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729. *The Crystal and Molecular Structure of Triphenylphosphorus.*

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The structure of triphenylphosphorus, PPh_3, has been determined by single-crystal *X*-ray diffraction methods. A three-dimensional least-squares refinement has been carried out. The molecule has the expected pyramidal configuration about the phosphorus atom but, owing to the unequal rotation of the benzene rings about the P–C bonds, possesses no symmetry. The mean P–C bond length is 1·828 Å; none of these three bonds differs significantly from the mean.

The determination of the correct structure of triphenylphosphorus in the solid state was reported recently.[1] The parameters obtained from this two-dimensional *X*-ray analysis have now been refined by the least-squares method, using three-dimensional data recorded photographically from Cu K_α radiation. The unit cell, space group, and density have been known for some time and the data have been summarised.[2]

Experimental and Results

$C_{18}H_{15}P$, $M = 262·3$, Monoclinic, $a = 11·413$, $b = 15·032$, $c = 8·500$ Å, $\beta = 92° 53'$, $U = 1456·4$ Å^3, $Z = 4$, $D_c = 1·196$ g./cc. Space group $P2_1/a(C_{2h}^5)$. Cu K_α radiation, single-crystal oscillation and Weissenberg photographs. The cell constants were determined from high-angle reflexions on oscillation photographs with asymmetric film mounting and are estimated to be

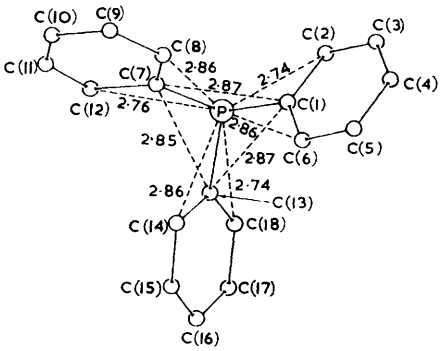

Fig. 1. The *a*-axis projection of the molecule, showing the numbering of the atoms and intramolecular distances less than 3·0 Å between non-bonded atoms, excluding C · · · C in benzene rings.

accurate to 1 part in 700. The cell dimensions are in reasonable agreement with previous values.[2,3] The axial ratio $a : b = 0·7592$ agrees with the value found by optical goniometry[4] (0·7590).

Multiple-film Weissenberg photographs were taken round all three principal axes. The relative intensities of the diffracted beams were estimated visually by comparison with a calibrated strip. All layers were brought to the same relative scale by correlation through common reflexions. 2290 reflexions were observed to be non-zero. Systematic absences were: $h0l$ absent if h odd, $0k0$ absent if k odd. Thus, the space group is $P2_1/a$. No correction has been made for absorption ($\mu = 15·7$ cm.$^{-1}$).

All three-dimensional calculations were done on an Elliott 803B computer using a programming system devised by Daly, Stephens, and Wheatley.[5] The quantity minimised in the least-squares refinement was $\Sigma w(|F_o| - |F_c|)$.[2] The anisotropic thermal parameters were used in the

[1] Daly, *Z. Krist.*, 1963, **118**, 332.
[2] *Structure Reports*, 1950, **13**, 551.
[3] Howells, Lovell, Rogers, and Wilson, *Acta Cryst.*, 1954, **7**, 298.
[4] Porter and Spiller, "Baker Index of Crystals," 1956, Vol. II, Part 3, M 2692.
[5] Daly, Stephens, and Wheatley, Monsanto Research S.A. Final Report No. 52 (1963).

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TABLE 1.

Co-ordinates, standard deviations, and orthogonal co-ordinations in Å.

	X	Y	Z	X'	Y'	Z'
P	2·4259(11)	0·5627(12)	1·2005(11)	2·3655	0·5627	1·1990
C(1)	3·5649(44)	1·9779(47)	1·4101(48)	3·4940	1·9779	1·4083
C(2)	3·3675(52)	2·8035(52)	2·5224(54)	3·2406	2·8035	2·5192
C(3)	4·1901(62)	3·9015(54)	2·7772(65)	4·0504	3·9015	2·7737
C(4)	5·1890(64)	4·2199(59)	1·9302(69)	5·0919	4·2199	1·9277
C(5)	5·4083(59)	3·3982(63)	0·8255(68)	5·3668	3·3982	0·8245
C(6)	4·5845(51)	2·2879(54)	0·5549(57)	4·5566	2·2879	0·5542
C(7)	3·4373(44)	−0·8618(48)	1·8018(45)	3·3467	−0·8618	1·7995
C(8)	4·7024(49)	−0·7426(51)	2·4490(51)	4·5792	−0·7426	2·4459
C(9)	5·3381(61)	−1·8812(58)	2·9977(63)	5·1873	−1·8812	2·9939
C(10)	4·7318(65)	−3·1393(63)	2·8811(70)	4·5869	−3·1393	2·8774
C(11)	3·4760(66)	−3·2609(62)	2·2399(73)	3·3633	−3·2609	2·2371
C(12)	2·8250(59)	−2·1321(57)	1·6851(64)	2·7402	−2·1321	1·6830
C(13)	2·3314(45)	0·2894(48)	−0·6123(46)	2·3622	0·2894	−0·6115
C(14)	3·3149(54)	−0·4223(66)	−1·2903(52)	3·3798	−0·4223	−1·2887
C(15)	3·1694(70)	−0·5393(72)	−2·6862(63)	3·3045	−0·5393	−2·6828
C(16)	2·0659(75)	0·0040(71)	−3·4012(60)	2·2370	0·0040	−3·3969
C(17)	1·0800(78)	0·6937(61)	−2·7178(64)	1·2167	0·6937	−2·7143
C(18)	1·2311(57)	0·8358(53)	−1·3122(55)	1·2971	0·8358	−1·3105

TABLE 2.

Anisotropic thermal parameters and their standard deviations in Å^2.

	U_{11}	U_{22}	U_{33}	$2U_{12}$	$2U_{23}$	$2U_{13}$
P	0·0504(5)	0·0626(6)	0·0584(6)	−0·0003(9)	−0·0077(10)	0·0005(9)
C(1)	0·0590(22)	0·0622(25)	0·0662(25)	0·0069(39)	−0·0100(41)	−0·0127(38)
C(2)	0·0780(30)	0·0656(30)	0·0749(29)	0·0084(47)	−0·0220(47)	−0·0173(48)
C(3)	0·0938(38)	0·0674(31)	0·0970(41)	−0·0045(55)	−0·0234(58)	−0·0326(63)
C(4)	0·0953(39)	0·0671(34)	0·1120(46)	−0·0097(59)	0·0028(62)	−0·0507(67)
C(5)	0·0801(34)	0·0819(36)	0·1100(47)	−0·0295(60)	0·0173(67)	0·0062(63)
C(6)	0·0671(26)	0·0712(30)	0·0900(35)	−0·0205(48)	−0·0001(54)	0·0125(48)
C(7)	0·0594(23)	0·0643(26)	0·0603(23)	−0·0090(39)	−0·0056(40)	−0·0020(37)
C(8)	0·0648(25)	0·0741(31)	0·0709(28)	0·0142(45)	−0·0031(47)	−0·0183(43)
C(9)	0·0895(35)	0·0762(35)	0·0943(39)	0·0248(58)	0·0093(58)	−0·0277(60)
C(10)	0·0978(40)	0·0771(36)	0·1054(45)	0·0213(63)	0·0172(66)	−0·0155(68)
C(11)	0·1019(42)	0·0660(34)	0·1200(52)	0·0080(61)	0·0119(66)	−0·0188(75)
C(12)	0·0849(34)	0·0671(31)	0·1013(41)	−0·0125(53)	−0·0030(57)	−0·0009(60)
C(13)	0·0596(23)	0·0679(28)	0·0601(22)	−0·0224(41)	−0·0063(41)	−0·0032(37)
C(14)	0·0754(32)	0·1085(42)	0·0671(29)	−0·0341(59)	−0·0471(55)	−0·0198(49)
C(15)	0·0999(43)	0·1223(52)	0·0794(35)	−0·0682(79)	−0·0472(72)	0·0351(63)
C(16)	0·1315(53)	0·1023(45)	0·0702(32)	−0·1054(86)	0·0150(66)	−0·0091(65)
C(17)	0·1360(55)	0·0822(39)	0·0830(37)	−0·0604(73)	0·0155(60)	−0·0655(74)
C(18)	0·0867(34)	0·0664(29)	0·0764(31)	−0·0248(49)	0·0096(47)	−0·0428(53)

form $\exp - 2\pi^2(\sum_{i,j=1}^{3} U_{ij}h_ib_ih_jb_j)$. The weighting scheme was the one described by Cruickshank:[6] $w = 1/(a + |F_o| + c|F_o|^2)$, with $a = 2|F_{min.}|$ and $c = 2/|F_{max.}|$.

The final values of R and R' were 0·101 and 0·018, respectively. The number of planes used in the final refinement cycle was 2260. The final co-ordinates, followed by their estimated standard deviations (e.s.d.) in parentheses, and the orthogonal co-ordinates are given in Table 1. Thus, 2·4259 (11) means that the co-ordinates of the atom (2·4259 Å) has an e.s.d. of 0·0011 Å. The transformation of the monoclinic co-ordinates (X, Y, Z) to orthogonal co-ordinates (X', Y', Z') is given by: $X' = X + Z\cos\beta$; $Y' = Y$; $Z' = Z\sin\beta$. The thermal parameters U_{ij} and their e.s.d.s' are listed in Table 2. F_o, F_c, and Δ, from the penultimate set of parameters, are given in Table 3. The maximum parameter shift in the final cycle was 0·3 of one e.s.d. [the Z-co-ordinate of C(4)]. The bond lengths and angles with their e.s.d.s' are given in Table 4. Fig. 1 shows the a-axis projection of the molecule, the numbering of the atoms and non-bonded intramolecular distances below 3 Å, excluding carbon–carbon distances across a benzene ring. Fig. 2 shows the a-axis projection of the unit-cell contents, and Fig. 3 the c-axis projection of

[6] Cruickshank *et al.*, "Symposium on Computer Methods," Pergamon, London, 1961.

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TABLE 3.

Observed and calculated structure factors. Planes marked with an asterisk were not included in the least-squares totals.

h	*k*	*l*	$100F_o$	$100F_c$	100Δ	*h*	*k*	*l*	$100F_o$	$100F_c$	100Δ	*h*	*k*	*l*	$100F_o$	$100F_c$	100Δ
2	0	0	-8099	-10740	2641	9	8	0	912	957	-45	10	1	1	-328	-251	-77
4	0	0	3591	3416	175	10	8	0	-670	-759	89	11	1	1	-1067	-1144	77
6	0	0	-1783	-1918	135	11	8	0	-635	-712	77	12	1	1	724	762	-38
8	0	0	-2046	-2091	45	13	8	0	299	398	-99	13	1	1	252	321	-69
10	0	0	2420	2632	-212	1	9	0	-637	-517	-120	1	1	-1	3652	4020	-368
12	0	0	-1229	-1305	76	2	9	0	-522	-587	65	2	1	-1	2074	1989	85
14	0	0	371	416	-45	3	9	0	-721	-498	-223	3	1	-1	-2353	-2501	148
1	1	0	-1270	-1043	-227	4	9	0	2056	1816	240	4	1	-1	3126	3116	10
2	1	0	611	598	13	5	9	0	-409	-331	-78	5	1	-1	3335	3183	152
3	1	0	-2106	-2266	160	6	9	0	-2221	-2131	-90	6	1	-1	1788	1666	122
4	1	0	540	656	-116	8	9	0	1238	1138	100	7	1	-1	-825	-882	57
5	1	0	677	453	224	9	9	0	-383	-393	10	13	1	-1	-229	-223	-6
6	1	0	-672	-522	-150	10	9	0	-779	-787	8	14	1	-1	227	235	-8
7	1	0	-506	-667	161	12	9	0	163	258	-95	0	2	1	3175	3272	-97
8	1	0	1166	1228	-62	1	10	0	-437	-249	-188	1	2	1	-3876	-4417	541
9	1	0	1068	1062	6	2	10	0	1276	1179	97	2	2	1	-7806	-7752	-54
10	1	0	249	160	89	3	10	0	1170	1137	33	3	2	1	-3893	-3879	-14
11	1	0	-656	-779	123	4	10	0	347	267	80	4	2	1	3329	3294	35
12	1	0	202	140	62	5	10	0	506	481	25	5	2	1	-1007	-1023	16
1	2	0	-1147	-1172	25	6	10	0	982	988	-6	6	2	1	-3605	-3967	362
2	2	0	-8513	-10193	1680	7	10	0	-548	-451	-97	7	2	1	467	402	65
3	2	0	-898	-546	-352	9	10	0	709	507	202	8	2	1	253	230	23
4	2	0	1267	1726	-459	10	10	0	-578	-572	-6	9	2	1	429	481	-52
5	2	0	1422	2015	-593	11	10	0	-368	-379	11	10	2	1	-265	-279	14
6	2	0	-1235	-1194	-41	12	10	0	187	253	-66	12	2	1	-346	-341	-5
7	2	0	123	171	-48	1	11	0	496	243	253	14	2	1	332	511	-179
8	2	0	-877	-1047	170	2	11	0	-1171	-1117	-54	1	2	-1	-2366	-2282	-84
9	2	0	1028	1036	-8	3	11	0	409	422	-13	2	2	-1	-2260	-2171	-89
10	2	0	1694	1710	-16	4	11	0	880	675	205	*3	2	-1	227	31	196
11	2	0	-648	-676	28	6	11	0	-542	-513	-29						
12	2	0	-724	-784	60	7	11	0	484	332	152	4	2	-1	-2608	-2207	-401
13	2	0	146	201	-55	8	11	0	588	533	55	6	2	-1	3096	3054	42
14	2	0	521	597	-76	9	11	0	-672	-588	-84	7	2	-1	-635	-552	-83
1	3	0	5796	6859	-1063	10	11	0	-377	-391	14	8	2	-1	-1342	-1485	143
2	3	0	-7258	-7784	526	11	11	0	443	501	-58	9	2	-1	1050	565	485
3	3	0	-4397	-4935	538	1	12	0	-1441	-1381	-60	10	2	-1	2011	2038	-27
4	3	0	550	272	278	2	12	0	1118	918	200	11	2	-1	-884	-809	-75
5	3	0	2465	2712	-247	3	12	0	1149	1139	10	12	2	-1	-1094	-1082	-12
6	3	0	-2457	-2805	348	4	12	0	-796	-931	135	14	2	-1	291	367	-76
7	3	0	-1976	-2033	57	6	12	0	491	377	114	0	3	1	4206	4437	-231
8	3	0	1189	1227	-38	7	12	0	-294	-286	-8	1	3	1	7080	7724	-644
9	3	0	1110	1166	-56	8	12	0	569	581	-12	2	3	1	5150	4972	178
10	3	0	-1307	-1314	7	10	12	0	-562	-581	19	3	3	1	-2545	-2449	-96
13	3	0	-240	-276	36	2	13	0	812	728	84	4	3	1	-790	-723	-67
1	4	0	-1675	-2009	334	3	13	0	531	411	120	5	3	1	838	1033	-195
2	4	0	-3681	-3484	-197	4	13	0	454	397	57	6	3	1	-2175	-2106	-69
3	4	0	-1760	-1235	-525	5	13	0	-343	-281	-62	7	3	1	-1090	-1141	51
4	4	0	618	516	102	6	13	0	-437	-342	-95	8	3	1	1471	1562	-91
5	4	0	-639	-626	-13	7	13	0	617	436	181	9	3	1	1028	1044	-16
6	4	0	303	153	150	8	13	0	-221	-241	20	10	3	1	-1022	-1002	-20
7	4	0	476	530	-54	9	13	0	-560	-502	-58	12	3	1	228	246	-18
8	4	0	-659	-691	32	2	14	0	868	872	-4	13	3	1	336	353	-17
10	4	0	841	791	50	3	14	0	-211	-240	29	14	3	1	-233	-217	-16
11	4	0	-257	-209	-48	4	14	0	-314	-260	-54	1	3	-1	-6031	-5729	-302
12	4	0	-909	-839	-70	5	14	0	-298	-233	-65	2	3	-1	-6490	-6295	-195
13	4	0	422	450	-28	1	15	0	-473	-393	-80	3	3	-1	-157	-419	262
14	4	0	469	517	-48	2	15	0	393	363	30	4	3	-1	2825	2819	6
1	5	0	915	642	273	3	15	0	222	677	-455	5	3	-1	327	254	73
2	5	0	-7348	-7613	265	4	15	0	639	546	93	6	3	-1	-1393	-1310	-83
3	5	0	-1291	-830	-461	5	15	0	-557	-617	60	7	3	-1	-1167	-1091	-76
4	5	0	4957	4899	58	7	15	0	536	430	106	*8	3	-1	361	27	334
5	5	0	1395	1361	34	1	16	0	302	263	39						
6	5	0	-2683	-2885	202	2	16	0	272	239	33	9	3	-1	1050	993	57
7	5	0	-151	-138	-13	3	16	0	-191	-207	16	12	3	-1	-235	-258	23
8	5	0	3977	4157	-180	4	16	0	-305	-330	25	13	3	-1	-418	-442	24
10	5	0	-295	-264	-31	5	16	0	303	356	-53	14	3	-1	293	360	-67
11	5	0	-276	-211	-65	6	16	0	183	201	-18	0	4	1	90	260	-170
12	5	0	-272	-261	-11	2	17	0	459	445	14	1	4	1	-306	-396	90
13	5	0	-163	-176	13	4	17	0	-389	-579	190	2	4	1	2717	2358	359
1	6	0	-278	-347	69	5	17	0	-541	-559	18	3	4	1	4053	3939	114
2	6	0	-4391	-3950	-441	2	18	0	410	425	-15	4	4	1	5141	4803	338
3	6	0	2141	1891	250	4	18	0	-203	-182	-21	5	4	1	-3164	-3198	34
4	6	0	1396	1477	-81	0	0	1	4415	6103	-1688	6	4	1	-1323	-1180	-143
5	6	0	-1170	-1064	-106	2	0	1	8401	8955	-554	7	4	1	1297	1257	40
6	6	0	-467	-450	-17	4	0	1	6011	5988	23	8	4	1	611	493	118
7	6	0	280	272	8	6	0	1	-548	-637	89	9	4	1	-292	-406	114
8	6	0	-288	-311	23	8	0	1	377	340	37	11	4	1	-457	-377	-80
9	6	0	-621	-660	39	10	0	1	239	202	37	12	4	1	-596	-567	-29
10	6	0	401	342	59	12	0	1	338	242	96	13	4	1	375	372	3
11	6	0	-750	-705	-45	14	0	1	157	142	15	14	4	1	305	273	32
13	6	0	409	441	-32	2	0	-1	-13187	-16836	3649	1	4	-1	-4195	-3493	-702
1	7	0	-802	-621	-181	4	0	-1	-1482	-907	-575	2	4	-1	-2016	-1583	-433
2	7	0	-4898	-4847	-51	*6	0	-1	440	20	420	3	4	-1	1841	1690	151
3	7	0	-1592	-1342	-250							4	4	-1	1184	1049	135
4	7	0	2353	2392	-39	8	0	-1	-1475	-1430	-45	5	4	-1	1888	2020	-132
5	7	0	1691	1719	-28	10	0	-1	2264	2239	25	6	4	-1	2065	2055	10
6	7	0	-2064	-2127	63	12	0	-1	-1639	-1632	-7	7	4	-1	-1349	-1232	-117
7	7	0	-419	-459	40	14	0	-1	351	335	16	8	4	-1	-1310	-1186	-124
8	7	0	2155	1991	164	0	1	1	-1406	-1607	201	9	4	-1	1173	1148	25
10	7	0	-807	-730	-77	1	1	1	-2906	-2721	-185	10	4	-1	690	617	73
11	7	0	162	203	-41	2	1	1	1736	1930	-194	11	4	-1	-443	-436	-7
1	8	0	-3523	-3350	-173	3	1	1	2048	1950	98	12	4	-1	-673	-665	-8
2	8	0	462	276	186	4	1	1	2301	2428	-127	13	4	-1	303	383	-80
3	8	0	-813	-670	-143	*5	1	1	324	63	261	14	4	-1	200	249	-49
4	8	0	952	726	226							0	5	1	-499	-619	120
5	8	0	488	307	181	6	1	1	-995	-1021	26	1	5	1	-706	-400	-306
6	8	0	969	1011	-42	7	1	1	-2450	-2324	-126	2	5	1	-1189	-1124	-65
7	8	0	-176	-153	-23	8	1	1	635	616	19	3	5	1	-1376	-1219	-157
8	8	0	365	396	-31												

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TABLE 3. (*Continued.*)

h	*k*	*l*	$100F_o$	$100F_c$	100Δ
4	5	1	-1691	-1829	138
5	5	1	553	599	-46
6	5	1	-1360	-1438	78
7	5	1	-1158	-830	-328
8	5	1	805	731	74
9	5	1	1036	946	90
10	5	1	210	152	58
11	5	1	-242	-239	-3
12	5	1	565	529	36
1	5	-1	-1041	-747	-294
2	5	-1	-5389	-4930	-459
3	5	-1	-1161	-1350	189
4	5	-1	6878	6508	370
5	5	-1	443	434	9
6	5	-1	-1345	-1190	-155
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TABLE 3. (*Continued.*)

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3	15	-2	-285	-290	5
4	15	-2	-546	-590	44
2	16	2	173	154	19
3	16	2	-169	-221	52
4	16	2	-275	-291	16
5	16	2	303	304	-1
6	16	2	178	174	4
1	16	-2	-228	-230	2
3	16	-2	481	463	18
4	16	-2	484	552	-68
5	16	-2	-463	-546	83
6	16	-2	-271	-286	15
7	16	-2	451	575	-124
0	17	2	467	571	-104
1	17	2	260	260	0
2	17	2	-562	-628	66
3	17	2	-291	-229	-62
3	18	2	-170	-155	-15
*4	18	2	245	54	191
3	18	-2	192	241	-49
2	0	3	4199	4246	-47
4	0	3	-1454	-1776	322
6	0	3	-1898	-2008	110
8	0	3	1496	1593	-97
10	0	3	-749	-775	26
12	0	3	789	905	-116
2	0	-3	6591	5647	944
4	0	-3	-4652	-4507	-145
6	0	-3	767	735	32
8	0	-3	-384	-277	-107
10	0	-3	-737	-646	-91
12	0	-3	607	501	106
14	0	-3	-400	-425	25
0	1	3	-1959	-2210	251
1	1	3	506	572	-66
2	1	3	1053	718	335
3	1	3	-550	-931	381
4	1	3	-1911	-2063	152
5	1	3	-726	-1035	309
6	1	3	-445	-469	24
7	1	3	1597	1726	-129
8	1	3	-831	-688	-143
9	1	3	-1353	-1704	351
11	1	3	402	448	-46
12	1	3	-273	-274	1
1	1	-3	-4457	-4134	-323
2	1	-3	-1611	-902	-709
3	1	-3	701	899	-198

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TABLE 3. (*Continued.*)

h	*k*	*l*	100F_o	100F_c	100Δ
4	1	-3	-1714	-1553	-161
5	1	-3	454	305	149
6	1	-3	-1050	-758	-292
7	1	-3	921	1010	-89
8	1	-3	-480	-410	-70
9	1	-3	-856	-820	-36
10	1	-3	712	737	-25
11	1	-3	643	624	19
13	1	-3	-289	-321	32
0	2	3	-4394	-4310	-84
1	2	3	2875	2869	6
2	2	3	3501	3843	-342
3	2	3	757	616	141
4	2	3	-1640	-1473	-167
5	2	3	-729	-803	74
6	2	3	294	178	116
7	2	3	730	603	127
8	2	3	827	945	-118
9	2	3	-415	-436	21
10	2	3	-1074	-1189	115
11	2	3	701	764	-63
12	2	3	757	788	-31
13	2	3	-126	-155	29
1	2	-3	-725	-363	-362
2	2	-3	3484	3066	418
3	2	-3	1131	1202	-71
4	2	-3	1279	1265	14
5	2	-3	962	1002	-40
*6	2	-3	-157	-27	-130
7	2	-3	471	490	-19
9	2	-3	-274	-297	23
10	2	-3	-660	-639	-21
12	2	-3	884	769	115
14	2	-3	-265	-295	30
0	3	3	-1608	-1847	239
1	3	3	1972	1847	125
2	3	3	1210	993	217
3	3	3	3294	3655	-361
4	3	3	-464	-804	340
5	3	3	-920	-978	58
6	3	3	2119	2227	-108
7	3	3	733	788	-55
8	3	3	-758	-681	-77
9	3	3	-707	-737	30
11	3	3	182	224	-42
1	3	-3	338	416	-78
2	3	-3	-1013	-921	-92
3	3	-3	-1370	-1451	81
4	3	-3	-996	-1045	49
5	3	-3	-768	-668	-100
6	3	-3	515	354	161
7	3	-3	318	247	71
8	3	-3	-1412	-1366	-46
9	3	-3	-507	-352	-155
10	3	-3	831	754	77
13	3	-3	-312	-296	-16
0	4	3	622	599	23
1	4	3	1886	1481	405
2	4	3	-1770	-1903	133
3	4	3	-2565	-2392	-173
4	4	3	-2483	-2481	-2
5	4	3	525	510	15
6	4	3	-247	-266	19
7	4	3	-337	-414	77
8	4	3	784	791	-7
9	4	3	-458	-417	-41
10	4	3	-397	-370	-27
11	4	3	841	847	-6
12	4	3	544	557	-13
13	4	3	-269	-306	37
1	4	-3	3195	3018	177
2	4	-3	-178	-213	35
3	4	-3	-885	-982	97
4	4	-3	-927	-851	-76
5	4	-3	1306	1406	-100
7	4	-3	-708	-620	-88
8	4	-3	-317	-331	14
10	4	-3	-335	-289	-46
11	4	-3	203	177	26
12	4	-3	472	448	24
13	4	-3	-227	-228	1
0	5	3	-1877	-1618	-259
1	5	3	962	1037	-75
2	5	3	2593	2381	212
3	5	3	-271	-183	-88
4	5	3	-3929	-3852	-77
5	5	3	-1567	-1410	-157
6	5	3	1255	1293	-38
7	5	3	1456	1507	-51
*8	5	3	-239	-3	-236
9	5	3	-660	-684	24
10	5	3	204	234	-30
12	5	3	296	289	7
1	5	-3	-1954	-1815	-139
2	5	-3	858	787	71
3	5	-3	2444	2287	157
4	5	-3	-2262	-1886	-376
*5	5	-3	-145	-15	-130
6	5	-3	2127	2010	117
7	5	-3	781	690	91
8	5	-3	-1588	-1336	-252
9	5	-3	245	210	35
10	5	-3	1150	1076	74
12	5	-3	-370	-366	-4
0	6	3	-314	-175	-139
1	6	3	3695	3469	226
2	6	3	1813	1877	-64
4	6	3	-462	-444	-18
5	6	3	728	891	-163
7	6	3	-1106	-1094	-12
8	6	3	-569	-579	10
9	6	3	-729	-689	-40
11	6	3	339	376	-37
13	6	3	-365	-396	31
1	6	-3	231	354	-123
2	6	-3	-1139	-1015	-124
3	6	-3	-1220	-1224	4
4	6	-3	718	586	132
5	6	-3	798	713	85
*6	6	-3	-544	-49	-495
7	6	-3	-1798	-1706	-92
8	6	-3	244	166	78
9	6	-3	333	264	69
10	6	-3	271	261	10
13	6	-3	-56	-123	67
0	7	3	-1335	-1106	-229
1	7	3	699	722	-23
2	7	3	987	953	34
3	7	3	-1646	-1403	-243
4	7	3	-1978	-2259	281
5	7	3	827	662	165
6	7	3	2899	2831	68
7	7	3	-259	-169	-90
8	7	3	-820	-828	8
9	7	3	622	617	5
10	7	3	396	352	44
12	7	3	177	172	5
1	7	-3	623	522	101
2	7	-3	631	546	85
3	7	-3	-568	-551	-17
4	7	-3	-2258	-2109	-149
5	7	-3	-587	-408	-179
6	7	-3	1871	1794	77
7	7	-3	-883	-912	29
8	7	-3	-1053	-1066	13
9	7	-3	-434	-381	-53
10	7	-3	1030	939	91
11	7	-3	217	217	0
1	8	3	260	312	-52
2	8	3	1651	1654	-3
3	8	3	-1384	-1495	111
4	8	3	-1132	-1085	-47
5	8	3	-567	-634	67
6	8	3	1346	1450	-104
7	8	3	684	648	36
9	8	3	-282	-372	90
11	8	3	544	670	-126
12	8	3	-205	-175	-30
1	8	-3	1163	1144	19
2	8	-3	-1095	-1121	26
3	8	-3	-1001	-1042	41
4	8	-3	844	687	157
5	8	-3	1701	1650	51
6	8	-3	-870	-802	-68
8	8	-3	810	684	126
9	8	-3	-337	-179	-158
0	9	3	-1069	-1201	132
1	9	3	737	830	-93
2	9	3	861	886	-25
3	9	3	-2193	-2173	-20
4	9	3	-968	-883	-85
6	9	3	1036	902	134
7	9	3	-507	-524	17
8	9	3	-722	-633	-89
9	9	3	233	221	12
10	9	3	231	226	5
12	9	3	-136	-174	38
1	9	-3	-492	-439	-53
3	9	-3	-338	-211	-127
4	9	-3	-247	-245	-2
5	9	-3	790	823	-33
6	9	-3	-257	-229	-28
7	9	-3	-288	-286	-2
8	9	-3	-846	-738	-108
9	9	-3	781	795	-14
10	9	-3	581	583	-2
12	9	-3	-187	-259	72
0	10	3	1603	1523	80
1	10	3	1987	2112	-125
2	10	3	-1170	-1241	71
3	10	3	-819	-575	-244
5	10	3	444	521	-77
6	10	3	600	571	29
7	10	3	629	500	129
8	10	3	-711	-663	-48
9	10	3	-577	-538	-39
10	10	3	445	447	-2
11	10	3	429	367	62
1	10	-3	1020	994	26
2	10	-3	-1957	-1888	-69
3	10	-3	-800	-819	19
4	10	-3	1653	1604	49
6	10	-3	-499	-476	-23
7	10	-3	284	281	3
9	10	-3	-113	-89	-24
10	10	-3	276	271	5
11	10	-3	264	292	-28
0	11	3	613	646	-33
1	11	3	942	963	-21
2	11	3	-374	-439	65
4	11	3	-810	-709	-101
5	11	3	688	562	126
6	11	3	431	407	24
8	11	3	-396	-385	-11
9	11	3	468	455	13
1	11	-3	-219	-204	-15
2	11	-3	-688	-710	22
*3	11	-3	361	20	341
4	11	-3	-332	-374	42
6	11	-3	665	602	63
7	11	-3	-873	-923	50
9	11	-3	463	443	20
11	11	-3	-308	-437	129
0	12	3	1076	1020	56
1	12	3	-798	-776	-22
2	12	3	-613	-668	55
3	12	3	-443	-387	-56
*4	12	3	-311	-69	-242
5	12	3	445	349	96
6	12	3	871	818	53
8	12	3	-608	-570	-38
10	12	3	283	312	-29
1	12	-3	781	692	89
2	12	-3	-2371	-2204	-167
3	12	-3	-561	-560	-1
4	12	-3	942	945	-3
5	12	-3	527	555	-28
6	12	-3	-328	-289	-39
7	12	-3	-284	-308	24
8	12	-3	184	251	-67
10	12	-3	199	246	-47
0	13	3	742	671	71
1	13	3	707	726	-19
3	13	3	-1372	-1230	-142
4	13	3	323	117	206
5	13	3	810	769	41
6	13	3	413	392	21
7	13	3	-524	-454	-70
8	13	3	-246	-202	-44
9	13	3	296	276	20
2	13	-3	1099	1025	74
5	13	-3	649	735	-86
6	13	-3	196	237	-41
7	13	-3	-558	-541	-17
9	13	-3	373	399	-26
10	13	-3	-148	-194	46
0	14	3	223	213	10
2	14	3	-194	-119	-75
*4	14	3	323	64	259
8	14	3	-433	-476	43
1	14	-3	-586	-562	-24
2	14	-3	-505	-592	87
4	14	-3	429	428	1
5	14	-3	-313	-304	-9
6	14	-3	-211	-237	26
1	15	3	371	382	-11
2	15	3	-343	-329	-14
3	15	3	-637	-628	-9
4	15	3	315	350	-35
5	15	3	737	740	-3
6	15	3	-198	-171	-27
7	15	3	-279	-348	69
1	15	-3	-553	-584	31
2	15	-3	-233	-219	-14
3	15	-3	-196	-206	10
4	15	-3	270	334	-64
5	15	-3	444	537	-93
7	15	-3	-359	-429	70
8	15	-3	170	236	-66
0	16	3	380	359	21
1	16	3	-264	-348	84
4	16	3	253	289	-36
1	16	-3	-264	-297	33
2	16	-3	-219	-249	30
3	16	-3	326	352	-26
4	16	-3	336	418	-82
5	16	-3	-267	-249	-18

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TABLE 3. (*Continued.*)

h	*k*	*l*	$100F_o$	$100F_c$	100Δ
7	16	-3	109	225	-116
0	17	3	416	458	-42
1	17	3	188	253	-65
2	17	3	-312	-308	-4
3	17	3	-241	-203	-38
3	17	-3	-218	-212	-6
4	17	-3	220	226	-6
5	17	-3	130	202	-72
0	18	3	100	108	-8
1	18	3	-199	-254	55
2	18	3	-294	-279	-15
1	18	-3	-183	-182	-1
3	18	-3	233	342	-109
0	0	4	-5139	-4915	-224
2	0	4	4650	4684	-34
4	0	4	-140	-85	-55
6	0	4	512	502	10
8	0	4	-1066	-1214	148
10	0	4	-199	-267	68
12	0	4	518	513	5
2	0	-4	-1145	-1174	29
4	0	-4	-2193	-1861	-332
6	0	-4	-823	-667	-156
8	0	-4	1208	1444	-236
10	0	-4	-1337	-1178	-159
12	0	-4	725	646	79
0	1	4	-889	-884	-5
1	1	4	1314	1217	97
2	1	4	1358	1320	38
3	1	4	-509	-269	-240
4	1	4	972	928	44
5	1	4	-862	-708	-154
6	1	4	626	591	35
7	1	4	1781	1995	-214
8	1	4	-977	-1047	70
9	1	4	-1300	-1437	137
10	1	4	350	270	80
11	1	4	371	461	-90
13	1	4	-313	-361	48
1	1	-4	-3642	-3439	-203
2	1	-4	-649	-670	21
3	1	-4	5697	5878	-181
4	1	-4	572	608	-36
5	1	-4	-1979	-1863	-116
6	1	-4	206	188	18
7	1	-4	1440	1198	242
8	1	-4	252	269	-17
9	1	-4	-739	-649	-90
10	1	-4	214	154	60
11	1	-4	-142	-159	17
13	1	-4	314	325	-11
0	2	4	-4043	-3925	-118
1	2	4	2358	2309	49
2	2	4	2948	2827	121
3	2	4	-1426	-1301	-125
4	2	4	-1286	-1276	-10
5	2	4	772	590	182
6	2	4	886	862	24
7	2	4	-739	-737	-2
10	2	4	-538	-606	68
12	2	4	490	521	-31
1	2	-4	1964	2087	-123
2	2	-4	4169	4421	-252
3	2	-4	-266	-221	-45
4	2	-4	-1642	-1507	-135
5	2	-4	-300	-465	165
6	2	-4	-888	-704	-184
7	2	-4	582	630	-48
8	2	-4	1153	1167	-14
9	2	-4	-941	-974	33
10	2	-4	-768	-719	-49
11	2	-4	463	410	53
12	2	-4	763	740	23
13	2	-4	-119	-123	4
0	3	4	1304	1370	-66
1	3	4	-575	-620	45
2	3	4	1353	1123	230
3	3	4	801	942	-141
4	3	4	-1291	-1359	68
6	3	4	1145	1191	-46
7	3	4	1234	1303	-69
8	3	4	-678	-682	4
9	3	4	-932	-990	58
10	3	4	970	962	8
11	3	4	677	697	-20
12	3	4	-181	-209	28
13	3	4	-221	-212	-9
1	3	-4	-4093	-4076	-17
2	3	-4	844	866	-22
3	3	-4	851	969	-118
4	3	-4	-1049	-1088	39
5	3	-4	-1878	-1902	24
6	3	-4	780	644	136
7	3	-4	976	973	3
8	3	-4	-234	-336	102
10	3	-4	495	488	7
11	3	-4	-461	-442	-19
13	3	-4	290	268	22
0	4	4	-1757	-1732	-25
1	4	4	2216	2086	130
2	4	4	3303	3248	55
3	4	4	-1556	-1509	-47
4	4	4	-1951	-1705	-246
5	4	4	1345	1400	-55
6	4	4	868	805	63
7	4	4	-1133	-1214	81
8	4	4	-886	-698	-188
9	4	4	-646	-645	-1
10	4	4	-270	-259	-11
11	4	4	401	362	39
12	4	4	302	307	-5
1	4	-4	2550	2543	7
2	4	-4	689	756	-67
3	4	-4	635	686	-51
4	4	-4	771	701	70
5	4	-4	-1103	-1005	-98
6	4	-4	-442	-482	40
7	4	-4	437	362	75
8	4	-4	464	359	105
9	4	-4	-986	-897	-89
10	4	-4	-491	-470	-21
11	4	-4	699	650	49
12	4	-4	297	286	11
13	4	-4	-311	-294	-17
0	5	4	1374	1428	-54
1	5	4	-955	-768	-187
2	5	4	631	513	118
3	5	4	1245	1235	10
4	5	4	-1206	-1135	-71
5	5	4	-1532	-1430	-102
6	5	4	-456	-416	-40
8	5	4	-1231	-1270	39
10	5	4	832	799	33
11	5	4	218	93	125
1	5	-4	873	728	145
2	5	-4	1596	1435	161
3	5	-4	1988	1633	355
4	5	-4	-1732	-1856	124
5	5	-4	-1370	-1202	-168
6	5	-4	2324	2363	-39
7	5	-4	937	843	94
8	5	-4	-765	-1058	293
9	5	-4	-237	-364	127
12	5	-4	-169	-169	0
0	6	4	-1070	-941	-129
1	6	4	2984	2751	233
2	6	4	1693	1323	370
3	6	4	-1149	-1047	-102
4	6	4	-845	-882	37
5	6	4	3249	3479	-230
6	6	4	720	615	105
7	6	4	-569	-584	15
8	6	4	-221	-208	-13
11	6	4	414	406	8
12	6	4	203	166	37
1	6	-4	1642	1662	-20
2	6	-4	695	588	107
3	6	-4	634	564	70
4	6	-4	325	262	63
5	6	-4	-1700	-1684	-16
6	6	-4	-778	-786	8
7	6	-4	1405	1245	160
8	6	-4	1180	1096	84
9	6	-4	-643	-617	-26
10	6	-4	-414	-342	-72
11	6	-4	841	808	33
0	7	4	772	781	-9
1	7	4	1024	779	245
2	7	4	1365	1280	85
3	7	4	-1122	-1209	87
4	7	4	-2173	-1988	-185
5	7	4	915	873	42
6	7	4	758	773	-15
7	7	4	-459	-412	-47
8	7	4	-1070	-1056	-14
9	7	4	287	254	33
10	7	4	697	663	34
12	7	4	-262	-197	-65
1	7	-4	-593	-560	-33
2	7	-4	1441	1427	14
3	7	-4	-467	-525	58
4	7	-4	-1656	-1619	-37
6	7	-4	1653	1552	101
7	7	-4	-377	-348	-29
8	7	-4	-958	-867	-91
9	7	-4	171	139	32
10	7	-4	436	406	30
0	8	4	-810	-770	-40
1	8	4	1744	1834	-90
3	8	4	-1960	-1944	-16
5	8	4	355	392	-37
6	8	4	-712	-727	15
7	8	4	-1084	-1124	40
8	8	4	493	456	37
10	8	4	401	397	4
11	8	4	276	249	27
1	8	-4	968	927	41
3	8	-4	354	502	-148
5	8	-4	-226	-217	-9
6	8	-4	-317	-364	47
7	8	-4	502	470	32
9	8	-4	-995	-1002	7
10	8	-4	-277	-253	-24
11	8	-4	355	335	20
0	9	4	796	810	-14
1	9	4	910	851	59
2	9	4	-565	-488	-77
3	9	4	371	473	-102
4	9	4	-585	-451	-134
5	9	4	-265	-281	-4
6	9	4	1477	1338	139
7	9	4	-1283	-1120	-163
8	9	4	-1259	-1191	-68
9	9	4	493	388	105
10	9	4	440	959	-519
1	9	-4	1424	1456	-32
2	9	-4	1266	1190	76
3	9	-4	-472	-374	-98
4	9	-4	-1608	-1523	-85
5	9	-4	696	737	-41
6	9	-4	484	453	31
9	9	-4	419	409	10
0	10	4	996	966	30
1	10	4	1073	922	151
2	10	4	-1187	-1096	-91
4	10	4	-397	-341	-56
5	10	4	333	333	0
6	10	4	477	356	121
1	10	-4	1070	1073	-3
2	10	-4	-319	-331	12
3	10	-4	-871	-891	20
4	10	-4	802	855	-53
6	10	-4	-431	-339	-92
7	10	-4	535	473	62
9	10	-4	-403	-378	-25
10	10	-4	184	184	0
11	10	-4	259	336	-77
0	11	4	1771	1588	183
1	11	4	-1259	-1152	-107
*2	11	4	347	39	308
3	11	4	421	351	70
4	11	4	-446	-340	-106
5	11	4	413	321	92
6	11	4	562	526	36
7	11	4	-774	-689	-85
8	11	4	-540	-424	-116
9	11	4	904	733	171
10	11	4	636	534	102
1	11	-4	1131	1085	46
2	11	-4	1224	1190	34
3	11	-4	-1772	-1846	74
4	11	-4	-321	-397	76
5	11	-4	182	156	26
6	11	-4	679	700	-21
7	11	-4	-457	-429	-28
9	11	-4	225	282	-57
0	12	4	807	814	-7
1	12	4	-383	-340	-43
2	12	4	-672	-685	13
3	12	4	-914	-749	-165
4	12	4	343	275	68
6	12	4	-362	-298	-64
7	12	4	-367	-252	-115
9	12	4	364	281	83
1	12	-4	-370	-406	36
2	12	-4	-452	-429	-23
3	12	-4	299	393	-94
4	12	-4	569	618	-49
5	12	-4	-393	-408	15
2	13	4	-402	-443	41
3	13	4	-374	-248	-126
5	13	4	318	278	40
6	13	4	305	254	51
7	13	4	-739	-499	-240
9	13	4	642	454	188
1	13	-4	528	536	-8
2	13	-4	504	492	12
3	13	-4	-362	-344	-18
4	13	-4	-812	-874	62
5	13	-4	490	509	-19
6	13	-4	225	230	-5
7	13	-4	-383	-406	23
0	14	4	904	761	143
2	14	4	-1091	-962	-129
3	14	4	326	209	117
4	14	4	980	813	167
6	14	4	-478	-294	-184
1	14	-4	-516	-503	-13
2	14	-4	-248	-336	88
6	14	-4	208	213	-5
7	14	-4	218	215	3
8	14	-4	-180	-180	0
2	15	4	-324	-355	31
3	15	4	-365	-276	-89
4	15	4	301	275	26
5	15	4	299	268	31

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TABLE 3. (*Continued.*)

h	k	l	100F_o	100F_c	100Δ
1	15	-4	231	270	-39
2	15	-4	209	249	-40
3	15	-4	-196	-201	5
5	15	-4	209	241	-32
6	15	-4	-258	-316	58
7	15	-4	-264	-315	51
0	16	4	153	179	-26
1	16	4	-385	-289	-96
2	16	4	-634	-641	7
4	16	4	492	446	46
5	16	4	-435	-344	-91
1	16	-4	-221	-275	54
3	17	4	205	200	5
0	0	5	-2236	-2121	-115
4	0	5	-2175	-2267	92
6	0	5	2800	3395	-595
8	0	5	-1585	-1556	-29
12	0	5	-180	-134	-46
2	0	-5	-1053	-1075	22
4	0	-5	3026	2764	262
6	0	-5	-1931	-1859	-72
8	0	-5	1980	1740	240
10	0	-5	-1325	-1148	-177
12	0	-5	468	356	112
1	1	5	1294	1369	-75
2	1	5	-2340	-2295	-45
3	1	5	-1449	-1596	147
4	1	5	585	552	33
6	1	5	729	877	-148
7	1	5	1331	1371	-40
8	1	5	-306	-374	68
9	1	5	-474	-476	2
11	1	5	439	532	-93
1	1	-5	-743	-813	70
2	1	-5	2107	1963	144
3	1	-5	2205	2231	-26
4	1	-5	-432	-294	-138
5	1	-5	-1491	-1400	-91
6	1	-5	-521	-545	24
7	1	-5	-369	-421	52
9	1	-5	174	170	4
10	1	-5	-347	-334	-13
11	1	-5	-431	-364	-67
13	1	-5	532	526	6
1	2	5	1274	1372	-98
2	2	5	872	1047	-175
4	2	5	-2358	-2495	137
5	2	5	886	906	-20
6	2	5	2609	2711	-102
7	2	5	-395	-283	-112
8	2	5	-1193	-1198	5
9	2	5	270	308	-38
10	2	5	431	454	-23
11	2	5	-165	-110	-55
12	2	5	-229	-258	29
1	2	-5	743	744	-1
2	2	-5	-1040	-1128	88
3	2	-5	-1092	-1115	23
4	2	-5	1670	1871	-201
5	2	-5	327	413	-86
6	2	-5	-1053	-1019	-34
7	2	-5	411	328	83
8	2	-5	1294	1315	-21
9	2	-5	-453	-406	-47
10	2	-5	-685	-632	-53
11	2	-5	658	370	288
12	2	-5	240	221	19
13	2	-5	-130	-133	3
0	3	5	1553	1381	172
2	3	5	-749	-823	74
3	3	5	-1270	-1287	17
4	3	5	1336	1236	100
5	3	5	-524	-635	111
7	3	5	554	602	-48
8	3	5	-1230	-1230	0
9	3	5	-671	-742	71
10	3	5	451	563	-112
11	3	5	393	476	-83
12	3	5	-285	-290	5
1	3	-5	-1009	-1212	203
2	3	-5	2798	2701	97
3	3	-5	1608	1457	151
4	3	-5	-1202	-1421	219
5	3	-5	-723	-686	-37
6	3	-5	579	471	108
7	3	-5	682	663	19
8	3	-5	346	342	4
10	3	-5	-309	-288	-21
11	3	-5	-314	-314	0
12	3	-5	310	326	-16
13	3	-5	324	344	-20
0	4	5	-1775	-1551	-224
1	4	5	-641	-623	-18
2	4	5	1392	1423	-31
3	4	5	-841	-807	-34
4	4	5	-2211	-2183	-28
5	4	5	1641	1647	-6
6	4	5	2753	2624	129
7	4	5	-461	-405	-56
8	4	5	-780	-639	-141
9	4	5	-209	-122	-87
10	4	5	244	192	52
11	4	5	-244	-230	-14
1	4	-5	857	838	19
4	4	-5	1231	1207	24
5	4	-5	-2159	-2116	-43
6	4	-5	-1950	-1910	-40
7	4	-5	993	890	103
8	4	-5	656	529	127
9	4	-5	-527	-513	-14
10	4	-5	-523	-449	-74
11	4	-5	511	484	27
12	4	-5	159	133	26
0	5	5	2644	2536	108
1	5	5	1117	1041	76
2	5	5	-1350	-1199	-151
4	5	5	1503	1558	-55
5	5	5	974	918	56
6	5	5	256	298	-42
7	5	5	-502	-361	-141
8	5	5	-1388	-1148	-240
9	5	5	-563	-459	-104
10	5	5	524	478	46
11	5	5	186	192	-6
12	5	5	-492	-510	18
1	5	-5	729	536	193
2	5	-5	2787	2655	132
3	5	-5	-201	-252	51
4	5	-5	-1125	-1069	-56
5	5	-5	183	214	-31
6	5	-5	626	656	-30
8	5	-5	-525	-452	-73
10	5	-5	-580	-537	-43
12	5	-5	417	401	16
0	6	5	231	279	-48
2	6	5	906	984	-78
3	6	5	-1745	-1660	-85
4	6	5	-560	-441	-119
5	6	5	1665	1484	181
*7	6	5	-269	-24	-245
9	6	5	109	50	59
11	6	5	298	265	33
1	6	-5	1145	1095	50
2	6	-5	-549	-516	-33
3	6	-5	528	493	35
5	6	-5	-1346	-1240	-106
7	6	-5	1762	1538	224
8	6	-5	695	622	73
9	6	-5	-837	-708	-129
10	6	-5	-532	-437	-95
11	6	-5	622	574	48
0	7	5	1585	1612	-27
1	7	5	256	331	-75
2	7	5	-1206	-1079	-127
3	7	5	-744	-731	-13
4	7	5	2308	1966	342
5	7	5	-431	-435	4
7	7	5	602	474	128
8	7	5	-992	-819	-173
9	7	5	-194	-193	-1
10	7	5	536	515	21
11	7	5	237	200	37
1	7	-5	-905	-952	47
2	7	-5	2317	2170	147
3	7	-5	-186	-79	-107
4	7	-5	-1516	-1439	-77
5	7	-5	163	147	16
6	7	-5	339	342	-3
7	7	-5	-406	-356	-50
10	7	-5	-307	-303	-4
11	7	-5	-145	-114	-31
12	7	-5	295	365	-70
0	8	5	1035	1021	14
1	8	5	958	973	-15
2	8	5	-850	-772	-78
3	8	5	-1206	-1085	-121
4	8	5	973	821	152
5	8	5	1088	998	90
6	8	5	-888	-802	-86
1	8	-5	502	621	-119
4	8	-5	-367	-432	65
5	8	-5	-1008	-970	-38
6	8	-5	397	348	49
0	9	5	1895	1783	112
1	9	5	203	266	-63
2	9	5	-1432	-1250	-182
3	9	5	1294	1220	74
5	9	5	607	561	46
6	9	5	676	605	71
1	9	-5	290	316	-26
2	9	-5	1773	1874	-101
3	9	-5	-1012	-1044	32
4	9	-5	-1355	-1383	28
5	9	-5	485	503	-18
6	9	-5	593	650	-57
0	10	5	495	475	20
2	10	5	166	235	-69
*4	10	5	-328	-58	-270
5	10	5	919	655	264
6	10	5	-874	-759	-115
1	10	-5	-323	-374	51
2	10	-5	402	434	-32
4	10	-5	-626	-642	16
0	11	5	747	676	71
1	11	5	-567	-542	-25
2	11	5	-183	-532	349
1	11	-5	415	402	13
2	11	-5	1268	1228	40
3	11	-5	-1221	-1325	104
4	11	-5	-504	-593	89
5	11	-5	673	744	-71
6	11	-5	344	430	-86
0	12	5	373	391	-18
1	12	5	367	366	1
2	12	5	-356	-312	-44
3	12	5	-449	-378	-71
4	12	5	854	731	123
6	12	5	-791	-698	-93
3	12	-5	231	225	6
4	12	-5	-514	-638	124
5	12	-5	-518	-583	65
6	12	-5	450	529	-79
0	13	5	464	505	-41
1	13	5	-389	-467	78
3	13	5	460	402	58
6	13	5	-305	-230	-75
1	13	-5	781	801	-20
2	13	-5	-363	-374	11
3	13	-5	-259	-334	75
5	13	-5	265	311	-46
6	13	-5	219	289	-70
0	14	5	578	564	14
2	14	5	-587	-600	13
6	14	5	-538	-475	-63
1	14	-5	-194	-174	-20
2	14	-5	-270	-253	-17
3	14	-5	333	385	-52
4	14	-5	-241	-272	31
5	14	-5	190	216	-26
6	14	-5	283	408	-125
3	15	5	188	165	23
1	15	-5	196	247	-51
3	15	-5	-365	-455	90
2	16	5	-524	-531	7
0	0	6	2189	2093	96
2	0	6	-472	-424	-48
4	0	6	-1741	-1559	-182
6	0	6	1189	1136	53
8	0	6	-320	-322	2
10	0	6	799	790	9
2	0	-6	-2009	-2009	0
4	0	-6	2109	2017	92
6	0	-6	-2470	-2072	-398
8	0	-6	937	819	118
10	0	-6	-260	-240	-20
12	0	-6	-184	-174	-10
0	1	6	962	945	17
1	1	6	1097	1078	19
2	1	6	-1202	-1253	51
3	1	6	-699	-654	-45
4	1	6	-391	-357	-34
5	1	6	-640	-663	23
11	1	6	128	140	-12
1	1	-6	-702	-636	-66
2	1	-6	616	717	-101
3	1	-6	606	800	-194
4	1	-6	-1682	-1721	39
5	1	-6	-811	-883	72
6	1	-6	-300	-323	23
7	1	-6	-281	-225	-56
8	1	-6	277	253	24
9	1	-6	777	666	111
10	1	-6	-308	-252	-56
11	1	-6	-331	-322	-9
12	1	-6	184	161	23
0	2	6	1383	1262	121
1	2	6	-819	-783	-36
2	2	6	301	338	-37
3	2	6	237	134	103
4	2	6	-1994	-1708	-286
*5	2	6	193	39	154
6	2	6	1167	1212	-45
8	2	6	-534	-651	117
9	2	6	550	580	-30
10	2	6	626	708	-82
11	2	6	-131	-166	35
1	2	-6	-355	-377	22
2	2	-6	-1395	-1296	-99
3	2	-6	615	609	6
4	2	-6	3087	3178	-91
5	2	-6	496	507	-11
6	2	-6	-2097	-2070	-27
8	2	-6	764	785	-21
10	2	-6	-270	-259	-11

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TABLE 3. (*Continued.*)

h	*k*	*l*	$100F_o$	$100F_c$	100Δ
0	3	6	1253	1182	71
1	3	6	1437	1247	190
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3	3	6	-309	-177	-132
4	3	6	1651	1618	33
5	3	6	230	226	4
6	3	6	371	386	-15
7	3	6	-360	-489	129
10	3	6	-240	-219	-21
1	3	-6	-588	-576	-12
2	3	-6	926	884	42
3	3	-6	363	366	-3
4	3	-6	-709	-672	-37
5	3	-6	-374	-429	55
6	3	-6	-306	-337	31
8	3	-6	804	817	-13
10	3	-6	-592	-548	-44
12	3	-6	499	445	54
1	4	6	-397	-347	-50
3	4	6	-760	-878	118
4	4	6	-1412	-1574	162
5	4	6	463	412	51
9	4	6	342	392	-50
10	4	6	261	261	0
11	4	6	-310	-344	34
1	4	-6	-953	-899	-54
2	4	-6	-634	-561	-73
3	4	-6	-393	-393	0
4	4	-6	906	838	68
5	4	-6	-741	-731	-10
6	4	-6	-1519	-1466	-53
7	4	-6	952	899	53
8	4	-6	908	803	105
0	5	6	1124	1032	92
1	5	6	1243	1133	110
2	5	6	-2331	-2203	-128
3	5	6	-437	-378	-59
4	5	6	1511	1257	254
5	5	6	588	555	33
6	5	6	-331	-340	9
7	5	6	780	678	102
8	5	6	312	289	23
10	5	6	239	231	8
1	5	-6	-1140	-1184	44
2	5	-6	1070	925	145
3	5	-6	719	709	10
6	5	-6	-1125	-1097	-28
7	5	-6	-285	-141	-144
8	5	-6	1044	855	189
9	5	-6	259	225	34
10	5	-6	-773	-741	-32
11	5	-6	-222	-217	-5
12	5	-6	303	465	-162
1	6	6	-404	-384	-20
2	6	6	259	165	94
3	6	6	-607	-468	-139
4	6	6	907	897	10
8	6	6	-336	-264	-72
1	6	-6	-571	-447	-124
2	6	-6	-690	-558	-132
4	6	-6	458	463	-5
5	6	-6	-651	-673	22
7	6	-6	749	621	128
9	6	-6	-274	-219	-55
10	6	-6	-241	-117	-124
0	7	6	1263	1280	-17
1	7	6	-429	-473	44
2	7	6	-2935	-2689	-246
3	7	6	593	546	47
4	7	6	1698	1547	151
5	7	6	-1369	-1175	-194
8	7	6	312	214	98
9	7	6	-216	-270	54
10	7	6	295	118	177
1	7	-6	-408	-412	4
2	7	-6	875	915	-40
3	7	-6	721	749	-28
4	7	-6	-341	-270	-71
5	7	-6	-388	-349	-39
6	7	-6	-513	-454	-59
8	7	-6	996	978	18
10	7	-6	-509	-632	123
2	8	6	233	237	-4
3	8	6	-402	-296	-106
4	8	6	614	602	12
5	8	6	451	399	52
1	8	-6	-553	-720	167
4	8	-6	-300	-351	51
5	8	-6	-387	-389	2
6	8	-6	473	449	24
0	9	6	946	862	84
1	9	6	-460	-506	46
2	9	6	-841	-835	-6
3	9	6	592	468	124
4	9	6	852	755	97
6	9	6	-551	-425	-126
1	9	-6	-644	-595	-49
2	9	-6	630	674	-44
3	9	-6	242	255	-13
4	9	-6	-409	-434	25
6	9	-6	-301	-366	65
0	10	6	-912	-883	-29
2	10	6	512	404	108
3	10	6	-579	-476	-103
4	10	6	908	826	82
5	10	6	639	514	125
6	10	6	-744	-696	-48
2	10	-6	647	714	-67
3	10	-6	736	890	-154
4	10	-6	-781	-914	133
5	10	-6	-344	-349	5
6	10	-6	463	475	-12
0	11	6	419	478	-59
1	11	6	-302	-264	-38
2	11	6	-333	-238	-95
3	11	6	395	362	33
5	11	6	-287	-205	-82
6	11	6	-367	-346	-21
1	11	-6	-332	-301	-31
3	11	-6	270	320	-50
0	12	6	-776	-742	-34
1	12	6	152	226	-74
2	12	6	235	214	21
4	12	6	389	304	85
5	12	6	196	192	4
6	12	6	-512	-442	-70
4	12	-6	-439	-541	102
5	12	-6	-220	-295	75
6	12	-6	496	592	-96
1	13	6	-411	-429	18
2	13	6	348	335	13
3	13	6	515	449	66
5	13	6	-222	-195	-27
6	13	6	-294	-255	-39
1	13	-6	486	511	-25
4	13	-6	288	436	-148
0	14	6	-454	-491	37
1	14	6	415	450	-35
2	14	6	207	211	-4
1	14	-6	214	234	-20
2	14	-6	281	339	-58
4	14	-6	-294	-435	141
0	15	6	-160	-213	53
1	15	6	-400	-443	43
0	0	7	1056	1208	-152
2	0	7	-925	-914	-11
4	0	7	505	464	41
6	0	7	-748	-666	-82
8	0	7	-460	-508	48
10	0	7	446	479	-33
2	0	-7	-1886	-1958	72
4	0	-7	206	170	36
6	0	-7	314	209	105
8	0	-7	-219	-179	-40
10	0	-7	592	503	89
1	1	7	349	445	-96
2	1	7	364	350	14
3	1	7	-261	-289	28
5	1	7	688	730	-42
6	1	7	-211	-211	0
7	1	7	-809	-798	-11
8	1	7	261	238	23
9	1	7	355	496	-141
10	1	7	-126	-208	82
1	1	-7	408	350	58
2	1	-7	-701	-767	66
3	1	-7	-490	-489	-1
4	1	-7	-362	-370	8
5	1	-7	306	364	-58
6	1	-7	264	242	22
7	1	-7	-192	-224	32
9	1	-7	391	351	40
11	1	-7	-227	-237	10
0	2	7	1605	1604	1
1	2	7	-802	-702	-100
2	2	7	-438	-428	-10
4	2	7	783	683	100
6	2	7	-739	-595	-144
7	2	7	-491	-569	78
10	2	7	177	186	-9
1	2	-7	-1150	-1160	10
2	2	-7	-184	-191	7
3	2	-7	1113	1126	-13
4	2	-7	-208	-188	-20
5	2	-7	-502	-524	22
6	2	-7	-474	-419	-55
10	2	-7	237	252	-15
11	2	-7	-213	-195	-18
1	3	7	365	499	-134
2	3	7	-601	-634	33
3	3	7	-764	-825	61
5	3	7	1205	1226	-21
6	3	7	-229	-232	3
7	3	7	-603	-627	24
8	3	7	615	967	-352
1	3	-7	-669	-686	17
2	3	-7	-397	-397	0
3	3	-7	-522	-563	41
4	3	-7	481	502	-21
5	3	-7	616	595	21
7	3	-7	-265	-223	-42
8	3	-7	646	571	77
9	3	-7	335	283	52
10	3	-7	-210	-196	-14
11	3	-7	-253	-214	-39
0	4	7	956	897	59
1	4	7	-391	-320	-71
2	4	7	-644	-696	52
3	4	7	387	482	-95
4	4	7	826	824	2
5	4	7	-262	-255	-7
6	4	7	-1012	-903	-109
9	4	7	339	273	66
1	4	-7	-971	-914	-57
2	4	-7	-270	-256	-14
3	4	-7	528	499	29
6	4	-7	186	192	-6
0	5	7	315	353	-38
*1	5	7	-237	-26	-211
2	5	7	-689	-585	-104
3	5	7	-248	-261	13
6	5	7	-948	-816	-132
8	5	7	339	310	29
2	5	-7	-1025	-1029	4
4	5	-7	675	665	10
5	5	-7	-239	-186	-53
6	5	-7	-828	-798	-30
8	5	-7	749	652	97
10	5	-7	-444	-442	-2
1	6	7	-780	-681	-99
2	6	7	-544	-525	-19
3	6	7	441	386	55
4	6	7	499	400	99
5	6	7	-211	-194	-17
6	6	7	512	432	80
9	6	7	466	386	80
1	6	-7	-876	-788	-88
3	6	-7	557	540	17
5	6	-7	-222	-229	7
6	6	-7	262	225	37
7	6	-7	321	256	65
8	6	-7	-245	-211	-34
0	7	7	225	146	79
1	7	7	-533	-448	-85
2	7	7	-548	-449	-99
3	7	7	550	429	121
6	7	7	-583	-471	-112
8	7	7	571	524	47
1	7	-7	522	535	-13
2	7	-7	-434	-609	175
3	7	-7	241	224	17
4	7	-7	474	631	-157
5	7	-7	-392	-408	16
6	7	-7	-457	-500	43
7	7	-7	220	273	-53
8	7	-7	381	534	-153
10	7	-7	-117	-294	177
0	8	7	-773	-762	-11
1	8	7	-203	-243	40
3	8	7	566	580	-14
5	8	7	-225	-155	-70
6	8	7	181	176	5
1	8	-7	-827	-789	-38
2	8	-7	295	282	13
3	8	-7	766	876	-110
5	8	-7	-164	-195	31
6	8	-7	306	379	-73
0	9	7	-227	-187	-40
1	9	7	-280	-279	-1
2	9	7	-314	-299	-15
3	9	7	396	302	94
4	9	7	619	484	135
5	9	7	-407	-380	-27
6	9	7	-522	-430	-92
2	9	-7	-542	-514	-28
3	9	-7	536	553	-17
4	9	-7	300	300	0
5	9	-7	-347	-398	51
6	9	-7	-296	-339	43
0	10	7	-576	-509	-67
1	10	7	-189	-207	18
2	10	7	-260	-244	-16
6	10	7	316	228	88
2	10	-7	458	525	-67
3	10	-7	241	258	-17
4	10	-7	-228	-274	46
5	10	-7	-239	-302	63
1	11	7	-354	-325	-29
2	11	7	314	310	4
3	11	7	276	239	37
5	11	7	-335	-316	-19
6	11	7	-380	-286	-94
3	11	-7	275	332	-57
4	11	-7	349	438	-89
5	11	-7	-314	-435	121
6	11	-7	-198	-275	77

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TABLE 3. (*Continued.*)

h	k	l	100Fo	100Fc	100Δ
0	12	7	-571	-592	21
2	12	7	363	397	-34
2	12	-7	545	694	-149
0	13	7	-264	-276	12
5	13	-7	-116	-284	168
0	14	7	-432	-513	81
2	14	-7	289	393	-104
0	0	8	-279	-289	10
2	0	8	-379	-321	-58
4	0	8	764	744	20
6	0	8	-435	-605	170
8	0	8	226	135	91
2	0	-8	380	193	187
4	0	-8	-170	-122	-48
6	0	-8	1071	962	109
8	0	-8	-481	-451	-30
10	0	-8	374	353	21
0	1	8	-364	-354	-10
1	1	8	-254	-218	-36
2	1	8	201	214	-13
3	1	8	-220	-137	-83
5	1	8	338	261	77
6	1	8	-218	-168	-50
7	1	8	-294	-379	85
8	1	8	242	322	-80
9	1	8	329	458	-129
1	1	-8	563	560	3
2	1	-8	-779	-808	29
3	1	-8	-906	-838	-68
4	1	-8	461	469	-8
5	1	-8	728	692	36
7	1	-8	-599	-529	-70
9	1	-8	191	130	61
0	2	8	329	269	60
2	2	8	-351	-377	26
3	2	8	319	280	39
4	2	8	1201	1190	11
6	2	8	-676	-746	70
8	2	8	387	486	-99
9	2	8	-146	-175	29
1	2	-8	-316	-342	26
2	2	-8	-297	-271	-26
3	2	-8	428	482	-54
4	2	-8	-836	-919	83
5	2	-8	-213	-248	35
6	2	-8	763	774	-11
8	2	-8	-507	-502	-5
10	2	-8	327	307	20
0	3	8	-848	-855	7
2	3	8	712	661	51
*3	3	8	-339	-88	-251
4	3	8	-508	-440	-68
5	3	8	-181	-99	-82
6	3	8	-613	-625	12
8	3	8	204	310	-106
2	3	-8	-642	-652	10
4	3	-8	660	704	-44
5	3	-8	718	718	0
7	3	-8	-425	-381	-44
0	4	8	306	274	32
1	4	8	-746	-843	97
2	4	8	-625	-627	2
3	4	8	652	607	45
4	4	8	763	643	120
5	4	8	-391	-368	-23
6	4	8	-420	-422	2
1	4	-8	-500	-490	-10
3	4	-8	193	233	-40
4	4	-8	-364	-323	-41
6	4	-8	473	418	55
7	4	-8	-345	-361	16
8	4	-8	-396	-343	-53
9	4	-8	349	336	13
0	5	8	-280	-215	-65
2	5	8	1083	947	136
3	5	8	240	234	6
1	5	-8	347	303	44
2	5	-8	-636	-682	46
3	5	-8	-263	-217	-46
4	5	-8	714	780	-66
5	5	-8	290	258	32
6	5	-8	-183	-180	-3
7	5	-8	-183	-124	-59
0	6	8	-234	-229	-5
1	6	8	-699	-643	-56
2	6	8	177	232	-55
3	6	8	541	430	111
4	6	8	-375	-305	-70
5	6	8	-648	-525	-123
8	6	8	129	213	-84
1	6	-8	-361	-324	-37
5	6	-8	247	253	-6
7	6	-8	-270	-276	6
9	6	-8	289	288	1
0	7	8	-745	-724	-21
2	7	8	837	757	80
4	7	8	-190	-138	-52
6	7	8	-308	-316	8
2	7	-8	-652	-786	134
4	7	-8	482	689	-207
5	7	-8	-144	-200	56
6	7	-8	-172	-234	62
*8	7	-8	195	8	187
1	8	8	-452	-495	43
3	8	8	760	624	136
4	8	8	-678	-490	-188
5	8	8	-450	-353	-97
6	8	8	327	222	105
3	8	-8	203	247	-44
4	8	-8	248	281	-33
6	8	-8	-155	-160	5
0	9	8	-461	-511	50
2	9	8	374	338	36
3	9	8	126	256	-130
4	9	8	-318	-241	-77
5	9	8	-251	-154	-97
2	9	-8	-508	-617	109
3	9	-8	203	223	-20
4	9	-8	367	443	-76
5	9	-8	-260	-330	70
2	10	8	345	348	-3
3	10	8	368	362	6
4	10	8	-813	-703	-110
5	10	8	-308	-275	-33
5	10	-8	112	143	-31
6	10	-8	-175	-340	165
0	11	8	-417	-416	-1
2	11	8	137	182	-45
1	11	-8	-236	-270	34
5	11	-8	-69	-174	105
0	12	8	-187	-211	24
2	12	8	259	267	-8
0	0	9	-402	-371	-31
2	0	9	-265	-237	-28
4	0	9	852	821	31
6	0	9	-671	-686	15
2	0	-9	952	962	-10
4	0	-9	-728	-679	-49
6	0	-9	699	683	16
8	0	-9	-410	-369	-41
1	1	9	-676	-619	-57
2	1	9	131	137	-6
3	1	9	675	659	16
5	1	9	-514	-464	-50
1	1	-9	635	647	-12
2	1	-9	-269	-276	7
3	1	-9	-365	-384	19
4	1	-9	217	193	24
7	1	-9	192	164	28
9	1	-9	-100	-170	70
0	2	9	-421	-420	-1
2	2	9	-436	-470	34
4	2	9	619	624	-5
5	2	9	-308	-332	24
6	2	9	-565	-534	-31
7	2	9	309	359	-50
1	2	-9	356	513	-157
2	2	-9	357	438	-81
3	2	-9	-198	-223	25
4	2	-9	-510	-569	59
5	2	-9	247	260	-13
6	2	-9	508	599	-91
7	2	-9	-149	-140	-9
8	2	-9	-324	-366	42
0	3	9	-648	-681	33
1	3	9	-841	-820	-21
2	3	9	445	455	-10
3	3	9	1013	933	80
5	3	9	-520	-537	17
1	3	-9	589	599	-10
2	3	-9	-553	-572	19
4	3	-9	374	358	16
5	4	9	-464	-402	-62
6	4	9	-574	-391	-183
2	4	-9	454	491	-37
3	4	-9	-408	-435	27
4	4	-9	-449	-502	53
5	4	-9	307	290	17
6	4	-9	401	398	3
7	4	-9	-190	-140	-50
8	4	-9	-155	-154	-1
0	5	9	-832	-764	-68
1	5	9	-374	-352	-22
2	5	9	823	794	29
3	5	9	277	313	-36
4	5	9	-212	-248	36
1	5	-9	293	302	-9
2	5	-9	-178	-177	-1
4	5	-9	221	258	-37
0	6	9	-426	-409	-17
3	6	9	268	224	64
4	6	9	243	159	84
5	6	9	-500	-457	-43
6	6	9	-373	-249	-124
1	6	-9	160	152	8
2	6	-9	354	348	6
3	6	-9	-421	-460	39
4	6	-9	-169	-220	51
5	6	-9	431	471	-40
0	7	9	-721	-648	-73
2	7	9	416	445	-29
4	7	9	-335	-304	-31
2	7	-9	-283	-369	86
4	7	-9	293	195	98
*6	7	-9	243	44	199
2	8	9	349	333	16
1	8	-9	241	218	23
2	8	-9	201	155	46
3	8	-9	-309	-427	118
5	8	-9	167	271	-104
0	9	9	-458	-524	66
2	9	9	538	531	7
2	9	-9	-296	-391	95
0	0	10	-295	-334	39
*2	19	9	-371	-41	-330
4	0	10	210	199	11
2	0	-10	432	459	-27
4	0	-10	-435	-421	-14
6	0	-10	357	330	27
1	1	10	-272	-342	70
2	1	10	100	73	27
3	1	10	543	581	-38
0	2	10	-236	-301	65
1	2	10	172	201	-29
2	2	10	363	134	229
1	2	-10	311	366	-55
2	2	-10	363	486	-123
3	2	-10	-290	-317	27
4	2	-10	-378	-419	41
5	2	-10	159	209	-50
6	2	-10	223	227	-4
1	3	10	-428	-490	62
3	3	10	339	365	-26
4	3	10	-281	-218	-63
0	4	10	-244	-128	-116
1	4	10	433	517	-84
2	4	10	365	306	59
1	4	-10	377	387	-10
2	4	-10	212	255	-43
3	4	-10	-371	-358	-13
4	4	-10	-280	-284	4
5	4	-10	374	379	-5
0	5	10	-389	-402	13
1	5	10	-200	-146	-54
2	5	10	359	370	-11
1	6	-10	236	288	-52
3	6	-10	-227	-261	34
0	7	10	-202	-245	43

the cell with all van der Waals contacts below 3·7 Å. There are 26 van der Waals contacts of less than 4 Å, only two of which involve the phosphorus atom (3·92 and 3·97 Å).

The equation of the least-squares planes through the three benzene rings are:

$$\text{Ring A [C(1)–C(6)]}\ 0{\cdot}60742X' - 0{\cdot}56709Y' + 0{\cdot}55627Z' = 1{\cdot}78303$$
$$\text{Ring B [C(7)–C(12)]}\ 0{\cdot}47599X' - 0{\cdot}15450Y' - 0{\cdot}86577Z' = 0{\cdot}17226$$
$$\text{Ring C [C(13)–C(18)]}\ 0{\cdot}51098X' + 0{\cdot}85259Y' - 0{\cdot}10953Z' = 1{\cdot}51638$$

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TABLE 4.

Bond lengths (Å) and angles (°), and their standard deviations.

P–C(1)	1·8221(48)	P–C(7)	1·8310(47)	P–C(13)	1·8310(48)
C(1)–C(2)	1·4071(70)	C(7)–C(8)	1·3968(68)	C(13)–C(14)	1·4144(74)
C(2)–C(3)	1·3878(80)	C(8)–C(9)	1·4023(79)	C(14)–C(15)	1·4011(89)
C(3)–C(4)	1·3790(88)	C(9)–C(10)	1·3989(90)	C(15)–C(16)	1·3945(97)
C(4)–C(5)	1·4029(90)	C(10)–C(11)	1·3863(94)	C(16–C(17)	1·4080(97)
C(5)–C(6)	1·4008(83)	C(11)–C(12)	1·4034(90)	C(17)–C(18)	1·4133(88)
C(6)–C(1)	1·3981(71)	C(12)–C(7)	1·4124(75)	C(18)–C(13)	1·3862(72)
C(1)–P–C(7)	103·57(21)	C(2)–C(1)–P	115·78(36)	C(6)–C(1)–P	124·94(37)
C(7)–P–C(13)	102·07(21)	C(12)–C(7)–P	116·27(37)	C(8)–C(7)–P	123·93(36)
C(13)–P–C(1)	103·34(21)	C(18)–C(13)–P	116·18(37)	C(14)–C(13)–P	123·17(38)
C(1)–C(2)–C(3)	120·26(49)	C(7)–C(8)–C(9)	119·62(47)	C(13)–C(14)–C(15)	118·67(53)
C(2)–C(3)–C(4)	120·72(56)	C(8)–C(9)–C(10)	120·77(55)	C(14)–C(15)–C(16)	121·21(61)
C(3)–C(4)–C(5)	119·68(58)	C(9)–C(10)–C(11)	119·75(60)	C(15)–C(16)–C(17)	119·82(63)
C(4)–C(5)–C(6)	120·18(57)	C(10)–C(11)–C(12)	120·24(60)	C(16)–C(17)–C(18)	119·31(60)
C(5)–C(6)–C(1)	119·83(50)	C(11)–C(12)–C(7)	120·01(54)	C(17)–C(18)–C(13)	120·33(52)
C(6)–C(1)–C(2)	119·28(45)	C(12)–C(7)–C(8)	119·59(45)	C(18)–C(13)–C(14)	120·64(46)

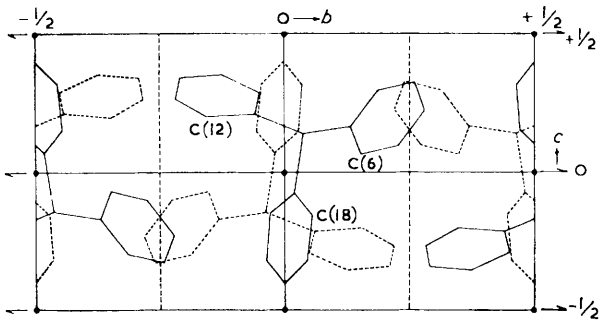

FIG. 2. *a*-Axis projection of the unit-cell contents.

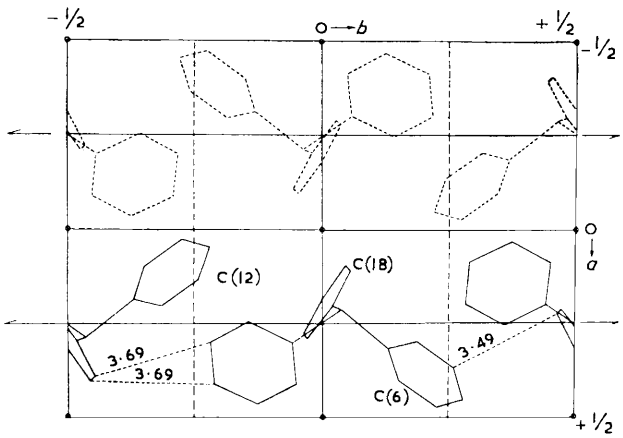

FIG. 3. *c*-Axis projection of the unit-cell contents and van der Waals contacts less than 3·7 Å

The bond lengths have not been corrected for torsional oscillation; any such correction, despite the large values of the U_{ij}'s, can only worsen the agreement between the mean C–C bond length and the standard value of 1·397 Å.

DISCUSSION

The rules used here to compare experimentally determined quantities follow those given by Cruickshank and Robertson.[7] All the carbon atoms lie within $1{\cdot}7\sigma_{rms}$ of the appropriate

[7] Cruickshank and Robertson, *Acta Cryst.*, 1953, **6**, 698.

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least-squares planes; $\sigma_{rms}^2 = [\sigma^2(X) + \sigma^2(Y) + \sigma^2(Z)]/3$. The mean bond lengths and angles in the benzene rings are:

Ring	A	B	C	All
Mean C–C length	1·3960(31)	1·4000(31)	1·4029(35)	1·3996(20) Å
Mean C–C–C angle	119·99(22)	120·00(22)	120·00(23)	120·00(13) Å

The most significant deviation from the mean C–C bond length is 0·0148 Å ($\Delta/\sigma = 1·92$) for C(13)–C(14); the most significant deviation from the mean C–C–C angle is 1·33° ($\Delta/\sigma = 2·42$) for C(13)–C(14)–C(15). The mean values of the aromatic C–C lengths agree well with standard values.[8] The angles are close to the theoretical value of 120°. The phosphorus atom displacements from the planes of the benzene rings are: 0·0017 Å from ring A, −0·1713 Å from ring B, and 0·0408 Å from ring C.

Although the three P–C bond lengths do not differ significantly from one another, one of the C–P–C angles [C(7)–P–C(13)] is considerably smaller than the other two: $\Delta/\sigma = 6·00$ and 5·08. Since this angle does not involve the P–C(1) bond, and since C(1) · · · C(7) = C(1) · · · C(13) ≠ C(7) · · · C(13), the symmetry of the P C(1) C(7) C(13) pyramid is closer to *m* than to 3*m*. The benzene rings adopt a configuration in which the molecule possesses no symmetry. This is best seen by comparing the angles that the normals to the rings A, B, and C make with the lines P–C(13) (117·8°), P–C(1) (85·6°), and P–C(7) (115·2°), respectively. These angles should all be equal if the symmetry of the molecule is to be 3. The B-ring is therefore twisted about 30° from the position which would give the molecule a threefold symmetry axis. This distortion cannot be due to intramolecular repulsions of the CH groups as twisting the B-ring to the symmetrical position would only reproduce contacts already present. Intermolecular repulsions may be the cause of the twisting, although the shortest of these contacts (3·49 Å) does not involve the B-ring. The shortest non-bonded intramolecular distances between atoms which are not bonded to a common atom are: 3·11 Å [C(1) · · · C(8)], 3·19 Å [C(6) · · · C(13)], 3·12 Å [C(7) · · · C(14)].

It has been postulated, from the vibrational spectrum of the melt, that the benzene rings in PPh_3 are perpendicular to the base of the phosphorus pyramid.[9] In the solid state the angles between the normals to the rings A, B, and C and the normal to the pyramid base ($0·90229X' - 0·10443Y' - 0·41830Z' = 2·35695$) are 68·0, 36·1, and 65·3°, respectively. In a personal communication Professor Steger points out that the vibrational spectrum might be explained by assuming free rotation of the phenyl rings about the P–C bonds.

The difference between the mean P–C bond length found here (1·828 ± 0·003 Å) and the P–C length in $P(CH_3)_3$ (1·841 ± 0·003 Å from microwave spectra [10] and 1·846 ± 0·003 Å from electron diffraction [11] with $\Delta/\sigma = 3·25$ and 4·5, respectively) indicates only a slight degree of conjugation in the phenyl derivative. The mean P–C bond length in PPh_3 is not significantly different from the P–Ph bond in *trans*-dimesitylbis(diethylphenylphosphine)cobalt(II) (1·835 ± 0·017 Å).[12]

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