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

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A very complete redetermination of the crystal structure of anthracene is described. All the reflexions that lie within the range of Cu $K\alpha$ radiation have been recorded on equi-inclination Weissenberg exposures, and the intensities have been estimated visually by independent observers. From these results a total of 691 structure factors have been evaluated out of a possible 1085 (64 %). The earlier two-dimensional determination of the structure has been further refined, by revising the ($h0l$) structure factors and the (010) projection, and from these results it has now been possible to assign phase constants to 667 of the structure factors. These are used in a new three-dimensional determination of the structure which is described in Part II.

1. Introduction

A very complete redetermination of the crystal and molecular structure of naphthalene has recently been described (Abrahams, Robertson & White, 1949*a*, *b*). The present papers deal with a similar redetermination of the structure of anthracene, carried out by the same methods, and we hope with about the same degree of precision.

A survey of the earlier work on the crystal structure of anthracene is given in the papers referred to above. The 1933 determination by double Fourier series methods, employing the axial zones of reflexion (Robertson, 1933), was used as the starting point for the present investigation, which now embraces all the X-ray reflexions within the range of Cu $K\alpha$ radiation at room temperature. A total of 691 structure factors has been evaluated out of a possible 1085 which are theoretically within the range of this wave-length. The previous two-dimensional structure determination, after some further refinement, has enabled us to make a reliable assessment of the phase constants for 667 of these structure factors, and their utilization in a three-dimensional determination of the structure is described in Part II.

The number of reflexions observed in the case of anthracene amounts to 63·7 % of those theoretically possible. For naphthalene the corresponding figure was 77·4 %. The smaller figure for anthracene is difficult to explain. It may be due in part to somewhat less intense exposures, although an attempt was made to keep these the same as for naphthalene, and the intensity range covered in the ($h0l$) zone is comparable for the two crystals (about 5000 to 1). Part of the difference will be due to the anthracene structure being more complex, with a larger number of small structure factors. For anthracene $F(000)$ is 188, while for naphthalene it is 136. The number of recorded structure factors might be increased by the use of larger crystals and longer exposures, but the present list appears to contain most of those whose sign (phase constant) can be determined with some measure of certainty from the 1933 approximation.

2. Crystal data

The crystal constants were redetermined by means of suitably calibrated oscillation and moving-film photographs. The following new values differ only slightly from the earlier measurements (Robertson, 1933):

Anthracene, $C_{14}H_{10}$; M, 178·2; m.p. 218° C.; d, calc. 1·24, found 1·25. Monoclinic prismatic,

$$a = 8{\cdot}561 \pm 0{\cdot}010, \quad b = 6{\cdot}036 \pm 0{\cdot}010,$$
$$c = 11{\cdot}163 \pm 0{\cdot}010 \text{ A.}, \quad \beta = 124^\circ\ 42' \pm 4'.$$

(The wave-length for Cu $K\alpha$ radiation was taken as 1·542 A.)

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, 474·2 A.^{3}. Absorption coefficient for X-rays, $\lambda = 1{\cdot}542$ A., $\mu = 6{\cdot}45$ cm.$^{-1}$. Total number of electrons per unit cell $= F(000) = 188$.

3. Experimental measurements

The X-ray work was carried out in a similar manner to that described for naphthalene (Abrahams *et al* 1949*a*) except that no special precautions were required to preserve the anthracene crystals. Suitable specimens were grown by slow cooling from amyl acetate solution. These were generally needle-shaped, elongated in the direction of the b axis.

The photographic surveys used for the intensity estimates were made exclusively on an instrument of the equi-inclination Weissenberg type. It was found that all the reflexions could be recorded, with sufficient overlap for correlation, on exposures of the equatorial and the first three, four or five layer lines for rotations about the [100], [010], [001] and [101] axes. Details of these layer lines, with the dimensions of the crystal specimens employed, are given in Table 1.

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

Layer line	Dimensions of crystal specimen (mm.). Cross-section × length along rotation axis
$0kl$, $1kl$, $2kl$, $3kl$, $4kl$	$0{\cdot}47 \times 0{\cdot}79 \times 0{\cdot}68$
$h0l$, $h1l$, $h2l$, $h3l$	$0{\cdot}37 \times 0{\cdot}66 \times 0{\cdot}68$
$hk0$, $hk1$, $hk2$, $hk3$, $hk4$, $hk5$	$0{\cdot}44 \times 0{\cdot}47 \times 0{\cdot}18$
$h.k.\overline{h}$, $h.k.\overline{h-1}$, $h.k.\overline{h-2}$, $h.k.\overline{h-3}$, $h.k.\overline{h-4}$, $h.k.\overline{h-5}$	$0{\cdot}75 \times 0{\cdot}47 \times 0{\cdot}39$

The intensities were estimated visually by two independent observers, employing the multiple-film technique for correlation of the strong and weak reflexions. The independent estimates generally agreed to within 10 %.

The correction factors applied to the intensities were the normal Lorentz and polarization factors, absorption corrections to allow for the shape of the crystal specimens (approximate corrections only, as for naphthalene, $e^{-\mu t}$ varying between 1·27 and 1·62 for extreme positions) and the Tunell (1939) geometrical correction factors for non-equatorial reflexions.

The structure factors were then evaluated by the usual formula for mosaic-type crystals, and placed on the absolute scale determined by Robertson (1933). They are listed in Table 3. Most of the structure factors were obtained from independent observations on two or more different layer lines and rotation axes. After correlation the discrepancies between the F values given by different settings and by different crystals were frequently of the order of 10 %. This result is similar to that obtained for naphthalene, and it is clear that the accuracy of the measured F values cannot be placed at much better than 10 %. There was some evidence of extinction effects amongst the stronger reflexions, and in such cases the highest observed value was usually adopted.

4. Determination of phase constants

The observed values of the structure factors are listed in Table 3 under '$F_{\text{meas.}}$'. For the calculated values, which determine the phase constant (+ or −) the Robertson (1933) structure was used as a starting point. On this basis a revised two-dimensional electron-density projection on (010) was prepared (Fig. 1) employing the 65 $F(h0l)$ terms now observed as against the 35 terms employed in 1933. The definition of the atoms is somewhat improved and the x and z co-ordinates estimated from this projection differed by up to 0·05 A. (average shift, 0·02 A.) from those obtained in the 1933 investigation.

The new x and z co-ordinates, together with the 1933 y co-ordinates, were now used to calculate all the $F(hkl)$ values. From these results the signs obtained for 667 of the F values in Table 3 were considered to be reasonably certain, and these were accordingly employed as coefficients in the triple Fourier series investigation described in Part II. Twenty-four small F values, marked with an asterisk in Table 3, were thought to be of doubtful sign and were omitted from the final synthesis.

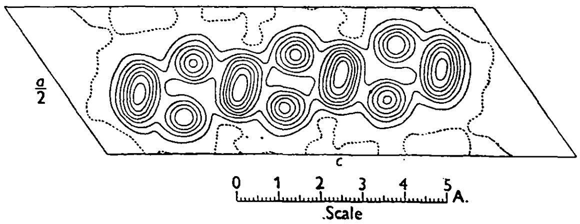

Fig. 1. Electron-density projection for one anthracene molecule on (010). Contour scale: 1 e.A.$^{-2}$, the one-electron line being dotted.

The values listed under '$F_{\text{calc.}}$' in Table 3 have been evaluated from the final co-ordinates of the atoms obtained as a result of the investigation described in Part II. This final recalculation of the structure factors shows that only four of the terms included in the triple Fourier synthesis have changed in sign, and these values are all small. They are marked with a double asterisk in Table 3.

A revised scattering curve for carbon was employed in the final recalculation of the structure factors, designed to give the best fit between the measured and calculated values. The data for this curve are listed in Table 2. It differs a little from the naphthalene curve (Abrahams *et al.* 1949*a*) presumably owing to a slightly different temperature factor.

Table 2. f_c *values for anthracene 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	100	100	99	98	97	95	94	92	91	89
0·1	87	85	83	80	78	76	74	72	70	68
0·2	66	64	62	60	59	57	56	54	53	51
0·3	50	48	47	45	44	42	41	40	39	37
0·4	36	35	34	33	31	30	29	28	27	27
0·5	26	25	24	23	23	22	21	21	20	19
0·6	19	18	18	17	16	16	15	15	14	14
0·7	13	13	12	12	12	12	11	11	11	10
0·8	10	10	9	9	9	9	9	8	8	8
0·9	8	7	7	7	7	7	7	7	6	6

The discrepancies finally obtained between the measured and calculated F values in Table 3, expressed as

$$\frac{\Sigma(|F_{\text{meas.}}|-|F_{\text{calc.}}|)}{\Sigma|F_{\text{meas.}}|},$$

amount to 19·6 % for all the values listed. This figure is reduced to 18·2 % if $\Sigma|F_{\text{calc.}}|$ is used as denominator, because the scales of the measured and calculated values are not exactly correlated, the measured scale being based on certain absolute measurements made in the 1933 investigation. Nevertheless, the discrepancies are clearly a little greater than in the naphthalene investigation. They could undoubtedly be improved if allowance were made for the hydrogen atoms and for the electron distribution between the carbon atoms in the rings.

References

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Table 3. *Measured and calculated values of the anthracene structure factors*

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

hkl	$F_{\text{meas.}}$	$F_{\text{calc.}}$	*hkl*	$F_{\text{meas.}}$	$F_{\text{calc.}}$	*hkl*	$F_{\text{meas.}}$	$F_{\text{calc.}}$	*hkl*	$F_{\text{meas.}}$	$F_{\text{calc.}}$
001	32·8	+38·4	40$\bar{9}$	26·6	+28·3	018	9·0	− 8·5	2.1.$\overline{12}$	<1·2	+ 1·0
002	23·7	−25·2	4.0.$\overline{10}$	10·3	+10·3	019	9·8	− 9·2	2.1.$\overline{13}$	1·7	− 1·8
003	16·4	+15·0	4.0.$\overline{11}$	3·7	− 3·7	0.1.10	<2·0	− 0·3	319	<0·9	− 2·1
004	24·6	−19·9	4.0.$\overline{12}$	2·0	+ 2·0	0.1.11	<1·3	− 0·3	318	<1·6	− 2·5
005	16·9	−14·7	4.0.$\overline{13}$	3·6	− 3·1	110	53·5	+65·0	317	2·0*	− 0·4
006	6·0	+ 6·0	605	<1·2	− 1·2	210	52·0	−47·8	316	2·1	− 0·3
007	<1·8	− 0·7	604	4·5	+ 3·5	310	11·7	+10·8	315	2·2	+ 1·4
008	4·1	− 4·4	603	<2·0	+ 0·1	410	28·3	−24·9	314	6·4	− 5·8
009	5·8	− 5·0	602	<2·1	− 0·7	510	5·0	− 5·6	313	4·8	− 3·9
0.0.10	<1·8	− 0·7	601	<2·1	+ 2·7	610	6·2	− 3·7	312	4·0	+ 5·4
0.0.11	1·5	+ 1·7	60$\bar{1}$	11·2	−12·8	710	3·0	− 2·5	311	8·1	−10·0
020	22·7	−22·5	60$\bar{2}$	2·9	− 3·1	810	<1·7	+ 0·6	31$\bar{1}$	31·5	+28·9
040	3·7	− 1·6	60$\bar{3}$	4·9	+ 5·1	910	<0·8	− 0·4	31$\bar{2}$	3·9	− 3·8
060	<1·8	+ 1·8	60$\bar{4}$	4·6*	− 2·4	1.1.11	<0·9	+ 0·3	31$\bar{3}$	2·6	+ 2·7
200	65·0	+73·8	60$\bar{5}$	20·6	−18·4	1.1.10	<1·5	0·0	31$\bar{4}$	14·3	− 9·3
400	3·9	− 1·8	60$\bar{6}$	5·3	− 4·0	119	2·4	− 2·4	31$\bar{5}$	25·8	−20·7
600	7·3	− 8·3	60$\bar{7}$	2·0	+ 2·3	118	<2·1	+ 0·4	31$\bar{6}$	<1·6	+ 2·7
800	2·5	− 1·5	60$\bar{8}$	2·4	− 4·0	117	<1·7	− 0·1	31$\bar{7}$	0·9	− 2·7
2.0.10	<1·0	+ 0·9	60$\bar{9}$	16·4	+19·0	116	<1·7	+ 0·8	31$\bar{8}$	3·8	+ 3·9
209	4·3	− 5·7	6.0.$\overline{10}$	16·6	+17·6	115	6·4	− 5·7	31$\bar{9}$	13·7	+13·0
208	5·5	− 7·5	6.0.$\overline{11}$	3·8	− 3·9	114	19·3	−17·1	3.1.$\overline{10}$	<1·4	− 0·4
207	<2·2	− 0·3	6.0.$\overline{12}$	<2·0	0·0	113	6·0	+ 7·1	3.1.$\overline{11}$	1·9	− 1·2
206	3·5	+ 4·0	6.0.$\overline{13}$	<1·7	+ 1·9	112	<1·0	− 1·1	3.1.$\overline{12}$	1·8	+ 1·8
205	9·3	− 8·3	6.0.$\overline{14}$	3·0	− 3·2	111	12·4	− 7·9	3.1.$\overline{13}$	3·5	− 2·7
204	25·5	−24·8	802	<1·0	− 1·1	11$\bar{1}$	26·9	+29·4	417	<1·5	+ 2·3
203	4·4	− 2·5	801	<1·5	+ 0·5	11$\bar{2}$	13·2	−14·5	416	1·9	− 2·6
202	4·3	+ 3·1	80$\bar{1}$	7·4	− 8·7	11$\bar{3}$	15·5	+12·6	415	3·3	+ 1·5
201	4·5	− 4·1	80$\bar{2}$	4·5	− 3·1	11$\bar{4}$	21·1	−17·0	414	10·5	+10·7
20$\bar{1}$	43·5	+52·8	80$\bar{3}$	2·1	+ 2·6	11$\bar{5}$	19·5	−16·7	413	5·0	+ 3·1
20$\bar{2}$	25·5	−28·8	80$\bar{4}$	<2·1	− 1·1	11$\bar{6}$	<1·4	+ 1·5	412	<2·0	− 1·0
20$\bar{3}$	14·5	+12·5	80$\bar{5}$	10·3	− 9·6	11$\bar{7}$	<1·6	− 1·0	411	2·4	+ 2·7
20$\bar{4}$	3·3*	+ 2·4	80$\bar{6}$	9·0	− 8·1	11$\bar{8}$	6·7	+ 5·3	41$\bar{1}$	33·1	−36·1
20$\bar{5}$	5·0	−10·5	80$\bar{7}$	2·2	+ 2·6	11$\bar{9}$	3·6	+ 2·3	41$\bar{2}$	2·7	+ 3·3
20$\bar{6}$	5·4	+ 7·4	80$\bar{8}$	<2·1	− 0·7	1.1.$\overline{10}$	2·8	− 2·8	41$\bar{3}$	5·2	+ 7·3
20$\bar{7}$	4·4	− 5·3	80$\bar{9}$	2·1	+ 1·9	1.1.$\overline{11}$	<1.4	+ 1·1	41$\bar{4}$	16·4	−16·8
20$\bar{8}$	2·6	+ 3·0	8.0.$\overline{10}$	9·0	+ 9·0	1.1.$\overline{12}$	<1·0	− 0·8	41$\bar{5}$	10·2	− 7·6
20$\bar{9}$	9·2	+10·4	8.0.$\overline{11}$	<1·9	− 0·4	2.1.10	<0·9	− 0·1	41$\bar{6}$	2·0	+ 2·0
2.0.$\overline{10}$	<1·6	+ 0·1	8.0.$\overline{12}$	1·4	− 1·4	219	<1·6	− 1·1	41$\bar{7}$	1·8	− 2·8
2.0.$\overline{11}$	<1·5	+ 0·8	8.0.$\overline{13}$	1·5	+ 2·8	218	<2·0	− 0·7	41$\bar{8}$	3·1	+ 4·2
2.0.$\overline{12}$	<1·2	− 0·2	8.0.$\overline{14}$	<1·0	− 1·3	217	<2·2	+ 1·7	41$\bar{9}$	9·4	+10·4
2.0.$\overline{13}$	<0·7	− 5·2	10.0.$\bar{3}$	<1·1	+ 0·9	216	<2·2	− 1·7	4.1.$\overline{10}$	3·1	+ 2·6
408	3·2	− 4·2	10.0.$\bar{4}$	<1·4	− 1·2	215	<1·5	− 1·9	4.1.$\overline{11}$	2·2	− 2·3
407	<1·5	0·0	10.0.$\bar{5}$	<1·5	− 0·9	214	1·9	+ 0·9	4.1.$\overline{12}$	<1·9	+ 0·8
406	<1·8	+ 0·8	10.0.$\bar{6}$	<1·7	− 3·3	213	4·0	− 4·0	4.1.$\overline{13}$	<1·5	− 1·6
405	<2·1	− 1·8	10.0.$\bar{7}$	<1·7	− 0·5	212	3·8	+ 5·3	516	<1·4	− 0·9
404	8·4	− 7·9	10.0.$\bar{8}$	<1·7	+ 1·7	211	1·7	+ 0·4	515	1·8	+ 1·5
403	7·6	− 8·0	10.0.$\bar{9}$	1·9	− 2·7	21$\bar{1}$	40·5	−42·3	514	2·9	+ 3·0
402	3·7	+ 5·1	10.0.$\overline{10}$	1·8	− 2·3	21$\bar{2}$	9·1	+ 8·5	513	3·1	− 3·2
401	<1·7	− 1·1	10.0.$\overline{11}$	<1·4	− 0·5	21$\bar{3}$	1·2	+ 3·0	512	<1·7	+ 0·5
40$\bar{1}$	3·5	+ 7·5	10.0.$\overline{12}$	<1·1	0·0	21$\bar{4}$	6·9	− 6·8	511	<2·1	+ 0·2
40$\bar{2}$	6·3	− 7·2	011	10·7	+10·4	21$\bar{5}$	13·2	+11·5	51$\bar{1}$	6·0	+ 5·4
40$\bar{3}$	6·2	+ 5·1	012	3·6	+ 3·4	21$\bar{6}$	2·4	+ 3·5	51$\bar{2}$	4·1	+ 2·9
40$\bar{4}$	1·8	+ 1·1	013	3·9	− 3·2	21$\bar{7}$	6·5	− 7·3	51$\bar{3}$	1·6*	− 0·8
40$\bar{5}$	12·3	−13·9	014	11·9	− 9·6	21$\bar{8}$	11·1	+11·0	51$\bar{4}$	3·8	− 3·2
40$\bar{6}$	5·0	+ 6·0	015	16·0	−13·6	21$\bar{9}$	16·5	+17·5	51$\bar{5}$	16·2	−15·2
40$\bar{7}$	5·2	− 5·0	016	<2·1	− 0·4	2.1.$\overline{10}$	2·9	+ 2·7	51$\bar{6}$	<1·3	− 0·3
40$\bar{8}$	1·6**	+ 0·6	017	3·6	− 4·4	2.1.$\overline{11}$	2·0	− 1·8	51$\bar{7}$	2·0	+ 2·2

Table 3 (*cont.*)

hkl	$F_{meas.}$	$F_{calc.}$
51$\bar{8}$	2·8	− 3·5
51$\bar{9}$	12·5	+13·3
5.1.$\overline{10}$	7·4	+ 7·7
5.1.$\overline{11}$	3·0	− 3·0
5.1.$\overline{12}$	2·9	+ 2·1
5.1.$\overline{13}$	<1·6	− 1·0
5.1.$\overline{14}$	3·2	− 3·5
615	<1·1	+ 0·3
614	8·2	+ 8·5
613	7·4	+ 6·3
612	<1·6	− 1·6
611	<2·2	+ 0·4
61$\bar{1}$	12·6	−10·9
61$\bar{2}$	<1·1	− 0·1
61$\bar{3}$	2·0	+ 3·2
61$\bar{4}$	6·0	− 7·2
61$\bar{5}$	5·9	− 6·3
61$\bar{6}$	1·8	− 1·5
61$\bar{7}$	1·5	+ 1·0
61$\bar{8}$	<2·0	+ 1·4
61$\bar{9}$	4·5	− 4·2
6.1.$\overline{10}$	6·1	− 5·4
6.1.$\overline{11}$	<0·8	− 0·9
6.1.$\overline{12}$	<2·0	+ 0·8
6.1.$\overline{13}$	<1·7	+ 0·5
6.1.$\overline{14}$	1·5	+ 1·8
713	2·0	+ 1·6
712	2·1	− 2·1
711	<2·0	+ 1·9
71$\bar{1}$	5·4	− 4·2
71$\bar{2}$	<1·7	+ 0·4
71$\bar{3}$	<1·2	− 0·3
71$\bar{4}$	<1·5	+ 0·3
71$\bar{5}$	6·9	− 5·8
71$\bar{6}$	3·7	− 4·1
71$\bar{7}$	2·7	+ 3·6
71$\bar{8}$	3·1	− 3·6
71$\bar{9}$	4·3	+ 2·9
7.1.$\overline{10}$	9·2	+ 9·4
7.1.$\overline{11}$	<1·2	− 0·2
7.1.$\overline{12}$	<0·8	− 0·2
7.1.$\overline{13}$	<1·6	+ 0·6
7.1.$\overline{14}$	5·2	− 3·4
812	<0·7	− 0·1
811	<1·5	− 0·6
81$\bar{1}$	<2·0	+ 0·8
81$\bar{2}$	2·1	+ 2·1
81$\bar{3}$	<2·0	− 0·1
81$\bar{4}$	<2·2	− 1·8
81$\bar{5}$	5·5	+ 3·7
81$\bar{6}$	3·5	+ 2·0
81$\bar{7}$	<2·1	− 0·5
81$\bar{8}$	<1·2	+ 1·8
81$\bar{9}$	7·1	− 6·1
8.1.$\overline{10}$	12·5	−11·6
8.1.$\overline{11}$	2·3	− 1·8
8.1.$\overline{12}$	2·1	+ 2·3
8.1.$\overline{13}$	1·7	− 1·8
8.1.$\overline{14}$	<0·7	− 0·9
91$\bar{1}$	4·3	− 3·6
91$\bar{2}$	1·7	− 1·4
91$\bar{3}$	<1·7	− 0·2
91$\bar{4}$	<2·0	+ 0·4
91$\bar{5}$	<2·1	+ 1·0
91$\bar{6}$	2·4	− 2·7
91$\bar{7}$	<2·0	+ 0·2
91$\bar{8}$	<1·9	+ 0·2
91$\bar{9}$	<1·1	− 2·4
9.1.$\overline{10}$	3·5	+ 3·6
9.1.$\overline{11}$	2·0	+ 2·2
9.1.$\overline{12}$	<1·0	− 0·9
9.1.$\overline{13}$	<0·7	+ 0·2
10.1.$\bar{3}$	<0·9	− 0·6
10.1.$\bar{4}$	<1·4	− 1·4
10.1.$\bar{5}$	5·1	+ 5·8
10.1.$\bar{6}$	8·4	+ 5·8
10.1.$\bar{7}$	<1·1	− 0·6
10.1.$\bar{8}$	<1·6	+ 0·2
10.1.$\bar{9}$	2·0	− 1·5
10.1.$\overline{10}$	7·6	− 7·3
10.1.$\overline{11}$	1·7	− 2·4
10.1.$\overline{12}$	<1·0	+ 2·1
11.1.$\bar{8}$	<0·5	+ 1·0
11.1.$\bar{9}$	<0·8	− 1·0
021	17·8	−18·9
022	8·7	+ 5·6
023	4·9*	0·0
024	17·9	−15·7
025	1·1	+ 1·8
026	<1·2	− 1·5
027	<1·4	− 1·1
028	12·4	+10·9
029	4·1	+ 3·3
0.2.10	2·0	− 2·2
0.2.11	<0·9	+ 0·8
120	20·5	−22·1
220	13·1	−12·3
320	28·1	−26·4
420	2·2	− 2·5
520	9·0	− 7·1
620	<1·3	− 1·0
720	<1·3	− 0·3
820	<0·9	− 1·0
1.2.10	<1·0	+ 1·2
129	3·2	− 3·6
128	8·0	− 7·4
127	2·4	− 1·6
126	1·7	+ 0·8
125	5·0	+ 5·0
124	9·0	+ 6·9
123	0·9*	0·0
122	<0·5	+ 0·7
121	10·6	−10·8
12$\bar{1}$	5·2*	+ 1·3
12$\bar{2}$	6·1	+ 8·6
12$\bar{3}$	9·4	− 9·8
12$\bar{4}$	13·5	− 9·4
12$\bar{5}$	3·0	+ 5·0
12$\bar{6}$	1·5	+ 2·9
12$\bar{7}$	1·8	− 2·6
12$\bar{8}$	11·3	+ 8·9
12$\bar{9}$	13·0	+10·9
1.2.$\overline{10}$	<1·2	− 0·5
1.2.$\overline{11}$	<0·9	− 0·3
1.2.$\overline{12}$	<0·6	+ 1·6
229	<0·8	+ 0·2
228	6·7	+ 7·4
227	<1·3	+ 1·1
226	2·1	− 3·4
225	11·2	+10·8
224	5·4	+ 4·2
223	2·8	− 1·9
222	6·2	+ 5·8
221	13·3	−16·1
22$\bar{1}$	4·4	+ 5·2
22$\bar{2}$	0·7	+ 2·0
22$\bar{3}$	<0·7	+ 1·1
22$\bar{4}$	23·8	−23·0
22$\bar{5}$	20·1	−20·6
22$\bar{6}$	<0·6	− 1·0
22$\bar{7}$	<0·7	− 0·3
22$\bar{8}$	5·5	+ 5·8
22$\bar{9}$	3·5	+ 2·5
2.2.$\overline{10}$	4·7	− 4·6
2.2.$\overline{11}$	<1·2	+ 0·4
2.2.$\overline{12}$	<0·8	+ 0·6
328	<1·0	− 2·2
327	1·2	− 1·1
326	<1·3	− 1·0
325	8·4	+ 6·5
324	11·6	+11·6
323	<1·2	− 2·2
322	1·2	− 1·7
321	2·1	+ 3·1
32$\bar{1}$	24·7	−25·0
32$\bar{2}$	4·7	+ 6·8
32$\bar{3}$	3·8**	+ 2·4
32$\bar{4}$	10·6	−13·4
32$\bar{5}$	6·3	+ 5·9
32$\bar{6}$	9·7	+ 9·1
32$\bar{7}$	3·2	− 3·7
32$\bar{8}$	1·3	+ 0·8
32$\bar{9}$	8·8	+10·6
3.2.$\overline{10}$	3·0	+ 3·9
3.2.$\overline{11}$	<1·2	− 1·0
3.2.$\overline{12}$	<0·9	+ 1·5
3.2.$\overline{13}$	<0·6	− 1·3
427	<0·8	+ 0·9
426	<1·0	− 2·3
425	6·7	+ 6·6
424	8·6	+ 8·3
423	<1·3	− 1·6
422	1·1	+ 2·0
421	4·7	− 4·5
42$\bar{1}$	20·8	+19·7
42$\bar{2}$	5·8	+ 5·7
42$\bar{3}$	4·2	− 4·4
42$\bar{4}$	4·5	− 4·3
42$\bar{5}$	19·3	−18·4
42$\bar{6}$	5·9	− 5·2
42$\bar{7}$	2·4	+ 3·7
42$\bar{8}$	2·3	− 2·5
42$\bar{9}$	2·7	− 3·6
4.2.$\overline{10}$	6·5	− 5·4
4.2.$\overline{11}$	<1·3	− 0·6
4.2.$\overline{12}$	<1·2	+ 1·4
4.2.$\overline{13}$	2·2	− 1·6
526	<0·7	− 1·0
525	2·9	+ 1·8
524	9·6	+ 9·4
523	4·5	+ 3·0
522	1·9	− 3·3
521	2·6	+ 4·1
52$\bar{1}$	26·7	−21·2
52$\bar{2}$	6·1	− 4·4
52$\bar{3}$	1·0	+ 2·4
52$\bar{4}$	1·0	− 3·0
52$\bar{5}$	5·6	+ 3·3
52$\bar{6}$	6·6	+ 5·7
52$\bar{7}$	<1·2	0·0
52$\bar{8}$	2·2	− 3·8
52$\bar{9}$	1·3**	− 0·5
5.2.$\overline{10}$	1·8	+ 2·8
5.2.$\overline{11}$	<1·3	+ 1·0
5.2.$\overline{12}$	<1·2	− 0·5
5.2.$\overline{13}$	<0·9	− 1·0
625	<0·5	+ 1·8
624	3·6	+ 3·9
623	<1·0	− 1·8
622	<1·3	− 0·7
621	<1·3	+ 0·9
62$\bar{1}$	13·4	+12·3
62$\bar{2}$	9·1	+ 7·9
62$\bar{3}$	4·7	− 6·3
62$\bar{4}$	5·3	+ 5·6
62$\bar{5}$	1·6	+ 2·0
62$\bar{6}$	3·4	− 4·5
62$\bar{7}$	<1·3	+ 3·4
62$\bar{8}$	2·8	− 3·3
62$\bar{9}$	4·8	− 6·4
6.2.$\overline{10}$	1·8	− 2·1
6.2.$\overline{11}$	<1·3	− 0·2
6.2.$\overline{12}$	<1·2	+ 1·2
6.2.$\overline{13}$	4·1	− 3·0
723	4·6	+ 4·0
722	<0·9	− 0·6
721	<1·2	+ 0·9
72$\bar{1}$	8·3	− 7·1
72$\bar{2}$	5·8	− 4·5
72$\bar{3}$	<1·3	0·0
72$\bar{4}$	3·9	+ 2·7
72$\bar{5}$	8·2	+ 6·9
72$\bar{6}$	2·5	+ 1·8
72$\bar{7}$	<1·3	− 0·9
72$\bar{8}$	<1·3	+ 0·3
72$\bar{9}$	5·4	− 5·9
7.2.$\overline{10}$	4·8	− 5·1
7.2.$\overline{11}$	1·2	+ 1·2
7.2.$\overline{12}$	<1·2	− 0·1
7.2.$\overline{13}$	3·0	− 2·6
821	<0·8	+ 1·5
82$\bar{1}$	2·3	+ 1·9
82$\bar{2}$	3·8	+ 4·6
82$\bar{3}$	<1·3	− 3·4
82$\bar{4}$	3·7	+ 3·4
82$\bar{5}$	8·4	+ 9·3
82$\bar{6}$	<1·4	− 0·4
82$\bar{7}$	<1·3	+ 0·4
82$\bar{8}$	<1·3	− 0·6
82$\bar{9}$	2·7	− 4·1
8.2.$\overline{10}$	2·5	+ 2·3
8.2.$\overline{11}$	2·3	+ 2·1
8.2.$\overline{12}$	<0·9	− 0·4
8.2.$\overline{13}$	2·2	− 1·5
92$\bar{1}$	<0·7	− 1·3
92$\bar{2}$	<0·9	− 0·3
92$\bar{3}$	<1·0	− 0·7
92$\bar{4}$	2·3*	+ 0·9
92$\bar{5}$	7·9	+ 7·5
92$\bar{6}$	4·8	+ 3·8
92$\bar{7}$	<1·2	− 2·4
92$\bar{8}$	<1·2	+ 1·7
92$\bar{9}$	2·5	− 1·8
9.2.$\overline{10}$	7·0	− 7·8
9.2.$\overline{11}$	2·1	− 2·2
9.2.$\overline{12}$	<0·8	+ 1·1
9.2.$\overline{13}$	<0·5	− 1·8
10.2.$\bar{4}$	<0·7	+ 0·7
10.2.$\bar{5}$	6·5	+ 5·7
10.2.$\bar{6}$	<0·9	+ 1·0
10.2.$\bar{7}$	<0·9	− 1·4
10.2.$\bar{8}$	<0·9	+ 0·9
10.2.$\bar{9}$	<0·9	− 1·3
10.2.$\overline{10}$	3·8	+ 3·3
10.2.$\overline{11}$	4·6	+ 4·2
031	20·9	−18·7
032	<1·3	− 0·4
033	8·0	+ 6·9
034	14·4	+12·9
035	16·6	+15·5
036	5·4	+ 2·9
037	2·2	− 2·2
038	3·5	− 2·7
039	2·0	− 2·0
0.3.10	<1·2	+ 0·8
130	21·5	−21·4
230	3·7*	− 2·5
330	7·5	− 6·5
430	1·8	− 1·7
530	1·2	− 3·1
630	<1·8	− 1·2
730	2·8	− 4·2
830	1·9	− 1·2
1.3.10	1·3	− 2·1
139	<1·0	− 0·1
138	8·0	+ 8·1
137	<1·8	− 0·9
136	2·9*	+ 0·8
135	16·0	+16·7
134	3·5*	− 2·3
133	13·4	−12·2
132	3·7	+ 4·6
131	8·4	− 7·1
13$\bar{1}$	12·9	−14·9

Table 3 (*cont.*)

hkl	$F_{meas.}$	$F_{calc.}$
$13\bar{2}$	< 1·3	− 0·1
$13\bar{3}$	3·4	− 3·6
$13\bar{4}$	10·1	− 10·3
$13\bar{5}$	8·9	+ 8·8
$13\bar{6}$	8·1	+ 7·0
$13\bar{7}$	4·3	− 4·6
$13\bar{8}$	2·6	+ 2·5
$13\bar{9}$	< 1·7	+ 1·2
$1.3.\overline{10}$	1·6	− 2·1
$1.3.\overline{11}$	< 1·1	+ 1·3
239	2·8	− 1·8
238	5·6	− 5·9
237	4·6	− 3·6
236	2·4	+ 1·6
235	11·4	+ 10·5
234	13·6	+ 12·3
233	5·5	+ 2·7
232	1·0*	+ 1·0
231	6·8	− 4·9
$23\bar{1}$	12·4	+ 15·5
$23\bar{2}$	2·2	+ 4·4
$23\bar{3}$	3·5	− 6·2
$23\bar{4}$	1·1	− 2·1
$23\bar{5}$	4·6	− 5·4
$23\bar{6}$	2·1	− 0·4
$23\bar{7}$	< 1·5	+ 0·5
$23\bar{8}$	3·2	− 4·1
$23\bar{9}$	< 1·6	− 0·3
$2.3.\overline{10}$	< 1·4	+ 0·8
$2.3.\overline{11}$	< 1·2	− 0·2
$2.3.\overline{12}$	< 0·8	+ 0·4
338	4·0	+ 5·0
337	4·1	+ 3·8
336	< 1·2	− 2·3
335	8·0	+ 7·9
334	5·5	+ 5·3
333	6·2	− 6·8
332	1·3	+ 2·7
331	0·9*	− 0·3
$33\bar{1}$	4·3	− 2·4
$33\bar{2}$	5·6	− 6·5
$33\bar{3}$	2·5	+ 3·1
$33\bar{4}$	3·3	+ 3·7
$33\bar{5}$	3·2	− 4·9
$33\bar{6}$	2·1	+ 1·1
$33\bar{7}$	< 1·3	− 0·9
$33\bar{8}$	4·5	− 4·2
$33\bar{9}$	3·7	− 3·9
$3.3.\overline{10}$	2·3	− 2·5
$3.3.\overline{11}$	1·1	+ 1·1
$3.3.\overline{12}$	1·8	− 1·8
437	2·4	− 2·8
436	< 1·3	+ 0·4
435	3·1	+ 3·0
434	6·5	+ 4·9
433	2·6*	+ 0·5
432	< 1·8	− 1·0
431	1·1	+ 2·1
$43\bar{1}$	< 1·4	− 0·1
$43\bar{2}$	< 1·3	+ 0·4
$43\bar{3}$	< 1·3	− 1·3
$43\bar{4}$	9·3	+ 9·7
$43\bar{5}$	10·4	+ 9·7
$43\bar{6}$	3·5	+ 3·8
$43\bar{7}$	< 1·7	+ 1·4
$43\bar{8}$	4·9	− 6·6
$43\bar{9}$	2·7	− 3·0
$4.3.\overline{10}$	3·6	+ 4·0
$4.3.\overline{11}$	< 1·7	+ 0·9
$4.3.\overline{12}$	< 1·3	− 1·1
$4.3.\overline{13}$	< 0·6	− 2·6
535	< 1·2	+ 0·7
534	2·2	+ 2·4
533	< 1·7	− 2·0
532	< 1·6	+ 1·8
531	< 1·8	− 0·2
$53\bar{1}$	8·7	+ 8·7
$53\bar{2}$	< 1·6	+ 0·6
$53\bar{3}$	< 1·5	− 2·3
$53\bar{4}$	13·1	+ 14·6
$53\bar{5}$	< 1·5	+ 0·9
$53\bar{6}$	8·1	− 8·9
$53\bar{7}$	< 1·2	+ 1·3
$53\bar{8}$	2·0	− 1·9
$53\bar{9}$	6·9	− 7·3
$5.3.\overline{10}$	4·8	− 4·9
$5.3.\overline{11}$	< 1·6	0·0
$5.3.\overline{12}$	< 1·4	− 0·8
$5.3.\overline{13}$	< 0·9	− 3·2
634	< 1·0	− 0·3
633	< 1·4	+ 0·5
632	< 1·4	− 0·8
631	< 1·8	+ 2·0
$63\bar{1}$	8·2	− 6·8
$63\bar{2}$	6·8	− 5·2
$63\bar{3}$	< 1·7	− 0·1
$63\bar{4}$	10·8	+ 9·1
$63\bar{5}$	14·3	+ 12·2
$63\bar{6}$	6·3	+ 4·3
$63\bar{7}$	< 1·3	+ 1·2
$63\bar{8}$	2·2	− 2·5
$63\bar{9}$	2·7	− 3·0
$6.3.\overline{10}$	4·0	+ 4·1
$6.3.\overline{11}$	2·8	+ 2·8
$6.3.\overline{12}$	2·0	− 1·9
$6.3.\overline{13}$	< 1·0	− 1·5
732	< 1·1	+ 1·1
731	< 1·4	+ 0·4
$73\bar{1}$	6·5	+ 5·8
$73\bar{2}$	8·2	+ 7·5
$73\bar{3}$	< 1·8	− 3·4
$73\bar{4}$	8·9	+ 7·5
$73\bar{5}$	8·1	+ 8·6
$73\bar{6}$	5·3	− 6·2
$73\bar{7}$	1·1	− 1·0
$73\bar{8}$	< 1·5	+ 0·2
$73\bar{9}$	3·7	− 4·5
$7.3.\overline{10}$	3·3	− 3·9
$7.3.\overline{11}$	1·5	− 1·5
$7.3.\overline{12}$	< 1·2	+ 0·1
$7.3.\overline{13}$	< 1·4	− 1·2
$83\bar{1}$	7·6	− 5·8
$83\bar{2}$	7·9	− 5·5
$83\bar{3}$	< 1·7	− 0·5
$83\bar{4}$	5·9	+ 4·0
$83\bar{5}$	8·4	+ 6·8
$83\bar{6}$	3·9	+ 2·6
$83\bar{7}$	< 1·4	− 0·4
$83\bar{8}$	< 1·1	+ 0·8
$83\bar{9}$	< 1·3	− 0·8
$8.3.\overline{10}$	< 1·5	+ 1·0
$8.3.\overline{11}$	1·4	+ 1·8
8.3.12	1·0	− 1·0
$93\bar{2}$	4·7	+ 5·6
$93\bar{3}$	< 1·2	− 0·2
$93\bar{4}$	< 1·4	+ 0·3
$93\bar{5}$	5·8	+ 5·7
$93\bar{6}$	< 1·1	− 1·0
$93\bar{7}$	1·5	− 1·2
$93\bar{8}$	< 1·1	+ 1·8
$93\bar{9}$	< 0·9	− 1·2
$9.3.\overline{10}$	< 1·0	+ 0·2
$9.3.\overline{11}$	< 1·1	+ 0·1
$10.3.\bar{5}$	< 0·6	+ 1·0
$10.3.\bar{6}$	< 0·9	+ 0·1
$10.3.\bar{7}$	< 1·0	− 0·6
$10.3.\bar{8}$	< 1·0	+ 0·7
$10.3.\bar{9}$	< 0·9	+ 0·5
$10.3.\overline{10}$	< 0·6	− 1·8
041	4·5	− 3·5
042	< 1·6	+ 0·8
043	1·4	− 0·7
044	1·9*	− 0·5
045	13·2	+ 12·5
046	6·8	+ 5·8
047	3·4	− 4·6
048	1·5	− 1·4
049	2·3	− 1·9
0.4.10	2·6	− 2·1
140	< 1·5	+ 1·7
240	1·9	− 1·8
340	1·5*	− 0·1
440	2·9	− 3·5
540	3·0	− 3·3
640	< 3·0	− 4·8
740	< 2·3	− 1·9
148	< 1·3	+ 0·8
147	5·0	+ 1·0
146	< 1·8	+ 1·4
145	8·7	+ 7·7
144	5·9	+ 4·3
143	1·1	+ 0·6
142	2·5	+ 4·2
141	3·8	− 4·8
$14\bar{1}$	8·6	+ 9·9
$14\bar{2}$	1·5	− 3·7
$14\bar{3}$	5·7	+ 6·1
$14\bar{4}$	5·0	+ 6·1
$14\bar{5}$	13·0	− 13·8
$14\bar{6}$	9·3	− 6·5
$14\bar{7}$	< 1·8	+ 0·2
$14\bar{8}$	4·7	− 5·3
$14\bar{9}$	< 1·5	− 1·0
$1.4.\overline{10}$	3·5	+ 2·9
248	< 1·2	+ 1·9
247	< 1·2	+ 0·3
246	< 1·4	− 0·6
245	5·1	+ 5·3
244	< 1·6	− 2·0
243	6·7	− 7·2
242	< 1·1	+ 1·0
241	1·4	+ 0·7
$24\bar{1}$	8·2	− 8·1
$24\bar{2}$	4·7	− 6·5
$24\bar{3}$	8·5	+ 9·1
$24\bar{4}$	9·4	+ 8·8
$24\bar{5}$	10·2	+ 10·0
$24\bar{6}$	10·5	+ 10·7
$24\bar{7}$	2·2	− 3·0
$24\bar{8}$	5·9	− 5·3
$24\bar{9}$	< 1·4	− 0·9
$2.4.\overline{10}$	< 1·2	− 0·7
$2.4.\overline{11}$	< 0·8	+ 0·2
347	< 0·7	− 1·3
346	< 1·0	+ 0·2
345	< 1·2	− 0·5
344	3·2	+ 2·0
343	5·8	+ 4·6
342	2·7	+ 4·6
341	2·2	− 3·9
$34\bar{1}$	10·0	+ 11·7
$34\bar{2}$	2·6*	+ 1·0
$34\bar{3}$	5·0	+ 10·0
$34\bar{4}$	15·1	+ 17·5
$34\bar{5}$	3·6	− 4·9
$34\bar{6}$	8·8	− 10·2
$34\bar{7}$	< 1·3	+ 2·0
$34\bar{8}$	3·7	− 3·9
$34\bar{9}$	3·5	− 4·0
$3.4.\overline{10}$	2·2	+ 2·2
$3.4.\overline{11}$	< 0·9	− 0·3
446	< 1·3	− 1·0
445	2·7	− 1·4
444	3·1	− 1·8
443	4·7	− 4·5
442	< 1·7	− 0·1
441	0·9	− 0·6
$44\bar{1}$	6·1	− 4·6
$44\bar{2}$	7·9	− 8·6
$44\bar{3}$	5·9	+ 5·3
$44\bar{4}$	15·4	+ 15·2
$44\bar{5}$	5·5	+ 4·9
$44\bar{6}$	5·0	+ 3·3
$44\bar{7}$	2·8	+ 1·5
$44\bar{8}$	3·8	− 3·5
$44\bar{9}$	1·2	− 1·0
$4.4.\overline{10}$	< 0·9	0·0
$4.4.\overline{11}$	< 1·9	0·0
$4.4.\overline{12}$	< 1·0	− 1·0
544	< 2·5	− 2·3
543	3·2	+ 2·5
542	< 1·5	+ 2·3
541	< 2·5	− 1·0
$54\bar{1}$	3·4	+ 7·4
$54\bar{2}$	4·3	+ 3·3
$54\bar{3}$	3·5*	+ 0·6
$54\bar{4}$	9·8	+ 11·0
$54\bar{5}$	6·4	+ 5·9
$54\bar{6}$	4·4	− 4·4
$54\bar{7}$	< 2·1	+ 1·7
$54\bar{8}$	< 1·4	− 0·4
$54\bar{9}$	1·9	− 3·0
$5.4.\overline{10}$	2·4	+ 2·3
$5.4.\overline{11}$	< 1·2	0·0
$5.4.\overline{12}$	< 1·4	− 0·5
643	< 1·0	− 1·5
642	< 1·2	+ 0·5
641	< 2·2	− 0·9
$64\bar{1}$	< 0·9	− 0·5
$64\bar{2}$	1·6	− 1·3
$64\bar{3}$	< 1·5	− 1·3
$64\bar{4}$	8·3	+ 8·5
$64\bar{5}$	3·2	+ 2·8
$64\bar{6}$	2·9	− 4·4
$64\bar{7}$	< 1·4	+ 0·7
$64\bar{8}$	< 2·0	+ 0·7
$64\bar{9}$	< 1·3	− 0·8
$6.4.\overline{10}$	1·4	− 1·4
$6.4.\overline{11}$	1·8	− 1·8
$6.4.\overline{12}$	< 1·1	+ 0·9
741	< 1·4	− 1·4
$74\bar{1}$	3·0	− 1·9
$74\bar{2}$	< 0·8	− 0·3
$74\bar{3}$	< 1·1	+ 0·1
$74\bar{4}$	2·7	+ 1·6
$74\bar{5}$	5·0	+ 4·1
$74\bar{6}$	2·8	+ 2·1
$74\bar{7}$	1·5	+ 2·0
$74\bar{8}$	< 1·3	+ 0·1
$74\bar{9}$	< 1·8	− 1·4
$7.4.\overline{10}$	3·1	+ 3·2
$7.4.\overline{11}$	0·8	+ 1·4
$7.4.\overline{12}$	< 0·4	− 0·1
$84\bar{1}$	< 1·3	+ 0·2
$84\bar{2}$	3·4	+ 4·3
$84\bar{3}$	< 0·7	− 0·7
$84\bar{4}$	< 1·0	0·0
$84\bar{5}$	2·3	+ 0·9
$84\bar{6}$	4·7	− 4·4
$84\bar{7}$	< 1·2	− 1·4
$84\bar{8}$	< 0·9	+ 1·3
$84\bar{9}$	< 1·0	− 1·0
$8.4.\overline{10}$	3·1	− 2·1
$8.4.\overline{11}$	2·5	− 3·0
$94\bar{4}$	< 0·4	− 0·9
$94\bar{5}$	< 1·6	− 1·2
$94\bar{6}$	< 0·9	+ 2·0
$94\bar{7}$	3·4	+ 2·5
$94\bar{8}$	< 0·8	− 0·5
$94\bar{9}$	1·4	− 1·8
$9.4.\overline{10}$	< 0·6	+ 2·0
051	< 1·8	− 1·1
052	< 1·8	+ 1·0
053	11·3	− 9·4

Table 3. (*cont.*)

hkl	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$
054	5·4	− 5·8	3.5.$\overline{10}$	1·2	− 1·8	064	3·3	+ 2·5	56$\bar{1}$	< 0·9	0·0
055	2·6	+ 3·2	455	< 1·2	− 3·7	065	4·3	− 4·3	56$\bar{2}$	< 1·1	+ 2·0
056	< 1·7	− 0·5	454	< 1·6	− 1·3	066	4·0	− 1·8	56$\bar{3}$	3·2	− 3·5
057	2·6	+ 1·8	453	2·2	+ 3·0	067	< 0·9	− 0·7	56$\bar{4}$	3·4	− 2·2
058	3·8	+ 4·0	452	< 1·5	+ 1·6	160	< 1·5	− 1·2	56$\bar{5}$	1·6	− 0·3
059	< 0·8	− 1·5	451	4·6	− 3·8	260	2·0*	+ 0·1	56$\bar{6}$	4·4	− 4·6
150	< 1·7	+ 2·9	45$\bar{1}$	3·7	+ 4·4	360	1·2	− 2·0	56$\bar{7}$	5·5	− 3·3
250	2·1	− 2·2	45$\bar{2}$	3·8	+ 2·5	460	1·0	− 0·5	56$\bar{8}$	2·4	− 1·4
350	2·0	− 1·3	45$\bar{3}$	2·8*	+ 0·3	560	< 0·6	− 0·1	56$\bar{9}$	< 0·4	− 1·0
450	4·1	− 4·3	45$\bar{4}$	7·5	+ 7·9	166	4·1	− 3·7	66$\bar{1}$	< 1·2	− 0·6
550	3·6	− 2·0	45$\bar{5}$	3·9	− 2·8	165	3·1	− 1·7	66$\bar{2}$	1·9	− 1·4
650	< 2·3	− 2·3	45$\bar{6}$	10·3	− 10·8	164	3·0	− 1·3	66$\bar{3}$	3·2	− 1·6
750	< 0·8	+ 0·5	45$\bar{7}$	< 1·5	+ 0·1	163	8·6	− 6·9	66$\bar{4}$	5·1	− 3·6
158	< 0·8	− 2·0	45$\bar{8}$	< 1·1	+ 0·8	162	6·6	− 4·5	66$\bar{5}$	< 1·0	− 1·5
157	3·1	− 2·6	459	0·7	− 1·3	161	3·5	− 2·6	66$\bar{6}$	3·8	+ 5·6
156	3·1	− 1·0	4.5.$\overline{10}$	< 1·6	+ 1·4	16$\bar{1}$	1·2	+ 2·3	66$\bar{7}$	2·8	+ 3·5
155	< 1·7	− 0·9	4.5.$\overline{11}$	< 1·0	+ 0·3	16$\bar{2}$	3·2	+ 1·6	66$\bar{8}$	3·1	− 3·8
154	2·6*	+ 0·6	553	< 1·3	− 2·0	16$\bar{3}$	5·9	+ 4·6	76$\bar{4}$	< 0·5	− 3·4
153	7·9	+ 7·4	552	1·7	− 1·9	16$\bar{4}$	2·8	+ 3·0	76$\bar{5}$	< 0·9	− 0·1
152	1·5*	+ 1·0	551	2·1	− 1·7	16$\bar{5}$	< 1·1	− 0·4	071	3·5	− 2·4
151	3·3	− 5·1	55$\bar{1}$	3·9	− 2·2	16$\bar{6}$	3·8	+ 3·2	072	1·6	− 0·9
15$\bar{1}$	1·2	− 2·4	55$\bar{2}$	4·0	− 4·0	16$\bar{7}$	< 1·2	+ 1·1	073	< 1·3	− 1·2
15$\bar{2}$	< 1·5	− 0·7	55$\bar{3}$	< 1·9	− 0·3	16$\bar{8}$	< 0·8	− 1·6	074	< 1·1	+ 0·8
15$\bar{3}$	11·3	+ 11·8	55$\bar{4}$	< 1·5	+ 2·0	265	3·2	− 3·0	075	1·4	− 0·6
15$\bar{4}$	8·2	+ 5·9	55$\bar{5}$	1·7	+ 1·0	264	< 1·2	+ 0·3	170	1·9	+ 0·9
15$\bar{5}$	4·5	+ 2·3	55$\bar{6}$	7·1	+ 6·5	263	7·5	+ 7·4	270	< 1·2	− 1·0
15$\bar{6}$	3·5	+ 4·1	55$\bar{7}$	4·7	+ 4·2	262	3·0	+ 2·3	370	< 0·8	+ 0·1
15$\bar{7}$	2·3	− 1·6	55$\bar{8}$	1·8	− 2·8	261	4·8	− 5·7	470	< 0·8	+ 0·9
15$\bar{8}$	2·8	− 2·4	55$\bar{9}$	< 1·0	+ 0·8	26$\bar{1}$	< 1·5	+ 0·4	174	< 0·8	+ 0·1
15$\bar{9}$	< 1·1	− 1·0	5.5.$\overline{10}$	5·8*	+ 0·1	26$\bar{2}$	1·7	− 2·7	173	2·3	+ 2·6
257	< 0·8	+ 3·1	652	< 1·7	+ 1·9	26$\bar{3}$	2·6	+ 3·5	172	< 1·0	+ 0·4
256	1·6	− 1·6	651	< 1·6	− 0·9	26$\bar{4}$	2·0	+ 1·6	171	1·5	− 1·8
255	4·7	− 3·5	65$\bar{1}$	< 0·8	+ 1·8	26$\bar{5}$	< 1·5	− 2·0	17$\bar{1}$	1·8	− 1·4
254	2·8	− 1·1	65$\bar{2}$	4·9	+ 5·2	26$\bar{6}$	< 1·1	+ 0·5	17$\bar{2}$	4·4	− 4·4
253	2·3	− 1·6	65$\bar{3}$	< 1·3	− 0·9	26$\bar{7}$	1·6	− 0·4	17$\bar{3}$	2·5	− 1·2
252	2·3*	− 0·3	65$\bar{4}$	2·6	− 1·4	26$\bar{8}$	< 0·9	− 0·2	17$\bar{4}$	< 1·0	+ 0·3
251	2·9	− 3·7	65$\bar{5}$	< 1·4	− 0·2	364	< 0·7	+ 0·2	17$\bar{5}$	1·6	− 1·4
25$\bar{1}$	< 1·6	+ 2·7	65$\bar{6}$	3·9	− 4·7	363	3·8	− 3·9	273	3·2	− 4·5
25$\bar{2}$	< 1·6	− 2·3	65$\bar{7}$	2·8	− 1·6	362	4·4	− 3·9	272	4·1	− 1·7
25$\bar{3}$	9·1	+ 7·9	65$\bar{8}$	< 1·6	+ 0·3	361	1·8	− 0·8	271	< 1·5	+ 1·7
25$\bar{4}$	10·1	+ 12·5	65$\bar{9}$	1·0	− 1·7	36$\bar{1}$	< 1·2	+ 1·2	27$\bar{1}$	1·5**	+ 2·1
25$\bar{5}$	6·5	− 7·1	6.5.$\overline{10}$	< 0·7	+ 0·3	36$\bar{2}$	< 1·3	+ 0·3	27$\bar{2}$	< 1·2	+ 1·8
25$\bar{6}$	7·0	− 7·0	6.5.$\overline{11}$	< 0·3	− 0·5	36$\bar{3}$	< 1·5	+ 1·7	27$\bar{3}$	2·1	− 2·7
25$\bar{7}$	< 1·5	+ 1·4	75$\bar{1}$	< 1·4	− 1·6	36$\bar{4}$	< 1·2	+ 1·5	27$\bar{4}$	1·9	− 2·2
25$\bar{8}$	2·7	− 2·7	75$\bar{2}$	2·7	− 2·2	36$\bar{5}$	2·0	− 1·2	27$\bar{5}$	1·2	+ 1·2
25$\bar{9}$	< 1·1	− 0·1	75$\bar{3}$	2·9	− 2·3	36$\bar{6}$	1·4	− 1·8	27$\bar{6}$	2·9	+ 3·5
2.5.$\overline{10}$	3·5	+ 3·1	75$\bar{4}$	3·1	− 1·7	36$\bar{7}$	< 0·9	+ 0·5	371	< 1·3	+ 1·7
356	< 0·6	− 2·1	75$\bar{5}$	2·2	− 1·5	36$\bar{8}$	1·4	− 1·3	37$\bar{1}$	< 0·9	+ 0·2
355	3·3	− 2·5	75$\bar{6}$	1·6	+ 1·5	36$\bar{9}$	< 0·5	+ 0·2	37$\bar{2}$	3·0	− 3·1
354	1·6	− 1·9	75$\bar{7}$	2·1	+ 2·5	463	< 0·9	+ 1·7	37$\bar{3}$	3·6	− 3·7
353	< 1·3	+ 0·5	75$\bar{8}$	1·4	− 2·4	462	2·6	+ 2·0	37$\bar{4}$	1·8	− 1·1
352	1·2	− 2·5	75$\bar{9}$	2·2	− 1·0	461	< 0·8	− 0·8	37$\bar{5}$	< 0·8	− 0·4
351	4·3	− 4·9	7.5.$\overline{10}$	< 0·7	+ 0·8	46$\bar{1}$	< 1·3	+ 1·0	37$\bar{6}$	2·7	− 1·8
35$\bar{1}$	3·2	− 1·4	85$\bar{3}$	< 0·4	+ 0·9	46$\bar{2}$	< 1·8	− 1·0	47$\bar{1}$	< 0·7	− 0·6
35$\bar{2}$	2·1	− 3·5	85$\bar{5}$	2·3	− 1·8	46$\bar{3}$	2·6	− 1·2	47$\bar{2}$	1·6	+ 1·9
35$\bar{3}$	5·8	+ 6·9	85$\bar{6}$	< 1·1	+ 1·0	46$\bar{4}$	3·0	− 2·5	47$\bar{3}$	2·2	− 2·9
35$\bar{4}$	7·1	+ 6·6	85$\bar{7}$	< 0·8	+ 0·3	46$\bar{5}$	< 1·4	− 0·5	47$\bar{4}$	1·5	− 2·7
35$\bar{5}$	4·4	+ 3·6	85$\bar{8}$	1·8	− 1·3	46$\bar{6}$	5·3	+ 5·1	47$\bar{5}$	< 1·3	+ 1·1
35$\bar{6}$	7·4	+ 8·7	85$\bar{9}$	< 0·6	− 2·6	46$\bar{7}$	< 1·1	+ 0·9	47$\bar{6}$	< 1·5	+ 1·3
35$\bar{7}$	2·3	+ 2·2	061	4·2	− 4·6	46$\bar{8}$	3·0	− 2·4			
35$\bar{8}$	2·0	− 2·5	062	< 1·8	− 1·6	46$\bar{9}$	< 1·9	+ 0·7			
35$\bar{9}$	< 1·0	+ 0·7	063	8·8	+ 8·9	561	< 1·3	+ 2·0			