1163. *The Crystal and Molecular Structure of Aspirin.*

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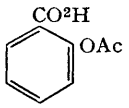
The crystal structure of aspirin (acetylsalicylic acid) has been determined by three-dimensional X-ray diffraction methods. The crystals are monoclinic, space group $P2_1/c$, with $a = 11{\cdot}446$, $b = 6{\cdot}596$, $c = 11{\cdot}388$ Å, $\beta = 95°\ 33'$. The final parameters were obtained by a least-squares refinement of 2055 intensities collected with a Hilger–Watts linear diffractometer. The eight hydrogen atoms were located from a three-dimensional difference synthesis and included in the refinement. The final R factor, including 267 planes of zero intensity, was 10·8%.

The crystal structure of aspirin (I) has not previously been determined, although it is known that a number of attempts have been made.[1] This investigation was undertaken to provide



(I)

adequate structural knowledge which might form a basis for an interpretation of the mode of operation of this remarkable drug.

Experimental.—$C_9H_8O_4$. $M = 180{\cdot}2$. Monoclinic. $a = 11{\cdot}446 \pm 0{\cdot}013$, $b = 6{\cdot}596 \pm 0{\cdot}006$, $c = 11{\cdot}388 \pm 0{\cdot}009$ Å, $\beta = 95°\ 33' \pm 2'$. $U = 855{\cdot}7$ Å^3. $D_m = 1{\cdot}40$. $Z = 4$. $D_c = 1{\cdot}398$. $F(000) = 376$. Space group $P2_1/c$ (C_{2h}^5, No. 14).

Excellent crystals (m. p. 143°) can be obtained from many common organic solvents with [b] as the axis of elongation. Those used in the present analysis were grown from benzene. The cell dimensions, obtained from oscillation photographs (Cu-K_α, $\lambda = 1{\cdot}5418$ Å), yield the axial ratio: $a:b:c :: 1{\cdot}7533:1:1{\cdot}7265$, $\beta = 95°\ 33'$. They may be compared with the optical results of Niini:[2] $a:b:c :: 1{\cdot}7322:1:1{\cdot}7322$, $\beta = 95°\ 42{\cdot}5'$, and with those of Nitta and Watanabe obtained by X-rays:[3] $a = 11{\cdot}37$, $b = 6{\cdot}54$, $c = 11{\cdot}37$ kX, $a:b:c :: 1{\cdot}7385:1:1{\cdot}7385$, $\beta = 95°\ 27'$.

The intensities were collected round [b] with Mo-K_α radiation on a Hilger–Watts linear diffracto-

[1] Private communication from Dr. J. H. Robertson.
[2] R. Niini, *Z. Krist.*, 1931, **79**, 532.
[3] I. Nitta and T. Watanabe, *Sci. Papers Inst. Phys. Chem. Res. (Tokyo)*, 1937, **31**, 125.

meter equipped with SrO–ZrO_2 balanced filters.[4] On the *h*0*l*–*h*2*l* layers, each reflexion was measured three times, and on *h*3*l*–*h*9*l* five times, with each filter. The *h*0*l*–*h*5*l* intensities were collected with a 3°, and the *h*6*l*–*h*9*l* with a 4° oscillation angle. About thirty reflexions had to be hand-measured. For these, a 4° oscillation was used. The maximum recording angle was $\theta = 30°$. A half-minute motor was used. The scale of the intensities so obtained was such that, when corrected for Lorentz and polarization factors, the resulting observed structure factors were on a scale slightly greater than absolute. In these circumstances it was felt justified to include all planes with the actual corrected count obtained, except when such a count was negative, in which case the reflexion was allotted zero intensity. In this manner 2055 independent reflexions (excluding 0*k*0) were obtained, of which 267 (13%) were zero. The analysis is based on these 2055 planes, and all values of *R* and *R'* include the zero reflexions.

The structure was solved from a sharpened three-dimensional Patterson synthesis. The

TABLE 1.

Final atomic co-ordinates in Å. Standard deviations are given as units in the last place.

Atom	*X*	*Y*	*Z*
O(1)	0·1209 (27)	1·2377 (28)	1·1004 (28)
O(2)	1·3764 (26)	0·9148 (28)	−0·5786 (27)
O(3)	3·2639 (23)	2·7176 (26)	−1·0070 (23)
O(4)	4·6127 (29)	1·4508 (33)	0·3906 (27)
C(1)	1·7513 (31)	2·8796 (34)	0·7679 (33)
C(2)	2·8180 (33)	3·3762 (34)	0·1047 (33)
C(3)	3·4249 (36)	4·5825 (39)	0·4774 (40)
C(4)	2·9845 (39)	5·3062 (40)	1·5338 (43)
C(5)	1·9428 (39)	4·8260 (40)	2·2077 (40)
C(6)	1·3357 (34)	3·6315 (37)	1·8242 (36)
C(7)	1·0279 (32)	1·5944 (34)	0·4241 (33)
C(8)	4·1795 (33)	1·7226 (39)	−0·7189 (36)
C(9)	4·5424 (45)	1·0675 (52)	−1·9791 (42)
H(1)	0·8160 (690)	−0·0133 (794)	−0·9209 (687)
H(3)	4·1336 (446)	4·8674 (491)	0·0158 (447)
H(4)	3·4349 (446)	6·1985 (501)	1·8538 (446)
H(5)	1·6477 (446)	5·3156 (498)	2·9276 (446)
H(6)	0·6357 (444)	3·3448 (494)	2·2671 (443)
H(7)	3·5432 (572)	0·7956 (657)	−2·6885 (574)
H(8)	4·9306 (572)	0·2440 (646)	−1·9332 (573)
H(9)	4·9193 (566)	1·5189 (643)	−2·4623 (573)

TABLE 2.

Thermal parameters in Å^2. Standard deviations are given as units in the last place.

Atom	U_{11}	U_{22}	U_{33}	$2U_{12}$	$2U_{23}$	$2U_{13}$
O(1)	0·0501 (15)	0·0458 (15)	0·0562 (16)	−0·0372 (25)	−0·0190 (26)	0·0416 (25)
O(2)	0·0465 (14)	0·0480 (15)	0·0518 (15)	−0·0169 (25)	−0·0285 (26)	0·0253 (24)
O(3)	0·0392 (12)	0·0416 (13)	0·0359 (12)	0·0016 (21)	0·0094 (21)	0·0136 (19)
O(4)	0·0589 (17)	0·0729 (21)	0·0413 (14)	0·0562 (32)	0·0125 (29)	0·0040 (25)
C(1)	0·0292 (15)	0·0332 (16)	0·0384 (16)	0·0005 (25)	0·0082 (27)	0·0032 (25)
C(2)	0·0366 (16)	0·0322 (16)	0·0375 (17)	0·0127 (27)	0·0084 (27)	0·0020 (26)
C(3)	0·0398 (18)	0·0394 (19)	0·0547 (22)	−0·0131 (31)	0·0127 (34)	0·0119 (32)
C(4)	0·0471 (20)	0·0380 (19)	0·0609 (24)	−0·0040 (33)	−0·0036 (36)	0·0058 (35)
C(5)	0·0483 (21)	0·0403 (19)	0·0510 (21)	0·0080 (33)	−0·0164 (34)	0·0124 (33)
C(6)	0·0341 (16)	0·0396 (18)	0·0436 (18)	−0·0022 (29)	−0·0030 (30)	0·0128 (28)
C(7)	0·0335 (16)	0·0339 (16)	0·0366 (16)	0·0057 (26)	0·0078 (27)	0·0027 (26)
C(8)	0·0309 (16)	0·0476 (20)	0·0431 (19)	−0·0029 (30)	0·0057 (32)	0·0112 (27)
C(9)	0·0582 (25)	0·0721 (30)	0·0481 (22)	0·0157 (45)	−0·0199 (43)	0·0236 (38)
H(1)	0·12 (6)	0·12 (7)	0·12 (6)	0·0 (1)	0·0 (1)	0·023 (99)
H(3)	0·04 (3)	0·04 (3)	0·04 (3)	0·0 (5)	0·0 (5)	0·008 (50)
H(4)	0·04 (3)	0·04 (3)	0·04 (3)	0·0 (5)	0·0 (5)	0·008 (50)
H(5)	0·04 (3)	0·04 (3)	0·04 (3)	0·0 (5)	0·0 (5)	0·008 (50)
H(6)	0·04 (3)	0·04 (3)	0·04 (3)	0·0 (5)	0·0 (5)	0·008 (50)
H(7)	0·08 (5)	0·08 (5)	0·08 (5)	0·0 (8)	0·0 (8)	0·015 (75)
H(8)	0·08 (5)	0·08 (5)	0·08 (5)	0·0 (8)	0·0 (8)	0·015 (75)
H(9)	0·08 (5)	0·08 (5)	0·08 (5)	0·0 (8)	0·0 (8)	0·015 (75)

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

TABLE 3.

h	k	l	F_o	F_c	Δ	h	k	l	F_o	F_c	Δ	h	k	l	F_o	F_c	Δ
0	0	14	−285	−259	−26	8	0	10	−379	−295	−84	1	1	−2	−1305	−1270	−38
0	0	12	125	66	59	8	0	8	0	11	−11	1	1	−3	2502	2438	64
0	0	10	−753	−721	−32	8	0	6	−469	−490	21	1	1	−4	461	495	−34
0	0	8	−2592	−2585	−7	8	0	4	−1237	−1308	71	1	1	−5	−2371	−2382	11
0	0	6	−597	−627	30	8	0	2	749	777	−28	1	1	−6	1114	988	126
0	0	4	−324	−141	−183	8	0	0	3109	3003	106	1	1	−7	−2904	−2738	−166
0	0	2	9561	10804	−1243	8	0	−2	2222	2091	131	1	1	−8	185	172	13
1	0	14	249	156	93	8	0	−4	387	362	25	1	1	−9	0	−61	61
1	0	12	−354	−218	−136	8	0	−6	659	642	17	1	1	−10	−110	−153	43
1	0	10	−1096	−1135	39	8	0	−8	0	58	−58	1	1	−11	170	168	2
1	0	8	−2568	−2470	−98	8	0	−10	−318	−88	−230	1	1	−12	−203	−160	−43
1	0	6	−2578	−2519	−59	8	0	−12	0	109	−109	1	1	−13	−191	−118	−73
1	0	4	−319	−297	−22	8	0	−14	−153	−299	146	1	1	−14	225	261	−36
1	0	2	−1661	−1621	−60	9	0	12	−219	−49	−170	1	1	−15	0	49	−49
1	0	0	3517	3628	89	9	0	10	0	68	−68	2	1	14	0	−43	43
1	0	−2	3242	3151	91	9	0	8	977	1035	−58	2	1	13	135	119	16
1	0	−4	−3033	−3164	131	9	0	6	1451	1595	−144	2	1	12	0	65	−65
1	0	−6	−279	−237	−42	9	0	4	1059	1061	−2	2	1	11	174	189	−15
1	0	−8	1921	1991	−70	9	0	2	−187	−226	39	2	1	10	114	77	37
1	0	−10	1467	1428	39	9	0	0	−894	−909	15	2	1	9	132	284	−152
1	0	−12	88	204	−116	9	0	−2	554	545	9	2	1	8	−299	−355	56
1	0	−14	−172	−98	−74	9	0	−4	−1033	−1100	67	2	1	7	151	75	76
2	0	12	0	−145	145	9	0	−6	−1545	−1538	−7	2	1	6	530	576	−46
2	0	10	1224	1263	−39	9	0	−8	−403	−392	−11	2	1	5	805	714	91
2	0	8	611	666	−55	9	0	−10	−623	−670	47	2	1	4	−3263	−3120	−143
2	0	6	0	142	−142	10	0	8	0	8	−8	2	1	3	5361	5374	−13
2	0	4	2654	2506	148	10	0	6	398	493	−95	2	1	2	−8846	−9211	365
2	0	2	−6704	−6850	146	10	0	4	−385	−280	−105	2	1	1	7444	7653	−209
2	0	0	−4631	−4609	−22	10	0	2	−141	−27	−114	2	1	0	2834	2841	−7
2	0	−2	4023	3913	110	10	0	0	979	1046	−67	2	1	−1	2975	2840	135
2	0	−4	−3897	−3723	−174	10	0	−2	946	965	−19	2	1	−2	2753	2655	98
2	0	−6	−1000	−942	−58	10	0	−4	114	70	44	2	1	−3	−1494	−1510	16
2	0	−8	−1183	−1218	35	10	0	−6	−819	−793	−26	2	1	−4	2628	2539	89
2	0	−10	−1940	−1942	2	10	0	−8	−904	−894	−10	2	1	−5	−2422	−2257	−165
2	0	−12	−301	−377	76	10	0	−10	−761	−663	−98	2	1	−6	1322	1305	17
2	0	−14	−225	−256	31	11	0	8	−288	−361	73	2	1	−7	−1386	−1367	−19
3	0	12	−266	−168	−98	11	0	6	−191	−180	−11	2	1	−8	−742	−780	38
3	0	10	325	317	8	11	0	4	0	−32	32	2	1	−9	592	641	−49
3	0	8	875	887	−12	11	0	2	747	683	64	2	1	−10	813	869	−56
3	0	6	−1883	−1727	−156	11	0	0	628	659	−31	2	1	−11	1264	1294	−30
3	0	4	−3222	−3172	−50	11	0	−2	−417	−411	−6	2	1	−12	777	831	−54
3	0	2	2934	2908	26	11	0	−4	−1026	−1026	0	2	1	−13	429	438	−9
3	0	0	2644	2573	71	11	0	−6	−1177	−1170	−7	3	1	14	405	353	52
3	0	−2	2671	2586	85	11	0	−8	0	167	−167	3	1	13	0	150	−150
3	0	−4	−203	−41	−162	11	0	−10	603	599	4	3	1	12	365	342	23
3	0	−6	−1892	−1834	−58	12	0	8	102	172	−70	3	1	11	−620	−600	−20
3	0	−8	189	178	11	12	0	6	767	892	−125	3	1	10	964	933	31
3	0	−10	700	728	−28	12	0	4	1260	1324	−64	3	1	9	−792	−835	43
3	0	−12	646	635	11	12	0	2	129	60	69	3	1	8	1208	1223	−15
3	0	−14	321	202	119	12	0	0	0	93	−93	3	1	7	312	286	26
4	0	12	271	445	−174	12	0	−2	0	24	24	3	1	6	−515	−569	54
4	0	10	1144	1194	−50	12	0	−4	−677	−812	135	3	1	5	−499	−566	67
4	0	8	1371	1413	−42	12	0	−6	0	−272	272	3	1	4	0	−133	133
4	0	6	−233	−345	112	12	0	−8	632	543	89	3	1	3	554	437	117
4	0	4	−839	−780	−59	12	0	−10	517	552	−35	3	1	2	−5101	−4913	−188
4	0	2	0	−218	218	13	0	4	−362	−348	−14	3	1	1	4017	3970	47
4	0	0	−4148	−4057	−91	13	0	2	−390	−403	13	3	1	0	−8607	−9138	531
4	0	−2	−1731	−1694	−37	13	0	0	233	250	−17	3	1	−1	−2927	−2884	−43
4	0	−4	−4293	−4058	−235	13	0	−2	1241	1335	−94	3	1	−2	−3931	−3899	−32
4	0	−6	−1822	−1807	−15	13	0	−4	1116	1205	−89	3	1	−3	−3749	−3590	−159
4	0	−8	4096	4185	−89	13	0	−6	0	95	−95	3	1	−4	−2866	−2685	−181
4	0	−10	2862	2759	103	14	0	4	−540	−674	134	3	1	−5	1008	980	28
4	0	−12	640	543	97	14	0	2	177	48	129	3	1	−6	−1084	−1070	−14
4	0	−14	339	229	110	14	0	0	−141	−34	−107	3	1	−7	211	246	−35
5	0	12	196	74	122	14	0	−2	570	610	−40	3	1	−8	492	505	−13
5	0	10	−121	−121	0	14	0	−4	499	316	183	3	1	−9	503	486	17
5	0	8	−653	−724	71	14	0	−6	−432	−442	10	3	1	−10	1459	1461	−2
5	0	6	332	308	24	15	0	4	−495	−617	122	3	1	−11	933	903	30
5	0	4	−1215	−1196	−17	15	0	2	−215	−273	58	3	1	−12	1464	1411	53
5	0	2	−1989	−1885	−104	15	0	0	−281	−335	54	3	1	−13	235	221	14
5	0	0	−1114	−1045	−69	15	0	−2	−350	−306	−44	4	1	12	0	59	−59
5	0	−2	−1051	−996	−55	15	0	−4	354	239	115	4	1	11	0	−76	76
5	0	−4	1896	1780	116	16	0	0	0	−29	29	4	1	10	386	450	−64
5	0	−6	901	820	81	16	0	−2	0	119	−119	4	1	9	198	236	−38
5	0	−8	1114	1115	−1	16	0	−4	403	535	−132	4	1	8	997	972	25
5	0	−10	1876	1887	−11	0	1	15	−261	−180	−81	4	1	7	507	446	61
5	0	−12	162	173	−11	0	1	14	−267	−294	27	4	1	6	769	696	73
5	0	−14	−273	−200	−73	0	1	13	−765	−716	−49	4	1	5	−1302	−1160	−142
6	0	12	−334	−277	−57	0	1	12	−530	−502	−28	4	1	4	1080	1005	75
6	0	10	0	115	−115	0	1	11	−682	−726	44	4	1	3	−4340	−4159	−181
6	0	8	0	114	−114	0	1	10	−1076	−1105	29	4	1	2	−288	−447	159
6	0	6	−1813	−1800	−13	0	1	9	−129	−212	83	4	1	1	−2924	−2899	−25
6	0	4	−2459	−2514	15	0	1	8	185	57	128	4	1	0	−77	−134	57
6	0	2	−1605	−1450	−155	0	1	7	267	261	6	4	1	−1	−459	−531	72
6	0	0	−1734	−1764	30	0	1	6	490	538	−48	4	1	−2	2848	2670	178
6	0	−2	−2025	−1719	−306	0	1	5	132	84	48	4	1	−3	−1090	−1116	26
6	0	−4	340	538	−198	0	1	4	−2792	−2696	−96	4	1	−4	263	290	−27
6	0	−6	−2358	−2330	−28	0	1	3	−1059	−1069	10	4	1	−5	−1148	−983	−165
6	0	−8	−2262	−2200	−62	0	1	2	4627	4977	−150	4	1	−6	1116	1155	−39
6	0	−10	1009	999	10	0	1	1	−3028	−3119	91	4	1	−7	−632	−518	−114
6	0	−12	702	720	−18	1	1	15	0	−80	80	4	1	−8	−662	−705	43
6	0	−14	406	413	−7	1	1	14	0	8	−8	4	1	−9	−1142	−1132	−10
7	0	12	310	355	−45	1	1	13	−256	−332	76	4	1	−10	−1929	−1930	1
7	0	10	939	956	−17	1	1	12	−182	−213	31	4	1	−11	−446	−451	5
7	0	8	385	547	−162	1	1	11	−244	−313	69	4	1	−12	−244	−231	−13
7	0	6	−1325	−1376	51	1	1	10	687	869	18	4	1	−13	93	276	−183
7	0	4	−1309	−1300	−9	1	1	9	1155	1097	38	5	1	12	−278	−58	−220
7	0	2	404	292	112	1	1	8	2172	2124	48	5	1	11	890	903	−13
7	0	0	4343	4261	82	1	1	7	1295	1305	−10	5	1	10	−877	−923	46
7	0	−2	1695	1779	−116	1	1	6	2637	2768	−69	5	1	9	266	345	−79
7	0	−4	−1308	−1206	−102	1	1	5	−723	−711	−12	5	1	8	0	−127	127
7	0	−6	−513	−491	−22	1	1	4	−1837	−1991	154	5	1	7	167	73	94
7	0	−8	−1622	−1660	38	1	1	3	2269	2159	110	5	1	6	−514	−456	−58
7	0	−10	−787	−774	−13	1	1	2	−7345	−7613	268	5	1	5	−959	−882	−77
7	0	−12	193	249	−56	1	1	1	1573	1650	−77	5	1	4	−3336	−3317	−19
7	0	−14	−511	−506	−5	1	1	0	−2693	−2664	−29	5	1	3	−3157	−3155	−2
8	0	12	523	534	−11	1	1	−1	−1092	−1097	5	5	1	2	−1092	−969	−124

TABLE 3—*continued.*

h	k	l	F_o	F_c	Δ	h	k	l	F_o	F_c	Δ	h	k	l	F_o	F_c	Δ
5	1	1	0	54	−54	9	1	−6	582	540	42	1	2	9	983	1012	−29
5	1	0	614	540	74	9	1	−7	−1439	−1448	9	1	2	8	−237	−245	8
5	1	−1	3358	3296	62	9	1	−8	−174	−54	−120	1	2	7	114	156	−42
5	1	−2	4136	3995	141	9	1	−9	0	178	−178	1	2	6	1339	1324	15
5	1	−3	688	584	104	9	1	−10	−162	−253	91	1	2	5	0	−22	22
5	1	−4	3274	3158	116	9	1	−11	196	222	−26	1	2	4	1229	1128	101
5	1	−5	−505	−362	−143	10	1	10	−435	−482	47	1	2	3	187	201	−14
5	1	−6	−491	−411	−80	10	1	9	0	94	−94	1	2	2	2104	2081	23
5	1	−7	0	−125	125	10	1	8	−193	−305	112	1	2	1	−2258	−2248	−10
5	1	−8	−435	−430	−5	10	1	7	0	124	−124	1	2	0	1541	1436	105
5	1	−9	−536	−561	25	10	1	6	−342	−311	−31	1	2	−1	781	822	−41
5	1	−10	−485	−501	16	10	1	5	376	383	−7	1	2	−2	−656	−577	−79
5	1	−11	0	40	−40	10	1	4	−310	−296	−14	1	2	−3	−2359	−2367	28
5	1	−12	0	−67	67	10	1	3	1090	1079	11	1	2	−4	630	404	226
5	1	−13	196	49	147	10	1	2	0	−11	11	1	2	−5	−5702	−5494	−208
6	1	12	285	316	−31	10	1	1	1061	1068	−7	1	2	−6	534	533	1
6	1	11	481	582	−101	10	1	0	−290	−258	−32	1	2	−7	−1295	−1243	−52
6	1	10	801	790	11	10	1	−1	240	112	128	1	2	−8	−617	−560	−57
6	1	9	83	165	−82	10	1	−2	564	651	−87	1	2	−9	261	369	−108
6	1	8	875	887	−12	10	1	−3	0	−13	13	1	2	−10	−1429	−1475	46
6	1	7	−235	−250	15	10	1	−4	509	523	−14	1	2	−11	524	539	−15
6	1	6	1434	1376	58	10	1	−5	325	243	82	1	2	−12	−437	−342	−95
6	1	5	0	−151	151	10	1	−6	−227	−178	−49	1	2	−13	859	801	58
6	1	4	516	580	−64	10	1	−7	−281	−382	101	1	2	−14	286	326	−40
6	1	3	−156	−41	−115	10	1	−8	−156	−140	−16	1	2	−15	370	264	106
6	1	2	−976	−1020	44	10	1	−9	0	−111	111	2	2	14	−327	−262	−65
6	1	1	−148	−211	63	10	1	−10	196	189	7	2	2	13	138	156	−18
6	1	0	−1379	−1389	10	10	1	−11	227	319	−92	2	2	12	−294	−260	−34
6	1	−1	461	475	−14	11	1	8	0	−159	159	2	2	11	233	70	163
6	1	−2	1225	1038	187	11	1	7	342	392	−50	2	2	10	−634	−679	45
6	1	−3	1027	952	75	11	1	6	0	44	−44	2	2	9	−362	−378	−4
6	1	−4	0	−193	193	11	1	5	−407	−424	17	2	2	8	−720	−765	45
6	1	−5	850	809	41	11	1	4	407	322	85	2	2	7	817	756	61
6	1	−6	−2891	−2952	61	11	1	3	−321	−398	77	2	2	6	833	878	−45
6	1	−7	1802	1758	44	11	1	2	276	291	−15	2	2	5	1706	1675	31
6	1	−8	−1068	−1058	−10	11	1	1	0	66	−66	2	2	4	−1942	−1893	−49
6	1	−9	1498	1436	62	11	1	0	−804	−833	29	2	2	3	114	162	−48
6	1	−10	−322	−246	−76	11	1	−1	−170	−82	−88	2	2	2	−4210	−3811	−399
6	1	−11	0	209	−209	11	1	−2	−118	−164	46	2	2	1	−1524	−1459	−65
6	1	−12	0	−113	113	11	1	−3	473	494	−21	2	2	0	−2716	−2535	−181
6	1	−13	−136	−136	−62	11	1	−4	409	343	66	2	2	−1	−924	−764	−160
7	1	12	−207	−193	−14	11	1	−5	526	651	−125	2	2	−2	−2766	−2680	−86
7	1	11	−198	−117	−81	11	1	−6	180	78	102	2	2	−3	97	24	73
7	1	10	−162	−51	−111	11	1	−7	−360	−316	−44	2	2	−4	586	555	31
7	1	9	0	74	−74	11	1	−8	213	227	−14	2	2	−5	0	21	−21
7	1	8	−574	−581	7	11	1	−9	−407	−365	−42	2	2	−6	507	521	−14
7	1	7	200	143	57	11	1	−10	0	−178	178	2	2	−7	−110	−103	−7
7	1	6	585	582	3	11	1	−11	0	123	−123	2	2	−8	256	311	−55
7	1	5	1043	1001	42	12	1	6	0	−167	167	2	2	−9	322	369	−47
7	1	4	1057	1051	6	12	1	5	−529	−574	45	2	2	−10	−474	−535	61
7	1	3	0	−93	93	12	1	4	−1122	−1217	95	2	2	−11	227	200	27
7	1	2	1560	1559	1	12	1	3	−674	−988	114	2	2	−12	−697	−772	75
7	1	1	−1469	−1470	1	12	1	2	−999	−1060	61	2	2	−13	−215	−215	0
7	1	0	2447	2438	5	12	1	1	−288	−299	11	3	2	14	0	1	−1
7	1	−1	−223	−134	−89	12	1	0	−180	−138	−42	3	2	13	0	19	−19
7	1	−2	1197	1192	5	12	1	−1	221	145	76	3	2	12	414	474	−60
7	1	−3	412	377	35	12	1	−2	200	282	−82	3	2	11	−253	−30	−223
7	1	−4	2313	2292	21	12	1	−3	0	−171	171	3	2	10	1641	1641	0
7	1	−5	319	264	55	12	1	−4	1323	1381	−58	3	2	9	−784	−738	46
7	1	−6	180	16	164	12	1	−5	0	−131	131	3	2	8	1060	1082	−22
7	1	−7	1120	1174	−54	12	1	−6	1209	1258	−49	3	2	7	208	307	−99
7	1	−8	−2092	−2088	−4	12	1	−7	−167	−171	4	3	2	6	1933	1963	30
7	1	−9	450	401	49	12	1	−8	360	325	35	3	2	5	−1956	−1942	−14
7	1	−10	−793	−804	11	12	1	−9	−423	−323	−100	3	2	4	2031	1949	82
7	1	−11	−336	−394	58	13	1	6	0	−184	184	3	2	3	−2619	−2641	178
7	1	−12	−718	−600	−118	13	1	5	229	114	115	3	2	2	−5253	−4796	−457
7	1	−13	0	25	−25	13	1	4	−378	−565	187	3	2	1	−5345	−4999	−346
8	1	10	−219	−316	97	13	1	3	−397	−363	−34	3	2	0	−3292	−3178	−114
8	1	9	−208	−160	−48	13	1	2	−648	−679	31	3	2	−1	−2892	−2795	−97
8	1	8	433	338	95	13	1	1	0	−193	193	3	2	−2	−1020	−997	−23
8	1	7	−322	−228	−94	13	1	0	−164	−5	−159	3	2	−3	6123	5805	318
8	1	6	164	257	−93	13	1	−1	−213	−326	113	3	2	−4	−671	−718	−153
8	1	5	−251	−370	119	13	1	−2	358	215	143	3	2	−5	3732	3422	310
8	1	4	671	651	20	13	1	−3	−562	−550	−12	3	2	−6	−476	−506	30
8	1	3	−372	−408	36	13	1	−4	350	154	196	3	2	−7	−114	−167	53
8	1	2	203	198	5	13	1	−5	0	60	−60	3	2	−8	−716	−610	−106
8	1	1	−187	−109	−78	13	1	−6	−346	−289	−57	3	2	−9	231	109	122
8	1	0	0	−182	182	13	1	−7	353	348	5	3	2	−10	−603	−583	−20
8	1	−1	586	617	−31	14	1	2	0	−224	224	3	2	−11	−288	−218	−70
8	1	−2	−416	−407	−9	14	1	1	0	−225	225	3	2	−12	−776	−821	45
8	1	−3	653	730	−77	14	1	0	−225	−205	−20	3	2	−13	−135	−48	−87
8	1	−4	464	456	8	14	1	−1	0	−71	71	4	2	12	−167	−256	89
8	1	−5	−835	−909	74	14	1	−2	0	19	−19	4	2	11	536	556	−20
8	1	−6	172	101	71	14	1	−3	0	−25	25	4	2	10	172	148	24
8	1	−7	−1380	−1348	−32	14	1	−4	−141	−118	−23	4	2	9	1021	1024	−3
8	1	−8	−875	−935	60	14	1	−5	102	193	−91	4	2	8	−416	−435	19
8	1	−9	−151	−215	64	0	2	15	−356	−342	−14	4	2	7	151	142	49
8	1	−10	−242	−316	74	0	2	14	708	636	72	4	2	6	352	322	70
8	1	−11	−135	−97	−38	0	2	13	−597	−609	12	4	2	5	−1926	−1766	−160
8	1	−12	0	−16	16	0	2	12	1203	1209	−6	4	2	4	4695	4438	257
8	1	−13	0	−75	75	0	2	11	−518	−589	71	4	2	3	−3596	−3468	−128
9	1	10	174	113	61	0	2	10	671	711	−40	4	2	2	3258	3051	207
9	1	9	0	−11	11	0	2	9	450	426	24	4	2	1	−1542	−1380	−162
9	1	8	759	817	−58	0	2	8	1081	1158	−77	4	2	0	2126	1991	135
9	1	7	−689	−656	−33	0	2	7	1150	1149	1	4	2	−1	1480	1356	124
9	1	6	765	871	−86	0	2	6	551	537	14	4	2	−2	1736	1726	10
9	1	5	−376	−364	−12	0	2	5	−283	−245	−38	4	2	−3	1715	1639	76
9	1	4	391	461	−70	0	2	4	−848	−822	−26	4	2	−4	1439	1322	117
9	1	3	991	1017	−26	0	2	3	−1586	−1749	163	4	2	−5	1991	1778	213
9	1	2	−1192	−1175	−17	0	2	2	−2269	−2284	15	4	2	−6	757	774	−17
9	1	1	934	882	52	0	2	1	−106	−46	−60	4	2	−7	0	−158	158
9	1	0	0	−17	17	1	2	15	0	132	−132	4	2	−8	−384	−449	65
9	1	−1	536	582	−46	1	2	14	0	−44	44	4	2	−9	−658	−689	31
9	1	−2	965	762	203	1	2	13	0	20	−20	4	2	−10	141	109	32
9	1	−3	72	158	−86	1	2	12	489	510	−21	4	2	−11	263	242	21
9	1	−4	−132	−237	105	1	2	11	336	364	−28	4	2	−12	−88	−80	−8
9	1	−5	−1436	−1496	60	1	2	10	0	2	−2	4	2	−13	339	276	63

TABLE 3—*continued.*

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
5	2	12	−1006	−954	−52	9	2	5	941	991	−50	0	3	1	−4695	−4943	248
5	2	11	−399	−361	−38	9	2	4	−1099	−1131	32	1	3	15	0	270	−270
5	2	10	−658	−738	80	9	2	3	422	415	7	1	3	14	−102	−131	29
5	2	9	−293	−376	83	9	2	2	−1425	−1340	−85	1	3	13	294	74	220
5	2	8	489	474	15	9	2	1	−306	−207	−99	1	3	12	−348	−323	−25
5	2	7	408	300	108	9	2	0	491	444	47	1	3	11	83	191	−108
5	2	6	0	−16	16	9	2	−1	261	221	40	1	3	10	−454	−478	24
5	2	5	−677	−687	10	9	2	−2	251	209	42	1	3	9	466	494	−28
5	2	4	2970	2682	288	9	2	−3	−392	−408	16	1	3	8	873	842	31
5	2	3	−819	−817	−2	9	2	−4	1749	1813	−64	1	3	7	0	36	−36
5	2	2	2668	2499	169	9	2	−5	−804	−726	−78	1	3	6	1267	1327	−60
5	2	1	1291	1223	68	9	2	−6	2721	2786	−65	1	3	5	680	670	10
5	2	0	−2676	−2599	−77	9	2	−7	118	25	93	1	3	4	1761	1735	26
5	2	−1	286	277	9	9	2	−8	626	627	−1	1	3	3	180	171	9
5	2	−2	−1668	−1688	20	9	2	−9	−274	−294	20	1	3	2	764	919	−155
5	2	−3	−189	−143	−46	9	2	−10	0	−191	191	1	3	1	−2023	−1938	−85
5	2	−4	−836	−808	−28	9	2	−11	−496	−493	−3	1	3	0	−2462	−2338	−124
5	2	−5	1262	1180	82	10	2	10	0	−30	30	1	3	−1	−2730	−2543	−187
5	2	−6	444	361	83	10	2	9	174	109	65	1	3	−2	−727	−679	−48
5	2	−7	97	16	81	10	2	8	−278	−146	−132	1	3	−3	−854	−907	53
5	2	−8	409	379	30	10	2	7	267	275	−8	1	3	−4	501	497	4
5	2	−9	240	193	47	10	2	6	−205	−146	−59	1	3	−5	2271	2292	−21
5	2	−10	−223	−112	−111	10	2	5	0	153	−153	1	3	−6	1181	1200	−19
5	2	−11	237	199	38	10	2	4	−397	−343	−54	1	3	−7	1337	1300	37
5	2	−12	208	93	115	10	2	3	−835	−750	−85	1	3	−8	225	99	126
5	2	−13	−466	−450	−16	10	2	2	−1812	−1736	−76	1	3	−9	−362	−371	11
6	2	12	−508	−474	−34	10	2	1	−1437	−1389	−48	1	3	−10	−542	−565	23
6	2	11	−613	−611	−2	10	2	0	−1225	−1208	−17	1	3	−11	−83	−74	−9
6	2	10	−901	−889	−12	10	2	−1	−621	−673	52	1	3	−12	−182	−24	−158
6	2	9	−489	−443	−46	10	2	−2	−974	−906	−68	1	3	−13	−336	−244	−92
6	2	8	0	−79	79	10	2	−3	1010	1092	−82	1	3	−14	0	−146	146
6	2	7	316	348	−32	10	2	−4	−1350	−1424	74	1	3	−15	−213	−264	51
6	2	6	−500	−420	−80	10	2	−5	1115	1150	−35	2	3	12	0	140	−140
6	2	5	1540	1512	28	10	2	−6	0	27	−27	2	3	11	−321	−285	−36
6	2	4	−865	−731	−134	10	2	−7	0	73	−73	2	3	10	385	384	1
6	2	3	716	711	5	10	2	−8	423	394	29	2	3	9	0	125	−125
6	2	2	470	424	46	10	2	−9	213	130	83	2	3	8	1775	1759	16
6	2	1	−956	−994	38	10	2	−10	97	38	59	2	3	7	959	983	−24
6	2	0	−454	−128	−326	10	2	−11	−205	−45	−160	2	3	6	1494	1487	7
6	2	−1	497	495	2	11	2	8	307	89	218	2	3	5	−566	−522	−44
6	2	−2	1326	1145	181	11	2	7	138	50	88	2	3	4	−894	−898	4
6	2	−3	1152	1146	6	11	2	6	386	355	31	2	3	3	−263	−297	34
6	2	−4	1222	1222	0	11	2	5	−167	−288	101	2	3	2	−97	−152	55
6	2	−5	358	359	−1	11	2	4	800	932	−132	2	3	1	72	72	0
6	2	−6	528	466	62	11	2	3	−369	−406	37	2	3	0	−1769	−1648	−121
6	2	−7	0	39	−39	11	2	2	−1304	−1345	41	2	3	−1	−1814	−1671	−143
6	2	−8	−377	−389	12	11	2	1	−1100	−1178	78	2	3	−2	−2119	−2069	−50
6	2	−9	−816	−801	−15	11	2	0	−983	−979	−4	2	3	−3	1336	1195	141
6	2	−10	−1117	−1104	−13	11	2	−1	−529	−581	52	2	3	−4	−1198	−1173	−25
6	2	−11	−593	−646	53	11	2	−2	−242	−315	73	2	3	−5	2307	2342	−35
6	2	−12	−687	−598	−89	11	2	−3	483	509	−26	2	3	−6	−102	−115	13
6	2	−13	0	−137	137	11	2	−4	−960	−916	−44	2	3	−7	1292	1247	45
7	2	12	102	267	−165	11	2	−5	283	306	−23	2	3	−8	121	221	−100
7	2	11	−221	−183	−38	11	2	−6	0	−84	84	2	3	−9	480	479	1
7	2	10	−668	−700	32	11	2	−7	0	−26	26	2	3	−10	−258	−150	−108
7	2	9	−375	−277	−98	11	2	−8	385	460	−75	2	3	−11	245	218	27
7	2	8	−691	−705	14	11	2	−9	138	177	−39	2	3	−12	391	435	−44
7	2	7	462	471	−9	12	2	6	0	−247	247	2	3	−13	−193	−7	−186
7	2	6	−470	−423	−47	12	2	5	0	28	−28	3	3	12	0	101	−101
7	2	5	759	796	−37	12	2	4	374	325	49	3	3	11	−339	−326	−13
7	2	4	−1091	−1038	−53	12	2	3	249	217	32	3	3	10	−823	−768	−55
7	2	3	−118	−125	7	12	2	2	625	584	41	3	3	9	−704	−645	−59
7	2	2	1038	891	147	12	2	1	290	228	62	3	3	8	−1443	−1415	−28
7	2	1	593	556	37	12	2	0	−341	−399	58	3	3	7	−65	−116	51
7	2	0	299	61	238	12	2	−1	−221	−221	0	3	3	6	−237	−328	91
7	2	−1	1465	1363	102	12	2	−2	340	264	76	3	3	5	879	830	49
7	2	−2	−58	−81	23	12	2	−3	−318	−274	−44	3	3	4	−313	−307	−6
7	2	−3	1026	991	35	12	2	−4	499	525	−26	3	3	3	1086	1120	−34
7	2	−4	893	902	−9	12	2	−5	421	394	27	3	3	2	2887	2627	260
7	2	−5	566	480	86	12	2	−6	0	44	−44	3	3	1	−41	−81	40
7	2	−6	−539	−570	31	12	2	−7	392	271	121	3	3	0	4051	3994	57
7	2	−7	−741	−848	107	12	2	−8	348	296	52	3	3	−1	994	964	30
7	2	−8	−325	−349	24	12	2	−9	0	60	−60	3	3	−2	398	442	−44
7	2	−9	−1314	−1378	64	13	2	4	174	199	−25	3	3	−3	1660	1503	177
7	2	−10	153	183	−30	13	2	3	0	−18	18	3	3	−4	−476	−385	−91
7	2	−11	132	190	−58	13	2	2	481	473	8	3	3	−5	−51	−131	80
7	2	−12	138	63	75	13	2	1	−274	−214	−60	3	3	−6	−227	−184	−43
7	2	−13	563	536	27	13	2	0	−135	−210	75	3	3	−7	0	−75	75
8	2	10	341	182	159	13	2	−1	−407	−387	−20	3	3	−8	700	771	−71
8	2	9	0	−9	9	13	2	−2	−271	−329	58	3	3	−9	−862	−838	−24
8	2	8	0	168	−168	13	2	−3	93	265	−172	3	3	−10	0	105	−105
8	2	7	−193	−76	−117	13	2	−4	0	−139	139	3	3	−11	−527	−535	8
8	2	6	1170	1080	90	13	2	−5	474	518	−44	3	3	−12	−346	−462	116
8	2	5	−278	−270	−8	13	2	−6	−415	−434	19	3	3	−13	0	−79	−79
8	2	4	1031	1022	9	13	2	−7	205	267	−62	4	3	12	−276	−169	−107
8	2	3	468	443	25	14	2	2	−102	−148	46	4	3	11	−370	−301	−69
8	2	2	835	865	−30	14	2	1	−97	−39	−58	4	3	10	−1007	−943	−64
8	2	1	739	677	62	14	2	0	0	−117	117	4	3	9	−1583	−1511	−72
8	2	0	−254	−7	−247	14	2	−1	200	217	−17	4	3	8	−2007	−2006	−1
8	2	−1	211	251	−40	14	2	−2	−405	−344	−61	4	3	7	−888	−909	21
8	2	−2	−1035	−1088	53	14	2	−3	249	290	−41	4	3	6	276	279	−3
8	2	−3	−387	−339	−48	14	2	−4	0	77	−77	4	3	5	−393	−358	−35
8	2	−4	785	774	11	14	2	−5	0	114	−114	4	3	4	1135	1069	66
8	2	−5	−1524	−1467	−57	0	3	15	0	50	−50	4	3	3	−223	−142	−81
8	2	−6	1215	1177	38	0	3	14	683	653	30	4	3	2	−422	−395	−27
8	2	−7	−925	−966	41	0	3	13	−217	−226	9	4	3	1	969	876	93
8	2	−8	306	260	46	0	3	12	530	563	−33	4	3	0	−41	−35	−6
8	2	−9	−279	−219	−60	0	3	11	−348	−273	−75	4	3	−1	−388	−416	28
8	2	−10	0	9	−9	0	3	10	457	501	−44	4	3	−2	−1381	−1320	−61
8	2	−11	135	103	32	0	3	9	215	149	66	4	3	−3	674	666	8
8	2	−12	−141	−89	−52	0	3	8	710	716	−6	4	3	−4	−764	−688	−76
8	2	−13	631	562	69	0	3	7	−633	−599	−34	4	3	−5	1932	1907	25
9	2	10	0	−166	166	0	3	6	135	191	−56	4	3	−6	896	917	−21
9	2	9	−278	−223	−55	0	3	5	189	69	120	4	3	−7	−97	−173	76
9	2	8	−454	−511	57	0	3	4	1677	1768	−91	4	3	−8	1346	1384	−38
9	2	7	0	57	−57	0	3	3	326	288	40	4	3	−9	−973	−1101	128
9	2	6	−339	−301	−38	0	3	2	1539	1600	−61	4	3	−10	679	752	−73

TABLE 3—*continued.*

h	k	l	F_o	F_c	Δ	h	k	l	F_o	F_c	Δ	h	k	l	F_o	F_c	Δ
4	3	−11	−467	−463	−4	9	3	2	271	289	−18	1	4	−6	1458	1539	−81
4	3	−12	−162	−102	−60	9	3	1	189	166	23	1	4	−7	−651	−719	68
4	3	−13	−296	−310	14	9	3	0	−296	−230	−6	1	4	−8	567	631	−64
5	3	12	−172	−166	−6	9	3	−1	−1112	−1121	9	1	4	−9	338	389	−51
5	3	11	231	116	113	9	3	−2	−1085	−1106	21	1	4	−10	430	505	−75
5	3	10	454	426	69	9	3	−3	−717	−714	−3	1	4	−11	196	76	120
5	3	9	208	41	167	9	3	−4	−335	−199	−136	1	4	−12	625	593	32
5	3	8	−114	−199	85	9	3	−5	256	325	−69	1	4	−13	−219	−265	46
5	3	7	132	43	89	9	3	−6	−695	−707	12	2	4	12	0	56	−56
5	3	6	−174	−66	−108	9	3	−7	148	256	−108	2	4	11	0	90	−90
5	3	5	0	20	−20	9	3	−8	−497	−476	−21	2	4	10	0	−134	134
5	3	4	1002	978	24	9	3	−9	−129	−125	−4	2	4	9	−159	−8	−151
5	3	3	376	373	3	9	3	−10	408	377	31	2	4	8	−581	−627	46
5	3	2	−883	−884	−99	9	3	−11	−198	−77	−121	2	4	7	−1905	−1901	−4
5	3	1	−296	−278	−18	10	3	8	138	101	37	2	4	6	−1927	−1985	58
5	3	0	557	539	18	10	3	7	213	116	97	2	4	5	−955	−1035	80
5	3	−1	−1916	−1878	−36	10	3	6	465	518	−53	2	4	4	−1089	−1100	11
5	3	−2	1903	1671	232	10	3	5	−312	−267	−45	2	4	3	1842	1953	−111
5	3	−3	−927	−836	−91	10	3	4	231	296	−65	2	4	2	−789	−729	−60
5	3	−4	1444	1322	122	10	3	3	225	142	83	2	4	1	596	610	−14
5	3	−5	213	226	−13	10	3	2	701	672	29	2	4	0	−180	−114	−66
5	3	−6	732	705	27	10	3	1	164	234	−70	2	4	−1	−1354	−1309	−45
5	3	−7	0	22	−22	10	3	0	470	503	−33	2	4	−2	1169	1058	131
5	3	−8	−448	−514	66	10	3	−1	0	−31	31	2	4	−3	−1040	−1125	85
5	3	−9	−430	−510	80	10	3	−2	−1760	−1793	33	2	4	−4	256	221	35
5	3	−10	−401	−410	9	10	3	−3	875	797	78	2	4	−5	−374	−358	−16
5	3	−11	−758	−814	56	10	3	−4	−1326	−1383	57	2	4	−6	329	307	22
5	3	−12	−415	−291	−124	10	3	−5	647	629	18	2	4	−7	253	297	−44
5	3	−13	97	101	−4	10	3	−6	−193	−176	−17	2	4	−8	0	55	−55
6	3	12	−174	−85	−89	10	3	−7	542	508	34	2	4	−9	302	345	−43
6	3	11	135	124	11	10	3	−8	0	26	−26	2	4	−10	−310	−274	−36
6	3	10	0	−45	45	10	3	−9	491	462	29	2	4	−11	−304	−350	46
6	3	9	196	172	24	10	3	−10	670	615	55	3	4	12	−191	−134	−57
6	3	8	−1152	−1149	−3	10	3	−11	−372	−208	−164	3	4	11	0	−61	61
6	3	7	1097	1074	23	11	3	8	−374	−315	−59	3	4	10	−743	−751	8
6	3	6	−2876	−2808	−68	11	3	7	−301	−288	−13	3	4	9	524	589	−65
6	3	5	2812	2738	74	11	3	6	0	43	−43	3	4	8	−1078	−1148	70
6	3	4	−986	−994	8	11	3	5	0	−73	73	3	4	7	498	497	1
6	3	3	1368	1368	0	11	3	4	0	49	−49	3	4	6	−1411	−1442	31
6	3	2	696	565	131	11	3	3	−125	−180	55	3	4	5	425	465	−40
6	3	1	978	1018	−40	11	3	2	−321	−369	48	3	4	4	170	69	101
6	3	0	2083	2075	8	11	3	1	0	38	−38	3	4	3	731	808	−77
6	3	−1	1100	1139	−39	11	3	0	260	195	65	3	4	2	1084	1016	68
6	3	−2	3108	3066	42	11	3	−1	0	176	−176	3	4	1	894	922	−28
6	3	−3	−1111	−1023	−88	11	3	−2	−416	−418	2	3	4	0	118	2	116
6	3	−4	1002	961	41	11	3	−3	392	377	15	3	4	−1	470	462	8
6	3	−5	−264	−192	−72	11	3	−4	−470	−534	64	3	4	−2	1523	1518	5
6	3	−6	141	101	40	11	3	−5	761	778	−17	3	4	−3	−407	−408	1
6	3	−7	338	428	−90	11	3	−6	442	478	−36	3	4	−4	616	651	−35
6	3	−8	−177	−42	−135	11	3	−7	400	388	12	3	4	−5	0	258	−258
6	3	−9	−417	−467	50	11	3	−8	193	138	55	3	4	−6	449	512	−63
6	3	−10	−83	−119	36	11	3	−9	0	−3	3	3	4	−7	217	233	−16
6	3	−11	−369	−423	54	12	3	6	227	184	43	3	4	−8	798	836	−38
6	3	−12	0	−16	16	12	3	5	−281	−303	22	3	4	−9	−304	−406	102
6	3	−13	304	135	169	12	3	4	487	480	7	3	4	−10	−375	−378	3
7	3	10	−93	−49	−44	12	3	3	−132	−215	83	3	4	−11	−356	−322	−34
7	3	9	−331	−454	123	12	3	2	−93	−21	−72	4	4	12	279	221	58
7	3	8	121	150	−29	12	3	1	−185	−121	−64	4	4	11	0	−155	155
7	3	7	0	−161	161	12	3	0	260	345	−85	4	4	10	88	43	45
7	3	6	−537	−509	−28	12	3	−1	−758	−771	13	4	4	9	−118	−50	−68
7	3	5	656	685	−29	12	3	−2	520	518	2	4	4	8	456	463	−7
7	3	4	302	138	164	12	3	−3	−490	−445	−45	4	4	7	0	−190	190
7	3	3	430	468	−38	12	3	−4	−458	−478	20	4	4	6	718	717	1
7	3	2	264	272	−8	12	3	−5	445	443	2	4	4	5	−1237	−1240	3
7	3	1	−735	−730	−5	12	3	−6	−361	−366	5	4	4	4	−227	−178	−49
7	3	0	−1770	−1719	−51	12	3	−7	−219	−72	−147	4	4	3	97	106	−9
7	3	−1	−619	−640	21	13	3	4	97	56	41	4	4	2	233	240	−7
7	3	−2	−1430	−1443	13	13	3	3	245	149	96	4	4	1	780	716	64
7	3	−3	235	302	−67	13	3	2	221	238	−17	4	4	0	0	−163	163
7	3	−4	−1339	−1343	4	13	3	1	167	98	69	4	4	−1	185	181	4
7	3	−5	748	703	45	13	3	0	307	350	−43	4	4	−2	240	259	−19
7	3	−6	−167	−79	−88	13	3	−1	0	12	−12	4	4	−3	979	987	−8
7	3	−7	574	612	−38	13	3	−2	836	811	25	4	4	−4	1096	1135	−39
7	3	−8	1083	1101	−18	13	3	−3	−526	−496	−30	4	4	−5	138	106	32
7	3	−9	838	827	11	13	3	−4	260	304	−44	4	4	−6	451	425	26
7	3	−10	471	488	−17	13	3	−5	−263	−159	−104	4	4	−7	−65	−125	60
7	3	−11	0	219	−219	0	4	13	−296	−185	−111	4	4	−8	321	349	−28
8	3	10	138	117	21	0	4	12	−207	−206	−1	4	4	−9	447	442	5
8	3	9	93	44	49	0	4	11	375	406	−31	4	4	−10	145	132	13
8	3	8	798	809	−11	0	4	10	−114	−35	−79	4	4	−11	153	239	−86
8	3	7	−657	−672	15	0	4	9	0	−31	31	5	4	12	245	57	188
8	3	6	675	704	−29	0	4	8	0	−66	66	5	4	11	0	50	−50
8	3	5	159	0	159	0	4	7	367	361	6	5	4	10	0	37	−37
8	3	4	0	19	−19	0	4	6	989	1039	−50	5	4	9	−286	−227	−59
8	3	3	362	379	−17	0	4	5	1913	2065	−152	5	4	8	−377	−428	51
8	3	2	−312	−238	−74	0	4	4	1307	1408	−101	5	4	7	−356	−406	50
8	3	1	−2067	−2019	−48	0	4	3	878	946	−68	5	4	6	−645	−672	27
8	3	0	−1950	−1997	47	0	4	2	970	985	−15	5	4	5	0	−119	119
8	3	−1	−2000	−2137	137	0	4	1	−487	−520	33	5	4	4	−678	−658	−20
8	3	−2	−852	−855	3	1	4	12	−132	−207	75	5	4	3	1247	1232	15
8	3	−3	−872	−908	36	1	4	11	281	286	−5	5	4	2	561	580	−19
8	3	−4	895	973	−78	1	4	10	0	121	−121	5	4	1	518	577	−59
8	3	−5	−460	−430	−30	1	4	9	−1081	−1108	27	5	4	0	1052	1097	−45
8	3	−6	427	457	−30	1	4	8	−381	−404	23	5	4	−1	−1549	−1613	64
8	3	−7	233	441	−208	1	4	7	−2204	−2296	92	5	4	−2	876	810	66
8	3	−8	437	467	−30	1	4	6	−354	−433	79	5	4	−3	−1565	−1622	57
8	3	−9	0	175	−175	1	4	5	−312	−358	46	5	4	−4	962	1015	−53
8	3	−10	207	53	154	1	4	4	−785	−836	51	5	4	−5	−435	−337	−98
8	3	−11	−93	−96	3	1	4	3	1638	1789	−151	5	4	−6	−569	−601	32
9	3	10	177	142	35	1	4	2	−3103	−3038	−65	5	4	−7	570	726	−156
9	3	9	0	68	−68	1	4	1	2473	2539	−66	5	4	−8	−172	−227	55
9	3	8	316	293	23	1	4	0	−254	−274	20	5	4	−9	443	521	−78
9	3	7	−231	−672	441	1	4	−1	1373	1289	84	5	4	−10	274	373	−99
9	3	6	174	225	−51	1	4	−2	633	648	−15	5	4	−11	342	359	−17
9	3	5	208	98	110	1	4	−3	434	420	14	6	4	10	0	25	−25
9	3	4	−483	−420	−63	1	4	−4	121	139	−18	6	4	9	−177	−228	51
9	3	3	254	417	−163	1	4	−5	−191	−217	26	6	4	8	−427	−508	81

TABLE 3—*continued.*

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
6	4	7	745	754	−9	11	4	−2	328	351	−23	3	5	−10	189	187	2
6	4	6	−106	−102	−4	11	4	−3	461	488	−27	3	5	−11	487	614	−127
6	4	5	422	474	−52	11	4	−4	310	251	59	4	5	10	153	29	124
6	4	4	321	368	−47	11	4	−5	0	−86	86	4	5	9	170	54	116
6	4	3	249	274	−25	11	4	−6	0	−31	31	4	5	8	240	238	2
6	4	2	−180	−135	−45	11	4	−7	0	−45	45	4	5	7	−364	−356	−8
6	4	1	881	901	−20	12	4	4	294	337	−43	4	5	6	302	343	−41
6	4	0	−567	−603	36	12	4	3	191	215	−24	4	5	5	−1562	−537	−1025
6	4	−1	−1873	−1956	83	12	4	2	456	450	6	4	5	4	839	973	−134
6	4	−2	−2323	−2471	148	12	4	1	0	−118	118	4	5	3	−319	−311	−8
6	4	−3	−2122	−2242	120	12	4	0	729	783	−54	4	5	2	621	706	−85
6	4	−4	−2258	−2292	34	12	4	−1	−618	−706	88	4	5	1	310	290	20
6	4	−5	641	670	−29	12	4	−2	436	436	0	4	5	0	−245	−206	−39
6	4	−6	−900	−928	28	12	4	−3	−187	−257	70	4	5	−1	182	282	−100
6	4	−7	1094	1173	−79	12	4	−4	327	252	75	4	5	−2	−276	−288	12
6	4	−8	−426	−530	104	12	4	−5	0	−281	281	4	5	−3	−1756	−1893	97
6	4	−9	536	625	−89	12	4	−6	135	137	−2	4	5	−4	−1285	−1372	87
6	4	−10	307	383	−76	12	4	−7	0	57	−57	4	5	−5	−1826	−1928	102
6	4	−11	207	267	−60	13	4	2	0	92	−92	4	5	−6	−882	−914	32
7	4	10	237	383	−146	13	4	1	357	412	−55	4	5	−7	−428	−470	42
7	4	9	−207	−48	−159	13	4	0	170	237	−67	4	5	−8	72	117	−45
7	4	8	806	836	−30	13	4	−1	−449	−514	65	4	5	−9	138	123	15
7	4	7	281	277	4	13	4	−2	310	433	−123	4	5	−10	−148	−227	79
7	4	6	754	793	−39	13	4	−3	−617	−721	104	4	5	−11	273	175	98
7	4	5	279	241	38	0	5	13	138	76	62	5	5	10	346	304	42
7	4	4	582	693	−111	0	5	12	0	152	−152	5	5	9	−263	−253	−10
7	4	3	−321	−329	8	0	5	11	153	206	−53	5	5	8	−114	−29	−85
7	4	2	−302	−161	−141	0	5	10	−187	−275	88	5	5	7	325	188	137
7	4	1	522	541	−19	0	5	9	0	113	−113	5	5	6	0	−36	36
7	4	0	−836	−835	−1	0	5	8	−592	−623	31	5	5	5	874	923	−49
7	4	−1	606	621	−15	0	5	7	−273	−308	35	5	5	4	651	685	−34
7	4	−2	−1469	−1434	25	0	5	6	−844	−926	82	5	5	3	600	870	−70
7	4	−3	−884	−931	47	0	5	5	−1570	−1694	124	5	5	2	421	518	−97
7	4	−4	−876	−886	10	0	5	4	−1153	−1317	164	5	5	1	366	385	−19
7	4	−5	−810	−825	15	0	5	3	−857	−1008	151	5	5	0	−170	−118	−52
7	4	−6	0	77	−77	0	5	2	145	111	34	5	5	−1	646	683	−37
7	4	−7	0	142	−142	0	5	1	729	871	−142	5	5	−2	489	460	29
7	4	−8	−276	−485	209	1	5	13	390	399	−9	5	5	−3	0	45	−45
7	4	−9	172	161	−9	1	5	12	382	401	−19	5	5	−4	−867	−898	31
7	4	−10	−129	−185	56	1	5	11	238	212	26	5	5	−5	−551	−576	25
7	4	−11	0	−144	144	1	5	10	118	186	−68	5	5	−6	−1192	−1223	31
8	4	10	302	380	−78	1	5	9	−399	−477	78	5	5	−7	−307	−294	−13
8	4	9	−520	−587	67	1	5	8	0	165	−165	5	5	−8	0	84	−84
8	4	8	358	520	−162	1	5	7	−238	−234	−4	5	5	−9	−205	−189	−16
8	4	7	−835	−980	145	1	5	6	312	335	−23	5	5	−10	−279	−252	−27
8	4	6	83	10	73	1	5	5	−411	−418	7	5	5	−11	0	−81	81
8	4	5	231	147	84	1	5	4	−1435	−1516	81	6	5	10	478	515	−37
8	4	4	0	80	−80	1	5	3	0	78	−78	6	5	9	364	379	−15
8	4	3	187	129	58	1	5	2	−894	−916	22	6	5	8	442	421	21
8	4	2	0	−135	135	1	5	1	412	460	−48	6	5	7	0	55	−55
8	4	1	823	844	−21	1	5	0	41	75	−34	6	5	6	260	263	−3
8	4	0	0	75	−75	1	5	−1	72	105	−33	6	5	5	−579	−622	43
8	4	−1	1715	1737	−22	1	5	−2	−919	−1091	172	6	5	4	0	−64	64
8	4	−2	756	758	−2	1	5	−3	0	−70	70	6	5	3	−271	−257	−14
8	4	−3	−180	−273	93	1	5	−4	1369	1508	−139	6	5	2	225	330	−105
8	4	−4	0	−151	151	1	5	−5	−953	−1095	142	6	5	1	−276	−271	−5
8	4	−5	−633	−702	69	1	5	−6	1636	1743	−107	6	5	0	−249	−181	−68
8	4	−6	196	81	115	1	5	−7	−235	−179	−56	6	5	−1	151	226	−75
8	4	−7	−114	−14	−100	1	5	−8	102	80	22	6	5	−2	−582	−570	−12
8	4	−8	172	170	2	1	5	−9	488	588	−100	6	5	−3	1189	1230	−41
8	4	−9	0	143	−143	1	5	−10	205	181	24	6	5	−4	−65	−49	−16
8	4	−10	−231	−89	−142	1	5	−11	−153	−110	−43	6	5	−5	299	266	33
8	4	−11	0	176	−176	1	5	−12	0	−217	217	6	5	−6	−514	−616	102
9	4	8	235	282	−47	1	5	−13	−263	−135	−68	6	5	−7	0	−72	72
9	4	7	−849	−910	61	1	5	−14	−348	−301	−47	6	5	−8	−138	−50	−88
9	4	6	310	385	−75	2	5	10	0	−143	143	6	5	−9	170	92	78
9	4	5	−613	−638	25	2	5	9	162	163	−1	6	5	−10	325	303	22
9	4	4	302	325	−23	2	5	8	−511	−551	40	6	5	−11	391	347	44
9	4	3	0	9	−9	2	5	7	97	91	6	7	5	8	88	38	50
9	4	2	517	505	12	2	5	6	−513	−552	39	7	5	7	121	97	24
9	4	1	−633	−581	−52	2	5	5	594	514	80	7	5	6	−515	−555	40
9	4	0	−132	−76	−56	2	5	4	−217	−285	68	7	5	5	−518	−570	52
9	4	−1	−472	−540	68	2	5	3	443	413	30	7	5	4	−479	−512	33
9	4	−2	−510	−518	8	2	5	2	0	−63	63	7	5	3	0	−89	89
9	4	−3	0	−215	215	2	5	1	510	625	−115	7	5	2	−97	−164	67
9	4	−4	−795	−876	81	2	5	0	1160	1209	−49	7	5	1	805	900	−95
9	4	−5	−77	−72	−5	2	5	−1	874	916	−42	7	5	0	−254	−214	−40
9	4	−6	−378	−386	8	2	5	−2	276	332	−56	7	5	−1	244	314	−70
9	4	−7	428	442	−14	2	5	−3	1393	1552	−159	7	5	−2	0	73	−73
9	4	−8	285	266	19	2	5	−4	−114	−78	−36	7	5	−3	−562	−564	2
9	4	−9	420	485	−65	2	5	−5	987	1130	−133	7	5	−4	716	733	−17
10	4	8	−245	−294	49	2	5	−6	532	574	−42	7	5	−5	−927	−1011	84
10	4	7	193	93	100	2	5	−7	0	44	−44	7	5	−6	205	81	124
10	4	6	−162	−247	85	2	5	−8	−148	−119	−29	7	5	−7	−552	−615	63
10	4	5	0	−121	121	2	5	−9	0	69	−69	7	5	−8	118	143	−25
10	4	4	−331	−298	−33	2	5	−10	0	−164	164	7	5	−9	−177	−85	−92
10	4	3	191	171	20	2	5	−11	0	6	−6	8	5	8	167	274	−87
10	4	2	118	118	0	3	5	10	−196	−117	−79	8	5	7	−125	−133	8
10	4	1	−276	−260	−16	3	5	9	332	285	47	8	5	6	211	223	−12
10	4	0	−298	−259	−39	3	5	8	−398	−344	−54	8	5	5	−203	−264	61
10	4	−1	164	12	152	3	5	7	−512	−567	55	8	5	4	211	191	20
10	4	−2	−141	−64	−77	3	5	6	397	358	39	8	5	3	−469	−455	−14
10	4	−3	0	8	−8	3	5	5	−1493	−1597	104	8	5	2	−151	−89	−62
10	4	−4	370	450	−80	3	5	4	832	796	36	8	5	1	316	342	−26
10	4	−5	−425	−363	−42	3	5	3	−1395	−1499	104	8	5	0	0	78	−78
10	4	−6	0	146	−146	3	5	2	−182	−243	61	8	5	−1	102	30	72
10	4	−7	0	92	−92	3	5	1	567	545	22	8	5	−2	−233	−325	92
10	4	−8	229	255	−26	3	5	0	177	182	−5	8	5	−3	−425	−524	99
10	4	−9	−435	−331	−104	3	5	−1	794	831	−37	8	5	−4	0	−30	30
11	4	6	0	−83	83	3	5	−2	−1280	−1375	95	8	5	−5	−354	−535	181
11	4	5	−135	−209	74	3	5	−3	532	568	−36	8	5	−6	306	375	−69
11	4	4	−208	−120	−88	3	5	−4	−2562	−2738	176	8	5	−7	−223	−260	37
11	4	3	0	94	−94	3	5	−5	854	916	−62	8	5	−8	−215	−192	−23
11	4	2	88	24	64	3	5	−6	−182	−141	−41	8	5	−9	290	253	37
11	4	1	562	531	31	3	5	−7	253	282	−29	9	5	6	0	−36	36
11	4	0	531	533	−58	3	5	−8	146	243	−95	9	5	5	0	−42	42
11	4	−1	412	461	−69	3	5	−9	527	577	−50	9	5	4	−83	−13	−70

TABLE 3—*continued.*

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
9	5	3	−627	−635	68	3	6	−5	559	518	41	10	6	2	−210	−28	−182
9	5	2	459	485	−26	3	6	−6	−184	−151	−33	10	6	1	−296	−254	−42
9	5	1	−745	−771	26	3	6	−7	−578	−603	25	10	6	0	0	−39	39
9	5	0	335	444	−109	3	6	−8	−516	−519	3	10	6	−1	430	368	62
9	5	−1	0	84	−84	3	6	−9	0	−134	134	10	6	−2	−166	−218	52
9	5	−2	379	381	−2	4	6	10	383	197	186	10	6	−3	908	840	68
9	5	−3	349	374	−25	4	6	9	609	504	105	10	6	−4	−323	−372	49
9	5	−4	683	655	28	4	6	8	459	386	73	10	6	−5	332	313	19
9	5	−5	141	178	−37	4	6	7	565	542	23	0	7	10	299	357	−58
9	5	−6	557	637	−80	4	6	6	100	103	−3	0	7	9	−566	−607	41
9	5	−7	−177	−161	−16	4	6	5	−91	−50	−41	0	7	8	801	828	−27
9	5	−8	88	107	−19	4	6	4	123	52	71	0	7	7	−742	−810	68
9	5	−9	−132	−49	−83	4	6	3	0	−163	163	0	7	6	180	198	−18
10	5	6	−573	−592	19	4	6	2	−219	−69	−130	0	7	5	−286	−304	18
10	5	5	0	59	−59	4	6	1	277	208	69	0	7	4	−219	−269	50
10	5	4	0	−349	349	4	6	0	1144	1077	67	0	7	3	−244	−313	69
10	5	3	0	110	−110	4	6	−1	−915	−822	−93	0	7	2	−81	−89	8
10	5	2	457	367	90	4	6	−2	1586	1484	102	0	7	1	274	448	−174
10	5	1	370	280	90	4	6	−3	−582	−424	−158	1	7	10	−116	−187	71
10	5	0	590	651	−61	4	6	−4	430	442	−12	1	7	9	197	40	157
10	5	−1	453	563	−110	4	6	−5	469	470	−1	1	7	8	407	373	34
10	5	−2	476	457	19	4	6	−6	321	325	−4	1	7	7	−174	−110	−64
10	5	−3	281	302	−21	4	6	−7	−495	−485	−10	1	7	6	160	150	10
10	5	−4	0	−140	140	4	6	−8	−153	−156	3	1	7	5	166	212	−46
10	5	−5	0	178	−178	4	6	−9	−283	−249	−34	1	7	4	0	77	−77
10	5	−6	125	95	30	5	6	8	396	317	79	1	7	3	433	377	56
10	5	−7	0	−221	221	5	6	7	838	714	124	1	7	2	586	563	23
11	5	4	0	−65	65	5	6	6	0	58	−58	1	7	1	244	256	−12
11	5	3	159	240	−81	5	6	5	0	217	−217	1	7	0	531	949	−418
11	5	2	377	407	−30	5	6	4	−367	−282	−85	1	7	−1	108	114	−6
11	5	1	469	432	37	5	6	3	−848	−790	−58	1	7	−2	739	793	−54
11	5	0	507	558	−51	5	6	2	−602	−506	−96	1	7	−3	−370	−403	33
11	5	−1	217	253	−36	5	6	1	−605	−503	−102	1	7	−4	−100	−43	−57
11	5	−2	−125	−189	64	5	6	0	479	465	14	1	7	−5	0	41	−41
11	5	−3	−298	−271	−27	5	6	−1	−459	−404	−55	1	7	−6	−180	−99	−81
11	5	−4	−376	−507	131	5	6	−2	742	711	31	1	7	−7	0	−2	2
11	5	−5	−371	−354	−17	5	6	−3	−791	−769	−22	1	7	−8	−261	−97	−164
12	5	0	187	245	−58	5	6	−4	−403	−399	−4	1	7	−9	−397	−353	−44
12	5	−1	263	293	−10	5	6	−5	−91	−45	−46	2	7	8	0	87	−87
12	5	−2	313	408	−95	5	6	−6	−197	−182	−15	2	7	7	631	575	56
12	5	−3	211	46	165	5	6	−7	−237	−149	−88	2	7	6	781	691	90
0	6	10	267	253	14	5	6	−8	0	−59	59	2	7	5	490	475	15
0	6	9	−299	−273	−26	5	6	−9	0	−134	134	2	7	4	193	67	126
0	6	8	845	793	52	6	6	8	0	−91	91	2	7	3	−237	−176	−61
0	6	7	−1063	−998	−65	6	6	7	512	456	56	2	7	2	−252	−244	−8
0	6	6	672	609	63	6	6	6	−460	−471	11	2	7	1	−741	−712	−29
0	6	5	−835	−790	−45	6	6	5	438	411	27	2	7	0	−100	−149	49
0	6	4	100	66	34	6	6	4	−352	−361	9	2	7	−1	237	235	2
0	6	3	−652	−611	−41	6	6	3	−306	−227	−79	2	7	−2	0	−6	6
0	6	2	−203	−206	3	6	6	2	0	43	−43	2	7	−3	91	123	−32
0	6	1	−452	−631	179	6	6	1	−445	−318	−127	2	7	−4	254	222	32
1	6	10	0	3	−3	6	6	0	−449	−282	−167	2	7	−5	0	158	−158
1	6	9	−108	−56	−52	6	6	−1	296	241	55	2	7	−6	277	260	17
1	6	8	383	402	−19	6	6	−2	326	340	−14	2	7	−7	613	698	−85
1	6	7	0	−131	131	6	6	−3	−346	−321	−25	2	7	−8	0	246	−246
1	6	6	−123	−191	68	6	6	−4	233	256	−23	2	7	−9	−197	−33	−164
1	6	5	−379	−407	28	6	6	−5	−244	−251	7	3	7	8	−277	−56	−215
1	6	4	−885	−817	−68	6	6	−6	0	−132	132	3	7	7	615	577	38
1	6	3	−332	−318	−14	6	6	−7	−153	−212	59	3	7	6	410	354	56
1	6	2	148	115	33	6	6	−8	197	246	−49	3	7	5	479	430	49
1	6	1	−1269	−617	−652	6	6	−9	−386	−350	−36	3	7	4	−81	−5	−76
1	6	0	0	45	−45	7	6	8	−312	−115	−197	3	7	3	171	168	−37
1	6	−1	309	301	8	7	6	7	116	33	83	3	7	2	−259	−228	−31
1	6	−2	410	438	−28	7	6	6	−309	−27	−282	3	7	1	−493	−463	−30
1	6	−3	0	−1	1	7	6	5	108	104	4	3	7	0	−180	−172	−8
1	6	−4	227	242	−15	7	6	4	0	−177	177	3	7	−1	−229	162	−67
1	6	−5	−958	−882	−76	7	6	3	292	160	132	3	7	−2	289	282	7
1	6	−6	−1075	−1029	−46	7	6	2	−170	−152	−18	3	7	−3	0	146	−146
1	6	−7	−136	−143	7	7	6	1	0	−45	45	3	7	−4	539	537	2
1	6	−8	−100	−145	45	7	6	0	0	−61	61	3	7	−5	−566	−526	−40
1	6	−9	−108	−221	113	7	6	−1	214	168	46	3	7	−6	−189	−210	21
1	6	−10	339	339	0	7	6	−2	339	265	74	3	7	−7	−247	−197	−50
2	6	10	116	33	83	7	6	−3	280	262	18	3	7	−8	−410	−464	54
2	6	9	−160	−35	−125	7	6	−4	370	329	41	3	7	−9	0	1	−1
2	6	8	−359	−357	−2	7	6	−5	426	251	175	4	7	8	−233	−111	−122
2	6	7	0	54	−54	7	6	−6	292	177	115	4	7	7	0	−69	69
2	6	6	0	−112	112	7	6	−7	449	374	75	4	7	6	292	211	81
2	6	5	0	73	−73	7	6	−8	241	200	41	4	7	5	0	33	−33
2	6	4	280	101	179	7	6	−9	219	37	182	4	7	4	203	139	64
2	6	3	510	450	60	8	6	6	493	346	147	4	7	3	329	262	67
2	6	2	547	494	53	8	6	5	−203	−284	81	4	7	2	0	20	−20
2	6	1	214	178	36	8	6	4	−280	−229	−51	4	7	1	−543	−464	−59
2	6	0	227	236	−9	8	6	3	−533	−473	−60	4	7	0	758	734	24
2	6	−1	997	915	82	8	6	2	0	−65	65	4	7	−1	−1051	−989	−62
2	6	−2	−1487	−1319	−168	8	6	1	−100	−260	160	4	7	−2	352	379	−27
2	6	−3	1662	1541	121	8	6	0	605	489	116	4	7	−3	0	−57	57
2	6	−4	−1925	−1785	−140	8	6	−1	254	90	164	4	7	−4	−81	−43	−38
2	6	−5	−492	−539	47	8	6	−2	333	370	−37	4	7	−5	−207	−222	15
2	6	−6	−1606	−1521	−85	8	6	−3	184	120	64	4	7	−6	0	−111	111
2	6	−7	−825	−804	−21	8	6	−4	569	459	110	4	7	−7	180	47	133
2	6	−8	−626	−520	−106	8	6	−5	0	−71	71	5	7	6	0	−86	86
2	6	−9	−108	−155	47	8	6	−6	−160	−37	−123	5	7	5	0	145	−145
3	6	10	123	122	1	8	6	−7	400	291	109	5	7	4	−214	−123	−91
3	6	9	116	97	19	9	6	4	−270	−225	−45	5	7	3	−203	−118	−85
3	6	8	416	329	87	9	6	3	−233	−205	−28	5	7	2	−430	−359	−71
3	6	7	−180	−253	73	9	6	2	−229	−37	−192	5	7	1	−116	−249	133
3	6	6	−752	−112	−640	9	6	1	299	236	63	5	7	0	321	305	16
3	6	5	−592	−582	0	9	6	0	465	475	−10	5	7	−1	−890	−925	35
3	6	4	623	518	105	9	6	−1	834	784	50	5	7	−2	595	578	17
3	6	3	0	−2	2	9	6	−2	649	591	58	5	7	−3	−483	−439	−44
3	6	2	766	732	36	9	6	−3	638	633	5	5	7	−4	227	307	−80
3	6	1	108	160	−52	9	6	−4	0	50	−50	5	7	−5	259	284	−25
3	6	0	520	527	−7	9	6	−5	−237	−219	−18	5	7	−6	460	380	80
3	6	−1	61	24	37	9	6	−6	−270	−306	36	5	7	−7	148	143	5
3	6	−2	−1231	−1115	−116	9	6	−7	−438	−402	−36	6	7	6	−379	−389	10
3	6	−3	1390	1292	98	10	6	4	0	53	−53	6	7	5	265	337	−72
3	6	−4	−649	−606	−43	10	6	3	0	−174	174	6	7	4	−252	−97	−155

TABLE 3—*continued.*

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
6	7	3	261	235	23	0	8	5	469	464	5	3	8	−5	0	−60	60
6	7	2	−870	−793	−77	0	8	4	619	674	−55	4	8	4	91	1	90
6	7	1	633	583	50	0	8	3	389	373	16	4	8	3	244	80	164
6	7	0	−662	−687	25	0	8	2	116	207	−91	4	8	2	−160	−47	−113
6	7	−1	600	498	102	0	8	1	136	284	−148	4	8	1	−321	−285	−36
6	7	−2	651	557	94	1	8	7	−143	−66	−77	4	8	0	−321	−306	−15
6	7	−3	436	358	78	1	8	6	233	214	19	4	8	−1	−197	−107	−90
6	7	−4	312	290	22	1	8	5	274	345	−71	4	8	−2	−283	−251	−32
6	7	−5	412	358	54	1	8	4	701	648	53	4	8	−3	390	213	177
6	7	−6	0	38	−38	1	8	3	−148	−33	−115	4	8	−4	445	408	37
6	7	−7	−108	−257	149	1	8	2	493	503	−10	4	8	−5	0	250	−250
7	7	6	−237	−78	−159	1	8	1	−314	−434	120	5	8	4	−656	−503	−153
7	7	5	−363	−335	−28	1	8	0	0	−108	108	5	8	3	−247	−141	−106
7	7	4	−153	−72	−81	1	8	−1	−223	−301	78	5	8	2	−312	−307	−5
7	7	3	−180	−202	22	1	8	−2	−352	−349	−3	5	8	1	−170	−25	−145
7	7	2	−174	−280	106	1	8	−3	130	80	50	5	8	0	0	69	−69
7	7	1	197	124	73	1	8	−4	0	70	−70	5	8	−1	−207	−194	−13
7	7	0	−721	−713	−8	1	8	−5	143	116	27	5	8	−2	193	20	173
7	7	−1	725	762	−37	1	8	−6	296	247	49	5	8	−3	283	339	−56
7	7	−2	0	−13	13	1	8	−7	−100	−46	−54	5	8	−4	465	418	47
7	7	−3	633	594	39	2	8	6	−277	−246	−31	5	8	−5	197	216	−19
7	7	−4	296	310	−14	2	8	5	0	48	−48	6	8	2	−749	−729	−20
7	7	−5	377	432	−55	2	8	4	−160	−109	−51	6	8	1	160	245	−85
7	7	−6	−339	−210	−129	2	8	3	−229	−173	−56	6	8	0	−363	−392	29
7	7	−7	0	62	−62	2	8	2	203	173	30	6	8	−1	184	46	138
8	7	4	−622	−489	−133	2	8	1	−123	−104	−19	6	8	−2	−455	−417	−38
8	7	3	−252	−189	−63	2	8	0	0	76	−76	6	8	−3	0	54	−54
8	7	2	0	−17	17	2	8	−1	116	103	13	7	8	0	−579	−658	79
8	7	1	−214	−178	−36	2	8	−2	−57	−48	−9	0	9	3	0	42	−42
8	7	0	−321	−281	−40	2	8	−3	−116	−43	−73	0	9	2	0	−3	3
8	7	−1	−184	−93	−91	2	8	−4	0	−68	68	0	9	1	91	17	74
8	7	−2	148	2	146	2	8	−5	81	97	−16	1	9	3	−219	−237	18
8	7	−3	153	23	130	3	8	6	0	−74	74	1	9	2	143	99	44
8	7	−4	449	534	−85	3	8	5	210	128	82	1	9	1	40	51	−11
8	7	−5	326	296	30	3	8	4	−148	−54	−94	1	9	0	0	−92	92
9	7	2	0	−38	38	3	8	3	440	486	−46	1	9	−1	180	241	−61
9	7	1	−306	−202	−104	3	8	2	−180	−85	−95	1	9	−2	−241	−276	35
9	7	0	0	−96	96	3	8	1	130	211	−81	1	9	−3	214	261	−47
9	7	−1	−301	−179	−122	3	8	0	−261	−272	11	2	9	2	184	170	14
9	7	−2	−430	−421	−9	3	8	−1	130	176	−46	2	9	1	0	148	−148
9	7	−3	0	38	−38	3	8	−2	0	−134	134	2	9	0	0	25	−25
0	8	7	143	136	7	3	8	−3	−100	−10	−90	2	9	−1	40	159	−119
0	8	6	207	294	−87	3	8	−4	−116	−78	−38	3	9	0	−148	−234	86

fourteen peaks within 2·8 Å of the origin due to the salicylic acid residue[5] were resolved and identified. This gave the orientation of the molecule. It was then assumed that the molecules would be linked into dimers across centres of symmetry by hydrogen bonds of length 2·65 Å. This assumption, which proved to be justified, yielded positions for ten of the thirteen heavier atoms, and the chosen co-ordinates gave $R = 45\%$ for the 182 $h0l$ reflexions. A Fourier synthesis with the $h0l$ phased structure factors showed plausible positions for the three heavier atoms of the acetyl group, and this projection was then rapidly refined to $R = 15\%$ by Fourier and difference syntheses. The y co-ordinates could be chosen from a model of the molecule, and immediately gave satisfactory agreement for the 300 planes with $\sin\theta/\lambda < 0{\cdot}35$. The structure was then refined by a least-squares procedure which uses the block diagonal approximation. At first only the nine carbon and four oxygen atoms were included until R for the 2055 planes fell to 13·3% and $R'[= \sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]$ to 1·33%. A three-dimensional difference map was then calculated with the 300 low-order planes and yielded positions for all eight hydrogen atoms, though the hydrogen atom involved in the hydrogen bond was a low peak showing considerable elongation towards the oxygen atoms with which it interacts. The hydrogen atoms were included in the refinement until R finally dropped to 10·6% and R' to 0·75%. Refinement was concluded when the maximum value of Δ/σ for a co-ordinate of a hydrogen atom had fallen to 0·3. By this time the heavier atoms had stopped moving completely. Constant weights were used, as we have found them more satisfactory for diffractometer intensities than a Cruickshank weighting scheme, which was devised for photographic intensities.[6] In all twenty-one three-dimensional least-squares refinement cycles were performed.

The least-squares programme necessarily refines the hydrogen atoms with anisotropic thermal factors if the heavier atoms are so refined. As might be expected, the thermal factors of the hydrogen atoms were often meaningless, merely reflecting the inadequacy of the data. Consequently a final set of structure factors was calculated with anisotropic thermal factors for the carbon and oxygen atoms, and mean isotropic thermal factors for the three different types of hydrogen atoms. The final value of R was 10·8%. The scattering factors were taken from International Tables. All

[5] H. Lipson and W. Cochran, "The Determination of Crystal Structures," 1953, G. Bell and Sons Ltd., London, p. 189.

[6] D. W. J. Cruickshank *et al.*, "Computing Methods and the Phase Problem in *X*-ray Crystal Analysis," 1961, Pergamon Press, London, p. 45.

TABLE 4.

Analysis of observed and calculated structure factors as a function of the index of the layer line. All figures are on an absolute scale.

k	$\Sigma\|F_o\|$	$\Sigma\|F_c\|$	$\Sigma\|\Delta\|$	N	R	$\Sigma\|\Delta\|/N$
0	1957·35	1959·25	142·02	182	0·073	0·780
1	2843·60	2868·88	229·90	332	0·081	0·693
2	2474·82	2400·10	221·04	328	0·089	0·674
3	1890·09	1873·04	179·53	304	0·095	0·591
4	1327·80	1405·83	165·09	269	0·124	0·614
5	921·21	988·13	154·60	231	0·168	0·669
6	711·04	649·85	132·69	181	0·187	0·733
7	418·06	407·14	91·04	140	0·218	0·650
8	163·78	157·69	48·87	73	0·298	0·670
9	15·00	20·55	8·19	15	0·546	0·546
All	12722·75	12730·46	1372·97	2055	0·108	0·668

calculations were carried out on an Elliott 803 computer with the programmes of Daly, Stephens, and Wheatley.[7]

Results.—The final atomic co-ordinates are given in Table 1, and the final thermal parameters in Table 2. Table 3 gives the observed and calculated structure factors obtained from the parameters given in Tables 1 and 2. In Table 4 an analysis is given of the structure factors in terms of the index of the layer. It will be seen that, although R increases substantially at higher equi-inclination angles, the absolute error in a structure factor remains approximately constant throughout.

TABLE 5.

Analysis of observed and calculated structure factors as a function of the magnitude of the observed structure factors. All figures are on an absolute scale.

Range of $\|F_o\|$	$\Sigma\|F_o\|$	$\Sigma\|F_c\|$	$\Sigma\|\Delta\|$	N	R	$\Sigma\|\Delta\|/N$
0	0	241·58	241·58	267	—	0·905
0·0— 5·0	2781·64	2637·72	616·60	1032	0·222	0·598
5·0— 10·0	2880·01	2885·18	212·61	405	0·074	0·525
10·0— 15·0	2021·92	2004·49	94·39	166	0·047	0·569
15·0— 20·0	1260·86	1237·35	63·31	72	0·050	0·879
20·0— 25·0	713·18	705·90	21·72	32	0·030	0·679
25·0— 30·0	969·72	938·46	37·44	35	0·039	1·070
30·0— 35·0	448·23	440·28	12·39	14	0·028	0·885
35·0— 40·0	228·22	219·30	8·92	6	0·039	1·487
40·0— 45·0	416·57	404·03	14·32	10	0·034	1·432
45·0— 50·0	188·48	189·67	6·77	4	0·036	1·693
50·0— 55·0	210·60	200·82	10·04	4	0·048	2·510
55·0— 60·0	57·02	54·94	2·08	1	0·036	2·080
60·0— 65·0	61·23	58·05	3·18	1	0·052	3·180
65·0— 70·0	67·04	68·50	1·46	1	0·022	1·460
70·0— 75·0	147·89	152·66	4·77	2	0·032	2·385
75·0— 80·0	—	—	—	—	—	—
80·0— 85·0	—	—	—	—	—	—
85·0— 90·0	175·43	183·49	8·96	2	0·051	4·480
90·0— 95·0	—	—	—	—	—	—
95·0—100·0	95·61	108·04	12·43	1	0·130	12·430

In Table 5 a similar analysis is given, but in terms of the magnitudes of the observed structure factors. R is poor for the very weak reflexions (and, of course, infinite, for those that are accidentally absent), but again, in terms of absolute errors, there is no reason to reject these weak planes. Indeed the evidence suggests that the twenty or thirty strongest planes should be down-weighted with respect to the weak planes. We feel that such satisfactory results for the weaker planes can be achieved with the diffractometer only if the size of the crystal or the counting time is so adjusted that the intensities yield structure factors that are on about absolute scale.

The bond lengths are given in Fig. 1, which also shows the labelling of the atoms. The bond angles are given in Table 6. Fig. 2 shows the structure as it appears when projected down the [b]

[7] J. J. Daly, F. S. Stephens, and P. J. Wheatley, 1963, *MRSA Final Report*, No. 52.

axis. The bond lengths are in fair agreement with those found in salicylic acid by Cochran,[8] though there are some very significant differences. The results for the two molecules are compared in Fig. 3. There are some very definite angular distortions within the molecule, both in the benzene ring and the carboxyl group, but, more particularly, in the acetyl group. The benzene

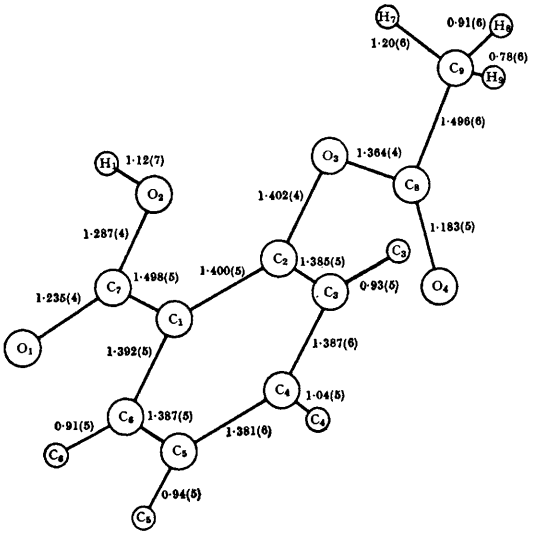


FIG. 1. Bond lengths in aspirin with their standard deviations, and the labelling of the atoms.

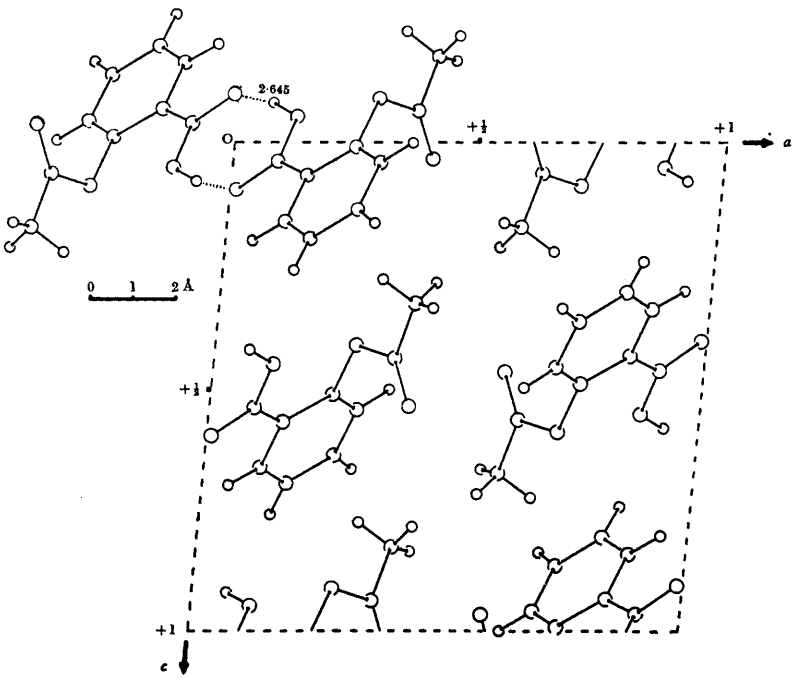


FIG. 2. The structure of aspirin as it appears in projection down [*b*].

[8] W. Cochran, *Acta Cryst.*, 1953, **6**, 260.

TABLE 6.

Bond angles (°). Standard deviations are given as units in the last place.

H(1)O(2)C(7)	120·7 (37)	O(3)C(8)O(4)	122·9 (3)	C(2)C(3)C(4)	119·8 (4)
O(2)C(7)O(1)	122·9 (3)	O(3)C(8)C(9)	110·7 (3)	C(3)C(4)H(4)	121·6 (26)
O(2)C(7)C(1)	118·1 (3)	O(4)C(8)C(9)	126·4 (4)	C(5)C(4)H(4)	118·4 (26)
O(1)C(7)C(1)	119·1 (3)	C(8)C(9)H(7)	110·0 (29)	C(3)C(4)C(5)	120·0 (4)
C(7)C(1)C(2)	124·6 (3)	C(8)C(9)H(8)	119·4 (38)	C(4)C(5)H(5)	120·0 (29)
C(7)C(1)C(6)	117·7 (3)	C(8)C(9)H(9)	115·9 (44)	C(6)C(5)H(5)	120·1 (29)
C(6)C(1)C(2)	117·7 (3)	H(7)C(9)H(8)	98·7 (48)	C(4)C(5)C(6)	119·9 (4)
C(1)C(2)O(3)	121·6 (3)	H(7)C(9)H(9)	100·9 (52)	C(5)C(6)H(6)	118·5 (29)
C(3)C(2)O(3)	117·3 (3)	H(8)C(9)H(9)	108·9 (58)	C(1)C(6)H(6)	119·9 (29)
C(1)C(2)C(3)	121·0 (3)	C(2)C(3)H(3)	118·0 (29)	C(5)C(6)C(1)	121·6 (3)
C(2)O(3)C(8)	115·7 (3)	C(4)C(3)H(3)	122·2 (29)		

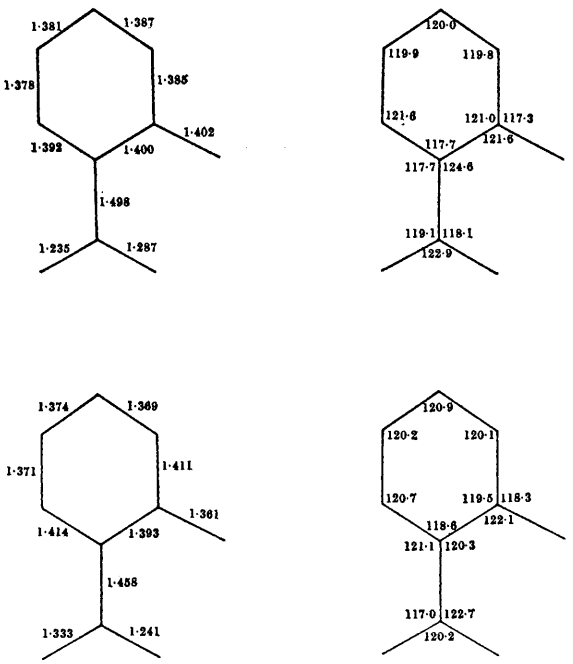


FIG. 3. Comparison of the bond lengths and angles in aspirin (above) and salicylic acid (below).

ring has the appearance of being pulled out by the carboxyl group so that the internal angles at C(2) and C(6) are greater than 120°, and that at C(1) is less. The carboxyl group is bent away from the acetyl group, possibly by repulsion between O(3) and O(2), so that there is a substantial increase in the angle C(2)C(1)C(7), and a decrease in C(6)C(1)C(7). The angle O(1)C(7)O(2) is greater than 120°, again suggesting repulsion between oxygen atoms. The angular distortions at the central atom of the acetyl group are enormous, the angles being 110·7, 122·9, and 126·4°, instead of the expected 120°. There appears to be no simple explanation for these distortions in terms of intramolecular contacts.

Except for hydrogen atoms on the methyl group, the molecule is composed of atoms lying approximately in two planes. The weighted least-squares equation for the plane of the four atoms in the acetyl group, referred to orthogonal axes a, b, and c', is

$$+0{\cdot}7512\,X+0{\cdot}6577\,Y-0{\cdot}0564\,Z'=4{\cdot}3680.$$

The departures of the atoms from this plane are O(3), +0·0007; O(4), +0·0009; C(8), −0·0030; C(9), +0·0011 Å, none of which is significant. Thus, despite the large angular distortions within the plane of this group, there is no out-of-plane bending. On the other hand no satisfactory plane can be constructed through all ten of the heavier atoms of the salicylic acid residue. A number of

planes were calculated, starting first with the benzene ring, and then adding one or more of the remaining four atoms. As soon as any other single atom was added, the departures from the plane increased, and these departures grew worse as more atoms were added. There seems to be no question that significant out-of-plane distortions do occur in the salicylic acid residue. It was particularly noticeable that one of the oxygen atoms of the carboxyl group always lay above the plane, and the other below, leading to the conclusion that the plane of the carboxyl group was twisted with respect to the plane of the benzene ring. In view of these various distortions it was felt that the most representative plane was the one through the six carbon atoms of the benzene ring, the equation of which is

$$+0{\cdot}5945\,X - 0{\cdot}4849\,Y + 0{\cdot}6415\,Z' = 0{\cdot}0941.$$

The departures of the atoms from this plane are given in Table 7. It will be seen that none of the carbon or hydrogen atoms of the benzene ring departs from this plane, whereas the other atoms,

TABLE 7.

Departure in Å of the atoms of the salicylic acid residue from the plane of the benzene ring.

Atom		Atom		Atom	
C(1)	−0·0031	H(1)	−0·138	O(1)	+0·1016
C(2)	+0·0050	H(3)	+0·012	O(2)	−0·0555
C(3)	−0·0026	H(4)	+0·019	O(3)	−0·0565
C(4)	−0·0016	H(5)	+0·009	C(7)	−0·0097
C(5)	+0·0034	H(6)	−0·021		
C(6)	−0·0011				

with the exception of C(7), do. The angle between the plane of the benzene ring and that of the acetyl group is 84° 45′.

The equation of the plane through the carboxyl group is

$$+0{\cdot}6091\,X - 0{\cdot}5022\,Y + 0{\cdot}6139\,Z' = 0{\cdot}0596.$$

H(1) departs from this plane by −0·064 Å, which is not significant. The angle between the plane of the benzene ring and that of the carboxyl group is 2° 2′.

Molecules of aspirin are, as expected, dimerized by hydrogen bonds across a centre of symmetry. The length of each hydrogen bond is 2·645 Å. The perpendicular distance between the two planes defined by the carboxyl groups in the dimer is 0·119 Å, which places aspirin roughly halfway down the table given by Jeffrey and Sax.[9] The weighted least-squares plane through the six heavier atoms of the eight-membered dimer ring is

$$+0{\cdot}5901\,X - 0{\cdot}5348\,Y + 0{\cdot}6084\,Z' = 0.$$

The departure of the atoms from this plane are O(1), +0·0089; O(2), +0·0077; C(7), −0·0151; H(1), −0·013 Å. Thus the eight atoms are very nearly coplanar, as would be expected from Robertson's arguments.[10]

All non-bonded intramolecular contacts were calculated in order to disclose any unusual features within the molecule. If hydrogen atoms are excluded, the two shortest intramolecular contacts are O(1)····O(2), 2·215; O(3)····O(4), 2·239 Å. Other distances of interest in connexion with the possibility of repulsion are O(2)····O(3), 2·674; O(3)····C(9), 2·354; O(4)····C(9), 2·395; C(2)····C(8), 2·342 Å. Inclusion of the hydrogen atoms results in a number of contacts of slightly less than 2 Å between hydrogen atoms on the benzene ring and next-nearest carbon atoms, and three shorter contacts between hydrogen atoms on the methyl group.

All van der Waals's contacts up to a limit of 4 Å were calculated both with and without hydrogen atoms. There is a large number of these distances, but no unusual features appear. If hydrogen atoms are excluded, the shortest contact, apart from the hydrogen bond, is 3·306 Å between two oxygen atoms. The shortest contact between hydrogen atoms is 2·50 Å.

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[9] G. A. Jeffrey and M. Sax, *Acta Cryst.*, 1963, **16**, 430.
[10] J. H. Robertson, *Acta Cryst.*, 1964, **17**, 316.