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408. *The Crystal and Molecular Structure of Pentaphenylphosphorus.*

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The structure of pentaphenylphosphorus, $P(C_6H_5)_5$, has been elucidated by three-dimensional *X*-ray diffraction methods. Unlike pentaphenylantimony which has a square pyramidal structure, pentaphenylphosphorus (and, presumably, the isomorphous pentaphenylarsenic) has a trigonal bipyramidal configuration. The molecule itself has no symmetry because of the asymmetric orientation of the benzene rings, which no doubt accounts for the finite dipole moment. The mean length of the two axial $P-C_6H_5$ bonds is 1·987 Å, and of the three equatorial $P-C_6H_5$ bonds 1·850 Å.

A recent communication listed the crystallographic constants and some of the physical properties of the pentaphenyls of phosphorus, arsenic, and antimony.[1] It was stated that the structure of pentaphenylantimony is based on a square pyramid and, from the regular trend in the dipole moments, it was concluded that the two lower homologues,

[1] Wheatley and Wittig, *Proc. Chem. Soc.*, 1962, 251.

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which are isomorphous, would have similar structures. Although it has now been demonstrated that the structure of pentaphenylantimony is indeed square pyramidal,[2] the extrapolation to the lower homologues, which has been questioned in the meantime,[3] is invalid. The present analysis shows that pentaphenylphosphorus (and, presumably the isomorphous pentaphenylarsenic) has a trigonal bipyramidal structure with only slight distortions.

Experimental

$C_{30}H_{25}P$. $M = 416{\cdot}5$. Monoclinic. $a = 10{\cdot}029 \pm 0{\cdot}015$, $b = 17{\cdot}215 \pm 0{\cdot}018$, $c = 14{\cdot}170 \pm 0{\cdot}017$ Å, $\beta = 112° 03' \pm 30'$. $U = 2267{\cdot}5$ Å^3. $D_m = 1{\cdot}22$. $Z = 4$. $D_c = 1{\cdot}220$. $F(000) = 880$. Space group Cc (C_s^4, No. 9). Cu-K_α radiation ($\lambda = 1{\cdot}542$ Å). Single crystal rotation and Weissenberg photographs.

The crystals, m. p. 124·5°, are initially white, but are photosensitive. When exposed in air to the *X*-ray beam they rapidly turn black, but the effect seems to be only a surface one since there is no observable change in the quality of the photographs nor in the intensities of the diffracted beams. Multiple-film Weissenberg photographs were taken round the three principal axes. Relative intensities were estimated visually by comparison with standard charts. All layer lines were brought to the same relative scale by correlation through common reflexions. 2140 independent reflexions were observed to be non-zero. No correction was made for absorption ($\mu = 12{\cdot}5$ cm.$^{-1}$). The following systematic absences were observed: hkl reflexions, absent for $h + k$ odd: $h0l$ reflexions, absent for h odd and l odd: $0k0$ reflexions, absent for k odd. These absences are consistent with either the centrosymmetric space group $C2/c$ or the non-centrosymmetric space group Cc. The general distribution of the intensities of the diffracted spectra suggested that the space group was non-centrosymmetric, and this conclusion was confirmed by applying the Wilson statistical test[4] to the $hk0$ and $0kl$ reflexions. Moreover, a test for pyroelectricity showed distinct positive results. The test was performed by a method which differs slightly from those usually used[5] and, since it is easy to carry out and the effects are very marked, will be briefly described.

A quantity (50—100 mg.) of the substance consisting of small crystals of approximately similar dimensions (0·05—0·3 mm.) is placed in a spoon made of anodized aluminium. The lip of the spoon is dipped below the surface of some liquid nitrogen so that about 0·5 c.c. runs on to the crystals. The spoon is lifted out and held firmly on a steady surface. As the liquid nitrogen evaporates, a circular motion sets in which rolls the crystals together into a sphere. When the last trace of liquid nirogen has disappeared, the sphere comes to rest at the centre of the spoon. If the sample is centrosymmetric, the sphere suddenly collapses within one or two seconds. On the other hand, if the crystals possess no symmetry centre, the sphere will remain intact apparently indefinitely. This technique has been applied to a number of samples of known and of unknown structure, and appears to yield very satisfactory results. It has the great merit that a number of samples can be tried one after another, and the results compared.

The solution of the crystal structure has a rather curious history. The y co-ordinate of the phosphorus atom was obtained from a sharpened Patterson synthesis calculated with the $0kl$ reflexions, and confirmed from the $hk0$ projection. Attempts were then made to solve the $0kl$ projection with only the phosphorus phases, and on the assumption that the molecule had a trigonal bipyramidal structure. These attempts were unsuccessful, partly because of the large amount of hand calculations that were necessary. At this stage crystals of pentaphenylantimony became available, and the structure of the antimony compound was shown to be based on a square pyramid. Attention was then turned again to the phosphorus compound, and immediately an adequate trial solution was found for the $0kl$ projection on the assumption that the molecule was a square pyramid. Although the R factor was 35%, the agreement amongst the low order planes left no doubt that the solution was essentially correct. At this stage, an Elliott 803B computer became available, and all subsequent work was carried out with the programming system devised by Daly, Stephens, and Wheatley.[6] Firstly the $0kl$

[2] Wheatley, *J.*, in the press.
[3] Muetterties, Mahler, and Schmutzler, *Inorg. Chem.*, 1963, **2**, 613.
[4] Wilson, *Acta Cryst.*, 1949, **2**, 318.
[5] Bunn, "Chemical Crystallography," Clarendon Press, 1st Edn., p. 292.
[6] Daly, Stephens, and Wheatley, MRSA Final Report No. 52.

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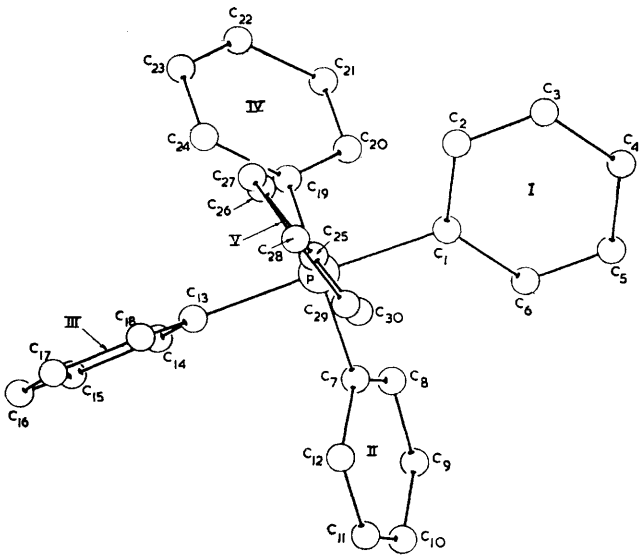
projection was refined to an R of 17% by means of successive difference maps. During this stage it became clear that the molecule was not a square pyramid, but a trigonal bipyramid. With the known y co-ordinates and a molecular model, a set of x co-ordinates were estimated and used to compute structure factors for the $hk0$ reflexions. The R factor was 32%. A three-dimensional Fourier synthesis was then calculated with the 1139 reflexions that had a value of sin θ/λ less than 0·5. The co-ordinates obtained from the Fourier synthesis were then used for two least-squares cycles on the 398 planes with sin θ/λ less than 0·35. For these planes R fell to 18%. The structure was then refined, all 2140 reflexions being used. Four cycles of least-squares analysis with isotropic temperature factors, and five cycles with anisotropic temperature factors were carried out. The final R factor for all observed reflexions was 8·7%.

Three planes (marked by asterisks in Table 3) were omitted from the refinement as the calculated values were less than 0·3 of the observed. The scattering factors were taken from International Tables.



Pentaphenylphosphorus as it appears when viewed down an axis normal to the yz plane, and the labelling of the atoms.

Results

The final atomic co-ordinates, and the orthogonal co-ordinates referred to a set of axes in which [b'] coincides with the original [b], [a'] is the projection of the monoclinic axis [a] on to the plane perpendicular to [b], and [c'] is perpendicular to [a'] and [b'], are given in Table 1. Standard deviations are given in parentheses after each co-ordinate, expressed as units in the last place. Thus 1·4638 (105) means 1·4638 $\pm$ 0·0105. The thermal factors and their standard deviations are given in Table 2. The observed and calculated structure factors, obtained from the co-ordinates listed in Table 1, are shown in Table 3. Table 4 shows the bond lengths and angles with their standard deviations. The Figure shows the molecule as it appears when projected down an axis normal to the yz plane, and also the labelling of the atoms.

The two axial P–C_6H_5 bonds have a mean length of 1·987 Å, and the three equatorial bonds a length of 1·850 Å. The difference between these is highly significant, and is the same as found in phosphorus pentachloride by electron diffraction.[7] It is also in the sense predicted on theoretical grounds.[8] The length of the equatorial bonds does not differ significantly from the P–C_6H_5 distance found in triphenylphosphorus.[9] The mean C–C distance is 1·390 Å and there are no significant departures from this mean, except for the

[7] Rouault, *Ann. physique*, 1940, **14**, 78.
[8] Cotton, *J. Chem. Phys.*, 1961, **35**, 228.
[9] Daly, private communication.

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TABLE 1.

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

	X	Y	Z	X'	Y'	Z'
P	−0·0128 (19)	1·9392 (12)	0·0267 (19)	−0·0228	1·9392	0·0247
C(1)	−0·1037 (66)	3·8384 (62)	−0·5911 (62)	0·1182	3·8384	−0·5479
C(2)	−0·1331 (76)	4·0547 (64)	−1·9717 (65)	0·6071	4·0547	−1·8275
C(3)	0·0072 (81)	5·3482 (73)	−2·4481 (72)	0·9262	5·3482	−2·2690
C(4)	0·1901 (86)	6·4436 (73)	−1·5348 (87)	0·7663	6·4436	−1·4225
C(5)	0·2216 (105)	6·2437 (78)	−0·1669 (95)	0·2843	6·2437	−0·1547
C(6)	0·0892 (74)	4·9497 (60)	0·3185 (59)	−0·0304	4·9497	0·2952
C(7)	−0·1245 (62)	2·3965 (60)	1·7902 (60)	−0·7966	2·3965	1·6593
C(8)	−1·3679 (66)	2·9578 (66)	1·8468 (71)	−2·0612	2·9578	1·7117
C(9)	−1·4603 (88)	3·2184 (76)	3·1827 (85)	−2·6551	3·2184	2·9499
C(10)	−0·2799 (91)	3·0048 (80)	4·4534 (81)	−1·9518	3·0048	4·1277
C(11)	0·9870 (90)	2·4636 (75)	4·3744 (76)	−0·6552	2·4636	4·0545
C(12)	1·0469 (72)	2·1496 (68)	3·0646 (68)	−0·1036	2·1496	2·8405
C(13)	0·1902 (60)	0·0583 (58)	0·7103 (61)	−0·0765	0·0583	0·6583
C(14)	−0·9565 (77)	−0·4959 (75)	1·0041 (88)	−1·3334	−0·4959	0·9307
C(15)	−0·8806 (101)	−1·7787 (83)	1·5713 (102)	−1·4705	−1·7787	1·4564
C(16)	0·3650 (100)	−2·5497 (82)	1·8099 (93)	−0·3145	−2·5497	1·6775
C(17)	1·4638 (100)	−2·0401 (77)	1·5111 (98)	0·8965	−2·0401	1·4006
C(18)	1·4051 (77)	−0·7353 (65)	0·9824 (76)	1·0363	−0·7353	0·9105
C(19)	−1·6854 (59)	1·5211 (60)	−1·5293 (61)	−1·1113	1·5211	−1·4174
C(20)	−2·8349 (63)	2·4387 (67)	−1·9738 (68)	−2·0939	2·4387	−1·8294
C(21)	−4·0997 (72)	2·0968 (80)	−3·1098 (76)	−2·9322	2·0968	−2·8823
C(22)	−4·2290 (72)	0·9014 (80)	−3·8305 (71)	−2·7910	0·9014	−3·5503
C(23)	−3·0784 (74)	0·0160 (73)	−3·4159 (73)	−1·7960	0·0160	−3·1661
C(24)	−1·8197 (68)	0·3247 (62)	−2·2638 (67)	−0·9698	0·3247	−2·0982
C(25)	1·6993 (64)	1·8556 (59)	−0·2380 (68)	1·7886	1·8556	−0·2206
C(26)	1·8263 (72)	1·1316 (74)	−1·3808 (66)	2·3447	1·1316	−1·2798
C(27)	3·1353 (81)	1·0105 (87)	−1·5654 (83)	3·7230	1·0105	−1·4509
C(28)	4·3795 (75)	1·5989 (104)	−0·5307 (94)	4·5787	1·5989	−0·4919
C(29)	4·2443 (74)	2·3132 (100)	0·5643 (93)	4·0325	2·3132	0·5230
C(30)	2·9215 (69)	2·4918 (78)	0·7057 (75)	2·6566	2·4918	0·6541

TABLE 2.

Thermal parameters in Å^2.

	U_{11}	U_{22}	U_{33}	$2U_{12}$	$2U_{23}$	$2U_{13}$
P	0·0377 (5)	0·0483 (5)	0·0388 (5)	0·0044 (11)	0·0038 (11)	0·0244 (9)
C(1)	0·0485 (27)	0·0556 (28)	0·0428 (25)	−0·0058 (46)	0·0072 (44)	0·0286 (47)
C(2)	0·0619 (33)	0·0597 (31)	0·0437 (28)	0·0015 (53)	0·0079 (48)	0·0396 (52)
C(3)	0·0639 (35)	0·0733 (37)	0·0511 (30)	0·0000 (61)	0·0148 (56)	0·0563 (58)
C(4)	0·0668 (39)	0·0636 (33)	0·0705 (41)	−0·0050 (60)	0·0197 (63)	0·0638 (69)
C(5)	0·0876 (51)	0·0620 (33)	0·0715 (44)	−0·0096 (71)	−0·0124 (65)	0·0630 (79)
C(6)	0·0635 (34)	0·0550 (26)	0·0415 (28)	−0·0080 (53)	0·0001 (41)	0·0381 (58)
C(7)	0·0458 (26)	0·0567 (27)	0·0406 (24)	0·0071 (44)	0·0123 (43)	0·0319 (44)
C(8)	0·0475 (28)	0·0619 (31)	0·0570 (30)	0·0018 (49)	0·0048 (54)	0·0483 (52)
C(9)	0·0737 (42)	0·0688 (36)	0·0680 (40)	−0·0110 (67)	0·0011 (63)	0·0840 (71)
C(10)	0·0800 (46)	0·0761 (39)	0·0606 (37)	−0·0030 (74)	0·0096 (66)	0·0788 (73)
C(11)	0·0803 (46)	0·0694 (38)	0·0480 (30)	0·0003 (71)	0·0004 (59)	0·0327 (65)
C(12)	0·0521 (31)	0·0642 (31)	0·0465 (29)	0·0083 (51)	0·0135 (51)	0·0229 (50)
C(13)	0·0412 (25)	0·0552 (28)	0·0448 (27)	0·0088 (43)	0·0088 (44)	0·0215 (44)
C(14)	0·0549 (32)	0·0668 (35)	0·0753 (43)	−0·0061 (59)	0·0273 (64)	0·0473 (65)
C(15)	0·0787 (50)	0·0662 (38)	0·0774 (50)	0·0008 (70)	0·0237 (72)	0·0450 (83)
C(16)	0·0824 (49)	0·0660 (37)	0·0694 (43)	0·0091 (72)	0·0207 (66)	0·0428 (79)
C(17)	0·0769 (47)	0·0687 (42)	0·0691 (44)	0·0327 (70)	0·0308 (67)	0·0405 (77)
C(18)	0·0581 (34)	0·0571 (31)	0·0612 (35)	0·0210 (57)	0·0144 (56)	0·0332 (57)
C(19)	0·0392 (23)	0·0582 (28)	0·0433 (25)	0·0045 (43)	0·0091 (47)	0·0253 (42)
C(20)	0·0420 (26)	0·0629 (32)	0·0507 (29)	0·0151 (47)	0·0051 (51)	0·0225 (48)
C(21)	0·0476 (32)	0·0847 (44)	0·0518 (33)	0·0106 (60)	0·0205 (62)	0·0143 (54)
C(22)	0·0484 (31)	0·0859 (43)	0·0480 (29)	−0·0157 (60)	0·0186 (63)	0·0133 (50)
C(23)	0·0574 (35)	0·0717 (37)	0·0517 (33)	−0·0225 (59)	−0·0070 (55)	0·0294 (57)
C(24)	0·0512 (28)	0·0559 (29)	0·0484 (27)	−0·0030 (49)	−0·0008 (49)	0·0262 (49)
C(25)	0·0405 (24)	0·0561 (28)	0·0502 (29)	−0·0038 (43)	−0·0011 (46)	0·0224 (44)
C(26)	0·0538 (31)	0·0766 (39)	0·0490 (30)	0·0039 (56)	−0·0153 (54)	0·0472 (53)
C(27)	0·0570 (36)	0·0921 (48)	0·0660 (37)	0·0082 (68)	−0·0091 (76)	0·0675 (64)
C(28)	0·0460 (35)	0·1081 (56)	0·0755 (45)	−0·0020 (70)	−0·0005 (84)	0·0663 (68)
C(29)	0·0462 (34)	0·1035 (53)	0·0712 (45)	−0·0210 (70)	−0·0178 (84)	0·0341 (66)
C(30)	0·0428 (27)	0·0826 (41)	0·0586 (35)	−0·0201 (57)	−0·0300 (64)	0·0322 (52)

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TABLE 3.

h	k	l	F_o	F_c	$\|F_o\|\|F_c\|$	A_c	B_c	h	k	l	F_o	F_c	$\|F_o\|\|F_c\|$	A_c	B_c
2	0	0	16254	18001	-1747	17968	1086	2	18	0	1096	1031	65	900	502
4	0	0	6044	4494	1550	4489	205	4	18	0	842	751	91	650	-377
6	0	0	7113	6744	369	6734	-367	6	18	0	986	807	179	806	48
8	0	0	1605	1549	56	1511	-340	1	19	0	674	549	125	391	365
10	0	0	2489	2567	-78	2545	332	3	19	0	790	685	105	685	3
1	1	0	6685	10734	-2049	10734	-99	5	19	0	488	416	72	393	-136
3	1	0	3301	2051	1210	-1364	-719	2	20	0	450	353	97	-211	283
5	1	0	1664	1686	-22	1503	-1140	1	21	0	204	173	31	-162	-61
7	1	0	4375	4803	-428	4791	343	3	21	0	334	255	79	155	203
9	1	0	825	760	65	715	257	1	1	1	6671	7843	-1172	-2365	7470
11	1	0	792	868	-76	852	-166	3	1	1	6704	6737	-33	2347	6315
0	2	0	3723	4480	-757	4480	0	5	1	1	4210	4165	45	563	4052
2	2	0	7875	8331	-456	-7861	2758	7	1	1	5143	5585	-442	256	5577
4	2	0	5204	4432	772	-4426	-235	9	1	1	2317	2300	17	615	2216
6	2	0	549	580	-31	-547	192	11	1	1	732	947	-215	334	856
8	2	0	2323	2341	-18	-2117	1000	-1	1	1	7969	9919	-1950	-362	9912
10	2	0	969	662	307	176	638	-3	1	1	10251	9994	257	4501	8923
1	3	0	3182	3834	-652	-3323	-1912	-5	1	1	8406	8646	-240	4480	7395
3	3	0	1052	834	218	820	-152	-7	1	1	3577	3459	118	1003	3310
5	3	0	693	612	81	507	343	-9	1	1	1342	1395	-53	-1354	44
7	3	0	2483	2528	-45	-2276	1100	-11	1	1	1033	1197	-164	1	1197
9	3	0	2174	2193	-19	-88	2191	0	2	1	8801	10464	-1663	665	10443
11	3	0	469	554	-85	-246	496	2	2	1	1486	944	542	863	-363
0	4	0	14853	17939	-3086	-17939	0	4	2	1	2386	1991	395	716	1857
2	4	0	6831	6580	251	-5784	-3137	6	2	1	3218	3336	-118	443	3306
4	4	0	663	471	192	-451	-135	8	2	1	687	565	122	-465	321
6	4	0	790	876	-86	-264	835	10	2	1	1245	1434	-189	-218	-1417
8	4	0	1016	988	28	-945	289	-2	2	1	10615	12425	-1810	-10931	-5515
10	4	0	928	829	99	-823	-98	-4	2	1	4240	4450	-210	-3282	3005
1	5	0	6639	6772	67	-455	-6757	-6	2	1	3058	3050	8	-2286	2019
3	5	0	1129	1036	93	345	-977	-8	2	1	2621	2868	-267	-2864	-369
5	5	0	3759	3299	460	-2763	1802	-10	2	1	1008	1035	-27	-582	656
7	5	0	2309	2110	199	-1582	-725	-12	2	1	1041	1176	-137	277	1145
9	5	0	980	970	10	-870	430	1	3	1	7240	7557	-317	-5407	-5260
11	5	0	1215	1061	154	-1043	194	3	3	1	5729	5707	22	-5354	-1977
0	6	0	4483	3167	1316	3167	0	5	3	1	3364	3203	161	-900	3074
2	6	0	1243	718	525	-395	-599	7	3	1	3326	3478	-152	113	3476
4	6	0	2091	1746	345	269	1725	9	3	1	1367	1173	194	4	1173
6	6	0	1665	1713	-48	-638	1590	11	3	1	881	1010	-129	-182	993
8	6	0	497	447	50	406	187	-1	3	1	1116	1143	-27	1063	419
10	6	0	273	235	38	1	235	-3	3	1	4511	4540	-29	-1066	-4413
1	7	0	3292	3004	288	2776	-1148	-5	3	1	4491	4668	-177	2575	3654
3	7	0	4469	4567	-98	3376	3075	-7	3	1	1505	1676	-171	1479	766
5	7	0	1370	1285	85	-1057	731	-9	3	1	1889	1834	55	-1741	-576
7	7	0	1461	1493	-32	1361	-613	-11	3	1	712	742	-30	-335	662
9	7	0	494	493	1	268	414	0	4	1	12621	13662	-1041	13174	3694
11	7	0	229	245	-16	236	-65	2	4	1	1118	966	152	-412	-674
0	8	0	7348	8335	-987	8335	0	4	4	1	5624	5058	566	-3240	3884
2	8	0	5737	6016	-279	4641	3571	6	4	1	1773	1974	-201	920	1747
4	8	0	3190	3305	-115	3231	-694	8	4	1	1165	1133	32	-171	-1120
6	8	0	1207	1139	68	1123	-152	-2	4	1	5508	5244	664	1880	4803
8	8	0	1223	1187	36	1055	458	-4	4	1	1758	2179	-381	-1428	1546
10	8	0	1574	1484	90	1421	429	-6	4	1	3414	3002	412	1180	2760
1	9	0	3751	3287	464	3151	-934	-8	4	1	585	533	52	-505	-170
3	9	0	2392	2511	-119	2273	1066	-10	4	1	657	655	2	361	547
5	9	0	2773	2525	248	2503	-332	1	5	1	3060	2925	135	2839	709
7	9	0	1585	1552	33	1398	-673	3	5	1	3563	3546	17	-1848	-3023
9	9	0	1002	1115	-113	1037	409	7	5	1	3196	3168	28	1016	-3001
0	10	0	1201	1035	166	1035	0	9	5	1	1667	1396	271	799	-1145
2	10	0	2879	2273	6	1603	-1611	-1	5	1	5384	5264	120	4786	-2191
4	10	0	1582	1670	-88	1076	-1277	-3	5	1	2167	2090	97	-2021	534
6	10	0	2232	2267	-35	2202	537	-5	5	1	1342	1150	192	-525	1023
8	10	0	513	575	-62	558	140	-7	5	1	845	859	-14	407	-756
10	10	0	320	287	33	265	111	-9	5	1	601	611	-10	520	622
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7	11	0	535	580	-45	-451	308	4	6	1	2276	2107	169	-2039	-277
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2	12	0	3447	3388	59	-2444	-2347	10	6	1	1058	1069	-11	402	-990
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3	13	0	1007	1054	-47	1393	651	-10	6	1	972	1060	-88	574	-891
5	13	0	1016	1041	-25	-352	960	1	7	1	2113	2391	-278	-643	-2303
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6	14	0	632	698	-66	-516	470	-3	7	1	4972	4831	141	-720	-4777
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1	15	0	2221	2105	116	-2058	443	-7	7	1	2828	2359	469	-717	-2247
3	15	0	864	919	-55	-143	908	-9	7	1	1547	1655	-108	361	-1611
5	15	0	958	1024	-66	-1023	48	-11	7	1	1088	1247	-159	354	-1062
7	15	0	370	361	9	-306	-192	0	8	1	4058	4370	-312	-2051	-3459
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4	16	0	414	358	56	297	199	6	8	1	1187	1281	-94	-832	-974
6	16	0	524	493	31	457	186	8	8	1	571	548	23	-497	-230
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1	17	0	1342	1258	84	1228	272	-4	8	1	1648	1666	182	1020	-1317
3	17	0	1190	1132	58	1068	-376	-6	8	1	2000	2420	-120	-466	-2143
5	17	0	1196	1092	104	1015	-404	-8	8	1	908	965	-57	-260	-924
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TABLE 3. (*Continued.*)

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-3	9	1	4433	4072	361	141	4070
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-9	9	1	784	918	-134	-706	-587
11	9	1	301	333	-32	-274	150
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4	10	1	2218	2275	-57	163	2269
6	10	1	1538	1700	-162	1292	1105
8	10	1	1046	939	107	821	455
-2	10	1	3502	3386	116	286	3374
-4	10	1	3022	3397	-375	-687	3327
-6	10	1	1069	1024	45	-470	910
-8	10	1	1022	997	25	-310	548
-10	10	1	1201	1142	59	-357	1095
1	11	1	1790	1987	-189	779	1828
3	11	1	2425	2519	-94	-1574	1967
5	11	1	2931	3006	-75	-106	3000
7	11	1	1270	1267	3	345	1219
-1	11	1	3671	3685	-13	649	3631
-3	11	1	3419	3688	-269	901	3576
-5	11	1	3094	3227	-133	953	3112
-7	11	1	1502	1476	26	-179	1465
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4	12	1	2174	2082	92	-1997	590
6	12	1	823	896	-73	-793	418
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2	14	1	1091	1104	-13	514	-977
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8	14	1	392	221	171	214	-54
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3	15	1	997	998	-1	-799	-611
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Table 3. (*Continued.*)

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2	10	2	2574	2703	-129	2690	268	-2	2	3	7246	7802	-556	-2437	7412
4	10	2	1977	2273	-296	2272	62	-4	2	3	9204	9521	-317	-6827	6937
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Table 3. (*Continued.*)

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TABLE 3. (*Continued.*)

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-5	13	4	1715	1623	-108	-1621	81
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-6	14	4	803	718	85	-655	-294
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-11	11	5	754	1010	-256	-187	953
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6	12	5	1041	1061	-20	-311	1014
-2	12	5	1033	1028	5	154	1016
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-6	12	5	1146	1177	-31	-381	1114
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5	13	5	383	363	20	-290	218
7	13	5	367	335	32	-177	285
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-3	13	5	408	525	-117	-313	-421
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TABLE 3. (*Continued.*)

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6	16	5	688	906	-238	-15	-906
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TABLE 3. (*Continued.*)

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-2	20	6	314	180	134	-20	-179	-1	11	7	2237	2232	5	-504	2174
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5	1	7	1522	1749	-227	939	1476	-1	11	7	1121	1437	-316	131	1431
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TABLE 3. (*Continued.*)

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-4	4	10	1107	1136	-29	-949	625	-9	3	11	1102	938	164	-660	667
-6	4	10	3096	2806	290	-2804	103	-11	3	11	361	528	-147	192	492
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5	5	10	1624	1385	239	-1380	123	-4	4	11	953	990	-37	-501	854
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-3	5	10	2889	3262	-373	-1646	-2816	-8	4	11	2400	2322	78	-1872	1374
-5	5	10	1403	1265	138	-1170	-482	-10	4	11	1251	1241	10	-1063	640
-7	5	10	1466	1555	-89	-1498	-416	1	5	11	881	929	-48	-134	-919
-9	5	10	2069	1681	388	-1389	-947	3	5	11	831	889	-58	403	-792
-11	5	10	1599	1164	435	-1079	-437	5	5	11	497	616	-119	109	-606
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2	6	10	1477	1550	-73	1296	851	-3	5	11	1571	1814	-243	-135	-1809
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-4	6	10	472	493	-21	143	472	-9	5	11	897	611	286	-396	465
-6	6	10	3798	3258	540	-2368	2236	0	6	11	331	324	7	286	-152
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-10	6	10	1041	956	85	-955	44	4	6	11	1469	1252	217	748	-1004
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-9	7	10	1417	1255	162	571	1118	1	7	11	1986	1713	273	-1015	-1380
-11	7	10	635	738	-103	123	728	3	7	11	864	823	41	779	-266
0	8	10	1102	1139	-37	551	-997	-1	7	11	2270	2334	-64	-524	-2274
2	8	10	1848	1626	222	1571	420	-3	7	11	1569	1855	-286	1478	-1121
6	8	10	574	610	-36	561	-240	-5	7	11	1395	1288	107	-1009	-600
-2	8	10	2500	2342	158	1961	-1281	-7	7	11	670	787	83	-392	-683
-4	8	10	845	969	-124	257	-934	-9	7	11	906	742	164	706	229
-6	8	10	1198	1090	108	-979	-479	-11	7	11	643	528	115	-338	-405
-8	8	10	2264	2070	206	2032	-437	0	8	11	2221	2287	-66	-1942	-1208
-10	8	10	919	864	55	651	146	-4	8	11	906	976	-70	561	-799
3	9	10	953	793	160	-628	-484	-6	8	11	1287	1185	102	-764	-906
5	9	10	991	849	142	297	-795	-8	8	11	544	519	25	165	-485
-1	9	10	1433	1392	41	1369	-93	3	9	11	1146	996	150	932	-351
-3	9	10	494	548	-54	512	194	-1	9	11	809	857	-48	-611	-601

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TABLE 3. (*Continued.*)

h	k	l	F_o	F_c	$\|F_o\|\|F_c\|$	A_c	B_c	h	k	l	F_o	F_c	$\|F_o\|\|F_c\|$	A_c	B_c
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-7	9	11	1146	1169	-23	644	-976	-4	10	12	1406	1510	-104	1479	-302
0	10	11	1008	920	88	-866	-311	-1	11	12	740	723	17	627	-361
2	10	11	859	712	147	476	530	-3	11	12	721	867	-146	859	-116
-2	10	11	845	1039	-194	-1037	69	-5	11	12	488	545	-57	-323	-439
-4	10	11	679	738	-59	-79	734	0	12	12	414	423	-9	-405	-122
1	11	11	1674	1370	304	-231	1350	-2	12	12	546	561	-15	-160	-538
-1	11	11	1262	1231	31	-509	1121	-4	12	12	325	417	-92	-383	-165
-3	11	11	1693	1761	-68	-277	1739	-1	13	12	1323	1389	-66	-1306	-84
-5	11	11	1411	1287	124	-135	1260	-5	13	12	1221	1267	-46	-1184	-450
0	12	11	928	967	-39	190	948	0	14	12	1138	1065	73	-1062	82
2	12	11	925	946	-21	240	915	-2	14	12	1107	1186	-79	-1176	-151
-2	12	11	544	547	-3	452	308	-4	14	12	1303	1606	-303	-1606	31
-4	12	11	1690	1888	-198	-179	1679	-1	15	12	696	631	65	-621	111
-3	13	11	704	338	366	333	56	-3	15	12	298	352	-54	-339	96
0	14	11	433	431	2	214	-374	-5	15	12	301	310	-9	-300	-80
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-3	15	11	1005	1166	-161	-44	-1165	-1	1	13	831	756	75	87	751
-5	15	11	798	887	-89	241	-854	-3	1	13	1265	1270	-5	-1127	585
0	16	11	740	718	22	-130	-706	-5	1	13	776	765	11	-737	-206
-2	16	11	469	434	35	-167	-401	-9	1	13	701	613	88	-38	612
-4	16	11	660	696	-36	34	-695	0	2	13	1248	1286	-38	445	1207
-1	17	11	339	322	17	20	-321	2	2	13	1502	1539	-37	-1305	815
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4	0	12	1287	1216	71	1177	307	-2	2	13	1770	1833	-63	-100	1830
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-4	0	12	1535	1788	-253	54	1767	-6	2	13	1624	1689	-65	796	1450
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-8	0	12	602	605	-3	605	-21	-10	2	13	1256	1315	-59	-484	1223
-10	0	12	1033	1079	-46	922	560	1	3	13	1878	2161	-283	871	1979
1	1	12	1378	1708	-330	1492	-831	3	3	13	930	961	-31	-211	538
3	1	12	569	547	22	-115	535	-1	3	13	1116	1355	-239	999	915
5	1	12	430	438	-8	310	-310	-3	3	13	1370	1263	107	-13	1263
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-5	3	12	969	1072	-103	21	-1072	-9	5	13	1080	953	127	-751	-566
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3	5	12	1679	1594	85	-1543	-401	-3	7	13	1430	1313	117	1152	-631
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-3	5	12	2295	2056	239	-1365	-1538	-9	7	13	480	428	52	-85	-419
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-7	5	12	2129	1946	183	-1935	-205	2	8	13	997	869	128	236	-836
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4	6	12	698	532	166	-277	-454	-3	9	13	1110	1062	48	978	-414
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-4	6	12	618	614	4	-611	-65	0	10	13	889	845	44	-166	829
-6	6	12	925	723	202	-236	683	-2	10	13	295	293	2	293	2
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-5	7	12	897	762	135	173	742	0	12	13	1069	1029	40	209	1008
-7	7	12	1428	1258	170	403	1162	-2	12	13	814	793	21	-518	600
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4	8	12	582	464	118	430	-175	0	14	13	339	375	-36	100	-361
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-4	8	12	574	600	-26	-276	-533	-3	15	13	364	405	-41	240	-326
-6	8	12	919	764	155	756	112	-5	15	13	516	611	-95	129	-597
-8	8	12	665	636	29	-586	-246	0	0	14	715	779	-64	410	-662
1	9	12	1176	921	255	896	-214	2	0	14	1000	1091	-91	571	930
3	9	12	1151	1062	89	1061	40	-2	0	14	991	915	76	915	1
-1	9	12	914	889	25	566	685	-4	0	14	745	683	62	563	-377
-3	9	12	621	464	157	249	391	-6	0	14	1240	1191	49	-399	-1126
-5	9	12	370	389	-19	-136	-364	-8	0	14	1215	1240	-25	756	953
-7	9	12	1038	1008	30	835	565	-10	0	14	599	662	-63	579	320
-9	9	12	497	433	64	305	307	1	1	14	875	1088	-213	919	-582

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TABLE 3. (*Continued*).

h	k	l	F_o	F_c	$\|F_o\|\|F_c\|$	A_c	B_c
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-7	1	14	530	456	74	437	-129
-9	1	14	640	578	62	575	-62
-11	1	14	508	577	-69	528	-232
0	2	14	795	872	-77	90	-871
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-2	2	14	823	783	40	706	-338
-4	2	14	665	731	-66	640	-353
-6	2	14	596	623	-27	-255	-568
-8	2	14	767	764	3	703	-299
1	3	14	751	806	-55	-803	-70
-1	3	14	1033	1074	-41	-340	-1019
-3	3	14	1698	1871	-173	-1864	159
-5	3	14	839	771	68	-721	274
-7	3	14	674	573	101	-463	337
-9	3	14	574	746	-172	-741	-85
0	4	14	900	894	6	-850	278
2	4	14	638	660	-22	-603	-269
-2	4	14	1475	1495	-20	-955	1150
-4	4	14	1756	1608	148	-1504	570
-6	4	14	1414	1187	227	-1005	632
-8	4	14	884	868	16	-777	-386
-10	4	14	1417	1411	6	-1380	-296
1	5	14	997	921	76	-895	-216
-1	5	14	549	856	-307	-771	-371
-3	5	14	417	327	90	-237	-225
-5	5	14	2533	2382	151	-2357	-342
-7	5	14	1712	1393	319	-1337	-390
-9	5	14	787	586	201	-371	-453
0	6	14	1607	1165	442	-1151	-177
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-2	6	14	1193	1109	84	-895	-655
-4	6	14	497	537	-40	-537	-9
-6	6	14	1977	1943	34	-1709	-925
-8	6	14	1154	1060	94	-550	-906
-10	6	14	983	854	89	-872	-196
-1	7	14	895	972	-77	-724	-648
-3	7	14	593	616	-23	556	260
-7	7	14	461	449	12	269	-360
0	8	14	1221	954	267	333	-892
2	8	14	1146	1151	-5	993	-573
-2	8	14	654	598	56	598	11
-4	8	14	1036	987	51	946	-280
-6	8	14	964	876	88	767	-427
-8	8	14	1077	845	228	842	110
1	9	14	958	879	79	423	771
-1	9	14	965	624	141	491	385
-3	9	14	977	954	23	928	-223
-5	9	14	1151	1172	-21	1172	-11
-7	9	14	1232	1099	133	1099	-27
-9	9	14	560	565	-5	521	-267
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-2	10	14	215	256	-41	-191	-171
-1	11	14	522	393	129	-271	285
-3	11	14	306	289	17	38	-286
0	12	14	334	333	1	-181	279
-1	13	14	726	782	-56	-693	-362
-3	13	14	582	678	-96	-652	-185
-5	13	14	505	643	-138	-522	-375
-4	14	14	853	994	-141	-994	-20
-1	1	15	350	398	-48	-237	-320
-3	1	15	693	834	-141	-781	292
-5	1	15	939	1003	-64	-388	925
-7	1	15	839	882	-43	-583	662
-9	1	15	488	574	-86	-261	511
0	2	15	668	721	-53	-467	549
2	2	15	864	871	-7	403	772
-2	2	15	831	1083	-252	-87	1080
-4	2	15	848	889	-41	150	876
-6	2	15	1895	1916	-21	277	1896
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-10	4	15	900	933	-33	-275	-892
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-3	5	15	585	632	-47	125	-620
-5	5	15	463	470	13	-448	-142
-1	7	15	1088	1235	-147	504	-1127
-1	7	15	1041	1163	-122	162	-1152
-3	7	15	1168	1012	156	-7	-1012
-5	7	15	820	751	69	405	-632
-7	7	15	544	333	211	80	-323
0	8	15	704	669	35	499	-446
-2	8	15	439	348	91	-198	-286
-4	8	15	527	502	25	-207	-457
-8	8	15	660	522	138	-511	-107
-1	9	15	491	471	20	116	456
-3	9	15	574	515	59	31	514
-5	9	15	442	383	59	177	340
-7	9	15	944	813	131	545	603
0	10	15	516	586	-70	316	494
-2	10	15	544	542	2	-30	541
-4	10	15	472	556	-84	-327	450
-1	11	15	436	513	-77	-23	512
-3	11	15	558	623	-65	-339	523
-5	11	15	414	428	-14	-277	326
-4	12	15	400	422	-22	-54	419
0	0	16	781	686	95	647	228
-2	0	16	825	791	34	676	410
-4	0	16	1649	1582	67	1477	568
-6	0	16	1237	1247	-10	852	910
-8	0	16	911	1017	-106	1001	180
1	1	16	798	1029	-231	1028	49
-1	1	16	723	813	-90	812	49
-3	1	16	1279	1419	-140	1408	-180
-5	1	16	436	394	42	388	-67
-7	1	16	367	375	-8	375	-9
-9	1	16	488	472	16	464	87
-2	2	16	698	798	-100	12	-796
-8	2	16	665	790	-125	250	-749
-1	3	16	687	794	-107	-791	-66
-3	3	16	596	477	119	-462	-120
-5	3	16	1138	1138	0	-999	-544
-9	3	16	558	563	-5	-290	-483
0	4	16	751	812	-61	-771	256
-2	4	16	1237	1206	31	-760	-936
-4	4	16	1861	1762	99	-1761	-52
-6	4	16	1279	1277	2	-1236	-321
-8	4	16	751	776	-25	-581	-514
-1	5	16	745	782	-37	-628	-466
-3	5	16	917	902	15	-735	-522
-5	5	16	1552	1337	215	-1161	-663
-7	5	16	942	731	211	-457	-571
-9	5	16	591	442	149	-257	-360
0	6	16	403	284	119	245	-137
*-2	6	16	596	182	414	160	-87
-4	6	16	690	550	140	-512	200
-1	7	16	221	187	34	186	23
-3	7	16	265	298	-33	226	155
-5	7	16	342	350	-8	258	236
-2	8	16	563	558	5	550	-93
-4	8	16	975	1006	-31	1005	-43
-6	8	16	1397	1233	164	981	-747
-3	9	16	693	717	-24	708	115
-5	9	16	806	778	28	773	-90
-4	10	16	555	746	-191	457	530
-1	1	17	406	483	-77	-444	191
-3	1	17	442	444	-2	-414	160
-5	1	17	411	475	-64	-392	269
-2	2	17	748	784	-36	-714	323
-4	2	17	814	853	-39	322	790
-6	2	17	701	749	-48	-412	626
-1	3	17	464	575	-111	-7	575
-3	3	17	856	834	22	81	830
-5	3	17	972	886	86	-264	846
-7	3	17	599	708	-109	-342	620
-4	4	17	980	855	125	16	855
-6	4	17	715	680	35	-379	565
-3	5	17	375	450	-75	406	-193
-5	5	17	629	480	149	128	-453
-4	6	17	734	670	64	121	-659
-6	6	17	825	709	116	333	-626
-3	7	17	406	450	-44	115	-434
-5	7	17	817	783	34	46	-782
-7	7	17	604	504	100	173	-473
-4	0	18	480	722	-242	357	-687
-5	1	18	621	701	-80	572	405
-4	2	18	414	627	-213	350	-520
-5	3	18	334	390	-56	-320	-223
-5	5	15	386	427	-41	351	-243
-7	5	15	1011	786	225	-607	-500
-9	5	15	792	523	269	181	-491
0	6	15	928	895	33	98	-890
-2	6	15	776	714	62	625	-345
-4	6	15	928	890	38	619	-639
-6	6	15	1450	1285	165	277	-1255
-8	6	15	895	803	92	286	-750

bond C(16)–C(17) which has the very low value of 1·343 Å. The angle between the axial P–C_6H_5 bonds is 176·9° and is significantly different from 180°. The angles between axial and equatorial bonds have a mean value of 90·0°, but there are some significant distortions.

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TABLE 4.

Bond lengths (Å) and angles (°).

P–C(1)	1·989	(7)	C(7)–C(8)	1·385	(9)	C(19)–C(20)	1·406	(9)
P–C(13)	1·986	(6)	C(7)–C(12)	1·392	(9)	C(19)–C(24)	1·384	(9)
P–C(7)	1·865	(6)	C(8)–C(9)	1·398	(11)	C(20)–C(21)	1·389	(10)
P–C(19)	1·855	(6)	C(9)–C(10)	1·388	(12)	C(21)–C(22)	1·377	(11)
P–C(25)	1·830	(7)	C(10)–C(11)	1·407	(12)	C(22)–C(23)	1·386	(10)
C(1)–C(2)	1·387	(9)	C(11)–C(12)	1·370	(11)	C(23)–C(24)	1·385	(10)
C(1)–C(6)	1·403	(9)	C(13)–C(14)	1·401	(10)	C(25)–C(26)	1·398	(10)
C(2)–C(3)	1·404	(10)	C(13)–C(18)	1·390	(9)	C(25)–C(30)	1·386	(10)
C(3)–C(4)	1·394	(11)	C(14)–C(15)	1·393	(13)	C(26)–C(27)	1·394	(11)
C(4)–C(5)	1·371	(12)	C(15)–C(16)	1·407	(13)	C(27)–C(28)	1·414	(12)
C(5)–C(6)	1·406	(11)	C(16)–C(17)	1·343	(13)	C(28)–C(29)	1·536	(13)
			C(17)–C(18)	1·401	(12)	C(29)–C(30)	1·394	(12)

C(1)PC(7)	92·7	(3)	PC(25)C(26)	121·3	(5)	C(13)C(18)C(17)	121·0	(7)
C(1)PC(19)	91·9	(3)	PC(25)C(30)	120·9	(5)	C(14)C(15)C(16)	118·9	(8)
C(1)PC(25)	86·3	(3)	C(2)C(1)C(6)	117·9	(6)	C(15)C(16)C(17)	120·0	(9)
C(7)PC(13)	86·6	(3)	C(1)C(2)C(3)	120·9	(6)	C(16)C(17)C(18)	121·0	(8)
C(13)PC(19)	91·1	(3)	C(1)C(6)C(5)	120·9	(7)	C(20)C(19)C(24)	119·4	(6)
C(13)PC(25)	91·5	(3)	C(2)C(3)C(4)	120·5	(7)	C(19)C(20)C(21)	118·9	(6)
C(7)P(C19)	119·6	(3)	C(3)C(4)C(5)	119·2	(8)	C(19)C(24)C(23)	120·7	(6)
C(7)PC(25)	122·6	(3)	C(4)C(5)C(6)	120·6	(8)	C(20)C(21)C(22)	121·3	(7)
C(19)PC(25)	117·8	(3)	C(8)C(7)C(12)	119·6	(6)	C(21)C(22)C(23)	119·6	(7)
PC(1)C(2)	116·1	(5)	C(7)C(8)C(9)	119·8	(6)	C(22)C(23)C(24)	120·0	(7)
PC(1)C(6)	125·2	(5)	C(7)C(12)C(11)	120·7	(7)	C(26)C(25)C(30)	117·8	(6)
PC(7)C(8)	120·8	(5)	C(8)C(9)C(10)	120·5	(7)	C(25)C(26)C(27)	122·1	(7)
PC(7)C(12)	119·6	(5)	C(9)C(10)C(11)	118·8	(8)	C(25)C(30)C(29)	120·0	(7)
PC(13)C(14)	117·5	(5)	C(10)C(11)C(12)	120·4	(7)	C(26)C(27)C(28)	118·6	(8)
PC(13)C(18)	125·3	(5)	C(14)C(13)C(18)	117·2	(6)	C(27)C(28)C(29)	118·9	(8)
PC(19)C(20)	119·4	(5)	C(13)C(14)C(15)	121·7	(7)	C(28)C(29)C(30)	122·4	(8)
PC(19)C(24)	121·2	(5)						

The angles between equatorial bonds have a mean value of 120·0° with again some significant departures. The mean PCC angle is 120·7°, and there are some highly significant distortions, particularly for the angles PC(13)C(18) and PC(1)C(6). The mean CCC angle is 120·0°. There are three angles that differ significantly from this mean, and they are all at atoms that are joined to the phosphorus atom.

The molecule has no symmetry. This is due to the different orientations of the benzene rings. The mean planes through the rings are given, in terms of the orthogonal axes, by the equations

$$\begin{array}{ll} \text{I} & -0{\cdot}9355X' + 0{\cdot}1189Y' - 0{\cdot}3327Z' = 0{\cdot}5239 \\ \text{II} & 0{\cdot}3873X' + 0{\cdot}9208Y' - 0{\cdot}0470Z' = 1{\cdot}8174 \\ \text{III} & 0{\cdot}0530X' + 0{\cdot}3595Y' + 0{\cdot}9317Z' = 0{\cdot}6293 \\ \text{IV} & 0{\cdot}6433X' + 0{\cdot}4300Y' - 0{\cdot}6334Z' = 0{\cdot}8468 \\ \text{V} & 0{\cdot}0231X' + 0{\cdot}8242Y' - 0{\cdot}5659Z' = 1{\cdot}7160 \end{array}$$

None of the carbon atoms departs significantly from its mean plane. On the other hand, the departure from these planes of the phosphorus atom is sometimes very significant, being −0·280, −0·042, +0·090, −0·043, and −0·132 Å, respectively. These departures serve to emphasise the distortions that do occur in this molecule.

The angle between the two axial rings, defined as the angle between their outward normals, is 108·5°. In order to define the positions of the equatorial rings, it is convenient to consider the angle of rotation round the P–C_6H_5 bond from a position in the equatorial plane through the atoms P, C(7), C(19), and C(25). The equation for the weighted mean plane through these four atoms is

$$0{\cdot}0020X' + 0{\cdot}9617Y' - 0{\cdot}2740Z' = 1{\cdot}8530$$

None of the atoms departs significantly from this plane. With respect to this plane, and looking towards the phosphorus atom, ring II must be rotated 25·9° anticlockwise, ring IV 53·9° clockwise, and ring V 18·6° anticlockwise. It will be seen that the normal " paddle-wheel " arrangement of benzene rings round a central atom is not adopted in the molecule, presumably because of interference from the axial rings.

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The shortest intramolecular contacts between non-bonded atoms, apart from distances across a benzene ring, are all between carbon atoms which are attached to the phosphorus atom in the axial position and carbon atoms that are attached to the phosphorus atom in the equatorial position. These distances are: C(1)–C(7), 2·791; C(1)–C(19), 2·764; C(1)–C(25), 2·613; C(13)–C(7), 2·643; C(13)–C(19), 2·742; C(13)–C(19), 2·735 Å. The next shortest set of non-bonded intramolecular contacts are between the phosphorus atom and the *ortho* carbon atoms. These distances range from 2·824 to 3·023 Å. The shortest intramolecular contact not in the above groups is between C(13) and C(24), 2·910 Å.

All intermolecular contacts are between benzene rings. There are 34 such contacts less than 4·0 Å, the lowest being 3·498 Å.

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