

### 1179. *The Crystal and Molecular Structure of Phosphobenzene A, (PC<sub>6</sub>H<sub>5</sub>)<sub>5</sub>.*

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Crystals of phosphobenzene A, m. p. 149—150°, are monoclinic with unit cell dimensions  $a = 9.742$ ,  $b = 10.139$ ,  $c = 27.488$  Å,  $\beta = 90.0^\circ$ . The space group is  $P2_1/n$ . The molecule is pentameric,  $(PC_6H_5)_5$ , and contains a five-membered ring of phosphorus atoms in the form of an equilateral pentagon with approximate symmetry  $m$ . To each phosphorus atom is attached one phenyl group. The structure has been refined by the least-squares method using three-dimensional intensity data collected on a Hilger and Watts Linear Diffractometer.

Four polyphosphines of formula  $(PC_6H_5)_n$  have been reported.<sup>1-9</sup> Of these, two are crystalline: A, m. p. 149—150°,<sup>1-9</sup> and B, m. p. 190°.<sup>2,3</sup> The other two forms have been presumed to be polymeric.<sup>3,8</sup> This paper describes the structure of form A, m. p. of a single crystal recrystallised from acetonitrile 154—156°. <sup>10</sup> Various molecular weight determinations in solution indicate that  $n = 2$  (refs. 2, 3, 8) or  $n = 4$  (refs. 4, 5, 9); however, in the crystalline state,  $n = 5$ , and compound A contains a five-membered ring of phosphorus atoms each of which also carries a phenyl group.<sup>10</sup>

#### EXPERIMENTAL

$C_{30}H_{25}P_5$ .  $M = 540.4$ . Monoclinic.  $a = 9.742$ ,  $b = 10.139$ ,  $c = 27.488$  Å,  $\beta = 90.0^\circ$ .  $U = 2715.1$  Å<sup>3</sup>.  $Z = 4$ .  $D_c = 1.322$ ,  $D_m = 1.324$  g./cc. Space group  $P2_1/n$ . The cell constants were determined from precession photographs recorded with Cu  $K_\alpha$  radiation. The intensities were measured with the aid of a Hilger and Watts Automatic Linear Diffractometer.<sup>11</sup> Mo $K_\alpha$  radiation with balanced filters was used, and data were recorded up to  $\theta = 27.5^\circ$ , the reciprocal lattice layers being perpendicular to the  $[a]$ -axis. Reflections whose measured intensity was less than twice the standard deviation of the measurement were omitted from the analysis. In this way 2614 intensities were recorded; these were then corrected for the Lorentz-polarization factors and reduced to a set of  $|F_o|$  values. The different layers were put on the same relative scale by correlation with  $|F_o(h0l)|$  which were determined from another crystal. No correction has been made for absorption,  $\mu = 3.67$  cm.<sup>-1</sup> for Mo  $K_\alpha$ -radiation. Wilson's<sup>12</sup> method was used to determine the overall scale and temperature factors. The scale factor so found for the  $|F_o|$  was 3.4, and at the end of refinement the scale factor was 3.38. The systematic absences were  $h0l$  absent for  $h + l$  odd,  $0k0$  absent for  $k$  odd. The space group is therefore  $P2_1/n$ .

*Determination of the Structure.*—The positions of the five phosphorus atoms in the asymmetric unit were obtained from a three-dimensional sharpened Patterson synthesis. These positions confirmed the existence of an equilateral pentagon of phosphorus atoms with a P-P bond length of 2.21 Å. The  $F_o^2$  coefficients were multiplied by the sharpening function

$$1/[|F_o|(\sum_f f_r \exp(-\sin^2\theta/\lambda^2))].$$

The 860 observed planes with  $\sin\theta/\lambda < 0.35$  Å<sup>-1</sup> were then selected from the data and used in subsequent calculations until the  $R$ -factor had fallen to 0.103. The approximate positions of all

<sup>1</sup> H. Köhler and A. Michaelis, *Ber.*, 1877, **10**, 807.

<sup>2</sup> Th. Weil, B. Prijs, and H. Erlenmeyer, *Helv. Chim. Acta*, 1952, **35**, 616.

<sup>3</sup> J. W. B. Reesor and G. F. Wright, *J. Org. Chem.*, 1957, **22**, 386.

<sup>4</sup> W. Kuchen and H. Buchwald, *Chem. Ber.*, 1958, **91**, 2296.

<sup>5</sup> F. Pass and H. Schmidbauer, *Monatsh.*, 1959, **90**, 148.

<sup>6</sup> L. Horner, H. Hoffmann, and P. Beck, *Chem. Ber.*, 1958, **91**, 1583.

<sup>7</sup> P. R. Bloomfield and K. Parvin, *Chem. and Ind.*, 1959, 541.

<sup>8</sup> W. A. Henderson, jun., M. Epstein, and F. S. Seichter, *J. Amer. Chem. Soc.*, 1963, **85**, 2462.

<sup>9</sup> E. Wiberg, M. Van Ghemen, and G. Müller-Schiedmayer, *Angew. Chem.*, 1963, **75**, 814.

<sup>10</sup> J. J. Daly and L. Maier, *Nature*, 1964, **203**, 1167.

<sup>11</sup> U. W. Arndt and D. C. Phillips, *Acta Cryst.*, 1961, **14**, 807.

<sup>12</sup> A. J. C. Wilson, *Nature*, 1942, **150**, 152.

the carbon atoms were found from the first three-dimensional electron-density synthesis and these positions were then improved from a second synthesis.  $R$  was then 0.354 and least-squares refinement was started. In seven cycles  $R$  had fallen to 0.103 and the structure was then refined with all 2614 observed planes; the final  $R$ -factor for all these planes was 0.105, and for the 2583 planes included in the refinement  $R'$  was 0.014. Planes were rejected from the refinement if  $3|F_o| < |F_c|$ .  $R$  and  $R'$  are defined by

$$R = \sum (|F_o| - |F_c|) / \sum |F_o|; R' = \sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2.$$

One thermal parameter, an isotropic temperature factor, was refined for each atom; the form used was  $\exp -2\pi^2 U(2\sin\theta/\lambda)^2$ . A constant weight was applied to all  $F_o$ . Refinement was stopped when  $(\Delta/\sigma)_{\max}$  was less than 0.3. Practically all of the calculations were done on our Elliott 803 computer using the programming system devised by Daly, Stephens, and Wheatley.<sup>13</sup> The least-squares refinement process uses a block diagonal approximation.

## RESULTS AND DISCUSSION

Final atomic parameters, with their corresponding standard deviations as units in the last place of decimals, are in Table 1. Table 2 lists  $F_o$ ,  $F_c$ , and  $\Delta$  from the penultimate set of

TABLE 1.

Co-ordinates and standard deviations in Å. Thermal parameters, and standard deviations in Å<sup>2</sup> in parentheses.

	$X$	$Y$	$Z$	$U = B/8\pi^2$
P1	-0.779 (3)	0.715 (3)	-3.729 (3)	0.0365 (7)
P2	-0.274 (3)	0.988 (4)	-1.581 (3)	0.0418 (8)
P3	1.731 (3)	1.926 (4)	-1.492 (3)	0.0425 (8)
P4	1.441 (3)	3.091 (3)	-3.344 (3)	0.0381 (7)
P5	1.031 (3)	1.450 (3)	-4.783 (3)	0.0347 (7)
C1	-0.586 (12)	-1.099 (13)	-3.909 (12)	0.0464 (32)
C2	-1.214 (14)	-1.945 (15)	-2.997 (14)	0.0589 (37)
C3	-1.203 (16)	-3.366 (17)	-3.231 (16)	0.0769 (48)
C4	-0.525 (15)	-3.861 (16)	-4.330 (15)	0.0683 (43)
C5	0.083 (16)	-3.071 (18)	-5.265 (16)	0.0763 (46)
C6	0.068 (14)	-1.655 (15)	-5.031 (14)	0.0584 (38)
C7	-1.266 (12)	2.503 (13)	-1.162 (12)	0.0438 (31)
C8	-2.428 (14)	2.881 (15)	-1.861 (14)	0.0576 (38)
C9	-3.251 (15)	3.961 (16)	-1.385 (15)	0.0660 (42)
C10	-2.832 (16)	4.687 (17)	-0.280 (16)	0.0740 (46)
C11	-1.684 (16)	4.330 (17)	0.411 (16)	0.0747 (46)
C12	-0.879 (15)	3.211 (16)	*0.012 (15)	0.0679 (42)
C13	2.912 (12)	0.526 (13)	-1.807 (12)	0.0446 (31)
C14	2.526 (14)	-0.773 (15)	-2.089 (14)	0.0567 (37)
C15	3.530 (16)	-1.774 (17)	-2.196 (16)	0.0750 (46)
C16	4.853 (16)	-1.470 (17)	-2.000 (16)	0.0733 (46)
C17	5.217 (15)	-0.146 (16)	-1.721 (15)	0.0639 (41)
C18	4.257 (14)	0.847 (15)	-1.604 (14)	0.0604 (39)
C19	3.126 (11)	3.583 (12)	-3.899 (12)	0.0395 (28)
C20	4.110 (12)	2.705 (13)	-4.364 (12)	0.0454 (32)
C21	5.341 (14)	3.214 (15)	-4.870 (14)	0.0586 (37)
C22	5.563 (15)	4.581 (16)	-4.940 (15)	0.0688 (43)
C23	4.606 (15)	5.447 (16)	-4.508 (15)	0.0697 (44)
C24	3.373 (14)	4.978 (15)	-3.955 (14)	0.0588 (38)
C25	0.323 (11)	2.504 (12)	-6.097 (11)	0.0353 (27)
C26	-1.016 (15)	2.559 (16)	-6.451 (15)	0.0671 (42)
C27	-1.469 (16)	3.385 (17)	-7.521 (16)	0.0773 (48)
C28	-0.594 (15)	4.158 (17)	-8.209 (15)	0.0712 (45)
C29	0.754 (16)	4.104 (17)	-7.901 (16)	0.0743 (46)
C30	1.232 (14)	3.257 (15)	-6.853 (14)	0.0573 (37)

parameters. The bond lengths and angles are in Table 3. The numbering of the atoms is shown in the  $[a]$ -axis projection of the molecule in Fig. 1. The packing of the molecules is shown in Fig. 2.

<sup>13</sup> J. J. Daly, F. Stephens, and P. J. Wheatley, Monsanto Research S.A., Final Report No. 52 (1963).

[1964]

Molecular Structure of Phosphobenzene A, (PC<sub>6</sub>H<sub>5</sub>)<sub>5</sub>.

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TABLE 2.  
100F<sub>o</sub>, 100F<sub>c</sub>, and 100Δ.

* Planes omitted from the least-squares analysis.			† Obscured by beam stop.								
k	h	l	100F <sub>o</sub>	100F <sub>c</sub>	100Δ	k	h	l	100F <sub>o</sub>	100F <sub>c</sub>	100Δ
2	0	0	16403	15080	1323	0	0	10	-13378	-14068	690
4	0	0	-7846	-7524	-322	2	0	10	-5744	-5099	-645
1	0	1	5815	15975	† -10160	4	0	10	-6197	-5546	-651
3	0	1	-6197	-6942	745	6	0	10	6213	604	609
5	0	1	-9209	-9376	107	8	0	10	6721	6777	-56
7	0	1	2277	2078	199	10	0	10	1507	1585	-78
1	0	-1	3642	5415	-1773	2	0	-10	2264	2011	253
3	0	-1	-554	-470	-144	4	0	-10	6849	6458	391
5	0	-1	3223	2898	325	6	0	-10	-2727	-3394	667
7	0	-1	1946	2331	-385	8	0	-10	-2379	-1896	-483
2	0	2	-18190	-17673	-517	10	0	-10	-1665	-1191	-474
4	0	2	-2466	-2837	371	1	0	11	-10465	-10117	-348
6	0	2	946	1210	-264	3	0	11	-1111	-1570	459
2	0	-2	-7643	-7400	-243	5	0	11	1382	1322	60
4	0	-2	10502	10598	-96	7	0	11	3761	3771	-10
6	0	-2	7687	7628	59	9	0	11	4818	4723	95
8	0	-2	-2696	-2743	47	1	0	-11	-2713	-1568	-1145
10	0	-2	-929	-1057	128	3	0	-11	-1578	-1215	-363
1	0	3	2078	1583	495	5	0	-11	-2912	-2975	63
3	0	3	-8752	-7684	-1068	0	0	12	-848	-1760	912
5	0	3	-3362	-2973	-339	2	0	12	8532	8747	-215
7	0	3	1780	1530	250	4	0	12	8894	8972	-78
9	0	3	-2882	-3850	985	6	0	12	-1432	-1346	-86
1	0	-3	-9423	-10096	668	10	0	12	1632	1848	-216
3	0	-3	6201	6072	129	2	0	-12	-7623	-7301	-322
5	0	-3	11030	11224	-194	4	0	-12	-4311	-4111	-200
7	0	-3	-952	-1390	438	6	0	-12	-5643	-5849	206
9	0	-3	-1098	-1080	-18	8	0	-12	2595	2823	-228
0	0	4	-10306	-10798	492	10	0	-12	1834	1701	133
2	0	4	-6849	-7050	201	1	0	13	-4501	-5061	560
4	0	4	-3311	-2903	-408	3	0	13	11824	11962	-138
6	0	4	1635	2142	-507	5	0	13	2297	2081	216
8	0	4	800	529	271	7	0	13	-6478	-6623	145
10	0	4	-2418	-2809	393	1	0	-13	-3974	-4512	538
2	0	-4	1108	465	643	3	0	-13	-2193	-1165	-1028
4	0	-4	11330	11101	229	5	0	-13	-6424	-6354	-70
6	0	-4	1067	892	175	0	0	14	5396	5201	195
10	0	-4	4095	4601	-506	2	0	14	-1959	-1895	-64
1	0	5	-2581	-2219	-362	4	0	14	8914	8761	153
3	0	5	4480	3396	1084	8	0	14	-4666	-4736	70
5	0	5	5035	5022	13	2	0	-14	1067	1314	-247
7	0	5	1284	1371	-87	*4	0	-14	1020	81	939
9	0	5	-1226	-1703	477	6	0	-14	-2385	-1928	-457
3	0	-5	3953	3195	758	8	0	-14	-1554	-1226	-328
5	0	-5	-1537	-1288	-249	10	0	-14	-1361	-1980	619
9	0	-5	5417	6565	-1148	3	0	15	1990	2359	-369
0	0	6	2446	2712	-266	5	0	15	3521	3697	-176
2	0	6	19819	17728	2091	1	0	-15	3102	3181	-79
4	0	6	-1709	-1850	141	3	0	-15	1199	1578	-379
6	0	6	-1804	-2270	466	5	0	-15	-3132	-2663	-469
8	0	6	-3119	-3416	297	7	0	-15	-1757	-1283	-474
10	0	6	-1419	-1383	-36	9	0	-15	-3956	-3086	130
2	0	-6	-3798	-2156	-1642	0	0	16	10519	11648	-1129
4	0	-6	-3690	-3396	-294	2	0	16	-5795	-5861	66
6	0	-6	-6589	-6386	-203	*4	0	16	1297	92	1205
10	0	-6	3771	4532	-761	6	0	16	1916	2505	-589
1	0	7	10026	10012	14	10	0	16	1557	1690	-133
3	0	7	-726	-469	-257	2	0	-16	7008	7357	-349
5	0	7	-8228	-8188	-40	6	0	-16	1321	1198	123
7	0	7	-5335	-5413	78	10	0	-16	-1841	-1893	52
9	0	7	-2953	-3604	651	1	0	17	6677	6932	-255
1	0	-7	6985	6629	356	3	0	17	-7042	-7027	-15
3	0	-7	-3784	-3900	116	5	0	17	-3538	-4446	908
5	0	-7	-6930	-5669	-261	7	0	17	3206	3413	-207
*7	0	-7	1209	370	839	9	0	17	2598	2730	-132
9	0	-7	3193	3383	-190	1	0	-17	5045	5202	-157
0	0	8	-11530	-10872	-658	3	0	-17	-1544	-2058	514
2	0	8	-8492	-7812	-680	5	0	-17	4989	4042	347
4	0	8	-15291	-14850	-441	7	0	-17	2618	2788	-170
6	0	8	-5048	-4515	-533	9	0	-17	-1493	-1523	30
8	0	8	-1317	-1914	597	0	0	18	6782	6746	36
2	0	-8	-6924	-6569	-355	2	0	18	5224	5736	-512
4	0	-8	-5677	-5989	312	8	0	18	1246	1068	178
6	0	-8	1213	878	335	2	0	-18	-3467	-3565	98
8	0	-8	1777	1904	-127	6	0	-18	3784	4130	-346
10	0	-8	-1436	-1528	92	1	0	19	2216	1875	341
1	0	9	3642	2357	1285	3	0	19	2493	2748	-255
3	0	9	-4122	-4440	318	5	0	19	2703	2495	208
5	0	9	-5160	-5317	157	9	0	19	-1713	-1335	-378
7	0	9	2429	3035	-606	1	0	-19	-2845	-3458	613
9	0	9	1189	873	316	3	0	-19	-2987	-3799	812
1	0	-9	4981	4627	354	5	0	-19	5123	4615	508
3	0	-9	2960	2531	429	7	0	-19	2449	2414	35
5	0	-9	1510	1364	146	2	0	20	2754	2953	-199
7	0	-9	-3315	-2731	-584	8	0	20	-2355	-2541	186
9	0	-9	-33319	-3090	-241	2	0	-20	-3342	-3259	-83

TABLE 2—continued

$h$	$k$		100F <sub>o</sub>	100F <sub>c</sub>	100Δ	$h$	$k$		100F <sub>o</sub>	100F <sub>c</sub>	100Δ
4	0	-20	3254	3506	-252	*6	1	-2	-456	-86	-370
6	0	-20	2473	2861	-388	7	1	-2	2713	3085	-372
1	0	21	2662	2360	302	10	1	-2	1794	2136	-342
3	0	21	2338	2899	-561	0	1	3	-1132	-948	-184
7	0	21	-1858	-1697	-161	1	1	3	11313	11579	-266
9	0	21	-2152	-2222	70	2	1	3	-3619	-3692	73
1	0	-21	1050	1388	-338	3	1	3	7089	6717	372
3	0	-21	2419	3321	-902	4	1	3	2145	2083	62
5	0	-21	1446	1636	-190	5	1	3	1733	1850	-117
7	0	-21	-2199	-2174	-25	6	1	3	2777	3047	-270
9	0	-21	2037	2291	-254	10	1	3	-1801	-2069	268
0	0	22	2297	2150	147	1	1	-3	9512	9499	13
2	0	22	-1206	-1214	8	2	1	-3	10742	7456	3286
4	0	22	-4264	-4244	-20	3	1	-3	5356	5787	-431
8	0	22	-1855	-1596	-259	4	1	-3	6859	5688	1171
2	0	-22	3511	3905	-394	5	1	-3	-6927	-6847	-80
4	0	-22	1277	1111	166	6	1	-3	5849	6203	-354
6	0	-22	-1665	-1709	44	7	1	-3	-4230	-3923	-307
1	0	23	1233	1054	179	9	1	-3	2041	2598	-557
3	0	23	-4548	-4373	-175	10	1	-3	-1186	-1122	-64
5	0	23	-3281	-3517	236	0	1	4	6015	6564	-549
1	0	-23	3284	3067	-383	1	1	4	-4413	-3100	-1313
3	0	-23	1709	1702	7	2	1	4	8671	6956	1715
4	0	24	-5200	-4851	-349	3	1	4	-6312	-5666	-646
6	0	24	-1804	-1311	-493	4	1	4	4886	4084	802
2	0	-24	-1848	-2552	704	5	1	4	1858	1423	435
3	0	25	-2118	-1718	-400	7	1	4	2649	2628	21
5	0	25	-1834	-1860	26	9	1	4	-932	-994	62
1	0	-25	-3534	-3744	210	1	1	-4	-15342	-15135	-207
3	0	-25	-2936	-3136	200	2	1	-4	8671	10670	-1999
5	0	-25	1750	1640	110	3	1	-4	7076	6254	822
7	0	-25	2044	1928	116	4	1	-4	-5160	-4616	-544
0	0	26	-3734	-4048	314	5	1	-4	5690	6023	-333
4	0	26	-1652	-2188	536	6	1	-4	-7890	-8482	592
8	0	26	1591	1637	-46	7	1	-4	1557	1745	-186
2	0	-26	-3362	-3691	329	8	1	-4	2449	2765	-316
4	0	-26	2183	2772	-589	9	1	-4	1747	1875	-128
1	0	27	-1544	-1373	-171	10	1	-4	2112	2266	-154
3	0	27	1449	1955	-506	0	1	5	-7322	-7120	-202
1	0	-27	-1922	-1870	-52	1	1	5	16700	16349	351
5	0	-27	-1784	-1566	-218	2	1	5	-5079	-4465	-614
6	0	-28	-3453	-3379	-74	3	1	5	3470	2743	727
3	0	29	1649	1393	256	4	1	5	-2233	-1787	-446
5	0	29	-1902	-2235	333	6	1	5	-675	-502	-173
5	9	-29	-4153	-3899	-254	7	1	5	1983	2030	-47
4	0	30	2125	2250	-125	10	1	5	-1665	-2140	475
2	0	-20	1476	1639	-163	1	1	-5	-8965	-9048	83
6	0	-30	-2321	-2208	-113	2	1	-5	4291	3524	767
1	0	31	-1818	-1880	62	3	1	-5	2551	1161	1390
1	0	-31	1503	1388	115	4	1	-5	-5450	-5364	-86
2	0	32	-1750	-1427	-323	5	1	-5	-6856	-6910	54
4	0	32	1872	1558	314	6	1	-5	1290	1301	-11
2	0	-32	1540	2194	-654	7	1	-5	756	550	206
1	0	-33	1186	1136	50	8	1	-5	2152	2627	-475
0	0	34	1371	1287	84	9	1	-5	1301	1708	-407
1	0	35	1618	1633	-15	10	1	-5	1943	2166	-223
1	0	0	6501	7063	-562	0	1	6	5109	5119	-10
2	1	0	-9350	-9417	67	1	1	6	18538	18701	-163
3	1	0	1233	1082	151	2	1	6	2537	2016	521
4	1	0	5474	4547	927	3	1	6	1132	1352	-220
6	1	0	2460	3065	-605	4	1	6	-3845	-3164	-681
7	1	0	-1726	-1413	-313	5	1	6	-2743	-3179	436
8	1	0	-1578	-1743	165	7	1	6	-2294	-2448	154
0	1	1	8874	9172	-298	9	1	6	-1581	-1435	-146
1	1	1	3362	3308	54	*1	1	-6	2960	325	2535
2	1	1	7366	6707	659						
3	1	1	-9549	-8246	-1303	2	1	-6	3467	2920	547
5	1	1	1848	1828	20	3	1	-6	-4227	-4354	127
6	1	1	-3328	-3432	104	4	1	-6	-5143	-4503	-640
9	1	1	1284	1643	-359	5	1	-6	-807	-412	-395
10	1	1	1067	1427	-360	8	1	-6	1524	1391	133
1	1	-1	-9242	-9548	306	9	1	-6	3051	3494	-443
2	1	-1	10418	10211	207	10	1	-6	-1574	-1742	168
3	1	-1	5629	5405	224	0	1	7	-17254	-17167	-87
4	1	-1	5988	6057	-69	1	1	7	-7647	-7197	-450
5	1	-1	6667	8520	-1853	2	1	7	3568	2911	657
7	1	-1	-2970	-2979	9	3	1	7	-4088	-3422	-666
0	1	2	11148	12859	-1711	4	1	7	-2247	-2041	-206
1	1	2	-1321	-1214	-107	5	1	7	-952	-993	41
2	1	2	-3331	-2814	-517	6	1	7	-6873	-6774	-99
3	1	2	-4977	-5326	349	8	1	7	-1233	-1219	-14
4	1	2	2372	2001	371	9	1	7	-1155	-973	-182
5	1	2	577	791	-214	*1	1	-7	1534	210	1315
7	1	2	-1564	-1464	-100						
8	1	2	-1611	-1583	-28	2	1	-7	-2429	-2619	190
9	1	2	-716	-1320	604	3	1	-7	993	992	1
10	1	2	966	1549	-583	4	1	-7	-4359	-3874	-485
1	1	-2	-3108	-2751	-357	5	1	-7	1794	1212	582
2	1	-2	6173	5738	435	6	1	-7	-2243	-2004	-239
3	1	-2	4149	4259	-110	7	1	-7	2051	1910	141
4	1	-2	12206	11639	567	9	1	-7	-3119	-3562	443
5	1	-2	3021	3090	-69	10	1	-7	1294	969	325

TABLE 2—continued

<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ
0	1	8	10827	10564	263	5	1	-13	1706	689	1017
1	1	8	-2970	-2487	-483	7	1	-13	-1209	-842	-367
2	1	8	1054	1008	46	8	1	-13	1645	1559	86
4	1	8	-5920	-5214	-706	9	1	-13	-1213	-1372	159
5	1	8	-1716	-1985	269	0	1	14	-6194	-6316	122
7	1	8	-4315	-4280	-35	1	1	14	-1165	-935	-230
8	1	8	-2497	-3024	527	2	1	14	9147	8741	406
10	1	8	-1540	-1539	-1	3	1	14	2943	2577	366
1	1	-8	577	479	98	4	1	14	2003	2444	-441
2	1	-8	3068	2570	498	5	1	14	2760	2871	-111
3	1	-8	1530	1577	-47	6	1	14	-5569	-5336	-233
4	1	-8	3950	3588	362	10	1	14	1625	1190	435
7	1	-8	-2757	-2973	216	2	1	-14	2700	2240	460
8	1	-8	-2649	-2971	322	3	1	-14	-3696	-3912	216
10	1	-8	-2605	-3157	552	5	1	-14	-2456	-2462	6
0	1	9	-7799	-7768	-31	6	1	-14	2902	2348	554
1	1	9	1730	1513	217	8	1	-14	-1554	-1896	342
2	1	9	-2014	-2424	410	9	1	-14	-1503	-1871	368
4	1	9	-4284	-4085	-199	10	1	-14	-1699	-1611	-88
*5	1	9	-875	-152	-723	0	1	15	5542	5680	-138
						1	1	15	-1415	-1222	-193
6	1	9	-1094	-1201	107	2	1	15	5379	5004	375
9	1	9	-4153	-4536	383	3	1	15	7255	7417	-162
1	1	-9	-1730	-1889	159	4	1	15	3582	3492	90
2	1	-9	3142	2770	372	5	1	15	2054	2718	-664
3	1	-9	1763	1076	687	7	1	15	-3375	-2823	-552
4	1	-9	2088	2201	-113	9	1	15	1517	569	948
5	1	-9	875	811	64	1	1	-15	2703	2699	4
6	1	-9	-2003	-2072	69	2	1	-15	4663	4598	65
7	1	-9	-3227	-2760	-467	3	1	-15	-2946	-2933	-13
8	1	-9	-1932	-2032	100	4	1	-15	2057	2161	-104
9	1	-9	-4224	-4499	275	5	1	-15	2720	2630	90
10	1	-9	-1456	-1432	-24	6	1	-15	-1723	-1976	253
1	1	10	-15078	-14919	-159	8	1	-15	-3423	-3877	454
*2	1	10	-892	-54	-838	0	1	16	-7451	-7161	-290
						1	1	16	-1341	-1113	-228
3	1	10	-2997	-2861	-136	2	1	16	-5133	-4947	-186
4	1	10	-4636	-2094	-2542	3	1	16	-2737	-2960	223
6	1	10	3828	3655	173	4	1	16	5842	6153	-311
7	1	10	1791	1692	99	6	1	16	2416	2102	314
8	1	10	902	853	49	9	1	16	1740	1807	-67
9	1	10	2085	2615	-530	1	1	-16	4298	4511	-213
10	1	-10	-1767	-2317	550	2	1	-16	-2409	-2129	-280
1	1	-10	2760	1153	1607	3	1	-16	5528	5817	-289
2	1	-10	-2767	-2466	-301	4	1	-16	2301	2479	-178
3	1	-10	4011	4387	-376	6	1	-16	3568	3694	-126
4	1	-10	-3514	-3701	187	7	1	-16	-1743	-1327	-416
5	1	-10	-1442	-1156	-286	9	1	-16	-1571	-2040	469
6	1	-10	-2335	-2243	-92	0	1	17	2723	2486	237
7	1	-10	-1595	-1847	252	1	1	17	-4173	-4054	-119
0	1	11	-6001	-5885	-116	2	1	17	-3122	-2679	-443
1	1	11	1486	1748	-262	5	1	17	3068	2485	583
2	1	11	-7978	-7082	-896	6	1	17	2108	1221	887
3	1	11	-1736	-1833	97	1	1	-17	-3149	-3730	581
5	1	11	-2291	-2385	94	2	1	-17	4061	4538	-477
6	1	11	2287	3280	-993	4	1	-17	1486	1923	-437
7	1	11	3257	3021	236	5	1	-17	6856	6779	77
8	1	11	2169	2752	-583	6	1	-17	2345	2193	152
1	1	-11	5646	5460	186	7	1	-17	1419	1275	144
2	1	-11	-3021	-2934	-87	0	1	18	2977	3392	-415
3	1	-11	-4977	-2467	-2510	1	1	18	1463	1379	84
4	1	-11	-3696	-3272	-424	2	1	18	-3227	-3348	121
7	1	-11	4747	4939	-192	5	1	18	2443	2537	-94
8	1	-11	2142	2557	-415	2	1	-18	-3440	-3885	445
9	1	-11	2176	2252	-76	3	1	-18	1196	1158	38
0	1	12	-8407	-8188	-219	4	1	-18	3277	3635	-358
1	1	12	1219	914	305	5	1	-18	1331	1437	-106
3	1	12	5373	5536	-163	6	1	-18	1736	1618	118
4	1	12	-5450	-5379	-71	7	1	-18	2649	2644	5
5	1	12	1426	1369	57	1	1	19	1409	1141	268
6	1	12	-2054	-1792	-262	3	1	19	-1500	-1189	-311
7	1	12	1412	870	542	4	1	19	2825	3036	-211
8	1	12	2743	2904	-161	1	1	-19	-3943	-4738	795
9	1	12	1064	1062	2	3	1	-19	1324	583	741
1	1	-12	-834	-778	-56	5	1	-19	-1314	-1085	-229
2	1	-12	1426	1170	256	6	1	-19	3308	3391	-83
3	1	-12	-5082	-4934	-148	7	1	-19	-1456	-1785	329
4	1	-12	-1777	-2030	253	9	1	-19	1652	1236	416
5	1	-12	-4234	-3752	-482	0	1	20	1105	1764	-659
6	1	-12	1622	1867	-245	1	1	20	2237	1917	320
0	1	13	2112	1061	1051	2	1	20	2308	2732	-424
1	1	13	-2385	-1284	-1101	4	1	20	4599	4041	558
2	1	13	3484	2824	660	5	1	20	2916	2894	22
3	1	13	-1030	-1078	48	9	1	20	-2287	-2698	411
4	1	13	5765	5523	242	1	1	-20	-1720	-2113	393
5	1	13	-6106	-5982	-124	2	1	-20	2372	2716	-344
7	1	13	-1987	-1719	-268	3	1	-20	-1763	-2299	536
9	1	13	2689	2613	76	5	1	-20	2980	2710	270
1	1	-13	7789	8551	-762	6	1	-20	-2612	-2569	-43
2	1	-13	-4102	-3817	-285	7	1	-20	2429	2197	232
3	1	-13	1257	960	297	*1	1	21	-881	-142	-739
4	1	-13	-5606	-5845	239						

TABLE 2—continued

<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ	
2	1	21	1622	1442	180	9	2	2	2382	2340	42	
3	1	21	4575	4947	-389	10	2	2	1000	858	142	
5	1	21	2308	2072	-236	1	2	2	-18315	-18415	100	
8	1	21	-1459	-917	-542	2	2	2	8113	8697	-584	
1	1	-21	2098	-901	-803	3	2	2	3473	3226	247	
2	1	-21	1807	1293	514	4	2	2	1814	1790	24	
3	1	-21	1757	1846	-39	5	2	2	3865	4055	-190	
5	1	-21	-4149	-3930	-219	6	2	2	1500	1550	-50	
1	1	22	2743	3305	-562	7	2	2	1280	1185	95	
3	1	22	-2524	-2735	211	8	2	2	2027	2040	-13	
4	1	22	2000	1632	368	9	2	2	1172	1481	-309	
5	1	22	-2132	-2191	59	0	2	2	6880	6026	854	
1	1	-22	3284	4495	-1211	1	2	2	1567	1403	164	
2	1	-22	1818	2151	-333	2	2	2	3649	3799	-150	
4	1	-22	-2095	-2257	162	3	2	2	-2466	-1623	-843	
6	1	-22	-2446	-2344	-102	5	2	2	3805	3045	760	
4	1	23	-5079	-4859	-220	6	2	2	-1429	-1248	-181	
6	1	23	-2909	-2938	29	7	2	2	1118	1458	-340	
*1	1	-23	-1169	-353	-816	8	2	2	-3054	-3475	421	
0	1	24	3730	4200	-470	10	2	2	2037	2139	-102	
1	1	24	-1405	-1050	-355	1	2	2	2967	3433	-466	
5	1	24	-2274	-1669	-605	2	2	2	-7975	-7251	-724	
1	1	-24	-1581	-1356	-225	3	2	2	5237	5035	202	
2	1	-24	-2477	-3145	668	4	2	2	-963	-508	-455	
0	1	25	-3521	-3832	311	5	2	2	-1301	-1054	-247	
1	1	25	2433	2855	-422	7	2	2	5744	5986	-242	
2	1	25	-2453	-2851	398	0	2	2	-1966	-1871	-95	
3	1	25	-2250	-2046	-204	1	2	2	-10215	-10149	-66	
1	1	-25	-1534	-2134	600	2	2	2	-3129	-3239	110	
2	1	-25	-1463	-1706	243	*3	2	2	831	220	611	
0	1	26	1469	1484	-15	4	2	2	1983	2147	-164	
1	1	26	-3190	-3127	-63	5	2	2	10590	10036	554	
4	1	26	-1628	-1774	146	7	2	2	1841	2046	-205	
1	1	-26	-3129	-3521	392	8	2	2	1483	1191	292	
2	1	-26	1953	1559	394	10	2	2	881	571	310	
6	1	-26	-1855	-1805	-50	1	2	2	-7289	-6893	-396	
0	1	27	-2098	-1936	-162	2	2	2	-6559	-5501	-1058	
3	1	27	-2037	-1843	-194	3	2	2	-3308	-2850	-458	
4	1	27	1490	1752	-262	4	2	2	-3348	-3040	-308	
1	1	-27	1426	1543	-117	5	2	2	-5842	-5674	-168	
4	1	-27	-1344	-1337	-7	6	2	2	3984	4022	-38	
5	1	-27	-2338	-2186	-152	7	2	2	-3788	-4430	642	
0	1	28	-1246	-1513	267	9	2	2	1767	1727	40	
1	1	28	1132	746	386	10	2	2	-1929	-2061	132	
4	1	28	-2314	-2430	116	*0	2	2	5	-821	-651	
3	1	-28	-1321	-1510	189	1	2	2	-2098	-952	-1146	
4	1	-28	-1497	-2426	929	2	2	2	-5048	-4405	-643	
5	1	-28	-2743	-2635	-108	3	2	2	-2869	-3007	138	
0	1	29	1581	1809	-228	4	2	2	2443	2387	56	
6	1	29	-1689	-1070	-619	5	2	2	1601	1446	155	
1	1	-29	2145	2089	56	6	2	2	8228	7536	692	
4	1	-29	-1557	-1500	-57	7	2	2	-2429	-2255	-174	
2	1	30	2220	1900	320	8	2	2	-1142	-1178	36	
2	1	-30	1767	1904	-137	9	2	2	-1777	-2210	433	
5	1	31	-1828	-1571	-257	10	2	2	-1169	-1312	143	
1	1	32	-1132	-1506	374	1	2	2	-8302	-8078	-224	
1	1	34	1240	522	718	2	2	2	-5106	-4404	-702	
0	2	0	-9178	-9071	-107	3	2	2	-8627	-7983	-644	
1	2	0	-4379	-4040	-339	4	2	2	-5227	-5281	54	
2	2	0	2183	2114	69	6	2	2	-3061	-3338	277	
4	2	0	7055	6814	241	7	2	2	6248	5963	285	
5	2	0	780	1348	-568	8	2	2	2906	3076	-170	
6	2	0	-3004	-3339	335	10	2	2	1338	1270	68	
7	2	0	912	748	164	0	2	2	6194	5507	687	
8	2	0	-2558	-2664	106	1	2	2	5575	5169	406	
9	2	0	1963	2308	-345	*2	2	2	6	-1490	-388	-1102
0	2	1	-4565	-4378	-187	3	2	2	6	-7306	-6963	-343
1	2	1	-9441	-9415	-26	4	2	2	6	-2014	-1788	-226
2	2	1	3960	3200	760	5	2	2	6	1932	1628	304
3	2	1	2030	2258	-228	6	2	2	6	-1439	-1675	236
4	2	1	5285	4732	553	7	2	2	6	5349	4932	417
5	2	1	-3135	-2713	-422	9	2	2	6	-2125	-2207	82
7	2	1	-3031	-2813	-218	1	2	2	-6	-11719	-11796	77
8	2	1	1081	1743	-662	2	2	2	-6	-7745	-6310	-1435
10	2	1	2602	3010	-408	3	2	2	-6	-3112	-2865	-247
1	2	-1	-6437	-5694	-743	4	2	2	-6	-3484	-3643	159
2	2	-1	-1662	-1523	-139	5	2	2	-6	-4575	-3824	-751
3	2	-1	12608	11839	769	6	2	2	-6	3713	3953	-240
4	2	-1	1814	4757	-2943	7	2	2	-6	-1713	-900	-813
5	2	-1	-1010	-1045	35	9	2	2	-6	-871	-402	-469
6	2	-1	5700	5374	326	0	2	2	7	9995	9833	162
8	2	-1	1622	1949	-327	1	2	2	7	4315	4098	217
10	2	-1	-1067	-1036	-31	3	2	2	7	969	1252	-283
0	2	2	5778	5477	301	4	2	2	7	-5041	-4614	-427
1	2	2	9982	9682	300	5	2	2	7	-1642	-1340	-302
2	2	2	-2713	-2086	-627	7	2	2	7	-3707	-3395	-312
3	2	2	2308	2232	76	1	2	2	-7	5264	5605	-341
4	2	2	3382	3780	-398	3	2	2	-7	2240	2051	189
5	2	2	1240	976	264	4	2	2	-7	3223	2725	498
6	2	2	-1571	-1166	-405							
7	2	2	-2956	-3079	123							



TABLE 2—continued

<i>h</i>	<i>k</i>	100F <sub>a</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>	100F <sub>a</sub>	100F <sub>c</sub>	100Δ		
5	2	-7	1091	1097	-6	7	2	13	4906	4548	358
6	2	-7	-3308	-3542	234	7	2	-13	1341	1125	216
7	2	-7	-3318	-3321	3	*2	2	-13	-1010	-44	-966
8	2	-7	-2737	-2693	-44						
9	2	-7	-1824	-2042	218	3	2	-13	-5170	-5084	-86
10	2	-7	-1118	-1455	337	4	2	-13	3031	3259	-228
0	2	8	-1794	-1691	103	5	2	-13	-1189	-1250	61
1	2	8	11090	11039	51	6	2	-13	-1388	-1557	-169
2	2	8	-4051	-3612	49	8	2	-13	-2169	-2201	32
3	2	8	1723	1174	549	0	2	-13	5802	5951	-149
4	2	8	1128	777	351	2	2	14	5281	5408	-127
5	2	8	-3903	-4275	372	2	2	14	1399	996	403
7	2	8	-2064	-1877	-187	4	2	14	-3595	-3963	368
8	2	8	912	-953	41	5	2	14	-1449	-961	-488
9	2	8	-2203	-2075	-128	1	2	-14	3838	4040	-202
10	2	8	1402	1477	-75	2	2	-14	-3696	-3912	216
1	2	-8	5670	5142	528	3	2	-14	6173	6261	-88
2	2	-8	-1419	-1107	-312	5	2	-14	2993	3245	-312
3	2	-8	3319	7796	523	7	2	-14	-2020	-1961	-59
4	2	-8	2318	2409	-91	9	2	-14	-1480	-1420	-60
5	2	-8	-2487	-2573	86	0	2	15	-3990	-4173	183
8	2	-8	-2857	-1472	185	1	2	15	3801	3729	72
9	2	-8	-2800	-2153	153	2	2	15	1953	2487	-584
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2	2	9	6062	5618	444	5	2	15	-4876	-4442	-434
3	2	9	-895	-827	-68	7	2	15	1175	1008	167
4	2	9	-2267	-2797	530	9	2	15	1638	1285	353
6	2	9	-6947	-6960	13	1	2	-15	-1645	-1984	339
8	2	9	-1966	-2380	414	2	2	-15	3696	3863	-167
1	2	-9	1050	1015	35	3	2	-15	2544	2313	231
*2	2	-9	-1341	-349	-992	4	2	-15	3835	3885	-50
						7	2	-15	-1669	-1700	31
						8	2	-15	-1287	-1387	100
						10	2	-15	1672	1341	331
3	2	-9	-2314	-2265	-49	0	2	16	-909	-774	-135
4	2	-9	-7137	-6919	-218	2	2	16	1818	2169	-351
5	2	-9	3791	3423	368	3	2	16	2243	1684	559
6	2	-9	-2750	-2250	-500	4	2	16	-979	-387	-592
7	2	-9	-1061	-1202	141	9	2	16	1355	1271	84
8	2	-9	-990	-935	-55	2	2	-16	2449	2584	-135
9	2	-9	-1169	-1090	-79	4	2	-16	4088	3782	306
0	2	10	-1564	-1268	-296	6	2	-16	-3095	-3180	85
1	2	10	-3872	-4024	152	8	2	-16	-2439	-2439	8
2	2	10	-7093	-6783	-310	9	2	-16	1736	2253	-517
3	2	10	-3696	-3403	-293	0	2	17	-2297	-2343	46
4	2	10	-3081	-3108	27	1	2	17	-4629	-4449	-180
5	2	10	-2345	-1963	-238	5	2	17	1236	1276	-40
6	2	10	1047	1075	-28	8	2	17	1638	1947	-309
7	2	10	-1858	-1921	63	1	2	-17	-2703	-3240	537
8	2	10	-1128	-1600	472	3	2	-17	5792	6279	-487
9	2	10	-1547	-1408	-139	4	2	-17	1213	1070	143
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1	2	-10	-3876	-3629	-247	8	2	-17	3555	3673	-118
2	2	-10	-3048	-3548	500	0	2	18	-3605	-3582	247
3	2	-10	-3970	-3924	-46	1	2	18	-3362	-2968	-394
4	2	-10	2331	2237	94	4	2	18	2578	2727	-149
5	2	-10	-3231	-3173	-75	9	2	18	2385	2957	-72
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2	2	11	-9536	-8604	-932	3	2	-18	-2284	-2236	-48
3	2	11	-2024	-1557	-467	4	2	-18	2493	2728	-235
4	2	11	-2277	-2211	-66	5	2	-18	3396	3432	-36
5	2	11	1297	1098	199	7	2	-18	2382	2198	184
6	2	11	2247	1821	426	8	2	-18	1307	1133	174
7	2	11	2568	2616	-48	0	2	19	2318	2564	-246
8	2	11	1378	1599	-221	1	2	19	-1625	-1876	251
9	2	11	-1693	-1952	259	10	2	19	2264	2279	-15
1	2	-11	692	970	-278	2	2	-19	-2571	-2086	-485
2	2	-11	-3365	-3059	-306	3	2	-19	2206	2264	-58
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5	2	-11	2372	2092	280	9	2	-19	1571	1762	-191
6	2	-11	2862	2931	-69	0	2	20	1182	1202	-20
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0	2	12	1415	1482	-67	3	2	20	3078	3026	52
1	2	12	-5873	-6151	278	4	2	20	1388	1214	174
2	2	12	1314	519	795	5	2	20	2297	2814	-517
3	2	12	-4920	-4610	-310	1	2	-20	-1510	-1707	197
4	2	12	-1135	-1117	-18	2	2	-20	1686	1439	247
5	2	12	-2970	-3260	290	4	2	-20	-1743	-1610	-133
6	2	12	5552	5713	-161	7	2	-20	-2078	-1675	-403
8	2	12	1138	931	207	8	2	-20	2098	1952	146
1	2	-12	1838	1496	342	0	2	21	1186	1564	-378
2	2	-12	-7424	-7586	162	4	2	21	5045	4970	75
3	2	-12	-5210	-4867	-343	6	2	21	2568	2713	-145
5	2	-12	2433	2594	-161	8	2	21	-1841	-1843	2
6	2	-12	1828	1993	-165	6	2	-21	-3129	-3367	238
7	2	-12	3010	3038	-28	8	2	22	966	119	847
0	2	13	-1615	-1922	307	*0	2				
1	2	13	3734	4117	-383	5	2	22	4139	4262	-123
2	2	13	-5021	-5289	268	6	2	22	-1807	-1962	155
4	2	13	-2882	-3105	223						
*6	2	13	-983	-5	-978						

TABLE 2—continued

<i>h</i>	<i>k</i>	<i>l</i>	100 <i>F</i> <sub>o</sub>	100 <i>F</i> <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>		100 <i>F</i> <sub>o</sub>	100 <i>F</i> <sub>c</sub>	100Δ	
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0	2	23	3666	3828	-162	8	3	3	3656	3465	191	
5	2	23	-1747	-1737	-10	9	3	3	1872	1923	-51	
7	2	23	-1943	-1484	-459	10	3	3	2777	2680	97	
2	2	-23	-1409	-1547	138	1	3	-3	-1007	-1365	358	
5	2	-23	1466	1397	-331	2	3	-3	1442	1349	93	
0	2	24	-1611	-1854	243	3	3	-3	-11286	-10408	-878	
1	2	24	4261	4604	-343	4	3	-3	-3399	-3256	-143	
3	2	24	-2508	-2235	-363	6	3	-3	-1253	-1299	-43	
2	2	24	-1997	-2396	399	7	3	-3	2321	2384	-13	
1	2	-24	-2436	-2244	-192	0	3	4	4605	4104	501	
2	2	-24	1892	2028	-136	1	3	4	-2798	-2435	-363	
4	2	-24	2784	3073	-289	2	3	4	5136	3656	1480	
0	2	25	2879	3008	-129	3	3	4	4899	4509	390	
1	2	25	-3309	-3167	-232	4	3	4	3669	3371	298	
2	2	25	2003	1890	113	5	3	4	986	1085	-99	
4	2	25	-2747	-2507	-240	6	3	4	1978	3109	-1133	
6	2	25	-1696	-1865	169	7	3	4	-4737	-4547	-190	
1	4	-25	1105	1454	-349	9	3	4	2000	1807	193	
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0	1	26	-1959	-2187	228	2	3	-4	-12942	-12127	-815	
1	1	26	1155	1385	-230	3	3	-4	-2524	-2621	97	
2	2	26	-1814	-1742	-72	4	3	-4	-1845	-2089	244	
2	2	-26	-1814	-1502	-312	5	3	-4	-3524	-3131	-393	
5	0	-26	-1642	-2026	384	6	3	-4	2017	1550	467	
0	5	27	-1838	-2093	255	7	3	-4	1395	678	717	
1	3	27	-1311	-1288	-23	8	3	-4	2544	2596	-52	
3	3	-27	-1838	-2136	298	9	3	-4	1601	855	746	
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5	1	-28	-1912	-1534	-378	4	3	5	8346	8114	232	
0	0	29	-1679	-2403	724	5	3	5	4812	4268	544	
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4	4	31	1412	1481	-69	4	3	-5	-3592	-3593	1	
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4	4	3	0	-1371	-543	-828	4	3	6	-871	-572	-299
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6	6	3	0	2524	3349	-825	7	3	6	-3223	-2893	-330
7	7	3	0	2199	2240	-41	9	3	6	-1831	-1800	-31
8	8	3	0	3088	3010	78	10	3	6	-1513	-1571	58
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8	8	3	1	2879	2912	-33						
9	9	3	1	1520	1412	108	6	3	-6	-4518	-4676	158
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5	5	3	-1	2088	2568	-480	1	3	7	5477	5114	363
6	6	3	-1	-1638	-1792	154	2	3	7	-6623	-6382	-241
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8	8	3	-1	-2189	-2569	380	4	3	7	-1642	-1040	-602
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							1	3	-7	-811	-337	-474
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2	3	2	7329	6655	674	3	3	-7	-2466	-1964	-502	
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6	3	-2	2743	3069	-326	7	3	8	1270	1229	41	
7	3	-2	-1469	-1717	248	8	3	8	-1571	-1536	-35	
8	3	-2	1412	1165	247	1	3	-8	12368	11816	552	
10	3	-2	-1713	-1800	87	2	3	-8	2159	1864	295	
1	3	3	1865	2431	-566	3	3	-8	-4095	-3887	-208	
2	3	3	5383	5173	210	4	3	-8	-1632	-830	-602	
3	3	3	4859	3750	1109	5	3	-8	-2118	-1930	-188	



TABLE 2—continued

<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ
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10	3	-8	-1895	-1249	-646	5	3	16	-2199	-1876	-323
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*1	3	9	-844	-240	-604	2	3	-16	4551	4786	-235
						3	3	-16	-1328	-1989	361
2	3	9	3281	2409	872	4	3	-16	2743	3167	-424
3	3	9	2345	2528	-183	5	3	-16	-1932	-2200	168
4	3	9	-4693	-4287	-406	6	3	-16	1277	1347	130
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4	3	-9	-3659	-3455	-204	9	3	17	3000	2255	745
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0	3	10	-3210	-3530	120	2	3	-17	-1839	-2221	332
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3	3	-10	-5383	-5532	149	1	3	-18	-3514	-3528	14
4	3	-10	-2490	-2916	426	2	3	-18	-3051	-3502	451
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3	3	11	-4977	-5119	142	7	3	19	2392	2091	301
5	3	11	-1949	-2163	214	8	3	19	2531	2426	105
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8	3	11	-1517	-1820	303	2	3	-19	2362	2768	-406
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3	3	-11	-2541	-2579	38	6	3	-19	-2436	-2327	-109
4	3	-11	4230	4227	3	0	3	20	-1301	-1475	174
6	3	-11	2902	2619	283	1	3	20	-1067	-416	-651
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1	3	-14	2274	2284	-10	1	3	24	-1294	-485	-809
2	3	-14	7937	8281	-344	3	3	24	-1912	-2292	380
3	3	-14	2375	2120	255	5	3	24	1875	1991	-116
4	3	-14	4176	4327	-151	6	3	24	-2760	-2635	-125
5	3	-14	-3179	-2351	-828	1	3	-24	3500	3871	-371
9	3	-14	2487	2716	-229	2	3	-24	-1554	-2724	1170
0	3	15	3250	3932	-682	0	3	25	2547	2928	-381
1	3	15	1510	1424	86	1	3	25	1148	1299	-151
3	3	15	-1415	-540	-875	2	3	25	-1273	-1285	12
4	3	15	-2967	-2337	-630	5	3	25	-1696	-2186	490
5	3	15	-1726	-1512	-214	7	3	25	-2247	-1547	-700
6	3	15	-1605	-1304	-301	1	3	-25	-2098	-1496	-602
1	3	-15	2368	2357	11	2	3	-25	1591	1121	470
3	3	-15	5616	6200	-584	3	3	-25	-2497	-2563	66
4	3	-15	-2014	-2063	49	1	3	26	1895	2530	-635
6	3	-15	-1388	-1017	-371	2	3	26	-1355	-1274	-81
8	3	-15	1733	2254	-521	6	3	26	-1584	-1550	-34

TABLE 2—continued

<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ
1	3	-26	2277	2408	-131	4	4	-5	-1328	-1934	606
2	3	-26	-1544	-1800	256	5	4	-5	1567	1407	160
3	3	-26	-1828	-1785	-43	7	4	-5	-1757	-1345	-412
4	3	-26	-2422	-2571	149	8	4	-5	-2402	-2156	-246
1	3	27	-2541	-2851	310	9	4	-5	-1142	-1195	53
1	3	-27	1446	905	541	0	4	6	-1905	-2071	166
2	3	-28	-1811	-2026	215	1	4	6	-4633	-4707	74
2	3	28	-2166	-2789	623	2	4	6	-3132	-3179	47
1	3	-28	-1571	-1688	-103	3	4	6	10769	10324	445
1	3	29	-2355	-2605	117	4	4	6	4004	4077	-73
3	3	-30	1378	1675	-297	6	4	6	4217	4581	-364
4	3	-30	1507	1995	-488	7	4	6	-2514	-2668	154
0	3	31	1473	1569	-96	8	4	6	1199	1031	168
3	3	-31	1682	1850	-168	2	4	-6	2689	2626	63
0	4	0	-6515	-6515	-2	1	4	-6	2686	2774	-88
2	4	0	-4869	-4458	-411	3	4	-6	-2544	-1878	-666
3	4	0	1916	1524	332	5	4	-6	-2706	-1969	-737
5	4	0	3940	4044	-104	6	4	-6	-936	-548	-388
9	4	0	-1497	-1711	214	7	4	-6	-1649	-1701	52
10	4	0	-1307	-954	-353	8	4	-6	-1578	-1455	-123
0	4	1	5934	6380	-446	9	4	-6	-1713	-1800	87
1	4	1	-5406	-4879	-527	10	4	-6	-1926	-1602	-324
2	4	1	7671	7785	-114	0	4	7	-6404	-6514	50
3	4	1	-2730	-2749	10	1	4	7	-7201	-7125	-76
4	4	1	871	633	238	2	4	7	932	921	11
5	4	1	2487	2132	355	3	4	7	881	-417	-464
6	4	1	4335	4211	124	4	4	7	9867	10017	-150
7	4	1	4413	4362	51	5	4	7	4693	4034	659
10	4	1	-2128	-212	-1916	6	4	7	-1812	-1697	-215
2	4	-1	-3680	-3541	-139	7	4	7	3382	3476	-94
3	4	-1	5977	5420	557	8	4	7	-3487	-3705	218
4	4	-1	-3190	-3801	611	2	4	-7	-3085	-3747	662
4	4	-1	3921	3631	-310	1	4	-7	-5048	-4731	-317
5	4	-1	-1564	-1596	32	3	4	-7	-2142	2552	-410
6	4	-1	3186	2393	793	4	4	-7	-2199	-1956	-248
7	4	-1	-2179	-2125	-54	7	4	-7	-1652	-1192	-460
8	4	-1	-1152	-1214	62	8	4	-7	-3281	-3409	128
9	4	-1	-1047	-1335	288	0	4	8	4467	4524	-57
1	4	2	3108	2596	512	1	4	8	-5707	-5681	-26
2	4	2	-2429	-3071	642	2	4	8	983	478	505
4	4	2	-827	-931	104	3	4	8	3612	3226	386
5	4	2	-2044	-1682	-362	5	4	8	3869	3735	154
6	4	2	1682	1701	-19	6	4	8	2277	2286	-9
7	4	2	1987	1432	555	7	4	8	-2203	-2268	65
8	4	2	2504	2190	314	8	4	8	-2237	-2357	120
1	4	-2	-2078	-1847	-231	9	4	8	-4741	-4514	-227
2	4	-2	-2422	-2196	-226	1	4	-8	4927	4978	-51
3	4	-2	-1162	-874	-288	3	4	-8	2591	2037	554
4	4	-2	-4268	-4101	-167	5	4	-8	4193	3531	662
5	4	-2	2879	3171	-292	6	4	-8	-1165	-1082	-83
6	4	-2	-5079	-4962	-117	7	4	-8	-2314	-2081	-233
8	4	-2	-1409	-1553	144	9	4	-8	-2821	-2594	-227
0	4	3	6532	6098	434	0	4	9	5447	5550	-103
1	4	3	5798	5258	540	1	4	9	9107	9091	16
2	4	3	5484	5400	84	2	4	9	-6758	-6042	-716
3	4	3	1554	1481	73	3	4	9	5383	5206	177
4	4	3	-5028	-4291	-737	6	4	9	-2243	-2344	101
5	4	3	-4230	-4301	71	8	4	9	-2855	-2896	41
8	4	3	3115	3368	-253	1	4	-9	5585	5916	-331
1	4	-3	4274	3815	459	2	4	-9	-8390	-8656	266
2	4	-3	-4551	-3928	-623	3	4	-9	1111	802	309
3	4	-3	-3886	-3674	-212	4	4	-9	5373	5402	-29
4	4	-3	-4278	-3985	-293	5	4	-9	-2409	-2174	-235
5	4	-3	-3629	-3704	75	6	4	-9	1388	1179	209
6	4	-3	1763	1894	-131	8	4	-9	-1791	-1902	111
7	4	-3	-1121	-948	-173	0	4	10	1652	1361	291
8	4	-3	1912	2349	-437	1	4	10	3061	2924	137
0	4	4	3281	3198	83	2	4	10	3389	3838	-449
1	4	4	1061	1124	-63	3	4	10	-3882	-3910	28
2	4	4	4927	4468	459	4	4	10	2977	2689	288
3	4	4	3798	3374	424	5	4	10	-1858	-1612	-246
4	4	4	3169	3123	46	7	4	10	-2483	-1940	-543
5	4	4	-3551	-3723	172	8	4	10	-2382	-2002	-380
6	4	4	-1189	-1216	27	1	4	-10	-7583	-8259	676
7	4	4	3538	3286	252	2	4	-10	-1246	-1024	-222
9	4	4	2781	3117	-336	3	4	-10	3987	4176	-189
10	4	4	1257	1651	-394	5	4	-10	2531	1989	542
2	4	-4	-1939	-1725	-214	6	4	-10	1540	1636	-96
3	4	-4	-4088	-4031	-57	7	4	-10	-1652	-1757	105
4	4	-4	-2659	-3091	432	0	4	11	-1223	-1023	-200
5	4	-4	-2889	-2788	-101	1	4	11	-1534	-1308	-226
6	4	-4	-1567	-1413	-154	2	4	11	-4099	-4154	55
0	4	5	-3666	-3120	-546	3	4	11	3494	3202	292
1	4	5	-1601	-1531	-70	4	4	11	-4072	-3996	-76
2	4	5	2304	2561	-257	6	4	11	-2250	-1821	-429
4	4	5	1703	1564	139	7	4	11	-2264	-2220	-44
6	4	5	-2078	-2237	209	1	4	-11	-2358	-2752	394
8	4	5	2331	2405	-74	2	4	-11	3429	3413	16
1	4	-5	1608	1736	-128	3	4	-11	3470	3496	-26
2	4	-5	-1077	-1067	-10	4	4	-11	3213	2930	283
3	4	-5	3703	3498	205	5	4	-11	2547	2675	-128
						6	4	-11	-4518	-4883	365

[1964]

Molecular Structure of Phosphobenzene A, (PC<sub>6</sub>H<sub>5</sub>)<sub>5</sub>.

6157

TABLE 2—continued

<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ
7	4	-11	1517	1379	138	8	4	20	1963	1850	113
10	4	-11	1723	1894	-171	1	4	-20	1574	2013	-439
*1	4	12	-804	-195	-609	2	4	-20	-1449	-1171	-278
						4	4	-20	-2406	-2303	-103
2	4	12	-1689	-1707	18	5	4	-20	-3386	-3087	-299
3	4	12	-5714	-5310	-404	1	4	21	1094	1271	-177
4	4	12	-1730	-1459	-271	2	4	21	3730	3662	68
6	4	12	-2645	-2224	-421	8	4	21	2101	1797	304
8	4	12	-2460	-2301	-159	1	4	-21	-942	-943	1
2	4	-12	2291	2175	116	2	4	-21	2088	2312	-224
3	4	-12	4518	4359	159	3	4	-21	-2602	-3034	432
4	4	-12	5021	5266	-245	4	4	-21	-1595	-1708	113
5	4	-12	-4061	-3879	-182	1	4	22	2345	2442	-97
6	4	-12	1480	1968	-488	3	4	22	5298	4949	349
7	4	-12	-2159	-1939	-220	4	4	22	1821	1674	147
9	4	-12	1834	2445	-611	1	4	-22	2017	2124	-107
0	4	13	-2872	-2337	-35	2	4	23	2933	2769	164
1	4	13	-3457	-3768	311	3	4	23	1622	976	646
*2	4	13	1121	81	1040	4	4	23	2301	2386	-85
						5	4	23	2345	2046	299
3	4	13	-2879	-2595	-284	6	4	23	-2963	-2572	-391
6	4	13	2453	2017	436	2	4	-23	-1638	-1492	-146
1	4	-13	1544	1882	-338	3	4	24	1963	1650	313
2	4	-13	4139	4306	-167	4	4	24	1706	1293	413
3	4	-13	4528	4151	377	6	4	24	2260	2234	26
6	4	-13	-3342	-3527	185	1	4	-24	-1856	-1846	-9
1	4	14	-2311	-2407	96	2	4	-24	1301	759	542
2	4	14	-2362	-3306	944	3	4	-24	-2399	-2747	348
4	4	14	-2872	-2716	-156	5	4	-24	1635	1708	-73
5	4	14	3250	3398	-148	1	4	25	1132	1266	-134
7	4	14	-2335	-1521	-814	2	4	25	-1382	-1350	-32
1	4	-14	4720	5030	-310	1	4	-25	1963	2151	-188
2	4	-14	1676	1593	83	2	4	-25	-3548	-4292	744
3	4	-14	3656	3100	556	0	4	26	2757	2750	7
4	4	-14	1375	985	390	1	4	26	-1618	-1504	-114
5	4	-14	-1331	-1466	135	3	4	26	-2551	-2675	124
3	4	15	1733	1680	53	4	4	26	-1611	-1637	26
6	4	15	2757	2358	399	1	4	-26	-1750	-1927	177
7	4	15	-2243	-1637	-606	2	4	-26	2051	1572	479
8	4	15	-1520	-1842	322	3	4	-26	-1463	-1097	-366
2	4	-15	3490	3606	-116	1	4	27	2159	2101	58
3	4	-15	-3122	-3380	258	2	4	27	-2007	-1589	-418
4	4	-15	2365	2340	25	1	4	-28	1132	964	168
5	4	-15	-1439	-1592	153	3	4	-28	1973	2113	-140
6	4	-15	2605	2371	234	2	4	-29	2127	2129	43
7	4	-15	1858	1097	761	0	4	33	1209	1040	169
8	4	-15	1591	1020	571	2	4	33	-1777	-1454	-323
10	4	-15	-1693	-2095	402	*1	4	34	1395	174	1221
0	4	16	-2159	-2304	145						
1	4	16	1473	1692	-219	1	5	0	-4531	-4144	-387
2	4	16	1564	717	847	2	5	0	9593	9258	335
3	4	16	-1297	-1135	-162	3	5	0	-1192	-1304	112
5	4	16	1297	1264	33	4	5	0	2304	2625	-321
6	4	16	-1429	-1679	250	5	5	0	2014	1833	181
7	4	16	-1544	-1553	9	6	5	0	-2622	-2647	25
8	4	16	-2105	-1862	-243	7	5	0	-1726	-2111	385
9	4	16	-1463	-1175	-288	8	5	0	-1652	-1995	343
1	4	-16	-2649	-2639	-10	0	5	1	-6045	-6102	57
2	4	-16	-6001	-5849	-152	1	5	1	6802	6449	353
3	4	-16	1926	1629	297	2	5	1	-4524	-4272	-252
4	4	-16	-1371	-1068	-303	3	5	1	4771	5203	-432
5	4	-16	3865	3725	140	5	5	1	1338	1086	252
7	4	-16	2169	2523	-354	6	5	1	4193	4690	-497
8	4	-16	1486	1114	372	7	5	1	-1469	-1669	200
0	4	17	3771	3807	-36	8	5	1	-1784	-1662	-122
1	4	17	-2480	-2970	490	9	5	1	-1557	-1342	-215
4	4	17	-2186	-1964	-222	1	5	-1	3325	3056	269
6	4	17	1804	1873	-69	2	5	-1	-4781	-4801	20
7	4	17	-1503	-1306	-197	3	5	-1	-2399	-1862	-537
8	4	17	-1500	-1208	-292	4	5	-1	-2923	-2713	-210
1	4	-17	-2189	-1893	-296	5	5	-1	-3024	-2155	-869
2	4	-17	1513	1435	78	10	5	-1	1507	1740	-233
3	4	-17	-2348	-1795	-553	0	5	2	3531	3475	56
4	4	-17	2223	2529	-306	1	5	2	-4014	-3578	-436
6	4	-17	1861	1715	146	2	5	2	3764	3091	673
1	4	18	2291	2599	-308	3	5	2	-4504	-4616	112
2	4	18	-1246	-795	-451	4	5	2	-1892	-1408	-484
7	4	18	2439	2034	405	5	5	2	4156	4059	97
3	4	-18	1321	991	330	7	5	2	1723	1338	385
5	4	-18	-1365	-1813	448	8	5	2	1223	1382	-159
0	4	19	1665	1671	-6	9	5	2	-1365	-1415	50
1	4	19	-1213	-1629	416	1	5	-2	-1203	-1423	220
2	4	19	1554	1612	-58	2	5	-2	-2608	-2850	242
3	4	19	-2358	-2353	-5	3	5	-2	-4433	-4689	256
4	4	19	-1223	-1234	11	4	5	-2	-2406	-2479	73
6	4	19	2754	3029	-275	5	5	-2	-3916	-3343	-573
8	4	19	1823	2184	-356	6	5	-2	2784	3084	-300
2	4	-19	1503	1407	96	8	5	-2	2801	3002	-201
4	4	-19	-2412	-2926	514	9	5	-2	1321	1383	-62
7	4	-19	-1953	-1893	-60	0	5	3	7738	7492	246
4	4	20	-1196	-1389	193	1	5	3	-3112	-2936	-176
7	4	20	4163	3487	676	2	5	3	3179	2687	492

TABLE 2—*continued*

<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ
3	5	3	-6380	-6204	-176	1	5	-9	-3446	-3505	59
4	5	3	-2020	-1763	-257	2	5	-9	2088	2057	31
5	5	3	-2967	-2802	-185	3	5	-9	-1020	-661	-359
6	5	3	4937	4504	433	4	5	-9	2166	1711	455
7	5	3	1818	1779	39	5	5	-9	2020	1712	308
8	5	3	1807	1510	297	6	5	-9	-2233	-2566	333
1	5	-3	-3027	-2854	-373	7	5	-9	1601	1978	-377
2	5	-3	-2645	-2600	-36	8	5	-9	1348	2083	-735
3	5	-3	-4798	-4427	-371	0	5	10	3085	3981	-896
4	5	-3	-5072	-5494	422	2	5	10	-2247	-2220	-27
5	5	-3	2338	2062	276	3	5	10	4024	3831	193
6	5	-3	-2993	-3901	368	4	5	10	-4403	-4438	35
7	5	-3	2135	2391	-256	5	5	10	1622	1929	-307
8	5	-3	-1351	-1716	365	6	5	10	-3240	-2984	-256
0	5	4	2122	1992	130	7	5	10	-2193	-1894	-299
1	5	4	4707	4823	-116	8	5	10	1794	1366	428
2	5	4	-4254	-3774	-480	9	5	10	-1382	-1299	-83
3	5	4	-3051	-2500	-551	1	5	-10	3555	4133	-578
4	5	4	-5153	-4730	-423	2	5	-10	-4700	-5133	433
5	5	4	-1469	-1320	-149	3	5	-10	3190	3018	172
7	5	4	1851	1724	127	4	5	-10	1483	1128	355
8	5	4	2466	2546	-80	5	5	-10	-3233	-3505	272
1	5	-4	-807	-640	-167	6	5	-10	2514	2149	365
2	5	-4	-2977	-3078	101	9	5	-10	2101	2405	-304
3	5	-4	-2666	-2180	-486	0	5	11	1277	1569	-292
4	5	-4	-1730	-1327	-403	1	5	11	1101	1036	65
7	5	-4	-1520	-1943	423	2	5	11	-1388	-778	-610
*8	5	-4	-1203	-354	-849	3	5	11	-2051	-1944	-107
						6	5	11	-2720	-2088	-632
9	5	-4	-1253	-1477	224	8	5	11	-1831	-1704	-127
2	5	5	1916	1775	141	9	5	11	1351	1275	76
4	5	5	-2605	-2306	-299	1	5	-11	-2835	-3232	397
5	5	5	-3963	-4074	111	2	5	-11	6082	6421	-339
6	5	5	3190	3371	-181	5	5	-11	1851	2018	-167
8	5	5	3315	3608	-293	8	5	-11	2500	2571	-71
1	5	-5	2659	2821	-162	0	5	12	-3494	-3849	355
2	5	-5	-6251	-5922	-329	*1	5	12	854	99	755
4	5	-5	1513	1798	-285						
7	5	-5	-1794	-1806	12	2	5	12	-2098	-1750	-348
8	5	-5	-2466	-2615	149	4	5	12	1909	1787	122
9	5	-5	-2145	-1658	-487	1	5	-12	3808	4012	-204
10	5	-5	-1503	-1521	18	2	5	-12	2372	2121	251
1	5	6	5393	5789	-396	3	5	-12	1777	1626	151
4	5	6	4176	4318	-142	6	5	-12	-2743	-2927	184
5	5	6	-1642	-1634	-8	7	5	-12	1537	1686	-149
7	5	6	4041	4088	-47	1	5	13	-3865	-4058	193
9	5	6	1804	1807	-3	2	5	13	-4663	-4174	-489
1	5	-6	-1720	-1659	-61	4	5	13	-3068	-3290	222
2	5	-6	1689	1628	61	5	5	13	4102	4202	-100
3	5	-6	2051	2162	-111	7	5	13	1743	1411	332
5	5	-6	4839	4122	717	1	5	-13	3406	3447	-41
6	5	-6	-3460	-3542	82	2	5	-13	5335	5963	-628
7	5	-6	-1233	-1470	237	3	5	-13	-1868	-2299	431
8	5	-6	-2169	-2174	5	4	5	-13	1371	1117	254
9	5	-6	-2926	-2383	-543	5	5	-13	-2848	-2614	-234
0	5	7	-3318	-3480	162	6	5	-13	3734	3665	69
2	5	7	6630	6217	413	7	5	-13	-2118	-1132	-986
3	5	7	4801	4672	129	1	5	14	-2088	-2065	-23
4	5	7	2669	2311	358	3	5	14	-2808	-3005	197
5	5	7	4484	3994	490	4	5	14	1165	963	202
6	5	7	-1382	-1205	-177	5	5	14	-4261	-2367	-1894
7	5	7	3301	2753	548	6	5	14	3663	3000	663
8	5	7	3325	3631	-306	3	5	-14	-1375	-1234	-141
9	5	7	-1831	-1596	-235	5	5	-14	2896	2831	65
1	5	-7	4562	4363	199	7	5	-14	2453	2055	398
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3	5	-7	1044	494	550	1	5	15	1074	782	292
4	5	-7	7941	8081	-140	3	5	15	-2081	-1494	-587
5	5	-7	-1635	-1670	35	6	5	15	-1649	-1509	-140
7	5	-7	-1608	-961	-647	1	5	-15	-1669	-1494	-175
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0	5	8	-2473	-2244	-229	5	5	-15	1943	2215	-272
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2	5	8	-932	-1012	80	7	5	-15	2088	1727	361
3	5	8	5028	5196	-168	0	5	16	2517	2450	67
4	5	8	2987	2537	450	1	5	16	-3085	-3285	200
5	5	8	1916	2078	-162	2	5	16	3044	3008	36
6	5	8	-1912	-1961	49	3	5	16	1456	1198	258
7	5	8	1378	1526	-148	4	5	16	-1544	-1121	-423
1	5	-8	-3740	-3953	213	7	5	16	-2750	-2512	-238
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3	5	-8	4535	4521	14	3	5	-16	-2291	-2840	549
4	5	-8	1128	1150	-22	4	5	-16	1355	1152	203
5	5	-8	1311	1629	-318	6	5	-16	1547	1756	-209
9	5	-8	1324	1753	-429	0	5	17	-1564	-1499	-65
0	5	9	-1013	-1420	407	1	5	17	1980	1895	85
1	5	9	3301	3098	203	2	5	17	-2669	-2488	-181
2	5	9	4768	5237	-469	4	5	17	1595	1457	138
3	5	9	-2507	-2301	-206	7	5	17	-2382	-2704	322
4	5	9	5501	5542	-41	7	5	17	-2929	-2610	-319
5	5	9	-2226	-2767	541	8	5	17	-2720	-2466	-254
6	5	9	-1490	-1213	-277	1	5	-17	1412	1206	206

TABLE 2—continued

<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ
3	5	-17	1561	1544	17	7	6	-3	-4197	-4379	182
4	5	-17	-2071	-1888	-183	9	6	-3	-1652	-2007	355
4	5	-18	-1520	-1322	-198	0	6	4	-2220	-1887	-388
4	5	-18	-3247	-2946	-301	1	6	4	-3585	-3682	97
5	5	-18	-2135	-2228	93	3	6	4	-5041	-5315	274
0	5	19	1257	2086	-829	*6	6	4	1159	231	928
1	5	19	-2835	-3255	420						
2	5	19	-3301	-3448	147	1	6	-4	-2446	-2742	296
6	5	19	1845	1788	57	3	6	-4	1192	858	334
7	5	19	2183	1748	435	4	6	-4	1763	2024	-261
2	5	-19	-1436	-308	-62	5	6	-4	2534	1965	569
3	5	-19	-4514	-4215	-299	6	6	-4	-5667	-5722	55
4	5	-19	-1841	-2245	404	8	6	-4	-3511	-3625	114
5	5	-19	-2054	-2048	-6	0	6	5	3112	2778	334
0	5	20	-1047	-1461	414	1	6	5	1074	1282	-208
3	5	20	-2747	-2399	-348	2	6	5	-2284	-2429	145
3	5	20	-5268	-5451	183	4	6	5	-3129	-2657	-472
6	5	20	1834	1718	116	5	6	5	-2189	-2385	196
3	5	-20	-1297	-1324	27	6	6	5	1544	1523	21
4	5	-20	-1638	-1511	-127	9	6	5	1635	1769	-134
4	5	21	-1902	-1633	-260	1	6	-5	3348	3152	196
6	5	21	2034	2162	-128	2	6	-5	1966	2345	-379
7	5	21	2645	1544	1101	3	6	-5	4105	4063	42
8	5	21	1615	1698	-83	4	6	-5	4639	4490	149
1	5	-21	1267	902	365	6	6	-5	-1469	-1507	38
2	5	-21	-2882	-3518	636	7	6	-5	-2740	-2500	-240
6	5	22	1175	1460	-285	8	6	-5	-1260	-736	-524
7	5	22	-2328	2471	-143	0	6	6	1946	1682	264
1	5	-22	-3315	-3115	-200	1	6	6	1902	1590	312
2	5	23	2345	2594	-249	2	6	6	2700	2667	33
2	5	23	3502	3513	79	3	6	6	-1760	-2351	591
3	5	23	2399	2348	51	5	6	6	1361	1608	-247
6	5	23	1659	1032	627	7	6	6	1774	1020	754
8	5	23	2037	1621	416	8	6	6	1395	2030	-635
2	5	-23	-3639	-3808	169	9	6	6	-1625	-1355	-270
4	5	-23	1578	1698	-120	10	6	6	1463	1364	99
1	5	24	1936	1800	136	1	6	-6	1213	1351	-138
2	5	24	1747	1684	63	3	6	-6	4741	4729	12
3	5	24	3622	3692	-70	4	6	-6	3369	3117	252
1	5	-24	-1662	-1773	111	5	6	-6	-1861	-1538	-323
3	5	-24	1591	1661	-70	7	6	-6	-2821	-2915	94
4	5	-24	-1534	-954	-580	1	6	7	1453	1570	-117
2	5	25	2551	2541	10	2	6	7	1017	820	197
3	5	-25	-1652	-1820	177	3	6	7	2781	2722	59
2	5	26	-2159	-1979	-180	4	6	7	-1057	-1321	264
3	5	26	1385	1370	15	6	6	7	3913	3786	127
3	5	-26	1807	2243	-436	7	6	7	3119	2719	400
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1	5	-28	1446	1249	197	2	6	-7	5879	6280	-401
2	6	0	-3301	-3790	489	3	6	-7	1865	1784	81
3	6	0	3240	3252	-12	6	6	-7	-2291	-2980	689
4	6	0	-3781	-3611	-170	7	6	-7	2429	2296	133
5	6	0	-3105	-2731	-374	1	6	8	3372	3254	118
6	6	0	4342	3971	371	2	6	8	1696	1509	187
7	6	0	-3467	-3477	10	4	6	8	3372	3361	11
8	6	0	1689	1714	-25	6	6	8	1463	1649	-186
0	6	1	-2041	-2440	399	7	6	8	2449	2023	426
1	6	1	1713	1459	254	1	6	-8	2517	2619	-102
2	6	1	1466	1110	356	2	6	-8	-6032	-3610	-2422
*3	6	1	-1534	-218	-1316	3	6	-8	1855	1789	66
						4	6	-8	-2122	-2563	441
						7	6	-8	3328	3058	270
4	6	1	3744	3599	145	8	6	-8	1524	1451	73
5	6	1	-1645	-1666	21	9	6	-8	1574	1465	109
8	6	1	-1848	-2579	731	1	6	9	3375	3089	286
1	6	-1	-5234	-5320	86	2	6	9	1770	1634	136
2	6	-1	1159	935	224	3	6	9	3615	4102	-487
3	6	-1	-6484	-6772	288	4	6	9	-2838	-2813	-25
4	6	-1	-1905	-1911	6	7	6	9	1456	1238	218
6	6	-1	-2017	-1790	-227	8	6	9	1503	1399	104
0	6	2	-1834	-1602	-232	1	6	-9	-2030	-2069	39
1	6	2	-4910	-5203	293	2	6	-9	963	678	285
2	6	2	4869	5147	-278	4	6	-9	-2622	-2151	-471
3	6	2	1578	1539	39	6	6	-9	2899	2886	13
4	6	2	2869	3153	-284	7	6	-9	1885	1461	424
7	6	2	-2737	-2443	-294	8	6	-9	2710	2775	-65
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1	6	-2	-1466	-1534	68	1	6	10	1672	1818	-146
2	6	-2	-4399	-4985	586	2	6	10	3673	3377	296
3	6	-2	-2517	-2149	-368	6	6	10	-3480	-3082	-398
4	6	-2	-4024	-3968	-56	9	6	10	1818	1788	30
6	6	-2	-1824	-1893	69	2	6	-10	3163	3595	-432
7	6	-2	1544	2162	-618	3	6	-10	-3102	-3153	51
9	6	-2	1358	1259	99	7	6	-10	3615	3498	117
1	6	3	1132	1281	-149	1	6	11	3108	3433	-325
2	6	3	-6799	-6806	7	2	6	11	3284	3107	177
4	6	3	-1422	-1631	209	4	6	11	1324	684	640
8	6	3	-2466	-1978	-488	5	6	11	-1578	-1335	-243
1	6	-3	-3375	-3482	107	6	6	11	-2517	-1899	-618
2	6	-3	-4646	-4479	-167	1	6	-11	6045	6471	-426
3	6	-3	-2588	-2181	-407	2	6	-11	-1659	-1706	47

TABLE 2—*continued*

<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ	2	6	-28	1787	2131	-344
3	6	-11	3061	3032	29	2	7	0	-4829	-4875	46
4	6	-11	-1324	-1533	209	3	7	0	-3294	-3258	-36
5	6	-11	-2970	-2659	-311	7	7	0	2034	1543	491
6	6	-11	2743	2843	-100	8	7	0	-1655	-1529	-126
0	6	12	2784	3084	-300	0	7	1	-1192	-1282	90
1	6	12	-1203	-1112	-91	1	7	1	-4271	-4137	-134
2	6	12	1513	941	572	2	7	1	5460	5466	-6
3	6	12	2321	2028	293	3	7	1	-2443	-2567	124
4	6	12	-2108	-2295	197	4	7	1	1074	993	81
5	6	12	1561	2015	-454	5	7	1	2101	2085	16
6	6	12	-3419	-3440	21	9	7	1	-1388	-1730	342
2	6	-12	6397	6521	-124	2	7	-1	-2639	-2498	-141
3	6	-12	-2203	-2398	195	3	7	-1	-5531	-5488	-43
4	6	-12	1767	1217	550	4	7	-1	2493	2854	-361
5	6	-12	-2324	-2101	-223	5	7	-1	-2108	-2051	-57
0	6	13	-3720	-4117	397	6	7	-1	3406	2705	701
1	6	13	-4839	-4977	138	7	7	-1	1459	1430	29
4	6	13	2226	2021	205	8	7	-1	-1990	-2327	337
6	6	13	2493	2548	-55	1	7	2	2395	2258	137
7	6	13	-3696	-3318	-378	1	7	2	-1925	-633	-292
2	6	-13	-1540	-1642	102	3	7	2	-3933	-4008	75
3	6	-13	1206	1620	-414	7	7	2	5511	5195	316
4	6	-13	-1882	-2863	981	8	7	2	-3166	-2529	-637
8	6	-13	-1987	-1692	-295	1	7	2	-2591	-2847	316
0	6	14	-4352	-4407	55	3	7	-2	-3713	-3570	-143
1	6	14	-2321	-1970	-351	4	7	-2	-6228	-5862	-366
2	6	14	-4927	-4565	-362	6	7	-2	2064	2395	-331
5	6	14	1520	1313	207	0	7	-2	-1530	-1547	17
1	6	-14	-2510	-1788	-722	1	7	3	-1071	-1480	409
6	6	-14	3203	3527	-324	2	7	3	892	839	53
0	6	15	2206	2404	-198	3	7	3	-3190	2123	-182
1	6	15	-4149	-4378	229	4	7	3	2818	-3287	97
2	6	15	1564	2202	-638	5	7	3	-2493	-2375	623
3	6	15	-1990	-1972	-18	7	7	3	-2416	-2024	-392
4	6	15	-1355	-1782	427	8	7	3	-1405	-1094	-311
2	6	-15	-1784	-1633	-151	9	7	3	-1365	-1279	-86
1	6	16	1905	2181	-276	1	7	-3	-1588	-1717	129
2	6	16	-2696	-2677	-19	2	7	-3	-2811	-2880	69
5	6	16	-3379	-3339	-40	*3	7	-3	1169	244	925
1	6	-16	-2639	-2435	-204	5	7	-3	-3291	-2679	-612
2	6	-16	2071	1859	212	6	7	-3	-1490	-1133	-357
4	6	-16	-2463	-2604	141	6	7	-3	-1510	-1714	204
1	6	17	1662	1771	-109	7	7	-3	-1426	-1437	11
2	6	17	2740	2942	-202	0	7	4	-1811	-2097	286
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6	6	17	-2804	-2702	-102	2	7	4	1111	1038	73
1	6	-17	1182	651	531	3	7	4	-2936	-2323	-608
3	6	-17	-5690	-6020	330	5	7	4	3903	3913	-10
5	6	-17	-2314	-1958	-356	1	7	-4	4382	4545	-163
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1	6	18	-1855	-2012	157	3	7	-4	-1240	-709	-531
4	6	18	-1598	-1488	-110	5	7	-4	-2416	-2140	-276
7	6	18	-2618	-2187	-431	6	7	-4	-3487	-3689	202
2	6	-18	-2274	-2921	647	7	7	-4	3031	3162	-131
3	6	-18	-1733	-2183	450	0	7	5	-3970	-3702	-268
4	6	-18	-2311	-2706	395	2	7	5	-1645	-1717	72
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0	6	19	-3598	-3708	110	10	7	5	4129	4480	-351
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3	6	19	-2145	-2328	183	2	7	-5	4109	4313	-209
5	6	19	-1839	-1759	-130	3	7	-5	-3470	-3021	-449
1	6	-19	1855	1844	11	6	7	-5	-2210	-2956	746
2	6	-19	-1943	-2535	592	0	7	6	-946	-475	-471
1	6	20	-3930	-4288	358	1	7	6	-1263	-938	-325
2	6	20	-1834	-1669	-165	2	7	6	-2527	-2521	-6
3	6	20	-1932	-2068	136	3	7	6	-1987	-1851	-136
5	6	20	1706	1980	-274	6	7	6	1868	1742	126
8	6	-20	-2193	-1672	-521	7	7	6	1814	1397	417
0	6	21	1469	633	836	9	7	6	1658	1105	483
1	6	21	-1665	-2177	512	10	7	6	4734	4886	-152
2	6	21	-3231	-3021	-260	1	7	-6	4437	4485	-48
5	6	21	2037	1872	165	2	7	-6	1334	750	584
7	6	21	2152	1882	270	3	7	-6	1429	1213	216
1	6	-21	-1040	-946	-94	7	7	-6	1747	1800	-53
2	6	-21	-1382	-621	-761	8	7	-6	936	520	416
3	6	-21	2064	2584	-520	1	7	7	-1057	-911	-146
4	6	-21	2297	2307	-10	2	7	7	1669	1718	-49
1	6	22	1361	1566	-205	4	7	7	1561	1594	-33
3	6	22	-1459	-1344	-115	5	7	7	3261	3758	-497
6	6	22	2531	2079	452	1	7	-7	-1649	-1266	-383
3	6	-22	2122	2476	-354	2	7	-7	1645	1649	-4
0	6	23	2000	2148	-148	3	7	-7	-1909	-1893	-16
1	6	23	1226	1005	221	4	7	-7	2470	1577	893
2	6	-23	2939	3012	-73	5	7	-7	1294	1166	128
4	6	-23	2199	2677	-478	6	7	-7	2382	2251	131
1	6	24	1922	2373	-451	7	7	-7	1196	1190	6
2	6	24	2669	2573	96	0	7	8	1199	1035	164
1	6	-24	1456	1240	216	3	7	8	1635	1558	77
1	6	25	3156	3128	23	4	7	8	5193	4578	615
3	6	25	1780	1889	-109	5	7	8	2885	2611	274
2	6	26	1834	1934	-100	6	7	8	-1635	-1869	234
3	6	-27	1828	2055	-227	9	7	8			



[1964]

Molecular Structure of Phosphobenzene A, (PC<sub>6</sub>H<sub>5</sub>)<sub>5</sub>.

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TABLE 2—continued

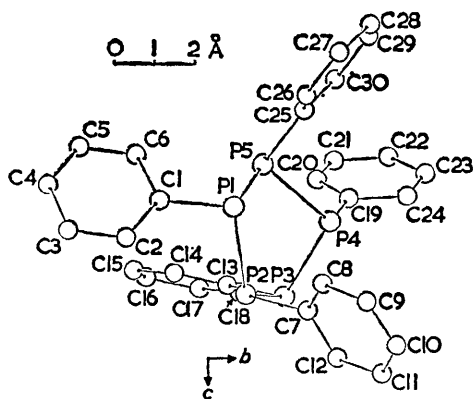
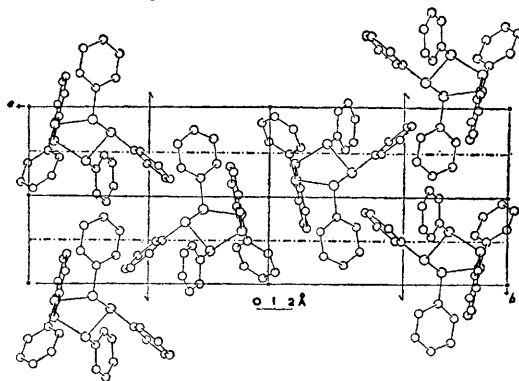
<i>h</i>			100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ
1	7	-8	-2216	-1958	-258	0	7	21	-2240	-2966	726
3	7	-8	-3031	-3098	67	2	7	21	-1605	-2075	470
4	7	-8	2375	2188	187	2	7	-21	1875	1962	-87
5	7	-8	1824	1789	35	4	7	-21	1980	2048	-88
6	7	-8	2098	2094	4	1	7	22	-2037	-2020	-17
7	7	-8	3261	3591	-330	2	7	-22	2024	1899	125
1	7	9	2983	3053	-70	1	7	23	-1128	-1183	55
6	7	9	2933	2686	-247	1	7	-23	1203	1450	-247
7	7	9	2091	1864	227	4	7	-23	-1730	-2198	468
10	7	9	-2372	-1951	-421	2	7	24	-1716	-1517	-199
1	7	-9	-1581	-1448	-133	0	7	25	1490	1418	72
2	7	-9	-4119	-3910	-209	1	7	26	1368	1121	247
3	7	-9	-2314	-1973	-341	1	7	27	1433	1321	162
6	7	-9	3406	2763	643	2	7	-27	1885	1957	-72
7	7	-9	1858	2082	-224	0	8	0	-4291	-4436	145
0	7	10	1645	1111	534	1	8	0	-1399	-1457	58
1	7	10	4146	4158	-12	2	8	0	1956	2081	-125
2	7	10	1993	2094	-101	3	8	0	-2652	-2944	292
6	7	10	1415	1463	-48	4	8	0	1686	1465	221
1	7	-10	1442	1093	349	5	8	0	-1818	-1371	-447
3	7	-10	1297	1616	-319	0	8	1	902	475	427
0	7	11	5836	5811	25	1	8	1	-2112	-2177	65
1	7	11	2926	2541	385	2	8	1	-2730	-2436	-294
2	7	11	2615	2277	338	3	8	1	4342	4704	-362
3	7	11	1270	1616	-346	4	8	1	-2669	-2804	135
4	7	11	-3061	-2873	-188	7	8	1	-2223	-1577	-646
6	7	11	-2480	-2008	-472	1	8	-1	-1730	-1660	-70
7	7	11	2149	1915	234	5	8	-1	-1905	-2151	246
1	7	-11	4281	4679	-398	6	8	-1	1889	1472	417
2	7	-11	1321	1798	-477	9	8	-1	2368	2076	292
5	7	-11	-1980	-1948	-32	0	8	2	-2389	-2336	-53
1	7	12	4017	4028	-11	2	8	2	1057	814	243
2	7	12	4017	3629	388	3	8	2	-1983	-1971	-12
5	7	12	-3220	-3180	-40	4	8	2	3315	3377	-62
1	7	-12	-1909	-1283	-626	5	8	2	-2595	-2327	-268
4	7	-12	-2291	-2121	-170	8	8	2	-2142	-1593	-549
0	7	13	-1382	-963	-419	2	8	-2	1838	2166	-328
1	7	13	2547	2313	234	3	8	-2	3548	3203	345
3	7	13	4065	3968	97	4	8	-2	-1997	-1815	-182
5	7	13	-1405	-1088	-317	8	8	-2	1797	3034	-1237
6	7	13	-2453	-1787	-666	0	8	3	-1297	-1481	184
1	7	-13	2000	1719	281	1	8	3	-2710	-2692	-18
4	7	-13	1388	1512	-124	2	8	3	-1088	-1240	152
0	7	14	-1297	-1345	48	4	8	3	-1855	-1972	117
1	7	14	-2537	-2603	66	6	8	3	-2125	-1420	-705
2	7	14	3947	4291	-344	1	8	-3	3375	2778	597
3	7	14	-1564	-1559	-5	2	8	-3	4082	4386	-304
4	7	14	2179	2729	-550	5	8	-3	-1480	-1491	11
5	7	14	1611	1644	-33	7	8	-3	2233	2481	-248
6	7	14	-1530	-989	-541	0	8	4	2247	2223	24
1	7	-14	-2443	-2551	108	3	8	4	2142	2278	-136
*2	7	-14	1341	336	1005	1	8	-4	1115	1535	-420
						2	8	-4	2000	2113	-113
5	7	-14	1767	1923	-156	4	8	-4	-2527	-2123	-404
0	7	15	-3081	-3574	493	0	8	5	-3132	-3124	-8
2	7	15	-2335	-2184	-151	1	8	5	-1628	-1292	-336
3	7	15	2983	3124	-141	2	8	5	-2460	-2311	-149
6	7	15	2649	2580	69	3	8	5	-3879	-3670	-209
7	7	15	-2054	-1832	-222	1	8	-5	6353	6899	-546
1	7	-15	-1527	-1503	-24	2	8	-5	3281	3103	178
3	7	-15	-3247	-3030	-217	8	8	-5	1591	1499	92
4	7	-15	2909	2967	-58	0	8	6	1929	1524	405
0	7	16	1804	1502	302	1	8	6	-3217	-2925	-292
1	7	16	-1223	-1102	-121	2	8	6	-2500	-2884	384
2	7	16	-1551	-1077	-474	3	8	6	-1581	-1519	-62
2	7	-16	-3365	-3640	275	4	8	6	-2520	-2449	-71
8	7	-16	-1784	-1833	49	5	8	6	-1503	-1480	-23
0	7	17	2449	2710	-261	8	8	6	1358	1337	21
1	7	17	-1811	-2071	260	1	8	-6	1132	631	501
2	7	17	1889	1910	-21	2	8	-6	-1152	-1267	115
4	7	17	-1402	-1855	453	3	8	-6	-1267	-1655	388
1	7	-17	-2639	-2666	27	5	8	-6	1946	1789	157
2	7	-17	-1601	-1473	-128	7	8	-6	2747	2821	-74
4	7	-17	-1720	-2046	326	1	8	7	-2331	-2261	-70
5	7	-17	2328	1862	466	2	8	7	-1355	-1296	-59
7	7	-17	-1892	-1948	56	3	8	7	1608	1882	-274
1	7	18	1858	1860	-2	1	8	-7	-2155	-2408	253
2	7	18	-2345	-2414	69	4	8	-7	2693	2744	-51
3	7	18	1415	1574	-159	5	8	-7	1899	2029	-130
5	7	18	-3916	-3729	-187	6	8	-7	3186	2486	700
3	7	-18	-1895	-1803	-92	7	8	-7	1953	1694	259
5	7	-18	-1831	-1073	-758	8	8	-7	-2311	-2189	-122
1	7	19	-1206	-1402	196	2	8	8	-2128	-1981	-147
2	7	19	1615	1596	19	4	8	8	3754	3595	159
3	7	19	-1703	-1519	-184	8	8	8	-1625	-2203	578
6	7	19	-2223	-2143	-80	3	8	-8	1997	1888	99
2	7	-19	-1551	-1820	269	4	8	-8	1987	1945	42
3	7	-19	1659	1351	308	6	8	-8	2101	2071	30
2	7	20	-1665	-1797	132	1	8	9	-1963	-1967	4
2	7	-20	1706	1754	-48	2	8	9	2372	2696	-324
3	7	-20	1780	1792	-12	4	8	9	1885	1768	117
5	7	-20	2010	1533	477	5	8	9	3811	3589	222

TABLE 2—*continued*

<i>h</i>	<i>k</i>		100F <sub>o</sub>	100F <sub>c</sub>	100Δ	<i>h</i>	<i>k</i>	<i>l</i>	100F <sub>o</sub>	100F <sub>c</sub>	100Δ
6	8	9	1578	974	604	6	9	5	-1368	-1135	-233
1	8	-9	-1591	-954	-37	1	9	-5	-1642	-1403	-239
5	8	-9	-1429	-923	506	3	9	-5	-1790	-1377	-403
2	8	10	-2504	-2561	57	5	9	-5	2987	2522	465
4	8	10	2162	2191	-29	1	9	6	1707	1354	413
5	8	10	3494	3384	110	1	9	6	-2608	-2275	-333
3	8	10	1513	1732	-219	2	9	6	-2216	-2268	-52
6	8	-10	1405	1332	73	3	9	6	-1453	-1256	-197
4	8	-10	-1540	-1861	321	4	9	6	-2024	-1851	-173
6	8	-10	-1750	-1812	62	1	9	-6	-1392	-1287	-105
1	8	11	1929	2400	-471	2	9	-6	-3406	-3349	-57
3	8	11	-2875	-2948	73	4	9	-6	1520	1988	-468
6	8	11	2473	2469	4	5	9	-6	1618	787	831
1	8	-11	1148	1603	-455	6	9	-6	2449	2479	-30
3	8	-11	-2453	-2194	-259	1	9	7	1497	590	907
5	8	-11	-2240	-1789	-451	2	9	7	-3085	-2891	-194
0	8	12	2264	2589	-325	3	9	7	-2199	-2191	-8
1	8	12	1165	1001	164	5	9	7	-1980	-1478	-502
4	8	12	-3683	-3268	-415	1	9	-7	-2291	-2338	47
1	8	-12	-2064	-2104	40	2	9	-7	-1595	-1651	56
0	8	13	1760	2499	-739	5	9	-7	2804	2407	397
1	8	13	2798	2890	-92	2	9	-8	2436	2154	282
2	8	13	2656	2735	-79	4	9	-8	1588	1878	-290
3	8	13	-1385	-1339	-46	0	9	9	1365	606	759
2	8	-13	-1385	-1326	-59	1	9	9	-1203	-1024	-179
5	8	-13	1926	1845	81	3	9	9	2740	2380	360
1	8	14	2152	2011	141	1	9	-9	2960	2997	-37
2	8	14	1260	1774	-514	2	9	-9	-1909	-2059	150
3	8	14	1246	1126	120	4	9	-9	-1740	-1490	-250
4	8	-14	2578	2930	-352	0	9	10	-1412	-1277	-135
6	8	-14	2057	2042	15	4	9	10	4673	4580	98
2	8	15	1513	1129	384	6	9	10	1757	1198	559
3	8	15	1344	1043	301	1	9	-10	-1503	-1888	385
1	8	-15	-4693	-4870	177	3	9	-10	-2088	-1950	-138
2	8	-15	-2341	-2178	-163	1	9	11	-1794	-2014	220
4	8	-15	-2858	-2616	-242	2	9	11	-1388	-994	-394
5	8	-15	2838	2619	219	5	9	11	3788	3245	543
0	8	16	-4051	-4040	-11	0	9	12	2845	2795	50
1	8	16	-1348	-862	-486	2	9	12	-1540	-1226	-314
5	8	-16	-2345	-2145	-200	2	9	-12	-3433	-3276	-157
2	8	17	-1784	-1863	79	1	9	13	1334	1256	78
3	8	17	1358	1877	-519	3	9	13	-2426	-2391	-35
4	8	-17	-1987	-1664	-323	1	9	-13	-5467	-5316	-151
5	8	-17	-1983	-1388	-595	5	9	-13	1956	1381	575
2	8	18	2189	2209	-20	0	9	14	4268	4378	-101
3	8	18	-1348	-1877	529	1	9	14	1223	713	510
6	8	18	-1655	-1451	-204	4	9	14	-1581	-1752	171
1	8	-18	-1953	-1932	-21	2	9	15	1571	1600	-29
0	8	19	1446	995	451	5	9	-15	-2737	-2589	-148
3	8	19	1540	1775	-235	6	9	16	1517	1565	-48
4	8	19	-2027	-1732	-295	2	9	-16	1895	1610	235
1	8	-19	1101	975	126	4	9	-16	-2845	-3037	192
4	8	-19	1581	1258	323	6	9	-16	-2071	-2122	51
1	8	-20	1693	1762	-69	2	9	17	2216	2171	45
1	8	21	-1818	-1780	-38	1	9	-17	2456	2486	-30
1	8	22	-1520	-1513	-7	5	9	-17	-2385	-2453	68
2	8	22	-1419	-1628	209	4	9	-18	-1574	-1064	-510
1	8	-22	1351	1163	188	1	9	19	1946	1918	28
0	8	23	-2064	-2313	249	2	9	22	-1513	-1495	-18
2	8	23	-1804	-1605	-199	1	9	-25	1203	1382	-179
1	8	24	-1371	-790	-581	0	10	0	1439	1241	198
4	8	24	1649	1625	24	3	10	0	-1314	-1286	-28
4	8	-25	1466	1208	258	6	10	0	2260	1898	362
1	8	-27	1581	1770	-189	1	10	1	1645	1575	70
4	9	0	-4899	-4624	-275	1	10	-1	1426	1356	70
6	9	0	-1723	-1116	-607	5	10	-1	3291	3250	41
0	9	1	-969	-657	-312	0	10	2	2270	2661	-391
2	9	1	1801	1986	-185	2	10	2	1824	1680	144
5	9	1	-3788	-3265	-523	4	10	2	-2318	-2211	-107
1	9	-1	1111	984	127	4	10	-2	1625	2041	-416
3	9	-1	-2666	-2680	14	0	10	3	-1784	-2230	446
5	9	-1	-2118	-1885	-233	1	10	3	1841	1965	-124
0	9	2	-1740	-1915	175	2	10	3	2338	2106	232
6	9	2	-1652	-1762	110	5	10	3	-2480	-1884	-596
1	9	-2	2287	2170	117	2	10	-3	3450	3345	105
2	9	-2	2230	1936	294	5	10	-3	1997	1100	897
3	9	-2	1517	1263	254	2	10	4	1797	2368	-571
0	9	3	1638	1596	42	3	10	4	2379	2128	251
2	9	3	1540	1125	415	1	10	-4	1943	1365	578
3	9	3	3291	3097	194	4	10	-4	1608	1733	-125
1	9	-3	3747	3957	-210	1	10	5	-1331	-1261	-70
2	9	-3	1503	1180	323	1	10	-5	-2419	-2545	126
5	9	-3	1622	1363	259	5	10	-5	1581	1114	467
0	9	4	-3987	-4402	415	0	10	6	-2257	-2439	182
2	9	4	-1426	-1803	377	4	10	-6	2017	1834	183
4	9	4	2179	2122	57	*0	10	7	-1263	-231	-1032
1	9	-4	1618	1564	54						
4	9	-4	1983	1368	615	1	10	7	-1382	-1241	-141
1	9	5	-1206	-1215	9	3	10	7	-2193	-2031	-162
2	9	5	-1392	-1546	154	2	10	-7	-3429	-2618	-811
3	9	5	-1469	-1441	-28	3	10	-7	1314	1305	9
4	9	5	-1605	-1180	-425	4	10	8	-2737	-2539	-198

TABLE 2—continued

$h$	$k$		100F <sub>o</sub>	100F <sub>c</sub>	100Δ	$h$	$k$		100F <sub>o</sub>	100F <sub>c</sub>	100Δ
4	10	-8	-2081	-1505	-576	0	11	4	2429	2172	257
0	10	9	-1838	-1807	-31	1	11	4	1453	1181	272
5	10	9	-2953	-2514	-439	2	11	4	1503	1582	-79
1	10	-9	-1402	-1635	233	1	11	5	2281	2075	206
3	10	-9	-2845	-2544	-301	2	11	5	2118	1193	925
1	10	10	-1412	-1251	-161	3	11	5	2172	1554	618
6	10	10	-2449	-2103	-346	2	11	-5	-1922	-1910	-12
1	10	-10	1395	970	425	1	11	-6	-2267	-2027	-240
2	10	-10	-2578	-2314	-264	0	11	7	-1385	-1607	222
3	10	11	2142	1847	295	3	11	-7	-1889	-2208	319
1	10	-11	-2101	-2242	141	4	11	-7	1649	1656	-7
0	10	12	-2564	-2715	151	2	11	8	-2014	-1745	-269
4	10	12	2132	2081	51	5	11	8	-1851	-1844	-7
0	10	13	2622	2748	-126	2	11	-8	-1730	-1291	-439
1	10	13	-1642	-1432	-210	5	11	-8	-1922	-1468	-454
3	10	-13	2061	1422	639	1	11	9	-1449	-1301	-148
2	10	14	-1595	-1089	-506	1	11	10	-1500	-1066	-434
2	10	-14	2632	2534	98	2	11	-10	1655	1690	-35
4	10	-14	-2108	-1874	-234	0	11	11	-1767	-1724	-43
1	10	-15	1713	2289	-576	4	11	11	1561	1492	69
0	10	16	1456	1997	-541	3	11	-11	1497	1989	-492
1	10	16	-1618	-1597	-21	1	11	12	-1385	-1527	162
4	10	16	1929	1100	829	1	11	13	1304	584	720
5	10	17	1716	1337	379	1	11	15	-1623	-1575	-53
0	10	18	1422	1000	421	0	11	19	1439	1310	129
0	10	20	1693	1600	93	1	11	-20	1507	1065	442
1	10	20	1436	1716	-280	0	12	1	-1611	-1491	-120
0	10	23	-1341	-1358	17	1	12	2	-1662	-1858	196
2	11	0	-2000	-2248	248	5	12	2	2591	2318	273
5	11	0	2230	1919	311	2	12	-2	1939	1546	393
1	11	1	-2115	-2047	-68	4	12	3	1659	1506	153
2	11	1	-1301	-1300	-1	1	12	-4	-2010	-1911	-99
2	11	-1	2041	2109	-68	0	12	5	2341	2460	-119
4	11	-1	2030	2041	-11	1	12	6	2446	2115	331
2	11	2	-2277	-1918	-359	1	12	-6	-1368	-1725	357
3	11	-2	-1524	-1492	-32	4	12	9	-1970	-1600	-370
1	11	-2	1885	2232	-347	1	12	-10	1794	1467	327
0	11	3	1186	1386	-200						

FIG. 1. View of molecule projected down  $[a]$ , and labelling of the atoms.FIG. 2. Packing of molecules projected down  $[a]$ .

The analysis shows that form A of  $(PPh)_n$  is a pentamer ( $n = 5$ ) with a five-membered ring of phosphorus atoms to each of which is attached a phenyl ring.

TABLE 3.

Bond lengths (in Å) and angles (in degrees), with their corresponding standard deviations.

P1-P2	2.223 (5)	P1-C1	1.833 (13)		
P2-P3	2.215 (5)	P2-C7	1.858 (13)		
P3-P4	2.207 (5)	P3-C13	1.858 (13)		
P4-P5	2.220 (5)	P4-C19	1.840 (12)		
P5-P1	2.219 (5)	P5-C25	1.828 (12)		
Average P-P	2.217 (6)*	Average P-C	1.843 (14)*		
C1-C2	1.394 (19)	C7-C8	1.409 (19)	C13-C14	1.384 (19)
C2-C3	1.440 (22)	C8-C9	1.439 (21)	C14-C15	1.422 (21)
C3-C4	1.383 (23)	C9-C10	1.387 (22)	C15-C16	1.372 (23)
C4-C5	1.366 (23)	C10-C11	1.387 (22)	C16-C17	1.401 (22)
C5-C6	1.436 (22)	C11-C12	1.435 (22)	C17-C18	1.386 (21)
C6-C1	1.413 (19)	C12-C7	1.424 (20)	C18-C13	1.398 (19)
C19-C20	1.399 (17)	C25-C26	1.387 (19)		
C20-C21	1.425 (19)	C26-C27	1.426 (23)		
C21-C22	1.386 (21)	C27-C28	1.355 (23)		
C22-C23	1.361 (22)	C28-C29	1.384 (23)		
C23-C24	1.430 (21)	C29-C30	1.429 (22)		
C24-C19	1.418 (19)	C30-C25	1.402 (18)		
Average C-C	1.403 (26)*				
P1-P2-P3	107.24 (19)	P3-P2-C7	97.41 (42)	P1-P2-C7	101.38 (42)
P2-P3-P4	94.05 (18)	P4-P3-C13	109.80 (42)	P2-P3-C13	104.45 (42)
P3-P4-P5	100.25 (18)	P5-P4-C19	99.89 (40)	P3-P4-C19	105.89 (40)
P4-P5-P1	95.05 (17)	P1-P5-C25	102.54 (39)	P4-P5-C25	96.40 (39)
P5-P1-P2	103.47 (18)	P2-P1-C1	101.12 (43)	P5-P1-C1	101.26 (42)
Average P-P-P	100.01 (544)*	Average P-P-C	102.01 (395)*		
P1-C1-C2	119.25 (98)	P3-C13-C18	114.45 (96)		
P1-C1-C6	121.08 (98)	P4-C19-C20	125.19 (92)		
P2-C7-C8	123.18 (97)	P4-C19-C24	115.78 (92)		
P2-C7-C12	116.51 (98)	P5-C25-C26	125.47 (98)		
P3-C13-C14	124.35 (99)	P5-C25-C30	116.57 (91)		
Average P-C-C	120.18 (421)*				
C1-C2-C3	119.25 (130)	C7-C8-C9	120.60 (126)	C13-C14-C15	118.66 (129)
C2-C3-C4	119.08 (144)	C8-C9-C10	118.95 (137)	C14-C15-C16	120.90 (145)
C3-C4-C5	123.73 (150)	C9-C10-C11	120.83 (149)	C15-C16-C17	119.25 (147)
C4-C5-C6	117.00 (144)	C10-C11-C12	121.75 (148)	C16-C17-C18	120.94 (139)
C5-C6-C1	121.50 (129)	C11-C12-C7	117.69 (133)	C17-C18-C13	119.31 (129)
C6-C1-C2	119.33 (120)	C12-C7-C8	119.99 (121)	C18-C13-C14	120.90 (121)
C19-C20-C21	120.13 (115)	C25-C26-C27	121.43 (136)		
C20-C21-C22	120.56 (129)	C26-C27-C28	120.42 (150)		
C21-C22-C23	119.90 (142)	C27-C28-C29	119.60 (150)		
C22-C23-C24	121.39 (141)	C28-C29-C30	120.77 (144)		
C23-C24-C19	119.19 (126)	C29-C30-C25	119.83 (126)		
C24-C19-C20	118.80 (113)	C30-C25-C26	117.85 (117)		
Average C-C-C	119.98 (141)*				

\* Standard deviation of individual values from the average.

The P-P bond lengths are all equal within the limits of error ( $2.217 \pm 0.006$  Å) and the P-P-P-P torsion angles are given in Table 4. Since one of these angles (P5-P1-P2-P3) is almost zero, the equilateral pentagon of phosphorus atoms possesses the approximate

TABLE 4.

P-P-P-P Torsion angles.

Atoms	Degrees
5-1-2-3	+ 2.2
1-2-3-4	+ 33.3
2-3-4-5	- 58.1
3-4-5-1	+ 60.6
4-5-1-2	- 36.5

symmetry  $m$ .<sup>14</sup> This plane passes through P4 and the mid-point of the P1–P2 bond. In an equilateral pentagon, if  $\phi_1$  be the angle at P1 then  $\phi_4$  is related to  $\phi_1$  ( $=\phi_2$ ) by the equation<sup>15</sup>  $\sin(\phi_4/2) = \frac{1}{2} - \cos\phi_1$ . Substitution of the average of  $\phi_1$  and  $\phi_2$  ( $105.35^\circ$ ) in this equation gives  $\phi_4 = 99.61^\circ$ ; the measured value of  $\phi_4$  is  $100.25^\circ$ . The angle  $\phi_3$  ( $=\phi_5$ ) is left free to assume values in a wide range, the maximum being  $3\pi/2 - (\phi_1 + \phi_4/2) = 114.5^\circ$  when the ring is planar. The values which  $\phi_3$  and  $\phi_5$  adopt are  $94.1^\circ$  and  $95.1^\circ$ , respectively, bringing the average P–P–P angle down to  $100.0^\circ$ . The least-squares plane through P1, P2, P3, and P5 is

$$-0.40841X + 0.91188Y - 0.04080Z = 1.10161$$

and the distances of the atoms from this plane are: P1, 0.020; P2,  $-0.024$ ; P3, 0.009; P5,  $-0.005$  Å.

Thus, although the deviations from  $m$  symmetry are statistically significant they are much smaller than those found in  $(PCF_3)_5$ <sup>16</sup> and  $(AsCH_3)_5$ <sup>15</sup> where the smallest torsion angles are  $+18$  and  $-10^\circ$ , respectively. The P–P bond lengths found in  $(PCF_3)_5$ <sup>14,16</sup> ( $2.213$  Å) and  $(PCF_3)_4$ <sup>14,17</sup> ( $2.223$  Å) agree well with the value reported here ( $2.217$  Å).

The P–P–P bond angles show a wide scatter but the average value ( $100.0^\circ$ ) is close to the value found in  $(PCF_3)_5$ <sup>16</sup> ( $101.3^\circ$ ); however the average P–P–C angles in the two compounds differ considerably, that for  $(PPh)_5$  being  $102.0^\circ$  while in  $(PCF_3)_5$  it is  $97.6^\circ$ . Thus the P–C valences in  $(PPh)_5$  are directed away from the ring centre relative to those in  $(PCF_3)_5$ , possibly to allow room for the phenyl group. The P–C–C bond angles deviate significantly from their average value ( $120.2^\circ$ ) as is also the case in  $PPh_3$ ;<sup>18</sup> their sum at each carbon atom is, however, close to  $360^\circ$ .

TABLE 5.

Least-squares planes through phenyl rings, mean C–C lengths, and mean C–C–C angles.

Ring	$l$	$m$	$n$	$p$	Average C–C length (Å)	Average C–C–C angle (degrees)
C1–C6	$-0.84796$	$0.06751$	$-0.52574$	$2.47813$	$1.405$	$119.98$
C7–C12	$0.53626$	$0.61904$	$-0.57377$	$1.53082$	$1.414$	$119.97$
C13–C18	$0.09319$	$0.19073$	$-0.97721$	$2.13260$	$1.394$	$119.99$
C19–C24	$-0.40214$	$0.02535$	$-0.91523$	$2.40068$	$1.403$	$120.00$
C25–C30	$0.12573$	$-0.75269$	$-0.64626$	$2.11413$	$1.397$	$119.98$

TABLE 6.

Non-bonded intramolecular contacts (in Å) of less than  $3.6$  Å (contacts across the benzene rings omitted)

P1–P3	3.57	P1–C7	3.17	P3–C7	3.07
P2–P4	3.24	P2–C13	3.23	P4–C13	3.33
P3–P5	3.40	P3–C19	3.24	P5–C19	3.12
P4–P1	3.27	P4–C25	3.03	P1–C25	3.17
P5–P2	3.49	P5–C1	3.14	P2–C1	3.14
	P1–C2	2.79	P3–C18	2.75	
	P1–C6	2.83	P4–C20	2.88	
	P2–C8	2.88	P4–C24	2.77	
	P2–C12	2.80	P5–C26	2.86	
	P3–C14	2.88	P5–C30	2.76	
P1–C8	3.30	P2–C2	3.39	P3–C12	3.27
P1–C26	3.30	P2–C14	3.35	C18–C20	3.33
P4–C7	3.53	P5–C6	3.26	C19–C30	3.52
P4–C30	3.52	P5–C20	3.35		

<sup>14</sup> J. Donohue, *Acta Cryst.*, 1962, **15**, 708.

<sup>15</sup> J. H. Burns and J. Waser, *J. Amer. Chem. Soc.*, 1957, **79**, 859.

<sup>16</sup> C. J. Spencer and W. N. Lipscomb, *Acta Cryst.*, 1961, **14**, 250.

<sup>17</sup> G. J. Palenik and J. Donohue, *Acta Cryst.*, 1962, **15**, 564.

<sup>18</sup> J. J. Daly, *J.*, 1964, 3799.

The average P–C bond length (1.843 Å) does not differ significantly from that found in PPh<sub>3</sub> (1.828 Å). The carbon atoms in the phenyl rings form planar, regular hexagons, within the limits of error; the equations of the least-squares planes through these rings, average C–C bond lengths, and average C–C–C bond angles are given in Table 5. The C–C bond lengths agree well with the standard value.<sup>19</sup>

The non-bonded intramolecular contacts of less than 3.6 Å (excluding distances across the phenyl rings) are listed in Table 6. The first 25 of these are base lines of the bond angles. There are 51 van der Waals contacts of less than 4 Å, the shortest being a C···C contact of 3.41 Å; the shortest contacts involving a P atom are 3.77 Å (to another P atom) and 3.87 Å (to a C atom).

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<sup>19</sup> L. E. Sutton *et al.*, "Interatomic Distances," *Chem. Soc. Special Publ.* No. 11., London, 1958.

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