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The Crystal and Molecular Structure of Naphthalene. I. X-ray Measurements

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A comprehensive X-ray investigation of the crystal structure of naphthalene is described, in which all the reflexions that lie within the reach of Cu $K\alpha$ radiation have been examined. Moving-film photographic methods and visual estimates of intensities by independent observers were employed. From the results a total of 644 structure factors out of a possible 832 have been evaluated, giving 129 structure factors per atom of the asymmetric unit. From the earlier two-dimensional approximation to the naphthalene structure it has been possible to assign phase constants to 612 of the factors with reasonable certainty. These results form the basis of a new three-dimensional determination of the structure which is described in Part II.

1. Introduction

Naphthalene and anthracene were among the first organic substances to be studied by the X-ray method, and the early measurements of Sir William Bragg (1921, 1927, 1928) on these crystals gave a clear indication of the existence of molecules of about the shape and size to be expected from the chemical evidence, and also showed how these molecules could be accommodated in the unit cells of the crystals. Later work based on optical and magnetic measurements as well as on X-ray data (Banerjee, 1930 *a*, *b*; Robertson, 1930) gave the positions and dimensions of the molecules more precisely, and finally the structures were determined in detail from a complete survey of all the axial zones by the application of the double Fourier series method (Robertson, 1933 *a*, *b*).

The results of this last investigation showed that in naphthalene the carbon atoms are arranged very accurately in the form of two regular, planar hexagonal rings. Ten out of the fifteen co-ordinates which determine the positions of the carbon atoms could be measured directly from the electron-density maps, and the other five values could be inferred with reasonable certainty. The average C–C distance (radius of the hexagon) was obtained as 1·41 A., and the individual C–C distances were placed at between 1·40 and 1·44 A.

These findings were in accord with theoretical expectations. The average C–C distance of 1·41 A. was a little less than the graphite value of 1·42 A. and a little greater than the benzene value of 1·39 A. Both theoretical calculations (Pauling, Brockway & Beach, 1935) and chemical properties indicated that the bond lengths in different parts of the molecule might vary slightly from the average value. The experimental results, however, were not capable of giving any reliable measure of this variation, apart from a slight indication that the central C–C bond might be rather longer than the others. The electron-density maps, obtained as projections of the crystal structure, also failed to give any reliable picture of the electron distribution in the regions between the carbon atoms, because the degree of resolution of the various atoms differed in different parts of the projections.

In the present papers we describe a redetermination of the naphthalene structure which employs all the X-ray reflexions that can be observed with copper radiation at room temperature. Special methods have been employed to preserve the volatile crystals during the long exposures which are necessary, and from the measurements a total of 644 structure factors have been evaluated out of a possible 832 which lie within the range of Cu $K\alpha$ radiation. Calculations employing the previously determined structure (Robertson, 1933 *b*) as a first approximation have led to a reliable determination of the phase constants for just over 600 of these structure factors. The utilization of these measurements in a new structure determination by the triple Fourier series method is described in Part II.

2. Crystal data

The lattice constants were redetermined by means of carefully calibrated oscillation and moving-film photographs. The new values, given below, differ only slightly from the earlier measurements (Bragg, 1921; Robertson, 1933 *b*). Naphthalene, $C_{10}H_8$; M, 128·2; m.p. 80·2° C.; d, calc. 1·172, found 1·152. Monoclinic prismatic,

$$a = 8{\cdot}235 \pm 0{\cdot}005, \qquad b = 6{\cdot}003 \pm 0{\cdot}010,$$
$$c = 8{\cdot}658 \pm 0{\cdot}010 \text{ A.}, \qquad \beta = 122° 55' \pm 5'.$$

Absent spectra, $(h0l)$ when h is odd; $(0k0)$ when k is odd. Space group, C_{2h}^5-$P2_1/a$. Two molecules per unit cell. Molecular symmetry, centre. Volume of the unit cell, 361·7 A.^{3}. Absorption coefficient for X-rays, $\lambda = 1{\cdot}54$ A., $\mu = 6{\cdot}05$ cm.$^{-1}$. Total number of electrons per unit cell $= F(000) = 136$.

3. Experimental measurements

Preservation of crystal specimens

In this work it was necessary to make a complete survey of all the reflexions within the range of Cu $K\alpha$ radiation ($\lambda = 1{\cdot}542$ A.). This was carried out by photographic methods, using small crystals (0·1–0·2 mg.) completely immersed in a uniform X-ray beam. Naphthalene is so volatile that crystals of this size, placed in the open, disappear within an hour or two. For the work on hand it was necessary to preserve the specimens for periods of up to 2 weeks. Several methods were tried, but the most effective consisted in mounting the specimen on an extremely fine glass fibre inside a thin gelatin capsule, about 15 mm. in length and 5 mm. in diameter. The capsules (size 2, manufactured by Messrs Parke, Davis and Co., Detroit) were of very uniform thickness (0·12 mm.), and so did not introduce appreciable intensity errors due to absorption of the X-ray beam. Some powdered naphthalene was kept in the base of the capsule, which was sealed off with Apiezon Sealing Compound Q. The capsule and crystal could then be mounted and set in the usual manner on the goniometer arcs. Crystals so mounted could be preserved on an accurate setting for several weeks.

Intensity measurements and corrections

The photographic surveys were carried out almost entirely by moving-film methods, with an instrument of the equi-inclination Weissenberg type. This method was preferred to that of the oscillation photograph, not only in giving a more reliable correlation between certain sets of reflexions, but especially because it permits the background around each reflexion to be reduced to a minimum by careful adjustment of the screens.

A consideration of the points which lie within the limiting sphere of the reciprocal lattice for naphthalene showed that all the reflexions could be recorded on conveniently accessible layer lines from rotation about the [100], [010], [001] and [110] axes. A list of the layer lines recorded, with dimensions of the crystal specimens employed, is given in Table 1.

A fairly reliable set of structure factors for the axial zones in naphthalene have already been determined on an absolute scale (Robertson, 1933*b*). For the present extended survey, the method of visual estimation by two independent observers was adopted. The multiple-film technique (Robertson, 1943) was used to correlate the strong and weak reflexions, the extreme range being about 5000 to 1. Kodak Industrex Type D film was used, for which the reduction factor from film to film (separated by two thicknesses of the inner black paper wrapping) was determined by photometer measurement as 3·1 for Cu $K\alpha$ radiation. Using this method, independent estimates of the various intensities generally agreed to better than 10 %.

Table 1. *Layer lines recorded and dimensions of specimen*

Layer line	Dimensions of crystal specimen (mm.) Cross-section × length along rotation axis
$0kl$, $1kl$	$0{\cdot}13 \times 0{\cdot}39 \times 0{\cdot}39$
$1kl$, $2kl$, $3kl$	$0{\cdot}24 \times 0{\cdot}53 \times 0{\cdot}79$
$h0l$, $h1l$, $h2l$	$0{\cdot}31 \times 0{\cdot}71 \times 0{\cdot}95$
$h3l$	$0{\cdot}28 \times 0{\cdot}61 \times 0{\cdot}90$
$hk0$, $hk1$, $hk2$, $hk3$, $hk4$	$0{\cdot}94 \times 1{\cdot}05 \times 0{\cdot}16$
hhl, $h, h\pm1, l$, $h, h\pm2, l$, $h, h\pm3, l$, $h, h\pm4, l$	$0{\cdot}26 \times 0{\cdot}61 \times 1{\cdot}00$
$h, h\pm1, l$, $h, h\pm2, l$	$0{\cdot}31 \times 0{\cdot}53 \times 1{\cdot}20$
$h, h\pm4, l$	$0{\cdot}44 \times 0{\cdot}50 \times 1{\cdot}30$

Three sets of correction factors were applied to the intensities: (*a*) The normal Lorentz and polarization factors. (*b*) Absorption corrections to allow for the shape of the crystal specimen. These were made very approximately by evaluating a mean path length for the ray through the specimen for each reflexion. As the coefficient for naphthalene is small ($\mu = 6{\cdot}05$ cm.$^{-1}$ for $\lambda = 1{\cdot}54$ A.) this rough correction is probably sufficient. (*c*) A geometrical correction factor applied to all reflexions other than those on equatorial layer lines, to allow for the angular velocity of rotation of the plane through the reflecting angle. For the equi-inclination Weissenberg type of camera employed, the factors described by Tunell (1939) were used.

The structure factors were calculated from the intensities by the usual formula for mosaic-type crystals, and placed on the absolute scale previously determined (Robertson, 1933*b*). The structure factors for planes whose reflexions appeared on different layer lines and which came from different crystal specimens were correlated by reflexions common to the different sets. The final values chosen were the average of the different sets after correlation, for each reflexion frequently occurred in several different sets examined. When variations occurred among very strong reflexions, the highest value was generally adopted, in view of the possibilities of extinction errors.

When the structure factors of reflexions which appeared on two or more different layer lines, given by different crystals, were correlated and compared, it was found that the discrepancy was frequently of the order of 10 %. The system adopted for estimating the intensities was generally good enough to provide F values correct to within about 5 %. There is, therefore, some apparent lack of constancy in the determination of the F values which may be due to variations in crystal

type or to inadequate corrections for absorption. The overall accuracy of the F values may perhaps be placed at between 5 and 10%.

Determination of phase constants

The values of the structure factor finally determined are shown in Table 3, under '$F_{meas.}$'. The phase constants of these structure factors were next calculated on the basis of the previous structure determination by the double Fourier series method (Robertson, 1933*b*). From these results the signs obtained for 612 of the 644 observed F values were considered to be reasonably certain, and these 612 values were accordingly employed as coefficients in the triple Fourier series investigation which is described in Part II. The remaining 32 F values, all small, and for which the geometrical structure factors were all less than 2% of the possible maximum (for all atoms in phase), were excluded from the triple Fourier summations as unreliable. These F values are marked with an asterisk in Table 3.

From the final co-ordinates obtained as a result of the investigation described in Part II, the structure factors have been recalculated, and these values are listed in Table 3 under '$F_{calc.}$'. From this final recalculation of the structure factors it was found that six of the terms included in the Fourier synthesis had changed in sign. The values involved are generally small, and are marked with a double asterisk in Table 3.

For the final evaluation of the structure factors an empirical scattering curve for carbon was employed which gave the best average correlation between the observed and calculated F values. This curve was found to differ somewhat from the f_C curve previously employed (Robertson, 1935*a*, *b*), which was based mainly on measurements from anthracene and graphite. The new f_C values are given in Table 2, and it should be noted that they are designed specifically for naphthalene at 20° C. and include the temperature factor. It is not to be expected that they will give an equally accurate fit for other crystals where the temperature factor will in general be different.

Table 2. f_C *values for naphthalene at* 20° C. *including temperature factors*

$\lambda = 1{\cdot}54$ A. Maximum = 100 for $\sin\theta = 0$.

$\sin\theta$	0·00	0·01	0·02	0·03	0·04	0·05	0·06	0·07	0·08	0·09
0·0			97	96	94	92	90	88	87	85
0·1	82	81	79	77	74	73	71	69	66	64
0·2	62	60	58	56	54	53	51	49	48	46
0·3	45	43	42	40	39	38	37	35	34	32
0·4	31	30	29	28	27	26	25	24	23	22
0·5	21	21	20	19	18	18	17	16	16	15
0·6	15	14	14	13	13	13	12	12	12	11
0·7	10	10	10	10	9	9	8	8	8	7
0·8	7	7	7	7	7	6	6	5	5	5
0·9	4	4	4	4	4	4	3	3	3	2

The agreement between the observed and finally calculated F values on this basis, expressed as

$$\frac{\Sigma\{|F_{meas.}|-|F_{calc.}|\}}{\Sigma|F_{meas.}|}$$

is 16·8% for all the structure factors. Part of this discrepancy will be due to errors in the measured F values, but a substantial portion must be attributed to lack of spherical symmetry in the atomic electron distributions, to the bridge values for the density in the aromatic rings, and to the hydrogen atoms.

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Table 3. *Measured and calculated value of the naphthalene structure factors*

* Values omitted from the Fourier synthesis.
** Values included in the Fourier synthesis with incorrect sign.

hkl	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$
001	33·5	+35·0	207	2·6	− 3·1	406	1·3	− 1·1	604	0·9	+ 0·2
002	18·2	−17·5	206	3·4	− 4·4	405	1·2*	+ 0·5	603	4·3	− 3·3
003	22·4	+16·0	205	1·1	− 0·6	404	<1·4	+ 1·0	602	1·9	− 1·0
004	16·5	+13·0	204	6·1	+ 6·2	403	1·7	+ 2·6	601	<1·5	+ 1·6
005	1·6	− 1·8	203	16·8	+16·2	402	5·7	+ 6·2	60$\bar{1}$	8·7	− 7·8
006	2·7	− 4·0	202	5·5	+ 4·3	401	1·2	− 1·8	60$\bar{2}$	3·6	− 3·4
007	3·9	− 4·9	201	4·9	− 3·1	40$\bar{1}$	2·9	+ 5·7	60$\bar{3}$	3·3	+ 2·3
008	1·3	− 1·7	20$\bar{1}$	37·5	+44·0	40$\bar{2}$	6·2	− 4·9	60$\bar{4}$	11·7	+ 9·7
009	<1·4	+ 1·0	20$\bar{2}$	17·3	−17·8	40$\bar{3}$	1·0*	− 1·8	60$\bar{5}$	3·9	+ 3·4
020	14·7	−11·8	20$\bar{3}$	0·6*	− 2·0	40$\bar{4}$	9·4	+10·6	60$\bar{6}$	1·9	− 2·7
040	0·8	+ 2·3	20$\bar{4}$	8·7	+10·5	40$\bar{5}$	3·9	− 3·4	60$\bar{7}$	11·2	+ 9·9
060	<1·6	+ 1·7	20$\bar{5}$	3·2	− 4·2	40$\bar{6}$	1·0*	+ 0·2	60$\bar{8}$	12·3	+11·0
200	43·9	+47·3	20$\bar{6}$	1·2	+ 0·6	40$\bar{7}$	13·3	+13·3	60$\bar{9}$	<1·4	− 0·2
400	4·6	− 6·4	20$\bar{7}$	3·5	+ 3·6	40$\bar{8}$	6·6	+ 6·7	6.0.$\bar{10}$	1·4	− 1·2
600	6·2	− 5·3	20$\bar{8}$	1·5	− 0·7	40$\bar{9}$	2·2	− 1·2	6.0.$\bar{11}$	2·1	+ 1·5
800	1·3*	− 0·3	20$\bar{9}$	<1·3	+ 0·8	4.0.$\bar{10}$	2·2	+ 1·6	801	<1·3	+ 0·3
208	<1·4	+ 0·4	2.0.$\bar{10}$	1·8	+ 1·5	4.0.$\bar{11}$	<1·0	+ 1·5	80$\bar{1}$	5·7	− 4·7

Table 3 (*cont.*)

hkl	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$
$80\bar{2}$	3·3	− 2·4	$31\bar{2}$	0·6*	+ 0·6	$81\bar{6}$	< 1·0	+ 0·4	323	6·9	− 6·7
$80\bar{3}$	1·8	+ 1·7	$31\bar{3}$	6·9**	+ 4·5	$81\bar{7}$	2·6	− 2·4	322	1·3*	+ 1·0
$80\bar{4}$	6·3	+ 4·6	$31\bar{4}$	15·7	+13·8	$81\bar{8}$	5·2	− 5·0	321	0·8	+ 1·8
$80\bar{5}$	6·1	+ 4·7	$31\bar{5}$	1·5*	0	$81\bar{9}$	2·3	− 2·1	$32\bar{1}$	15·1	−16·9
$80\bar{6}$	< 1·7	+ 1·6	$31\bar{6}$	2·5	+ 2·4	$8.1.\bar{10}$	0·6	+ 0·6	$32\bar{2}$	2·7	+ 3·2
$80\bar{7}$	1·9	+ 0·5	$31\bar{7}$	8·0	+ 6·8	$91\bar{1}$	2·6	− 1·6	$32\bar{3}$	8·3	+ 9·3
$80\bar{8}$	6·5	+ 5·6	$31\bar{8}$	< 1·0	− 0·1	$91\bar{2}$	0·9	− 0·7	$32\bar{4}$	2·3	− 2·3
$80\bar{9}$	1·2	+ 1·3	$31\bar{9}$	1·0	− 1·0	$91\bar{3}$	0·8	− 0·2	$32\bar{5}$	6·9	− 6·8
$8.0.\bar{10}$	1·4	− 1·5	$3.1.\bar{10}$	1·5	+ 1·2	$91\bar{4}$	< 0·9	− 0·8	$32\bar{6}$	2·2	+ 1·0
$10.0.\bar{3}$	< 1·2	+ 0·5	416	< 0·9	+ 0·2	$91\bar{5}$	0·9	+ 1·2	$32\bar{7}$	6·5	+ 6·8
$10.0.\bar{4}$	< 1·2	+ 0·2	415	0·9	+ 1·6	$91\bar{6}$	< 1·0	+ 0·2	$32\bar{8}$	2·0	+ 3·0
$10.0.\bar{5}$	< 1·2	+ 0·6	414	3·0	− 2·7	$91\bar{7}$	< 1·2	− 1·3	$32\bar{9}$	0·6	− 0·9
$10.0.\bar{6}$	< 1·2	+ 0·7	413	8·0	− 7·3	$91\bar{8}$	1·5	+ 1·4	$3.2.\bar{10}$	0·9	+ 0·4
$10.0.\bar{7}$	< 1·2	− 1·1	412	3·4	− 2·6	$91\bar{9}$	1·4	+ 1·2	426	< 0·9	− 0·7
$10.0.\bar{8}$	< 1·2	− 0·4	411	1·0	+ 1·0	$9.1.\bar{10}$	0·7	− 0·3	425	0·7	+ 0·4
$10.0.\bar{9}$	< 1·2	− 0·1	$41\bar{1}$	23·5	−23·5	$10.1.\bar{3}$	0·8	+ 0·3	424	4·3	− 4·4
011	6·4	+ 6·7	$41\bar{2}$	3·0	− 3·5	$10.1.\bar{4}$	2·9	− 1·3	423	3·8	− 4·6
012	3·8	+ 4·1	$41\bar{3}$	11·7	+12·8	$10.1.\bar{5}$	3·0	− 1·3	422	1·8	+ 2·3
013	6·7	+ 4·7	$41\bar{4}$	5·0	+ 4·2	$10\,1.\bar{6}$	< 0·9	− 0·1	421	2·8	− 2·6
014	9·4	+ 7·6	$41\bar{5}$	2·5	− 3·4	$10.1.\bar{7}$	< 0·9	− 0·3	$42\bar{1}$	14·2	+13·2
015	1·4	+ 2·8	$41\bar{6}$	2·9	+ 3·0	$10.1.\bar{8}$	2·7	− 2·0	$42\bar{2}$	7·0	+ 7·6
016	4·1	− 4·4	$41\bar{7}$	8·4	+ 8·0	021	15·8	−14·3	$42\bar{3}$	1·5	+ 1·4
017	3·5	− 3·8	$41\bar{8}$	3·9	+ 3·6	022	5·3	+ 2·4	$42\bar{4}$	10·0	+ 9·6
018	0·7*	− 0·4	$41\bar{9}$	0·9	− 0·9	023	11·2	+10·8	$42\bar{5}$	4·6	+ 4·8
019	< 1·1	− 0·4	$4.1.\bar{10}$	0·7	− 0·6	024	4·0	− 4·0	$42\bar{6}$	1·4*	− 1·1
110	37·0	+45·0	515	< 1·0	+ 0·1	025	1·4**	− 0·8	$42\bar{7}$	< 0·9	− 0·2
210	28·9	−31·0	514	1·4	− 1·2	026	8·2	+ 8·4	$42\bar{8}$	2·7	− 2·5
310	5·4	+ 5·0	513	2·0	− 2·6	027	2·5	+ 2·3	$42\bar{9}$	1·3	− 1·6
410	14·4	−14·2	512	1·5	+ 2·0	028	0·9	− 1·1	$4.2.\bar{10}$	1·1	+ 0·9
510	4·7	− 4·2	511	1·1	+ 0·6	029	< 0·9	+ 0·5	525	0·7	+ 0·7
610	1·6	− 1·5	$51\bar{1}$	3·0	+ 2·9	120	13·2	−13·5	524	1·5	− 1·0
710	1·3	− 1·4	$51\bar{2}$	3·5	+ 3·5	220	6·9	− 7·0	523	4·9	− 5·0
810	< 1·4	+ 0·3	$51\bar{3}$	1·6	+ 0·9	320	15·0	−15·1	522	3·4	− 2·2
118	0·7*	− 0·1	$51\bar{4}$	10·2	+ 9·1	420	2·3	− 1·5	521	1·8	+ 2·8
117	2·0	− 1·6	$51\bar{5}$	1·9	+ 2·1	520	3·1	− 3·4	$52\bar{1}$	14·3	−11·5
116	0·9	+ 0·2	$51\bar{6}$	1·4	− 2·3	620	< 1·3	− 1·2	$52\bar{2}$	6·4	− 5·3
115	1·0*	+ 0·1	$51\bar{7}$	7·1	+ 6·9	720	< 1·2	− 0·2	$52\bar{3}$	1·0**	− 2·4
114	2·9	+ 2·8	$51\bar{8}$	5·0	+ 6·1	820	1·1	− 0·8	$52\bar{4}$	1·4	− 0·6
113	11·3	+12·2	$51\bar{9}$	2·3	− 1·6	128	0·6	+ 0·4	$52\bar{5}$	5·1	− 4·3
112	3·3	− 4·2	$5.1.\bar{10}$	0·7	+ 0·4	127	1·7	− 1·9	$52\bar{6}$	2·0	− 1·7
111	8·9	− 5·7	$5.1.\bar{11}$	< 1·0	+ 0·9	126	3·9	− 3·4	$52\bar{7}$	1·3	+ 0·9
$11\bar{1}$	19·5	+23·5	614	< 0·8	− 0·8	125	4·2	− 3·0	$52\bar{8}$	1·6	+ 1·7
$11\bar{2}$	12·6	−11·8	613	4·3	− 4·2	124	4·5	− 4·1	$52\bar{9}$	< 0·9	+ 0·9
$11\bar{3}$	14·8	+12·6	612	4·4	− 3·6	123	4·0	− 4·8	$5.2.\bar{10}$	1·0	+ 0·2
$11\bar{4}$	12·2	+12·8	611	0·8	+ 0·4	122	1·5	− 1·3	624	< 0·7	− 0·5
$11\bar{5}$	1·0*	+ 0·2	$61\bar{1}$	6·1	− 5·7	121	7·5	− 7·2	623	0·8	− 1·2
$11\bar{6}$	3·4	+ 6·0	$61\bar{2}$	1·1	− 1·4	$12\bar{1}$	2·3*	− 2·1	622	< 0·3	+ 1·7
$11\bar{7}$	1·3	+ 0·8	$61\bar{3}$	3·6	+ 4·7	$12\bar{2}$	11·8	+ 9·9	621	1·5	+ 1·2
$11\bar{8}$	1·9	− 1·7	$61\bar{4}$	2·7	+ 3·5	$12\bar{3}$	9·2	+ 6·2	$62\bar{1}$	7·7	+ 6·4
$11\bar{9}$	0·8	+ 0·8	$61\bar{5}$	1·0	+ 0·5	$12\bar{4}$	1·2	− 2·4	$62\bar{2}$	8·3	+ 7·8
218	< 0·9	− 0·1	$61\bar{6}$	< 1·0	+ 0·2	$12\bar{5}$	1·2	− 0·9	$62\bar{3}$	3·3	− 4·3
217	0·9*	− 0·1	$61\bar{7}$	1·2	− 0·5	$12\bar{6}$	7·8	+ 6·1	$62\bar{4}$	1·7	− 1·9
216	0·9	+ 0·9	$61\bar{8}$	1·4	− 1·4	$12\bar{7}$	6·2	+ 6·6	$62\bar{5}$	3·2	+ 3·9
215	1·0	+ 2·0	$61\bar{9}$	0·9	− 1·1	$12\bar{8}$	1·0*	+ 0·2	$62\bar{6}$	1·6	− 1·9
214	2·2*	− 1·1	$6.1.\bar{10}$	< 1·0	− 1·0	$12\bar{9}$	1·4	− 0·6	$62\bar{7}$	2·4	− 3·6
213	4·0	− 2·9	$6.1.\bar{11}$	< 0·8	− 0·4	227	< 1·0	− 0·4	$62\bar{8}$	1·9	− 1·6
212	2·2	+ 3·4	713	< 1·3	− 1·4	226	3·8	+ 3·9	$62\bar{9}$	1·1	− 0·9
211	1·3	− 1·0	712	1·3	− 1·2	225	1·3	+ 1·3	$6.2.\bar{10}$	2·0	+ 1·0
$21\bar{1}$	28·1	−32·0	711	0·8	+ 1·8	224	8·4	− 8·1	722	2·0	− 1·4
$21\bar{2}$	1·1*	− 0·5	$71\bar{1}$	2·6	− 2·8	223	2·2	− 2·3	721	< 1·4	− 0·7
$21\bar{3}$	6·9	+ 6·7	$71\bar{2}$	1·0	+ 0·6	222	3·1	+ 3·5	$72\bar{1}$	3·5	− 2·9
$21\bar{4}$	10·0	− 7·9	$71\bar{3}$	< 1·0	+ 0·3	221	11·5	−12·0	$72\bar{2}$	4·2	− 3·3
$21\bar{5}$	6·2	− 6·2	$71\bar{4}$	2·7	+ 2·3	$22\bar{1}$	4·0	+ 4·7	$72\bar{3}$	2·9	− 3·0
$21\bar{6}$	8·4	+ 7·3	$71\bar{5}$	2·9	+ 3·3	$22\bar{2}$	1·9	+ 2·7	$72\bar{4}$	3·6	− 2·8
$21\bar{7}$	10·2	+10·2	$71\bar{6}$	1·9	− 2·4	$22\bar{3}$	16·3	+15·2	$72\bar{5}$	2·2	− 1·6
$21\bar{8}$	2·2	+ 2·5	$71\bar{7}$	1·7	+ 1·0	$22\bar{4}$	12·2	+11·0	$72\bar{6}$	1·5	− 0·7
$21\bar{9}$	1·1	− 0·8	$71\bar{8}$	5·5	+ 5·6	$22\bar{5}$	1·1	+ 1·0	$72\bar{7}$	2·2	− 2·2
$2.1.\bar{10}$	0·9	+ 0·9	$71\bar{9}$	0·8	+ 0·7	$22\bar{6}$	4·9	+ 5·5	$72\bar{8}$	2·5	− 2·0
317	0·7	− 0·9	$7.1\,\bar{10}$	0·7	− 0·2	$22\bar{7}$	4·6	+ 3·4	$72\bar{9}$	1·3	+ 1·4
316	1·1	− 1·2	$7.1.\bar{11}$	< 0·7	+ 0·9	$22\bar{8}$	2·5	− 2·4	$7.2.\bar{10}$	2·0	+ 1·0
315	1·0*	− 0·1	811	< 0·7	+ 0·1	$22\bar{9}$	1·3**	− 0·5	821	1·1	+ 0·9
314	2·0	− 0·8	$81\bar{1}$	< 0·8	+ 0·6	$2.2.\bar{10}$	0·6*	+ 0·1	$82\bar{1}$	< 1·2	+ 0·1
313	3·2	+ 3·5	$81\bar{2}$	0·9	+ 1·5	327	0·7	− 0·6	$82\bar{2}$	2·1	+ 3·1
312	5·0	+ 4·4	$81\bar{3}$	< 1·0	+ 0·7	326	< 0·8	− 0·2	$82\bar{3}$	2·8	− 2·2
311	6·5	− 7·2	$81\bar{4}$	2·3	− 2·0	325	1·6	− 0·7	$82\bar{4}$	4·8	− 5·6
$31\bar{1}$	20·3	+21·0	$81\bar{5}$	1·8	− 1·2	324	5·6	− 5·1	$82\bar{5}$	< 1·2	+ 0·5

Table 3 (*cont.*)

hkl	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$
$82\bar{6}$	<1·1	− 0·2	$33\bar{3}$	1·8	− 1·8	$93\bar{7}$	<0·6	− 0·7	543	0·8	+ 1·0
$82\bar{7}$	1·5	− 2·3	$33\bar{4}$	2·0	+ 3·6	$93\bar{8}$	<0·6	− 0·3	542	1·8	− 1·4
$82\bar{8}$	<0·9	+ 0·1	$33\bar{5}$	3·3	− 2·7	041	3·3	− 2·5	541	3·7	− 3·6
$82\bar{9}$	<0·9	+ 0·8	$33\bar{6}$	2·7	− 2·4	042	1·6	− 0·6	$54\bar{1}$	1·3	+ 2·3
8.2.$\bar{1}\bar{0}$	<0·7	+ 0 6	$33\bar{7}$	<0·8	− 0·4	043	0·9	+ 2·5	$54\bar{2}$	<1·3	+ 0·2
$92\bar{1}$	0·8	− 0·4	$33\bar{8}$	1·8	− 1·5	044	7·0	− 5·5	$54\bar{3}$	6·0	− 5·4
$92\bar{2}$	<0·9	+ 0·1	$33\bar{9}$	1·3	+ 0·4	045	5·4	− 6·2	$54\bar{4}$	2·7	− 2·8
$92\bar{3}$	1·3	− 1·1	3.3.$\bar{1}\bar{0}$	0·4	+ 0·6	046	0·7	− 0·2	$54\bar{5}$	2·3	+ 2·6
$92\bar{4}$	4·8	− 3·0	435	1·4	− 1·5	047	<0·7	− 0·6	$54\bar{6}$	1·0	+ 0·5
$92\bar{5}$	2·6	− 1·8	434	1·4	− 1·2	048	<0·7	− 0·6	$54\bar{7}$	1·1	− 1·8
$92\bar{6}$	<1·2	+ 0·7	433	2·0	− 1·2	140	1·0	+ 0·8	$54\bar{8}$	1·1	+ 0·3
$92\bar{7}$	<1·2	− 1·2	432	1·5	− 0·4	240	<1·0	− 0·9	$54\bar{9}$	0·9	+ 0·6
$92\bar{8}$	3·3	− 2·4	431	<1·0	+ 0·9	340	<1·0	+ 0·7	642	1·6	+ 0·2
$92\bar{9}$	0·8	− 1·0	$43\bar{1}$	1·0	+ 0·6	440	1·0	− 2·2	641	0·7	− 0·5
10.2.$\bar{4}$	3·0	− 2·0	$43\bar{2}$	0·8	− 0·9	540	1·5	− 1·6	$64\bar{1}$	1·1	− 0·1
10.2.$\bar{5}$	<1·1	− 0·5	$43\bar{3}$	5·5	− 5·8	640	2·0	− 2·5	$64\bar{2}$	2·1	− 0·7
10.2.$\bar{6}$	<1·1	+ 0·5	$43\bar{4}$	4·8	− 4·0	740	0·9	− 0·6	$64\bar{3}$	5·7	− 5·5
10.2.$\bar{7}$	<1·0	− 0·6	$43\bar{5}$	2·4	− 1·9	147	2·7	− 0·4	$64\bar{4}$	1·1	− 1·2
10.2.$\bar{8}$	<1·0	+ 0·4	$43\bar{6}$	2·5	− 4·1	146	<1·0	+ 0·4	$64\bar{5}$	2·1	+ 2·7
031	13·7	−12·1	$43\bar{7}$	1·9	− 2·3	145	1·2	− 1·1	$64\bar{6}$	0·8	− 0·5
032	8·0	− 7·5	$43\bar{8}$	1·1	+ 1·2	144	3·3	− 2·5	$64\bar{7}$	<0·8	− 0·3
033	7·8	− 6·5	$43\bar{9}$	1·2	+ 1·3	143	3·8	− 1·4	$64\bar{8}$	<0·8	− 1·1
034	8·9	− 8·2	4.3.$\bar{1}\bar{0}$	0·5	+ 0·7	142	1·8	− 1·2	$64\bar{9}$	<0·8	− 0·8
035	6·8	− 5·7	534	<0·4	+ 0·1	141	3·3	− 3·8	741	0·7	− 0·5
036	3·2	− 2·5	533	0·5	− 1·2	$14\bar{1}$	5·8	+ 5·1	$74\bar{1}$	1·0	− 0·5
037	1·3	− 1·2	532	0·8	+ 1·7	$14\bar{2}$	3·0	− 3·8	$74\bar{2}$	1·1	− 0·7
038	<1·0	+ 0·1	531	1·1	− 1·1	$14\bar{3}$	2·9	− 3·3	$74\bar{3}$	1·3	− 0·5
130	10·0	−10·2	$53\bar{1}$	5·3	+ 5·6	$14\bar{4}$	6·0	+ 4·1	$74\bar{4}$	1·3	+ 1·4
230	1·6*	− 0·5	$53\bar{2}$	1·3	+ 1·1	$14\bar{5}$	4·6	+ 3·9	$74\bar{5}$	1·1	− 0·6
330	4·3	− 3·7	$53\bar{3}$	8·9	− 9·2	$14\bar{6}$	1·1	− 1·6	$74\bar{6}$	<1·0	− 0·8
430	<1·1	− 0·3	$53\bar{4}$	0·7	− 0·5	$14\bar{7}$	1·0	− 1·3	$74\bar{7}$	<1·0	− 0·9
530	1·1	− 2·7	$53\bar{5}$	4·1	+ 4·7	$14\bar{8}$	1·1	+ 1·0	$74\bar{8}$	<0·8	+ 0·6
630	0·9	− 0·7	$53\bar{6}$	1·3	− 1·3	246	0·5	+ 1·0	$74\bar{9}$	<0·8	+ 0·3
730	1·4	− 2·7	$53\bar{7}$	3·1	− 3·0	245	2·4	+ 1·0	$84\bar{1}$	<0·8	− 0·3
830	0·6	− 0·6	$53\bar{8}$	2·1	− 2·0	244	1·9	− 2·2	$84\bar{2}$	1·9	+ 1·9
138	<0·6	− 0·5	$53\bar{9}$	0·8*	− 0·1	243	<1·5	+ 1·8	$84\bar{3}$	1·2	+ 0·5
137	0·6	− 0·1	5.3.$\bar{1}\bar{0}$	1·3	+ 1·3	242	5·0	+ 2·9	$84\bar{4}$	0·8	− 0·6
136	5·8	+ 5·6	633	<0·8	+ 0·5	241	1·5*	+ 0·4	$84\bar{5}$	1·9	+ 1·8
135	1·1	− 1·3	632	<0·7	− 0·3	$24\bar{1}$	5·5	− 3·6	$84\bar{6}$	1·2	+ 1·0
134	9·8	− 9·9	631	0·5**	− 0·2	$24\bar{2}$	10·5	−10·2	$84\bar{7}$	<1·0	− 0·3
133	3·0	+ 2·6	$63\bar{1}$	3·6	− 3·3	$24\bar{3}$	4·5	− 5·8	$84\bar{8}$	<0·8	− 0·1
132	10·8	+ 9·3	$63\bar{2}$	6·1	− 4·9	$24\bar{4}$	4·7	− 2·7	$94\bar{4}$	<0·9	+ 0·3
131	6·5	− 5·3	$63\bar{3}$	7·5	− 6·5	$24\bar{5}$	9·9	− 9·0	$94\bar{5}$	<0·9	− 0·3
$13\bar{1}$	8·9	− 8·4	$63\bar{4}$	6·7	− 5·9	$24\bar{6}$	5·1	− 4·2	$94\bar{6}$	<0·9	− 0·9
$13\bar{2}$	0·6*	+ 1·1	$63\bar{5}$	3·7	− 2·5	$24\bar{7}$	<1·0	+ 0·4	051	3·1	+ 4·6
$13\bar{3}$	8·8	+ 8·1	$63\bar{6}$	2·7	− 2·8	$24\bar{8}$	<1·0	− 0·4	052	6·3	+ 5·2
$13\bar{4}$	5·2	− 6·7	$63\bar{7}$	2·1	− 2·1	$24\bar{9}$	<0·7	+ 0·3	053	1·8	+ 1·9
$13\bar{5}$	7·8	− 7·3	$63\bar{8}$	1·3	+ 1·4	345	<1·0	− 1·2	054	<2·3	− 0·3
$13\bar{6}$	2·7	+ 3·2	$63\bar{9}$	2·1	+ 1·9	344	0·9	+ 0·7	055	<2·0	+ 2·5
$13\bar{7}$	1·5	+ 1·9	6.3.$\bar{1}\bar{0}$	0·8	+ 0·8	343	<1·1	+ 0·1	056	<2·0	+ 1·2
$13\bar{8}$	1·7	− 1·7	732	0·7	+ 0·8	342	4·4	− 3·4	057	<1·8	− 0·9
$13\bar{9}$	0·4	+ 0·5	731	1·2	− 0·2	341	4·2	− 5·2	150	1·3	+ 3·4
237	1·0	− 0·8	$73\bar{1}$	2·7	+ 2·6	$34\bar{1}$	5·2	+ 5·7	250	<0·9	− 1·0
236	3·3	− 3·2	$73\bar{2}$	4·7	+ 5·3	$34\bar{2}$	1·8	− 2·6	350	0·9	+ 0·1
235	5·1	− 4·7	$73\bar{3}$	4·0	− 4·6	$34\bar{3}$	8·7	− 8·6	450	2·5	− 2·5
234	6·1	− 5·7	$73\bar{4}$	5·2	− 5·2	$34\bar{4}$	1·2	+ 1·7	550	1·3	− 0·6
233	5·7	− 5·7	$73\bar{5}$	3·2	+ 3·3	$34\bar{5}$	6·8	+ 6·2	650	0·9	− 1·1
232	4·6	− 2·7	$73\bar{6}$	1·7	+ 2·1	$34\bar{6}$	1·4	− 0·9	156	<0·8	+ 0·4
231	5·3	− 4·0	$73\bar{7}$	2·4	− 2·2	$34\bar{7}$	2·0	− 2·7	155	<0·8	− 0·5
$23\bar{1}$	9·7	+ 9·5	$73\bar{8}$	1·7	− 1·5	$34\bar{8}$	1·1	+ 1·2	154	0·8	+ 0·4
$23\bar{2}$	5·4	+ 6·6	$73\bar{9}$	0·7	− 0·6	$34\bar{9}$	1·2	+ 1·2	153	0·7	+ 0·8
$23\bar{3}$	0·8*	+ 0·6	7.3.$\bar{1}\bar{0}$	1·0	+ 0·8	445	<1·0	+ 1·5	152	6·1	− 5·5
$23\bar{4}$	2·9	+ 3·4	$83\bar{1}$	2·7	− 1·8	444	2·0	+ 1·3	151	4·6	− 5·2
$23\bar{5}$	2·7	+ 2·0	$83\bar{2}$	4·6	− 3·1	443	0·9	+ 0·4	$15\bar{1}$	3·8	− 3·3
$23\bar{6}$	1·0	− 2·1	$83\bar{3}$	4·6	− 3·2	442	2·2	+ 2·2	$15\bar{2}$	10·2	− 9·1
$23\bar{7}$	<0·8	− 0·6	$83\bar{4}$	4·7	− 2·7	441	1·0*	− 1·4	$15\bar{3}$	3·3	− 1·3
$23\bar{8}$	<0·8	+ 0·1	$83\bar{5}$	2·2	− 1·2	$44\bar{1}$	2·7	− 1·5	$15\bar{4}$	1·0	+ 0·8
$23\bar{9}$	0·5	+ 0·1	$83\bar{6}$	0·9	− 0·5	$44\bar{2}$	9·8	− 9·0	$15\bar{5}$	3·2	− 3·0
336	2·1	+ 1·9	$83\bar{7}$	<0·9	− 0·6	$44\bar{3}$	9·3	− 8·5	$15\bar{6}$	1·8	− 1·2
335	3·4	+ 2·7	$83\bar{8}$	<0·9	+ 0·4	$44\bar{4}$	1·9*	− 0·5	157	<0·8	− 0·1
334	4·0	− 4·7	$83\bar{9}$	<0·9	+ 0·9	$44\bar{5}$	4·0	− 2·6	255	3·3	+ 2·8
333	3·0	− 2·6	$93\bar{2}$	1·8	+ 1·9	$44\bar{6}$	5·1	− 4·3	254	2·8	+ 2·3
332	4·5	+ 5·4	$93\bar{3}$	0·5	+ 0·5	$44\bar{7}$	<1·3	+ 0·1	253	<1·1	− 0·4
331	0·9	− 1·3	$93\bar{4}$	2·2	− 2·3	$44\bar{8}$	<1·0	+ 0·4	252	1·9	− 0·7
$33\bar{1}$	0·8*	+ 0·9	$93\bar{5}$	<0·5	+ 0·2	$44\bar{9}$	<0·8	+ 0·1	251	<1·1	+ 0·4
$33\bar{2}$	5·6	− 5·9	$93\bar{6}$	1·3	+ 1·4	544	0·4	+ 0·4	$25\bar{1}$	1·5	− 3·0

Table 3 (*cont.*)

hkl	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$
$25\bar{2}$	6·6	− 5·4	$55\bar{6}$	4·8	− 4·2	$16\bar{1}$	0·9	− 0·7	$56\bar{4}$	<0·8	− 0·5
$25\bar{3}$	6·0	− 5·6	$55\bar{7}$	<1·0	+ 0·3	$16\bar{2}$	1·7	− 1·0	$56\bar{5}$	<0·8	+ 0·3
$25\bar{4}$	2·7	+ 2·1	$55\bar{8}$	1·1	+ 0·4	$16\bar{3}$	<0·9	− 0·3	$56\bar{6}$	<0·8	+ 0·8
$25\bar{5}$	3·6	+ 3·3	651	0·8	− 0·5	$16\bar{4}$	2·7	+ 0·2	$66\bar{1}$	<0·4	+ 0·1
$25\bar{6}$	1·1	+ 1·0	$65\bar{1}$	0·8	+ 0·5	$16\bar{5}$	0·9	− 1·5	$66\bar{2}$	0·4	+ 0·4
$25\bar{7}$	0·7*	+ 0·8	$65\bar{2}$	3·4	+ 3·4	$16\bar{6}$	<0·9	− 0·9	$66\bar{3}$	0·4	+ 0·4
$25\bar{8}$	<0·7	+ 0·6	$65\bar{3}$	2·2	+ 2·5	264	1·1	+ 0·1	$66\bar{4}$	<0·4	+ 0·4
355	<0·8	+ 0·5	$65\bar{4}$	0·7*	− 0·2	263	<0·8	+ 0·1	$66\bar{5}$	2·0	− 1·4
354	<0·9	+ 0·1	$65\bar{5}$	1·7	+ 1·3	262	4·8	− 3·6	$66\bar{6}$	2·6	− 2·2
353	<0·8	+ 0·1	$65\bar{6}$	1·3	+ 1·8	261	7·4	− 5·7	071	0·7	− 0·7
352	0·8	− 0·5	$65\bar{7}$	0·5	+ 0·7	$26\bar{1}$	<1·0	+ 1·0	072	<0·5	+ 0·3
351	2·7	− 3·1	$65\bar{8}$	<0·5	− 0·7	$26\bar{2}$	3·5	− 3·4	073	<0·5	+ 0·4
$35\bar{1}$	1·6	+ 1·4	$75\bar{1}$	<0·8	− 0·3	$26\bar{3}$	0·7	− 0·9	074	<0·5	− 0·6
$35\bar{2}$	7·9	− 6·3	$75\bar{2}$	<0·8	− 0·6	$26\bar{4}$	<1·2	+ 1·5	170	<0·6	+ 0·6
$35\bar{3}$	4·3	− 3·2	$75\bar{3}$	<0·9	− 0·1	$26\bar{5}$	<1·0	+ 0·2	270	0·7*	+ 0·1
$35\bar{4}$	1·0	+ 0·9	$75\bar{4}$	<0·9	+ 0·3	$26\bar{6}$	<0·8	+ 0·4	370	0·6	− 0·7
$35\bar{5}$	5·5	− 4·3	$75\bar{5}$	<1·0	− 0·5	363	<0·8	− 0·4	173	<0·8	+ 0·6
$35\bar{6}$	4·1	− 3·3	$75\bar{6}$	2·5	− 2·2	362	1·8	+ 0·9	172	<1·0	− 0·1
$35\bar{7}$	<1·0	+ 0·6	$75\bar{7}$	<0·8	− 0·5	361	2·5	+ 1·9	171	1·8	− 1·4
$35\bar{8}$	<0·9	− 0·4	$85\bar{3}$	<0·7	+ 1·5	$36\bar{1}$	<0·8	+ 0·1	$17\bar{1}$	1·8	+ 0·4
454	0·4	+ 0·7	$85\bar{4}$	<0·7	+ 0·1	$36\bar{2}$	1·3	+ 1·1	$17\bar{2}$	<1·0	− 1·0
453	<0·6	− 0·5	$85\bar{5}$	<0·9	− 0·9	$36\bar{3}$	<0·9	− 0·5	$17\bar{3}$	<0·8	− 0·4
452	1·8	− 1·8	$85\bar{6}$	<0·7	− 0·4	$36\bar{4}$	0·9	+ 0·4	$17\bar{4}$	<0·8	+ 0·1
451	3·6	− 3·3	061	3·6	− 4·0	$36\bar{5}$	0·8	− 0·6	272	2·3	+ 2·0
$45\bar{1}$	0·9	+ 1·5	062	7·5	− 6·7	$36\bar{6}$	<0·7	− 0·4	271	2·1	+ 2·2
$45\bar{2}$	0·8	+ 1·0	063	1·4	− 0·6	$36\bar{7}$	<0·7	+ 0·1	$27\bar{1}$	1·9	+ 1·0
$45\bar{3}$	2·8	− 3·2	064	<2·0	+ 1·4	462	0·7	+ 0·1	$27\bar{2}$	3·2	+ 2·0
$45\bar{4}$	1·1	+ 0·5	065	<2·0	+ 0·5	461	<0·8	− 1·0	$27\bar{3}$	1·3	+ 1·2
$45\bar{5}$	5·9	+ 3·6	066	<1·5	+ 0·3	$46\bar{1}$	1·0	+ 1·4	$27\bar{4}$	<0·8	− 0·8
$45\bar{6}$	2·5	+ 2·0	160	<1·0	− 0·1	$46\bar{2}$	0·9	+ 0·6	371	2·2	− 1·0
$45\bar{7}$	<0·6	+ 0·6	260	1·1**	+ 0·2	$46\bar{3}$	<0·9	− 0·2	$37\bar{1}$	0·7	+ 1·1
$45\bar{8}$	0·4*	+ 0·3	360	<0·9	− 0·9	$46\bar{4}$	<0·9	+ 0·7	$37\bar{2}$	<0·7	+ 0·2
552	0·4	+ 0·5	460	<0·9	− 0·7	$46\bar{5}$	2·5	− 1·7	$37\bar{3}$	<0·7	− 0·5
551	1·0	+ 0·6	560	<0·9	+ 0·1	$46\bar{6}$	1·7	− 1·6	$37\bar{4}$	<0·7	− 0·3
$55\bar{1}$	1·0	− 0·3	165	<0·9	+ 1·2	$46\bar{7}$	<0·8	+ 0·4	$47\bar{1}$	<0·8	− 0·3
$55\bar{2}$	2·6	− 2·1	164	<0·9	+ 0·4	561	0·7	+ 0·6	$47\bar{2}$	<0·8	+ 0·1
$55\bar{3}$	1·8	− 1·9	163	<1·0	− 0·8	$56\bar{1}$	<0·8	− 0·2	$47\bar{3}$	1·3	+ 1·3
$55\bar{4}$	0·7	+ 1·0	162	2·4	+ 1·7	$56\bar{2}$	2·4	+ 1·9	$47\bar{4}$	<0·7	− 0·4
$55\bar{5}$	3·2	− 2·4	161	2·7	+ 1·9	$56\bar{3}$	2·1	+ 0·7			

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The Crystal and Molecular Structure of Naphthalene. II. Structure Investigation by the Triple Fourier Series Method

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A triple Fourier series investigation of the naphthalene structure is described, based on the 612 structure factors listed in Part I. The series for the electron density has been evaluated at 54,000 points over the asymmetric crystal unit (half the chemical molecule), and the results are expressed by giving a number of sections through separate atoms at different levels, and also by giving a section through the plane of the molecule. From this map the bond lengths can be determined by direct measurement and are found to vary from 1·36 A. in the $\alpha\beta$ bond to 1·42 A. in the $o\alpha$ bond. The $\beta\beta$ bond and the central bond, oo, are both measured at 1·395 A. These figures are probably correct to within about 0·01 A., and appear to be in reasonably good agreement with the latest theoretical calculations. The rings are also found to be coplanar to within 0·01 A. The bridge value of the electron density varies in the different bonds; the electron distribution and the effect of the hydrogen atoms are briefly discussed.

1. Introduction

In Part I we have described the measurement and listed the values of all the structure factors of naphthalene that lie within the range of copper radiation. The signs, or phase constants, of 612 of these factors can be determined from the previous approximate structure