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The Crystal and Molecular Structure of 9-Fluorenone

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The crystal structure of 9-fluorenone, $C_{13}H_8O$, a molecule with interesting spectroscopic and photochemical properties, has been determined from counter-recorded, single-crystal X-ray diffraction data. The crystals are orthorhombic; space group *Pcab*, with $a=16·068$ (4), $b=18·650$ (6), $c=12·550$ (4) Å and $Z=16$. The structure was solved by direct methods and refined by least squares. Hydrogen atoms were located and refined. The final value of the agreement index is 0·056. The molecules are planar to 0·025 Å. The C–C bonds of the benzo rings average 1·383 (1) Å, but can be divided into two sets of alternate bonds which average 1·378 (1) and 1·388 (1) Å. The angles of the benzo rings can be divided into three distinct sets which average 118·0 (2), 120·4 (2), and 121·7 (2)°, the low average being at the C(1) and C(4) positions. The C–C bonds between the benzo rings are consistent with single bonds between sp^2 carbon atoms.

Introduction

The spectroscopic properties and photochemistry of 9-fluorenone have attracted increased attention in recent years (Kuboyama, 1964; Yoshihara & Kearns, 1966; Kuroda & Kunii, 1967; Liptay, Weisenberger, Tiemann, Eberlein & Konopka, 1968; Davis, Carapellucci, Szoc & Gresser, 1969; Singer, 1969; Caldwell, 1969; Marchetti, 1971). The first X-ray investigation of 9-fluorenone was by Iball (1936), in which he established the space group and lattice constants and suggested a possible molecular packing arrangement. Griffiths & Hine (1970) have reported the crystal structure of a bromine derivative, 2-bromo-9-fluorenone. The present structure determination of 9-fluorenone was undertaken to determine more accurate bond lengths and to describe the molecular packing.

Crystal data

9-Fluorenone $C_{13}H_8O$ M.W. 180·21
Yellow, long prismatic (*c*) crystals
Orthorhombic (Mo $K\alpha_1=0·70926$ Å)
$a=16·068\pm0·004$, $b=18·650\pm0·006$,
$c=12·550\pm0·004$ Å
Volume of unit cell, $3760·8\pm2·0$ Å^3
Density, calculated ($Z=16$), 1·273 g.cm^{-3}
measured (flotation), 1·24 g.cm^{-3}
Linear absorption coefficient, $\mu=0·86$ cm^{-1} (Mo $K\alpha$)
Total number of electrons per unit cell, $F(000)=1504$
Absent spectra: $0kl$ for l odd, $h0l$ for h odd, $hk0$ for k odd
Space group, *Pcab* (D_{2h}^{15})
General positions: $\pm(x,y,z;\ \tfrac{1}{2}+x,\tfrac{1}{2}-y,z;\ x,\tfrac{1}{2}+y,\tfrac{1}{2}-z;\ \tfrac{1}{2}+x,-y,\tfrac{1}{2}-z)$

Experimental

Single crystals grown from methanol were supplied by S. J. Marino of these laboratories. Space-group extinctions and preliminary lattice dimensions were obtained from precession photographs. A small crystal, $0·28\times0·35\times0·47$ mm, was mounted on a thin glass rod with G. E. varnish cement and covered with a glass capillary to prevent sublimation. This crystal was used for intensity data collection on an automatic Picker 4-circle goniostat. To minimize the effect of multiple reflections (Zachariasen, 1965), the *c* axis was oriented 4° from the φ axis. Twenty reflections, at moderately high Bragg angles (Mo $K\alpha_1$ radiation), were accurately centered through very narrow vertical and horizontal slits at a take-off angle of 0·5°. These observations were used as input for the computer program *PICK*2 (Ibers, 1966), which refined the cell and orientation parameters by the least-squares method and generated the cards to control the automated goniostat.

Intensity data were collected with Zr-filtered Mo radiation at a 1·5° take-off angle. A scintillation detector was used, and the pulse-height analyzer was set for an approximately 90% window. All 3719 unique reflections $2\theta < 52°$ were measured by the θ–2θ scan technique at a 2θ scan rate of 1·0° min^{-1}. The scan range varied from 1·0° at low 2θ to 1·4° at high 2θ. Stationary-crystal stationary-counter background counts were taken for 20 sec at each end of the scan. For count rates above 13,000 cycles per sec, brass attenuators were automatically inserted in the diffracted beam. To check electronic and crystal stability during the data collection, the intensity of the 355 reflection was measured every 50th reflection. No systematic variation was observed for these standard intensities. The standard deviation of 355, calculated for 81 observations, was the same as that which one would expect on the basis of counting statistics.

The background for a reflection was approximated by a straight line between the two measured background points. The intensities were corrected for background and for Lorentz and polarization effects and were reduced to structure amplitudes, $|F_o|$. Absorption corrections were not applied, because of the low absorption coefficient and the small size and regularity of the crystal. The maximum error caused by absorption is estimated to be less than 1% of the intensity. Standard deviations $\sigma(I)$ were based on counting statistics and were corrected to $\sigma(F)$. Of the 3719 measured reflections, 2057 were less than $2\sigma(I)$ and were considered unobserved. The structure determination and refinement were based on the 1662 observed reflections.

Determination and refinement of structure

The observed structure factors were converted to normalized structure-factor magnitudes, $|E_H|$ (Hauptman & Karle, 1953), which were then phased by the multiple-solution computer program of Long (1965), modified by Tsai (1968), based on the reiterative application of Sayre's (1952) equation. An E map, calculated from the most consistent set of phases, yielded all 28 heavy atoms for the two molecules in the asymmetric unit. Refinement was by a block-diagonal least-squares program (Trotter, 1965), which utilized a 3×3 block for coordinates and was diagonal in temperature factors. This program minimized $\sum w(F_o^* - F_c)^2$, where

$$F_o^* = K\left[1 + g\,\frac{(1+\cos^4 2\theta)}{(1+\cos^2 2\theta)\sin 2\theta}\,F_c^2\right]^{1/2} F_o$$

in which K is the scale factor, g is the extinction parameter (Zachariasen, 1963; Larson, 1967) and F_c is the usual calculated structure factor. Weights were defined as

$$w = \{[qK\sigma(F_o)]^2 + (rF_o^*)^2\}^{-1},$$

where q and r were chosen by inspection to make the average of $\sum w(F_o^* - F_c)^2$ approximately constant for groups of increasing F_o's (Cruickshank, 1965). The usual agreement index was defined as $R_1 = \sum|F_o^* - F_c|/\sum|F_o^*|$ and the weighted agreement index as $R_2 = [\sum w(F_o^* - F_c)^2/\sum wF_o^{*2}]^{1/2}$. The atomic scattering factors for carbon and oxygen were obtained from *International Tables for X-ray Crystallography* (1962) and for hydrogen from Stewart, Davidson & Simpson (1965).

Table 1. *Final atomic parameters for nonhydrogen atoms*

E.s.d.'s are given in parentheses. Anisotropic thermal parameters are in the form: $\exp[-0{\cdot}25(h^2a^{*2}B_{11} + \ldots 2klb^*c^*B_{23})]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O	0.41219(13)	0.40676(12)	0.51933(16)	7.78(12)	7.78(14)	6.00(11)	1.48(11)	-2.37(10)	-1.18(11)
C(1)	0.34430(19)	0.30441(17)	0.34444(25)	5.92(17)	5.93(17)	6.57(17)	0.46(14)	-0.72(16)	-0.79(15)
C(2)	0.30381(19)	0.27315(17)	0.25914(28)	6.64(18)	6.17(18)	8.42(20)	-0.19(16)	-0.79(18)	-1.65(18)
C(3)	0.24890(20)	0.31184(17)	0.19882(26)	6.51(18)	7.75(18)	6.68(18)	-0.82(17)	-0.96(16)	-1.80(17)
C(4)	0.23212(18)	0.38352(16)	0.21982(24)	5.76(17)	6.58(17)	5.69(17)	-0.20(14)	-0.59(15)	-0.08(16)
C(5)	0.22267(19)	0.54729(16)	0.31575(24)	5.53(15)	5.71(15)	5.92(16)	-0.46(14)	-0.37(15)	0.98(15)
C(6)	0.23051(19)	0.61052(16)	0.37357(27)	5.93(17)	5.10(15)	8.58(20)	-0.24(14)	0.33(18)	1.23(16)
C(7)	0.28439(19)	0.61530(16)	0.45877(27)	6.43(18)	4.95(15)	8.38(20)	-0.96(14)	0.94(17)	-0.97(17)
C(8)	0.33165(19)	0.55689(17)	0.49043(25)	5.89(17)	5.69(17)	6.12(16)	-0.23(14)	0.10(16)	-0.41(15)
C(9)	0.36245(18)	0.42316(16)	0.45033(22)	4.94(14)	6.73(17)	4.33(14)	-0.25(14)	-0.18(14)	-0.29(15)
C(10)	0.32847(16)	0.37558(16)	0.36566(22)	4.41(13)	5.51(15)	4.55(14)	0.15(13)	-0.11(13)	-0.24(14)
C(11)	0.27332(16)	0.41501(15)	0.30438(21)	4.57(13)	5.28(14)	4.27(14)	-0.75(13)	0.30(13)	-0.28(14)
C(12)	0.26882(17)	0.48868(15)	0.34679(22)	4.02(13)	5.54(15)	4.37(14)	-0.46(13)	0.11(13)	0.90(13)
C(13)	0.32209(17)	0.49408(15)	0.43412(23)	4.76(14)	4.61(14)	4.70(14)	-0.17(13)	0.38(13)	-0.01(14)
O'	0.56374(13)	0.36589(11)	0.29626(16)	7.14(11)	7.51(13)	6.20(11)	-0.76(10)	-1.78(10)	1.72(11)
C(1')	0.50260(19)	0.27187(16)	0.10678(25)	5.03(15)	5.27(17)	7.70(19)	0.01(14)	0.23(16)	0.21(15)
C(2')	0.46595(19)	0.24363(17)	0.01638(26)	5.79(18)	5.08(17)	8.84(20)	-0.57(14)	1.11(17)	-1.38(17)
C(3')	0.41633(20)	0.28671(17)	-0.04657(25)	6.75(19)	7.11(18)	6.50(18)	-0.59(16)	0.22(17)	-2.28(16)
C(4')	0.40261(18)	0.35854(17)	-0.02258(24)	5.59(17)	6.54(18)	5.27(16)	0.11(15)	-0.31(15)	-0.86(15)
C(5')	0.39719(19)	0.52049(16)	0.08107(25)	5.68(17)	5.33(15)	5.91(16)	0.53(14)	-0.16(15)	-0.26(15)
C(6')	0.40632(19)	0.58163(18)	0.14246(27)	6.91(19)	5.46(17)	7.82(20)	0.49(16)	0.64(18)	-0.04(17)
C(7')	0.45301(19)	0.58174(16)	0.23447(27)	7.22(18)	5.48(15)	7.31(18)	-1.13(16)	1.69(17)	-1.85(16)
C(8')	0.49265(19)	0.51990(15)	0.26935(24)	6.04(15)	6.06(17)	5.30(16)	-1.36(14)	0.57(16)	-0.50(15)
C(9')	0.51885(17)	0.38612(15)	0.22362(22)	4.51(13)	6.09(15)	4.75(14)	-0.98(13)	-0.08(13)	1.15(14)
C(10')	0.48855(17)	0.34301(15)	0.13218(22)	4.25(13)	4.67(14)	4.99(14)	-0.37(13)	-0.12(14)	0.18(13)
C(11')	0.43906(16)	0.38628(14)	0.06813(22)	4.13(12)	4.93(14)	4.27(13)	-0.22(13)	0.28(12)	-0.41(14)
C(12')	0.43667(16)	0.45884(15)	0.11481(21)	4.20(13)	4.58(14)	4.34(14)	-0.08(12)	0.31(13)	-0.09(13)
C(13')	0.48391(17)	0.45911(14)	0.20789(21)	4.42(13)	4.96(14)	4.34(14)	-0.86(13)	0.09(13)	-0.05(13)

All computations were performed on an IBM 360/65 computer.

Five cycles of refinement with isotropic temperature factors and two with anisotropic temperature factors reduced R_1 to 0·12. The largest structure factors were obviously affected by extinction, so the 223 largest F's were used with unit weighting to refine g. Three further cycles of anisotropic refinement were followed by the calculation of a difference Fourier, which revealed all 16 hydrogen atoms. The hydrogen atoms were assigned isotropic temperature factors, and all atomic parameters were refined for several cycles. The largest F's were again used to adjust g, after which two final cycles of atomic parameter refinement ($q=1·3$, $r=0·02$, $g=1·27\times10^{-6}$) yielded the final agreement indices $R_1=0·056$ and $R_2=0·045$ for the 1662 observed reflections. The standard deviation of an observation of unit weight was 1·13. The maximum parameter shift on the last cycle was 0·24σ. A final difference Fourier was featureless, with residual electron density between $-0·21$ and $+0·21$ e.Å^{-3}, and verified the structure.

The final positional and thermal parameters, with standard deviations estimated from the least-squares process, are given in Tables 1 and 2. The average standard deviation of the positional parameters expressed in Å are 0·0029 for oxygen (range, 0·0023–0·0033), 0·0035 for carbon (range, 0·0027–0·0048), and 0·025 for hydrogen (range, 0·022–0·028). Another parameter that was refined was the scale factor, $K=0·8926\pm0·0011$. The final values of the observed and calculated structure factors and $\sigma(F_o)$, based on counting statistics, are given in Table 3.

Table 2. *Final atomic parameters for hydrogen atoms*

E.s.d.'s are given in parentheses.

	x	y	z	B
H(1)	0.3859(16)	0.2773(14)	0.3897(19)	8.5(8)
H(2)	0.3117(15)	0.2210(13)	0.2437(20)	8.3(8)
H(3)	0.2202(15)	0.2895(14)	0.1351(19)	8.0(8)
H(4)	0.1937(14)	0.4156(13)	0.1765(19)	6.7(7)
H(5)	0.1827(14)	0.5448(12)	0.2510(22)	7.3(7)
H(6)	0.1976(15)	0.6529(14)	0.3512(19)	7.3(7)
H(7)	0.2886(14)	0.6597(12)	0.5005(19)	6.4(7)
H(8)	0.3716(14)	0.5606(13)	0.5550(19)	6.8(7)
H(1')	0.5376(15)	0.2426(14)	0.1536(18)	7.2(7)
H(2')	0.4761(17)	0.1892(14)	-0.0024(22)	9.6(9)
H(3')	0.3912(15)	0.2659(14)	-0.1118(18)	7.9(8)
H(4')	0.3683(16)	0.3896(13)	-0.0714(21)	8.2(8)
H(5')	0.3598(16)	0.5185(13)	0.0147(21)	7.5(7)
H(6')	0.3808(16)	0.6265(14)	0.1211(20)	8.0(8)
H(7')	0.4559(15)	0.6243(13)	0.2762(20)	7.3(7)
H(8')	0.5294(17)	0.5198(14)	0.3379(21)	8.6(8)

Description of structure

Fig. 1 shows the atomic labeling and the intramolecular distances and angles, uncorrected for thermal motion, for the two molecules in the asymmetric unit. The values shown in Fig. 1(c) are averages for equivalent bonds and angles assuming C_{2v} symmetry. The cell-parameter errors and the coordinate standard deviations obtained from the least-squares refinement were used to calculate estimated standard deviations for the distances and angles. These e.s.d.'s average 0·004 Å for C–O, 0·005 Å for C–C, and 0·025 Å for C–H. The e.s.d.'s for the angles are 0·33° for C–C–O, 0·31° for C–C–C, and 1·5° for C–C–H.

The 24 C–C bond distances of the benzo rings average 1·383 Å, slightly shorter than the accepted value of 1·394 Å (Sutton, 1965). All of the bonds are within ± 3σ of the average, but there is an apparent systematic alternation of bond lengths around the rings. The 12 bonds of the type C(1)–C(2), C(3)–C(4), and C(10)–C(11) range from 1·382 to 1·394 Å and average 1·388 Å.

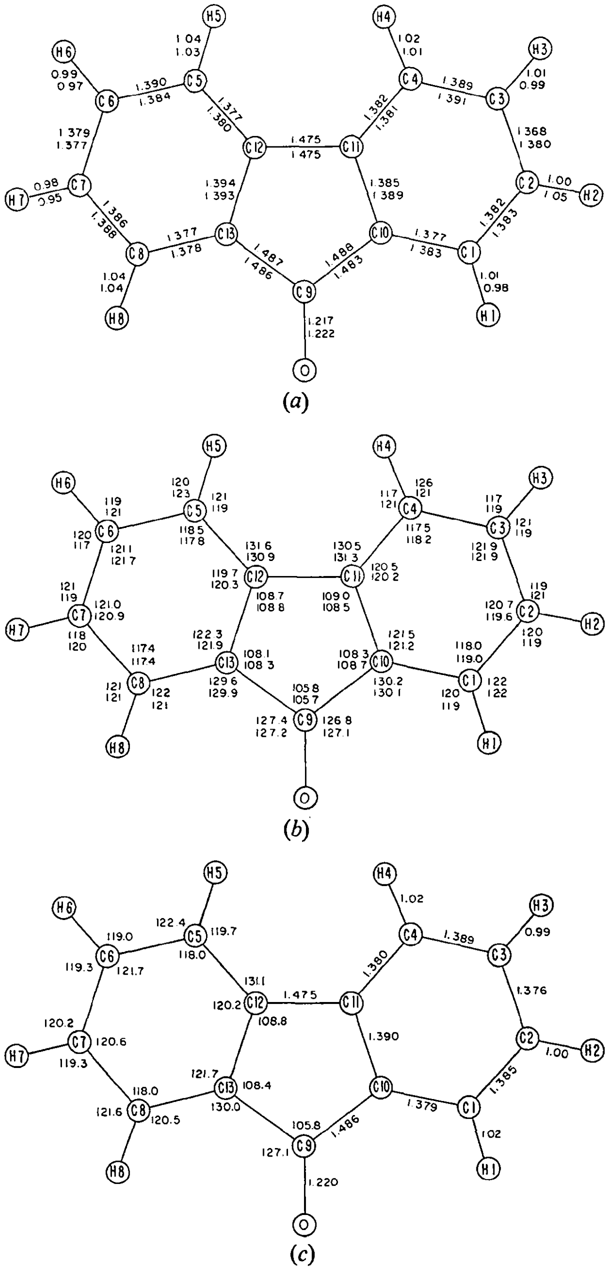

Fig. 1. Atomic labeling and bond lengths (a) and angles (b) for the two molecules in the asymmetric unit. Upper numbers are for the unprimed molecule, lower ones are for the primed molecule. Averages for equivalent bonds are given in (c).

The 12 alternating bonds of the type C(2)–C(3), C(4)–C(11) and C(1)–C(10) range from 1·368 to 1·383 Å and average 1·378 Å. The two ranges overlap only slightly and the 0·010 Å difference in the averages appears significant when compared to the calculated standard deviation of 0·001 Å for the averages. The angles of the benzo rings average the expected 120·0° but also show systematic variation. The 24 angles can be grouped into three nonoverlapping sets of eight angles each, the angles of each set being in *para* positions. The angles at C(5), C(8), and their equivalents average 118·0° (range, 117·4–119·0°), those at C(7) and C(12) average 120·4° (range 119·6–121·0°) and those at C(6) and C(13) average 121·7° (range, 121·1–122·3°). These differences of 2·4 and 1·3° appear significant when compared to calculated standard deviations of 0·2° for the averages. The variations in distances and angles are consistent with the less precise values found by Griffiths & Hine (1970) for 2-bromo-9-fluorenone, and with the SCF MO CI calculations of Kuroda & Kunii (1967) who

Table 3. *Observed and calculated structure factors*

Column headings are h, k, $10F_o$*, $10\vert F_c\vert$, and $10K\sigma(F_o)$.

h	k	$10F_o$*	$10\vert F_c\vert$	$10K\sigma(F_o)$
••••••• L= 0 •••••••				
0	2	1995	1882	3
0	4	975	974	1
0	6	1204	1214	3
0	8	1094	1082	2
0	10	443	436	3
0	12	244	279	4
0	14	62	34	14
1	2	927	985	1
1	4	1108	1135	2
1	6	315	315	2
1	8	677	673	2
1	12	192	190	4
1	14	174	167	5
1	16	211	212	5
2	0	537	556	1
2	2	418	427	1
2	4	278	280	2
2	6	251	249	2
2	8	279	242	3
2	10	662	669	3
2	12	77	64	9
2	16	271	280	5
2	18	150	147	7
3	2	296	297	2
3	4	213	211	1
3	10	153	150	4
3	12	63	52	11
3	14	274	283	4
3	16	317	312	4
3	18	247	251	5
4	0	1774	1846	2
4	2	77	79	6
4	4	178	174	1
4	6	80	82	6
4	8	535	538	2
4	10	61	65	10
4	12	110	106	7
4	14	345	344	4
4	18	170	161	6
5	2	385	352	2
5	4	192	184	3
5	6	680	683	2
5	8	325	324	3
5	10	88	94	9
5	12	89	84	9
5	16	85	84	11
5	18	107	115	10
6	0	575	579	2
6	2	287	285	2
6	4	1025	1037	4
6	6	340	336	3
6	8	69	74	9
6	10	354	355	3
6	16	91	82	10
6	18	129	119	8
7	2	445	447	2
7	4	87	84	6
7	6	158	153	4
7	8	348	344	3
7	10	221	219	4
7	12	86	101	10
8	0	92	96	7
8	4	222	220	3
8	6	228	229	4
8	8	165	165	5
8	10	85	67	9
8	12	143	150	7
8	16	63	79	15
9	6	122	121	7
9	8	300	301	4
9	10	315	306	4
9	12	76	50	11
9	16	125	99	8
10	0	174	171	4
10	4	227	225	4
10	6	79	68	10
10	8	181	170	5
10	12	66	63	13
10	14	65	77	14
10	16	192	194	6
11	2	273	270	4
11	6	64	68	13
11	8	147	147	7
11	10	137	140	7
11	12	268	260	5
11	14	67	79	15
11	16	56	87	12
12	0	462	476	3
12	6	215	211	5
12	10	65	79	13
13	2	138	133	7
13	4	260	262	5
13	6	155	154	6
13	8	119	129	8
14	0	134	130	8
14	4	103	98	9
14	6	137	101	9
14	8	65	80	13
14	14	78	42	13
14	16	85	86	13
15	8	75	80	13
15	10	106	117	10
15	12	88	54	12
15	14	71	65	15
16	6	87	75	11
17	2	75	61	13
17	4	94	83	10
17	6	131	130	8
17	10	70	36	15
18	0	145	152	8
18	2	117	114	10
18	8	80	62	14
••••••• L= 1 •••••••				
1	1	321	346	1
1	2	1165	1211	1
1	3	398	396	2
1	4	517	521	2
1	5	496	492	2
1	6	275	285	2
1	7	289	287	2
1	8	334	330	3
1	10	471	462	3
1	11	405	401	3
1	12	196	187	4
1	13	58	64	13
1	14	275	274	4
1	15	125	143	8
1	16	257	259	5
1	19	96	82	10
2	0	1358	1476	1
2	1	248	254	2
2	2	482	487	1
2	3	724	735	2
2	4	505	518	2
2	5	324	328	2
2	6	242	242	3
2	7	95	100	5
2	8	219	217	3
2	9	505	516	2
2	10	265	269	3
2	11	112	121	6
2	12	142	145	6
2	13	365	360	3
2	15	239	237	5
2	17	148	152	7
3	1	1491	1557	1
3	2	106	106	4
3	3	170	171	3
3	4	127	127	4
3	5	107	111	4
3	6	536	546	2
3	7	215	217	3
3	8	212	210	3
3	9	101	99	6
3	10	110	99	6
3	12	133	114	6
3	14	86	85	10
3	16	202	200	5
3	17	110	107	4
3	18	95	109	12
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4	2	1068	1090	2
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4	8	543	574	2
4	9	484	494	3
4	10	211	201	4
4	11	221	192	4
4	12	72	57	13
4	13	111	128	9
4	14	238	222	5
4	15	71	66	15
4	16	134	124	7
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5	2	953	964	2
5	3	271	278	3
5	4	221	222	3
5	5	395	403	2
5	6	325	329	3
5	7	384	376	3
5	8	264	212	4
5	9	296	289	4
5	10	126	122	6
5	12	55	88	4
5	14	127	131	8
5	15	158	165	7
5	16	74	79	13
6	0	170	162	4
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6	2	157	155	4
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6	7	145	145	4
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6	9	88	87	7
6	12	186	195	5
6	13	80	89	11
6	15	91	87	9
6	16	126	131	8
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7	8	260	287	3
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7	15	72	82	13
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8	4	166	162	4
8	5	507	512	3
8	6	115	121	6
8	8	146	140	6
8	10	167	159	6
8	11	125	133	7
8	12	215	214	5
8	13	224	224	5
8	14	87	81	10
8	20	83	44	12
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9	2	96	67	6
9	3	78	77	8
9	4	212	211	4
9	5	254	243	4
9	6	243	242	4
9	7	55	49	13
9	8	154	150	6
9	9	55	80	14
9	10	233	239	5
9	11	137	136	7
9	12	128	122	8
9	13	129	136	7
9	14	158	157	7
9	16	64	66	15
9	18	77	87	14
10	0	95	75	7
10	2	77	65	9
10	3	196	189	4
10	4	182	171	5
10	5	183	184	5
10	6	155	149	5
10	7	110	113	8
10	8	115	121	7
10	10	98	94	9
10	12	169	183	6
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10	14	136	129	8
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10	18	115	105	10
11	3	183	183	5
11	4	247	245	4
11	5	132	139	7
11	6	150	147	6
11	7	65	73	13
11	12	117	119	8
11	13	155	144	7
11	15	82	12	12
11	16	56	93	11
12	0	142	146	6
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12	6	116	97	9
12	8	76	75	13
12	10	178	171	6
12	11	156	159	7
12	12	98	90	12
12	18	67	19	16
13	2	195	206	5
13	4	56	104	10
13	6	44	74	9
13	11	55	100	10
13	15	70	73	15
14	1	62	50	14
14	2	104	102	9
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14	6	151	155	7
14	7	110	102	9
14	11	113	135	12
15	1	81	82	11
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15	9	84	46	11
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15	12	78	86	14
16	10	82	93	13
16	11	98	85	11
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17	7	71	75	15
18	2	65	80	16
18	6	90	64	12
18	7	72	62	14
19	1	76	66	14
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1	8	162	161	4
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1	14	76	65	11
1	15	125	129	8
1	16	110	105	9
1	17	106	111	9
1	18	57	95	10
1	19	70	60	14
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2	4	452	463	2
2	5	463	475	2
2	6	537	525	2
2	7	230	231	3
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2	11	64	71	11
2	12	105	103	7
2	13	127	133	7
2	15	147	153	7
2	16	70	15	13
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3	3	826	835	2
3	4	130	133	4
3	5	485	447	2
3	6	947	949	2
3	7	352	358	2
3	8	837	835	2
3	9	208	209	4
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3	15	89	110	11
3	16	104	105	9
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4	10	187	193	4
4	11	181	169	5
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5	2	448	461	2
5	3	557	555	2
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5	11	86	75	9
5	12	124	110	7
5	13	143	154	7
5	14	93	104	10
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6	12	177	161	5
6	14	118	118	8
6	15	331	340	4
6	16	152	162	7
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7	2	77	65	7
7	4	68	56	8
7	5	127	123	5
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7	8	60	40	11
7	9	140	136	6
7	11	129	132	7
7	12	287	295	4
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7	18	85	94	11
7	19	74	68	14
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8	1	425	425	3
8	2	406	407	3
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8	4	135	141	5
8	5	340	328	3
8	6	115	146	5
8	7	114	117	6
8	9	97	101	8
8	10	175	179	5
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8	13	67	46	13
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8	16	63	54	15
8	18	95	67	11
9	1	228	222	4
9	2	281	282	3
9	3	156	154	5
9	4	164	162	5
9	5	230	229	4
9	6	65	56	11
9	7	166	167	5
9	8	68	56	12
9	9	74	74	11
9	11	58	88	10
10	0	164	169	5
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10	2	110	105	7
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10	4	321	324	4
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10	6	145	142	6
10	10	116	139	7
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11	8	61	51	14
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12	6	102	58	9
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13	4	85	99	11
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13	7	105	109	9
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13	11	89	88	11
13	13	77	75	13
13	15	67	49	16
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14	10	92	71	11
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15	7	86	87	12
15	13	94	76	11
16	0	63	40	15
16	1	107	105	10
16	2	71	85	14
17	3	68	57	15
17	4	66	53	15
17	6	68	51	16
17	9	69	40	15
18	5	70	41	14
18	6	66	43	16
19	2	71	25	15
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1	13	128	127	7
1	14	120	115	8
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2	13	135	141	7
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2	15	86	83	14
2	16	134	137	7
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3	4	84	56	6
3	5	380	385	2
3	6	424	426	2
3	7	55	47	10
3	9	152	148	5
3	10	76	75	10
3	12	111	113	8
3	14	231	240	5
3	15	85	54	11
3	22	65	6	16
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4	8	157	155	4
4	9	85	91	7
4	10	235	227	4
4	11	212	209	4
4	12	127	134	7
4	13	111	109	5
4	14	135	144	7
4	15	126	141	9
4	16	67	79	14
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5	7	320	314	3
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5	14	198	200	5
5	16	209	213	5
5	17	117	95	8
5	19	102	114	10
5	20	65	52	15
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6	7	448	463	3
6	8	345	348	3
6	9	72	65	10
6	10	80	38	9
6	12	218	222	5
6	13	193	187	6
6	14	145	140	7
6	15	75	75	12
6	16	139	132	7
6	18	116	111	9
6	19	76	47	14
6	21	81	36	14
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7	2	205	203	3
7	3	148	151	4
7	4	316	306	3
7	5	72	82	9
7	6	254	256	3
7	7	163	169	5
7	8	91	90	8
7	11	157	148	6
7	12	215	222	5
7	13	219	222	5
7	14	206	155	5
7	15	155	161	7
8	0	157	161	4
8	1	110	102	6
8	2	378	386	3
8	3	462	472	3
8	4	196	195	4
8	6	133	135	5
8	7	134	122	6
8	9	40	101	10
8	10	91	90	9
8	12	66	37	14
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9	1	77	73	9
9	2	316	316	3
9	3	511	508	3
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9	12	146	143	7
9	13	179	177	6
9	14	68	63	14
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10	7	194	153	5
10	9	67	62	13
10	11	74	84	12
10	13	140	133	7
11	1	175	165	5
11	2	245	244	4
11	3	62	72	14
11	4	198	198	5
11	8	143	135	7
11	11	166	176	7
11	12	76	45	12
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12	0	195	189	5
12	3	98	102	9
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12	11	107	109	10
12	12	167	172	7
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13	7	74	45	12
13	9	91	117	11
13	10	143	147	8
13	11	85	89	12
13	15	75	57	14
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14	3	121	133	8
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17	10	113	119	11
17	11	69	34	16
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18	3	64	20	16
18	4	66	71	16
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1	7	171	170	4
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1	14	147	165	7
1	15	135	146	7
1	17	65	83	15
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3	7	292	289	3
3	9	233	226	4
3	10	154	161	5
3	11	197	204	5
3	13	351	346	4
3	14	165	164	6
3	16	176	163	6
3	17	129	144	8
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4	12	141	129	6
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5	12	79	72	11
5	13	128	141	8
5	14	162	175	6
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6	6	122	107	6
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6	9	85	53	9
6	13	130	134	8
6	14	127	140	8
6	15	64	72	15
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7	2	1043	1067	2
7	3	717	735	3
7	4	327	337	3
7	5	168	166	4
7	6	243	236	4
7	7	111	106	7
7	8	107	105	8
7	11	74	75	12
7	13	168	172	6
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8	1	427	427	3
8	2	362	370	3
8	3	548	553	3
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8	6	137	142	6
8	9	88	56	13
8	11	100	112	9
8	12	200	197	5
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8	15	110	126	9
8	16	64	56	15
8	18	82	49	12
9	2	212	215	4
9	4	67	51	11
9	5	102	85	8
9	6	65	47	12
9	7	125	134	7
9	8	126	125	7
9	9	130	129	7
9	12	81	35	11
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10	12	178	170	5
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11	6	163	166	6
11	8	93	99	10
11	10	77	69	12
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17	8	84	60	13
18	0	101	121	11
18	1	84	81	13
18	3	74	61	15
19	2	83	50	14
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1	14	85	79	11
1	15	68	77	14
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2	6	119	123	5
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2	9	409	410	3
2	12	175	172	5
2	13	148	140	7
2	17	102	102	10
2	19	68	51	15
3	1	126	124	4
3	2	301	303	3
3	3	157	150	4
3	4	97	99	6
3	5	424	429	3
3	6	437	422	3
3	7	317	308	3
3	8	92	80	7
3	9	142	140	6
3	10	205	199	4
3	11	123	119	7
3	12	256	252	4
3	13	149	163	7
3	14	330	335	4
3	16	95	99	11
4	0	433	437	2
4	1	140	145	4
4	3	384	380	3
4	4	93	76	7
4	5	75	62	8
4	6	84	94	8
4	8	56	63	13
4	9	261	263	4
4	11	65	98	10
4	14	131	136	9
4	15	72	73	13
4	16	82	82	12
4	17	64	83	15
4	18	68	82	12
4	19	65	41	15
5	1	312	307	3
5	2	377	384	3
5	3	398	405	3
5	4	210	206	4
5	5	73	51	7
5	6	239	234	4
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5	8	101	97	7
5	9	67	44	11
5	10	98	59	9
5	13	232	234	5
5	18	79	57	13
6	0	467	478	3
6	2	190	200	4
6	3	376	386	3
6	4	94	89	7
6	5	123	118	6
6	6	281	278	4
6	7	66	64	11
6	8	58	87	9
6	9	103	100	8
6	10	64	67	13
6	12	75	62	12
7	1	562	492	3
7	2	231	229	4
7	3	119	136	5
7	4	406	411	3
7	5	557	511	3
7	7	68	71	9
7	8	121	135	7
7	9	151	155	6
7	12	64	65	14
7	13	175	191	6
7	14	67	49	15
7	18	71	8	14
8	0	291	281	4
8	1	129	127	6
8	2	245	241	4
8	3	167	173	5
8	4	179	173	5
8	5	425	426	3
8	6	157	143	7
8	11	78	74	12
8	12	210	211	5
8	14	171	146	9
8	15	64	69	15
8	19	87	70	14
9	2	163	179	5
9	6	141	132	6
9	8	130	136	7
9	9	285	286	4
9	10	203	197	5
9	11	262	257	4
9	12	125	128	8
9	13	172	173	6
9	14	89	101	11
9	15	80	46	12
9	17	70	20	14
10	0	159	159	6
10	1	101	97	8
10	2	71	89	12
10	3	178	172	6
10	4	103	77	8
10	5	162	162	6
10	6	223	220	5
10	8	119	124	8
10	10	78	81	12
10	12	104	119	10
10	13	91	85	11
10	18	81	58	14
11	3	131	139	7
11	4	111	111	9
11	5	161	161	6
11	7	133	127	7
11	8	60	42	14
11	11	61	4	15
11	12	65	71	14
11	13	62	71	12
11	16	65	24	15
12	1	51	58	10
12	3	192	188	5
12	4	433	442	4
12	5	275	270	4
12	6	200	194	5
12	7	153	146	7
13	1	177	176	6
13	2	140	118	7
13	3	103	85	9
13	5	64	81	12
13	6	61	45	12
13	10	102	100	10
13	13	70	26	15
14	0	293	295	5
14	4	115	135	9
14	5	107	109	9
14	7	75	63	14
14	9	134	76	10
14	10	119	111	9
15	2	168	168	7
15	7	74	73	14
15	11	95	89	11
17	1	85	81	13
••••••• L= 6 •••••••				
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0	6	76	78	9
0	7	111	106	6
0	8	357	359	3
0	10	191	190	5
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0	12	138	127	7
0	13	94	94	10
0	15	337	336	4
0	16	73	59	13
0	19	80	78	13
0	20	115	59	10
1	1	93	92	6
1	2	40	36	9
1	3	441	444	3
1	4	195	192	4
1	5	52	30	11
1	6	91	95	7
1	7	336	328	3
1	9	223	219	4
1	11	62	59	14
1	12	158	153	5
1	13	217	226	5
1	14	92	45	10
1	15	118	146	9
1	20	68	31	16
1	21	76	15	15
2	0	592	591	2
2	1	440	438	3
2	2	525	531	3
2	3	171	173	4
2	5	421	416	3
2	6	65	64	10
2	7	233	224	4
2	8	172	171	5
2	9	135	149	6
2	10	87	105	10
2	12	81	87	11
2	13	222	214	5
2	14	64	62	15
3	1	62	55	9
3	2	155	155	4
3	3	105	111	6
3	4	92	57	7
3	5	336	336	3
3	14	61	64	15
4	1	73	67	8
4	2	180	181	4
4	3	172	173	4
4	4	322	314	3
4	5	134	143	5
4	6	202	209	4
4	7	258	251	4
4	9	214	222	5
4	11	207	219	5
4	12	113	113	8
4	15	117	125	9
5	1	231	239	4
5	3	55	52	12
5	4	259	261	4
5	5	150	151	5
5	6	117	107	7
5	7	120	108	7
5	9	93	49	9
5	10	156	153	6
5	11	181	180	6
5	14	164	173	7
5	15	89	66	11
5	16	81	96	12
5	18	79	38	13
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6	1	104	104	7
6	2	178	176	4
6	3	194	187	4
6	4	115	118	7
6	6	65	65	11
6	8	135	140	6
6	9	228	231	5
6	10	112	122	8
6	11	142	153	7
6	12	215	211	5
6	13	158	164	7
6	14	84	85	11
6	18	67	6	16
7	2	63	71	12
7	3	67	68	12
7	5	154	144	6
7	6	80	66	10
7	7	94	99	9
7	8	120	134	8
7	9	97	102	10
7	10	125	131	6
7	11	95	111	10
7	14	78	73	13
7	15	91	58	11
7	17	105	98	10
8	1	59	53	13
8	5	97	112	9
8	6	159	143	6
8	7	214	211	5
8	9	160	153	6
8	10	62	47	14
8	11	150	148	7
9	3	89	80	10
9	5	266	269	4
9	6	121	117	8
9	13	95	80	11
10	0	133	142	7
10	1	82	94	11
10	2	94	77	9
10	3	360	363	4
10	4	361	354	4
10	5	184	188	6
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10	13	72	47	14
11	1	142	133	7
11	3	338	351	4
11	4	142	149	7
11	5	156	160	7
11	7	140	147	7
11	8	65	87	11
11	9	148	158	7
11	10	77	81	13
11	15	66	35	16
12	3	153	164	7
12	4	136	148	7
12	6	113	106	9
12	9	65	101	11
13	2	173	165	6
13	3	86	64	11
13	6	70	66	14
13	7	123	130	8
13	10	114	107	9
14	1	145	149	7
14	2	82	65	12
14	6	76	49	13
14	8	66	26	15
15	1	84	68	12
15	2	80	63	13
15	3	135	146	8
15	5	84	81	12
15	6	63	26	16
16	0	168	170	7
16	2	70	21	14
••••••• L= 7 •••••••				
1	1	151	154	5
1	2	164	181	4
1	3	65	65	10
1	4	220	218	4
1	5	146	134	5
1	7	291	295	4
1	8	133	125	7
1	9	195	194	5
1	10	161	168	6
1	12	112	138	9
1	13	273	276	5
1	16	150	136	7
1	18	75	62	13
2	0	372	369	3
2	1	255	253	3
2	3	64	102	8
2	5	295	302	3
2	7	226	220	4
2	8	112	107	8
2	9	172	127	7
2	10	65	84	13
2	11	173	174	6
2	12	135	131	8
2	13	77	76	12
2	15	88	49	11
2	16	84	83	12
3	1	104	51	6
3	3	151	145	5
3	4	54	74	7
3	5	251	249	4
3	6	159	162	5
3	7	142	128	6
3	9	167	174	6
3	10	97	90	10
3	11	93	92	10
3	14	78	72	12
4	0	624	613	3
4	1	121	124	6
4	2	307	296	3
4	3	322	322	3
4	4	210	210	4
4	5	112	104	7
4	7	82	77	10
4	9	96	84	9
4	10	105	100	9
5	2	67	67	11
5	4	175	188	5
5	5	143	151	6
5	6	114	122	8
5	7	90	85	9
5	8	143	135	6
5	9	171	168	6
5	10	70	62	13
5	11	193	195	6
5	12	68	59	14
5	13	63	81	15
5	15	72	57	14
5	16	108	88	10
5	18	87	69	13
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6	1	80	67	9
6	3	117	119	7
6	4	145	130	6
6	5	88	69	9
6	7	61	79	13
6	8	218	227	5
6	9	138	138	7
6	10	151	148	7
6	11	123	127	8
6	14	65	64	14
6	19	75	40	15
7	2	57	73	14
7	3	163	190	5
7	4	172	159	6
7	6	92	75	9
7	11	149	152	7
7	12	62	55	15
7	13	120	124	9
8	0	195	197	5
8	2	79	50	10
8	4	158	154	6
8	7	132	135	8
8	8	87	86	11
8	9	44	57	10
8	11	64	101	11
8	13	76	34	13
9	1	111	125	8
9	2	97	79	9
9	3	326	336	4
9	4	238	238	5
9	5	305	312	4
9	6	236	248	5
9	7	130	137	8
9	8	163	164	6
9	13	67	19	14
10	0	264	271	5
10	1	264	281	5
10	2	64	34	14
10	3	135	141	7
10	4	97	88	10
10	5	210	220	5
10	6	140	145	7
10	7	257	261	5
10	8	111	103	9
10	9	66	73	15
10	16	65	75	14
11	2	274	272	5
11	3	87	107	11
11	5	210	218	6
11	7	148	150	7
11	8	126	120	8
11	12	71	82	15
11	13	108	121	11
12	0	137	136	7
12	1	88	102	11
12	4	101	105	10
12	5	160	165	7
12	8	63	43	15
12	9	55	107	11
12	10	116	107	9
12	14	67	49	16
13	5	102	96	10
14	0	65	74	16
14	3	64	35	15
14	5	120	123	9
14	10	71	22	15
15	3	63	57	16
15	5	97	109	11
15	6	100	110	11
16	5	92	94	12
16	7	90	57	12
••••••• L= 8 •••••••				
0	0	135	133	6
0	1	217	218	4
0	2	234	226	4
0	6	148	148	6
0	7	186	185	5
0	10	200	208	6
0	11	284	280	5
0	13	87	98	12
0	16	114	80	9
1	1	432	423	3
1	2	138	135	6
1	3	137	128	6
1	4	114	111	7
1	5	107	97	6
1	7	139	138	7
1	8	163	169	6
1	9	85	103	11
1	10	235	238	5
1	12	95	95	10
1	13	117	114	9
1	15	103	84	10
2	0	354	343	3
2	2	140	145	6
2	3	108	115	7
2	4	150	145	6
2	5	233	223	4
2	8	196	195	5
2	12	242	243	5
2	16	86	60	12
2	17	105	95	10
2	18	85	62	13
3	2	113	123	7
3	5	137	138	7
3	6	90	73	9
3	8	135	131	7
3	9	120	124	8
3	11	204	202	5
3	13	83	73	12
4	0	56	59	14
4	2	82	76	10
4	3	134	135	6
4	4	131	125	7
4	5	103	111	8
4	6	66	70	13
4	8	158	147	6
4	9	181	183	6
4	10	65	62	14
4	11	244	248	5
4	12	87	100	11
4	13	78	86	13
5	1	152	133	6
5	4	148	152	6
5	5	74	71	11
5	6	130	133	7
5	7	125	131	8
5	8	210	210	5
5	9	77	88	12
5	11	91	76	10
5	12	135	122	7
6	0	296	308	4
6	1	83	84	10
6	2	207	214	5
6	3	165	153	6
6	4	76	106	12
6	7	74	65	12
6	11	107	87	9
6	12	141	117	7
7	2	44	53	9
7	4	192	182	6
7	5	170	155	6
7	6	122	117	8
7	7	272	220	5
7	8	92	49	10
7	9	45	108	10
8	1	163	166	6
8	3	125	111	8
8	4	98	69	9
8	6	158	170	7
8	8	232	252	5
8	10	101	97	10
8	12	77	31	13
9	1	77	42	12
9	2	166	167	6
9	3	84	92	12
9	4	115	126	8
9	7	139	145	7
9	11	110	115	10
10	0	151	141	7
10	2	108	123	9
10	4	139	146	7
10	5	66	28	14
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10	11	68	74	15
11	1	105	110	10
11	3	122	124	8
11	4	85	96	11
12	0	104	110	9
12	1	133	127	8
12	2	85	67	11
12	4	136	129	7
12	6	79	52	12
13	5	126	127	8
13	6	132	153	9
14	4	107	111	10
14	5	122	125	9
14	6	116	123	10
••••••• L= 9 •••••••				
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1	3	60	58	10
1	4	201	159	5
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1	10	67	76	14
2	2	95	80	9
2	3	67	80	13
2	5	147	145	7
2	6	85	78	11
2	7	247	253	5
2	8	83	90	12
2	9	70	75	14
2	10	84	74	12
2	11	116	103	9
3	2	83	84	11
3	3	78	96	11
3	5	108	117	9
3	7	101	118	10
3	9	91	86	11
3	10	178	179	6
3	11	195	201	6
3	15	98	91	11
4	0	212	201	5
4	3	87	89	10
4	7	63	40	14
4	9	227	223	5
4	10	66	34	14
4	12	142	144	8
5	1	102	94	9
5	2	195	204	5
5	3	106	98	9
5	4	175	191	6
5	6	260	260	5
5	7	63	33	14
5	8	96	101	10
5	9	174	163	6
6	0	183	187	6
6	1	114	128	8
6	3	125	127	8
6	5	122	132	8
6	6	94	89	10
6	7	243	254	5
6	8	92	96	11
6	9	136	149	8
6	10	90	101	11
7	1	127	123	8
7	2	300	309	4
7	3	243	256	5
7	5	116	105	8
7	6	168	177	6
7	7	119	132	9
7	8	86	107	12
7	9	76	56	12
8	0	257	256	5
8	1	98	117	10
8	4	149	155	7
8	9	75	53	13
9	2	73	56	12
9	3	132	125	7
9	5	121	119	8
9	6	64	45	14
9	11	77	59	14
10	4	108	99	9
10	5	91	82	11
11	3	70	48	13
12	2	118	117	9
12	6	101	104	11
14	0	65	14	15
14	6	75	72	15
••••••• L=10 •••••••				
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0	3	165	162	6
0	5	168	169	6
0	6	67	45	14
0	7	80	92	12
0	8	71	78	14
0	9	75	54	13
0	10	232	232	5
0	11	151	155	8
0	12	108	91	10
0	13	139	150	8
0	14	124	115	9
1	1	84	76	11
1	3	112	126	9
1	5	74	56	13
1	6	121	101	8
1	7	68	54	14
1	10	136	126	8
1	11	91	81	11
2	0	127	127	8
2	1	66	67	14
2	4	126	134	8
2	5	131	124	8
2	6	72	77	13
2	7	156	156	7
2	8	208	198	6
2	9	110	132	10
2	12	72	68	14
3	1	73	38	13
3	2	184	168	6
3	4	135	140	8
3	6	136	143	7
3	7	106	118	9
3	8	130	131	8
3	9	85	95	12
3	11	85	77	11
4	0	215	224	5
4	1	200	204	6
4	2	80	71	12
4	3	100	96	10
4	5	103	120	10
4	6	158	166	7
4	7	112	111	9
4	8	140	140	8
4	9	122	134	9
4	10	64	18	15
4	11	82	59	13
5	1	74	98	13
5	2	175	178	6
5	4	164	158	6
5	6	136	135	8
5	8	67	88	11
5	9	131	134	8
5	10	113	127	10
5	11	69	59	15
5	12	73	27	14
6	0	155	153	7
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6	4	123	125	8
6	7	73	77	13
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6	16	73	8	16
7	2	135	130	7
7	3	85	102	11
7	4	79	80	12
7	5	181	186	6
7	6	74	82	13
7	7	97	79	10
7	8	85	60	12
7	9	82	84	13
8	1	144	155	7
8	2	107	102	9
8	5	70	75	14
8	7	95	107	11
8	11	69	68	16
8	13	78	28	13
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9	10	84	65	13
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10	13	74	69	16
11	2	73	56	14
11	4	65	29	15
11	9	71	38	15
12	5	80	60	13
13	1	80	39	13
14	6	78	13	14
••••••• L=11 •••••••				
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1	5	108	109	9
1	6	142	135	7
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2	7	80	96	13
2	8	124	128	9
2	10	102	100	11
3	1	161	166	7
3	2	159	145	7
3	3	143	134	7
3	4	65	36	14
3	5	97	114	11
3	6	140	146	8
3	8	78	74	13
4	4	303	303	5
4	6	132	125	8
4	11	70	35	15
5	2	117	116	9
5	9	107	92	10
5	10	68	15	15
5	11	73	35	14
6	3	95	70	10
6	7	75	66	13
6	8	95	104	11
6	9	68	46	15
6	11	85	65	13
7	7	110	108	10
7	8	65	20	15
7	13	72	52	16
8	0	107	114	10
8	1	77	83	13
8	8	73	66	14
8	10	73	58	14
9	1	80	68	13
9	3	104	108	10
9	5	66	52	15
10	0	76	59	13
10	2	66	22	15
10	7	90	71	12
11	9	72	36	16
12	7	75	39	15
••••••• L=12 •••••••				
0	0	233	233	5
0	4	207	212	6
0	5	223	229	6
0	7	128	118	9
0	11	80	45	14
0	12	96	87	12
1	2	91	79	11
1	4	78	77	13
1	5	138	143	8
1	11	75	63	15
2	0	76	67	13
2	3	72	49	14
2	4	97	104	11
2	5	82	70	13
2	6	113	102	9
2	9	103	104	11
2	10	106	108	11
2	11	78	76	15
3	5	93	79	11
3	6	116	117	9
3	7	105	103	10
3	13	74	68	16
4	0	124	112	8
4	3	168	169	7
4	6	68	55	15
4	9	98	65	11
4	11	70	41	15
5	5	76	80	14
5	6	104	128	11
6	5	82	40	12
6	7	94	93	11
7	1	100	65	10
7	4	66	55	15
7	8	80	69	14
8	0	95	83	11
8	3	65	55	15
8	6	74	59	14
9	1	72	24	14
10	7	85	68	13
11	2	75	17	14
••••••• L=13 •••••••				
1	2	191	193	7
1	4	72	67	15
1	5	170	159	7
1	12	76	18	16
2	0	101	111	11
2	2	65	69	15
2	4	67	78	16
4	3	104	98	10
4	5	73	76	15
5	1	84	86	13
5	5	97	90	12
7	6	80	61	14
7	8	74	36	15
••••••• L=14 •••••••				
0	0	145	143	9
0	2	85	69	13
0	3	94	75	12
0	6	80	70	15
0	7	125	126	10
0	8	85	91	14
1	4	75	3	15
1	5	80	93	15
3	2	82	58	13
3	5	68	68	17
4	3	74	19	15

predicted that the longest benzo bond would be the C(10)–C(11) bond and the shortest would be C(2)–C(3).

The relatively low values for the angles at the C(1)- and C(4)-type positions are similar to those found in the photodimer of 1,4-epoxy-1,4-dihydronaphthalene (118°) (Bordner, Stanford & Dickerson, 1970), 2-acetyl-3-indazolinone (117·5°) (Smith & Barrett, 1969), 3-(*p*-bromophenyl)phthalide (113°) (Kalyani & Vijayan, 1969), and *meso*-3,3′-di(*p*-bromophenyl)bi-3-phthalidyl (116·4°) (Kalyani, Manohar & Mani, 1967), where benzo rings are fused to five-membered rings, and in biphenylene (115·2°) (Fawcett & Trotter, 1966), and 3,4:7,8-dibenzotricyclo[4·2·0·$0^{2,5}$]octa-3,7-diene (115·4°) (Barnett & Davis, 1970), where benzo rings are fused to four-membered rings. For these otherwise unsubstituted benzo rings, the four- and five-membered fused rings impose bond angles of approximately 90 and 108° at sp^2 carbon atoms, and cause the benzo angles at the points of fusion to become greater than 120° to relieve the strain. The effect of the enlargement of the benzo angles at the fusion points is to reduce the angles at the C(1)- and C(4)-type positions below 120°. A striking example of this effect is found in benzo-[1,2:4,5]dicyclobutene (Lawrence & MacDonald, 1969), where four-membered rings are fused to opposite sides of a benzo ring and the angle at C(1) is reduced to 108°.

The averages of four C(9)–C(13)-type bonds (1·486 Å) and of two C(11)–C(12)-type bonds (1·475 Å) are close to the 1·48 Å expected for a single bond between sp^2 carbon atoms (Lide, 1962; Dewar & Schmeising, 1960), and indicate little, if any, conjugation interaction

Table 4. *Equations of least-squares planes and distances* (Å × 10³) *of atoms from these planes*

X, *Y*, and *Z* are expressed in Å units relative to the crystallographic axes. Planes were calculated by the method of Schomaker, Waser, Marsh & Bergman (1959) as modified by Blow (1960).

Unprimed molecule *A*: $0{\cdot}7440X+0{\cdot}2751Y-0{\cdot}6089Z=3{\cdot}0584$
B: $0{\cdot}7374X+0{\cdot}2858Y-0{\cdot}6120Z=3{\cdot}1236$
C: $0{\cdot}7468X+0{\cdot}2716Y-0{\cdot}6070Z=3{\cdot}0611$
D: $0{\cdot}7470X+0{\cdot}2685Y-0{\cdot}6082Z=3{\cdot}0317$

Primed molecule *A′*: $0{\cdot}8081X+0{\cdot}2563Y-0{\cdot}5304Z=7{\cdot}0983$
B′: $0{\cdot}8117X+0{\cdot}2528Y-0{\cdot}5265Z=7{\cdot}0995$
C′: $0{\cdot}8082X+0{\cdot}2578Y-0{\cdot}5294Z=7{\cdot}1110$
D′: $0{\cdot}8028X+0{\cdot}2605Y-0{\cdot}5363Z=7{\cdot}0822$

	Unprimed molecule				Primed molecule			
Plane:	*A*	*B*	*C*	*D*	*A′*	*B′*	*C′*	*D′*
O	12	61*	10*	12*	2	−20*	−1*	27*
C(1)	12	68*	11*	4	−16	−32*	−14*	−3
C(2)	5	59*	6*	−4	−7	−18*	−3*	−2
C(3)	2	40*	9*	1	12	10*	16*	5
C(4)	−5	18*	7*	3	7	9*	9*	−5
C(5)	1	−6	22*	29*	−7	1	−11*	−24*
C(6)	25	8	48*	60*	−9	0	−16*	−26*
C(7)	7	−1	26*	39*	−3	−2	−11*	−9*
C(8)	−16	−7	−4*	6*	10	3	3*	15*
C(9)	−5	33*	−1	0*	5	−10*	2	19*
C(10)	−2	39*	2	0	−5	−16*	−5	4
C(11)	−13	11*	−3	−3	5	2*	5	1
C(12)	−13	−2	1	6*	0	0	−3	−7*
C(13)	−10	9	0	6*	5	−2	1	9*

* Not included in calculation of the plane

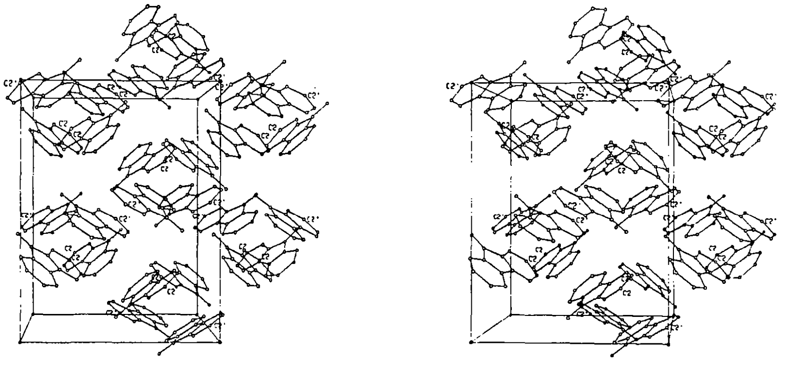

Fig. 2. Stereoscopic view of the molecular packing down the *b* axis. The *c* axis is horizontal and *a* is vertical.

across the central ring. The C–O distances average 1·220 Å, comparable to the 1·215 Å found for aliphatic and conjugated aldehydes and ketones (Sutton, 1965). As is typical of X-ray structures, the C–H bonds average 1·01 Å, less than the true 1·08 Å separation.

Equations of least-squares planes for the molecules and for the rings of the molecules, along with deviations of the atoms from the planes, are given in Table 4. Both molecules are approximately planar with maximum deviations of 0·025 Å for the unprimed molecule (Plane *A*) and 0·016 Å for the primed molecule (Plane *A'*). The deviations from the molecular planes appear to be systematic, particularly for the unprimed molecule, but the dihedral angles between the planes of the individual rings are only about 1° and are not very significant in terms of bonding in the molecules.

The molecular packing is shown stereoscopically (Johnson, 1965) in Fig. 2. The molecules pack on end in layers perpendicular to **b**. The two molecules in the asymmetric unit are almost parallel (dihedral angle, 5·9°) and average 3·6 Å apart. Two asymmetric units are related by a center of symmetry to form a stack of four molecules in which the two inner (primed) molecules are parallel and 3·57 Å apart. These stacks of four are tilted in the *ac* plane and combine with stacks related by the **c** translation to form zigzag chains. Neighboring chains are nested along **a**, but with the axis of the stacks in the opposite direction. There are no intermolecular contacts shorter than would be expected from van der Waals radii.

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