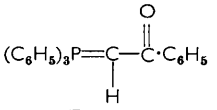
1051. *The Crystal and Molecular Structure of Benzoyl(triphenylphosphoranylidene)methyl Chloride*

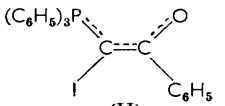
By F. S. Stephens

The crystal structure of benzoyl(triphenylphosphoranylidene)methyl chloride has been determined by *X*-ray diffraction methods; refinement has been carried out by an isotropic least-squares procedure with three-dimensional data. There are four molecules in the monoclinic unit cell (space group $P2_1/a$) with cell dimensions $a = 11{\cdot}130$, $b = 12{\cdot}641$, $c = 15{\cdot}470$ Å, $\beta = 97°\ 32'$. The phosphorus-carbon double bond length is 1·736 Å with an estimated standard deviation of 0·014 Å. The carbonyl group is almost coplanar with the plane containing the phosphorus-carbon double bond and the benzoyl ring is twisted 57·7° from the plane containing the carbonyl group.

It has been shown [1] that as the hydrogen is replaced in structure (I) by halogen atoms the carbonyl stretching frequency decreases in the infrared solid-state spectrum. In the iodo-compound [2] it is indicated that delocalisation of the phosphorus-carbon double bond



(I)



(II)

and the carbonyl bond occurs (structure (II)). Thus, as predicted,[1] the decrease in the ν_{CO} stretch can be accounted for in terms of a field effect lengthening the C–O bond. The $(C_6H_5)_3P$ and benzoyl ring, in this compound, are found to be *trans* to one another and the benzoyl ring is rotated 63° from the plane containing the phosphorus and iodine atoms, the carbonyl group being rotated 21° from the latter plane.

The chloro- and bromo-compounds are isomorphous (see Table 1) and it is uncertain what effects on the overcrowding occurs when the iodine is replaced by the other halogens.

Table 1

Unit cell dimensions of the chloro- and bromo-compounds

	Chloro	Bromo		Chloro	Bromo
a	11·130 Å	11·149 Å	*U*	2157·8 Å^3	2195·8 Å^3
b	12·641	12·663	Space group	$P2_1/a$	$P2_1/a$
c	15·470	15·686	D_c	1·277	1·389
	97° 32′	97° 27′	D_m	1·279	1·380

The structure analysis of the chloro-compound was undertaken to investigate this and to obtain information of the delocalisation of the double bonds.

Experimental

$C_{26}H_{20}ClOP$. $M = 414{\cdot}9$. Monoclinic. $a = 11{\cdot}130 \pm 0{\cdot}019$, $b = 12{\cdot}641 \pm 0{\cdot}025$, $c = 15{\cdot}470 \pm 0{\cdot}030$ Å, $\beta = 97°\ 32' \pm 15'$. $U = 2157{\cdot}8$ Å^3. $Z = 4$, $D_m = 1{\cdot}279$ g. cm.$^{-3}$ (by flotation). $D_c = 1{\cdot}277$ g. cm.$^{-3}$. F(000) = 864. Space group $P2_1/a$ (C_{2h}^5, No. 14). Cu-K_α radiation ($\lambda = 1{\cdot}5418$ Å) for cell dimensions. Mo-K_α ($\lambda = 0{\cdot}71069$ Å) for intensity measurements.

Crystals of the compound were obtained from ethanol solution as colourless hexagonal plates elongated in the [*a*] direction. Cell dimensions were obtained from single crystal oscillation and Weissenberg photographs. The intensities were collected on a Hilger-Watts linear diffractometer [3] equipped with SrO–ZrO_2 balanced filters. Each reflection in the 0*kl* to 12*kl* layers, to a maximum angle of $\theta = 30°$, was measured six times, thrice with the SrO(α) filter in position and thrice with the $ZrO_2(\beta)$ filter. For all measurements a half-minute oscillation

[1] A. J. Speziale and K. W. Ratts, *J. Org. Chem.*, 1963, **28**, 465; *J. Amer. Chem. Soc.*, 1963, **85**, 2790.

[2] F. S. Stephens, *J.*, 1965, 5640.

[3] U. W. Arndt and D. C. Phillips, *Acta Cryst.*, 1961, **14**, 807.

TABLE 2

Co-ordinates (Å) and isotropic thermal parameters (Å²) (estimated standard deviations are given in parentheses)

	X	*Y*	*Z*	*U*
Cl	4·147(4)	6·123(4)	1·201(4)	0·0492(9)
P	3·797(4)	5·554(4)	4·081(3)	0·0321(7)
O	4·674(12)	8·247(13)	4·506(12)	0·0782(36)
C(1)	2·304(13)	6·060(14)	4·819(13)	0·0393(31)
C(2)	1·672(14)	5·077(15)	5·556(14)	0·0455(34)
C(3)	0·515(16)	5·484(17)	6·141(15)	0·0569(40)
C(4)	0·047(17)	6·777(17)	5·950(16)	0·0632(45)
C(5)	0·605(17)	7·709(18)	5·193(17)	0·0659(46)
C(6)	1·795(16)	7·350(16)	4·598(15)	0·0556(40)
C(7)	3·386(13)	3·951(12)	3·320(12)	0·0315(28)
C(8)	4·196(14)	2·872(14)	3·554(13)	0·0434(34)
C(9)	3·881(15)	1·639(15)	2·962(15)	0·0517(38)
C(10)	2·651(15)	1·507(16)	2·073(14)	0·0514(38)
C(11)	1·817(16)	2·590(16)	1·839(15)	0·0532(39)
C(12)	2·145(14)	3·831(14)	2·425(13)	0·0432(34)
C(13)	5·158(13)	5·272(13)	5·416(12)	0·0358(30)
C(14)	4·926(15)	4·837(15)	6·678(14)	0·0487(36)
C(15)	6·105(17)	4·520(17)	7·667(16)	0·0613(44)
C(16)	7·386(17)	4·648(18)	7·336(17)	0·0647(46)
C(17)	7·590(19)	5·099(19)	6·093(19)	0·0739(51)
C(18)	6·471(16)	5·379(16)	5·097(15)	0·0539(39)
C(19)	4·232(14)	6·671(14)	2·881(13)	0·0410(32)
C(20)	4·736(15)	7·897(15)	3·263(14)	0·0489(37)
C(21)	5·241(14)	8·912(14)	2·362(13)	0·0394(32)
C(22)	4·652(16)	10·121(16)	2·235(15)	0·0519(38)
C(23)	5·142(17)	11·109(17)	1·395(17)	0·0651(46)
C(24)	6·230(16)	10·813(16)	0·736(15)	0·0573(42)
C(25)	6·828(17)	9·587(17)	0·873(16)	0·0614(44)
C(26)	6·329(17)	8·585(17)	1·688(16)	0·0608(44)

motor was used; the oscillation angle was increased from 3·5° to 4·0° for the layers 7*kl* to 12*kl*. Of the 4759 reflections measured the counts for only 2212 reflections were significant (a count was considered significant if it exceeded twice the standard deviation of its measurement) and these were used in subsequent calculations. The intensities were corrected for Lorentz and polarisation effects but no correction for absorption or extinction was applied. Wilson's method [4] was used to put the observed data on an approximately absolute scale. However, during the refinement it was necessary to rescale the data layerwise by comparison with the calculated structure factor values. The scattering factor curves for all atoms are those given in International Tables. All calculations were carried out on an Elliott 803B computer with programmes of Daly, Stephens, and Wheatley.[5]

Structure Determination. Positions for the chlorine and phosphorus atoms were obtained from a sharpened three-dimensional Patterson synthesis. A subsequent three-dimensional Fourier synthesis using the phases of the contributions of these heavy atoms to the structure factors enabled all the other atoms to be obtained (excluding hydrogen atoms). The structure factors calculated with the co-ordinates for all atoms with an overall temperature factor of $U = 0{\cdot}035$ Å² ($U = B/8\pi^2$) for planes $\sin\theta/\lambda < 0{\cdot}35$ gave an R value of 0·228. The structure was refined by an isotropic least-squares procedure in which the function minimised was $\Sigma w(|F_o| - |F_c|)^2$. Each reflection was weighted as follows: $|F_o| \leq F_m$, $w = 0{\cdot}005$; $|F_o| > F_m$, $w = 1/c|F_o|^2$ where c is given by $1/cF_m = 0{\cdot}005$. Reflections, the calculated structure factors of which were less than one-third of the observed values, were omitted from the least-squares analysis. The number of planes used in the final cycle of refinement was 2189. The final values for R and R'* were 0·167 and 0·028, respectively. The final atomic co-ordinates and isotropic thermal parameters together with their estimated standard deviations (in brackets

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

[4] A. J. C. Wilson, *Nature*, 1942, **150**, 151.

[5] J. J. Daly, F. S. Stephens, and P. J. Wheatley, Monsanto Research S.A., Final Report No. 52, 1963.

TABLE 3

Observed and calculated structure factors (scale: 100 × absolute)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
0	0	1	1467	4330	-2863	0	4	11	748	420	328
0	0	2	-5311	-10183	4872	0	4	12	2095	1723	372
0	0	4	-9153	-7767	-1386	0	4	13	3256	2870	386
0	0	5	-8196	-7134	-1062	0	4	15	802	315	487
0	0	6	-2320	-2516	196	0	4	16	644	523	121
0	0	7	-4547	-3714	-833	0	5	1	-7643	-7000	-643
0	0	8	-1410	-848	-562	0	5	2	2058	1323	735
0	0	9	-3552	-3126	-424	0	5	3	3175	2583	592
0	0	11	1056	402	654	0	5	4	-8418	-7895	-523
0	0	12	1541	1178	363	0	5	5	-3643	-3474	-169
0	0	14	2732	1573	1159	0	5	6	1674	1410	264
0	0	15	2129	1938	191	0	5	7	4020	3796	224
0	0	17	-2050	-1556	-494	0	5	10	1224	681	543
0	0	18	-705	-333	-372	0	5	11	1870	1815	55
0	1	1	-2875	-4186	1311	0	5	12	-818	-956	138
0	1	2	5053	5986	-933	0	5	13	-893	-1015	122
0	1	3	2900	2191	709	0	5	16	-1636	-1283	-353
0	1	4	10040	8909	1131	0	6	0	-578	-394	-184
0	1	5	-759	-109	-650	0	6	1	4895	5905	-1010
0	1	6	-1481	-1397	-84	0	6	2	2893	3556	-663
0	1	7	3390	2598	792	0	6	3	-4840	-5314	474
0	1	8	3039	2712	327	0	6	4	-649	-88	-561
0	1	9	-2246	-2033	-213	0	6	5	-2574	-2521	-53
0	1	11	699	310	389	0	6	7	-1391	-1265	-126
0	1	12	-1015	-738	-277	0	6	8	-3243	-2827	-416
0	1	13	-1084	-784	-300	0	6	9	-745	-159	-586
0	1	14	1064	784	280	0	6	10	2791	2560	231
0	2	0	5312	6928	-1616	0	6	13	2309	1940	369
0	2	1	-6528	-7644	1116	0	6	14	1101	790	311
0	2	2	-1638	-1569	-69	0	6	15	-703	-693	-10
0	2	3	10848	12340	-1492	0	6	16	-657	-357	-300
0	2	4	-1152	-1143	-9	0	7	2	-2447	-2460	13
0	2	5	-2613	-2340	-273	0	7	3	1883	1762	121
0	2	6	-5390	-4380	-1010	0	7	4	-4535	-4620	85
0	2	7	-3586	-3028	-558	0	7	5	-3715	-3775	60
0	2	8	-2966	-2344	-622	0	7	8	1259	1089	170
0	2	9	-2886	-2531	-355	0	7	9	1949	1820	129
0	2	10	1811	1524	287	0	7	10	775	815	-40
0	2	11	4778	4182	596	0	7	11	1103	1162	-59
0	2	12	3543	2813	730	0	7	12	974	767	207
0	2	15	2414	2009	405	0	7	13	-647	-360	-287
0	2	16	1443	1104	339	0	7	16	-1329	-1189	-140
0	2	17	-1401	-1100	-301	0	8	1	1316	1291	25
0	2	18	-1639	-1192	-447	0	8	2	4551	5082	-531
0	2	19	-909	-557	-352	0	8	3	-1029	-708	-321
0	3	1	-6141	-6421	280	0	8	7	-3709	-3995	286
0	3	2	5380	5332	48	0	8	8	-3912	-3848	-64
0	3	3	-6534	-6252	-282	0	8	9	876	988	-112
0	3	4	-540	-1229	689	0	8	10	1654	1508	146
0	3	6	1317	1116	201	0	8	11	-799	-492	-307
0	3	7	1534	1570	-36	0	8	13	1462	1133	329
0	3	8	-2311	-2241	-70	0	8	14	994	916	78
0	3	9	-3943	-3121	-822	0	8	17	864	730	134
0	3	10	3028	2653	375	0	9	1	1350	1822	-472
0	3	11	3800	3207	593	0	9	2	-1588	-2176	588
0	3	12	-1543	-1196	-347	0	9	3	-1237	-1172	-65
0	3	13	-706	-795	89	0	9	6	2672	2838	-166
0	3	14	2392	2299	93	0	9	9	928	1209	-281
0	3	16	-2041	-1659	-382	0	9	12	1224	1235	-11
0	3	17	-1221	-809	-412	0	9	14	-1067	-1128	61
0	3	18	973	743	230	0	9	17	-989	-992	3
0	4	0	-7126	-6401	-725	0	10	0	571	1234	-663
0	4	1	8745	9196	-451	0	10	1	1231	1496	-265
0	4	4	-568	-1018	450	0	10	2	943	595	348
0	4	5	-509	-506	-3	0	10	3	-1364	-1185	-179
0	4	6	-4891	-4138	-653	0	10	4	-3988	-4400	412
0	4	7	-1410	-992	-418	0	10	6	1272	1459	-187
0	4	8	-1601	-1542	-59	0	10	7	-741	-549	-192
0	4	9	-1941	-1559	-382	0	10	8	-596	-734	138

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_o	Δ	*h*	*k*	*l*	F_o	F_o	Δ
0	10	9	1642	1760	-118	1	2	-9	1930	1461	469
0	10	13	1456	1462	-6	1	2	-3	494	48	446
0	10	14	1055	1253	-198	1	2	-6	-4705	-4956	251
0	11	1	565	779	-214	1	2	-5	3896	3159	737
0	11	2	-746	-1527	779	1	2	-4	5205	5686	-481
0	11	3	-2155	-2758	603	1	2	-3	8244	8699	545
0	11	4	-1291	-1311	20	1	2	-2	-5683	-5697	-186
0	11	7	-1039	-875	-164	1	2	-1	3479	4350	-871
0	11	8	703	900	-197	1	2	0	-2655	-3917	1222
0	11	9	1699	1752	-53	1	2	1	-2522	-1535	-987
0	11	12	1032	1051	-59	1	2	2	2548	2673	-125
0	11	13	880	1019	-139	1	2	3	-3977	-3963	-14
0	11	14	-1097	-1060	-37	1	2	4	-7659	-5470	-2229
0	12	0	-837	-1204	367	1	2	5	-1816	-1621	-195
0	12	1	-733	-480	-253	1	2	6	-2612	-2431	-181
0	12	3	2373	2694	-321	1	2	7	-1026	-582	-444
0	12	7	-804	-1042	238	1	2	8	3497	2843	654
0	12	8	-527	-535	9	1	2	9	-1549	-1836	-113
0	13	1	733	685	48	1	2	10	-2540	-2274	-266
0	13	3	-1601	-1908	307	1	2	11	5091	4308	773
0	13	4	-657	-937	280	1	2	12	1552	1317	235
0	13	6	-798	-1066	268	1	2	13	-1641	-1106	-535
0	13	7	-669	-761	92	1	2	14	1784	1473	311
0	13	8	1026	1113	-85	1	2	16	-967	-861	-106
0	13	9	1039	1061	-22	1	2	17	-1456	-1072	-424
0	13	12	954	1087	-133	1	3	-18	-1408	-1216	-272
0	14	5	-551	-882	331	1	3	-17	-1553	-1650	-263
0	14	9	-767	-700	-67	1	3	-16	-1013	-883	-130
0	15	3	-1188	-1319	131	1	3	-15	613	1709	-1096
0	15	4	-747	-1208	461	1	3	-12	2711	1970	741
0	15	6	796	1273	-475	1	3	-11	2692	2043	649
0	16	0	648	1067	-219	1	3	-8	-1530	-1472	-58
0	16	2	-719	-681	-38	1	3	-7	-1970	-1466	-502
1	1	-17	-1949	-1419	-530	1	3	-4	-4590	-3706	-884
1	1	-16	-1340	-976	-364	1	3	-3	-2714	-2345	-369
1	1	-14	1731	1199	532	1	3	-2	-4054	-4173	119
1	1	-13	-1043	-1043	0	1	3	-1	3490	4135	-645
1	1	-12	1421	897	524	1	3	0	-312	-84	-228
1	1	-11	5163	4349	834	1	3	1	12592	14119	-1527
1	1	-10	3385	2658	727	1	3	2	3949	4984	-1035
1	1	-9	3117	2396	721	1	3	3	6843	6073	770
1	1	-8	-2317	-1669	-648	1	3	4	2997	1913	1084
1	1	-7	-1552	-979	-573	1	3	5	468	994	-526
1	1	-6	-2562	-2304	-258	1	3	6	-4354	-4462	108
1	1	-5	-11220	-9729	-1491	1	3	7	-5524	-4606	-918
1	1	-4	-2873	-3246	373	1	3	8	-5006	-4015	-991
1	1	-2	-717	-165	-552	1	3	9	-2219	-1878	-341
1	1	-1	-8343	-9979	1636	1	3	10	-5240	-4209	-1031
1	1	0	7126	6763	-1635	1	3	11	979	1416	-437
1	1	1	10146	12574	-2428	1	3	12	2666	2073	593
1	1	2	-3127	-3006	-121	1	3	13	1953	1494	459
1	1	3	-9053	-7889	-1164	1	3	14	-701	-489	-212
1	1	4	11476	11727	-251	1	3	15	882	422	460
1	1	6	-2702	-1737	-965	1	3	16	1479	1127	352
1	1	7	-1377	-1453	76	1	3	17	1477	1167	310
1	1	8	-668	-560	-328	1	3	18	-831	-531	-300
1	1	9	-2670	-1790	-880	1	4	-16	1035	1437	-402
1	1	10	-4200	-3662	-538	1	4	-15	1692	1501	191
1	1	12	3301	3054	247	1	4	-13	-826	-748	-78
1	1	13	-1010	-1080	70	1	4	-12	2274	2089	185
1	1	14	2137	1311	826	1	4	-10	-2679	-2799	80
1	1	15	1776	1578	208	1	4	-9	-1212	-1025	-183
1	1	16	1666	1221	445	1	4	-8	1943	1878	65
1	1	18	-705	-860	151	1	4	-7	-908	-1213	305
1	2	-18	1249	1214	35	1	4	-6	-7797	-6628	-1169
1	2	-16	-781	-474	-307	1	4	-5	-3723	-3424	-299
1	2	-14	-943	-551	-392	1	4	-4	8105	7548	557
1	2	-12	2616	2227	389	1	4	-3	1167	1628	-461
1	2	-10	-2955	-2398	-257	1	4	-2	-2450	-2517	67

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
1	4	-1	8559	8540	19	1	7	-15	-716	-607	-109
1	4	0	1317	2927	-1610	1	7	-13	1847	2025	-178
1	4	1	-6868	-7379	511	1	7	-12	973	1147	-174
1	4	2	2685	1945	740	1	7	-10	966	614	352
1	4	3	4194	4902	-708	1	7	-9	1683	1818	-135
1	4	4	-644	-1204	560	1	7	-8	664	904	-240
1	4	5	-4951	-3505	-1446	1	7	-7	-1163	-1449	286
1	4	6	-2319	-1798	-521	1	7	-6	-1505	-2043	538
1	4	7	2049	1169	880	1	7	-4	-802	-1332	530
1	4	8	2208	2098	110	1	7	-3	-3859	-4842	983
1	4	9	-2252	-1780	-472	1	7	0	1451	1337	114
1	4	11	3968	3616	352	1	7	1	-2201	-2003	-198
1	4	13	-2092	-2037	-55	1	7	2	2854	3176	-322
1	5	-16	-1009	-1033	24	1	7	3	1605	1287	318
1	5	-12	2482	2523	-41	1	7	4	2561	2323	238
1	5	-11	1898	1682	216	1	7	7	-914	-507	-407
1	5	-10	3003	2792	211	1	7	8	-3373	-2738	-635
1	5	-9	2430	2299	131	1	7	9	-3329	-2895	-434
1	5	-8	-936	-919	-17	1	7	10	3773	3273	500
1	5	-7	-3670	-3764	94	1	7	12	-1963	-1488	-475
1	5	-6	-2724	-2734	10	1	7	13	1310	1374	-64
1	5	-5	-2988	-2974	-14	1	7	14	3021	2220	801
1	5	-4	-2202	-2336	134	1	8	-16	825	501	324
1	5	-3	-2751	-2994	243	1	8	-13	1056	1047	9
1	5	-2	-2481	-2587	106	1	8	-11	-988	-1283	295
1	5	-1	4250	3922	328	1	8	-9	1067	1076	-9
1	5	0	2393	2220	173	1	8	-7	-1543	-1386	-157
1	5	1	7013	7250	-237	1	8	-4	-616	-787	171
1	5	2	5560	5112	448	1	8	-3	2616	2577	39
1	5	3	2219	2484	-265	1	8	-2	1520	1492	28
1	5	4	-4152	-3469	-683	1	8	0	1685	1636	49
1	5	5	-2439	-2642	203	1	8	1	1733	2204	-471
1	5	8	-2441	-1968	-473	1	8	2	-2064	-1628	-436
1	5	9	-3644	-2908	-736	1	8	5	-3524	-3406	-118
1	5	11	1143	1019	124	1	8	6	-3633	-3480	-153
1	5	12	-1422	-1463	41	1	8	7	870	949	-79
1	5	13	1400	1110	290	1	8	10	1534	1754	-220
1	5	14	1049	790	259	1	8	12	2038	1422	616
1	5	15	1117	533	584	1	8	13	1235	994	241
1	5	16	1159	849	310	1	9	-13	938	1284	-346
1	5	17	909	481	428	1	9	-9	1339	1399	-60
1	5	19	-791	-354	-437	1	9	-7	-1781	-2029	248
1	6	-17	-792	-809	17	1	9	-6	-1023	-1511	488
1	6	-16	-764	-934	-170	1	9	-5	2425	2807	-382
1	6	-15	1522	1510	12	1	9	-4	-2125	-2673	548
1	6	-12	745	1032	-287	1	9	-3	-3375	-3827	452
1	6	-11	-752	666	-86	1	9	-2	2125	2689	-564
1	6	-10	-1213	-1554	341	1	9	-1	1973	2256	-283
1	6	-9	-2072	-1858	-214	1	9	0	-887	-1016	129
1	6	-7	-1320	-1357	37	1	9	1	-1556	-1935	379
1	6	-5	-513	-942	429	1	9	2	2646	2760	-114
1	6	-4	3349	3382	-33	1	9	3	1793	1681	112
1	6	-3	-3367	-3784	417	1	9	4	-599	-570	-29
1	6	-2	-2174	-2005	-169	1	9	6	1368	704	664
1	6	-1	2185	2239	-54	1	9	7	1218	1555	-337
1	6	0	6818	7310	-492	1	9	8	-3214	-2618	-596
1	6	1	-1312	-671	-641	1	9	9	-2050	-1926	-124
1	6	2	-2548	-2504	-44	1	9	11	-1190	-887	-303
1	6	3	1548	1361	187	1	9	12	-1283	-821	-462
1	6	5	-2324	-2413	89	1	9	13	1043	729	314
1	6	6	-949	-1304	355	1	9	14	1988	1531	457
1	6	7	2450	2226	224	1	10	-13	990	1469	-479
1	6	9	-1553	-1747	194	1	10	-8	-1660	-1963	303
1	6	10	1201	965	236	1	10	-7	-1017	-1125	108
1	6	13	1128	1029	99	1	10	-6	-588	-566	-22
1	6	14	808	922	-114	1	10	-5	-999	-810	-89
1	6	15	1281	1327	-46	1	10	-3	5029	6290	-1261
1	6	16	-1507	-1317	-190	1	10	-2	2544	2705	-161
1	6	17	-1776	-1565	-211	1	10	-1	-1012	-1297	285

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
1	10	0	-1732	-1794	62	2	0	-1	-9158	-11242	2086
1	10	1	1398	1281	117	2	0	0	5200	7456	-2256
1	10	2	915	1160	-245	2	0	1	5920	6096	-176
1	10	3	-2105	-2001	-104	2	0	2	13686	16100	-2414
1	10	4	-2077	-2398	321	2	0	3	-7612	-6246	-1366
1	10	5	-2526	-2392	-134	2	0	4	-3887	-3312	-575
1	10	7	1191	752	439	2	0	5	9172	8312	860
1	10	8	-1316	-1574	258	2	0	6	1732	2127	-395
1	10	9	841	675	166	2	0	7	-5615	-5840	225
1	10	10	1540	1260	280	2	0	8	-1787	-1533	-254
1	10	12	1036	1132	-96	2	0	9	-3605	-2780	-825
1	10	13	1231	1121	110	2	0	10	-3616	-3440	-176
1	10	15	-1092	-670	-422	2	0	11	-3501	-3355	-146
1	11	-8	838	937	-99	2	0	12	2645	2682	-37
1	11	-7	-1446	-2007	561	2	0	13	-894	-456	-438
1	11	-6	-1068	-1299	231	2	0	14	999	403	596
1	11	-4	-716	-943	227	2	0	15	753	843	-90
1	11	-1	846	631	215	2	0	16	1657	1668	-11
1	11	1	1739	1736	3	2	0	17	981	1137	-156
1	11	2	1456	1240	216	2	1	-18	900	1051	-151
1	11	3	820	1041	-221	2	1	-17	762	590	172
1	11	4	-1357	-1548	191	2	1	-14	-729	-280	-449
1	11	7	-706	-553	-153	2	1	-12	1515	1194	321
1	11	8	-1696	-1749	-147	2	1	-10	-1185	-953	-232
1	12	-14	888	1544	-656	2	1	-9	-3741	-3128	-613
1	12	-8	-1446	-2249	803	2	1	-7	-2914	-2751	-163
1	12	-7	-910	-2055	1145	2	1	-6	-3835	-3931	96
1	12	-6	688	1103	-415	2	1	-5	5257	4561	696
1	12	-4	-878	-1057	179	2	1	-4	7481	6009	1472
1	12	-2	820	1226	-406	2	1	-3	2990	2085	905
1	12	0	910	1091	-181	2	1	-2	-11260	-10949	-310
1	12	1	936	987	-51	2	1	-1	-6202	-7246	1044
1	12	2	754	869	-115	2	1	0	-461	-647	186
1	12	3	-1033	-1434	401	2	1	1	11930	14532	-2602
1	12	4	-951	-780	-171	2	1	2	8846	7710	1136
1	12	7	-1405	-1244	-161	2	1	3	6618	5327	1291
1	12	9	2042	1911	131	2	1	4	5197	4626	571
1	12	11	-691	-863	-28	2	1	6	-6766	-6091	-675
1	13	-6	847	1332	-485	2	1	7	-3180	-2963	-217
1	13	-5	-908	-1161	253	2	1	8	-1045	-1076	31
1	13	-4	-915	-1609	694	2	1	9	2142	1901	241
1	13	3	1345	1407	-62	2	1	10	-692	-678	-14
1	13	5	-900	-699	-201	2	1	11	957	826	131
1	13	11	797	475	322	2	1	13	-1529	-1486	-43
1	14	-6	842	1159	-317	2	1	15	711	579	132
1	14	-4	-900	-760	-140	2	1	16	934	906	28
1	14	-3	793	1083	-290	2	1	17	-761	-392	-369
1	14	-2	1258	1717	-459	2	2	-17	-1024	-639	-385
1	14	2	802	785	17	2	2	-16	-2153	-1830	-323
1	14	3	-771	-653	82	2	2	-14	1240	1506	-266
1	14	4	-1433	-1523	90	2	2	-13	-1272	-775	-497
1	14	7	-1411	-1281	-130	2	2	12	-2413	-2516	103
1	15	-3	769	1066	-297	2	2	11	3346	2641	705
1	15	8	982	940	42	2	2	10	5964	5362	602
2	0	-19	-1000	-638	-362	2	2	-9	3061	2246	815
2	0	-18	972	1091	-119	2	2	-8	1840	1135	705
2	0	-17	-1666	-1122	-544	2	2	-7	-1265	-737	-528
2	0	-16	-4281	-3432	-849	2	2	-6	-453	-96	-357
2	0	-15	-3452	-2670	-782	2	2	-5	-526	-1105	579
2	0	-12	-1532	-1364	-168	2	2	-4	-9009	-7765	-1244
2	0	-11	2562	2587	375	2	2	-3	-7328	-6565	-764
2	0	-10	5194	3858	1336	2	2	-2	-6745	-6767	22
2	0	-9	4601	3335	1266	2	2	-1	-4905	-4662	-243
2	0	-7	1410	580	830	2	2	0	-421	-1089	668
2	0	-6	-2232	-1174	-1058	2	2	1	-904	-463	-441
2	0	-5	-9495	-8300	-1195	2	2	2	10617	11136	-519
2	0	-4	-2653	-262	-2391	2	2	3	7990	6518	1472
2	0	-3	11702	13270	-1568	2	2	4	1802	2077	-275
2	0	-2	-5274	-5129	-145	2	2	5	10304	9227	1077

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
2	2	6	1170	54	1116	2	5	-16	-818	-719	-99
2	2	7	-5098	-4247	-851	2	5	-15	1250	1442	-198
2	2	10	-4036	-3790	-246	2	5	-14	1508	1020	488
2	2	11	-2813	-2455	-358	2	5	-11	2144	2289	-145
2	2	12	1469	1612	-143	2	5	-9	-3461	-3069	-392
2	2	13	1006	806	200	2	5	-8	728	618	110
2	2	14	-1427	-1326	-101	2	5	-7	1158	1009	149
2	2	16	1201	855	346	2	5	-6	-3676	-3679	-197
2	2	17	1486	1248	238	2	5	-5	-5405	-5950	501
2	3	-17	-1218	-1541	323	2	5	-4	6313	6105	208
2	3	-15	1659	1808	-149	2	5	-3	1979	2468	-489
2	3	-14	638	856	-218	2	5	-2	-533	-16	-517
2	3	-13	-1379	-1655	476	2	5	-1	2330	2231	99
2	3	-12	1032	951	81	2	5	0	5277	5697	-420
2	3	-11	1559	1540	19	2	5	1	-1021	-1525	504
2	3	-10	-675	-734	59	2	5	2	-4299	-3340	-959
2	3	-9	-1946	-1961	15	2	5	4	4704	4233	471
2	3	-8	881	912	-31	2	5	5	-4013	-3653	-360
2	3	-7	7305	6672	633	2	5	6	-4609	-4556	-53
2	3	-6	-2403	-2149	-254	2	5	7	-1316	-1339	23
2	3	-5	-6556	-6139	-417	2	5	8	2872	3086	-194
2	3	-4	-1367	-965	-402	2	5	9	-1450	-1586	136
2	3	-3	660	1075	-415	2	5	10	-1885	-2110	225
2	3	-2	-3357	-3150	-207	2	5	11	590	534	56
2	3	-1	1185	1648	-464	2	5	12	1556	1332	224
2	3	1	4600	4000	600	2	5	13	1019	712	307
2	3	2	-2683	-2793	-90	2	5	14	1222	1047	175
2	3	3	-1914	-1680	-234	2	5	15	-1017	-635	-382
2	3	4	3226	2696	530	2	6	-16	-665	-548	63
2	3	5	-894	-1506	612	2	6	-17	-860	-650	-210
2	3	6	-1214	-1179	-35	2	6	-15	-882	-918	36
2	3	7	3056	2940	116	2	6	-14	-1102	-1083	-19
2	3	8	-1122	-1351	229	2	6	-12	894	1051	-157
2	3	10	-3063	-2993	-70	2	6	-10	1738	1391	347
2	3	11	3057	2913	144	2	6	-9	1625	1621	4
2	3	12	1981	1742	239	2	6	-8	2126	2520	-394
2	3	13	-1060	-986	-74	2	6	-6	-3312	-3350	38
2	3	16	1075	1012	63	2	6	-4	-1106	-1442	334
2	3	17	-745	-648	-97	2	6	-3	-4979	-4695	-284
2	4	-18	-852	-676	-84	2	6	-1	-1064	-1448	384
2	4	-17	-795	-279	-516	2	6	0	537	140	397
2	4	-16	-893	-512	-381	2	6	1	3485	3259	226
2	4	-14	-883	-773	-110	2	6	2	1055	528	527
2	4	-11	2208	1680	528	2	6	3	2351	2875	-524
2	4	-10	1588	1597	-9	2	6	4	4207	4128	79
2	4	-9	-1757	-1941	184	2	6	5	-2032	-2136	104
2	4	-8	5358	4493	865	2	6	7	3515	2932	583
2	4	-7	2408	2296	112	2	6	9	-5328	-4871	-457
2	4	-6	-945	-1028	83	2	6	10	-1310	-933	-377
2	4	-5	3024	2165	859	2	6	12	-1756	-1756	0
2	4	-4	-5104	-4543	-561	2	6	13	-1120	-1174	54
2	4	-3	-6606	-6663	75	2	6	14	812	633	179
2	4	-2	-1670	-1021	-649	2	6	16	1228	806	423
2	4	-1	-2254	-1450	-794	2	7	-11	1231	1611	-380
2	4	0	-3385	-3044	559	2	7	-7	-2063	-2146	77
2	4	1	2684	2752	-68	2	7	-6	-2235	-2584	349
2	4	3	1323	1411	-88	2	7	-5	-1533	-1565	-32
2	4	4	538	638	-100	2	7	-4	569	431	138
2	4	5	3389	3259	130	2	7	-3	1443	1496	-53
2	4	6	1721	1290	431	2	7	-2	1055	1468	-413
2	4	9	-801	-759	-42	2	7	-1	-1433	-1408	-25
2	4	10	-3232	-2600	-632	2	7	1	2229	2604	-375
2	4	11	-1502	-1164	-418	2	7	2	672	533	139
2	4	12	-2245	-1890	-355	2	7	3	-1015	-1157	142
2	4	13	1712	1498	214	2	7	6	-4067	-3840	-227
2	4	15	1704	1423	281	2	7	7	-2109	-2054	-55
2	4	16	908	558	350	2	7	8	2514	2331	183
2	4	17	934	575	359	2	7	11	1402	1179	223
2	5	-17	-1052	-1194	142	2	7	12	973	532	441

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
2	7	14	700	814	-114	2	11	8	-1618	-1859	241
2	7	15	765	715	50	2	11	10	1536	1458	78
2	8	-14	-1056	-1125	69	2	11	13	1072	921	151
2	8	-9	3076	3534	-458	2	11	14	1153	903	250
2	8	-8	1773	1574	199	2	12	-1	696	1100	-404
2	8	-7	-1068	-943	-145	2	12	1	-965	-900	-65
2	8	-6	-2717	-2563	-154	2	13	-11	-754	-1145	391
2	8	-5	1208	1204	4	2	13	-9	1035	1298	-263
2	8	-4	2658	3138	-460	2	13	-7	-857	-1211	354
2	8	-3	-2886	-3450	564	2	13	-4	-1106	-1597	491
2	8	-2	-2668	-3052	384	2	13	-3	-860	-1106	246
2	8	0	1118	1003	115	2	13	-2	2151	2823	-632
2	8	2	948	1169	-221	2	13	-1	1731	1745	-16
2	8	3	2989	3000	-11	2	13	2	1163	1216	-53
2	8	4	2492	2474	18	2	13	4	-1338	-1267	-71
2	8	5	-1056	-1282	226	2	13	5	-1000	-1075	75
2	8	8	-2354	-2224	-130	2	13	7	-964	-888	-76
2	8	9	-3636	-3460	-176	2	13	8	-979	-1162	183
2	8	10	629	506	123	2	13	10	1062	891	171
2	8	11	1085	1132	-47	2	14	5	773	515	258
2	8	13	-1214	-734	-480	2	14	7	-711	-938	227
2	8	14	1973	1712	261	2	14	11	-1050	-527	-153
2	9	-12	816	863	-47	2	15	-2	886	962	-76
2	9	-11	-823	-919	96	2	15	-1	883	1324	-441
2	9	-10	-1038	-1129	91	2	16	-1	-850	-907	57
2	9	-7	-1532	-1672	140	3	1	-20	1425	1113	316
2	9	-6	-1320	-1703	383	3	1	-17	1277	1125	152
2	9	-4	-4071	-4989	918	3	1	-16	-1291	-715	-576
2	9	-2	3559	4347	-788	3	1	-15	-4113	-3665	-453
2	9	-1	1754	2129	-375	3	1	-14	1046	1539	-493
2	9	0	849	1187	-338	3	1	-13	983	694	89
2	9	1	2611	3111	-500	3	1	-12	-2624	-2295	-329
2	9	4	-826	-1044	218	3	1	-11	-1519	-1184	-335
2	9	5	546	267	281	3	1	-10	2601	2231	370
2	9	8	-919	-1200	281	3	1	-9	4878	4412	466
2	9	9	-1294	-1209	-85	3	1	-8	-2652	-2620	-32
2	9	10	-1368	-1216	-152	3	1	-7	2585	2384	201
2	9	12	877	759	118	3	1	-6	6985	6145	840
2	9	13	957	1002	-45	3	1	-5	-1075	-1605	530
2	10	-12	1512	2152	-640	3	1	-4	-848	-1002	154
2	10	-10	-934	-1369	435	3	1	-3	-4084	-3744	-340
2	10	-9	984	1440	-456	3	1	-2	-2325	-2442	117
2	10	-8	1243	1243	0	3	1	-1	-8382	-8421	103
2	10	-6	-1137	-1379	242	3	1	0	-7653	-8201	543
2	10	-3	-2577	-2792	215	3	1	1	3378	2736	642
2	10	-2	-2049	-2471	422	3	1	2	-3084	-1453	-1631
2	10	-1	1486	1905	-439	3	1	3	4868	4105	763
2	10	1	-1791	-1638	-153	3	1	5	2130	2977	-847
2	10	2	881	1079	-198	3	1	6	10508	9465	1043
2	10	3	2401	2577	-176	3	1	7	880	478	402
2	10	6	1259	1111	148	3	1	8	-1807	-1441	-366
2	10	7	1635	1696	-61	3	1	9	2011	1916	95
2	10	12	-782	-647	-135	3	1	10	-1460	-1674	214
2	10	13	-1141	-809	-332	3	1	11	-3672	-3065	-607
2	10	15	855	840	15	3	1	12	-1101	-1153	52
2	11	-13	830	1086	-256	3	1	13	-557	-754	197
2	11	-12	1126	1582	-456	3	1	14	719	439	280
2	11	-9	761	873	-112	3	1	15	-1687	-1712	25
2	11	-7	-1608	-2207	599	3	1	17	1552	1794	-242
2	11	-5	1429	2157	-728	3	2	-16	-1050	-1080	-30
2	11	-2	1158	1710	-552	3	2	-12	1701	1589	112
2	11	-1	-1374	-1789	415	3	2	-7	6622	6056	566
2	11	0	-1323	-1498	175	3	2	-5	-6268	-4620	-1648
2	11	1	1291	1458	-167	3	2	-4	-7364	-7065	-319
2	11	2	2478	2680	-202	3	2	-2	4902	4308	594
2	11	3	1163	1693	-530	3	2	-1	-271	-616	345
2	11	4	-1244	-1132	-112	3	2	0	-2545	-2436	-109
2	11	5	-2301	-2350	49	3	2	1	3328	2866	462
2	11	7	-1069	-1054	-15	3	2	2	5805	5171	634

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
3	2	3	-5773	-4199	-1574	3	5	-17	-1002	-1182	180
3	2	4	-6945	-4156	-2789	3	5	-16	-905	-1009	104
3	2	5	5253	4311	942	3	5	-14	-1732	-1941	209
3	2	6	-9003	-7455	-1548	3	5	-13	-977	-535	-442
3	2	7	-691	-1119	428	3	5	-10	1490	1574	-84
3	2	8	4782	4570	212	3	5	-9	886	671	215
3	2	9	1106	1322	-216	3	5	-8	2493	2337	156
3	2	10	-2020	-1817	-203	3	5	-7	3382	3179	203
3	2	11	2353	2147	206	3	5	-5	-1764	-2159	375
3	2	16	1359	1391	-32	3	5	-4	-1738	-1635	-103
3	2	18	-1018	-1040	22	3	5	-3	-2183	-1899	-284
3	3	-16	-1230	-1029	-201	3	5	-2	-1947	-2754	807
3	3	-15	-1198	-1218	20	3	5	-1	2371	2457	-86
3	3	-14	-1253	-1183	-70	3	5	0	-1588	-1476	-112
3	3	-13	-2042	-1371	-671	3	5	1	-4485	-4726	241
3	3	-12	-2565	-2456	-109	3	5	2	1030	1146	-116
3	3	-11	-1742	-1566	-176	3	5	3	-446	-1	-445
3	3	-10	3442	3007	435	3	5	4	3205	3670	-465
3	3	-9	5096	4374	722	3	5	5	2171	2101	70
3	3	-8	3168	2816	352	3	5	6	1554	1362	192
3	3	-7	4073	3550	523	3	5	7	4005	3810	195
3	3	-6	623	633	-10	3	5	8	1137	1108	29
3	3	-5	-1575	-1225	-350	3	5	9	-3007	-3178	171
3	3	-4	3542	2597	945	3	5	10	-4222	-3696	-526
3	3	-3	-1130	-1753	623	3	5	11	-1654	-1836	182
3	3	-2	-6456	-5694	-762	3	5	13	1371	1343	28
3	3	-1	-1976	-2623	647	3	5	14	-1259	-1051	-208
3	3	0	-6065	-6178	113	3	6	-16	-1284	-1295	11
3	3	1	-2401	-1657	-744	3	6	-14	1306	1436	-130
3	3	2	8472	7390	1082	3	6	-12	-1384	-1821	437
3	3	3	4968	4960	8	3	6	-11	1472	1856	-384
3	3	4	-551	-294	-257	3	6	-10	1907	1580	327
3	3	6	3103	2900	203	3	6	-9	-512	-587	75
3	3	7	-1630	-1623	-7	3	6	-7	560	519	41
3	3	8	-2105	-1964	-141	3	6	-5	-3292	-3628	336
3	3	9	2559	2176	383	3	6	-4	-1257	-1275	18
3	3	10	-1507	-1171	-336	3	6	-3	742	857	-115
3	3	11	-2894	-2671	-223	3	6	-2	-1956	-1830	-126
3	3	12	-2418	-1921	-497	3	6	-1	-2850	-3282	432
3	3	17	1383	1013	370	3	6	1	3602	4004	-402
3	4	-16	-1676	-1956	320	3	6	2	3597	3186	411
3	4	-14	1715	1894	-179	3	6	3	1329	1240	89
3	4	-13	-624	-853	229	3	6	4	2636	3315	-679
3	4	-11	1901	1902	-1	3	6	5	498	851	-353
3	4	-10	2602	2359	243	3	6	6	-1372	-1243	-129
3	4	-9	-2500	-2225	-275	3	6	7	-3857	-3261	-596
3	4	-8	-3543	-3210	-333	3	6	10	-651	-445	-206
3	4	-7	1142	1505	-363	3	6	11	-1275	-1083	-192
3	4	-6	-768	-533	-235	3	6	12	1832	1710	122
3	4	-5	-4709	-4294	-415	3	6	14	-808	-868	60
3	4	-4	-1297	-193	-1104	3	6	15	790	901	-111
3	4	-3	4595	3746	849	3	7	-14	-1411	-1660	249
3	4	-2	1235	782	453	3	7	-13	-1078	-1610	532
3	4	-1	-2397	-2131	-266	3	7	-11	824	828	-4
3	4	0	4423	3633	790	3	7	-8	2683	2913	-230
3	4	1	788	1240	-452	3	7	-7	1694	1478	216
3	4	2	-463	-56	-407	3	7	-6	-983	-1566	583
3	4	3	-2550	-2803	253	3	7	-4	2043	1671	372
3	4	4	2482	3211	-729	3	7	-2	-5094	-5163	69
3	4	5	6375	6050	325	3	7	-1	-4391	-4429	38
3	4	6	-4050	-3923	-127	3	7	1	472	244	228
3	4	7	-3839	-3241	-598	3	7	2	-514	-332	-182
3	4	8	3650	3512	138	3	7	4	3055	3397	-342
3	4	9	-1449	-1417	-32	3	7	5	1203	1650	-447
3	4	10	-3100	-2829	-271	3	7	6	-1212	-1496	284
3	4	11	-1050	-1282	192	3	7	7	2662	2611	51
3	4	12	701	498	203	3	7	8	1571	1451	120
3	4	13	1644	1582	62	3	7	9	-1292	-1248	-44
3	5	-18	876	711	165	3	7	10	1138	1038	100

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
3	7	12	-880	-839	-41	3	11	-8	1240	1660	-420
3	7	13	-3075	-2673	-402	3	11	-7	610	1361	-751
3	7	14	-894	-886	-8	3	11	1	-957	-1377	420
3	7	15	926	1394	-468	3	11	2	-1016	-1157	141
3	7	16	698	1038	-140	3	11	3	527	1307	-780
3	8	-15	-773	-847	74	3	11	5	-714	-809	95
3	8	-13	943	978	-35	3	11	7	796	752	44
3	8	-12	661	339	322	3	11	10	-1436	-1315	-123
3	8	-11	1461	1838	-377	3	12	-9	726	1163	-435
3	8	-8	1731	2025	-294	3	12	-8	764	1337	-573
3	8	-6	-1939	-1989	50	3	12	-7	-751	-978	227
3	8	-5	-1096	-1410	312	3	12	-6	-1694	-1923	229
3	8	-4	-1423	-1560	137	3	12	-5	-692	-959	267
3	8	-3	-651	-547	-104	3	12	-3	-1401	-1564	163
3	8	-2	579	236	343	3	12	-2	-742	-460	-282
3	8	-1	1748	1742	6	3	12	-1	1874	2179	-305
3	8	0	-875	-798	-77	3	12	0	1119	1146	-27
3	8	1	1581	1437	144	3	12	2	2089	2749	-660
3	8	2	861	651	210	3	12	3	1460	1532	-72
3	8	4	555	832	-277	3	12	4	-752	-467	-285
3	8	6	-1017	-792	-225	3	12	5	-1086	-1060	-26
3	8	7	-1799	-1380	-419	3	12	6	607	310	297
3	8	8	-1872	-2047	175	3	12	8	-1298	-1475	177
3	8	9	1136	1080	56	3	12	9	-1094	-1158	64
3	8	10	-699	-853	154	3	12	12	-1038	-775	-263
3	8	11	-1319	-1445	126	3	14	-9	983	1209	-226
3	8	12	1723	1313	410	3	14	-7	-1029	-1457	428
3	8	13	866	734	132	3	14	-3	-1136	-1559	423
3	8	15	1310	1197	113	3	14	-1	1084	1440	-356
3	9	-13	-734	-677	-57	3	14	1	-1033	-725	-308
3	9	-11	1043	1127	-84	3	14	2	1066	1041	25
3	9	-10	-1160	-1712	552	3	14	3	1152	1426	-274
3	9	-8	2301	2499	-198	3	14	7	-678	-455	-223
3	9	-7	865	915	-50	3	15	0	-697	-777	80
3	9	-6	-887	-894	7	3	15	3	-898	-700	-198
3	9	-5	1368	1802	-434	3	15	5	998	1017	-19
3	9	-4	2568	2163	405	3	15	6	962	962	0
3	9	-3	-1129	-1444	315	4	0	-18	1213	831	382
3	9	-2	-3592	-4194	202	4	0	-16	1063	779	284
3	9	-1	-1221	-1810	589	4	0	-15	-3367	-2922	-445
3	9	0	1681	2119	-438	4	0	-14	-4117	-3190	-927
3	9	1	-916	-668	-248	4	0	-13	2653	2176	477
3	9	2	-2277	-2332	55	4	0	-11	-4916	-3834	-1082
3	9	3	1770	2185	-415	4	0	-10	-3315	-2869	-446
3	9	4	2032	2410	-378	4	0	-9	3010	2166	844
3	9	5	623	764	-141	4	0	-8	1970	1652	318
3	9	7	1688	1560	128	4	0	-7	1807	1389	418
3	9	8	651	282	369	4	0	-6	10854	9581	1273
3	9	9	-1401	-1363	-38	4	0	-5	9366	8991	375
3	9	10	-1021	-894	-127	4	0	-4	-2433	-1977	-456
3	9	13	-1447	-1279	-168	4	0	-3	-3096	-3553	457
3	10	-12	763	1200	-437	4	0	-2	3909	3249	660
3	10	-11	854	985	-131	4	0	-1	-6411	-8765	2354
3	10	-8	686	632	54	4	0	0	-9842	-10556	714
3	10	-6	-756	-971	215	4	0	1	-3461	-2137	-1324
3	10	-4	-1545	-1553	8	4	0	2	3061	3215	-154
3	10	-3	-1601	-2460	859	4	0	3	5082	2919	2163
3	10	-2	894	163	731	4	0	4	-7824	-6545	-1279
3	10	-1	2415	3007	-592	4	0	5	-2351	-1777	-574
3	10	1	-1243	-1660	417	4	0	6	1195	647	548
3	10	2	1545	2412	-867	4	0	7	4795	4729	66
3	10	3	2362	2678	-316	4	0	8	3480	2946	534
3	10	5	-1748	-1908	160	4	0	9	627	781	-154
3	10	6	-639	-774	135	4	0	10	1147	737	410
3	10	7	697	916	-219	4	0	11	-1626	-1902	276
3	10	8	-1478	-1552	74	4	0	12	-2368	-2430	62
3	10	14	971	872	99	4	0	13	-1404	-1064	-340
3	11	-13	-934	-907	-27	4	0	14	1517	1880	-363
3	11	-11	876	1293	-417	4	0	16	-1055	-1740	685

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
4	0	18	843	1025	-182	4	3	3	1846	2043	-197
4	1	-17	998	1231	-233	4	3	4	-880	-524	-356
4	1	-14	-1588	-1285	-303	4	3	5	5573	4824	749
4	1	-13	-1868	-1632	-236	4	3	6	3411	3314	97
4	1	-11	573	441	132	4	3	7	-2364	-1978	-386
4	1	-10	-1359	-1269	-90	4	3	8	-1084	-702	-382
4	1	-9	566	475	91	4	3	9	2314	1835	479
4	1	-8	2027	1730	297	4	3	10	-4013	-3626	-387
4	1	-7	1006	1417	-411	4	3	11	-1830	-2131	301
4	1	-4	-4663	-3610	-1053	4	3	13	1356	1265	91
4	1	-3	2555	2722	233	4	3	16	858	732	126
4	1	-2	6821	6090	731	4	4	-13	-1836	-1555	-281
4	1	-1	-2075	-1559	-516	4	4	-12	-1124	-1154	30
4	1	0	-537	-948	411	4	4	-9	-570	-451	-115
4	1	1	3244	2047	1197	4	4	-8	825	480	345
4	1	2	4770	5579	-809	4	4	-7	785	935	-150
4	1	3	551	591	-40	4	4	-6	3352	3484	-132
4	1	4	-5881	-5399	-482	4	4	-5	4917	4927	-10
4	1	6	570	444	126	4	4	-4	481	111	370
4	1	7	-962	-1316	354	4	4	-3	1971	2344	-373
4	1	8	-1382	-1011	-371	4	4	-2	-4530	-4827	297
4	1	9	2060	1690	390	4	4	-1	-4121	-4870	749
4	1	10	-2103	-2001	-102	4	4	0	-4588	-4062	-526
4	1	14	-758	-594	-204	4	4	1	-6230	-6823	593
4	2	-17	742	905	-163	4	4	4	1790	2020	-230
4	2	-16	999	1245	-246	4	4	5	556	294	262
4	2	-15	-742	-1014	272	4	4	6	3819	3433	386
4	2	-14	-1733	-1564	-169	4	4	-7	4376	3802	574
4	2	-12	-2698	-2316	-382	4	4	-8	1559	1480	79
4	2	-11	-5465	-4935	-530	4	4	10	1019	1259	-240
4	2	-10	-1291	-1151	-140	4	4	12	-1957	-1874	-83
4	2	-9	4686	4207	479	4	4	14	-1502	-1098	-404
4	2	-8	5531	4941	590	4	4	15	-1012	-1245	233
4	2	-7	-940	-642	-298	4	5	-16	-1071	-1274	203
4	2	-6	-875	-797	-78	4	5	-15	-1411	-1609	198
4	2	-5	2144	1878	266	4	5	-14	1122	1143	-21
4	2	-4	-1974	-1875	-99	4	5	-13	1069	871	198
4	2	-2	2856	2172	684	4	5	-12	-934	-889	-45
4	2	0	-2912	-2943	31	4	5	-10	2565	2837	-272
4	2	1	-5726	-5775	47	4	5	-6	-1345	-1542	197
4	2	2	-898	-1313	415	4	5	-7	1360	1347	13
4	2	3	1427	1513	-86	4	5	-6	2774	3455	-681
4	2	5	3196	3003	193	4	5	-5	-1688	-1506	-182
4	2	6	4360	3994	366	4	5	-4	-1010	-1695	685
4	2	7	3097	2460	637	4	5	-2	-844	-297	-547
4	2	8	-762	-781	19	4	5	-1	-1829	-2566	737
4	2	10	1661	1346	315	4	5	0	-1199	-1750	551
4	2	11	-1225	-1122	-103	4	5	1	2562	2788	-226
4	2	12	-2428	-2329	-99	4	5	3	-2482	-2157	-325
4	2	13	-758	-766	8	4	5	4	651	1110	-459
4	2	15	-1028	-1114	86	4	5	5	2401	2157	244
4	2	16	-875	-1027	152	4	5	6	1517	941	576
4	2	18	933	1082	-149	4	5	7	-6285	-4910	-1375
4	3	-16	-1264	-1562	298	4	5	8	-1388	-797	-591
4	3	-15	-797	-674	-123	4	5	9	2101	2011	90
4	3	-14	1915	2003	-88	4	5	10	1681	1213	468
4	3	-12	-1311	-1623	312	4	5	11	-1785	-1657	-132
4	3	-10	1496	1379	117	4	5	12	-807	-728	-79
4	3	-9	1489	1363	126	4	5	13	998	938	60
4	3	-8	-880	-575	-305	4	5	16	956	913	43
4	3	-7	-470	-256	-214	4	6	-13	-1329	-1922	593
4	3	-6	2144	1564	580	4	6	-7	1326	1238	88
4	3	-5	-487	-161	-326	4	6	-6	2447	2760	-313
4	3	-4	-7007	-6855	-152	4	6	-5	638	428	210
4	3	-2	4798	4384	414	4	6	-4	1391	1641	-250
4	3	-1	-3160	-3441	281	4	6	-3	3464	3620	-156
4	3	0	-2325	-2269	-56	4	6	-2	-1277	-1652	375
4	3	1	-459	-1328	869	4	6	-1	-3269	-3355	86
4	3	2	3609	2909	700	4	6	0	-906	-28	-878

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_o	Δ	*h*	*k*	*l*	F_o	F_o	Δ
4	6	1	-961	-826	-135	4	10	-1	-1736	-2331	595
4	6	2	-3321	-3236	-85	4	10	1	1426	1923	-497
4	6	3	-634	-1134	500	4	10	2	-1401	-1256	-145
4	6	4	3011	3202	-191	4	10	4	1005	1447	-442
4	6	5	577	1017	-440	4	10	8	2095	1780	315
4	6	6	-1584	-1438	-146	4	10	9	965	847	118
4	6	7	1564	1433	131	4	10	10	-1389	-1322	-67
4	6	8	3670	3061	609	4	10	11	-757	-757	0
4	6	9	744	146	598	4	11	-9	720	523	197
4	6	10	-1226	-1383	157	4	11	-7	1122	1455	-333
4	6	11	-1579	-1534	-45	4	11	-6	-953	-1300	347
4	6	12	-1045	-828	-217	4	11	-5	-1174	-1131	-43
4	6	14	-1334	-987	-347	4	11	-3	-723	-1325	602
4	6	15	-926	-680	-246	4	11	-2	-1377	-1816	439
4	7	-15	-876	-998	122	4	11	0	1413	1951	-538
4	7	-10	2099	2496	-397	4	11	1	-1450	-1757	277
4	7	-8	-853	-1325	472	4	11	3	3141	3623	-482
4	7	-7	937	1483	-546	4	11	4	1726	1637	89
4	7	-6	694	1039	-345	4	11	5	-912	-1046	134
4	7	-5	-2267	-2733	466	4	11	7	1534	1297	237
4	7	-4	-2382	-2685	303	4	11	9	-1574	-1267	-307
4	7	-3	-2914	-3008	94	4	11	10	-832	-647	-185
4	7	-1	1666	1604	62	4	12	-5	705	534	171
4	7	0	-1915	-2168	253	4	12	-3	728	441	287
4	7	1	2548	2516	32	4	12	-2	660	732	-72
4	7	2	1449	1608	-159	4	12	1	-848	-874	26
4	7	3	1141	1027	114	4	12	2	-1603	-1803	200
4	7	4	1486	1542	-46	4	12	3	-1320	-1203	-117
4	7	7	-1808	-1378	-430	4	12	4	974	1365	-391
4	7	9	847	562	285	4	12	6	770	884	-114
4	7	11	-1818	-1113	-705	4	13	-8	813	1409	-596
4	8	-13	-1081	-1821	740	4	13	-6	-748	-848	100
4	8	-12	-791	-956	165	4	13	-3	-863	-1162	299
4	8	-8	1866	2836	-970	4	13	-2	-1081	-1471	390
4	8	-7	4383	5181	-798	4	13	0	1608	1736	-128
4	8	-5	-3777	-4369	592	4	13	1	-948	-1347	399
4	8	-4	1303	1230	73	4	13	2	-1134	-915	-219
4	8	-3	2283	1991	292	4	13	3	1861	2107	-246
4	8	-1	-3311	-3514	203	4	13	4	1043	782	261
4	8	1	1145	1245	-100	4	13	5	-820	-485	-335
4	8	2	-3390	-3409	19	4	14	2	795	950	-155
4	8	3	-1052	-999	-53	4	15	-2	-910	-1580	670
4	8	4	1231	854	377	4	15	0	705	452	253
4	8	5	1355	1453	-98	4	16	-1	925	1003	-78
4	8	6	-776	-332	-444	5	1	-18	826	533	293
4	8	7	1227	784	443	5	1	-17	1529	1245	284
4	8	8	1610	1329	281	5	1	-16	1478	1029	450
4	8	12	854	669	185	5	1	-15	767	625	142
4	8	13	-847	-844	-3	5	1	-13	-1038	-997	-41
4	8	14	-1353	-1264	-89	5	1	-11	-3341	-2622	-719
4	9	-9	718	767	-49	5	1	-10	-6345	-5486	-863
4	9	-7	1122	1597	-475	5	1	-9	618	325	293
4	9	-6	-725	-1060	335	5	1	-8	3440	3491	-51
4	9	-5	-869	-937	68	5	1	-7	-1825	-1593	-232
4	9	-3	-858	-806	-52	5	1	-6	-2912	-2364	-548
4	9	-2	-606	-844	238	5	1	-5	5014	4670	344
4	9	3	1878	2286	-408	5	1	-4	7736	6735	1001
4	9	4	1783	1807	-24	5	1	-3	-3090	-2878	-212
4	9	5	769	578	191	5	1	-2	5311	5263	48
4	9	7	737	320	417	5	1	-1	1946	1549	397
4	9	8	-1768	-1730	-38	5	1	0	-3887	-4699	812
4	9	9	-1338	-976	-362	5	1	1	-5166	-4339	-827
4	9	10	-1294	-1096	-198	5	1	2	-4354	-4057	-297
4	9	11	-899	-983	84	5	1	4	-3490	-2845	-645
4	9	12	-844	-698	-146	5	1	5	-830	-694	-136
4	10	-9	-1361	-1681	320	5	1	6	2469	2455	14
4	10	-7	1097	1906	-809	5	1	7	4054	3998	56
4	10	-4	1351	1596	-205	5	1	8	2843	2866	-23
4	10	-2	-1703	-2027	324	5	1	10	1108	1074	34

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
5	1	11	1390	1221	169	5	4	1	-2269	-2418	149
5	1	12	-1246	-1566	318	5	4	2	2633	1728	905
5	1	13	-1559	-1723	164	5	4	3	-1415	-618	-797
5	1	16	-1231	-1680	449	5	4	4	835	586	249
5	2	-15	-968	-946	-22	5	4	5	4908	3962	946
5	2	-14	-1159	-1187	28	5	4	6	2897	2897	0
5	2	-11	2693	2592	101	5	4	8	-5328	-4790	-530
5	2	-10	2583	2196	387	5	4	9	-2599	-2080	-519
5	2	-9	1807	1520	287	5	4	10	3022	2745	277
5	2	-8	-2861	-2639	-222	5	4	12	-1261	-1080	-181
5	2	-7	-2461	-1704	-757	5	4	13	914	937	-23
5	2	-5	4031	3790	241	5	4	15	-1015	-1060	45
5	2	-4	-4960	-3857	-1103	5	5	-12	-1062	-1334	272
5	2	-3	-3750	-4082	332	5	5	-11	-1928	-2063	135
5	2	-2	2390	1900	490	5	5	-10	-1061	-956	-95
5	2	-1	1216	2197	-981	5	5	-9	-630	-606	-24
5	2	0	-1348	-1637	289	5	5	-8	-955	-1040	85
5	2	1	-3989	-3911	-78	5	5	-7	947	1602	-655
5	2	2	3683	3723	-40	5	5	-6	2617	3044	-427
5	2	3	-532	-311	-221	5	5	-5	1920	2440	-520
5	2	4	-2354	-2217	-137	5	5	-4	1074	813	261
5	2	5	607	394	213	5	5	-3	1512	1650	-138
5	2	6	-1704	-970	-734	5	5	-2	-1453	-1223	-230
5	2	7	2291	1953	338	5	5	0	-1119	-1429	310
5	2	8	-1216	-841	-375	5	5	2	-959	-1686	727
5	2	9	1621	1729	-108	5	5	3	-4816	-4079	-737
5	2	10	2038	2314	-276	5	5	4	1682	2001	-319
5	2	11	-1479	-1573	94	5	5	6	-2098	-1467	-631
5	2	12	-1032	-1103	71	5	5	7	-638	-692	54
5	2	13	1027	1034	-7	5	5	8	2629	1992	637
5	3	-17	898	753	145	5	5	9	3996	3350	646
5	3	-14	-835	-1051	216	5	5	11	-724	-649	-75
5	3	-13	-1603	-1419	-184	5	5	12	-872	-795	-77
5	3	-11	-820	-533	-287	5	6	-15	-1118	-1624	506
5	3	-10	-2363	-2280	-83	5	6	-11	-1248	-1651	403
5	3	-9	-1522	-1279	-243	5	6	-10	959	1218	-259
5	3	-8	1462	909	553	5	6	-9	1517	1888	-371
5	3	-7	3591	3658	-67	5	6	-6	3586	4294	-708
5	3	-6	567	1129	-562	5	6	-5	1134	1803	-669
5	3	-5	3944	3541	403	5	6	-4	-2819	-2948	129
5	3	-4	2366	2783	-417	5	6	-3	-1801	-1514	-287
5	3	-2	1141	474	667	5	6	-2	-1136	-1211	75
5	3	-1	2759	2881	-122	5	6	0	-583	-883	300
5	3	0	-4764	-4599	-165	5	6	1	874	762	112
5	3	1	-4747	-5806	1059	5	6	2	2011	1778	233
5	3	2	-2263	-2168	-95	5	6	3	2097	1731	366
5	3	3	773	683	90	5	6	4	-799	-533	-266
5	3	4	1210	315	895	5	6	5	-771	-495	-276
5	3	5	-4149	-3368	-781	5	6	6	1159	1097	62
5	3	6	-547	-229	-318	5	6	8	1140	971	169
5	3	7	1551	1401	150	5	6	9	815	939	-124
5	3	8	1004	1239	-235	5	6	11	-2921	-2769	-152
5	3	9	932	1070	-138	5	6	12	-2943	-2666	-277
5	3	10	1176	1228	-52	5	6	14	989	643	346
5	3	11	1706	1645	61	5	7	12	-1018	-1541	523
5	3	13	-1203	-1220	17	5	7	-8	-1512	-1602	90
5	4	-17	813	921	-108	5	7	-6	2595	2907	-312
5	4	-15	-1478	-1607	129	5	7	-5	-1742	-1539	-203
5	4	-13	1374	1613	-239	5	7	-3	4168	4303	-135
5	4	-12	-725	-682	-43	5	7	-2	2843	3235	-392
5	4	-11	-2611	-2660	49	5	7	-1	-2737	-3155	418
5	4	-9	1610	1506	104	5	7	0	-2718	-3471	753
5	4	-6	2889	3175	-286	5	7	3	-3944	-3749	-195
5	4	-5	1010	972	38	5	7	5	2351	2495	-144
5	4	-4	-3169	-3499	330	5	7	7	1411	1286	125
5	4	-3	762	768	-6	5	7	8	2150	1767	383
5	4	-2	2463	2398	65	5	7	9	932	1056	-124
5	4	-1	-1309	-1701	392	5	7	10	-753	-608	-145
5	4	0	-2753	-2347	-446	5	7	12	1434	989	445

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
5	7	14	-1433	-1571	138	6	0	8	2178	2007	171
5	7	15	-914	-866	-48	6	0	9	-648	-541	-307
5	8	-9	733	1270	-537	6	0	10	1159	1103	56
5	8	-8	1102	1360	-258	6	0	11	2078	2731	-653
5	8	-6	1374	1725	-351	6	0	12	1069	1453	-384
5	8	-4	-2008	-2035	26	6	0	13	-1327	-1905	578
5	8	-3	-1060	-1157	117	6	1	-14	-1344	-1114	-230
5	8	0	-1226	-2042	816	6	1	-13	-2016	-1676	-340
5	8	2	-1004	-856	-148	6	1	-11	1221	1360	-159
5	8	4	1032	732	300	6	1	-9	3512	3034	478
5	8	5	2042	2174	-132	6	1	-8	-677	-655	-22
5	8	6	2414	2083	331	6	1	-7	-1524	-1014	-510
5	8	8	-1461	-1093	-368	6	1	-5	1322	1472	-150
5	9	-12	-1002	-1642	640	6	1	-3	3352	1996	1356
5	9	-7	752	1159	-407	6	1	-2	1630	2343	-713
5	9	-6	1426	1970	-544	6	1	-1	2960	3010	-50
5	9	-5	-709	-906	197	6	1	0	-2577	-2745	168
5	9	-3	2515	2845	-330	6	1	1	-7036	-5882	-1154
5	9	-2	1114	921	193	6	1	2	-1481	-1384	-97
5	9	-1	-2525	-2536	11	6	1	3	2200	2416	-216
5	9	1	1613	1473	140	6	1	4	786	953	-167
5	9	2	-792	-757	-35	6	1	12	-1153	-1217	64
5	9	3	-2363	-2822	459	6	1	13	-814	-822	8
5	9	4	-1072	-1564	492	6	2	-16	1883	1873	10
5	9	5	1676	1545	131	6	2	-15	1050	758	292
5	9	8	1154	1157	-3	6	2	-12	-1325	-826	-499
5	9	9	1354	1066	288	6	2	-10	-3525	-2834	-791
5	9	14	-1106	-1024	-162	6	2	-9	-5541	-5095	-446
5	10	-7	744	1135	-391	6	2	-8	1517	1356	161
5	10	-2	-936	-1637	701	6	2	-7	522	915	-393
5	10	-1	-698	-1189	291	6	2	-6	-2478	-1938	-540
5	10	2	-1000	-1157	157	6	2	-5	513	646	-133
5	10	4	3313	3297	21	6	2	-4	4133	4075	58
5	10	5	1214	1298	-84	6	2	-3	4979	4766	213
5	10	6	-1010	-726	-284	6	2	-2	816	901	-85
5	10	9	-643	-366	-277	6	2	-1	2307	2824	-517
5	10	10	-377	-701	-276	6	2	0	2951	3133	-182
5	10	13	-1027	-882	-145	6	2	1	-3606	-3746	-160
5	11	-2	636	320	316	6	2	2	-5114	-3554	-1560
5	11	3	-1017	-870	-147	6	2	4	-1136	-830	-306
5	11	5	1174	963	191	6	2	5	-2734	-2569	-165
5	11	7	-966	-721	-247	6	2	6	-2963	-2662	-301
5	11	9	1143	904	239	6	2	8	1440	1261	179
5	12	-7	1095	1612	-517	6	2	10	954	1162	-208
5	12	-2	-1113	-1350	237	6	2	11	1351	1567	-216
5	12	4	2123	2352	-229	6	3	-14	-636	-705	131
5	12	6	-1488	-1231	-257	6	3	-12	1547	1720	227
5	12	7	988	1124	-136	6	3	-11	-1516	-1125	-393
5	12	8	1226	970	256	6	3	-10	-5163	-5122	-41
5	14	-8	820	1384	-564	6	3	-9	2264	2314	-50
5	14	-2	-1319	-1679	360	6	3	-8	-503	-401	-102
6	0	-15	999	1036	-37	6	3	-7	-2168	-1650	-518
6	0	-16	1924	1310	614	6	3	-6	4247	3752	495
6	0	-13	1631	1385	246	6	3	-5	4795	4220	575
6	0	-11	3046	2546	500	6	3	-4	-1796	-1293	-503
6	0	-10	-3541	-2497	-1044	6	3	-3	-2624	-2775	151
6	0	-9	-5467	-4668	-799	6	3	-2	-1663	-1704	173
6	0	-8	3775	3274	501	6	3	-1	1057	1457	-400
6	0	-6	-2001	-1786	-215	6	3	1	-1361	-2072	691
6	0	-5	2473	2075	398	6	3	2	1643	1104	539
6	0	-4	4298	3561	737	6	3	3	3577	3442	135
6	0	-3	1090	1297	-207	6	3	4	-595	-524	-71
6	0	0	3219	2676	543	6	3	5	-1270	-1047	-223
6	0	1	-6650	-5554	-1096	6	3	6	1334	1146	188
6	0	2	-5110	-4253	-857	6	3	12	-1054	-1459	405
6	0	3	-967	-753	-214	6	3	13	-982	-853	-129
6	0	5	-505	-1000	495	6	3	14	1023	1326	-303
6	0	6	-2353	-2055	-298	6	3	-13	1245	1030	215
6	0	7	1710	976	734	6	3	-14	1694	1873	-179

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
6	4	-11	-1689	-1926	234	6	7	0	-1010	-884	-126
6	4	-10	-885	-1188	303	6	7	2	-2047	-2207	160
6	4	-9	-2132	-1847	-285	6	7	4	1058	501	557
6	4	-8	-2193	-2255	62	6	7	5	1071	812	259
6	4	-4	688	939	-251	6	7	6	1783	2043	-260
6	4	-3	1267	1356	-89	6	7	12	-1298	-1430	132
6	4	-1	3273	3454	-181	6	8	-10	840	1082	-242
6	4	0	826	1552	-726	6	8	-8	-2007	-2589	582
6	4	1	-1139	-1637	498	6	8	-6	1788	2521	-733
6	4	2	-1158	-1409	251	6	8	-4	-1361	-1006	-373
6	4	3	-537	-977	440	6	8	-2	3294	3379	-85
6	4	4	-1520	-1591	71	6	8	0	-2123	-2537	414
6	4	5	-1838	-1909	71	6	8	2	1598	1214	384
6	4	6	-714	-653	-61	6	8	4	-2060	-2427	367
6	4	7	824	1462	-638	6	8	5	677	645	28
6	4	8	2073	2019	54	6	8	7	-2211	-1881	-330
6	4	9	2387	2370	17	6	8	9	1354	1407	-53
6	5	-15	-959	-645	-310	6	8	13	1054	1049	5
6	5	-14	-980	-995	5	6	8	15	-553	-521	-32
6	5	-12	962	1167	-205	6	9	-9	-1633	-2209	576
6	5	-11	-1140	-1389	249	6	9	-7	3745	4252	-507
6	5	-9	2319	2054	265	6	9	-6	994	1082	-288
6	5	-8	2312	2041	271	6	9	-5	1684	2322	-638
6	5	-7	-1804	-2273	469	6	9	-3	-1602	-1478	-324
6	5	-6	1542	1851	-309	6	9	-1	-658	-923	265
6	5	-5	2239	2342	-103	6	9	0	-1793	-1681	-102
6	5	-3	-3103	-3133	30	6	9	5	845	790	55
6	5	-2	803	458	345	6	9	8	842	719	123
6	5	-1	-1490	-1320	-170	6	10	-8	-966	-1057	91
6	5	0	-2731	-2598	-133	6	10	-2	1218	1537	-319
6	5	1	-842	-1046	204	6	10	4	-2136	-1934	-204
6	5	2	-550	-637	87	6	10	7	-1331	-845	-486
6	5	4	-877	-790	-87	6	10	8	-864	-477	-387
6	5	5	-1243	-974	-269	6	10	9	1374	1006	368
6	5	6	4023	3577	446	6	11	-7	1331	1518	-187
6	5	7	2252	2022	230	6	11	-3	774	939	-165
6	5	8	-771	-581	-190	6	11	-1	-1545	-1909	364
6	5	9	-1275	-1115	-160	6	11	2	-561	-637	-24
6	5	10	990	1415	-425	6	11	4	1660	1370	290
6	5	11	1565	2051	-486	6	11	5	2116	2386	-270
6	5	12	-1372	-1353	-19	6	11	8	1357	1427	-70
6	5	13	-1173	-1111	-62	6	12	-2	803	431	372
6	6	-11	-2100	-2369	269	6	13	-2	-1299	-1150	-149
6	6	-10	-806	-1226	420	6	13	-1	-1246	-1543	297
6	6	-8	-2097	-2537	440	6	13	3	-1488	-1744	256
6	6	-6	1007	1563	-556	6	13	5	1497	1694	-197
6	6	-5	886	1261	-375	6	14	5	-1261	-1159	-102
6	6	-4	1626	1713	-87	7	1	-15	1864	1481	383
6	6	-3	1429	1922	-493	7	1	-14	921	420	501
6	6	-2	3367	3520	-153	7	1	-13	977	691	286
6	6	-1	1666	1349	317	7	1	-12	1765	1413	352
6	6	0	-1892	-2124	232	7	1	-11	2177	2053	124
6	6	3	-4006	-3878	-128	7	1	-10	-2798	-2593	-205
6	6	4	-3422	-3679	257	7	1	-9	-5533	-4621	-912
6	6	5	1181	1062	119	7	1	-8	-2398	-2335	-63
6	6	6	1004	873	131	7	1	-7	1049	498	551
6	6	7	-1571	-2272	701	7	1	-6	-1940	-1473	-467
6	6	9	1843	2175	-332	7	1	-5	-1923	-1682	-241
6	6	10	1058	1346	-288	7	1	-4	1062	1002	60
6	7	-10	1081	1455	-374	7	1	-3	2700	3084	-384
6	7	-9	930	670	260	7	1	-2	3228	3660	-432
6	7	-8	1370	1390	-20	7	1	-1	905	211	694
6	7	-7	-936	-1270	334	7	1	0	1861	1745	116
6	7	-6	-2216	-2594	378	7	1	1	5933	4834	1099
6	7	-5	2056	2483	-427	7	1	2	-3548	-2885	-663
6	7	-4	1717	1559	158	7	1	3	-2014	-2012	-2
6	7	-3	-2650	-2631	-19	7	1	4	1672	1346	326
6	7	-2	853	1120	-267	7	1	5	-3455	-3136	-319
6	7	-1	1958	2053	-95	7	1	6	-3050	-3105	55

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
7	1	8	1075	1291	-216	7	6	-10	-932	-1174	242
7	1	12	1596	2038	-442	7	6	-9	871	1076	-205
7	2	-11	2054	1864	190	7	6	-7	-1078	-1832	754
7	2	-10	-2523	-2579	56	7	6	-5	1378	1894	-516
7	2	-8	1795	1629	166	7	6	-4	3839	4670	-831
7	2	-7	-1993	-1654	-339	7	6	-3	1334	1936	-602
7	2	-6	-3625	-3805	180	7	6	-2	-2133	-2034	-99
7	2	-5	2877	2734	143	7	6	0	1229	1071	158
7	2	-4	857	1153	-296	7	6	1	-3503	-3510	-353
7	2	-3	-831	-1141	310	7	6	2	-1569	-1242	-327
7	2	-2	-2184	-2455	271	7	6	4	1545	752	793
7	2	-1	792	1301	-509	7	6	5	647	273	374
7	2	0	1660	1796	-136	7	6	6	1265	805	461
7	2	2	-2664	-2452	-212	7	6	7	878	534	344
7	2	3	1725	2398	-673	7	6	9	-896	-736	-160
7	2	5	-1317	-1425	108	7	6	10	1032	978	54
7	2	7	2465	2215	250	7	7	-13	1214	1060	-646
7	3	-15	938	1280	-342	7	7	-9	837	1210	-373
7	3	-14	1436	1638	-202	7	7	-8	-1524	-2022	498
7	3	-10	1616	1829	-213	7	7	-7	-2095	-2736	641
7	3	-8	-1776	-1848	72	7	7	-2	1767	2056	-289
7	3	-6	-1143	-1044	-99	7	7	-1	3403	3827	-424
7	3	-5	-1834	-2160	326	7	7	0	-782	-552	-230
7	3	-3	1018	1364	-346	7	7	1	-3065	-2627	-441
7	3	-2	453	898	-445	7	7	2	1836	1572	264
7	3	-1	2122	1994	128	7	7	3	2650	2103	547
7	3	0	3939	4320	-381	7	7	4	-895	-1179	284
7	3	2	-4408	-4373	-35	7	7	5	-1088	-1072	72
7	3	3	-728	-1198	470	7	7	7	-2170	-1570	-600
7	3	4	1677	1653	24	7	7	8	-1539	-1501	-38
7	3	6	-3700	-3079	-621	7	7	10	1791	1643	148
7	3	7	-2463	-2103	-360	7	8	-4	994	1103	-109
7	3	8	-956	-924	-32	7	8	-2	-2126	-1794	-332
7	3	9	837	812	25	7	8	-1	933	1469	-536
7	3	10	932	1251	-319	7	8	1	-1411	-1725	314
7	3	11	1796	1937	-141	7	8	4	-956	-1144	188
7	3	12	979	1089	-110	7	8	7	2105	1836	273
7	4	-16	1187	1533	-346	7	9	-7	-1193	-1777	584
7	4	-14	-1000	-880	-120	7	9	-1	1297	1638	-341
7	4	-13	-1548	-1763	215	7	9	2	1483	1144	339
7	4	-10	-2315	-2648	333	7	9	4	-2295	-2295	-6
7	4	-8	3101	3057	44	7	9	5	-2438	-2312	-126
7	4	-6	746	665	83	7	9	8	-1242	-966	-276
7	4	-5	1974	2224	-250	7	9	10	2140	1718	422
7	4	-3	-1462	-1614	152	7	10	-6	932	1014	-82
7	4	-2	-1028	-832	-196	7	10	0	-1010	-1131	121
7	4	-1	1134	1253	-119	7	10	3	-1348	-1360	12
7	4	0	2099	2088	11	7	10	5	1207	670	537
7	4	1	-3262	-2747	-515	7	10	8	1191	628	563
7	4	2	-1280	-1064	-216	7	10	9	1041	1030	11
7	4	3	2582	1723	859	7	11	-5	967	1130	-163
7	4	5	-3772	-2958	-814	7	11	-3	-908	-557	-351
7	4	7	3061	2334	727	7	11	3	-1106	-856	-250
7	4	9	-1108	-1002	-106	7	12	0	-939	-812	-127
7	4	13	-1246	-1280	34	7	12	3	-1660	-1616	56
7	5	-12	1164	1617	-633	7	12	5	1219	756	463
7	5	-11	-875	-648	-227	8	0	-15	1102	753	349
7	5	-8	-1860	-2534	674	8	0	-14	1754	1309	445
7	5	-5	-616	-407	-209	8	0	-12	-1044	-718	-326
7	5	-3	566	707	-139	8	0	-11	5002	4364	638
7	5	-1	2064	2123	-59	8	0	-10	947	774	173
7	5	0	2346	3005	-659	8	0	-9	-2064	-1642	-422
7	5	2	1373	1045	328	8	0	-8	-2126	-1601	-525
7	5	3	-1354	-1560	206	8	0	-7	-2033	-1585	-451
7	5	4	-4965	-4357	-608	8	0	-5	-2282	-1211	-1071
7	5	5	-1526	-1254	-272	8	0	-4	-2527	-2182	-345
7	5	6	1344	974	370	8	0	-3	2022	1188	834
7	5	14	1360	1456	-96	8	0	0	-2024	-1438	-586
7	6	-14	-1018	-1421	403	8	0	1	4830	4755	75

TABLE 3 (*Continued*)

h	k	l	F_o	F_o	Δ
8	0	[illegible]	2636	[illegible]	[illegible]
8	0	3	-1873	-1476	-397
8	0	4	1558	922	636
8	0	5	641	684	-43
8	0	6	-1940	-2446	506
8	0	7	-1710	-2404	694
8	1	-13	-954	-801	-153
8	1	-11	880	810	70
8	1	-9	-1222	-1250	28
8	1	-7	903	765	138
8	1	-4	2114	2388	-274
8	1	-3	594	676	-82
8	1	-2	-767	-1500	733
8	1	2	-3641	-3211	-430
8	1	3	1192	1540	-348
8	1	7	1247	1277	-30
8	2	-14	1548	1784	-236
8	2	-11	1792	1783	9
8	2	-9	-1485	-1491	6
8	2	-8	1167	667	400
8	2	-5	-1923	-2080	157
8	2	-4	-2914	-3203	289
8	2	-2	1069	1437	-368
8	2	0	1720	2367	-647
8	2	1	4602	4457	145
8	2	2	747	670	77
8	2	3	-3775	-3112	-663
8	2	5	748	452	296
8	2	6	-1508	-1819	311
8	2	7	-1524	-1986	462
8	3	-15	1433	1556	-123
8	3	-13	-2083	-2157	74
8	3	-10	-1618	-1315	-303
8	3	-7	1926	2109	-183
8	3	-6	-730	-560	-170
8	3	-5	-1130	-1388	258
8	3	-4	2909	3181	-272
8	3	-3	1147	1444	-297
8	3	-2	-854	-1266	412
8	3	0	3654	3838	-184
8	3	1	1029	617	412
8	3	2	-6068	-5562	-506
8	3	3	647	529	118
8	3	5	-931	-1056	125
8	4	-12	1461	1724	-263
8	4	-10	898	922	-24
8	4	-8	-1615	-1916	301
8	4	-7	-2777	-3399	622
8	4	-6	-2172	-1865	-307
8	4	-5	-644	-1038	394
8	4	-4	-850	-743	-107
8	4	-2	1781	2441	-660
8	4	0	3712	4499	-787
8	4	4	695	1070	-375
8	4	5	898	279	619
8	4	6	-1634	-1918	284
8	4	7	-1455	-1593	138
8	4	8	-1019	-1146	127
8	5	-15	1275	1518	-243
8	5	-12	1006	727	279
8	5	-5	-1213	-1046	-167
8	5	-4	1295	1373	-78
8	5	-3	635	645	-10
8	5	-2	-1333	-928	-405
8	5	-1	-2173	-2200	27
8	5	0	1878	2071	-193
8	5	2	-2083	-1747	-336
8	5	3	1205	729	476
8	5	4	2492	1936	556
8	5	5	-2518	-2404	-114
8	5	6	1536	1504	32
8	6	-12	1763	2094	-331
8	6	-5	1017	792	225
8	6	-4	-784	-759	-25
8	6	-3	-657	-376	-281
8	6	1	-1512	-1176	-336
8	6	3	2394	1858	536
8	6	4	-784	-1284	500
8	6	5	-1203	-1191	-12
8	6	9	-1342	-1333	-9
8	6	11	1276	1516	-240
8	7	-9	-1080	-1573	493
8	7	-6	-784	-1385	601
8	7	-5	917	492	425
8	7	-4	1619	2082	-463
8	7	-3	2365	2810	-445
8	7	-1	-1731	-1290	-441
8	7	0	724	854	-130
8	7	1	1305	964	341
8	7	2	-1011	-544	-467
8	7	3	-1336	-1170	-166
8	7	5	-1940	-1762	-178
8	7	7	850	578	272
8	7	11	1180	1102	78
8	8	-9	921	1363	-442
8	8	-3	-2242	-2303	61
8	8	-1	2149	2770	-621
8	8	0	1644	1836	-192
8	8	3	966	1226	-260
8	8	5	-1232	-1297	65
8	8	9	-1534	-1508	-26
8	9	-5	1366	1436	-70
8	9	-2	908	805	103
8	9	-1	967	1468	-501
8	9	2	-1150	-1116	-34
8	9	3	-1372	-906	-466
8	10	-1	1030	1244	-214
8	10	1	-850	-666	-184
8	10	3	1506	1259	247
8	10	5	-1084	-1422	338
8	11	0	-1232	-959	-273
8	11	2	988	528	460
8	11	4	-1213	-1571	358
9	1	-11	1406	1442	-36
9	1	-10	2702	2533	169
9	1	-8	-2218	-1943	-275
9	1	-7	-812	-596	-216
9	1	-6	774	242	532
9	1	-4	-3327	-3894	567
9	1	-3	-1154	-1700	546
9	1	-2	1665	1900	-235
9	1	0	-1278	-650	-628
9	1	1	4163	3452	711
9	1	3	806	1112	-306
9	1	6	920	1061	-141
9	1	7	-1934	-2242	308
9	1	8	-1321	-1976	655
9	2	-11	1849	1875	-26
9	2	-7	-981	-1170	189
9	2	-5	-1776	-2294	518
9	2	-3	2839	3637	-798
9	2	-2	651	809	-158
9	2	-1	-3025	-2566	-459
9	2	2	-1627	-1284	-343
9	2	3	2505	1743	762
9	2	6	-1704	-2074	370
9	3	-10	1560	2048	-488
9	3	-9	1303	1748	-445

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
9	3	-6	-1468	-1492	24	10	2	-7	-827	-1002	175
9	3	-5	-1412	-2269	857	10	2	-4	-1424	-2228	804
9	3	-4	-902	-847	-55	10	2	-3	-1564	-1516	32
9	3	-3	-1007	-1642	635	10	2	0	-1999	-1502	-457
9	3	-2	644	134	510	10	2	1	-795	-2[illegible]0	-507
9	3	-1	-1263	-1588	325	10	2	2	1681	171[illegible]	-30
9	3	1	2337	2406	-69	10	2	3	1643	1529	114
9	3	2	3153	2821	332	10	2	6	1435	1788	-352
9	3	3	-2268	-1353	-915	10	3	-10	1116	1468	-352
9	3	6	-1079	-1287	208	10	3	-8	-910	-1102	192
9	4	-14	1191	1449	-258	10	3	-3	1164	1140	24
9	4	-6	870	1088	-218	10	3	-2	1636	1502	134
9	4	-4	-854	-1556	702	10	3	-1	-3090	-2354	-736
9	4	-3	1377	1841	-464	10	3	1	1176	1395	-219
9	4	-2	-724	-519	-205	10	3	4	-2916	-1845	-1071
9	4	-1	-1119	-1189	70	10	3	7	-1596	-1889	293
9	4	0	3845	3578	267	10	4	-2	-1153	-1624	471
9	4	1	2104	2395	-291	10	4	-1	-860	-1536	676
9	4	2	-2135	-1611	-574	10	4	0	2552	2317	235
9	4	3	-3675	-2884	-791	10	4	2	2010	1670	340
9	4	6	1726	1537	189	10	5	-5	-1023	-1345	322
9	4	10	-1359	-1463	104	10	5	-4	-1259	-2031	772
9	5	-8	-666	-563	-303	10	5	-2	1280	1519	-239
9	5	-4	944	919	25	10	5	1	1945	2086	-141
9	5	-3	-1612	-2192	580	10	5	7	-2394	-2138	-256
9	5	-2	-2156	-2307	151	10	6	-2	-3368	-3454	86
9	5	-1	808	337	471	10	6	0	1890	1605	285
9	5	1	-718	-438	-280	10	6	5	1073	1116	-43
9	5	2	3361	3071	290	10	7	-2	1071	1227	-156
9	5	6	-1620	-1328	-292	10	7	-1	920	606	314
9	5	9	-1164	-1166	2	10	8	-3	1528	1264	264
9	6	-9	-1054	-1162	108	10	8	2	-1277	-621	-656
9	6	-4	968	1006	-38	10	9	-4	1433	1408	25
9	6	-3	3100	3638	-538	10	11	-1	1483	1140	343
9	6	-1	-1423	-1693	270	11	1	-9	1632	1722	-90
9	6	0	-1210	-851	-359	11	1	-8	1379	1473	-94
9	6	2	1224	1320	-96	11	1	-7	-1271	-963	-308
9	6	3	-2225	-1732	-493	11	1	-5	1649	2326	-677
9	6	4	846	342	504	11	1	-2	-1039	-2057	1018
9	6	6	-1605	-1486	-119	11	1	3	2059	2145	-86
9	6	7	-1109	-680	-429	11	2	-7	-687	-1333	446
9	7	-8	936	1310	-374	11	2	-6	1075	1745	-670
9	7	-6	-1470	-2331	861	11	2	-4	-661	-1143	482
9	7	-5	-1052	-1335	283	11	2	-1	678	316	362
9	7	-2	-2259	-2231	-28	11	2	2	1503	770	733
9	7	-1	3119	3171	-52	11	3	-2	746	575	171
9	7	0	1791	1808	-17	11	3	1	-2072	-1149	-923
9	7	6	-1117	-812	-305	11	3	7	1244	1759	-515
9	7	9	-1103	-1050	-53	11	4	-4	-1153	-1724	571
9	8	-1	1524	1730	-206	11	4	0	-1018	-961	-57
9	8	1	965	843	122	11	4	2	2649	2008	641
9	8	3	-1819	-1270	-549	11	4	4	-1263	-1275	12
9	8	7	1327	1013	314	11	5	-2	-933	-1245	312
9	9	-2	-982	-1148	166	11	5	-1	-1996	-2663	667
9	9	2	-962	-703	-259	11	5	0	-1116	-1187	71
9	9	3	1648	1233	415	11	5	1	1489	1187	302
9	9	5	-1056	-1164	106	11	5	4	1637	1129	508
9	9	9	-1242	-845	-397	11	6	-4	-1151	-1523	332
9	11	4	1308	1045	263	11	7	3	-1196	-1039	-157
10	0	-13	1164	1201	-37	11	7	5	1354	1333	21
10	0	-10	1721	1551	170	12	0	-8	1122	2587	-1465
10	0	-9	1852	1679	173	12	2	1	-1157	-1316	159
10	0	-7	-1157	-712	-445	12	2	2	-1162	-1316	154
10	0	-5	1726	2157	-431	12	3	-3	-977	-1636	659
10	0	0	-2135	-2548	753	12	3	-2	645	628	17
10	0	1	1744	1249	495	12	3	-1	1122	728	394
10	1	-6	677	643	34	12	3	0	-683	-606	-77
10	2	-10	1577	2013	-436	12	3	1	-1287	-810	-477
10	2	-9	1681	2457	-776	12	3	6	1111	1148	-37

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
12	4	4	-1096	-996	-100	12	6	-1	-914	-632	-282
12	5	4	-1143	-450	-693	12	6	5	1456	1328	128

after each parameter) are given in Table 2. Thus **4·147(4)** means that the co-ordinate of the atom (**4·147** Å) has an estimated standard deviation of 0·004 Å. The calculated and observed structure factor values are given in Table **3**.

DISCUSSION

The Figure shows the molecule as it appears when projected down the [*c*] axis, and also the labelling of the atoms. The bond lengths and bond angles, together with their estimated standard deviations, are given in Table 4. The bond lengths and angles invoving

TABLE 4

Bond lengths (Å) and bond angles (°), (estimated standard deviations are given in parentheses)

Cl–C(19)	1·759(14)	P–C(1)	1·822(14)
O–C(20)	1·301(19)	P–C(7)	1·798(13)
C(19)–C(20)	1·361(20)	P–C(13)	1·800(13)
C(20–C(21)	1·489(20)	P–C(19)	1·736(14)
C(1)–C(2)	1·425(19)	C(7)–C(8)	1·351(19)
C(2)–C(3)	1·423(21)	C(8)–C(9)	1·386(21)
C(3)–C(4)	1·380(23)	C(9)–C(10)	1·427(21)
C(4)–C(5)	1·364(24)	C(10)–C(11)	1·368(22)
C(5)–C(6)	1·443(23)	C(11)–C(12)	1·393(21)
C(6)–C(1)	1·393(21)	C(12)–C(7)	1·437(18)
C(13)–C(14)	1·383(19)	C(21)–C(22)	1·344(20)
C(14)–C(15)	1·470(22)	C(22)–C(23)	1·424(23)
C(15)–C(16)	1·370(24)	C(23)–C(24)	1·377(24)
C(16)–C(17)	1·363(25)	C(24)–C(25)	1·363(23)
C(17)–C(18)	1·425(24)	C(25)–C(26)	1·422(24)
C(18)–C(13)	1·395(20)	C(26)–C(21)	1·392(21)
C(1)–P–C(7)	105·4(5)	P–C(1)–C(2)	117·4(10)
C(1)–P–C(13)	108·9(6)	P–C(1)–C(6)	119·7(11)
C(7)–P–C(13)	106·4(6)	P–C(7)–C(8)	122·7(10)
C(1)–P–C(19)	113·2(6)	P–C(7)–C(12)	117·9(9)
C(7)–P–C(19)	110·2(6)	P–C(13)–C(14)	121·7(10)
C(13)–P–C(19)	112·3(6)	P–C(13)–C(18)	117·5(10)
		C(20)–C(21)–C(22)	119·4(13)
		C(20)–C(21)–C(26)	118·8(13)
Cl–C(19)–P	118·3(8)	O–C(20)–C(19)	116·6(13)
Cl–C(19)–C(20)	121·2(11)	O–C(20)–C(21)	117·2(13)
P–C(19)–C(20)	120·2(11)	C(19)–C(20)–C(21)	126·0(13)
C(6)–C(1)–C(2)	122·9(13)	C(12)–C(7)–C(8)	119·4(12)
C(1)–C(2)–C(3)	117·0(13)	C(7)–C(8)–C(9)	122·7(13)
C(2)–C(3)–C(4)	119·4(14)	C(8)–C(9)–C(10)	118·5(13)
C(3)–C(4)–C(5)	124·0(16)	C(9)–C(10)–C(11)	119·3(14)
C(4)–C(5)–C(6)	118·6(15)	C(10)–C(11)–C(12)	121·9(14)
C(5)–C(6)–C(1)	117·9(14)	C(11)–C(12)–C(7)	118·2(13)
C(18)–C(13)–C(14)	120·6(13)	C(26)–C(21)–C(22)	121·8(14)
C(13)–C(14)–C(15)	117·8(13)	C(21)–C(22)–C(23)	120·0(14)
C(14)–C(15)–C(16)	120·7(15)	C(22)–C(23)–C(24)	119·1(15)
C(15)–C(16)–C(17)	120·5(16)	C(23)–C(24)–C(25)	120·6(15)
C(16)–C(17)–C(18)	120·3(16)	C(24)–C(25)–C(26)	120·6(15)
C(17)–C(18)–C(13)	120·1(14)	C(25)–C(26)–C(21)	117·8(15)

the phosphorus atom and the phenyl rings of the triphenylphosphorus group do not differ significantly from their mean values of 1·807 Å and 106·9°, respectively. These values are in good agreement with the corresponding values reported in similar compounds.[2,6]

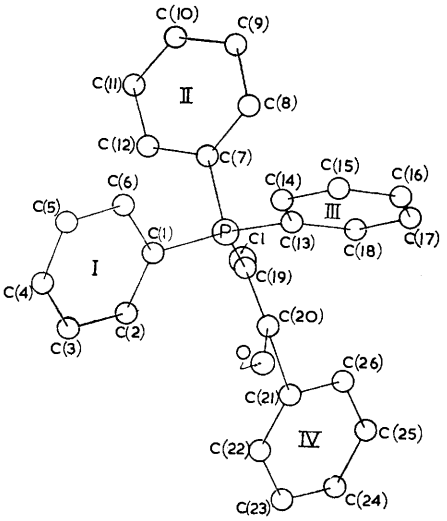
[6] P. J. Wheatley, in preparation.

The lengths are rather shorter than the values found in phosphorus triphenyl (1·828 Å) [7] but not significantly so. The mean values in the phenyl rings for the C–C bond and C–C–C angle are 1·397 Å and 120·0°, respectively. The mean planes through the phenyl rings are given in Table 5, and none of the carbon atoms departs significantly from its mean plane.

TABLE 5

Weighted least-squares planes in terms of the orthogonal axes where $X' = X + Z\cos\beta$, $Y' = Y$, $Z' = Z\sin\beta$ and the equations of the planes given by $lX' + mY' + nZ' - p = 0$.

	l	m	n	p
Ring I	0·4757	0·2986	0·8274	6·5387
II	0·5797	0·2544	−0·7741	0·1684
III	−0·0174	0·9472	0·3202	6·6286
IV	0·5257	0·3309	0·7838	7·3726
P, C(19), C(20), O	0·9243	−0·3243	0·2012	2·0197
P,Cl,C(19),C(20)	0·9220	−0·3500	0·1655	1·7283
O,C(19),C(20),C(21)	0·8952	−0·3750	0·2408	1·6457



The molecule as it appears when projected down [*c*], and also the labelling of the atoms

The bond lengths show that resonance is present in the grouping P, C(19), C(20), O as is indicated in the iodo-compound.[2] The C–C length (1·361 Å) more closely agrees with a C=C length (1·337 Å) [8] than an (sp^2) C–C (sp^2) (1·460 Å) [8] and the C–O distance (1·301 Å) is considerably longer than that expected for C=O (1·23 Å).[8] The P–C distance (1·736 Å), although rather longer than that found in *p*-tolyl (triphenylphosphoranylidene)methyl sulphone (1·709 Å) [6] and the iodo-compound (1·71 Å),[2] is found to be between P–C (1·863 Å) [9] and P=C (1·665 Å),[10] the latter being the sum of the covalent radii. The mean plane through the atoms P, C(19), C(20), O shows that the atoms C(19) and C(20) depart significantly from this plane, though this departure is small C(19), −0·046 Å (3·4 σ), C(20, 0·052 Å (3·6 σ). The chlorine and C(21) atoms are both significantly out of the mean plane (Cl, −0·078 Å, C(21), −0·205 Å). The C–Cl bond is lengthened compared with that found for =C–Cl (1·72 Å).[9] However, the accuracy of the determination does not permit this difference to be considered significant. This elongation is also apparent in the iodo-compound.[2] There appears to be no significant effect on the C(20)—C(21) length and the value found is in agreement with that expected.[9] Thus the resonance indicated is in accord with the postulations to account for the decrease in the ν_{CO} stretching frequency.[1]

[7] J. J. Daly, *J.*, 1964, 3799.
[8] L. E. Sutton *et al.*, " International Distances and Configuration in Molecules and Ions," *Chem. Soc. Special Publ.* No. 11, London, 1958.
[9] T. Kojima, E. L. Breig, and C. C. Lim, *J. Chem. Phys.*, 1961, **35**, 2139.
[10] L. Pauling, " Nature of the Chemical Bond," Cornell Univ. Press Ithaca, New York, 1942, p. 192.

As expected the benzoyl ring is twisted with respect to the plane containing the carbonyl group, the latter plane being rotated from the plane of the phosphorus and chlorine atoms. The planes of both the benzoyl ring and that containing the carbonyl group are rotated in the same direction from the plane containing the phosphorus and chlorine atoms. The equations of the respective mean planes are given in Table 5, and Table 6 gives the various angles of rotation for these mean planes together with those for the iodo-compound [2] for comparison. The carbonyl group is more closely planar to the phosphorus and halogen atoms in the chloro- than in the iodo-compound and this may account for the very marked

TABLE 6

	Chloro	Iodo
C(19),C(20),O,C(21)/Ring IV	57·7°	52°
P,X,C(19),C(20)/C(19),C(20),O,C(21)	4·8	12
P,X,C(19),C(20)/Ring IV	60·1	63

elongation of the C–I bond in the latter compound. The closest approach of a carbon atom of the benzoyl ring to the halogen atom is C(26) at a distance of 3·28 Å for the chloro- and 3·44 Å for the iodo-compound.[2] This is in accord with the increase in size of the atom when the chlorine is replaced by iodine.

Of the 51 van der Waals' contacts less than 4·0 Å the shortest contact is that of 3·27 Å between an oxygen atom of one molecule and carbon atom C(15) of an adjacent molecule.

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MONSANTO RESEARCH S.A., BINZSTRASSE 39, 8045 ZÜRICH, SWITZERLAND.

[Present address: DEPARTMENT OF CHEMISTRY, THE UNIVERSITY, MANCHESTER 13.]

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