1090. *An X-Ray Determination of the Molecular Structure of a Wittig Reagent:* p-*Tolyl Triphenylphosphoranylidenemethyl Sulphone*

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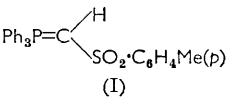
The structure of *p*-tolyl triphenylphosphoranylidenemethyl sulphone has been determined and refined with three-dimensional intensities collected on a Hilger–Watts linear diffractometer. There are eight molecules of PTT in a monoclinic cell, space group $C2/c$, with $a = 25{\cdot}633$, $b = 8{\cdot}981$, $c = 20{\cdot}733$ Å, $\beta = 111°\ 54'$. The mean P–C_6H_5 length is 1·808 Å. The length of the bond written as P=C is 1·709 Å, with a standard deviation of 0·019 Å, which is rather longer than expected from interpolation between the known single- and triple-bond lengths, or from the sum of the covalent radii.

A structure analysis of *p*-tolyl triphenylphosphoranylidenemethyl sulphone (PTT) (I) was undertaken to provide details of the molecular geometry of a Wittig reagent,[1] and as part of a wider study of several phosphorus ylids.[2] The structural analyses of two further phosphorus ylids will be described by Stephens,[3] and a full interpretation of the structural results in terms of the chemical and physico-chemical properties will appear in a Paper by Speziale and Ratts.[4] This Paper is concerned solely with the results of the *X*-ray structure determination of PTT.



(I)

Experimental.—$C_{26}H_{23}O_2PS$, $M = 430{\cdot}5$. Monoclinic, $a = 25{\cdot}633 \pm 0{\cdot}087$, $b = 8{\cdot}981 \pm 0{\cdot}008$, $c = 20{\cdot}733 \pm 0{\cdot}071$ Å, $\beta = 111°\ 54' \pm 10'$, $U = 4428{\cdot}5$ Å^3, $D_m = 1{\cdot}30$, $Z = 8$. $D_c = 1{\cdot}291$, $F(000) = 1808$. Space group $C2/c(C_{2h}^6$, No. 15). Cu-K_α radiation ($\lambda = 1{\cdot}542$ Å) for cell dimensions, Mo-K_α radiation ($\lambda = 0{\cdot}71069$ Å) for intensity measurements.

The crystals, m. p. 185—186°, were well-formed needles with [*b*] as the direction of elongation. Cell dimensions were measured from single crystal oscillation photographs. Intensities were collected in a Hilger–Watts linear diffractometer [5] equipped with SrO/ZrO_2 balanced filters. All reflexions in the *h*0*l* to *h*,12,*l* layers were measured twice with a half-minute motor. In the first seven layers the oscillation angle was 2°: in the rest 3°. In this way a total of 6249 independent reflexions, up to a maximum $\theta = 32{\cdot}5°$, was recorded, of which 1750 were deemed significant in that they had a corrected count more than twice the standard deviation of the total counts. The analysis is based on these 1750 reflexions.

The structure was solved in projection down [*b*] from a sharpened Patterson synthesis which served to locate the phosphorus and sulphur atoms. The positions of the 28 lighter atoms, excluding hydrogen atoms, were fixed by a succession of Fourier approximations. The *y* co-ordinates of the two heavier atoms were then found from a series of three-dimensional Patterson sections. With these known positions and a model of the molecule, the remaining *y* co-ordinates could be chosen, and the atomic positions and isotropic thermal factors refined by a least-squares analysis using the block-diagonal approximation. All calculations were carried out on an Elliott 803 computer with the programmes of Daly, Stephens, and Wheatley.[6] A Cruickshank weighing scheme was used.[7] The scattering factors were obtained from International Tables. In the refinement cycles, reflexions with a calculated value less than 0·3 times the observed were omitted from the least-squares totals, though not from the *R* factors.

The final *R* factor was 16·4%, which is considerably worse than would have been expected with photographic intensities, and is an indication of our inexperience with the diffractometer. This was our first structure analysis carried out with diffractometer intensities. Our techniques

[1] G. Wittig and U. Schöllkopf, *Chem. Ber.*, 1954, **97**, 1318.
[2] A. J. Speziale and K. W. Ratts, *J. Org. Chem.*, 1963, **28**, 465; *J. Amer. Chem. Soc.*, 1963, **85**, 2790.
[3] F. S. Stephens, *J.*, in the press.
[4] A. J. Speziale and K. W. Ratts, *J. Amer. Chem. Soc.*, in the press.
[5] U. Arndt and D. C. Phillips, *Acta Cryst.*, 1961, **14**, 807.
[6] J. J. Daly, F. S. Stephens, and P. J. Wheatley, unpublished results.
[7] D. W. J. Cruickshank *et al.*, "Computing Methods and the Phase Problem in *X*-Ray Analysis," Pergamon Press, London, 1961.

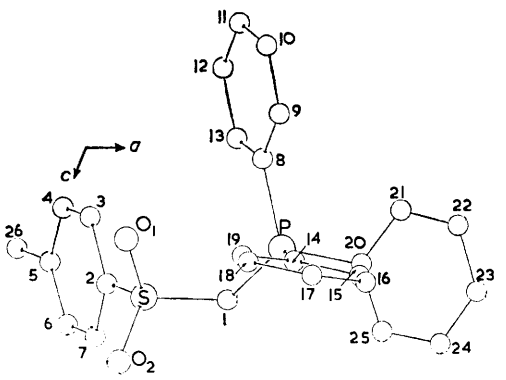
TABLE 1

Atomic co-ordinates (Å) and individual isotropic temperature factors (Å²). Standard deviations are given in parentheses as units in the last place

Atom	*X*	*Y*	*Z*	U_{iso}
S	2·3432(46)	0·4922(43)	3·1895(47)	0·0271(8)
P	4·7545(45)	1·0774(42)	2·1856(45)	0·0215(8)
O(1)	1·5387(131)	1·3127(122)	1·9259(132)	0·0381(30)
O(2)	2·3356(142)	0·9170(136)	4·5665(146)	0·0492(35)
C(1)	4·0430(184)	0·2684(168)	3·2727(187)	0·0311(39)
C(2)	1·5113(168)	−1·0977(169)	2·8945(171)	0·0270(35)
C(3)	0·6598(190)	−1·4992(182)	1·4729(193)	0·0354(42)
C(4)	0·0100(189)	−2·7040(174)	1·2598(190)	0·0331(42)
C(5)	0·1859(190)	−3·5863(176)	2·4138(196)	0·0356(42)
C(6)	1·0195(216)	−3·2001(210)	3·7570(218)	0·0485(52)
C(7)	1·6924(207)	−1·9802(200)	4·0200(209)	0·0420(46)
C(8)	3·6649(178)	0·8587(163)	0·2676(180)	0·0290(39)
C(9)	3·6726(198)	1·8869(189)	−0·7043(200)	0·0400(46)
C(10)	2·8886(217)	1·6566(206)	−2·1627(220)	0·0464(49)
C(11)	2·1733(217)	0·4862(215)	−2·6439(217)	0·0455(49)
C(12)	2·1886(226)	−0·4888(224)	−1·6955(231)	0·0516(52)
C(13)	2·9955(192)	−0·3125(184)	−0·1739(197)	0·0355(43)
C(14)	5·0922(159)	2·8214(152)	2·4462(165)	0·0207(33)
C(15)	6·5152(192)	3·3413(185)	2·7772(195)	0·0366(42)
C(16)	6·7309(278)	4·6797(245)	2·9295(275)	0·0671(67)
C(17)	5·5756(224)	5·5897(228)	2·7587(225)	0·0522(54)
C(18)	4·2312(228)	5·1389(224)	2·4305(230)	0·0524(54)
C(19)	3·9847(196)	3·7269(179)	2·3289(198)	0·0355(44)
C(20)	6·4773(170)	0·2728(149)	2·5272(169)	0·0245(35)
C(21)	6·8337(193)	−0·2253(177)	1·3938(193)	0·0345(43)
C(22)	8·1286(254)	−0·9196(240)	1·7084(253)	0·0602(62)
C(23)	9·0012(214)	−1·2064(207)	3·1198(217)	0·0478(51)
C(24)	8·6522(217)	−0·6775(206)	4·2535(220)	0·0481(52)
C(25)	7·3877(203)	0·0209(192)	3·9590(203)	0·0388(45)
C(26)	−0·5799(278)	−4·9444(277)	2·1324(279)	0·0712(70)

have improved sufficiently to give intensities as reliable as those obtained photographically, but with a great saving of time.

Results.—The final atomic co-ordinates and individual isotropic temperature factors are given in Table 1, with the standard deviations as units in the last place. The observed and



Projection of the molecule viewed down the [*b*] axis

calculated structure factors are shown in Table 2. Table 3 gives the bond lengths and angles with their standard deviations. Figure 1 shows the molecule as it appears in projection down [*b*], and also the labelling of the atoms.

The bond lengths agree well with expected values.[8] The P=C length is 1·709 Å, in agreement with the values obtained by Stephens,[3] and by Mak and Trotter.[9] It is, however, longer than

[8] L. E. Sutton *et al.*, " Tables of Interatomic Distances," *Chem. Soc. Special Publ.*, No. 11, 1958.
[9] T. C. W. Mak and J. Trotter, *Acta Cryst.*, 1965, **18**, 81.

TABLE 2

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
0	0	24	-5404	-3443	-1961	8	0	-16	4428	4364	64
0	0	22	-4042	-4468	426	8	0	-18	9844	9544	300
0	0	10	7463	8581	-1118	10	0	16	-4492	-4782	290
0	0	8	19527	15190	4337	10	0	12	4954	4594	360
0	0	4	-53847	-60214	367	10	0	6	-11076	-10688	-388
0	0	2	7001	7065	-64	10	0	4	-4225	-4125	-100
2	0	12	7527	6333	1194	10	0	2	12267	13652	-1385
2	0	10	-8235	-5813	-2422	10	0	-2	-20524	-18385	-2139
2	0	8	-9265	-10760	1495	10	0	-4	4225	480	3745
2	0	6	7152	10104	-2952	10	0	-6	-3238	-618	-2620
2	0	4	26187	21550	4637	10	0	-8	3774	1992	1782
2	0	2	-24845	-21852	-2993	10	0	-10	-4267	-2692	-1575
2	0	0	-2595	-6343	3748	10	0	-14	-4074	-4466	392
2	0	-2	20964	22225	-1261	10	0	-18	10390	12669	-2279
2	0	-4	-1704	-1927	223	10	0	-22	-8621	-9059	438
2	0	-6	-21307	-17013	-4294	10	0	-26	5050	4905	145
2	0	-8	-13500	-11934	-1566	12	0	10	-4525	-5602	1077
2	0	-12	7570	6956	614	12	0	8	2991	2052	939
2	0	-14	6422	7450	-1028	12	0	4	-6481	-9849	1368
2	0	-16	-5950	-7025	1075	12	0	2	-10080	-9978	-102
2	0	-18	-4139	-4771	632	12	0	0	20064	17692	2392
2	0	-20	4096	5190	-1094	12	0	-4	-15023	-15764	741
2	0	-22	3977	5041	-1064	12	0	-8	9456	7886	1570
4	0	12	6294	5064	1230	12	0	-10	-6980	-5278	-1702
4	0	10	6991	8280	-1289	12	0	-12	-8621	-8748	127
4	0	8	-11162	-11622	460	12	0	-14	5125	4532	593
4	0	6	-33800	-30958	-2842	12	0	-16	-8922	-8535	-387
4	0	4	9253	6100	3153	12	0	-20	5478	5384	95
4	0	2	-3913	-2867	-1046	12	0	-22	-3969	-3376	-613
4	0	0	-4203	-6392	2189	14	0	12	4203	3213	990
4	0	-2	3045	5375	-2330	14	0	10	-3088	-1698	-1188
4	0	-4	-35237	-35463	246	14	0	8	-9339	-9233	-106
4	0	-6	11891	11146	745	14	0	4	10552	10554	-402
4	0	-8	2455	1721	734	14	0	-2	-4911	-3534	-1377
4	0	-10	-15441	-14400	-1041	14	0	-6	7420	5445	-2025
4	0	-12	-17157	-17801	644	14	0	-8	7163	4625	2538
4	0	-14	4256	2854	1402	14	0	-10	-6851	-5505	-1346
4	0	-16	18551	20365	-1814	14	0	-12	-8760	-8996	236
4	0	-18	-4825	-4421	-404	14	0	-14	8922	9007	-85
4	0	-20	-7731	-9700	1969	14	0	-18	-7442	-6224	-1218
6	0	14	-6241	-7439	1198	14	0	-20	3646	3050	596
6	0	12	-6723	-7183	460	16	0	14	-4235	-3949	-286
6	0	10	3946	5728	-1782	16	0	10	3756	5801	-2045
6	0	8	3870	3659	211	16	0	8	3710	3621	89
6	0	6	-2659	-1879	-780	16	0	6	-7956	-7844	-112
6	0	2	-2111	-2869	758	16	0	4	-3934	-3404	-530
6	0	0	-1918	-3685	1767	16	0	2	5200	5349	-149
6	0	-2	30894	31496	-602	16	0	-2	9822	10008	-186
6	0	-4	13671	10585	3086	16	0	-6	-12599	-10990	-1609
6	0	-6	-21543	-19909	-1634	16	0	-8	5328	4844	484
6	0	-8	-5297	-6346	1049	16	0	-10	12726	12687	41
6	0	-10	15656	15912	-256	16	0	-12	-5769	-5816	47
6	0	-12	7013	5603	1410	16	0	-14	-8428	-7524	-904
6	0	-14	-15280	-13737	-1543	16	0	-16	6615	7683	-1068
6	0	-16	4426	5921	-1493	16	0	-20	6272	4768	1504
6	0	-22	-3591	-2928	-663	16	0	-22	5018	3476	1542
6	0	-26	-4074	-2064	-2010	18	0	12	-4053	-4693	640
8	0	16	-5500	-5540	40	18	0	8	-4559	-5281	682
8	0	14	6820	8013	-1193	18	0	-2	-3505	-3332	-173
8	0	12	-5457	-7101	1644	18	0	-4	7152	6875	277
8	0	10	-4675	-4966	291	18	0	-8	-10411	-11148	737
8	0	8	8503	6514	1989	18	0	-12	8900	8440	460
8	0	6	6905	8274	-1369	18	0	-14	-5190	-3504	-1686
8	0	2	3098	4257	-1159	20	0	4	-6143	-6222	79
8	0	0	-2638	-5068	2430	20	0	0	5993	5912	81
8	0	-2	18337	17506	831	20	0	-2	-3538	-2163	-1375
8	0	-4	27655	24833	2822	20	0	-8	5812	4952	860
8	0	-10	-19698	-16901	-2797	20	0	-10	-5972	-4610	-1362
8	0	-12	7828	7115	713	20	0	-12	-6723	-7114	391

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
26	0	-14	-4642	-4399	-243	3	1	-4	-19055	-16466	-589
26	0	-16	6615	6206	409	3	1	-5	6527	4554	2373
20	0	-20	-5050	-5167	117	3	1	-6	-13207	-11643	-2264
20	0	-22	-6305	-7397	1092	3	1	-8	6056	4503	1555
22	0	0	3098	3698	-600	3	1	-9	4749	2687	2062
22	0	-6	-3570	-2644	-926	3	1	-12	-16352	-14685	-1667
22	0	-8	-4985	-5360	375	3	1	-14	8857	10870	-2013
22	0	-12	9608	8657	951	3	1	-15	4170	5125	-955
22	0	-16	-5619	-6661	1042	3	1	-16	6980	6567	413
24	0	2	-6477	-7234	757	3	1	-18	-9308	-10739	1431
24	0	-12	-6122	-5481	-641	3	1	-19	-4578	-4463	-115
24	0	-14	6401	6452	-51	3	1	-21	-3956	-3977	21
24	0	-16	4761	5576	-815	5	1	14	-4117	-4018	-99
24	0	-18	-4053	-3500	-553	5	1	13	-6701	-7161	460
24	0	-24	4053	4291	-238	5	1	11	-4664	-5610	946
26	0	-6	-3741	-2481	-1260	5	1	8	3312	3070	242
26	0	-8	5371	4302	1069	5	1	7	7016	6607	1209
26	0	-6	-4461	-3370	-1091	5	1	6	-3088	-3683	595
26	0	-10	5157	5401	-244	5	1	5	4042	5190	-1148
26	0	-14	-4665	-5665	980	5	1	4	-2841	-444	-2397
26	0	-26	-4020	-3486	-534	5	1	1	7130	8708	-1578
30	0	-2	-4256	-6570	2314	5	1	0	-42990	-39521	-3469
30	0	-8	-6036	-5353	-683	5	1	-1	13757	8317	5440
32	0	-4	-4406	-5072	666	5	1	-2	4482	4332	150
32	0	-10	4503	3878	625	5	1	-3	3913	6763	-2850
1	1	16	-4696	-5057	361	5	1	-4	23463	21523	1940
1	1	12	4042	5411	-1369	5	1	-5	-2519	-460	-2059
1	1	9	-10723	-8776	-1947	5	1	-6	-5511	-5842	331
1	1	8	6820	6990	-170	5	1	-7	-13553	-9534	-4159
1	1	7	6251	3854	2397	5	1	-8	-9897	-9228	-669
1	1	6	-4256	-2414	-1842	5	1	-9	-2573	-3390	817
1	1	5	9983	10896	-913	5	1	-11	10776	11438	-662
1	1	4	4900	3520	1380	5	1	-13	3045	403	2642
1	1	3	4814	3136	1678	5	1	-14	-7452	-8504	1052
1	1	2	-11517	-10440	-1077	5	1	-15	-5361	-5282	-79
1	1	1	-14240	-10275	-3965	7	1	17	-4032	-4177	145
1	1	0	20311	15921	990	7	1	13	3824	4351	-767
1	1	-1	-11259	-13384	2125	7	1	12	-3253	-3614	355
1	1	-2	17608	16399	1209	7	1	9	-6712	-6174	-538
1	1	-3	-5371	-2134	-3237	7	1	7	-2991	-4032	1041
1	1	-4	-6272	-7130	856	7	1	6	7034	7217	-183
1	1	-5	11088	6916	4172	7	1	5	11431	12304	-873
1	1	-6	20342	15575	4767	7	1	4	7645	7204	441
1	1	-7	-14541	-11020	-3521	7	1	3	5511	2812	2699
1	1	-9	-10433	-9033	-1400	7	1	2	-2457	-1329	-1168
1	1	-10	-10665	-10878	209	7	1	1	2390	5638	-3248
1	1	-12	6112	6039	73	7	1	0	-13668	-10661	-3007
1	1	-13	8567	8660	-93	7	1	-1	6937	3159	3778
1	1	-14	10283	10594	-311	7	1	-2	17136	14547	2589
1	1	-15	9811	10596	-785	7	1	-3	-26947	-21568	-5379
1	1	-16	-5757	-6433	676	7	1	-4	34432	29520	4912
1	1	-17	-6251	-5623	-428	7	1	-5	-6548	-6034	-514
1	1	-18	-3977	-4555	578	7	1	-6	2659	2205	454
1	1	-20	4375	5857	-1482	7	1	-7	2090	5015	-2925
3	1	24	3753	1924	1829	7	1	-8	-16321	-15075	-1246
3	1	13	-3538	-3552	54	7	1	-11	-5607	-3278	-2329
3	1	12	6744	6204	540	7	1	-12	9897	8937	960
3	1	11	3066	2057	1009	7	1	-13	2680	1683	997
3	1	10	-4192	-4064	-128	7	1	-15	3119	4925	-1806
3	1	9	-6465	-3904	-2561	7	1	-16	7120	6896	224
3	1	8	-15130	-14889	-241	7	1	-19	-3495	-4155	660
3	1	5	-2497	-1378	-1119	7	1	-20	-4320	-4421	101
3	1	4	13533	13045	488	9	1	18	-3670	-4239	569
3	1	3	9725	8336	3389	9	1	14	3784	4893	-1109
3	1	2	-15527	-14395	-1132	9	1	7	-6927	-7274	347
3	1	1	13757	15974	-2217	9	1	6	3227	2583	644
3	1	0	-4385	-3707	-678	9	1	5	-5371	-3619	-1752
3	1	-1	-17618	-16527	1309	9	1	4	-2969	-3500	531
3	1	-3	-20127	-15912	-4215	9	1	3	3367	2088	1279

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
9	1	2	4375	4189	186	15	1	-11	2776	4847	-2071
9	1	1	8009	8126	-117	15	1	-12	-6245	-7962	-283
9	1	-1	2948	1322	1626	15	1	-16	8725	7925	800
9	1	-2	-9243	-10450	1207	15	1	-17	3495	1823	1672
9	1	-3	-28534	-23893	-4641	15	1	-19	4285	3775	510
9	1	-4	17886	15283	2603	15	1	-22	4032	3779	253
9	1	-5	-6869	-9330	441	17	1	12	-5522	-5309	-213
9	1	-6	7709	7101	608	17	1	10	3324	3311	13
9	1	-7	7580	8402	-822	17	1	8	4589	5927	-1338
9	1	-8	3892	1507	2385	17	1	4	-5886	-5264	-622
9	1	-9	8095	6680	1415	17	1	0	-2755	-2560	-195
9	1	-11	-3527	-758	-2769	17	1	-1	-5586	-6622	1036
9	1	-17	5779	4738	1041	17	1	-3	2991	3386	-395
9	1	-18	6755	7170	-415	17	1	-4	5371	4675	696
9	1	-21	-3860	-2940	-920	17	1	-5	6863	7041	-178
9	1	-22	-3849	-4482	633	17	1	-6	-3238	-5628	2390
11	1	8	3324	2278	1046	17	1	-7	-4363	-3815	-548
11	1	4	-9811	-9765	-46	17	1	-9	-6680	-7606	926
11	1	3	3536	2498	1038	17	1	-10	10068	10215	-147
11	1	2	-5812	-5104	-708	17	1	-12	3784	4491	-707
11	1	1	-6894	-5353	-1541	17	1	-13	6093	7508	1415
11	1	0	14444	12683	1761	17	1	-14	-7720	-7275	-445
11	1	-1	13114	10818	2296	17	1	-20	3670	3276	394
11	1	-2	-9940	-8432	-1508	17	1	-22	4835	4425	410
11	1	-3	7206	6849	357	19	1	2	3195	3721	-526
11	1	-4	-5940	-6001	61	19	1	1	5769	6166	-397
11	1	-5	-3281	-5498	2217	19	1	0	-6186	-6108	-78
11	1	-7	-2166	-1472	-694	19	1	-1	2916	2457	459
11	1	-8	-5157	-5214	57	19	1	-3	-6873	-6604	-269
11	1	-10	-3505	-3311	-194	19	1	-4	6927	7627	-700
11	1	-11	3024	3159	-135	19	1	-6	3463	3700	-237
11	1	-12	4042	3172	870	19	1	-7	6916	6964	-48
11	1	-13	5190	4721	469	19	1	-8	-7194	-6105	911
11	1	-16	-6465	-7017	552	19	1	-9	3710	3271	439
11	1	-18	3849	3056	791	19	1	-10	-8670	-7575	905
11	1	-19	-3741	-3763	22	19	1	-11	-7516	-6574	-942
13	1	19	-4589	-460	-4129	19	1	-12	7678	6954	724
13	1	15	-4363	-2815	-1548	19	1	-20	-4997	-5764	767
13	1	12	3753	4151	-398	19	1	-21	-3624	-3688	64
13	1	11	4203	5579	-1376	19	1	-24	4053	3581	472
13	1	10	-4182	-4758	576	21	1	5	3591	2961	630
13	1	7	-5886	-7041	1155	21	1	3	-3827	-3120	-707
13	1	6	5533	6425	-892	21	1	1	-3699	-3784	85
13	1	3	12375	12249	126	21	1	0	5833	6575	-742
13	1	2	-8578	-8849	271	21	1	-1	4127	3147	980
13	1	-6	8310	7231	1079	21	1	-2	-4353	-4240	-113
13	1	-7	-2938	-1765	-1173	21	1	-4	-5328	-6493	1165
13	1	-10	-7430	-7842	412	21	1	-6	4771	3855	916
13	1	-14	8996	8437	559	21	1	-8	5447	5131	316
13	1	-15	3634	4093	-459	21	1	-13	3024	1753	1271
13	1	-16	-6787	-6173	-614	21	1	-15	3261	1116	2145
13	1	-18	-9179	-9263	84	21	1	-21	3536	3666	-128
13	1	-21	-3174	-2677	-497	21	1	-22	-3534	-2483	-1051
15	1	10	5511	6764	-1253	21	1	-23	-4461	-1278	-3183
15	1	8	-5436	-7299	1863	23	1	2	-5629	-5820	191
15	1	6	-8460	-9332	872	23	1	-2	4814	4736	78
15	1	5	-8021	-7058	-963	23	1	-6	-3441	-3628	187
15	1	4	9361	9974	-613	23	1	-7	3677	3365	312
15	1	3	-3956	-5290	1334	23	1	-14	5822	5379	443
15	1	2	5478	5442	37	23	1	-15	5114	5819	-705
15	1	1	2841	4779	-1938	23	1	-22	4020	1100	2920
15	1	-1	2636	2017	621	25	1	4	4847	5155	-348
15	1	-4	-10840	-8651	-2189	25	1	2	-3474	-437	-3037
15	1	-5	-10552	-11599	1047	25	1	-6	3634	3228	406
15	1	-6	3367	3085	282	25	1	-9	5928	5628	301
15	1	-7	-8653	-6912	-1741	25	1	-13	-5297	-6459	1162
15	1	-8	3918	3959	-41	25	1	-17	3934	3552	382
15	1	-9	4203	3804	399	25	1	-18	-4654	-4107	-547
15	1	-10	3764	4230	-466	27	1	-3	3624	2596	1028

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
27		-13	4235	4865	-630	4	2	-10	4556	2462	2094
27	1	-12	-6467	-5465	-1002	4	2	-11	6122	5843	279
27	1	-14	-4203	-3588	-615	4	2	-12	-11388	-9740	-1648
29	1	0	-3934	-3673	-261	4	2	-15	-4149	-4571	422
29	1	-1	-5147	-3189	-1958	4	2	-16	-3667	-3553	-114
31	1	-2	-5726	-5977	251	6	2	19	-3527	-2573	-954
31	1	-6	4825	4117	708	6	2	16	-3024	-35	-2965
35	1	-10	-4085	-1120	-2965	6	2	15	7666	8791	-1125
0	2	17	6412	6370	42	6	2	14	-4462	-4661	379
0	2	14	5972	5159	813	6	2	12	5254	118	5136
0	2	13	-7173	-7532	359	6	2	11	-10712	-11263	551
0	2	12	2680	2638	42	6	2	10	7420	6842	578
0	2	8	6670	8396	-1726	6	2	9	-6627	-6215	-412
0	2	7	4182	3626	556	6	2	7	8900	7944	956
0	2	6	9854	8808	1046	6	2	5	10080	10305	-225
0	2	5	2776	2016	760	6	2	3	-3710	-3883	173
0	2	4	-17918	-15387	-2531	6	2	2	7302	11522	-4220
0	2	2	-3527	-4707	1180	6	2	1	2390	2863	-473
0	2	1	-9618	-9861	243	6	2	0	-14208	-11882	-2326
2	2	20	-3441	-1327	-2114	6	2	-1	-10304	-9102	-1202
2	2	19	-3692	-4675	983	6	2	-2	-25253	-22741	-2512
2	2	18	3692	4928	-1036	6	2	-3	6477	7705	-1228
2	2	15	3474	3685	-211	6	2	-5	6015	6163	-148
2	2	14	-5286	-5883	597	6	2	-10	14519	12758	1761
2	2	12	4599	4531	68	6	2	-12	-3956	-2310	-1646
2	2	11	2412	2529	-117	6	2	-13	5093	5503	-410
2	2	10	-3999	-2925	-1074	6	2	-14	-4182	-5361	1179
2	2	9	-2262	-2899	637	6	2	-15	-4578	-5169	591
2	2	8	-3624	-1929	-1695	8	2	13	6487	8230	-1743
2	2	7	-5576	-5826	250	8	2	12	-4749	-3672	-1077
2	2	6	6364	6733	1631	8	2	9	-4235	-5459	1224
2	2	4	1854	3826	-1972	8	2	8	3398	3865	-467
2	2	3	20965	17197	3768	8	2	7	-4585	-5795	810
2	2	1	-26224	-26931	-1293	8	2	6	3119	2071	1048
2	2	0	-18690	-14428	-4262	8	2	5	-3195	-2611	-584
2	2	-1	-17972	-16643	-1329	8	2	4	-5447	-4896	-551
2	2	-2	8922	4793	4129	8	2	3	3870	2779	1091
2	2	-3	16106	14221	1885	8	2	1	3774	3344	430
2	2	-4	-4761	-1577	-3184	8	2	0	2359	4046	-1687
2	2	-5	7141	5561	1580	8	2	-1	-7742	-6454	-1288
2	2	-6	-8595	-4447	1652	8	2	-2	10509	4111	6398
2	2	-7	2873	3185	-312	8	2	-3	-11667	-12599	932
2	2	-8	16116	17615	-1499	8	2	-4	2004	2942	-938
2	2	-9	-9511	-8577	-934	8	2	-5	-3195	-2342	-853
2	2	-11	-4406	-4604	198	8	2	-6	4718	3174	1544
2	2	-12	-4225	-2869	-1356	8	2	-7	10015	8939	1076
2	2	-14	5062	3928	1134	8	2	-8	5316	5600	-282
2	2	-15	6734	7936	-1202	8	2	-9	4792	4260	532
2	2	-16	-7430	-7054	-376	8	2	-10	6300	6557	1743
2	2	-17	-4415	-4777	359	8	2	-11	-10467	-10260	-207
4	2	15	4921	5649	-728	8	2	-12	3720	3509	211
4	2	14	-4139	-4269	130	8	2	-13	-3174	-2277	-897
4	2	10	2991	2680	311	8	2	-14	-3474	-3855	381
4	2	9	3603	3653	-50	8	2	-16	3460	2961	502
4	2	7	2316	1853	463	8	2	-17	6467	6166	301
4	2	6	-4461	-5548	1087	8	2	-18	4254	4697	-57
4	2	5	-3913	-3010	-903	8	2	-21	-3152	-2580	-572
4	2	4	2166	3356	-1190	10	2	11	3505	2483	1022
4	2	3	-2041	-531	-2310	10	2	6	4074	2698	1376
4	2	2	6291	1667	4564	10	2	3	-4720	-5167	447
4	2	1	6278	7625	443	10	2	1	-4514	-5431	917
4	2	0	-4554	-4308	-646	10	2	-1	16677	16577	1502
4	2	-1	13018	10164	2854	10	2	-2	-6673	-8533	1660
4	2	-3	5662	5483	179	10	2	-4	4900	5117	-217
4	2	-4	-13640	-10622	-3018	10	2	-5	-9275	-9623	648
4	2	-5	-11058	-9517	-1161	10	2	-6	9618	8059	1559
4	2	-6	-4053	-5395	1342	10	2	-7	-6465	-5579	-886
4	2	-7	-2433	-2362	-71	10	2	-9	-9222	-7798	-1424
4	2	-8	2111	3288	-1177	10	2	-9	10356	9871	487

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
10	2	-10	2337	730	1607	18	2	5	6091	6920	-829
10	2	-12	7066	7261	-195	18	2	3	-2895	-3772	877
10	2	-13	-3710	-3559	-151	18	2	2	6091	5367	724
10	2	-16	-4310	-4641	331	18	2	0	-2991	-2536	-455
10	2	-17	-5822	-4845	-977	18	2	-1	-4342	-3644	-698
10	2	-25	-4375	-3049	-1326	18	2	-2	-4042	-4879	837
12	2	17	3827	2086	1741	18	2	-4	4053	4643	-590
12	2	9	-3956	-5271	1315	18	2	-5	12899	12261	638
12	2	5	5726	5938	-212	18	2	-6	3634	2221	1413
12	2	4	-6326	-6148	-178	18	2	-8	-6434	-4988	-1446
12	2	2	-5328	-5087	-241	18	2	-9	-6444	-6809	365
12	2	1	-4997	-5935	938	18	2	-10	2948	1766	1182
12	2	0	11753	12127	-374	18	2	-11	-6241	-6158	-83
12	2	-1	2873	1396	1477	18	2	-13	5383	4198	1185
12	2	-2	3195	397	2798	18	2	-14	-3045	-4577	1532
12	2	-3	15259	13169	2090	18	2	-21	-3281	-2926	-355
12	2	-4	-22379	-18722	-3657	18	2	-22	-3989	-1559	-2430
12	2	-5	8503	7523	980	20	2	9	3345	2260	1085
12	2	-8	3956	5352	-1396	20	2	6	4085	4081	4
12	2	-9	-5586	-5387	-199	20	2	4	-4847	-4386	-461
12	2	-10	-5886	-6407	521	20	2	1	4310	4474	-164
12	2	-11	-2991	-2969	-22	20	2	-1	4954	5135	-181
12	2	-12	-5790	-4093	-1697	20	2	-7	6058	5576	482
12	2	-13	3560	4437	-877	20	2	-8	-3505	-2100	-1405
12	2	-15	7334	6716	618	20	2	-11	-3903	-3295	-608
12	2	-17	-5533	-5940	407	20	2	-14	-2873	-1386	-1487
12	2	-21	3012	1673	1339	20	2	-16	-4139	-3012	-1127
14	2	15	-4964	-3916	-1048	20	2	-18	3570	2928	642
14	2	11	6701	7697	-996	20	2	-19	4170	4093	77
14	2	8	-4599	-4726	127	20	2	-22	-3753	-3630	-123
14	2	7	-7249	-6574	-675	22	2	5	4096	3796	300
14	2	5	-9296	-8919	-377	22	2	3	-5328	-5188	-140
14	2	4	4857	5576	-719	22	2	1	-9479	-9318	-161
14	2	3	5812	5668	144	22	2	-1	3946	4346	-400
14	2	2	-5361	-5005	-356	22	2	-3	3152	2808	344
14	2	0	-5071	-4091	-980	22	2	-6	2969	1791	1178
14	2	-1	-3860	-3975	115	22	2	-12	4642	3466	1176
14	2	-3	10840	9981	859	22	2	-14	3796	3097	699
14	2	-4	-6894	-6631	-263	22	2	-17	-3999	-2671	-1328
14	2	-5	-2390	-2988	598	22	2	-21	3903	4243	-340
14	2	-7	-8138	-8188	50	24	2	-1	-3817	-3307	-510
14	2	-8	5082	5023	59	24	2	-7	3410	2895	515
14	2	-10	4975	2833	2142	24	2	-8	3141	3140	1
14	2	-11	7259	6642	617	24	2	-11	-4718	-4536	218
14	2	-13	-5135	-6452	1317	24	2	-12	-3495	-3296	-199
14	2	-14	4032	3184	848	24	2	-13	-4149	-3831	-318
14	2	-17	6101	6605	-504	24	2	-15	3892	2540	1352
14	2	-18	-3324	-3555	231	26	2	9	4042	2862	1180
16	2	13	-3699	-4323	624	26	2	-5	-3774	-2900	-874
16	2	9	3591	4749	-1158	26	2	-11	5726	4069	1657
16	2	5	-5190	-7149	1959	26	2	-15	-4556	-4891	335
16	2	3	-6841	-7866	1025	28	2	0	-3849	-3062	-787
16	2	2	4418	3996	422	28	2	-3	4568	3144	1424
16	2	0	-8750	-8587	-163	28	2	-5	3527	3902	-375
16	2	-2	4256	3344	912	28	2	-9	-3946	-2720	-1226
16	2	-3	6294	5763	531	28	2	-14	-3892	-3448	-444
16	2	-4	4514	5220	-706	30	2	0	-3860	-1960	-1900
16	2	-7	-14905	-14144	-761	30	2	-4	4053	3281	772
16	2	-8	7538	7407	131	30	2	-9	3312	592	2720
16	2	-9	-6337	-5966	-371	34	2	-9	-3634	-1001	-2633
16	2	-10	4127	2574	1553	1	3	27	-4418	-1360	-3058
16	2	-11	10733	10924	-191	1	3	25	3817	2102	1715
16	2	-12	-4514	-4205	-309	1	3	14	5607	6131	-524
16	2	-15	-6755	-6525	-230	1	3	12	3999	4020	-21
16	2	-16	4289	5095	-806	1	3	10	-7334	-7501	167
18	2	15	3710	2784	926	1	3	8	-4525	-4850	325
18	2	12	-3441	-2682	-759	1	3	7	-7538	-7313	-225
18	2	9	-4406	-5090	684	1	3	6	12866	10523	2343
18	2	7	3324	3037	287	1	3	4	4492	4177	315

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o–F_c	*h*	*k*	*l*	F_o	F_c	F_o–F_c
1	3	3	1768	1483	305	7	3	5	4182	3474	708
1	3	2	-9415	-8279	-1136	7	3	4	6691	6850	-159
1	3	1	-13886	-16226	2340	7	3	3	-12439	-11119	-1320
1	3	0	-1415	-1518	103	7	3	2	9210	8338	872
1	3	-1	11324	12544	-1220	7	3	1	5662	4151	1511
1	3	-2	4246	2779	1467	7	3	0	5919	4804	1115
1	3	-3	15473	11490	3983	7	3	-2	-13414	-13090	-324
1	3	-4	-4900	-4522	-378	7	3	-3	-9725	-8963	-762
1	3	-5	4654	5386	-732	7	3	-4	-9501	-7626	-1875
1	3	-6	13232	11946	1286	7	3	-5	3119	4091	-972
1	3	-8	4503	5474	-971	7	3	-6	5533	5936	-403
1	3	-9	-8750	-7789	-961	7	3	-7	7249	6646	603
1	3	-10	-7066	-7649	583	7	3	-9	4042	4175	-133
1	3	-13	2873	4117	-1244	7	3	-10	3195	3530	-335
1	3	-15	9157	10220	-1063	7	3	-11	-5361	-4397	-964
1	3	-17	-3527	-4960	1433	9	3	19	3710	3367	343
1	3	-19	-4985	-5474	489	9	3	15	-3410	-5550	2140
3	3	18	5865	6142	-277	9	3	12	-4182	-4711	529
3	3	16	4320	3949	371	9	3	8	9350	9433	-83
3	3	14	-8846	-9051	205	9	3	4	-8310	-7014	-1296
3	3	12	-2595	-3100	505	9	3	3	-7302	-6690	-612
3	3	11	7044	7256	-212	9	3	1	9554	8242	1312
3	3	10	7056	6475	581	9	3	0	7280	6134	1146
3	3	9	4954	3907	1047	9	3	-1	2938	2832	106
3	3	8	-7377	-7347	-30	9	3	-2	10530	9676	854
3	3	7	-3367	-2324	-1043	9	3	-3	-12449	-12905	456
3	3	5	-6465	-7605	1140	9	3	-6	-5479	-2444	-3035
3	3	4	8235	8123	112	9	3	-7	5983	5040	943
3	3	3	6369	15000	-8631	9	3	-9	3977	4457	-480
3	3	2	11098	8926	2172	9	3	-10	3741	3780	-39
3	3	1	14648	8911	5737	9	3	-11	-9372	-8807	-565
3	3	-1	-17296	-14003	-3293	9	3	-12	5040	5016	24
3	3	-2	-8803	-7657	-1146	9	3	-13	-2916	-2464	-452
3	3	-3	4814	2503	2311	9	3	-16	-3977	-4336	359
3	3	-5	-7430	-4429	-3001	9	3	-17	-3152	-1431	-1721
3	3	-6	-3667	-4237	570	9	3	-19	5168	6266	-1098
3	3	-8	2798	2948	-150	11	3	11	4235	3860	375
3	3	-13	-9468	-9643	175	11	3	10	-3259	-4265	1006
3	3	-17	4568	5419	-851	11	3	7	3527	4123	-596
3	3	-18	-3463	-3088	-375	11	3	5	2540	1910	630
3	3	-22	3367	1753	1614	11	3	3	-3827	-3513	-314
5	3	12	-3646	-4377	731	11	3	0	5586	5104	482
5	3	11	-2819	-566	-2253	11	3	-1	14208	13742	466
5	3	9	5500	5960	-460	11	3	-2	10787	9268	1519
5	3	7	5190	6521	-1331	11	3	-4	-4127	-3980	-147
5	3	5	-7356	-9397	2041	11	3	-5	-6241	-6024	-217
5	3	4	3431	3525	-94	11	3	-6	-5619	-4290	-1329
5	3	3	-3591	-1454	-2137	11	3	-7	2540	1347	1193
5	3	1	9897	7384	2513	11	3	-8	-8653	-7295	-1358
5	3	0	-2776	-3874	1098	11	3	-10	-4718	-4797	79
5	3	-1	-8781	-7182	-1599	11	3	-12	5050	5227	-177
5	3	-2	2476	360	2116	11	3	-14	3088	3577	-489
5	3	-3	12610	9015	3595	11	3	-15	5297	4487	810
5	3	-6	-5490	-5673	183	11	3	-18	-3410	-3817	407
5	3	-8	2938	2243	695	11	3	-19	-3892	-2819	-1073
5	3	-9	-6658	-5162	-1496	13	3	14	-3281	-1986	-1295
5	3	-11	3667	6046	-2381	13	3	11	6712	7878	-1166
5	3	-12	-3024	-2566	-458	13	3	7	-12117	-12044	-73
5	3	-14	-2455	-2772	317	13	3	4	-4127	-4476	349
5	3	-15	-6487	-6775	288	13	3	3	10766	10431	335
5	3	-19	2841	1090	1751	13	3	1	-4804	-5595	791
7	3	18	-4074	-1527	-2547	13	3	0	3398	4116	-718
7	3	17	-3205	-4201	996	13	3	-3	4568	3947	621
7	3	13	4599	4236	363	13	3	-4	-10640	-10569	-271
7	3	11	-6251	-7915	1664	13	3	-6	-6284	-6916	632
7	3	10	2712	2060	652	13	3	-8	5779	5961	-182
7	3	9	-7270	-7218	-52	13	3	-11	3088	2457	631
7	3	8	-6572	-6541	-31	13	3	-13	-5554	-5492	-62
7	3	6	-7785	-7452	-333	13	3	-15	6701	6112	589

TABLE 2 (*Continued*)

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13	3	-17	3463	2516	947	25	3	8	4235	61	4174
13	3	-13	-3066	-533	-2533	25	3	0	4127	4780	-653
15	3	13	-5361	-5474	113	25	3	-2	4728	4978	-250
15	3	10	3045	427	2618	25	3	-4	-3710	-3300	-410
15	3	9	3753	4922	-1169	25	3	-6	-3667	-2923	-744
15	3	7	-3441	-2897	-544	25	3	-11	3281	573	2708
15	3	5	-7871	-9022	1151	25	3	-13	-8257	-7683	-574
15	3	1	4900	4482	418	27	3	-7	-3570	-4216	646
15	3	0	-2991	-2068	-923	27	3	-11	4525	5835	-1310
15	3	-1	-4556	-3199	-1357	27	3	-14	3817	3702	115
15	3	-2	7763	7349	414	27	3	-16	4964	2402	2562
15	3	-5	-3796	-3491	-305	29	3	-7	4203	2810	1393
15	3	-6	-9136	-7804	-1332	31	3	-8	-3774	-2781	-993
15	3	-7	-2815	-3018	199	33	3	-14	4320	2050	2270
15	3	-11	5414	5082	332	0	4	16	3088	2476	612
15	3	-13	-5683	-4800	-883	0	4	15	-3205	-3964	759
15	3	-14	3367	4231	-864	0	4	14	2948	2859	89
15	3	-15	-4492	-5694	1202	0	4	12	2595	1441	1154
15	3	-17	3281	3607	-326	0	4	10	-7699	-7055	-644
17	3	5	-3570	-2282	-1288	0	4	9	-8374	-8281	-93
17	3	4	7013	6927	86	0	4	8	-8224	-8956	732
17	3	2	5361	5165	196	0	4	6	8739	8719	20
17	3	0	-4921	-5983	1062	0	4	5	9661	9069	592
17	3	-1	-5168	-5598	430	0	4	4	14412	12301	2111
17	3	-3	3474	2700	774	0	4	3	-4997	-5196	199
17	3	-4	11302	11033	269	0	4	2	-3024	-437	-2587
17	3	-5	5790	5459	331	0	4	1	-7001	-11805	4804
17	3	-7	-2798	-2765	-13	2	4	20	2969	3053	-84
17	3	-9	-11324	-11025	-299	2	4	15	-4032	-4453	421
17	3	-10	4462	3957	505	2	4	13	-2798	-2969	171
17	3	-11	3152	1813	1339	2	4	12	5769	5217	552
17	3	-13	4418	5500	-1082	2	4	11	7602	7685	-83
17	3	-15	-7130	-6805	-325	2	4	10	7645	7566	79
17	3	-20	-3024	-2853	-171	2	4	9	5007	4605	402
17	3	-21	-3591	-1695	-1896	2	4	8	-2262	-2131	-131
19	3	12	-3152	-19	-3133	2	4	7	-7688	-7952	264
19	3	4	-4042	-3280	-762	2	4	6	-4762	-3245	-1517
19	3	2	5511	5653	-142	2	4	5	-6562	-5607	-955
19	3	1	6079	6794	-715	2	4	4	5340	3505	1835
19	3	0	3060	3802	-742	2	4	3	15045	12792	2253
19	3	-1	3603	3190	413	2	4	2	11570	11098	472
19	3	-3	-8235	-9336	1101	2	4	0	-1973	-2062	89
19	3	-7	10047	10307	-260	2	4	-1	-5827	-4446	-1443
19	3	-8	-3796	-2669	-1127	2	4	-2	-6460	-6426	-2572
19	3	-9	4353	4139	214	2	4	-3	7592	8198	-607
19	3	-11	-4932	-5459	527	2	4	-4	-8460	-8407	-53
19	3	-16	3098	46	3052	2	4	-8	12074	11557	517
19	3	-18	3538	3960	-422	2	4	-10	-4965	-3756	-1229
19	3	-23	-3495	-2627	-868	2	4	-12	-7313	-7015	-298
21	3	7	3463	1924	1539	2	4	-14	-3410	-2148	-1262
21	3	3	-3660	-5314	1454	2	4	-16	2967	467	2500
21	3	2	-4020	-3581	-439	2	4	-22	-3692	-1784	-1908
21	3	-1	5050	5139	-89	4	4	16	3646	3893	-247
21	3	-7	3281	2361	920	4	4	15	3741	4192	-451
21	3	-8	-5715	-6172	457	4	4	12	-5506	-6636	1130
21	3	-9	4149	4627	-478	4	4	9	4707	5653	-946
21	3	-11	-4503	-3977	-526	4	4	5	-2210	-2700	490
21	3	-18	4246	3078	1168	4	4	3	8503	7418	1085
21	3	-20	2969	2683	286	4	4	2	-3174	-2931	-243
21	3	-23	-3720	-1035	-2685	4	4	1	6916	6759	157
23	3	6	-4696	-3634	-1062	4	4	0	3560	1656	1904
23	3	0	3227	4094	-867	4	4	-1	-4042	-3605	-437
23	3	-2	-3152	-2659	-493	4	4	-2	6530	70	6460
23	3	-8	2938	2145	793	4	4	-4	5276	3504	1772
23	3	-10	-3098	-2471	-627	4	4	-5	-8300	-6384	-1916
23	3	-11	-7270	-7180	-90	4	4	-6	-8031	-6327	-1704
23	3	-12	-3152	-2644	-508	4	4	-7	-10798	-10449	-349
23	3	-15	6026	6136	-110	4	4	-9	3431	3156	275
23	3	-19	-4875	-5182	307	4	4	-10	4020	4975	-955

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
4	4	-11	9318	9449	-131	12	4	11	3[illegible]	4818	[illegible]
4	4	-12	6272	6574	-302	12	4	8	-3495	-4642	1147
4	4	-13	-5122	-5698	-224	12	4	5	9983	10042	-59
4	4	-16	-4299	-4097	-202	12	4	3	4954	4730	224
6	4	14	3259	2285	974	12	4	1	-7109	-8570	1461
6	4	11	-3784	-4138	354	12	4	0	-2187	-2689	-1898
6	4	10	-5082	-5908	826	12	4	-3	4020	4372	-352
6	4	9	-3227	-3967	740	12	4	-6	2841	3648	-807
6	4	8	-4857	-4453	-404	12	4	-8	4449	3135	1314
6	4	7	4782	4257	525	12	4	-9	2412	2544	-132
6	4	6	-5340	-4330	-1010	12	4	-10	-5650	-5743	93
6	4	5	3538	2043	1495	12	4	-11	-2755	-2102	-653
6	4	4	5908	5997	-89	12	4	-12	-2641	-2086	-755
6	4	3	-5361	-3382	-1979	12	4	-15	6946	6657	291
6	4	2	6214	5532	-1318	12	4	-16	4428	5364	-936
6	4	1	2359	2216	143	14	4	8	-3227	-3871	644
6	4	0	-10423	-9633	-790	14	4	7	-4353	-4771	418
6	4	-1	-15956	-14055	-1901	14	4	3	7152	7751	-599
6	4	-2	-19860	-17766	-2094	14	4	2	-4235	-4238	3
6	4	-4	10583	8848	1735	14	4	1	-3312	-3685	373
6	4	-5	8267	8525	-258	14	4	0	3410	3303	107
6	4	-6	9025	9880	-851	14	4	-1	-7452	-6783	-669
6	4	-8	2111	145	1966	14	4	-3	2519	2347	172
6	4	-9	-3227	-2506	-721	14	4	-6	-7806	-7172	-634
6	4	-10	-4032	-3959	-73	14	4	-10	3441	3542	-101
6	4	-13	4127	5143	-1016	14	4	-12	3699	2349	1350
6	4	-14	4085	4604	-519	14	4	-17	3527	3781	-254
6	4	-15	-4921	-4677	-244	14	4	-19	-5211	-4867	-344
8	4	15	-3377	-2654	-723	14	4	-22	3934	2547	1387
8	4	9	-3842	-4882	1040	16	4	11	-5426	-6218	792
8	4	8	3441	2689	552	16	4	8	-3410	-1996	-1414
8	4	7	5114	5718	-604	16	4	4	6229	6461	-232
8	4	6	-6712	-7669	957	16	4	0	-5093	-4922	-171
8	4	4	-2519	-2961	442	16	4	-1	-4642	-5299	657
8	4	3	-6723	-7120	397	16	4	-4	8364	7408	956
8	4	1	2058	200	1858	16	4	-7	-8425	-8475	47
8	4	0	12513	11309	1204	16	4	-8	-2412	-2079	-333
8	4	-1	2037	895	1142	16	4	-9	-4256	-4688	432
8	4	-2	5822	6897	-1075	16	4	-10	-4406	-4353	-53
8	4	-3	-4020	-4959	939	16	4	-11	8342	9505	-1163
8	4	-4	-10895	-12438	1543	16	4	-14	3646	4298	-652
8	4	-6	-7763	-6008	-1755	16	4	-15	-7345	-7329	-16
8	4	-7	4568	4850	-282	16	4	-22	3527	1551	1976
8	4	-8	3710	2819	891	18	4	15	3560	717	2843
8	4	-9	-2776	-2140	-636	18	4	6	-4353	-4485	132
8	4	-10	4525	5261	-736	18	4	4	4353	4146	207
8	4	-11	-2862	-2959	97	18	4	2	5586	4755	831
8	4	-12	-3474	-3221	-253	18	4	1	4192	4461	-269
8	4	-13	3560	3941	-381	18	4	-2	-4342	-4047	-295
8	4	-14	-3238	-3674	436	18	4	-3	-5586	-5819	233
10	4	10	-4621	-4617	-4	18	4	-6	5093	5688	-595
10	4	8	3474	3283	191	18	4	-13	5457	6040	-583
10	4	7	5447	6677	-1230	18	4	-15	-4461	-3416	-1045
10	4	6	7871	9394	-1523	18	4	-18	3903	5366	-1463
10	4	5	7130	7406	-276	18	4	-22	-4032	-3444	-588
10	4	3	-6658	-7103	445	20	4	-1	4532	5301	-769
10	4	1	-4353	-3222	-1131	20	4	-5	-4535	-5026	491
10	4	-1	10594	8974	1620	20	4	-9	2551	3714	-723
10	4	-2	-3141	-243	-2898	20	4	-12	3345	3245	100
10	4	-3	-5522	-5815	293	20	4	-13	4726	4393	333
10	4	-4	4857	3761	1096	20	4	-17	-3538	-2165	-1373
10	4	-7	2916	2296	618	22	4	4	4074	3331	743
10	4	-8	-6186	-7477	1291	22	4	0	-3291	-3503	212
10	4	-11	-3495	-2946	-549	22	4	-8	3527	2803	724
10	4	-12	6069	6050	19	22	4	-10	-7087	-7386	299
10	4	-14	4299	5249	-950	22	4	-15	4696	4069	627
10	4	-17	-3312	-4941	1628	22	4	-17	-4418	-4695	277
10	4	-18	-6165	-7179	1014	22	4	-20	-4020	-2651	-1369
10	4	-21	3913	3310	603	24	4	7	-3570	-1247	-2323

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
24	4	0	4170	4339	-169	5	5	-4	4761	5231	-470
24	4	-7	-5855	-5709	-146	5	5	-5	2965	3400	-505
24	4	-19	-3591	-2467	-1124	5	5	-6	5822	5775	47
24	4	-21	-4192	-1025	-3167	5	5	-9	-4985	-4822	-163
26	4	3	3324	2880	444	5	5	-10	-3667	-3991	324
26	4	-1	-3324	-2791	-533	5	5	-12	3860	4391	-531
26	4	-6	-3205	-1733	-1472	5	5	-14	5114	4523	591
26	4	-7	-3505	-4142	637	7	5	18	2819	714	2105
26	4	-12	4117	2957	1160	7	5	14	-3720	-3103	-617
26	4	-14	4042	5266	-1224	7	5	13	-3238	-3760	522
26	4	-22	5114	3342	1772	7	5	11	-5221	-5356	135
26	4	-12	-4814	-5246	432	7	5	9	6541	7220	-679
30	4	-15	-3624	-1850	-1774	7	5	7	6036	5931	105
1	5	15	-3710	-3909	199	7	5	6	-5135	-5110	-25
1	5	13	-3410	-2978	-432	7	5	5	-6235	-7848	-387
1	5	12	4363	2945	1418	7	5	3	-5693	-6244	551
1	5	11	8932	9828	-896	7	5	2	2262	1707	555
1	5	10	4074	4548	-474	7	5	0	9415	9637	-222
1	5	9	3741	4302	-561	7	5	-1	2991	1841	1150
1	5	8	-3152	-3503	351	7	5	-2	-2969	-6037	3068
1	5	7	-9651	-11168	1517	7	5	-3	-6251	-5456	-795
1	5	3	2755	2774	-19	7	5	-4	-10047	-10445	398
1	5	2	2841	4244	-1403	7	5	-6	2111	2538	-427
1	5	1	-2540	-2590	50	7	5	-7	-2680	-1659	-1021
1	5	-1	5683	7809	-2126	7	5	-8	5168	6168	-1000
1	5	-2	-3312	-3094	-218	7	5	-11	3495	5953	-2458
1	5	-3	3753	5199	-1446	7	5	-12	-5168	-5694	526
1	5	-4	-6229	-5293	-936	7	5	-15	-7270	-7631	361
1	5	-5	-6701	-8196	1495	7	5	-16	-3205	-606	-2599
1	5	-9	8395	8731	-336	7	5	-19	5908	5724	184
1	5	-12	-3505	-3726	221	9	5	11	-3398	-3405	7
1	5	-13	-3024	-3844	820	9	5	9	-4235	-3449	-786
1	5	-14	-5693	-5716	23	9	5	8	10883	10809	74
1	5	-15	4096	3879	217	9	5	7	6615	7508	-893
1	5	-16	3088	2348	740	9	5	6	5371	5491	-120
1	5	-26	3903	2093	1810	9	5	5	2938	3659	-721
1	5	-27	3796	764	3032	9	5	4	-4911	-5064	153
3	5	19	-2938	-2359	-579	9	5	3	-7763	-8444	681
3	5	18	3174	2419	755	9	5	2	-5286	-5361	75
3	5	15	3377	2754	623	9	5	1	-6143	-5412	-731
3	5	13	-3431	-4575	1144	9	5	-1	3913	2484	1429
3	5	11	3238	2933	305	9	5	-2	11624	11210	414
3	5	10	7473	8043	-570	9	5	-3	3324	4320	-996
3	5	9	6348	6827	-479	9	5	-5	3324	2370	954
3	5	8	4299	4365	-66	9	5	-6	-6214	-7357	857
3	5	7	-3849	-3715	-134	9	5	-7	2916	3102	-186
3	5	4	-2090	-3025	935	9	5	-10	4149	3508	641
3	5	3	4625	3756	869	9	5	-11	-5082	-4942	-140
3	5	2	2948	2944	4	9	5	-13	6637	6943	-305
3	5	1	-6551	-5128	-1423	9	5	-16	-3946	-5357	1411
3	5	-2	-3827	-3826	1	9	5	-20	4749	3842	907
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3	5	-7	-13018	-12026	-992	11	5	8	-3312	-3145	-167
3	5	-9	6284	5825	459	11	5	4	4461	4113	348
3	5	-11	6138	6133	5	11	5	2	3259	3762	-503
3	5	-14	-4342	-4336	-4	11	5	0	-5276	-5639	363
3	5	-20	3195	994	2201	11	5	-2	-2573	-2376	-197
5	5	21	3410	3696	-286	11	5	-3	-3088	-2021	-1067
5	5	13	4149	4352	-203	11	5	-6	6765	7028	-263
5	5	10	-5297	-4593	-704	11	5	-7	9672	10616	-944
5	5	-7	-2355	-2652	293	11	5	-9	5404	4229	1175
5	5	-5	-5800	-5733	-67	11	5	-10	-2455	-1956	-499
5	5	3	4707	4703	+76	11	5	-11	-7666	-7591	-75
5	5	2	-9662	-8269	-1393	11	5	-14	3345	3340	5
5	5	1	4285	4032	257	11	5	-15	3141	3905	-764
5	5	0	-2219	-2256	37	11	5	-16	5779	6439	-660
5	5	-1	-2728	-3332	534	13	5	14	-4074	-3061	-1013
5	5	-3	-2595	-1625	-970	13	5	9	2862	2768	

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
13	5	8	6412	560	5852	23	5	-9	-5623	-5929	-164
13	5	4	-8149	-8112	-37	23	5	-7	-3119	-1746	-1373
13	5	0	4353	3420	933	23	5	-8	3141	2982	159
13	5	-1	2294	1328	966	23	5	-14	-3291	-1771	-1520
13	5	-3	4020	5466	-1446	23	5	-19	-3398	-1643	-1755
13	5	-4	-3570	-3109	-461	25	5	2	-3560	-2485	-1075
13	5	-5	-2616	-2721	105	25	5	-3	4310	3491	819
13	5	-6	-2659	-2812	153	25	5	-9	-3463	-2478	-985
13	5	-7	-4449	-4057	-392	27	5	-1	-3934	-1863	-2071
13	5	-8	9715	9239	476	27	5	-5	3646	2122	1524
13	5	-9	5221	4478	743	27	5	-17	4020	3273	747
13	5	-10	5082	5407	-325	29	5	-15	-4235	-2738	-1497
13	5	-12	-6422	-5198	-1224	31	5	-7	3627	2509	918
13	5	-13	-4267	-4232	-35	0	6	15	-5886	-6516	630
13	5	-14	-5769	-6445	676	0	6	11	10776	11609	-833
13	5	-18	4203	4431	-228	0	6	9	-8055	-7405	-650
13	5	-21	3410	3337	73	0	6	8	-3634	-4088	454
15	5	14	4246	542	3704	0	6	7	-7087	-7715	628
15	5	6	2916	4461	-1545	0	6	5	7270	7077	193
15	5	3	7163	6974	189	0	6	2	1573	1505	68
15	5	2	-6369	-6692	323	2	6	15	-3012	-524	-2488
15	5	0	-2948	-3186	238	2	6	17	3870	4443	-573
15	5	-1	-11677	-12757	1080	2	6	13	-3624	-3205	-419
15	5	-2	3141	4755	-1614	2	6	11	5522	6779	-1257
15	5	-4	6058	5781	277	2	6	10	5307	4216	1091
15	5	-5	5243	5142	101	2	6	9	6005	6338	-334
15	5	-6	-5316	-5446	128	2	6	7	-4720	-4875	147
15	5	-7	-5812	-6939	1127	2	6	6	-4985	-4613	-372
15	5	-8	-6294	-6584	290	2	6	5	-3710	-3901	191
15	5	-11	3977	3235	742	2	6	2	6894	6189	705
15	5	-12	4525	4740	-215	2	6	1	3238	2458	780
15	5	-13	-4792	-3690	-1102	2	6	-3	5007	6441	-1434
15	5	-16	-4139	-4232	93	2	6	-7	-5157	-5478	321
17	5	4	3088	4008	-920	2	6	-8	-3670	-3672	-198
17	5	1	6315	6359	-44	2	6	-9	7924	8053	-129
17	5	-2	-4804	-5695	891	2	6	-11	4170	3986	184
17	5	-3	-7785	-6877	-908	2	6	-21	3527	3550	-23
17	5	-6	4449	5193	-744	4	6	15	3627	4343	-716
17	5	-7	4192	2683	1309	4	6	14	2948	2501	447
17	5	-9	3698	2167	1532	4	6	12	-2969	-2973	4
17	5	-10	3377	2364	1013	4	6	11	-3045	-2228	-817
17	5	-13	-3227	-3023	-204	4	6	9	-3291	-3149	-142
17	5	-15	-5876	-4763	-1113	4	6	7	-5082	-5449	367
17	5	-16	2916	2814	102	4	6	5	3367	3648	-281
17	5	-17	3560	2910	650	4	6	4	-5061	-4652	-409
17	5	-20	-2895	-2008	-887	4	6	3	6422	6823	-401
19	5	5	-3152	-1987	-1165	4	6	1	-4032	-4104	72
19	5	4	-3358	-3199	-159	4	6	0	8021	8245	-224
19	5	3	-2916	-3569	653	4	6	-1	-7999	-7736	-263
19	5	0	2776	3702	-926	4	6	-2	2690	1594	1096
19	5	-1	5479	5331	148	4	6	-3	5254	5806	-552
19	5	-3	-3699	-3829	130	4	6	-5	12267	12356	-89
19	5	-4	-4042	-4351	309	4	6	-7	-9308	-9262	-46
19	5	-8	4482	4799	-317	4	6	-8	-4020	-3478	-542
19	5	-10	4718	5788	-1070	4	6	-9	-3398	-3033	-365
19	5	-11	3012	4282	-1270	4	6	-11	6294	6524	-230
19	5	-14	-3560	-3382	-178	4	6	-12	3377	2986	391
19	5	-15	-4074	-3201	-873	6	6	16	-3441	-1530	-1911
19	5	-16	-3152	-2131	-1021	6	6	15	-3024	-2461	-563
19	5	-17	-3903	-3583	-320	6	6	10	-4482	-5168	686
19	5	-18	3312	3803	-491	6	6	9	4792	5601	-809
21	5	5	4320	3197	1123	6	6	6	4599	4360	239
21	5	-7	3677	4065	-388	6	6	5	-9339	-10479	1140
21	5	-8	-3903	-3974	71	6	6	2	-4762	-5946	1184
21	5	-11	-3667	-4240	573	6	6	1	9243	9058	185
21	5	-12	3324	2464	860	6	6	0	-2755	-2145	-610
21	5	-18	-4096	-4035	-61	6	6	-3	-11763	-11437	-326
23	5	2	5950	4455	1495	6	6	-4	4975	4852	123
23	5	-2	-5135	-3606	-1529	6	6	-6	2873	1960	913

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
6	6	-7	3948	3888	-140	16	6	1	5325	4363	965
6	6	-8	-4875	-4872	-303	18	6	-1	3521	2844	-53
6	6	-9	-3410	-2556	-852	16	6	-9	2776	1794	982
6	6	-10	-5564	-5604	40	18	6	-11	4139	4513	-374
6	6	-12	2433	2669	-236	18	6	-15	-4053	-5235	1182
6	6	-13	-6412	-6540	128	18	6	-16	-4139	-1837	-2302
6	6	-14	5157	5485	-328	18	6	-19	4085	5361	-1276
6	6	-15	-4589	-4297	-292	20	6	5	6348	5446	902
8	6	7	7013	7063	-50	20	6	-4	-2776	-1564	-1212
8	6	6	-2916	-4339	1423	20	6	-9	-3066	-3037	-29
8	6	5	3570	1621	1949	20	6	-11	-4246	-3888	-358
8	6	4	2497	2456	41	20	6	-12	-3431	-3494	63
8	6	3	-6562	-7169	607	22	6	0	-3634	-3487	-147
8	6	1	-5264	-4397	-867	22	6	-1	2519	505	2014
8	6	-1	5586	5788	-202	22	6	-3	-3119	-3190	71
8	6	-2	4718	3331	1387	22	6	-7	3474	3622	-148
8	6	-3	2166	1769	397	22	6	-8	-3603	-1909	-1694
8	6	-4	-5833	-5484	-349	22	6	-11	-3410	-3942	532
8	6	-6	3710	3258	452	22	6	-12	-3441	-902	-2539
8	6	-9	-6015	-5668	-347	24	6	-3	5286	5754	-468
8	6	-10	-3977	-4820	843	24	6	-7	-4267	-5634	1367
8	6	-11	5426	5705	-279	24	6	-11	3710	3723	-13
8	6	-13	4246	4571	-325	26	6	-5	3741	4004	-263
10	6	0	-2755	-2221	-534	26	6	-15	3570	2366	1204
10	6	-1	-4020	-4281	261	26	6	-19	-3591	-2804	-787
10	6	-3	-4492	-5122	630	28	6	-2	-3152	-1957	-1195
10	6	-5	10745	10656	89	28	6	-15	-5490	-3417	-2073
10	6	-7	18959	17855	1104	1	7	16	3522	3921	-399
10	6	-9	-6519	-6962	443	1	7	12	-3860	-4881	1021
10	6	-10	3141	3542	-401	1	7	11	4021	5142	-1121
10	6	-11	-11848	-11181	-667	1	7	8	5506	4758	748
10	6	-13	5697	5467	410	1	7	7	-4872	-5046	174
10	6	-15	6498	7864	-1366	1	7	6	-4291	-4375	84
12	6	3	-3205	-2060	-1145	1	7	5	3967	4606	-639
12	6	2	3045	1716	1329	1	7	4	-6167	-5588	-579
12	6	0	-6980	-7126	146	1	7	3	2752	4236	-1484
12	6	-1	7109	7537	-428	1	7	-2	3603	6499	-2896
12	6	-2	3624	2514	1110	1	7	-3	3266	4022	-756
12	6	-3	7613	6514	1099	1	7	-4	2915	3005	-90
12	6	-4	4685	4668	17	1	7	-5	-6167	-5845	-322
12	6	-5	-8729	-8518	-211	1	7	-6	-8031	-8519	488
12	6	-6	2476	1144	1332	1	7	-8	-3441	-2465	-976
12	6	-9	7956	7044	912	1	7	-9	6492	6636	-144
12	6	-11	-2916	-3201	285	1	7	-10	4454	3927	527
12	6	-13	-3860	-4234	374	1	7	-15	4413	801	3612
12	6	-23	-3463	-1809	-1654	1	7	-26	-5897	-2028	-3869
14	6	9	3398	2804	594	3	7	14	4184	3350	834
14	6	6	-3667	-2978	-689	3	7	12	3415	1594	1821
14	6	3	2969	2156	813	3	7	10	-5075	-5584	509
14	6	1	-4685	-5616	931	3	7	9	3886	4642	-756
14	6	-1	-3946	-5190	1244	3	7	5	2752	2618	134
14	6	-2	-5050	-4852	-198	3	7	4	-3117	-2342	-775
14	6	-3	5318	4935	383	3	7	2	2456	2998	-542
14	6	-5	3345	2962	383	3	7	1	-4184	-4239	55
14	6	-7	-5093	-4484	-609	3	7	-3	6816	8389	-1573
14	6	-9	-3977	-3643	-334	3	7	-4	6302	7048	-746
14	6	-11	-4375	-3500	-875	3	7	-7	-9327	-8779	-548
14	6	-17	-3827	-4001	174	3	7	-8	-3292	-3744	452
14	6	-19	-4406	-4530	124	3	7	-9	3117	2144	973
14	6	-23	3977	5105	-1128	3	7	-11	7882	6903	979
16	6	0	2519	2763	-244	5	7	16	-4319	-3471	-848
16	6	-1	-3710	-4236	526	5	7	13	4319	4396	-77
16	6	-3	-3870	-3101	-769	5	7	9	-4710	-5116	406
16	6	-5	2755	3444	-689	5	7	8	3347	4188	-841
16	6	-13	-4127	-5308	1181	5	7	4	-5762	-7241	1479
16	6	-17	6379	7283	-904	5	7	3	2969	3664	-695
16	6	-21	-4954	-6314	1360	5	7	2	3171	3944	-773
18	6	5	-4353	-3903	-450	5	7	0	7289	8470	-1181
18	6	3	-3741	-3859	150	5	7	-1	-3927	-3196	-731

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
[illegible]	7	-2	[illegible]	-2772	288	2	8	-4	6560	7503	-943
5	7	-3	-2831	-2953	122	2	8	-8	-3660	-5719	1059
5	7	-7	-5196	-4939	-257	2	8	-23	4102	1881	2221
5	7	-9	-3765	-2912	-853	4	8	14	3644	2763	881
5	7	-10	-4170	-2457	-1713	4	8	3	3967	4519	-552
5	7	-11	3468	2256	1212	4	8	0	4710	4863	-153
7	7	9	3967	3046	921	4	8	-1	-3495	-3760	265
7	7	6	4926	5867	-941	4	8	-4	-3292	-3701	409
7	7	5	-5925	-5543	-382	6	8	6	4900	4415	485
7	7	2	-7936	-8601	665	6	8	5	-4710	-4574	164
7	7	1	5196	4165	1031	6	8	2	-4143	-3305	-838
7	7	0	3466	3681	-213	6	8	0	3198	2881	317
7	7	-1	2186	491	1695	6	8	-1	-2591	-2810	219
7	7	-2	2942	2863	79	6	8	-2	2631	2871	-240
7	7	-3	-5331	-5762	431	6	8	-3	-5331	-5377	46
7	7	-5	-4630	-4379	-251	6	8	-4	-3603	-4374	771
7	7	-6	-4062	-4242	180	6	8	-6	-2591	-2093	-498
7	7	-11	4035	4298	-263	6	8	-7	2658	1695	963
7	7	-15	-3632	-5449	1617	6	8	-12	3576	3315	261
9	7	15	4278	2607	1671	6	8	-16	-5182	-4568	-614
9	7	8	-4953	-5570	617	8	8	6	3036	2828	208
9	7	7	4360	4496	-136	8	8	4	4751	4869	-118
9	7	4	5182	5489	-307	8	8	0	-3495	-3776	281
9	7	3	-3090	-3147	57	8	8	-6	3239	3476	-237
9	7	0	-5493	-4968	-525	8	8	-8	3117	3315	-198
9	7	-1	4616	3604	1012	8	8	-9	2793	1448	1345
9	7	-3	3292	3066	226	8	8	-10	-4332	-4705	373
9	7	-4	2887	2597	290	8	8	-12	-3468	-1416	-2052
9	7	-9	-3967	-3280	-687	8	8	-14	4561	4231	330
9	7	-13	5075	5077	-2	10	8	8	-4237	-3674	-563
11	7	6	-5007	-4357	-650	10	8	4	3415	4665	-1270
11	7	2	4021	3208	813	10	8	1	4291	4487	-196
11	7	-3	-3171	-2714	-457	10	8	0	-2887	-3632	745
11	7	-7	4670	4589	81	10	8	-6	-4319	-3528	-791
11	7	-10	3550	3454	96	10	8	-7	5345	5076	269
11	7	-14	-5466	-5556	90	10	8	-8	3900	3155	745
11	7	-16	3550	3568	-18	10	8	-10	4656	5370	-714
13	7	9	4035	3211	824	10	8	-12	-4035	-3712	-323
13	7	1	-3198	-2236	-962	10	8	-14	-3955	-2977	-978
13	7	-1	4580	3543	1037	10	8	-15	3955	3469	486
13	7	-2	-4143	-3530	-613	12	8	6	4481	5090	-609
13	7	-3	4630	3890	740	12	8	0	-3171	-3173	2
13	7	-5	-6155	-4359	-1796	12	8	-2	3090	2580	510
13	7	-7	-4751	-5857	1106	12	8	-4	4251	3527	724
13	7	-18	4360	3175	1185	12	8	-5	-4102	-4851	749
15	7	3	3927	3284	643	12	8	-6	-4495	-4249	-246
15	7	-7	-5592	-6688	696	14	8	-2	-6290	-6068	-222
15	7	-11	3632	3513	119	14	8	-6	6600	5907	693
15	7	-18	5075	3654	1421	14	8	-8	-3576	-3213	-363
17	7	0	6006	6442	-436	14	8	-19	-4400	-3440	-960
17	7	-4	-3671	-3224	-447	16	8	4	-4372	-5943	1571
17	7	-8	3266	840	2426	16	8	0	4980	6070	-1090
17	7	-19	4251	3670	581	16	8	-4	-3711	-4922	1211
19	7	2	-3320	-1830	-1990	16	8	-8	4319	3315	1004
19	7	-14	4413	3757	656	18	8	-2	4724	3956	768
21	7	-8	3036	1652	1384	18	8	-10	-3955	-2112	-1843
21	7	-9	-4332	-1888	-2444	20	8	0	-3117	-1274	-1843
23	7	-8	-3632	-3025	-607	20	8	-3	3441	1372	2069
25	7	-13	3955	1967	1988	20	8	-8	3765	3852	-87
27	7	-15	4184	304	3880	20	8	-9	-3415	-1326	-2089
0	8	16	3697	2145	1552	20	8	-13	3792	611	3181
0	8	5	3010	3550	-540	20	8	-17	4076	74	4002
2	8	13	-3387	-2035	-1352	22	8	-6	-4143	-3740	-403
2	8	9	3765	4234	-469	22	8	-10	5844	5111	733
2	8	6	3644	5310	-1666	1	9	25	4751	170	4581
2	8	7	-2602	-2624	-75	1	9	12	-6087	-6180	93
4	8	3	4583	5324	-841	1	9	8	4561	5056	-495
4	8	0	-3232	-5640	2548	1	9	6	-2375	-492	-1883
4	8	-3	2564	3869	-1305	1	9	-6	-3002	-4072	10

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	F_o-F_c	*h*	*k*	*l*	F_o	F_c	F_o-F_c
1	9	-10	3974	3937	-563	19	9	-14	4372	3915	453
1	9	-20	3576	533	3043	0	10	10	3603	3181	422
3	9	18	-4966	-3862	-1104	0	10	7	3860	4312	-452
3	9	14	4765	4142	623	2	10	13	3671	1786	1885
3	9	10	-3495	-4353	858	2	10	12	-3671	-2849	-822
3	9	7	2969	2025	944	2	10	11	3198	1814	1384
3	9	6	-1565	-3187	1622	2	10	9	-2887	-247	-2640
3	9	-2	-2482	-4404	1922	2	10	5	2523	502	2021
3	9	-6	3617	4122	-505	2	10	-5	4184	5714	-1530
3	9	-8	-4360	-3621	-739	4	10	8	2887	710	2177
3	9	-17	3617	1899	1718	4	10	-1	3347	4164	-817
5	9	2	3347	2762	585	4	10	-5	-2915	-3938	1023
5	9	0	4400	4584	-184	4	10	-9	3603	2845	758
5	9	-2	-2335	-1965	-370	6	10	5	3644	3394	250
5	9	-4	-5657	-7327	1430	6	10	4	-3145	-3426	281
5	9	-6	2752	3546	-796	6	10	1	-3832	-5425	1593
5	9	-8	3671	3962	-291	6	10	0	4102	5274	-1172
5	9	-10	-2752	-436	-2316	6	10	-2	2307	2226	81
7	9	6	4845	5837	-992	6	10	-4	-2969	-3367	398
7	9	2	-4440	-4372	-68	6	10	-9	-3617	-3344	-273
7	9	-2	5587	4916	671	8	10	4	3374	2055	1319
7	9	-6	-2820	-1771	-1049	8	10	-2	2658	2417	241
9	9	8	-5007	-5582	575	10	10	-6	-4400	-3853	-547
9	9	7	-3765	-1529	-2236	10	10	-11	4143	3898	245
9	9	4	6627	5645	982	12	10	-4	3036	3454	-418
9	9	2	3171	3231	-60	12	10	-5	3415	2224	1191
9	9	0	-4319	-5139	820	12	10	-8	-4278	-3260	-1018
9	9	-2	-3063	-2769	-294	12	10	-12	3292	1414	1878
9	9	-8	4616	4665	-69	16	10	4	-4035	-2848	-1187
11	9	6	-3711	-3569	-142	16	10	0	2820	2812	8
11	9	-1	3036	2380	656	1	11	11	-3644	-1693	-1951
11	9	-6	-4872	-4562	-310	1	11	-4	2226	2471	-245
11	9	-10	3550	5598	-2048	1	11	-9	-3860	-3509	-351
13	9	-2	-2887	-2040	-847	3	11	12	-3468	-1470	-1998
13	9	-4	5506	7508	-2002	3	11	2	1930	1499	431
13	9	-8	-4724	-5849	1125	3	11	-2	-2186	-1960	-226
15	9	5	-4251	-2835	-1416	5	11	3	-2942	-3510	568
15	9	2	5088	4051	1037	5	11	-1	3320	3908	-588
15	9	0	2887	2586	301	7	11	0	1635	2668	-833
15	9	-2	-4076	-3979	-97	7	11	-4	-2699	-2743	44
15	9	-6	4912	4547	365	7	11	-11	-3617	-2598	-1019
15	9	-9	3522	818	2704	9	11	8	-3415	-832	-2583
17	9	2	-4400	-3301	-1099	9	11	-6	-3468	-2538	-930
17	9	0	4076	3364	712	11	11	-3	2699	1216	1483
17	9	-3	4481	3114	1367	15	11	-5	-3644	-3574	-70
17	9	-4	-3927	-3879	-48	4	12	-5	-2375	-1880	-495
19	9	-8	3550	1790	1760	12	12	0	-2699	-1549	-1150

expected for a true double bond by an interpolation between the known single (1·843 Å) [10] and triple (1·542 Å) [11] bond lengths, or from the sum of the covalent radii (1·665 Å),[12] a situation that is comparable to that generally found with CN bonds. The mean P–C_6H_5 length is 1·808 Å, which is rather shorter than that found [13] in triphenylphosphorus (1·828 Å) but not significantly so. The mean C–C length in the four benzene rings is 1·390 Å. There is a significant difference in the lengths of the two C–S bonds, that to the doubly-bonded carbon atom being 0·08 Å shorter than that to the benzene ring. This difference is in the same sense as, but rather greater than, that found by Bullough and Wheatley in comparable circumstances.[14] The bond joining the methyl group to the benzene ring has a length of 1·535 Å. The four bonds to the phosphorus atom are tetrahedrally arranged, as are the four bonds to the sulphur atom, but some

[10] D. R. Lide and D. E. Mann, *J. Chem. Phys.*, 1958, **29**, 914; L. S. Bartell and L. O. Brockway, *ibid.*, 1960, **32**, 512.
[11] J. K. Tyler, *J. Chem. Phys.*, 1964, **40**, 1170.
[12] L. Pauling, "Nature of the Chemical Bond," 1st edn., Cornell University Press, 1948.
[13] J. J. Daly, *J.*, 1964, 3799.
[14] R. K. Bullough and P. J. Wheatley, *Acta Cryst.*, 1957, **10**, 233.

TABLE 3

Bond lengths (Å) and angles (°)

S–O(1)	1·469(14)	C(2)–C(3)	1·416(25)	C(9)–C(10)	1·393(29)	C(17)–C(18)	1·338(32)
S–O(2)	1·444(15)	C(2)–C(7)	1·388(27)	C(10)–C(11)	1·363(31)	C(18)–C(19)	1·430(30)
S–C(1)	1·686(19)	C(3)–C(4)	1·348(26)	C(11)–C(12)	1·356(31)	C(20)–C(21)	1·400(25)
S–C(2)	1·767(18)	C(4)–C(5)	1·411(26)	C(12)–C(13)	1·443(30)	C(20)–C(25)	1·404(26)
P–C(1)	1·709(19)	C(5)–C(6)	1·347(29)	C(14)–C(15)	1·433(25)	C(21)–C(22)	1·398(31)
P–C(8)	1·832(18)	C(6)–C(7)	1·370(30)	C(14)–C(19)	1·401(25)	C(22)–C(23)	1·385(33)
P–C(14)	1·777(16)	C(8)–C(9)	1·412(26)	C(15)–C(16)	1·355(33)	C(23)–C(24)	1·408(30)
P–C(20)	1·815(17)	C(8)–C(13)	1·340(26)	C(16)–C(17)	1·430(35)	C(24)–C(25)	1·377(29)
C(5)–C(26)	1·533(34)						

O(1)SO(2)	117·4(8)	PC(8)C(9)	118·6(13)	C(10)C(11)C(12)	120·2(21)
O(1)SC(1)	109·6(8)	PC(8)C(13)	118·6(14)	C(11)C(12)C(13)	120·4(20)
O(2)SC(1)	110·9(9)	PC(14)C(15)	120·5(13)	C(15)C(14)C(19)	118·1(16)
O(1)SC(2)	106·6(8)	PC(14)C(19)	121·4(13)	C(14)C(15)C(16)	119·1(19)
O(2)SC(2)	104·7(8)	PC(20)C(21)	121·0(13)	C(14)C(19)C(18)	121·5(18)
C(1)SC(2)	107·0(9)	PC(20)C(25)	118·7(13)	C(15)C(16)C(17)	121·8(23)
PC(1)S	123·9(11)	C(3)C(2)C(7)	118·8(17)	C(16)C(17)C(18)	120·5(22)
C(1)PC(8)	112·6(9)	C(2)C(3)C(4)	119·1(17)	C(17)C(18)C(19)	118·7(20)
C(1)PC(14) ...	118·2(8)	C(2)C(7)C(6)	120·3(19)	C(21)C(20)C(25)	119·9(16)
C(1)PC(20) ...	105·2(8)	C(3)C(4)C(5)	121·6(17)	C(20)C(21)C(22)	119·3(18)
SC(2)C(3)	119·5(13)	C(4)C(5)C(6)	118·6(18)	C(20)C(25)C(24)	120·3(18)
SC(2)C(7)	121·7(14)	C(5)C(6)C(7)	121·6(20)	C(21)C(22)C(23)	120·7(21)
C(8)PC(14) ...	106·1(8)	C(9)C(8)C(13)	122·6(17)	C(22)C(23)C(24)	119·5(20)
C(8)PC(20) ...	107·2(8)	C(8)C(9)C(10)	116·9(18)	C(23)C(24)C(25)	120·1(19)
C(14)PC(20) ...	107·0(8)	C(8)C(13)C(12)	117·9(18)	C(4)C(5)C(26)	120·2(18)
		C(9)C(10)C(11)	121·9(20)	C(6)C(5)C(26)	121·2(19)

considerable distortions from a regular tetrahedral distribution do occur at both atoms. The mean of the three C_6H_5–P–C_6H_5 angles (106·8°) is rather greater than that found [13] in triphenylphosphorus (103·0°).

The equations for the mean least-squares planes through the four benzene rings were calculated in terms of orthogonal axes in which [*a*′] and [*b*′] coincide with the original monoclinic [*a*] and [*b*] axes, and [*c*′] is normal to them. These equations are:

Ring I	$+0{\cdot}9087X' - 0{\cdot}4012Y' - 0{\cdot}1153Z' = 0{\cdot}5343$
Ring II	$+0{\cdot}9169X' - 0{\cdot}3885Y' - 0{\cdot}0914Z' = 2{\cdot}9284$
Ring III	$-0{\cdot}1964X' - 0{\cdot}0700Y' + 0{\cdot}9780Z' = 1{\cdot}2147$
Ring IV	$+0{\cdot}5304X' + 0{\cdot}8477Y' + 0{\cdot}0053Z' = 3{\cdot}1770$

The distance of the methyl-group carbon atoms from the first plane is −0·029 Å, which is not significant. The distances of the phosphorus atom from the last three planes are +0·080, −0·080, and −0·164 Å, respectively. Each of these is highly significant, a phenomenon found elsewhere.[13–15]

It was noticeable from the molecular model that the four atoms P, S, O(1), and C(1) were almost coplanar. The weighted least-squares plane through these four atoms is given by the equation,

$$+0{\cdot}0276X' + 0{\cdot}8001Y' + 0{\cdot}5992Z' = 2{\cdot}1732.$$

None of the four atoms departs significantly from this plane, the greatest deviation being −0·061 Å for C(1). All three benzene rings attached to the phosphorus atoms are twisted in the same sense round the P–C_6H_5 bonds, so that the distribution is of the familiar "paddle-wheel" form.

There are 52 van der Waals' contacts less than 4 Å, the two shortest being O(1) . . . C(4), 3·287, and O(1) . . . C(3), 3·293 Å.

I thank Drs. A. J. Speziale and K. W. Ratts of the Monsanto Company, St. Louis, for suggesting this problem and supplying the sample.

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[*Received, February* 1*st*, 1965.]

[15] P. J. Wheatley, *J.*, 1964, 2206.