954
		-10	-4047	- 3912	- 999		0	1011	1978	499			-37	1011	-1725	- 504
		11	954	679	275		-8	2377	2473	- 96		_	-4	·913	-726	-187
		12	1684	1699	-15		9	-3785	- 3854	69			5 -	2733	-2459	-274
		14	1004	1035	- 10			- 5100	- 3004	000			<u> </u>	100	- 2400	- 110
		-12	3007	2700	307		-9	1632	1254	378			-ð .	1805	1657	148
		13	-1641	-1381	-260		10	-1830	-1788	-42			6 1	938	1994	- 56
		14	1401	1.001	10		ĩŏ	1500	1000	200			č .	070	2002	50
		14	1431	-1421	~~ 10		-10	-1989	-1226	- 303		_	.0	318	322	- 00
		-14	-1647	-1666	19		11	1560	2074	-514			7 5	2884	3186	- 302
		15	909	1012	911		11	-1425	1914	991			7 -	997	029	
		10	804	1015	- 211			- 1455	-1214	221		_		441	- 334	- 200
		16	884	899			12	2100	1663	437			8 ~	663	- 530	-133
0	9	0	906	619	- 288		-12	990	749	248		_	.8	.413	- 379	34
. '	-	4	10.000	-010	- 200		- 12	0140	0177	0.07			0	110	- 010	40
•		1	10,809	-7380	- 3429		13	- 2142	- 2477	330			9 - 2	199		49
		-1	4559	5065	506		-13	821	716	105		1	10 2	1547	1476	71
		ō	10 207	16 576	9751		15	1064	1240	995		-	11	1597	1492	167
		4	-15,327	-10,070	-2751		10	1004	1049	- 200				1001	1440	104
*		-2	-6073	-4193	-1880		17	-958	-1003	45			12 - 1	1223	-1120	-103
		3	9603	10 202	- 599	0	5 0	2344	2341	3		1	13 _	1210	-1350	140
			1000	10,202	000	0		0050	07.07					210	- 1000	
		3	-1306	-1383	77		1	- 2978	- 3967	989			14	567	367	200
		4	5048	5276	-228		-1	3092	3434	342		1	15	848	857	-9
		â	4020	2840	100		-	9129	9150	91	0	0	ŏ	1007	- 050	197
		-4	4039	3849	190		4	2138	- 2109	41	0	9	0 -	1087	- 950	-15/
		5	-3051	-3154	103		-2	-1612	-1460	-152			1 -1	924	-1829	95
		- 5	5630	5967	- 337		3	3721	4044	- 323		-	.1 1	574	1406	168
		-0	0000	0001	- 001			0121	1011	-020		-		011	1400	100
		6	-4413	-4852	439		- 3	- 3404	- 3444	40			2.	010	998	12
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		-10	-1726	1797	71			- 904	-895	- 9			8 ~	-809	-877	68
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photographs were taken round [a] and [b]. Relative intensities were obtained visually by comparison with a standard chart, and no correction was made for absorption ($\mu = 101.8 \text{ cm}.^{-1}$). 262 0kl and 263 hol reflexions were observed to be non-zero. The co-ordinates of the antimony

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atom were found from sharpened Patterson syntheses, and Fourier projections calculated with the antimony phases sufficed to define the approximate positions of the carbon atoms. The original h0l electron density projection, calculated with the antimony phases only, is reproduced in Fig. 1, since it shows, despite the severe overlapping, that the molecule cannot be a trigonal bipyramid. Refinement of the two projections was carried out initially by hand calculations of successive Fourier and difference maps. It soon became apparent that many of the stronger low-order reflexions were suffering badly from extinction. These planes are marked by asterisks in Table 2. 10 0kl reflexions and 21 h0l reflexions were so affected. Extinction corrections were applied to these planes,² but they were omitted completely from the subsequent refinement cycles.

The hand calculations had reduced the R factor to about 15% for each projection. At this stage an Elliott 803B computer became available, and the later refinement was carried out with the programming system constructed by Daly, Stephens, and Wheatley.³ Several more difference maps were calculated for each projection with the non-extinguished planes only, and finally the co-ordinates and individual isotropic temperature factors were refined by a least-squares analysis, each projection being treated quite independently. The final R factor for the 0kl projection was $6\cdot5\%$, and for the h0l projection $8\cdot4\%$. The z co-ordinates were then meaned and, since it was felt that the number of variables was too large, an overall isotropic temperature factors was calculated which gave an R factor of $11\cdot1\%$ for the 0kl and $12\cdot3\%$ for the h0l projection. These figures include the extinguished planes but omit non-observed reflexions. The scattering factors were taken from International Tables, with the antimony curve corrected for the real part of the dispersion. The temperature factors used for the antimony atom were $3\cdot77$ and $2\cdot98$, and for the carbon atoms $5\cdot68$ and $4\cdot90$ Å² for the 0kl and h0l projections respectively.

RESULTS

The co-ordinates of the atoms are given in Table 1, together with the orthogonal coordinates referred to a set of axes in which [b'] coincides with the original triclinic axis [b]; [a'] is the projection of the triclinic axis [a] on the plane perpendicular to [b']; and [c'] is perpendicular to [a'] and [b']. Table 2 gives the observed and calculated structure

TABLE 3.

C(1)SbC(19) 104

C(7)SbC(25)

163

E	Bond lengths (Å) and bond angles (°) a	t the a	ntimony atom.	
Sb-C(1)	$\dots 2.23$	C(1)SbC(7)	89	C(7)SbC(19)	101
Sb-C(7)	2.12	C(1)SbC(25)	91	C(13)SbC(19)	109
Sb-C(13)	2.17	C(7)SbC(13)	88	C(19)SbC(25)	95
Sb-C(19)	2·13	C(13)SbC(25)	84	C(1)SbC(13)	147

factors. Fig. 2 shows the molecule and the labelling of the atoms. Table 3 gives the bond lengths and angles at the antimony atom. The standard deviation of the co-ordinates of the antimony atoms are 0.003 Å, and of the carbon atoms about 0.07 Å. Thus the standard deviation of the Sb-C bond lengths is about 0.07 Å and of the C-C lengths about 0.10 Å. Angles involving antimony have a standard deviation of about 3° and those involving only carbon atoms about 6°. These standard deviations were obtained by normal least squares procedure from the residuals, but, since they involve projections, may well be over-optimistic. The C-C bond lengths vary between 1.15 and 1.71 Å, and have a mean value of 1.37 Å with a standard deviation of 0.02 Å. The mean value of the Sb-C bond length is 2.14 Å which agrees well with the distance found in dichlorotris-2-chlorovinylstibine, (ClCH=CH)₃SbCl₂.⁴ It should be noticed, however, that the configuration of the bonds round the antimony atom found in this stibine is trigonal bipyramidal. There is no evidence that the axial bond in antimony pentaphenyl differs in length from the other four Sb-C bonds.

² James, "The Optical Principle of the Diffraction of X-rays," G. Bell and Sons, Ltd., London, p. 292.

³ Daly, Stephens, and Wheatley, in course of publication.

Sb-C(25)

2.05

⁴ Struchkov and Khotsanova, Doklady Akad. Nauk S.S.S.R., 1953, 91, 565.

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The molecule has, within the limits of error, a two-fold axis of symmetry through the axial bond, as can be seen in Fig. 2. However the description of the molecule as being a square pyramid is a slight over-simplification, as there does seem to be a significant difference between the angles C(1)SbC(13) and C(7)SbC(25). The difference is such that the two atoms C(1) and



FIG. 2. Drawing of the molecule and labelling of the atoms.

C(13) lie further below the antimony atom than the two atoms C(7) and C(25). The mean least-squares plane through the four atoms forming the base of the pyramid is given, in terms of the orthogonal co-ordinates listed in Table 1, by the equation

$$-0.5452X' + 0.1144Y' + 0.8305Z' = 1.7483.$$

The departure of the four carbon atoms from this plane are: C(1), 0.16; C(7), -0.14; C(13), 0.16; C(25), -0.18 Å. The distance of the antimony atom from this plane is 0.46 Å.

The benzene rings are all planar within the limits of error. The mean planes through the five rings are given by the equations

I	0.8407X' - 0.1930Y' - 0.5060Z' = 0.3862
II	0.2605X' + 0.7793Y' + 0.5700Z' = 2.5039
III	-0.0769X' - 0.0111Y' + 0.9970Z' = 2.9546
\mathbf{IV}	0.6412X' - 0.6622Y' + 0.3877Z' = 2.8557
v	0.6926X' + 0.7110Y' - 0.1219Z' = 1.6556

The greatest departure of any carbon atom from its mean plane is 0.07 Å. The angles between the rings I and III is 124° , and between the rings II and V 48° .

The intermolecular contacts are all between benzene rings. There are 27 contacts less than 4.0 Å, the shortest being 3.55 Å.

I thank Professor G. Wittig of the University of Heidelberg who kindly provided the samples of the pentaphenyls of phosphorus, arsenic, and antimony.

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