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The Crystal Structures of Fluorene Derivatives. I. 2-Bromoketofluorene

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2-Bromoketofluorene ($C_{13}H_7OBr$) crystallizes in the orthorhombic system, space group $P2_12_12_1$, with a unit cell of dimensions $a=3{\cdot}97\pm0{\cdot}01$, $b=7{\cdot}64\pm0{\cdot}01$, $c=33{\cdot}22\pm0{\cdot}03$ Å containing four molecules. The crystal structure was determined by means of the heavy-atom technique and refined by electron-density and difference syntheses, and finally by least-squares methods using three-dimensional data.

Introduction

Parry & Warren (1965) have investigated experimentally the effect of 2-substituents upon the reactivity at the 9 position of 9-ketofluorene (fluorenone) and find that the substituents have less effect in this case than when substituted in 9-diazofluorene. They suggest that the cyclopentadiene ring in 9-diazofluorene is more aromatic in character than in 9-ketofluorene. Both these compounds have one canonical form which has a formal negative charge at the 9-carbon. Delocalization of this negative charge over the cyclopentadiene ring might be expected in 9-diazofluorene, but not in 9-ketofluorene where an electron displacement opposite to that usual for carbonyl linkages would be required. The electron count on the cyclopentadiene ring of 9-diazofluorene would, if delocalization occurs, satisfy Hückel's rule requiring $(4n+2)$ π electrons for an aromatic system, where n is the number of atoms, and the ring would be expected to show increased aromatic character and greater stability. The aromatic character of the ring has been studied theoretically by Warren (1966) who has calculated bond lengths for the 2-substituents CH_2^+, as an extreme example of an electron-withdrawing group, and CH_2^-, for electron-supplying.

Two of the 2-substituted derivatives studied by Parry & Warren were 2-bromoketofluorene and 2-bromodiazofluorene. Both these have been studied crystallographically. The intensity data allow the establishment of only the main features of the crystal structures. Those of 2-bromoketofluorene are reported here; those of 2-bromodiazofluorene will be reported later.

Experimental

2-Bromoketofluorene ($C_{13}H_7OBr$, Fig. 1) crystallizes from benzene as thin yellow needles having rhombohedral cross section and elongated parallel to [100]. The melting point is 145 °C.

Oscillation and Weissenberg photographs uniquely determined the space group as $P2_12_12_1$ with principal axial lengths $a=3{\cdot}97\pm0{\cdot}01$, $b=7{\cdot}64\pm0{\cdot}01$, $c=33{\cdot}22\pm0{\cdot}03$ Å, $\varrho_o=1{\cdot}72\pm0{\cdot}02$ g.cm^{-3}, $\varrho_c=1{\cdot}71$ g.cm^{-3} (four molecules per unit cell). Cu $K\alpha$ radiation was used for all the intensity measurements.

The linear absorption coefficient of 57 cm^{-1} for Cu $K\alpha$ radiation is uncomfortably high, but because of the bromine atom very little advantage would be gained by the use of Mo $K\alpha$. The crystals were thin

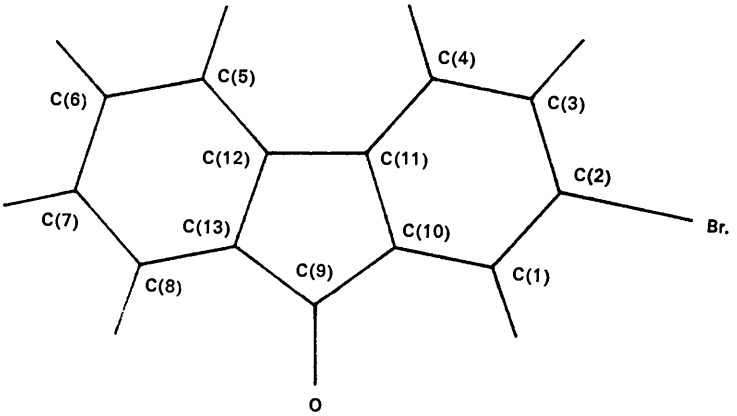

Fig. 1. Schematic diagram of the molecule showing the atom numbering.

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and did not grind into good spheres. The intensity data were therefore collected from a small unshaped crystal. The intensities used for this study were obtained by visual estimation from zero and upper-layer equi-inclination Weissenberg photographs taken about [100], by comparison with a graded wedge prepared from the same crystal. In this way approximately 0·75 of the total number of reflexions within the Cu *Kα* sphere were covered. These were distributed reasonably symmetrically in reciprocal space but with some curtailment parallel to [100]*. The data obtained contain, beside the random errors of visual-intensity measurement amounting to about ±0·1 times the intensity, at least one important systematic error arising from the neglect of absorption. The method of data collection – reciprocal layers normal to [100]* – coupled with the very regular crystal cross section normal to [100]*, mainly confines this error to a systematic variation of scale factor from one layer to another. Some allowance for this was made by introducing the scale factor for each layer as an adjustable parameter. This was thought to be preferable to the experimental determination of a scale factor from correlation photographs obtained from a second crystal and showing a different spot shape, but it causes difficulties during anisotropic temperature-factor refinement. The maximum variation in absorption possible in a given layer of reflexions for the crystals used is rather less than the magnitude of the random errors. A second factor which must be borne in mind when assessing the results is the presence of the bromine atom which, though convenient for phase determination, dominates the light-atom contributions.

Structure determination and refinement

The crystal structure was solved by conventional heavy-atom methods. The (y,z) coordinates of the bromine atom were obtained from the (100) Patterson projection and the fourteen light atoms other than hydrogen, positioned from the first (100) electron-density synthesis based on the bromine phases. The reliability index for the first set of structure factors calculated with all atom contributions except those of the hydrogen atoms was 0·22. The x coordinates of the atoms were obtained by three-dimensional methods: that of the bromine atom from the three-dimensional Patterson function and those of the oxygen and carbon atoms from a three-dimensional electron-density synthesis based on the bromine phases. This electron-density synthesis contained additional symmetry to that of the space group, but careful study of the map gave the x coordinates of eleven carbon atoms. The x coordinates

Table 1. *Final parameters*

Coordinate standard deviations are enclosed in brackets.

	X (Å)	Y (Å)	Z (Å)	B (Å^2)
C(1)	0·622 (0·023)	4·542 (0·017)	3·568 (0·013)	2·13
C(2)	1·048 (0·022)	4·553 (0·019)	2·222 (0·017)	2·85
C(3)	1·684 (0·023)	5·643 (0·018)	1·671 (0·017)	2·48
C(4)	1·952 (0·022)	6·806 (0·019)	2·398 (0·017)	2·41
C(5)	2·147 (0·023)	1·482 (0·017)	4·747 (0·017)	2·36
C(6)	2·062 (0·024)	2·249 (0·026)	5·963 (0·023)	4·81
C(7)	1·512 (0·026)	1·790 (0·019)	7·076 (0·017)	2·81
C(8)	0·981 (0·021)	0·476 (0·014)	7·096 (0·013)	1·94
C(9)	0·535 (0·026)	5·947 (0·017)	5·720 (0·013)	2·02
C(10)	0·835 (0·019)	5·668 (0·013)	4·272 (0·013)	0·98
C(11)	1·531 (0·020)	6·812 (0·017)	3·747 (0·013)	1·82
C(12)	1·573 (0·021)	0·220 (0·015)	4·800 (0·013)	1·63
C(13)	1·004 (0·021)	7·355 (0·014)	5·956 (0·013)	1·59
O	3·906 (0·017)	5·233 (0·013)	6·458 (0·013)	3·24
Br	0·720 (0·003)	2·998 (0·002)	1·166 (0·002)	Anisotropic

Heavy atom anisotropic B values

$B(1,1)$	0·0528
$B(2,2)$	0·0186
$B(3,3)$	0·0009
$B(1,2)$	0·0008
$B(1,3)$	0·0014
$B(2,3)$	0·0019

Calculated hydrogen positions

	X	Y	Z
H(1)	0·159 Å	3·754 Å	3·973 Å
H(3)	1·995	5·634	0·721
H(4)	2·415	7·594	1·993
H(5)	2·563	9·480	3·910
H(6)	2·448	10·812	5·966
H(7)	1·490	9·998	7·899
H(8)	0·566	7·758	7·767

Table 2. *Final observed and calculated structure factors*

H	K	L	|FO|	|FC|	AC	BC
0	0	6	58.2	55.3	+55.3	+0.0
0	0	8	84.2	80.5	-80.5	-0.0
0	0	10	54.1	52.2	-52.2	-0.0
0	0	12	132.1	124.9	-124.9	-0.0
0	0	14	87.4	82.6	-82.6	-0.0
0	0	16	32.2	37.3	-37.3	-0.0
0	0	18	33.3	37.3	-37.3	-0.0
0	0	20	29.1	30.2	-30.2	-0.0
0	0	22	5.2	6.6	+6.6	+0.0
0	0	24	15.6	15.4	+15.4	+0.0
0	0	26	27.0	27.4	+27.4	+0.0
0	0	28	68.6	69.8	+69.8	+0.0
0	0	30	20.8	22.2	+22.2	+0.0
0	0	32	7.3	7.6	+7.6	+0.0
0	0	34	7.3	11.0	+11.0	+0.0
0	0	38	5.2	8.2	-8.2	-0.0
0	1	3	52.0	54.0	-0.0	+54.0
0	1	4	104.0	111.8	+0.0	-111.8
0	1	5	75.9	73.5	-0.0	+73.5
0	1	6	100.9	93.1	+0.0	-93.1
0	1	7	18.7	17.5	-0.0	+17.5
0	1	8	81.1	76.4	+0.0	-76.4
0	1	9	7.3	5.2	-0.0	-5.2
0	1	10	59.3	57.8	+0.0	-57.8
0	1	11	65.5	70.5	+0.0	-70.5
0	1	12	68.6	63.4	+0.0	-63.4
0	1	13	15.6	17.9	-0.0	-17.9
0	1	14	5.2	4.1	-0.0	+4.1
0	1	15	65.5	61.1	+0.0	-61.1
0	1	16	34.3	31.6	-0.0	+31.6
0	1	17	74.9	73.2	+0.0	-73.2
0	1	18	38.5	35.7	-0.0	+35.7
0	1	19	10.4	10.6	+0.0	-10.6
0	1	20	46.8	45.6	-0.0	+45.6
0	1	22	30.2	32.4	-0.0	+32.4
0	1	23	26.0	26.2	+0.0	+26.2
0	1	24	42.6	44.7	-0.0	+44.7
0	1	25	9.4	8.5	+0.0	+8.5
0	1	26	9.4	8.6	+0.0	+8.6
0	1	27	32.2	33.5	-0.0	+33.5
0	1	28	10.4	11.2	+0.0	+11.2
0	1	29	20.8	25.0	-0.0	+25.0
0	1	30	7.3	9.4	-0.0	+9.4
0	1	32	25.0	29.9	+0.0	-29.9
0	1	33	18.7	22.1	-0.0	+22.1
0	1	34	13.5	15.3	+0.0	-15.3
0	1	36	9.4	11.9	+0.0	-11.9
0	1	38	9.4	12.8	+0.0	-12.8
0	1	39	7.3	14.6	+0.0	-14.6
0	1	40	5.2	11.1	-0.0	-11.1
0	1	41	5.2	11.1	+0.0	-11.1
0	2	0	23.9	22.4	-22.4	-0.0
0	2	2	41.6	40.5	+40.5	+0.0
0	2	3	79.0	73.1	+73.1	+0.0
0	2	4	15.6	15.6	+15.6	-0.0
0	2	5	90.5	89.1	+89.1	+0.0
0	2	6	21.8	19.6	-19.6	-0.0
0	2	7	110.2	103.2	+103.2	+0.0
0	2	8	20.8	18.1	+18.1	-0.0
0	2	9	90.5	81.8	+81.8	+0.0
0	2	11	36.4	38.2	+38.2	+0.0
0	2	12	11.4	9.7	+9.7	-0.0
0	2	13	62.4	56.1	+56.1	+0.0
0	2	14	10.4	9.4	-9.4	-0.0
0	2	15	39.5	33.9	-33.9	-0.0
0	2	16	34.3	31.1	-31.1	+0.0
0	2	17	41.6	39.9	-39.9	-0.0
0	2	18	16.6	12.2	-12.2	+0.0
0	2	19	30.2	30.9	-30.9	-0.0
0	2	20	17.7	11.6	-11.6	+0.0
0	2	21	77.0	71.9	-71.9	-0.0
0	2	22	18.7	18.7	-18.7	+0.0
0	2	23	57.2	53.7	-53.7	-0.0
0	2	24	15.6	17.2	-17.2	+0.0
0	2	25	23.9	25.9	-25.9	-0.0
0	2	26	11.4	12.1	+12.1	+0.0
0	2	27	5.2	5.7	-5.7	-0.0
0	2	28	22.9	24.6	+24.6	+0.0
0	2	29	9.4	10.1	+10.1	-0.0
0	2	31	14.6	15.9	+15.9	+0.0
0	2	32	9.4	8.7	+8.7	-0.0
0	2	33	12.5	15.8	+15.8	+0.0
0	2	34	7.3	13.3	+13.3	-0.0
0	2	35	19.8	24.2	+24.2	+0.0
0	2	37	9.4	13.2	+13.2	+0.0
0	2	39	5.2	7.4	+7.4	+0.0
0	2	41	5.2	7.1	+7.1	+0.0
0	3	1	63.4	64.6	-0.0	+64.6
0	3	2	40.6	38.8	-0.0	+38.8
0	3	3	68.6	68.2	-0.0	+68.2
0	3	5	69.7	69.3	-0.0	+69.3
0	3	6	72.8	69.5	-0.0	+69.5
0	3	7	29.1	26.9	+0.0	+26.9
0	3	8	40.6	35.8	-0.0	+35.8
0	3	9	39.5	37.0	+0.0	-37.0
0	3	10	9.4	10.9	-0.0	+10.9
0	3	11	81.1	74.4	+0.0	-74.4
0	3	12	22.9	22.5	-0.0	+22.5
0	3	13	66.6	65.1	+0.0	-65.1
0	3	14	27.0	22.7	-0.0	-22.7
0	3	15	59.3	55.8	+0.0	-55.8
0	3	16	19.8	19.1	-0.0	-19.1
0	3	17	64.5	59.5	+0.0	-59.5
0	3	18	20.8	21.9	+0.0	-21.9
0	3	19	29.1	30.8	-0.0	-30.8
0	3	20	38.5	37.9	+0.0	-37.9
0	3	21	5.2	5.5	-0.0	+5.5
0	3	23	31.2	32.9	-0.0	+32.9
0	3	24	5.2	6.0	+0.0	-6.0
0	3	25	26.0	27.5	-0.0	+27.5
0	3	28	9.4	9.8	-0.0	+9.8
0	3	29	13.5	15.3	-0.0	+15.3
0	3	30	5.2	8.2	+0.0	+8.2
0	3	31	26.0	28.9	-0.0	+28.9
0	3	32	9.4	10.9	+0.0	+10.9
0	3	33	12.5	13.5	-0.0	+13.5
0	3	34	10.4	14.9	-0.0	+14.9
0	3	35	5.2	5.2	+0.0	+5.2
0	4	0	36.4	41.5	-41.5	-0.0
0	4	1	9.4	10.2	+10.2	+0.0
0	4	2	89.4	83.7	-83.7	-0.0
0	4	3	12.5	16.6	+16.6	+0.0
0	4	4	37.4	37.8	-37.8	-0.0
0	4	5	18.7	18.4	+18.4	+0.0
0	4	6	29.1	22.3	+22.3	+0.0
0	4	7	38.5	37.9	+37.9	+0.0
0	4	8	12.5	13.4	+13.4	-0.0
0	4	9	29.1	26.1	+26.1	+0.0
0	4	10	18.7	19.6	+19.6	+0.0
0	4	11	42.6	33.5	+33.5	+0.0
0	4	12	43.7	38.3	+38.3	+0.0
0	4	13	10.4	11.3	+11.3	-0.0
0	4	14	54.1	53.7	+53.7	+0.0
0	4	16	46.8	40.8	+40.8	+0.0
0	4	17	15.6	14.3	+14.3	-0.0
0	4	18	20.8	21.6	+21.6	+0.0
0	4	19	26.0	23.9	-23.9	-0.0
0	4	20	5.2	4.4	+4.4	+0.0
0	4	21	18.7	18.7	-18.7	-0.0
0	4	22	12.5	15.2	+15.2	+0.0
0	4	23	16.6	15.3	-15.3	-0.0
0	4	24	9.4	10.1	-10.1	+0.0
0	4	25	23.9	22.8	-22.8	-0.0
0	4	26	41.6	48.0	-48.0	-0.0
0	4	27	5.2	2.8	-2.8	+0.0
0	4	28	29.1	31.7	-31.7	-0.0
0	4	29	11.4	11.8	-11.8	+0.0
0	4	30	22.9	26.4	-26.4	-0.0
0	4	31	5.2	4.3	-4.3	+0.0
0	4	32	7.3	9.4	-9.4	-0.0
0	5	1	18.7	20.4	+0.0	-20.4
0	5	2	27.0	27.9	-0.0	+27.9
0	5	3	13.5	13.7	+0.0	-13.7
0	5	4	42.6	40.3	-0.0	+40.3
0	5	5	11.4	8.7	+0.0	+8.7
0	5	6	35.4	38.3	-0.0	+38.3
0	5	7	7.3	7.3	+0.0	-7.3
0	5	8	68.6	63.5	-0.0	+63.5
0	5	9	33.3	31.7	+0.0	+31.7
0	5	10	45.8	40.4	-0.0	+40.4
0	5	11	12.5	11.3	+0.0	+11.3
0	5	12	7.3	10.8	-0.0	+10.8
0	5	13	21.8	22.8	-0.0	+22.8
0	5	14	20.8	18.1	+0.0	+18.1
0	5	15	14.6	15.8	-0.0	+15.8
0	5	16	11.4	13.0	+0.0	-13.0
0	5	17	18.7	21.4	-0.0	-21.4
0	5	18	30.2	32.3	+0.0	-32.3
0	5	20	29.1	31.7	+0.0	-31.7
0	5	21	15.6	16.9	-0.0	-16.9
0	5	22	30.2	27.8	+0.0	-27.8
0	5	23	28.1	25.8	+0.0	-25.8
0	5	24	15.6	16.2	+0.0	-16.2
0	5	25	12.5	12.5	-0.0	-12.5
0	5	26	26.0	27.8	+0.0	-27.8
0	5	28	10.4	13.7	+0.0	-13.7
0	5	30	7.3	13.5	-0.0	+13.5
0	5	32	7.3	7.9	-0.0	+7.9
0	5	33	7.3	8.9	-0.0	+8.9
0	5	34	7.3	12,3	-0.0	+12.3
0	5	35	5.2	8.8	+0.0	+8.8
0	6	0	48.9	50.9	-50.9	-0.0
0	6	1	15.6	18.4	-18.4	-0.0
0	6	2	29.1	31.9	-31.9	-0.0
0	6	3	25.0	28.6	-28.6	-0.0
0	6	4	11.4	12.6	-12.6	-0.0
0	6	5	28.1	33.0	-33.0	-0.0
0	6	7	14.6	20.5	-20.5	-0.0
0	6	9	36.4	36.4	-36.4	-0.0
0	6	10	5.2	4.9	+4.9	+0.0
0	6	11	23.9	24.0	-24.0	-0.0
0	6	12	23.9	26.7	+26.7	+0.0
0	6	13	26.0	24.5	+24.5	+0.0
0	6	14	19.8	19.4	+19.4	+0.0
0	6	15	7.3	4.8	-4.8	-0.0
0	6	16	23.9	19.3	+19.3	+0.0
0	6	17	18.7	17.1	+17.1	+0.0
0	6	18	33.3	36.2	+36.2	+0.0
0	6	20	23.9	24.4	+24.4	+0.0
0	6	21	9.4	12.2	+12.2	-0.0
0	6	22	14.6	15.4	+15.4	+0.0
0	6	23	13.5	18.4	+18.4	+0.0
0	6	24	9.4	8.8	-8.8	-0.0
0	6	25	7.3	12.2	+12.2	+0.0
0	6	27	5.2	5.0	-5.0	+0.0
0	6	28	11.4	15.4	-15.4	-0.0
0	6	29	11.4	13.0	-13.0	+0.0
0	6	30	10.4	12.8	-12.8	-0.0
0	6	31	7.3	11.0	-11.0	-0.0
0	7	1	7.3	7.6	+0.0	-7.6
0	7	3	25.0	27.7	+0.0	-27.7
0	7	4	7.3	8.7	-0.0	+8.7
0	7	5	38.5	38.0	+0.0	-38.0
0	7	6	5.2	6.4	-0.0	-6.4
0	7	9	12.5	13.0	-0.0	+13.0
0	7	12	11.4	9.8	+0.0	+9.8
0	7	13	32.2	30.5	-0.0	+30.5
0	7	15	28.1	31.3	-0.0	+31.3
0	7	16	9.4	6.8	+0.0	+6.8
0	7	17	21.8	23.2	-0.0	+23.2
0	7	18	12.5	12.9	+0.0	+12.9
0	7	19	12.5	14.4	-0.0	+14.4
0	7	22	5.2	7.3	-0.0	+7.3
0	7	23	7.3	11.4	+0.0	-11.4
0	7	24	9.4	10.8	+0.0	-10.8
0	7	25	10.4	14.2	+0.0	-14.2
0	7	26	9.4	7.9	-0.0	-7.9
0	7	27	7.3	11.0	+0.0	-11.0
0	7	28	5.2	7.2	+0.0	-7.2
0	8	2	18.7	21.8	+21.8	+0.0
0	8	3	5.2	7.6	-7.6	-0.0
0	8	6	7.3	7.7	-7.7	-0.0
0	8	7	16.6	16.7	-16.7	-0.0
0	8	9	16.6	17.8	-17.8	-0.0
0	8	10	11.4	15.6	-15.6	-0.0
0	8	11	5.2	7.9	-7.9	+0.0
0	8	12	12.5	16.7	-16.7	-0.0
0	8	13	12.5	11.8	-11.8	-0.0
0	8	14	7.3	13.2	-13.2	-0.0
0	8	19	5.2	9.7	+9.7	+0.0
0	8	21	9.4	11.2	+11.2	+0.0
0	8	23	7.3	14.5	+14.5	+0.0
0	8	25	7.3	13.9	+13.9	+0.0
0	9	4	7.3	11.3	+0.0	-11.3
0	9	5	5.2	5.5	+0.0	-5.5
0	9	6	9.4	14.2	+0.0	-14.2
1	0	3	15.3	15.4	+0.0	-15.4
1	0	4	49.6	61.0	-61.0	-0.0
1	0	5	25.4	30.0	-0.0	+30.0
1	0	6	101.7	106.6	-106.6	-0.0
1	0	7	31.8	40.8	-0.0	+40.8
1	0	8	61.0	72.2	-72.2	-0.0
1	0	9	8.9	11.3	-0.0	+11.3
1	0	10	76.3	83.3	-83.3	-0.0
1	0	11	53.4	53.4	-0.0	+53.4
1	0	12	30.5	34.1	-34.1	-0.0
1	0	13	35.6	36.7	-0.0	+36.7
1	0	14	11.4	9.6	+9.6	+0.0
1	0	15	28.0	26.6	+0.0	-26.6
1	0	16	38.1	37.5	+37.5	+0.0
1	0	17	16.5	15.9	+0.0	-15.9
1	0	18	39.4	33.9	+33.9	+0.0
1	0	19	31.8	28.8	+0.0	-28.8
1	0	20	31.8	30.9	+30.9	+0.0
1	0	21	24.2	22.8	+0.0	-22.8
1	0	22	64.8	62.0	+62.0	+0.0
1	0	23	28.0	26.2	+0.0	-26.2
1	0	24	28.0	24.5	+24.5	+0.0
1	0	25	8.9	7.2	+0.0	-7.2
1	0	26	30.5	32.2	+32.2	+0.0
1	0	27	6.4	9.5	-0.0	+9.5
1	0	28	8.9	10.5	+10.5	+0.0
1	0	29	15.3	18.8	+0.0	-18.8
1	0	30	16.5	22.3	-22.3	-0.0
1	0	31	8.9	11.0	-0.0	+11.0
1	0	32	8.9	8.7	-8.7	-0.0
1	0	33	15.3	20.4	-0.0	+20.4
1	0	34	20.3	24.6	-24.6	-0.0
1	0	36	12.7	12.8	-12.8	-0.0
1	0	37	6.4	8.4	-0.0	+8.4
1	0	38	6.4	10.7	-10.7	-0.0
1	0	39	5.1	5.1	-0.0	+5.1
1	0	40	5.1	9.8	-9.8	-0.0
1	1	0	49.6	50.7	+0.0	-50.7
1	1	1	72.5	75.9	-74.7	+13.3
1	1	2	114.4	119.9	+29.4	-116.2
1	1	3	20.3	15.9	-1.6	+15.8
1	1	4	119.5	121.3	-112.0	-46.7
1	1	5	80.1	81.2	+9.5	-80.6
1	1	6	28.0	25.8	-22.5	+12.7
1	1	7	59.7	59.2	-3.3	-59.1
1	1	8	22.9	23.4	-22.5	+6.5
1	1	9	34.3	38.9	+3.9	-38.7
1	1	10	49.6	50.3	-21.9	+45.3
1	1	11	49.6	49.9	+28.8	-40.8
1	1	12	53.4	48.2	+10.7	+47.0
1	1	13	29.2	27.7	+27.4	-3.8
1	1	14	55.9	53.2	-2.3	+53.2
1	1	15	24.2	23.3	+8.9	-21.5
1	1	16	47.0	47.3	+22.7	+41.5
1	1	17	43.2	40.0	+24.5	+31.6
1	1	18	40.7	36.2	+14.6	+33.1
1	1	19	50.8	47.1	+6.6	+46.6
1	1	20	6.4	10.1	+2.2	-9.9
1	1	21	26.7	25.2	-1.7	+25.1
1	1	22	15.3	17.3	+15.0	+8.6
1	1	23	29.2	29.0	+8.3	+27.8
1	1	24	15.3	17.8	+14.8	-9.9
1	1	25	21.6	19.7	-10.5	+16.7
1	1	26	28.0	28.9	-4.0	-28.6
1	1	27	28.0	25.2	-24.9	+4.0
1	1	28	16.5	17.1	-7.9	-15.2
1	1	29	16.5	16.7	-14.5	-8.2
1	1	30	36.9	34.7	-1.8	-34.7
1	1	31	5.1	4.1	-2.0	-3.6
1	1	32	15.3	17.7	-6.4	-16.5
1	1	33	14.0	13.9	+1.4	-13.8
1	1	34	6.4	5.7	-5.7	+0.5
1	1	35	11.4	13.4	-4.1	-12.8
1	1	37	6.4	10.3	+1.9	-10.1
1	1	39	5.1	11.2	+7.4	-8.4
1	1	40	5.1	6.5	-3.1	+5.7
1	2	0	5.1	6.1	+0.0	-6.1
1	2	1	78.8	73.2	+73.1	+3.4
1	2	2	53.4	41.3	-14.5	-38.7
1	2	3	67.4	65.0	+64.6	+7.3
1	2	4	38.1	31.2	-4.1	-30.9
1	2	5	55.9	50.9	+43.4	+26.5
1	2	6	34.3	30.0	-18.2	-23.9
1	2	7	30.5	24.0	+23.2	+6.3
1	2	8	16.5	15.7	-12.6	-9.3
1	2	9	49.6	41.8	-37.7	+18.0
1	2	10	64.8	54.8	-8.2	+54.2
1	2	11	49.6	44.4	-43.5	+9.1
1	2	12	40.7	34.7	-18.7	+29.2
1	2	13	81.4	73.3	-73.3	-2.2
1	2	14	20.3	20.3	-15.2	+13.5
1	2	15	80.1	70.2	-70.2	+0.6
1	2	16	45.8	41.4	-6.2	+40.9
1	2	17	45.8	42.6	-39.4	-16.3
1	2	18	15.3	17.6	+6.4	+16.4
1	2	19	41.9	34.9	-34.9	-0.4
1	2	20	11.4	8.6	+8.5	-1.0
1	2	21	6.4	5.5	+2.6	-4.9
1	2	22	16.5	19.3	-1.3	-19.3
1	2	23	15.3	18.1	+18.1	+0.1
1	2	24	21.6	22.7	+15.9	-16.2
1	2	25	28.0	31.8	+31.6	+3.3
1	2	26	28.0	29.0	+29.0	-1.5
1	2	27	30.5	30.0	+29.1	-7.2
1	2	28	8.9	12.3	+0.4	-12.3
1	2	29	22.9	22.6	+21.9	+5.6
1	2	30	8.9	9.7	-5.4	-8.1
1	2	31	15.3	17.5	+16.6	-5.6
1	2	32	8.9	10.3	+8.2	-6.2
1	2	33	6.4	10.1	+10.0	-1.7
1	2	34	6.4	7.6	-2.6	+7.1
1	2	35	6.4	9.0	+8.9	+1.1
1	2	36	6.4	9.2	-8.5	+3.5
1	2	37	5.1	8.1	-7.2	-3.8
1	2	38	6.4	9.8	-6.9	+7.0
1	2	39	6.4	10.3	-7.5	+7.0
1	2	40	5.1	4.9	-2.1	+4.4
1	3	0	58.5	50.3	-0.0	+50.3
1	3	1	31.8	27.2	+21.7	-16.4
1	3	2	55.9	45.1	-38.3	+23.9
1	3	3	33.0	29.9	+2.9	-29.8
1	3	4	16.5	13.8	-1.1	+13.8
1	3	5	53.4	45.2	+6.2	-44.8
1	3	6	40.7	34.1	-33.3	+7.5
1	3	7	86.4	72.5	-15.3	-70.9
1	3	8	21.6	19.2	-16.2	-10.3
1	3	10	35.6	31.9	-12.0	-29.6
1	3	11	44.5	40.4	-11.0	-38.9
1	3	12	40.7	32.1	-15.7	-28.0
1	3	13	22.9	20.6	-20.2	-3.9
1	3	14	19.1	19.5	+0.3	-19.5
1	3	15	6.4	7.0	+4.8	-5.1
1	3	16	20.3	17.4	+0.0	-17.4
1	3	17	28.0	23.7	-13.7	+19.4
1	3	18	14.0	12.8	+0.3	-12.8
1	3	19	45.8	40.6	-0.6	+40.6
1	3	20	15.3	13.6	+13.3	+3.0
1	3	21	49.6	50.4	+6.7	+50.0
1	3	22	34.3	34.1	+29.5	+17.1
1	3	23	31.8	33.1	-3.8	+32.9
1	3	24	25.4	20.0	+17.3	+10.1
1	3	25	16.5	14.8	+14.3	+4.0
1	3	26	16.5	17.3	+11.7	+12.7
1	3	27	15.3	13.3	+10.1	+8.6
1	3	28	15.3	20.1	+3.3	+19.8
1	3	29	8.9	10.1	+3.3	+9.5
1	3	30	8.9	9.7	-8.5	+4.6
1	3	31	6.4	6.6	+5.5	-3.7
1	3	32	6.4	8.1	-7.7	+2.6
1	3	33	12.7	15.4	-6.1	-14.1
1	3	34	6.4	10.8	-10.8	-0.3
1	3	35	11.4	13.1	-3.8	-12.5
1	3	36	11.4	12.8	-8.6	-9.5
1	3	37	11.4	9.8	-0.4	-9.8
1	3	38	6.4	7.4	-4.9	-5.5
1	3	39	6.4	9.1	-6.3	-6.6
1	3	39	6.4	9.1	-6.3	-6.6
1	4	0	10.2	10.0	-0.0	-10.0
1	4	1	21.6	19.9	+16.8	-10.6
1	4	2	17.8	15.1	+14.9	+2.6
1	4	3	34.3	29.6	+28.0	-9.7
1	4	5	35.6	29.7	+16.1	-24.9
1	4	6	59.7	49.0	+46.4	-15.7
1	4	7	45.8	36.7	+13.0	-34.3
1	4	8	41.9	37.8	+35.5	+13.1
1	4	9	34.3	27.5	-6.9	-26.6
1	4	10	36.9	35.3	+34.8	-6.2
1	4	11	20.3	16.9	-4.1	-16.4
1	4	12	30.5	26.1	+24.8	+8.1
1	4	13	30.5	27.4	-26.5	+6.9
1	4	14	16.5	13.6	+1.8	+13.5
1	4	15	28.0	24.5	-24.3	+3.4
1	4	16	25.4	21.8	-21.8	+1.0
1	4	17	29.2	25.9	-13.1	+22.4
1	4	18	40.7	38.1	-32.5	+19.9
1	4	19	40.7	39.4	-26.4	+29.3
1	4	20	24.2	22.6	-22.4	+2.6
1	4	21	15.3	13.1	-7.9	+10.4
1	4	22	16.5	19.1	-19.1	-0.3
1	4	24	43.2	37.9	-37.9	+1.9
1	4	26	17.8	18.9	-17.3	-7.6
1	4	27	5.1	5.1	+4.9	+1.5
1	4	29	6.4	8.7	+3.5	-8.0
1	4	30	11.4	12.6	+10.6	-6.8
1	4	31	8.9	12.1	+12.0	-1.9
1	4	32	20.3	20.7	+17.6	-10.9
1	4	33	11.4	12.6	+12.1	-3.4
1	4	34	11.4	11.0	+10.6	-2.8
1	4	35	10.2	8.4	+6.8	-4.9
1	4	36	11.4	14.1	+14.1	-1.1
1	5	1	34.3	28.2	+27.5	+6.3
1	5	2	47.0	42.1	+10.0	+40.9
1	5	3	39.4	31.7	+24.4	+20.3
1	5	4	30.5	27.1	-1.3	+27.1
1	5	6	15.3	14.9	-3.4	+14.5
1	5	7	16.5	18.7	-6.6	+17.5
1	5	8	20.3	17.5	+2.2	-17.4
1	5	9	12.7	12.7	-9.9	+7.9
1	5	10	21.6	22.8	+3.9	-22.5
1	5	11	6.4	6.3	-2.6	-5.7
1	5	12	25.4	24.0	-4.6	-23.6
1	5	13	21.6	20.2	-19.9	+3.6
1	5	14	43.2	39.2	+1.3	-39.2
1	5	15	45.8	44.0	-30.2	-32.0
1	5	16	34.3	31.5	-2.9	-31.4
1	5	17	5.1	8.2	+6.9	-4.4
1	5	18	24.2	22.1	-4.0	-21.7
1	5	19	8.9	7.5	-5.0	-5.6
1	5	20	15.3	13.9	-0.6	-13.9
1	5	21	26.7	24.1	-14.9	-19.0
1	5	22	5.1	8.9	-8.9	-0.6
1	5	23	10.2	6.4	+6.2	+1.7
1	5	25	8.9	13.0	+10.3	+7.9
1	5	26	6.4	14.3	-2.4	+14.1
1	5	27	14.0	16.2	+12.1	+10.7
1	5	28	26.7	26.2	+2.1	+26.1
1	5	29	14.0	12.2	+11.9	+2.5
1	5	30	24.2	23.7	+10.3	+21.4
1	5	31	10.2	12.2	+2.6	+11.9
1	5	32	11.4	10.8	+2.3	+10.6
1	5	33	5.1	9.0	+0.8	+9.0
1	5	34	5.1	9.1	+4.5	+7.9
1	6	1	28.0	27.1	-27.0	+1.9
1	6	2	28.0	27.6	+26.8	+6.7
1	6	3	28.0	23.6	-22.7	-6.5
1	6	4	29.2	25.6	+17.3	+18.9
1	6	5	5.1	8.6	+7.1	+4.8
1	6	6	21.6	20.8	+20.4	+4.2
1	6	7	5.1	4.8	+3.0	-3.7
1	6	8	17.8	16.8	+12.7	-11.0
1	6	9	21.6	19.5	+0.8	-19.5
1	6	10	24.2	27.2	+27.2	-0.2
1	6	11	35.6	36.4	+36.2	-3.4
1	6	12	16.5	16.8	+13.0	-10.6
1	6	13	22.9	25.4	+23.4	-9.8
1	6	14	21.6	19.1	-0.4	-19.1
1	6	15	15.3	16.1	+15.1	-5.5
1	6	17	22.9	24.1	+23.9	+2.7
1	6	18	5.1	7.8	-3.9	-6.7
1	6	19	5.1	10.6	-3.1	+10.1
1	6	22	21.6	21.8	-20.4	+7.6
1	6	23	6.4	11.7	-11.3	+3.0
1	6	24	14.0	15.9	-12.5	+9.9
1	6	25	17.8	19.5	-18.6	+5.9
1	6	26	16.5	15.3	-13.0	+8.0
1	6	27	17.8	17.8	-14.8	+9.9
1	6	28	12.7	13.2	-12.7	-3.7
1	6	29	5.1	8.3	-8.0	+2.3
1	6	30	5.1	8.3	-8.0	+2.3
1	7	2	24.2	20.2	+18.1	+8.9
1	7	4	8.9	12.0	+10.9	-4.9
1	7	5	22.9	23.7	-0.7	+23.7
1	7	6	8.9	12.6	+12.6	-0.3
1	7	7	41.9	34.9	+2.2	+34.8
1	7	8	22.9	19.1	+15.4	+11.3
1	7	9	22.9	18.8	+10.4	+15.7
1	7	10	6.4	4.8	+4.8	+0.6
1	7	11	8.9	12.1	-1.1	+12.0
1	7	13	14.0	15.4	+1.2	+15.4
1	7	14	6.4	5.7	-5.7	-0.0
1	7	17	15.3	14.3	-8.1	-11.8
1	7	18	6.4	11.9	-6.6	-9.9
1	7	19	17.8	18.9	-2.3	-18.8
1	7	20	11.4	13.4	-12.3	-5.3
1	7	21	20.3	22.7	-3.1	-22.5
1	7	22	8.9	9.0	+0.8	-9.0
1	7	23	12.7	14.3	-6.9	-12.5
1	7	24	12.7	16.5	-10.0	-13.1
1	7	25	5.1	9.4	-2.1	-9.2
1	7	26	5.1	6.8	-6.8	-0.2
1	7	27	5.1	5.8	+0.5	-5.8
1	8	0	5.1	2.1	+0.0	+2.1
1	8	1	6.4	9.4	-9.2	-1.8
1	8	2	6.4	12.5	-12.1	+3.3
1	8	3	6.4	11.9	-11.7	+2.4
1	8	4	15.3	17.3	-12.9	+11.5
1	8	5	6.4	8.1	-7.9	-1.9
1	8	6	5.1	6.6	-3.9	+5.3
1	8	7	6.4	9.7	-9.2	+3.2
1	8	8	11.4	14.0	-13.0	-5.3
1	8	9	10.2	11.3	+2.8	+10.9
1	8	10	10.2	11.1	-10.4	-3.9
1	8	11	6.4	9.1	+9.0	-1.6
1	8	12	5.1	4.5	+0.1	-4.5
1	8	13	6.4	7.0	+6.9	+1.0
1	8	14	6.4	11.3	+9.6	-5.9
1	8	15	11.4	14.4	+14.4	-0.5
1	8	16	8.9	11.0	+8.5	-7.0
1	8	17	14.0	16.9	+16.5	-3.7
1	8	18	5.1	7.0	+6.4	-2.9
1	8	19	6.4	10.1	+8.1	-6.1
1	8	20	8.9	12.3	+11.8	-3.3
1	8	21	6.4	9.0	+4.0	-8.1
1	9	0	8.9	15.9	+0.0	-15.9

Table 2 (*cont.*)

H	K	L	|FO|	|FC|	AC	BC
1	9	1	5.1	7.7	-7.5	+1.8
1	9	2	8.9	10.6	-1.9	-10.4
1	9	3	5.1	5.0	-4.7	-1.7
1	9	4	5.1	7.4	+0.3	-7.4
1	9	7	5.1	5.5	+2.1	+5.1
1	9	9	5.1	5.1	-3.7	+3.5
1	9	10	5.1	8.0	+3.8	+7.0
1	9	11	6.4	8.6	+5.4	+6.7
1	9	12	5.1	13.1	-0.9	+13.1
2	0	5	19.1	21.2	-0.0	+21.2
2	0	7	17.2	16.2	-0.0	+16.2
2	0	9	31.6	29.6	+0.0	-29.6
2	0	10	17.2	19.6	+19.6	+0.0
2	0	11	19.1	22.6	+0.0	-22.6
2	0	12	40.2	39.7	+39.7	+0.0
2	0	13	45.0	48.8	+0.0	-48.8
2	0	14	42.1	42.3	+42.3	+0.0
2	0	15	56.4	56.3	+0.0	-56.3
2	0	16	36.3	38.4	+38.4	+0.0
2	0	17	23.9	21.1	+0.0	-21.1
2	0	19	28.7	27.6	+0.0	-27.6
2	0	20	30.6	30.9	+30.9	+0.0
2	0	21	2.9	3.4	+0.0	-3.4
2	0	22	0.0	1.2	+1.2	-0.0
2	0	23	21.0	20.1	-0.0	+20.1
2	0	24	23.0	20.7	-20.7	-0.0
2	0	25	23.0	19.2	-0.0	+19.2
2	0	27	15.3	15.9	-0.0	+15.9
2	0	28	23.0	22.7	-22.7	-0.0
2	0	29	36.3	27.5	-0.0	+27.5
2	0	30	21.0	17.9	-17.9	-0.0
2	0	31	23.0	21.9	-0.0	+21.9
2	0	32	23.9	22.3	-22.3	-0.0
2	0	34	8.6	7.4	-7.4	-0.0
2	1	0	29.6	32.4	-32.4	-0.0
2	1	5	34.4	38.8	+25.6	-29.2
2	1	6	17.2	18.5	-0.7	+18.5
2	1	7	32.5	40.2	+29.5	+27.3
2	1	8	34.4	41.1	+13.2	+38.9
2	1	9	45.0	44.9	+44.0	+9.0
2	1	10	37.3	40.8	+30.4	+27.2
2	1	11	39.2	38.8	+36.3	+13.6
2	1	12	36.3	33.0	+33.0	-0.8
2	1	13	33.5	32.6	+9.8	+31.1
2	1	14	36.3	32.5	+31.2	+9.1
2	1	15	23.9	22.8	-8.4	+21.2
2	1	16	12.4	14.6	+14.5	+1.5
2	1	17	37.3	35.2	-24.3	+25.5
2	1	18	21.0	20.9	+16.9	-12.3
2	1	19	26.8	25.8	-25.8	+0.2
2	1	20	21.0	18.6	-8.6	-16.5
2	1	21	23.0	18.7	-18.7	+0.3
2	1	22	19.1	16.6	-8.1	-14.5
2	1	23	21.0	19.9	-19.5	+3.8
2	1	24	28.7	30.6	-4.5	-30.3
2	1	25	32.5	30.6	-23.0	-20.2
2	1	26	30.6	30.2	-25.6	-16.0
2	1	27	15.3	15.0	-8.0	-12.7
2	1	28	12.4	11.4	-8.9	-7.1
2	1	29	12.4	12.9	+12.3	-3.9
2	1	30	8.6	4.6	-3.9	+2.4
2	1	31	17.2	12.8	+9.7	-8.3
2	1	32	17.2	14.4	-2.8	+14.1
2	1	35	12.4	8.4	+8.2	-1.9
2	1	36	8.6	9.8	-0.5	+9.8
2	1	37	12.4	11.1	+10.8	-2.6
2	2	0	43.0	41.5	-41.5	-0.0
2	2	1	8.6	10.6	-8.4	+6.5
2	2	2	15.3	15.1	+5.9	+13.9
2	2	3	32.5	31.7	-10.7	+29.8
2	2	4	32.5	35.7	-18.9	+30.3
2	2	5	21.0	23.8	-19.3	+13.9
2	2	6	70.8	70.9	-17.3	+68.8
2	2	7	61.2	61.5	-55.1	-27.4
2	2	8	67.9	66.5	+29.2	+59.8
2	2	9	52.6	48.0	-47.2	+8.6
2	2	10	23.0	24.0	-6.4	+23.1
2	2	11	34.4	36.2	-35.2	-8.6
2	2	12	8.6	9.6	+4.9	+8.3
2	2	13	23.9	24.5	-18.8	-15.7
2	2	14	15.3	13.4	+13.4	+0.6
2	2	15	15.3	14.0	+9.4	-10.4
2	2	16	15.3	11.2	+6.9	-8.8
2	2	17	21.0	16.8	+13.6	-9.8
2	2	18	30.6	28.4	+6.2	-27.7
2	2	19	44.0	42.3	+41.8	+6.7
2	2	20	45.0	39.1	+0.3	-39.1
3	2	21	33.3	28.8	+28.3	-5.5
2	2	22	34.4	31.8	-0.5	-31.8
2	2	23	12.4	12.0	+11.6	-3.0
2	2	24	15.3	15.2	+10.4	-11.1
2	2	25	15.3	14.7	+13.8	+5.2
2	2	26	8.6	4.3	+1.9	-3.9
2	2	28	12.4	12.9	-12.6	-2.7
2	2	31	8.6	6.4	-3.0	+5.6
2	2	32	8.6	12.7	-0.8	+12.7
2	2	33	8.6	5.9	-2.7	+5.3
2	2	34	23.0	21.2	+19.6	-8.2
2	2	36	15.3	12.9	-3.6	+12.4
2	2	37	17.2	16.4	-13.8	+8.8
2	3	0	52.6	49.9	-49.9	-0.0
2	3	1	34.4	36.4	+1.4	-36.4
2	3	2	30.6	29.9	-26.5	-13.9
2	3	3	23.0	23.2	-14.1	-18.4
2	3	4	34.4	36.1	-28.2	-22.6
2	3	5	36.3	34.8	-30.2	-17.2
2	3	6	15.3	15.3	-12.8	-8.4
2	3	7	15.3	13.6	-10.5	-8.7
2	3	8	17.2	18.1	+8.0	-16.2
2	3	9	8.6	8.9	-8.6	-2.1
2	3	10	19.1	18.9	+12.9	-13.8
2	3	11	33.5	35.1	-17.9	+30.2
2	3	12	33.5	32.0	+31.2	+7.2
2	3	13	21.0	20.6	-1.7	+20.5
2	3	14	29.6	32.7	+32.6	-2.8
2	3	15	26.8	26.0	+14.8	+21.4
2	3	16	30.6	27.9	+26.9	+7.5
2	3	17	35.4	35.9	+18.0	+31.1
2	3	18	19.1	16.3	+14.1	+8.1
2	3	19	23.0	22.3	+6.7	+21.3
2	3	20	28.7	26.2	+25.0	+7.8
2	3	21	17.2	19.9	+10.3	+17.0
2	3	22	21.0	17.2	+3.2	+16.9
2	3	23	21.0	19.1	+14.3	-12.6
2	3	24	21.0	22.9	-22.9	+1.2
2	3	25	12.4	10.5	+1.6	-10.4
2	3	26	12.4	14.6	-11.7	+8.7
2	3	27	15.3	12.1	-6.1	-10.5
2	3	28	23.0	17.9	-17.9	-0.7
2	3	29	19.1	17.0	-5.9	-15.9
2	3	30	21.0	20.2	-16.1	-12.2
2	3	31	15.3	14.1	-5.8	-12.9
2	3	32	15.3	13.4	-13.2	-2.5
2	3	33	15.3	15.3	-11.5	-10.1
2	3	34	12.4	11.2	-5.7	-9.6
2	4	0	23.9	27.3	+27.3	+0.0
2	4	1	36.3	36.8	+9.9	-35.4
2	4	2	35.4	31.7	+31.7	+0.8
2	4	3	35.4	31.8	-5.4	-31.3
2	4	4	29.6	28.2	+25.2	+12.7
2	4	5	21.0	19.5	-2.6	-19.3
2	4	6	12.4	9.7	+5.1	+8.2
2	4	7	21.0	18.2	-15.8	+9.1
2	4	8	25.8	26.0	-8.9	+24.4
2	4	9	25.8	25.6	-19.8	+16.3
2	4	10	28.7	26.9	-20.4	+17.5
2	4	11	38.3	35.5	-6.9	+34.8
2	4	12	23.0	24.0	-23.8	-2.8
2	4	13	39.2	36.6	-26.0	+25.8
2	4	14	25.8	26.0	-24.8	+7.7
2	4	15	26.8	25.0	+6.0	+24.3
2	4	16	33.5	30.7	-27.5	+13.7
2	4	17	34.4	29.9	+1.8	+29.8
2	4	18	15.3	11.2	-9.3	-6.2
2	4	20	19.1	19.0	+6.4	-17.9
2	4	21	25.8	23.0	+19.1	-12.8
2	4	23	12.4	11.9	+5.3	-10.6
2	4	24	12.4	10.4	+2.8	-10.0
2	4	25	12.4	11.3	+4.4	-10.4
2	4	26	17.2	16.5	+12.5	-10.7
2	4	27	19.1	20.0	+6.9	-18.8
2	4	28	15.3	14.8	+13.7	-5.5
2	4	29	12.4	13.2	+5.6	-12.0
2	4	30	8.6	9.2	+8.1	-4.3
2	4	31	8.6	6.3	+5.6	-2.9
2	4	34	8.6	8.0	+5.7	+5.6
2	4	35	8.6	8.2	-7.1	+4.1
2	5	0	23.0	21.2	+21.2	+0.0
2	5	1	23.0	18.7	-14.7	+11.5
2	5	2	23.0	22.3	-2.6	-22.1
2	5	3	30.6	28.8	-27.7	-7.7
2	5	4	23.0	23.8	-5.9	-23.1
2	5	5	23.0	22.9	-22.9	-1.1
2	5	6	37.3	37.7	+4.5	-37.4
2	5	7	23.9	24.4	-24.1	+3.8
2	5	8	15.3	18.6	-0.0	-18.6
2	5	9	25.8	25.5	-23.5	-9.9
2	5	10	12.4	6.6	-6.0	-2.7
2	5	11	23.0	22.7	-22.7	+0.5
2	5	12	23.9	24.4	-10.8	-21.9
2	5	13	23.9	19.4	-15.6	-11.5
2	5	15	15.3	15.9	+15.9	-0.0
2	5	16	12.4	9.8	-4.5	+8.7
2	5	17	15.3	20.3	+19.2	+6.6
2	5	19	15.3	16.6	+12.2	-11.2
2	5	20	12.4	12.0	+2.5	+11.7
2	5	21	15.3	15.7	+14.3	+6.4
2	5	23	19.1	19.2	+17.6	+7.6
2	5	24	23.9	22.7	+8.8	+20.9
2	5	26	19.1	13.9	+3.3	+13.5
2	5	27	8.6	6.9	+4.3	+5.4
2	5	28	12.4	10.0	+9.3	+3.6
2	5	29	8.6	6.3	-4.5	+4.4
2	5	31	8.6	11.7	-10.9	+4.3
2	5	32	8.6	9.3	-4.1	-8.3
2	6	0	25.8	26.4	+26.4	+0.0
2	6	1	15.3	14.7	-4.2	-14.1
2	6	2	8.6	6.1	+5.1	+3.4
2	6	3	8.6	6.2	+2.5	-5.7
2	6	4	23.9	19.7	+3.1	-19.5
2	6	5	15.3	17.0	+16.2	-5.1
2	6	6	17.2	20.9	+7.9	-19.4
2	6	7	15.3	14.4	+9.4	-10.9
2	6	8	15.3	17.4	+4.6	-16.8
2	6	9	12.4	16.7	+16.6	+1.7
2	6	10	12.4	11.5	+0.0	-11.5
2	6	11	12.4	15.4	+15.1	+2.9
2	6	12	15.3	15.2	-15.2	-1.0
2	6	13	12.4	11.3	+0.7	+11.3
2	6	15	17.2	14.2	-1.6	+14.1
2	6	16	8.6	8.7	-7.4	+4.6
2	6	17	21.0	19.4	-15.8	+11.3
2	6	18	21.0	17.9	-13.6	+11.7
2	6	19	21.0	17.4	-9.9	+14.3
2	6	20	23.0	20.9	-9.2	+18.8
2	6	21	17.2	12.6	-11.8	+4.3
2	6	22	17.2	12.4	-5.7	+11.0
2	6	23	17.2	13.0	-12.9	+1.7
2	6	24	12.4	6.0	-1.3	+5.9
2	7	0	19.1	17.5	+17.5	+0.0
2	7	1	15.3	16.2	+2.4	+16.0
2	7	2	23.0	20.6	+20.6	+0.5
2	7	3	12.4	12.6	+2.8	+12.3
2	7	4	12.4	9.9	+8.9	-4.4
2	7	5	8.6	7.7	-1.4	+7.6
2	7	6	8.6	9.2	+2.5	+8.9
2	7	7	8.6	7.0	+6.4	+2.9
2	7	8	8.6	4.5	-3.3	-3.1
2	7	9	12.4	14.4	+0.7	-14.4
2	7	10	15.3	16.2	-15.8	-3.4
2	7	11	8.6	11.4	-9.4	-6.4
2	7	12	12.4	13.6	-13.6	-1.0
2	7	13	8.6	8.0	-3.3	-7.3
2	7	14	12.4	14.9	-14.3	-4.2
2	7	15	19.1	18.3	-6.5	-17.1
2	7	16	15.3	13.2	-11.6	-6.2
2	7	17	8.6	9.9	-4.6	-8.8
2	7	18	12.4	9.9	-7.6	-6.4
2	7	19	12.4	8.8	-3.2	-8.2
2	8	0	8.6	7.7	-7.7	-0.0
2	8	1	8.6	7.3	-5.7	+4.5
2	8	2	8.6	4.4	-4.1	+1.7
2	8	4	8.6	4.5	+3.2	-3.2
2	8	6	23.0	20.4	-5.6	-19.6
2	8	7	8.6	6.3	+6.3	+0.1
2	8	12	8.6	9.9	+8.4	-5.3
2	8	13	8.6	8.1	+3.6	-7.3
2	8	14	8.6	8.0	+6.8	-4.3
2	8	15	8.6	7.2	+5.1	-5.1
3	0	7	44.4	45.6	+0.0	-45.6
3	0	8	15.5	11.6	+11.6	+0.0
3	0	9	47.7	47.6	+0.0	-47.6
3	0	11	15.5	17.2	+0.0	-17.2
3	0	13	15.5	16.2	+0.0	-16.2
3	0	15	15.5	10.2	-0.0	+10.2
3	0	17	15.5	20.9	-0.0	+20.9
3	0	18	15.5	9.1	+9.1	+0.0
3	0	19	25.5	19.9	-0.0	+19.9
3	0	20	15.5	12.6	-12.6	-0.0
3	0	21	34.4	38.1	-0.0	+38.1
3	1	0	15.5	13.7	-0.0	+13.7
3	1	1	28.9	38.7	+38.6	+2.0
3	1	2	25.5	21.7	+9.6	+19.5
3	1	3	25.5	29.4	+27.5	+10.4
3	1	4	15.5	16.1	+16.1	-1.2
3	1	5	15.5	13.1	+10.7	+7.5
3	1	6	28.9	33.4	+33.4	-0.3
3	1	7	15.5	15.5	+9.3	+12.4
3	1	8	28.9	31.3	+30.5	+6.9
3	1	9	15.5	11.9	-4.9	+10.8
3	1	10	25.5	20.5	+17.4	-10.8
3	1	11	25.5	26.2	-26.1	+2.5
3	1	12	15.5	16.4	+15.4	-5.5
3	1	13	37.7	38.4	-37.3	+9.1
3	1	15	37.7	37.5	-37.3	-3.8
3	1	16	15.5	8.3	-6.3	-5.4
3	1	17	25.5	23.7	-20.2	-12.3
3	1	18	25.5	23.5	-20.5	-11.5
3	1	19	15.5	7.2	-5.5	-4.6
3	1	20	25.5	26.8	-26.7	-2.0
3	2	0	41.1	49.0	-0.0	+49.0
3	2	2	34.4	37.4	-0.5	+37.4
3	2	3	15.5	13.9	-13.6	+2.8
3	2	4	34.4	35.5	+0.5	+35.5
3	2	5	25.5	24.0	-11.2	-21.2
3	2	6	34.4	31.5	+28.9	+12.5
3	2	8	28.9	28.4	-3.6	-28.2
3	2	10	28.9	27.4	-7.3	-26.4
3	2	11	15.5	16.9	+2.5	-16.7
3	2	12	28.9	28.4	+6.3	-27.7
3	2	13	15.5	10.8	+9.8	-4.5
3	2	14	25.5	27.9	+2.9	-27.7
3	2	15	15.5	17.1	+16.2	-5.6
3	2	16	25.5	26.4	-11.1	-23.9
3	2	17	15.5	11.6	+10.9	+3.9
3	2	18	25.5	26.3	-1.3	-26.3
3	3	1	15.5	13.7	-12.9	+4.6
3	3	2	15.5	14.4	+14.3	+1.3
3	3	3	15.5	19.9	-19.9	-1.2
3	3	4	15.5	23.8	+22.9	-6.6
3	3	6	28.9	33.7	+33.7	-1.4
3	3	8	34.4	37.3	+35.7	+10.9
3	3	10	28.9	34.8	+33.4	-9.6
3	3	11	28.9	33.5	+15.1	+29.9
3	3	12	15.5	14.5	+14.2	+2.9
3	3	13	25.5	19.0	+19.0	-0.5
3	3	14	15.5	13.2	+0.2	+13.2
3	3	15	25.5	21.4	+19.5	+8.9
3	4	2	25.5	20.3	-2.1	+20.2
3	4	3	25.5	20.9	+5.2	+20.2
3	4	4	15.5	12.5	-8.4	+9.2
3	4	5	28.9	35.0	-3.7	+34.8
3	4	6	15.5	19.6	-19.5	+2.2
3	4	7	25.5	30.6	-16.0	+26.1
3	4	8	15.5	13.6	-11.4	+7.4
3	4	9	15.5	21.2	+7.3	+19.9
3	4	10	15.5	17.4	-3.2	-17.1

of the oxygen atom and two remaining carbon atoms were obtained from a second three-dimensional electron-density synthesis.

The structure was refined by least-squares using the Busing, Martin & Levy *ORFLS* program which uses the full matrix of the normal equations for each atom. Coordinate and temperature parameters were refined for all atoms except the hydrogen atoms which were positioned with respect to their bonded neighbours by the usual stereochemical considerations. The hydrogen contributions were included in the calculation of the structure factors. The initial three cycles of refinement were of the coordinate and isotropic temperature parameters and the layer scale factors. The next two cycles were of all coordinates and the bromine anisotropic temperature parameters only. Refinement was terminated with two similar cycles of refinement in which thirteen terms for which the agreement between observed and calculated structure factors was poor, and which had been measured from elongated spots on the photographs, were removed. The final reliability index for all observed terms was 0·11, when the calculated shifts for all parameters obtained were less than the corresponding standard deviations. The final parameters are listed in Table 1 and the observed and calculated structure factors in Table 2.

Crystal structure

The structure consists of planar molecules symmetrically placed about the screw axes with their planes inclined at about 28° to (100). The molecular dimen-

Table 3. *Molecular geometry of* 2-*bromoketofluorene*

Standard deviations are enclosed in brackets.

C(1)—C(2)	1·411 (0·023) Å	C(7)—C(8)	1·417 (0·026) Å
C(2)—C(3)	1·378 (0·027)	C(8)—C(13)	1·370 (0·020)
C(3)—C(4)	1·398 (0·026)	C(13)-C(12)	1·384 (0·022)
C(4)—C(11)	1·413 (0·021)	C(13)-C(9)	1·503 (0·023)
C(11)-C(12)	1·486 (0·021)	C(9)—C(10)	1·505 (0·019)
C(12)-C(5)	1·388 (0·025)	C(10)-C(11)	1·438 (0·023)
C(5)—C(6)	1·440 (0·029)	C(10)-C(1)	1·345 (0·021)
C(6)—C(7)	1·324 (0·031)	C(2)—Br	1·908 (0·013)
C(9)-O	1·189 (0·023) Å		
C(1)—C(2)—C(3)	121·8 (1·4)°	C(12)-C(5)—C(6)	115·6 (1·6)°
C(2)—C(3)—C(4)	122·6 (1·4)	C(5)—C(6)—C(7)	123·3 (1·9)
C(3)—C(4)—C(11)	116·3 (1·5)	C(6)—C(7)—C(8)	119·3 (1·7)
C(4)—C(11)-C(10)	119·3 (1·3)	C(7)—C(8)—C(13)	119·8 (1·3)
C(11)-C(10)-C(1)	123·5 (1·2)	C(8)—C(13)-C(12)	119·9 (1·3)
C(10)-C(1)—C(2)	116·4 (1·4)	C(13)-C(12)-C(5)	122·3 (1·3)
C(11)-C(12)-C(13)	108·9 (1·5)	C(13)-C(9)—O	128·5 (1·3)
C(12)-C(13)-C(9)	109·8 (1·2)	C(10)-C(9)—O	125·9 (1·3)
C(13)-C(9)—C(10)	105·2 (1·2)	C(1)—C(2)—Br	118·0 (1·2)
C(9)—C(10)-C(11)	107·6 (1·2)	C(3)—C(2)—Br	120·2 (1·1)
C(10)-C(11)-C(12)	108·4 (1·2)	C(5)—C(12)-C(11)	128·7 (1·3)
C(4)-C(11)-C(12)	132·1 (1·4)°		

sions are listed in Table 3. The best plane through all atoms is given in Table 4 and no atom departs significantly from this. Intermolecular bonding is entirely of the van der Waals type and there are no intermolecular distances less than the sum of the van der Waals radii. The individual atomic temperature factors are smaller for the atoms of the cyclopentadiene ring and increase with distance of the atom from the ring, indicating a pronounced rigid body motion. Atom C(6) is an exception, in that it has been given by the least-squares refinement a temperature factor which appears to be abnormally large even for its position furthest from the cyclopentadiene ring. The most likely explanation is that this atom is slightly misplaced owing to some artefact in the intensity data. This atom is not involved in any bonds of interest here.

Table 4. *Deviations of atoms from the best plane*

Best plane through all atoms

$$+0{\cdot}883x-0{\cdot}371y+0{\cdot}287z+0{\cdot}126=0\,.$$

Deviations from the plane

C(1)	+0·013 Å
C(2)	−0·001
C(3)	−0·001
C(4)	+0·012
C(5)	−0·001
C(6)	−0·011
C(7)	−0·007
C(8)	+0·017
C(9)	+0·034
C(10)	−0·014
C(11)	+0·026
C(12)	−0·024
C(13)	−0·007
Br	−0·016
O	−0·019

The dimensions of the cyclopentadiene ring are included in Table 3. The bond angles are regular and not significantly different to those found for fluorene (Burns & Iball, 1954). The bond lengths show some fluctuation, but at the accuracy of the present study none departs significantly from the fluorene values.

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