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The Crystallography of Acridine. Part III. The Structure of Acridine II

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A three-dimensional analysis of a second crystalline form of acridine is described. Acridine II is monoclinic with

$$a = 16{\cdot}292,\ b = 18{\cdot}831,\ c = 6{\cdot}072\ \text{Å},\ \beta = 95°\ 4',\ Z = 8$$

and space group $P2_1/a$. There are two molecules in the asymmetric unit. The structure has been determined by trial-and-error and refined by successive calculations of differential syntheses from the three-dimensional data. Termination-of-series errors have been corrected by Booth's back-shift method.

Determination of the best mean isotropic temperature factors for each atom has shown that one of the molecules in the asymmetric unit is subject to more intense apparent thermal motion than the other. It has also been shown that the atomic thermal motion in each molecule is anisotropic and that it increases with the distance of an atom from its molecular centre. This anisotropic thermal motion, which arises from rigid-body vibrations and librations of the molecules, has not been allowed for in detail in the present refinement.

The two molecules in the asymmetric unit exhibit significant and different departures from planarity, but at this stage of refinement there are no significant differences in bond lengths (r.m.s. deviation 0·011 Å). The weighted mean bond lengths (estimated standard deviation between 0·003 and 0·005 Å) agree well with those observed in acridine III (r.m.s. deviation 0·008 Å) and in anthracene (r.m.s. deviation 0·005 Å).

Introduction

Acridine, $C_{13}H_9N$, is a heterocyclic molecule derived from anthracene by the replacement of one *meso*-CH group by nitrogen. Fig. 1 shows the structural formula with the atoms numbered in the order preferred by Albert (1951). The numbers in brackets are used to refer to a second molecule.

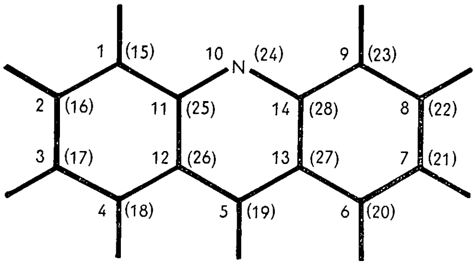

Fig. 1. Structural formula of acridine with numbering adopted for two molecules.

Three distinct crystalline forms of acridine have been described in Part I (Lowde, Phillips & Wood, 1953) and the structure of the simplest of these forms, acridine III, has been reported in detail in Part II (Phillips, 1956*a*). This paper describes a second of these forms, designated acridine II. This form is more complex crystallographically than acridine III, in particular because the asymmetric unit in acridine II consists of two molecules.

The objects of the work now to be described were to determine the crystal structure of acridine II with sufficient accuracy to discover its relations with the other polymorphic forms of acridine, and to make further measurements of the molecular dimensions for comparison with those determined quite independently from acridine III. It is clear from the results obtained, however, that acridine II is a suitable structure in which to investigate directly the effects of molecular interactions on intramolecular dimensions. The two molecules in the asymmetric unit have markedly different environments and it is possible that sufficiently accurate measurements would reveal the different effects of these environments on them.

The possibility of measuring the effects of molecular interactions in crystals with more than one molecule per asymmetric unit has already been noted, for example by de Lange, Robertson & Woodward (1939) in their study of *trans*-azobenzene, but no thorough investigation has yet been made. There is, however, a growing body of evidence, for example from studies of crystal fluorescence (e.g. Sangster & Irvine, 1956), that molecular states are modified by interactions in the crystalline state. In particular it is known that 'fluorescence in aromatic compounds is associated with planarity' (Birks & Cameron, 1959) being determined by the presence and configuration of π-electrons in the molecule and that crystals of many normally

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planar molecules, including acridine, exhibit less than the expected fluorescence. In view of this evidence it is encouraging to find as the result of the present investigation that the two molecules in the asymmetric unit in acridine II exhibit significant and different departures from planarity. Their observed dimensions, on the other hand, are not significantly different at the present level of accuracy and the detailed investigation of the effects of molecular interactions on molecular dimensions, which are expected to be small, must await more accurate intensity measurements.

Crystal data

The crystals are monoclinic prismatic (Lowde *et al.*, 1953). The cell dimensions have been re-determined by the Straumanis method using Cr $K\alpha_1$ radiation, $\lambda = 2{\cdot}28962$ Å, with the following results:

$$a = 16{\cdot}292 \pm 0{\cdot}004,\quad b = 18{\cdot}831 \pm 0{\cdot}002,$$
$$c = 6{\cdot}072 \pm 0{\cdot}002\ \text{Å};\quad \beta = 95^\circ\ 4' \pm 2';$$
$$U = 1855{\cdot}6\ \text{Å}^3;\quad Z = 8\ .$$

This gives the calculated density as 1·283 g.ml.$^{-1}$ which may be compared with the measured value of 1·278 g.ml.$^{-1}$. Linear absorption coefficient, for X-rays with wavelength 1·542 Å; $\mu = 6{\cdot}92$ cm.$^{-1}$.

Reflexions $h0l$ are absent when h is odd and reflexions $0k0$ are absent when k is odd. No other reflexions are systematically absent. The space group thus is $P2_1/a\text{–}C_{2h}^5$.

Intensity measurements

Roughly cylindrical crystals about 0·5 mm. in diameter were mounted on glass fibres with 'Duco' cement for rotation about the [001], [010] and [100] axes. The reflexions from these were recorded on equi-inclination Weissenberg photographs of the layers $l = 0\text{–}5$, $k = 0\text{–}7$ and $h = 0\text{–}12$. Each exposure was made with a set of three sheets of Kodak no-screen X-ray film. Exposure times varied up to 100 hr. All the estimations of reflexion intensity were made by visual comparison of the reflexion spots with those obtained by timed exposures of a single reflexion. Only the extended spots were measured on upper-level photographs and the intensities were corrected for extension (Phillips, 1956*b*). The Lorentz-polarization factors were derived from charts due to Lu (1943). No absorption corrections were applied.

The measurements from the various layer lines were brought to the same relative scale by the method described in Part II (Phillips, 1956*a*). In calculation of the average intensity for each reflexion the various estimations were weighted according to the inverse of the conversion factors required to bring them to the same scale. These conversion factors, after being adjusted to give a nearly absolute scale, varied from 1·72 to 5·32 with a mean value of 3·10. They were smallest for the densely populated [001]-axis photographs.

Within the Cu sphere of reflexion there are 4225 possible reflexions but only 2679, i.e. 63·4%, were estimated. This is a slightly smaller proportion than was observed for acridine III, but is about the same as that observed for anthracene. The intensities of 803 reflexions were estimated once, 1263 twice (i.e. on separate photographs taken about different axes) and 613 three times. A determination of the accuracy of these measurements made by the range-estimate method (Ibers, 1956) showed that $\sigma(F)$ varies roughly as $0{\cdot}09F$ with a minimum value of 0·6. The final comparison of observed and calculated structure factors has shown, however, that the very largest amplitudes, which were estimated only once, are subject to rather larger errors. The observed structure amplitudes together with the final calculated values are listed in Table 1.

Structure determination

The projection of the structure on (001) was considered first since it was expected to show the molecules resolved from one another and projected in much the same way as those in acridine III and anthracene. The Patterson projection was calculated and found to have narrow rows of peaks near the origin lying near the intersections with the {420} planes. These peaks were interpreted as arising from intramolecular vectors and showing the two molecules in the asymmetric unit in projection on (001) to be nearly parallel to (420). Bragg–Lipson charts were prepared for the relatively strong reflexions 060, 080, 410, 420 and 430, and the weak one 440, and the positions of the molecules, projected as in acridine III, were adjusted to give good agreement for these structure factors. The structure factors for all $hk0$ reflexions with $\sin\theta < 0{\cdot}4$ were then calculated and their signs were used in a calculation of $\varrho(xy)$. In this first synthesis the individual atoms were not resolved but adjustments to the atomic positions derived from difference (error) syntheses in several cycles of refinement improved the map slowly until the atoms were resolved in one molecule (A) but not in the other. A partial difference synthesis, calculated by taking out the contribution from the well-resolved molecule, then showed the second molecule resolved and clearly in a rather different orientation from that assumed. The two molecules in the asymmetric unit are rather differently inclined to (001) as may be seen in Fig. 4. Further refinement by the difference synthesis technique quickly reduced R, the residual error index (cf. Sutton, 1958, p. 27) of the $hk0$ reflexions, to 0·23.

The z-coordinates also were determined by trial-and-error. Several models based on the type of packing found in acridine III were tested by the calculation of hkl structure factors and the one which gave satis-

Table 1. *Observed and calculated structure factors*

h	k	l	10|Fo|	10Fc
00	00	00		7520
02	00	00	230	192
04	00	00	212	178•
06	00	00	134	110•
08	00	00	129	84•
10	00	00	104	86•
12	00	00	216	188•
14	00	00	92	68•
16	00	00	36	32
18	00	00	97	94•
20	00	00	9•	1•
00	02	00	927	822
00	04	00	441	376
00	06	00	819	694•
00	08	00	482	422
00	12	00	118	88
00	14	00	57	40•
00	16	00	131	146•
00	18	00	195	198•
00	20	00	36	30
00	00	01	66	68•
00	00	02	1216	986•
00	00	03	367	370•
00	00	04	44	8•
00	00	05	11•	16•
00	00	06	81	74•
00	00	07	18	16•
00	01	07	18	6
00	01	06	29	38
00	01	05	45	54•
00	01	04	52	56•
00	01	03	208	218
00	01	02	159	180•
00	01	01	148	148•
00	02	07	32	44
00	02	06	22•	22
00	02	05	39	68
00	02	04	9•	31
00	02	03	102	130
00	02	02	276	290•
00	02	01	30	24
00	03	07	32	24
00	03	06	29	10•
00	03	05	11•	13•
00	03	04	35	28
00	03	03	19	6•
00	03	02	116	122•
00	03	01	7•	15•
00	04	07	11•	5•
00	04	06	37	30
00	04	05	41	60•
00	04	04	29	46•
00	04	03	131	142•
00	04	02	26	14•
00	04	01	82	78
00	05	07	31	38•
00	05	06	116	124
00	05	05	54	50•
00	05	04	36	18•
00	05	03	102	106
00	05	02	148	128•
00	05	01	31	2
00	06	07	14•	2
00	06	06	32	32•
00	06	05	28	54
00	06	04	62	84•
00	06	03	139	146•
00	06	02	141	136
00	06	01	68	72
00	07	07	52	42•
00	07	06	32	16
00	07	05	65	76
00	07	04	164	164
00	07	03	312	314
00	07	02	280	268•
00	07	01	240	240•
00	08	07	22	28
00	08	06	55	28
00	08	05	123	150•
00	08	04	190	188•
00	08	03	199	216•
00	08	02	408	394
00	08	01	18	38
00	09	07	47	50•
00	09	06	19•	13
00	09	05	200	208
00	09	04	182	188
00	09	03	9•	22
00	09	02	154	158•
00	09	01	166	160•
00	10	07	13•	30•
00	10	06	29	44
00	10	05	178	194
00	10	04	138	132
00	10	03	10•	14•
00	10	02	196	182•
00	10	01	125	106•
00	11	06	29	38
00	11	05	97	108
00	11	04	156	148
00	11	03	217	228•
00	11	02	40	36•
00	11	01	160	138
00	12	06	37	34•
00	12	05	52	52
00	12	04	185	160
00	12	03	184	194•
00	12	02	45	38
00	12	01	94	94
00	13	06	26	18•
00	13	05	12•	30•
00	13	04	130	130
00	13	03	121	122•
00	13	02	74	38
00	13	01	41	44•
00	14	06	81	80•
00	14	05	94	102
00	14	04	46	40
00	14	03	62	50•
00	14	02	12•	1•
00	14	01	29	20•
00	15	05	12•	23•
00	15	04	13•	31•
00	15	03	96	104
00	15	02	49	46•
00	15	01	36	46
00	16	05	11•	14•
00	16	04	13•	4
00	16	03	47	44•
00	16	02	83	106
00	16	01	77	80•
00	17	05	10•	7
00	17	04	12•	5
00	17	03	46	54
00	17	02	69	68•
00	17	01	151	148•
00	18	05	17	18
00	18	04	27	36
00	18	03	87	114
00	18	02	12•	11•
00	18	01	154	184•
00	19	04	22	18
00	19	03	22	12
00	19	02	12•	7
00	19	01	121	126•
00	20	04	28	22
00	20	03	34	26•
00	20	02	36	32
00	20	01	38	48•
00	21	03	24	26•
00	21	02	9•	24
00	21	01	11•	2•
00	22	03	6•	6
00	22	02	8•	8•
00	22	01	11•	3
00	23	02	25	22
00	23	01	9•	12
01	01	07•	18•	19
01	01	06•	25•	38
01	01	05•	29	8•
01	01	04•	26	30
01	01	03•	134	136•
01	01	02•	21•	24
01	01	01•	803	1046
01	01	00•	332	294
01	01	01	812	1122
01	01	02	429	484•
01	01	03	400	396•
01	01	04	65	68•
01	01	05	28	44•
01	01	06	62	50•
01	02	07•	52	50
01	02	06•	36	32
01	02	05•	50	72
01	02	04•	69	54
01	02	03•	162	166•
01	02	02•	447	478
01	02	01•	244	230
01	02	00•	806	704•
01	02	01	290	344
01	02	02	204	224
01	02	03	125	146•
01	02	04	95	114
01	02	05	17	10
01	02	06	29	2
01	02	07	18•	3•
01	03	07•	14•	38
01	03	06•	104	128
01	03	05•	94	118•
01	03	04•	75	56
01	03	03•	96	94•
01	03	02•	510	506
01	03	01•	57	50•
01	03	00•	528	436•
01	03	01	151	162•
01	03	02	101	90•
01	03	03	213	224
01	03	04	73	70•
01	03	05	12•	8
01	03	06	59	58•
01	03	07	52	50
01	04	07•	34	34
01	04	06•	56	62•
01	04	05•	129	160
01	04	04•	36	20
01	04	03•	174	156•
01	04	02•	57	54
01	04	01•	204	184
01	04	00•	598	486
01	04	01	110	120•
01	04	02	45	44•
01	04	03	18	4
01	04	04	49	52
01	04	05	40	40
01	04	06	32	20•
01	04	07	11•	8
01	05	07•	22	26•
01	05	06•	94	106
01	05	05•	138	178•
01	05	04•	12•	17•
01	05	03•	159	140
01	05	02•	73	46•
01	05	01•	185	160•
01	05	00•	198	170
01	05	01	277	260•
01	05	02	87	94•
01	05	03	11	8•
01	05	04	54	80
01	05	05	60	76
01	05	06	87	126•
01	05	07	39	60
01	06	07•	14	24
01	06	06•	57	56•
01	06	05•	97	108
01	06	04•	108	106
01	06	03•	270	252•
01	06	02•	20	16
01	06	01•	96	92•
01	06	00•	47	40•
01	06	01	14	32•
01	06	02	8•	51•
01	06	03	30	38
01	06	04	69	72•
01	06	05	54	50•
01	06	06	32	24
01	06	07	12•	13
01	07	07•	32	38
01	07	06•	47	54•
01	07	05•	129	146•
01	07	04•	227	226•
01	07	03•	81	80
01	07	02•	216	204
01	07	01•	172	150
01	07	00•	108	100•
01	07	01	170	170
01	07	02	209	232
01	07	03	102	80
01	07	04	237	246•
01	07	05	178	158•
01	07	06	40	46
01	07	07	16•	41
01	08	07•	40	30•
01	08	06•	19•	2•
01	08	05•	131	96
01	08	04•	230	220
01	08	03•	78	78
01	08	02•	371	366•
01	08	01•	224	208•
01	08	00•	206	172•
01	08	01	72	84•
01	08	02	195	208•
01	08	03	111	92
01	08	04	223	250•
01	08	05	134	108•
01	08	06	65	66
01	09	07•	13•	8•
01	09	06•	65	40
01	09	05•	70	68
01	09	04•	60	44•
01	09	03•	123	78•
01	09	02•	40	26
01	09	01•	291	246
01	09	00•	258	212•
01	09	01	123	126•
01	09	02	9•	22•
01	09	03	130	124
01	09	04	49	42•
01	09	05	12•	5
01	09	06	19•	12
01	10	07•	11•	14•
01	10	06•	52	56
01	10	05•	133	140
01	10	04•	139	122
01	10	03•	235	240•
01	10	02•	182	182•
01	10	01•	105	92
01	10	00•	482	418•
01	10	01	64	74
01	10	02	42	50
01	10	03	96	114•
01	10	04	118	82
01	10	05	124	134•
01	10	06	29	36•
01	11	06•	19•	12
01	11	05•	91	104
01	11	04•	166	152
01	11	03•	143	152•
01	11	02•	56	50•
01	11	01•	74	68
01	11	00•	101	82•
01	11	01	148	138•
01	11	02	68	64•
01	11	03	262	222•
01	11	04	81	98•
01	11	05	95	92
01	11	06	18	44
01	12	06•	17•	13•
01	12	05•	70	54
01	12	04•	13•	7•
01	12	03•	19	24
01	12	02•	86	82•
01	12	01•	11•	18
01	12	00•	78	74
01	12	01	26	30
01	12	02	32	6
01	12	03	172	158•
01	12	04	100	98
01	12	05	35	28•
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01	13	05•	26	46•
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01	13	02•	27	16
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01	13	00•	87	72•
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01	14	03•	31	30
01	14	02•	78	78
01	14	01•	22	18
01	14	00•	13•	3
01	14	01	12•	8•
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01	14	03	11•	26
01	14	04	26	28
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01	15	06•	11•	1
01	15	05•	46	36•
01	15	04•	13•	30•
01	15	03•	60	82•
01	15	02•	13•	6
01	15	01•	36	32
01	15	00•	13•	4•
01	15	01	21	6•
01	15	02	28	28•
01	15	03	102	118
01	15	04	13•	20•
01	15	05	42	54•
01	16	05•	22	12•
01	16	04•	39	30
01	16	03•	76	94
01	16	02•	69	58•
01	16	01•	14•	26
01	16	00•	52	40
01	16	01	14•	6
01	16	02	123	140•
01	16	03	112	130
01	16	04	39	24•
01	16	05	11•	8•
01	17	05•	10•	6•
01	17	04•	12•	1•
01	17	03•	10•	8•
01	17	02•	113	114
01	17	01•	161	192•
01	17	00•	248	254•
01	17	01	36	20•
01	17	02	42	16•
01	17	03	146	194
01	17	04	22	16
01	17	05	10•	1
01	18	05•	13	4•
01	18	04•	12•	17
01	18	03•	10•	21
01	18	02•	112	118•
01	18	01•	140	138•
01	18	00•	81	94
01	18	01	42	56
01	18	02	53	54
01	18	03	22	18
01	18	04	19	32•
01	18	05	17	16
01	19	04•	11•	1•
01	19	03•	10•	16
01	19	02•	12•	8
01	19	01•	12•	33•
01	19	00•	152	154•
01	19	01	12•	12•
01	19	02	53	46
01	19	03	38	58
01	19	04	11•	3•
01	20	04•	36	44•
01	20	03•	19	4
01	20	02•	34	30
01	20	01•	29	32
01	20	00•	34	34•
01	20	01	31	32•
01	20	02	11•	9
01	20	03	27	24•
01	20	04	6•	10
01	21	03•	24	20
01	21	02•	9•	7•
01	21	01•	11•	15
01	21	01	11•	10•
01	21	02	9•	5
01	21	03	8•	7
01	22	03•	22	28
01	22	02•	8•	5•
01	22	01•	11•	13•
01	22	01	11•	1•
01	22	02	8•	7
01	22	03	17	20•
01	23	02•	8•	7•
01	23	01•	9•	6•
01	23	01	9•	3
02	00	07•	13•	3•
02	00	06•	28	46•
02	00	05•	13	26•
02	00	04•	34	22•
02	00	03•	27	34•
02	00	02•	11	22•
02	00	01•	458	580
02	00	01	1002	1456
02	00	02	700	704•
02	00	03	978	816•
02	00	04	36	48•
02	00	05	12•	61•
02	00	06	131	182•
02	00	07	28•	16•
02	01	07•	34	36
02	01	06•	42	50
02	01	05•	11	8•
02	01	04•	69	60
02	01	03•	102	106
02	01	02•	108	92
02	01	01•	29	20
02	01	00•	156	126
02	01	01	190	206•
02	01	02	113	130•
02	01	03	225	254•
02	01	04	125	154•
02	01	05	12•	1•
02	01	06	17•	21
02	02	07•	26	24
02	02	06•	28	6•
02	02	05•	56	54
02	02	04•	189	192
02	02	03•	340	398
02	02	02•	226	236•
02	02	01•	896	992•
02	02	00•	6•	25
02	02	01	302	320•
02	02	02	98	100
02	02	03	238	256•
02	02	04	154	164
02	02	05	18	22•
02	02	06	17•	9
02	02	07	16•	36•
02	03	07•	47	42
02	03	06•	112	170
02	03	05•	141	138•
02	03	04•	148	156
02	03	03•	468	518
02	03	02•	328	324•
02	03	01•	382	376•
02	03	00•	64	62•
02	03	01	190	198
02	03	02	69	64
02	03	03	80	70
02	03	04	42	36•
02	03	05	21	42
02	03	06	27	18
02	03	07	12•	9
02	04	07•	12•	12
02	04	06•	85	130•
02	04	05•	207	210
02	04	04•	83	114•
02	04	03•	189	170
02	04	02•	159	146•
02	04	01•	465	404
02	04	00•	62	60
02	04	01	291	304
02	04	02	63	58•
02	04	03	66	54•
02	04	04	12•	9
02	04	05	14•	17•
02	04	06	77	78
02	04	07	36	54•
02	05	07•	48	34
02	05	06•	52	35•
02	05	05•	121	104•
02	05	04•	65	58•
02	05	03•	207	146
02	05	02•	130	112•
02	05	01•	181	164
02	05	00•	139	130
02	05	01	77	84
02	05	02	45	58
02	05	03	21	30•
02	05	04	60	60•
02	05	05	59	68•
02	05	06	94	122
02	05	07	14•	42•
02	06	07•	13•	15•
02	06	06•	17•	10
02	06	05•	42	62
02	06	04•	48	48
02	06	03•	28	14
02	06	02•	105	108
02	06	01•	31	20
02	06	00•	30	36•
02	06	01	177	172•
02	06	02	184	178
02	06	03	161	158
02	06	04	84	40•
02	06	05	115	76•
02	06	06	97	148
02	06	07	39	22•
02	07	07•	14	10
02	07	06•	26	36•
02	07	05•	81	58
02	07	04•	69	54
02	07	03•	90	86•
02	07	02•	85	70•
02	07	01•	251	226•
02	07	00•	84	82
02	07	01	452	472•
02	07	02	166	172•
02	07	03	48	48
02	07	04	28	68
02	07	05	12•	5
02	07	06	65	60
02	07	07	16•	7
02	08	07•	12•	11
02	08	06•	16•	8•
02	08	05•	73	78•
02	08	04•	168	150•
02	08	03•	9•	6•
02	08	02•	214	198
02	08	01•	309	270
02	08	00•	179	158•
02	08	01	485	522
02	08	02	124	130
02	08	03	46	64•
02	08	04	200	244•
02	08	05	100	78•
02	08	06	16•	15
02	09	07•	10•	12•
02	09	06•	16•	3•
02	09	05•	98	102
02	09	04•	101	78
02	09	03•	129	134•
02	09	02•	260	238•
02	09	01•	92	56•
02	09	00•	249	228
02	09	01	625	686•
02	09	02	85	98•
02	09	03	165	170
02	09	04	11•	7
02	09	05	27	8
02	09	06	20	18•
02	10	06•	34	40
02	10	05•	97	108
02	10	04•	91	128
02	10	03•	112	100•
02	10	02•	265	242•
02	10	01•	311	266•
02	10	00•	73	70
02	10	01	152	152•
02	10	02	44	66•
02	10	03	91	104•
02	10	04	278	286
02	10	05	27	44
02	10	06	31	20•
02	11	06•	13•	7
02	11	05•	21	20
02	11	04•	13•	1•
02	11	03•	84	72
02	11	02•	258	226•
02	11	01•	157	128•
02	11	00•	212	188
02	11	01	270	248•
02	11	02	134	126•
02	11	03	222	190
02	11	04	13•	10•
02	11	05	18•	14
02	11	06	13•	12•
02	12	06•	17	38•
02	12	05•	12•	27•
02	12	04•	96	90•
02	12	03•	256	234
02	12	02•	271	230•
02	12	01•	36	40•
02	12	00•	97	92
02	12	01	19	0
02	12	02	42	26
02	12	03	40	42•
02	12	04	22	60•
02	12	05	16•	6•
02	13	06•	13•	0•
02	13	05•	34	28•
02	13	04•	47	30•
02	13	03•	115	106
02	13	02•	115	70•
02	13	01•	54	34
02	13	00•	77	70
02	13	01	60	52
02	13	02	12•	20•
02	13	03	28	42•
02	13	04	13•	14
02	13	05	16•	14•
02	13	06	12•	•
02	14	06•	12•	18•
02	14	05•	25	24•
02	14	04•	40	40
02	14	03•	24	12
02	14	02•	204	212•
02	14	01•	63	48
02	14	00•	58	72
02	14	01	12•	13
02	14	02	12•	6
02	14	03	57	56•
02	14	04	36	46
02	14	05	12•	12•
02	14	06	34	42
02	15	06•	10•	16
02	15	05•	60	66
02	15	04•	13•	1•
02	15	03•	27	20•
02	15	02•	213	264
02	15	01•	97	88•
02	15	00•	132	156•
02	15	01	14•	35•
02	15	02	13•	36
02	15	03	11•	5
02	15	04	13•	13
02	15	05	12•	7
02	16	05•	11•	11•
02	16	04•	13•	20•
02	16	03•	18	28
02	16	02•	233	244•
02	16	01•	175	146
02	16	00•	132	134
02	16	01	14•	22
02	16	02	25	60
02	16	03	22	32•
02	16	04	13•	9
02	16	05	28	30
02	17	05•	10•	6•
02	17	04•	12•	18
02	17	03•	10•	21
02	17	02•	55	76
02	17	01•	130	154•
02	17	00•	119	122•
02	17	01	157	176
02	17	02	151	142
02	17	03	136	154•
02	17	04	12•	13
02	17	05	39	40
02	18	05•	8•	14
02	18	04•	18	4
02	18	03•	17	16•
02	18	02•	37	22
02	18	01•	52	62•
02	18	00•	130	152•
02	18	01	45	36•
02	18	02	162	182
02	18	03	10•	13•
02	18	04	55	72
02	18	05	36	42
02	19	04•	22	30•
02	19	03•	10•	18•
02	19	02•	31	8
02	19	01•	20	38
02	19	00•	116	88•
02	19	01	19	42
02	19	02	46	68
02	19	03	34	42•
02	19	04	11•	3
02	20	04•	24	38•
02	20	03•	9•	15•
02	20	02•	11•	26
02	20	01•	42	58
02	20	00•	13•	7•
02	20	01	27	24
02	20	02	11•	8•
02	20	03	9•	17
02	20	04	32	30•
02	21	03•	14	10•
02	21	02•	9•	19
02	21	01•	36	42
02	21	01	11•	1•
02	21	02	9•	15•
02	21	03	8•	1•
02	22	03•	18	30•
02	22	02•	8•	5
02	22	01•	20	8•
02	22	01	11•	7
02	22	02	8•	4•
02	23	01•	8•	22•
02	23	01	8•	5
03	01	07•	45	38
03	01	06•	39	22
03	01	05•	28	20•
03	01	04•	42	14
03	01	03•	146	130
03	01	02•	86	96•
03	01	01•	449	498•
03	01	00•	525	438
03	01	01	1045	1328•
03	01	02	44	40•
03	01	03	220	252
03	01	04	124	128•
03	01	05	35	70•
03	01	06	94	114•
03	01	07	13•	8
03	02	07•	17	26
03	02	06•	49	46•
03	02	05•	103	114
03	02	04•	129	174
03	02	03•	272	264
03	02	02•	329	332•
03	02	01•	767	850•
03	02	00•	228	216
03	02	01	493	578•
03	02	02	241	256
03	02	03	72	90•
03	02	04	39	32
03	02	05	28	6
03	02	06	17•	2•
03	02	07	13•	6•
03	03	07•	24	24
03	03	06•	59	72
03	03	05•	39	50•
03	03	04•	137	128
03	03	03•	255	230
03	03	02•	65	62
03	03	01•	757	736•
03	03	00•	609	580•
03	03	01	150	134
03	03	02	148	152
03	03	03	46	36
03	03	04	12•	2
03	03	05	22	24
03	03	06	27	18•
03	03	07	12•	1
03	04	07•	25	26
03	04	06•	22	20•
03	04	05•	96	94•
03	04	04•	32	30
03	04	03•	92	70
03	04	02•	152	116
03	04	01•	399	350•
03	04	00•	175	168•
03	04	01	39	36•
03	04	02	67	64
03	04	03	92	100•
03	04	04	12•	5•
03	04	05	19	6•
03	04	06	14•	25•
03	04	07	20	32
03	05	07•	47	60•
03	05	06•	67	92
03	05	05•	209	212
03	05	04•	82	96
03	05	03•	306	258•
03	05	02•	288	288
03	05	01•	69	68
03	05	00•	123	114
03	05	01	58	66•
03	05	02	122	114•
03	05	03	22	24
03	05	04	42	64
03	05	05	48	76
03	05	06	14•	51•
03	05	07	11•	11•
03	06	07•	13	28
03	06	06•	25	30
03	06	05•	217	240•
03	06	04•	54	62•
03	06	03•	217	208
03	06	02•	261	262•
03	06	01•	149	124
03	06	00•	29	26•
03	06	01	47	38•
03	06	02	189	170•
03	06	03	50	72
03	06	04	136	148
03	06	05	84	70
03	06	06	75	102•
03	06	07	45	52
03	07	07•	11•	4
03	07	06•	67	78
03	07	05•	35	34•
03	07	04•	46	24•
03	07	03•	19	10•
03	07	02•	326	286
03	07	01•	152	114
03	07	00•	136	124
03	07	01	58	72
03	07	02	271	256
03	07	03	161	170•
03	07	04	72	68•
03	07	05	87	64•
03	07	06	50	62•
03	07	07	78	80
03	08	07•	11•	6•
03	08	06•	22	16
03	08	05•	27	4•
03	08	04•	74	44
03	08	03•	9•	10•
03	08	02•	139	110•
03	08	01•	50	26•
03	08	00•	114	92•
03	08	01	11•	15
03	08	02	332	372•
03	08	03	68	64•
03	08	04	363	410
03	08	05	103	120
03	08	06	34	36•
03	08	07	10•	2•
03	09	07•	11	12
03	09	06•	15•	1•
03	09	05•	12•	27
03	09	04•	45	22•
03	09	03•	48	28•
03	09	02•	69	66•
03	09	01•	22	26
03	09	00•	45	40
03	09	01	265	268•
03	09	02	96	108
03	09	03	40	64
03	09	04	13•	13
03	09	05	18•	16•
03	09	06	15•	2
03	09	07	5•	14•
03	10	07•	8•	19
03	10	06•	15•	33
03	10	05•	12•	7•
03	10	04•	29	24•
03	10	03•	59	50•
03	10	02•	90	90•
03	10	01•	13	20
03	10	00•	138	114•
03	10	01	284	296•
03	10	02	28	30•
03	10	03	246	260
03	10	04	178	180
03	10	05	39	26
03	10	06	22	20•
03	11	06•	17	26•
03	11	05•	28	28•
03	11	04•	13•	37•
03	11	03•	88	82•
03	11	02•	30	24•
03	11	01•	25	28
03	11	00•	154	132•
03	11	01	142	128•
03	11	02	52	64•
03	11	03	76	68
03	11	04	172	178
03	11	05	54	45•
03	11	06	53	42•
03	12	06•	50	54•
03	12	05•	65	84•
03	12	04•	82	86
03	12	03•	156	122•
03	12	02•	175	160
03	12	01•	41	34•
03	12	00•	116	102•
03	12	01	32	32
03	12	02	18	16•
03	12	03	24	4
03	12	04	52	48•
03	12	05	45	48
03	12	06	25	30
03	13	06•	67	74•
03	13	05•	21	16
03	13	04•	13•	16•
03	13	03•	254	230•
03	13	02•	319	288
03	13	01•	11•	5
03	13	00•	101	76•
03	13	01	57	68•
03	13	02	29	32•
03	13	03	11•	34
03	13	04	13•	7•
03	13	05	14•	1
03	13	06	36	22•
03	14	06•	36	34•
03	14	05•	12•	18•
03	14	04•	72	96
03	14	03•	60	24•
03	14	02•	44	80•
03	14	01•	12•	29
03	14	00•	66	88•
03	14	01	56	54•
03	14	02	13•	6•
03	14	03	11•	26
03	14	04	13•	26•
03	14	05	14•	17
03	14	06	10•	2•
03	15	05•	18	22
03	15	04•	48	44•
03	15	03•	203	212•
03	15	02•	154	128
03	15	01•	22	24
03	15	00•	222	238
03	15	01	85	106
03	15	02	44	66•
03	15	03	22	50•

* In the l and F_c columns indicates a negative sign and in the F_o column indicates the most probable amplitude of an unobserved reflexion.

Table 1 (*cont.*)

h	k	l	$10\lvert F_o\rvert$	$10F_c$
03	15	04	13•	6•
03	15	05	26	34
03	16	05•	29	24
03	16	04•	13•	3
03	16	03•	70	98
03	16	02•	13•	13
03	16	01•	38	42•
03	16	00•	113	144•
03	16	01	54	70•
03	16	02	45	56
03	16	03	34	30•
03	16	04	13•	8
03	16	05	10•	22
03	17	05•	13	2
03	17	04•	12•	5
03	17	03•	32	42•
03	17	02•	28	30•
03	17	01•	86	68
03	17	00•	45	60
03	17	01	14•	3•
03	17	02	32	44
03	17	03	10•	21
03	17	04	12•	18
03	17	05	34	47
03	18	05•	8•	19
03	18	04•	20	16•
03	18	03•	10•	14•
03	18	02•	19	28•
03	18	01•	21	32•
03	18	00•	14•	27
03	18	01	47	76
03	18	02	12•	19•
03	18	03	50	48
03	18	04	13	22•
03	19	04•	47	46•
03	19	03•	9•	13•
03	19	02•	40	30
03	19	01•	73	80
03	19	00•	77	94
03	19	01	56	74•
03	19	02	11•	21•
03	19	03	41	56
03	19	04	19	26
03	20	04•	27	42•
03	20	03•	38	50•
03	20	02•	78	82
03	20	01•	60	76
03	20	00•	85	92
03	20	01	81	76•
03	20	02	11•	34•
03	20	03	29	34
03	20	04	34	32•
03	21	03•	11	16•
03	21	02•	26	42
03	21	01•	21	6
03	21	01	26	44•
03	21	02	9•	14•
03	21	03	20	14•
03	22	03•	8	26•
03	22	02•	25	4•
03	22	01•	11•	8
03	22	01	11•	17
03	22	02	8•	2•
03	23	02•	8•	20
03	23	01•	8•	3•
03	23	01	8•	0•
04	00	07•	39	64•
04	00	06•	21•	10
04	00	05•	35	96•
04	00	04•	52	48
04	00	03•	32	24•
04	00	02•	54	58•
04	00	01•	70	32•
04	00	01	560	574
04	00	02	73	54•
04	00	03	209	218•
04	00	04	103	88•
04	00	05	46	64•
04	00	06	55	72•
04	00	07	16•	3•
04	01	07•	16•	10
04	01	06•	71•	0
04	01	05•	65	90•
04	01	04•	35	12
04	01	03•	210.	200
04	01	02•	24•	38
04	01	01•	543	556•
04	01	00•	927	912•
04	01	01	795	798
04	01	02	58	58•
04	01	03	134	172•
04	01	04	62	52
04	01	05	14•	27•
04	01	06	19•	14
04	01	07	16•	4
04	02	07•	17	28
04	02	06•	28	32
04	02	05•	13	18•
04	02	04•	112	118
04	02	03•	246	260
04	02	02•	30	14
04	02	01•	1063	1272•
04	02	00•	1900	1930•
04	02	01	1037	1374
04	02	02	158	170
04	02	03	85	68
04	02	04	12•	7•
04	02	05	36	66
04	02	06	19•	4•
04	02	07	13•	14
04	03	07•	25	8•
04	03	06•	45	56•
04	03	05•	86	108
04	03	04•	30	56•
04	03	03•	84	86
04	03	02•	240	246
04	03	01•	1056	1156•
04	03	00•	1467	1474•
04	03	01	567	622
04	03	02	174	178
04	03	03	60	66
04	03	04	12•	21•
04	03	05	29	30
04	03	06	50	62
04	03	07	31	52•
04	04	07•	20	28•
04	04	06•	87	88
04	04	05•	54	68•
04	04	04•	198	192
04	04	03•	29	10•
04	04	02•	195	162•
04	04	01•	361	322•
04	04	00•	70	60
04	04	01	8•	24
04	04	02	144	144•
04	04	03	46	62•
04	04	04	12•	39•
04	04	05	16•	41•
04	04	06	14•	5•
04	04	07	34	36
04	05	07•	16•	2
04	05	06•	67	82•
04	05	05•	131	156•
04	05	04•	234	226•
04	05	03•	49	32•
04	05	02•	636	656
04	05	01•	166	154•
04	05	00•	39	32•
04	05	01	46	52
04	05	02	60	60
04	05	03	26	10•
04	05	04	29	46•
04	05	05	16•	41•
04	05	06	18•	32•
04	05	07	11•	14
04	06	07•	50	42•
04	06	06•	19•	30
04	06	05•	216	262
04	06	04•	174	110
04	06	03•	20	18
04	06	02•	458	398•
04	06	01•	53	44•
04	06	00•	85	72•
04	06	01	69	62
04	06	02	84	90•
04	06	03	24	24
04	06	04	52	48•
04	06	05	16•	6•
04	06	06	31	4•
04	06	07	38	22
04	07	07•	13•	5
04	07	06•	58	60•
04	07	05•	21	18•
04	07	04•	44	44
04	07	03•	46	28
04	07	02•	72	78
04	07	01•	124	98•
04	07	00•	130	110
04	07	01	261	266•
04	07	02	16•	21•
04	07	03	123	160
04	07	04	133	166
04	07	05	126	128
04	07	06	18•	6
04	07	07	47	64•
04	08	07•	29	22•
04	08	06•	36	36•
04	08	05•	12•	3•
04	08	04•	30	16•
04	08	03•	47	44•
04	08	02•	206	158
04	08	01•	83	72
04	08	00•	96	102
04	08	01	29	30
04	08	02	152	174
04	08	03	27	40
04	08	04	245	232•
04	08	05	93	116•
04	08	06	65	76
04	08	07	10•	15
04	09	07•	17	18•
04	09	06•	17•	8•
04	09	05•	35	22
04	09	04•	13•	13
04	09	03•	10•	8
04	09	02•	9•	29•
04	09	01•	148	132
04	09	00•	40	32
04	09	01	55	50•
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06	20	03	37	40
06	21	03•	7•	3
06	21	02•	9•	3•
06	21	01•	21	32
06	21	01	45	70•
06	21	02	28	28•
06	21	03	12•	22
06	22	02•	8•	9
06	22	01•	9•	29•
06	22	01	8•	8•
06	23	01•	12•	24•
07	01	07•	47	60•
07	01	06•	19•	14•
07	01	05•	78	58
07	01	04•	34	14•
07	01	03•	50	54•
07	01	02•	46	44•
07	01	01•	103	102
07	01	00•	27	20
07	01	01	101	96
07	01	02	159	144•
07	01	03	91	96•
07	01	04	102	98
07	01	05	18•	24
07	01	06	19	18
07	01	07	25	34•
07	02	07•	14•	22•
07	02	06•	92	110
07	02	05•	108	90
07	02	04•	48	22•
07	02	03•	30	20•
07	02	02•	65	64
07	02	01•	9•	23•
07	02	00•	93	106•
07	02	01	529	528
07	02	02	279	264•
07	02	03	47	36
07	02	04	112	134
07	02	05	36	56
07	02	06	19	10
07	02	07	38	60•
07	03	07•	18	18•
07	03	06•	98	104•
07	03	05•	186	186•
07	03	04•	109	94
07	03	03•	64	56
07	03	02•	9•	35•
07	03	01•	152	148
07	03	00•	78	64•
07	03	01	539	568
07	03	02	260	254•
07	03	03	10•	13•
07	03	04	78	68
07	03	05	35	38
07	03	06	16	34
07	03	07	18	30•
07	04	07•	9•	9•
07	04	06•	69	80
07	04	05•	29	38
07	04	04•	238	202•
07	04	03•	54	52•
07	04	02•	525	654
07	04	01•	52	38
07	04	00•	110	102
07	04	01	370	388
07	04	02	190	194•

Table 1 (*cont.*)

h	k	l	$10\vert F_o\vert$	$10F_c$
07	04	03	125	128•
07	04	04	90	68•
07	04	05	16•	30
07	04	06	35	38
07	05	07•	13•	31•
07	05	06•	17•	12•
07	05	05•	13	22•
07	05	04•	121	122•
07	05	03•	129	92•
07	05	02•	136	112
07	05	01•	696	595
07	05	00•	156	132•
07	05	01	273	272•
07	05	02	212	178•
07	05	03	253	280
07	05	04	133	156
07	05	05	18•	14
07	05	06	25	29•
07	06	07•	11•	2
07	06	06•	17•	28•
07	06	05•	72	54•
07	06	04•	91	74•
07	06	03•	54	38
07	06	02•	174	148
07	06	01•	224	178
07	06	00•	131	128
07	06	01	36	28
07	06	02	164	176
07	06	03	216	224•
07	06	04	176	196•
07	06	05	18•	6
07	06	06	14•	33
07	07	07•	11•	9
07	07	06•	17•	16•
07	07	05•	30	28
07	07	04•	30	34•
07	07	03•	10•	15•
07	07	02•	42	22•
07	07	01•	28	22
07	07	00•	42	26•
07	07	01	11•	8
07	07	02	18	28•
07	07	03	103	100
07	07	04	46	56
07	07	05	18•	10•
07	07	06	14•	27
07	08	06•	17•	25•
07	08	05•	87	96
07	08	04•	47	66•
07	08	03•	69	52•
07	08	02•	25	26•
07	08	01•	58	42•
07	08	00•	58	66
07	08	01	11•	16
07	08	02	30	38•
07	08	03	78	38•
07	08	04	22	24•
07	08	05	16•	1•
07	08	06	15•	28
07	09	06•	15•	7
07	09	05•	77	62
07	09	04•	32	6•
07	09	03•	45	46•
07	09	02•	25	34
07	09	01•	77	64•
07	09	00•	52	38
07	09	01	11•	11•
07	09	02	31	44
07	09	03	11•	13•
07	09	04	111	138•
07	09	05	110	118
07	09	06	13•	2
07	10	06•	15•	3•
07	10	05•	25	32
07	10	04•	52	72•
07	10	03•	25	30
07	10	02•	20	20•
07	10	01•	11•	8•
07	10	00•	83	86•
07	10	01	11•	18
07	10	02	12•	39
07	10	03	28	14
07	10	04	22	62•
07	10	05	29	44•
07	10	06	13•	17
07	11	06•	15•	7
07	11	05•	12•	23•
07	11	04•	87	112
07	11	03•	11•	32•
07	11	02•	98	102•
07	11	01•	11•	12
07	11	00•	80	76
07	11	01	159	158
07	11	02	78	96•
07	11	03	72	102•
07	11	04	80	82•
07	11	05	37	44
07	11	06	11•	8•
07	12	06•	13•	18•
07	12	05•	12•	7
07	12	04•	56	86•
07	12	03•	17	30
07	12	02•	205	180
07	12	01•	34	24
07	12	00•	233	266
07	12	01	94	98
07	12	02	153	154•
07	12	03	146	166•
07	12	04	48	50•
07	12	05	21	20
07	12	06	7•	5
07	13	06•	11•	22
07	13	05•	17	24
07	13	04•	100	110
07	13	03•	125	122
07	13	02•	199	192•
07	13	01•	14•	0•
07	13	00•	58	100•
07	13	01	22	42
07	13	02	44	14•
07	13	03	134	134•
07	13	04	20	36•
07	13	05	30	26
07	14	06•	7•	27
07	14	05•	11•	6
07	14	04•	21	36•
07	14	03•	11•	21•
07	14	02•	81	50•
07	14	01•	220	186
07	14	00•	138	174
07	14	01	14•	21•
07	14	02	13•	43•
07	14	03	11•	22•
07	14	04	12•	9•
07	14	05	19	18
07	15	05•	11	2•
07	15	04•	22	2
07	15	03•	101	84
07	15	02•	244	210•
07	15	01•	40	14
07	15	00•	62	54
07	15	01	14•	37
07	15	02	34	34•
07	15	03	10•	14•
07	15	04	12•	13
07	15	05	30	36•
07	16	05•	38	36•
07	16	04•	36	26
07	16	03•	60	58
07	16	02•	87	60•
07	16	01•	67	58
07	16	00•	25	36•
07	16	01	14•	27•
07	16	02	67	80
07	16	03	10•	13•
07	16	04	12•	14
07	16	05	9•	1•
07	17	05•	7•	8•
07	17	04•	34	20
07	17	03•	10•	6
07	17	02•	44	34•
07	17	01•	14•	13•
07	17	00•	14•	2
07	17	01	37	44
07	17	02	11•	29•
07	17	03	9•	21
07	17	04	22	30•
07	18	04•	48	44
07	18	03•	9•	1
07	18	02•	52	42•
07	18	01•	12•	13•
07	18	00•	13•	10•
07	18	01	12•	1
07	18	02	11•	1•
07	18	03	9•	21
07	18	04	8•	12•
07	19	04•	19	24•
07	19	03•	17	10•
07	19	02•	25	22
07	19	01•	11•	1•
07	19	00•	13•	9
07	19	01	11•	16•
07	19	02	9•	10•
07	19	03	8•	15
07	20	03•	7•	11
07	20	02•	9•	18
07	20	01•	11•	10•
07	20	01	11•	14•
07	20	02	9•	5•
07	20	03	13	18•
07	21	02•	29	40•
07	21	01•	11•	27•
07	21	01	34	35
07	21	02	25	22•
07	22	01•	18	28•
07	22	01	27	24
08	00	07•	36	36•
08	00	06•	17•	16•
08	00	05•	30	53
08	00	04•	67	122•
08	00	03•	9•	21
08	00	02•	9•	44
08	00	01•	21	18
08	00	01	280	246•
08	00	02	47	38
08	00	03	42	34•
08	00	04	94	78
08	00	05	45	80•
08	00	06	18•	23
08	01	07•	36	32
08	01	06•	19•	6•
08	01	05•	81	76•
08	01	04•	159	148
08	01	03•	63	76•
08	01	02•	9•	5•
08	01	01•	149	138
08	01	00•	215	174
08	01	01	37	48•
08	01	02	65	70•
08	01	03	63	72•
08	01	04	13•	13•
08	01	05	18•	1
08	01	06	18•	10
08	02	07•	16•	4•
08	02	06•	90	114•
08	02	05•	12•	30
08	02	04•	182	214•
08	02	03•	272	260
08	02	02•	162	148
08	02	01•	251	260•
08	02	00•	73	54•
08	02	01	49	54
08	02	02	88	58
08	02	03	10•	0
08	02	04	53	54•
08	02	05	49	58
08	02	06	18•	12
08	03	07•	25	28
08	03	06•	98	130
08	03	05•	103	136
08	03	04•	13•	10
08	03	03•	281	252•
08	03	02•	154	154•
08	03	01•	468	444
08	03	00•	85	82•
08	03	01	543	524•
08	03	02	273	268
08	03	03	17	2•
08	03	04	27	14•
08	03	05	54	62
08	03	06	14•	2•
08	04	07•	16•	15•
08	04	06•	78	74•
08	04	05•	137	140•
08	04	04•	75	52•
08	04	03•	35	14
08	04	02•	490	468
08	04	01•	517	462
08	04	00•	122	110
08	04	01	683	668•
08	04	02	285	274
08	04	03	39	58
08	04	04	36	28
08	04	05	14•	22•
08	04	06	32	26•
08	05	07•	12•	11•
08	05	06•	19•	26
08	05	05•	12•	16•
08	05	04•	157	144•
08	05	03•	19	4
08	05	02•	289	250
08	05	01•	824	738
08	05	00•	98	88
08	05	01	334	308•
08	05	02	29	44•
08	05	03	190	212•
08	05	04	172	180•
08	05	05	39	58•
08	05	06	58	56
08	06	07•	12•	5
08	06	06•	17•	9
08	06	05•	52	44
08	06	04•	35	26•
08	06	03•	10•	19•
08	06	02•	45	38
08	06	01•	482	438
08	06	00•	109	104•
08	06	01	255	242•
08	06	02	76	94•
08	06	03	248	258
08	06	04	159	178
08	06	05	46	18•
08	06	06	42	64•
08	07	07•	11•	8•
08	07	06•	19•	7
08	07	05•	24	32
08	07	04•	34	18•
08	07	03•	10•	3•
08	07	02•	42	46•
08	07	01•	38	24
08	07	00•	98	88•
08	07	01	75	68
08	07	02	52	74
08	07	03	106	86•
08	07	04	109	98•
08	07	05	78	94
08	07	06	18	16
08	08	07•	11•	28
08	08	06•	17•	10•
08	08	05•	27	24•
08	08	04•	32	36
08	08	03•	31	30
08	08	02•	30	14
08	08	01•	11•	11
08	08	00•	18	20
08	08	01	11•	10
08	08	02	26	34•
08	08	03	11•	15
08	08	04	113	124
08	08	05	116	118•
08	08	06	18	42
08	09	06•	17•	0•
08	09	05•	81	94•
08	09	04•	40	52
08	09	03•	17	18•
08	09	02•	88	80
08	09	01•	19	16
08	09	00•	18	26
08	09	01	20	36
08	09	02	18	26•
08	09	03	11•	49•
08	09	04	80	84•
08	09	05	75	82
08	09	06	13•	17•
08	10	06•	17•	10•
08	10	05•	25	10
08	10	04•	87	106•
08	10	03•	40	52
08	10	02•	59	52•
08	10	01•	11•	16•
08	10	00•	37	30•
08	10	01	20	34
08	10	02	12•	22•
08	10	03	42	4•
08	10	04	53	54
08	10	05	84	78•
08	10	06	13•	7•
08	11	06•	16•	4•
08	11	05•	12•	21•
08	11	04•	74	78
08	11	03•	47	50•
08	11	02•	19	2•
08	11	01•	29	46
08	11	00•	44	20
08	11	01	30	46•
08	11	02	25	36•
08	11	03	98	80•
08	11	04	22	26
08	11	05	14•	3
08	11	06	11•	13
08	12	06•	13•	10•
08	12	05•	12•	1•
08	12	04•	34	14
08	12	03•	17	34
08	12	02•	13•	33•
08	12	01•	205	202•
08	12	00•	75	84
08	12	01	24	14•
08	12	02	13•	7
08	12	03	170	188•
08	12	04	22	34•
08	12	05	20	22
08	13	06•	11•	12
08	13	05•	12•	3
08	13	04•	66	56•
08	13	03•	17	30•
08	13	02•	13•	47
08	13	01•	230	220
08	13	00•	317	286
08	13	01	78	88•
08	13	02	130	168•
08	13	03	144	180•
08	13	04	20	42•
08	13	05	13	18
08	14	05•	11•	16
08	14	04•	29	14•
08	14	03•	11•	3•
08	14	02•	80	82•
08	14	01•	36	34•
08	14	00•	149	174•
08	14	01	14•	0
08	14	02	87	110
08	14	03	29	24•
08	14	04	12•	37•
08	14	05	22	28
08	15	05•	30	26
08	15	04•	42	52•
08	15	03•	58	56•
08	15	02•	38	54
08	15	01•	57	52•
08	15	00•	14•	9
08	15	01	21	34
08	15	02	48	66•
08	15	03	42	50
08	15	04	12•	6
08	15	05	7•	0
08	16	05•	38	30
08	16	04•	69	54•
08	16	03•	45	48•
08	16	02•	137	106
08	16	01•	77	56•
08	16	00•	22	2•
08	16	01	14•	9•
08	16	02	65	66
08	16	03	10•	18•
08	16	04	11•	14
08	17	04•	59	46•
08	17	03•	10•	22•
08	17	02•	67	56
08	17	01•	12•	11
08	17	00•	13•	3
08	17	01	11•	5•
08	17	02	36	32•
08	17	03	9•	9
08	17	04	9•	5
08	18	04•	40	26•
08	18	03•	9•	11•
08	18	02•	11•	8•
08	18	01•	29	28
08	18	00•	13•	9
08	18	01	11•	7
08	18	02	11•	11
08	18	03	8•	8•
08	18	04	6•	35
08	19	03•	36	34
08	19	02•	9•	4•
08	19	01•	21	32•
08	19	00•	13•	19•
08	19	01	11•	10
08	19	02	9•	13
08	19	03	7•	10•
08	20	03•	7•	13•
08	20	02•	13	30•
08	20	01•	11•	7•
08	20	00•	18•	7•
08	20	01	11•	16•
08	20	02	8•	22•
08	21	02•	8•	7•
08	21	01•	9•	38•
08	21	01	9•	26
08	21	02	6•	14
09	01	07•	41	30
09	01	06•	54	64•
09	01	05•	137	162•
09	01	04•	364	364
09	01	03•	83	110•
09	01	02•	156	130•
09	01	01•	11•	32•
09	01	00•	18	6•
09	01	01	62	66
09	01	02	16	10
09	01	03	10•	31
09	01	04	88	82•
09	01	05	65	60
09	01	06	18•	16•
09	02	07•	20	24
09	02	06•	29	36
09	02	05•	74	82
09	02	04•	143	136•
09	02	03•	68	38•
09	02	02•	9•	22
09	02	01•	187	160•
09	02	00•	178	164•
09	02	01	96	72•
09	02	02	95	88
09	02	03	10•	1•
09	02	04	45	66•
09	02	05	44	54
09	02	06	18•	2•
09	03	07•	35	34•
09	03	06•	82	96•
09	03	05•	83	82•
09	03	04•	53	66
09	03	03•	187	158
09	03	02•	90	60
09	03	01•	175	140
09	03	00•	140	128
09	03	01	11•	9
09	03	02	16•	3
09	03	03	87	28•
09	03	04	68	68•
09	03	05	16•	3•
09	03	06	12•	8
09	04	07•	12•	17
09	04	06•	58	56
09	04	05•	49	40
09	04	04•	44	58•
09	04	03•	170	142•
09	04	02•	144	128
09	04	01•	308	262
09	04	00•	210	182•
09	04	01	154	148•
09	04	02	210	180•
09	04	03	10•	22•
09	04	04	68	78•
09	04	05	21	18•
09	04	06	26	22
09	05	07•	10•	0•
09	05	06•	19•	16•
09	05	05•	12•	10
09	05	04•	31	34•
09	05	03•	90	76
09	05	02•	333	280
09	05	01•	126	94
09	05	00•	53	44
09	05	01	142	142•
09	05	02	162	132•
09	05	03	59	74
09	05	04	54	64
09	05	05	60	66•
09	05	06	25	32•
09	06	07•	25	32
09	06	06•	19•	11•
09	06	05•	12•	11•
09	06	04•	13•	14
09	06	03•	10•	8•
09	06	02•	289	220
09	06	01•	166	136•
09	06	00•	90	86
09	06	01	81	74
09	06	02	263	240•
09	06	03	11•	13•
09	06	04	41	52•
09	06	05	52	66•
09	06	06	57	58
09	07	06•	19•	30
09	07	05•	19	38
09	07	04•	76	68
09	07	03•	10•	20•
09	07	02•	46	20
09	07	01•	182	148•
09	07	00•	104	96
09	07	01	25	4
09	07	02	133	120
09	07	03	17	30•
09	07	04	53	56•
09	07	05	63	92
09	07	06	54	58•
09	08	06•	17•	22•
09	08	05•	21	18•
09	08	04•	80	68
09	08	03•	17	8
09	08	02•	41	28
09	08	01•	45	54
09	08	00•	13•	13
09	08	01	47	52•
09	08	02	12•	15
09	08	03	11•	28
09	08	04	58	58
09	08	05	57	62•
09	08	06	20	30
09	09	06•	17•	13
09	09	05•	21	30•
09	09	04•	47	46
09	09	03•	48	58•
09	09	02•	41	38
09	09	01•	28	16•
09	09	00•	25	18•
09	09	01	12•	13•
09	09	02	12•	1•
09	09	03	11•	38
09	09	04	35	28•
09	09	05	14•	5
09	09	06	10•	13•
09	10	06•	15•	10
09	10	05•	25	24
09	10	04•	13•	20
09	10	03•	42	58
09	10	02•	12•	8•
09	10	01•	35	34•
09	10	00•	27	30•
09	10	01	12•	11•
09	10	02	13•	12
09	10	03	11•	12
09	10	04	30	30
09	10	05	14•	2•
09	11	06•	12•	12•
09	11	05•	12•	12•
09	11	04•	73	60•
09	11	03•	17	16•
09	11	02•	12•	10
09	11	01•	56	62•
09	11	00•	31	46
09	11	01	74	86
09	11	02	32	14•
09	11	03	69	84•
09	11	04	50	52•
09	11	05	48	52
09	12	06•	10•	9
09	12	05•	12•	18
09	12	04•	22	44
09	12	03•	49	38•
09	12	02•	39	56•
09	12	01•	260	276
09	12	00•	54	70•
09	12	01	25	6•
09	12	02	134	142•
09	12	03	96	96•
09	12	04	46	52•
09	12	05	29	26
09	13	05•	11•	2•
09	13	04•	13•	6
09	13	03•	48	52
09	13	02•	13•	7•
09	13	01•	381	368•
09	13	00•	14•	32
09	13	01	160	174
09	13	02	94	90•
09	13	03	38	42•
09	13	04	20	2•
09	13	05	73	72
09	14	05•	10•	2•
09	14	04•	81	76•
09	14	03•	101	72•
09	14	02•	98	72
09	14	01•	14•	21
09	14	00•	84	88•
09	14	01	21	20
09	14	02	13•	9•
09	14	03	29	62•
09	14	04	26	26•
09	15	05•	27	18
09	15	04•	72	64•
09	15	03•	94	84•
09	15	02•	95	72
09	15	01•	154	140•
09	15	00•	40	30•
09	15	01	109	90
09	15	02	12•	4
09	15	03	31	40
09	15	04	11•	4
09	16	05•	7•	11
09	16	04•	30	30•
09	16	03•	10•	14•
09	16	02•	12•	31
09	16	01•	78	64•
09	16	00•	14•	6•
09	16	01	12•	28•
09	16	02	18	20
09	16	03	9•	5
09	16	04	12	16•
09	17	04•	9•	12
09	17	03•	9•	3•
09	17	02•	11•	17•
09	17	01•	12•	9
09	17	00•	13•	10
09	17	01	11•	8
09	17	02	11•	7•
09	17	03	9•	10•
09	17	04	17	6•
09	18	04•	26	18
09	18	03•	9•	15
09	18	02•	11•	9•
09	18	01•	11•	18•
09	18	00•	13•	19
09	18	01	11•	6•
09	18	02	9•	1
09	18	03	8•	6
09	19	03•	44	42•
09	19	02•	9•	3•
09	19	01•	11•	6
09	19	00•	34	2•
09	19	01	11•	1•
09	19	02	9•	9
09	19	03	7•	14
09	20	03•	62	68
09	20	02•	8•	21
09	20	01•	11•	3
09	20	00•	18•	14•
09	20	01	24	46
09	20	02	8•	30
09	21	02•	45	54•
09	21	01•	38	42•
09	21	01	47	30•
10	00	07•	41	30
10	00	06•	105	112
10	00	05•	119	128
10	00	04•	330	318•
10	00	03•	200	220
10	00	02•	56	48•
10	00	01•	39	32•
10	00	01	11•	13•
10	00	02	83	84
10	00	03	54	72
10	00	04	50	42
10	00	05	40	54•
10	00	06	22	4•
10	01	07•	41	62•
10	01	06•	19	0
10	01	05•	21	2
10	01	04•	119	88•
10	01	03•	60	44
10	01	02•	48	44
10	01	01•	39	38
10	01	00•	48	48•
10	01	01	67	54•
10	01	02	11•	8•
10	01	03	11•	13•
10	01	04	13•	4•
10	01	05	26	34•
10	01	06	13•	9
10	02	07•	11	26•
10	02	06•	22	22
10	02	05•	49	10•
10	02	04•	65	52
10	02	03•	17	26
10	02	02•	11•	22•
10	02	01•	148	122
10	02	00•	143	124
10	02	01	42	28•
10	02	02	111	84•
10	02	03	109	100•
10	02	04	20	34
10	02	05	40	56•
10	02	06	22	38
10	03	07•	9•	19•
10	03	06•	69	76
10	03	05•	54	46
10	03	04•	94	58•
10	03	03•	141	144•
10	03	02•	97	60•
10	03	01•	288	246•
10	03	00•	154	140•
10	03	01	94	82•
10	03	02	93	60•
10	03	03	242	242
10	03	04	86	96
10	03	05	84	106•
10	03	06	11•	5
10	04	06•	31	22•
10	04	05•	36	24•
10	04	04•	22	14
10	04	03•	78	62
10	04	02•	22	10
10	04	01•	238	224
10	04	00•	85	76
10	04	01	134	118
10	04	02	502	484•
10	04	03	85	72
10	04	04	49	56•
10	04	05	65	56•
10	04	06	16	6•
10	05	06•	18•	7•
10	05	05•	13	14
10	05	04•	13•	4•
10	05	03•	10•	2•
10	05	02•	90	80
10	05	01•	81	78
10	05	00•	78	62•
10	05	01	112	108•
10	05	02	41	28•
10	05	03	80	96•
10	05	04	74	104•
10	05	05	14•	2•
10	05	06	11•	29
10	06	06•	16•	16
10	06	05•	19	22
10	06	04•	84	80
10	06	03•	94	90•
10	06	02•	105	98•
10	06	01•	25	26
10	06	00•	27	24
10	06	01	87	90•
10	06	02	116	112•
10	06	03	50	48
10	06	04	13•	16
10	06	05	80	78•
10	06	06	18	8
10	07	06•	16	38
10	07	05•	78	90
10	07	04•	62	44
10	07	03•	91	60•
10	07	02•	251	220•
10	07	01•	52	42
10	07	00•	68	50•
10	07	01	19	34•
10	07	02	90	76
10	07	03	35	40
10	07	04	35	4
10	07	05	19	14
10	07	06	9•	0•
10	08	06•	22	2•
10	08	05•	92	78
10	08	04•	13•	10•
10	08	03•	11•	3
10	08	02•	208	160•
10	08	01•	19	18
10	08	00•	13•	21•
10	08	01	28	46
10	08	02	42	40•
10	08	03	11•	14•
10	08	04	13•	12
10	08	05	25	40
10	09	06•	13•	0
10	09	05•	72	66
10	09	04•	34	40•
10	09	03•	63	84
10	09	02•	12•	10
10	09	01•	41	8
10	09	00•	13•	11•
10	09	01	12•	4
10	09	02	13•	3•
10	09	03	11•	6•
10	09	04	13•	15•
10	09	05	12•	3
10	10	05•	12•	5•
10	10	04•	68	70•
10	10	03•	65	84•
10	10	02•	161	146
10	10	01•	166	174
10	10	00•	22	28•
10	10	01	65	76•
10	10	02	28	34
10	10	03	17	4
10	10	04	12•	4
10	10	05	31	28
10	11	05•	29	46
10	11	04•	32	36
10	11	03•	77	92
10	11	02•	101	82•
10	11	01•	325	316•
10	11	00•	88	102
10	11	01	14•	12
10	11	02	13•	13
10	11	03	11•	8•
10	11	04	28	16•
10	11	05	40	57
10	12	05•	11•	19•
10	12	04•	29	34•
10	12	03•	11•	11•
10	12	02•	29	22
10	12	01•	177	184
10	12	00•	180	194•
10	12	01	41	66
10	12	02	40	54
10	12	03	25	26•
10	12	04	12•	1•
10	12	05	68	70
10	13	05•	11•	2
10	13	04•	20	20•
10	13	03•	40	38•
10	13	02•	27	44
10	13	01•	30	36•
10	13	00•	70	96
10	13	01	41	70•
10	13	02	48	88•
10	13	03	29	20•
10	13	04	22	24•
10	13	05	8	22•
10	14	05•	10•	2•
10	14	04•	57	58•
10	14	03•	19	16•
10	14	02•	27	26•
10	14	01•	52	16•
10	14	00•	96	100•
10	14	01	37	30•
10	14	02	139	142
10	14	03	32	38
10	14	04	11•	22
10	15	05•	8•	9•
10	15	04•	12•	26•
10	15	03•	16	34•
10	15	02•	157	106•
10	15	01•	34	34
10	15	00•	128	116•
10	15	01	35	34•
10	15	02	125	124
10	15	03	26	32
10	15	04	11•	5•
10	16	04•	11•	14•
10	16	03•	21	18•
10	16	02•	136	102•
10	16	01•	138	110
10	16	00•	72	64•
10	16	01	12•	37•
10	16	02	16	22
10	16	03	19	34
10	16	04	8•	1
10	17	04•	40	44
10	17	03•	9•	18•
10	17	02•	74	54•
10	17	01•	103	88
10	17	00•	29	18•
10	17	01	11•	3•
10	17	02	9•	29•
10	17	03	8•	11•
10	18	03•	8•	26
10	18	02•	9•	2
10	18	01•	11•	8•
10	18	00•	41	6
10	18	01	11•	3•
10	18	02	9•	6•
10	18	03	7•	11•
10	19	03•	16	20•
10	19	02•	9•	18
10	19	01•	11•	1
10	19	00•	11•	9
10	19	01	11•	10
10	19	02	8•	5
10	20	02•	8•	27•
10	20	01•	9•	8
10	20	00•	13•	36•
10	20	01	8•	16•
11	01	06•	139	110
11	01	05•	12•	19
11	01	04•	136	128•
11	01	03•	108	116
11	01	02•	40	40
11	01	01•	102	108•
11	01	00•	80	68
11	01	01	40	52
11	01	02	12•	34•
11	01	03	11•	9
11	01	04	13•	10•
11	01	05	13•	2
11	02	06•	52	62•
11	02	05•	11•	0•
11	02	04•	130	90
11	02	03•	133	100•
11	02	02•	86	80•
11	02	01•	151	142
11	02	00•	215	186•

Table 1 (*cont.*)

h	k	l	$10\lvert F_o\rvert$	$10F_c$
11	02	01	31	38•
11	02	02	172	156
11	02	03	138	130
11	02	04	13•	13
11	02	05	26	28•
11	03	06•	69	62•
11	03	05•	27	16•
11	03	04•	67	46
11	03	03•	103	82
11	03	02•	11•	12
11	03	01•	134	132•
11	03	00•	297	292
11	03	01	28	50
11	03	02	12•	24•
11	03	03	304	286•
11	03	04	87	92•
11	03	05	45	54
11	03	06	21	30
11	04	06•	12•	6•
11	04	05•	12•	16
11	04	04•	42	58•
11	04	03•	11•	18
11	04	02•	11•	11
11	04	01•	11•	18
11	04	00•	221	188•
11	04	01	160	164•
11	04	02	293	274
11	04	03	85	88
11	04	04	46	50•
11	04	05	36	40•
11	05	06•	21•	1•
11	05	05•	12•	18
11	05	04•	13•	12•
11	05	03•	46	40•
11	05	02•	63	28•
11	05	01•	49	50
11	05	00•	64	55•
11	05	01	213	182•
11	05	02	213	192
11	05	03	189	184•
11	05	04	55	64•
11	05	05	14•	12•
11	06	06•	18•	4
11	06	05•	52	46
11	06	04•	58	65
11	06	03•	90	76•
11	06	02•	225	180•
11	06	01•	74	0•
11	06	00•	60	56•
11	06	01	31	28•
11	06	02	177	160
11	06	03	45	50•
11	06	04	13•	40•
11	06	05	14•	12
11	07	06•	18•	6•
11	07	05•	72	64
11	07	04•	52	38
11	07	03•	114	90•
11	07	02•	296	258•
11	07	01•	84	66•
11	07	00•	29	14
11	07	01	47	54
11	07	02	13•	13
11	07	03	11•	13
11	07	04	13•	12
11	07	05	57	68•
11	08	06•	17•	43
11	08	05•	36	34
11	08	04•	53	72
11	08	03•	141	140•
11	08	02•	143	116•
11	08	01•	87	60•
11	08	00•	125	112
11	08	01	14•	14
11	08	02	47	62•
11	08	03	11•	9
11	08	04	13•	7
11	08	05	34	36
11	09	05•	12•	9•
11	09	04•	13•	12•
11	09	03•	48	78
11	09	02•	13•	0
11	09	01•	69	14•
11	09	00•	14•	5•
11	09	01	14•	9•
11	09	02	13•	12
11	09	03	11•	7
11	09	04	13•	6
11	09	05	32	28•
11	10	05•	12•	1
11	10	04•	156	158
11	10	03•	87	96•
11	10	02•	150	132•
11	10	01•	27	36•
11	10	00•	116	126•
11	10	01	56	78
11	10	02	13•	36
11	10	03	17	18
11	10	04	12•	0
11	10	05	11•	11•
11	11	05•	49	44•
11	11	04•	13•	32•
11	11	03•	19	34
11	11	02•	180	146
11	11	01•	81	92
11	11	00•	73	100
11	11	01	32	66•
11	11	02	13•	17•
11	11	03	25	38
11	11	04	12•	14
11	11	05	11	36•
11	12	05•	11•	14
11	12	04•	45	50
11	12	03•	11•	5
11	12	02•	94	92•
11	12	01•	26	46•
11	12	00•	14•	10•
11	12	01	14•	5
11	12	02	29	16
11	12	03	10•	6•
11	12	04	18	30
11	12	05	30	46•
11	13	05•	10•	2•
11	13	04•	12•	1•
11	13	03•	10•	15
11	13	02•	64	70
11	13	01•	37	24•
11	13	00•	95	96•
11	13	01	14•	6•
11	13	02	113	134
11	13	03	10•	1•
11	13	04	25	26
11	14	05•	8•	6•
11	14	04•	18	30•
11	14	03•	19	18•
11	14	02•	22	24•
11	14	01•	37	32•
11	14	00•	36	24•
11	14	01	45	6•
11	14	02	81	76
11	14	03	88	96
11	14	04	9•	23•
11	15	04•	11•	5•
11	15	03•	9•	13•
11	15	02•	11•	3•
11	15	01•	95	86•
11	15	00•	45	50•
11	15	01	12•	36
11	15	02	109	128
11	15	03	24	32
11	16	04•	30	30•
11	16	03•	9•	18
11	16	02•	92	70
11	16	01•	119	102•
11	16	00•	13•	1
11	16	01	32	38
11	16	02	31	30
11	16	03	29	34
11	17	04•	6•	15
11	17	03•	8•	1•
11	17	02•	65	54
11	17	01•	115	98•
11	17	00•	13•	1•
11	17	01	11•	14
11	17	02	9•	1
11	17	03	7•	3•
11	18	03•	7•	10
11	18	02•	41	32
11	18	01•	49	40•
11	18	00•	25	6
11	18	01	11•	16•
11	18	02	8•	18•
11	19	02•	8•	12
11	19	01•	9•	7•
11	19	00•	11•	13•
11	19	01	9•	14•
11	19	02	6•	21
11	20	01•	8•	1
11	20	00•	20	30
11	20	01	7•	16
12	00	06•	105	124
12	00	05•	12•	9•
12	00	04•	111	124
12	00	03•	475	488•
12	00	02•	109	126
12	00	01•	189	162
12	00	01	138	114•
12	00	02	75	74
12	00	03	29	34
12	00	04	34	40
12	00	05	14•	14•
12	01	06•	87	86•
12	01	05•	25	28•
12	01	04•	113	108
12	01	03•	52	38
12	01	02•	91	70
12	01	01•	16•	17•
12	01	00•	193	148
12	01	01	12•	2
12	01	02	46	54•
12	01	03	17	14
12	01	04	13•	21•
12	01	05	13•	4
12	02	06•	25	42
12	02	05•	12•	5
12	02	04•	13•	3•
12	02	03•	48	66•
12	02	02•	12•	23•
12	02	01•	143	126
12	02	00•	48	16
12	02	01	38	36
12	02	02	174	162•
12	02	03	115	102•
12	02	04	39	34•
12	02	05	56	70
12	03	06•	12•	11
12	03	05•	12•	7
12	03	04•	13•	29
12	03	03•	45	54•
12	03	02•	12•	7
12	03	01•	35	34•
12	03	00•	85	117•
12	03	01	12•	23
12	03	02	174	158
12	03	03	196	182
12	03	04	18	30
12	03	05	40	28•
12	04	06•	9•	13
12	04	05•	31	30•
12	04	04•	13•	10
12	04	03•	11•	8•
12	04	02•	12•	21•
12	04	01•	12•	9•
12	04	00•	81	70
12	04	01	25	48
12	04	02	109	80•
12	04	03	125	124•
12	04	04	31	29•
12	04	05	24	18
12	05	06•	19•	15•
12	05	05•	12•	1
12	05	04•	46	48
12	05	03•	34	22•
12	05	02•	52	32•
12	05	01•	12•	6•
12	05	00•	92	70
12	05	01	32	26
12	05	02	137	130•
12	05	03	187	166
12	05	04	30	26•
12	05	05	97	94•
12	06	06•	17•	16
12	06	05•	41	32
12	06	04•	13•	3
12	06	03•	70	44•
12	06	02•	193	150•
12	06	01•	131	104•
12	06	00•	187	154
12	06	01	146	126
12	06	02	187	168•
12	06	03	44	32
12	06	04	13•	0
12	06	05	50	68
12	07	06•	16•	14•
12	07	05•	46	66
12	07	04•	13•	5
12	07	03•	128	102•
12	07	02•	320	282•
12	07	01•	231	172•
12	07	00•	223	182
12	07	01	149	126
12	07	02	67	60•
12	07	03	69	66
12	07	04	40	42
12	07	05	62	54•
12	08	05•	19	16
12	08	04•	103	102
12	08	03•	164	144•
12	08	02•	126	72•
12	08	01•	206	164•
12	08	00•	161	142
12	08	01	29	32
12	08	02	13•	11
12	08	03	11•	3•
12	08	04	12•	20
12	08	05	53	50
12	09	05•	12•	18•
12	09	04•	13•	8•
12	09	03•	11•	11
12	09	02•	110	108•
12	09	01•	96	72•
12	09	00•	88	96
12	09	01	14•	9
12	09	02	13•	7•
12	09	03	38	52•
12	09	04	12•	6•
12	09	05	10•	6•
12	10	05•	11•	15•
12	10	04•	56	42•
12	10	03•	22	12
12	10	02•	132	142
12	10	01•	188	138
12	10	00•	14•	30•
12	10	01	65	78•
12	10	02	18	38•
12	10	03	17	6
12	10	04	11•	28•
12	10	05	8•	16•
12	11	05•	27	28
12	11	04•	12•	13
12	11	03•	31	34•
12	11	02•	125	130•
12	11	01•	139	114•
12	11	00•	78	76•
12	11	01	101	106
12	11	02	63	72
12	11	03	10•	16
12	11	04	12•	0
12	11	05	7•	17
12	12	05•	10•	10
12	12	04•	38	32•
12	12	03•	10•	2•
12	12	02•	45	56
12	12	01•	31	36
12	12	00•	85	100
12	12	01	101	102•
12	12	02	32	48•
12	12	03	49	46
12	12	04	11•	2•
12	13	05•	8•	3•
12	13	04•	12•	0•
12	13	03•	10•	5
12	13	02•	12•	2
12	13	01•	12•	29
12	13	00•	60	72•
12	13	01	60	68
12	13	02	49	52
12	13	03	9•	8•
12	13	04	12	10•
12	14	04•	11•	2•
12	14	03•	9•	3
12	14	02•	11•	4
12	14	01•	12•	19•
12	14	00•	47	48•
12	14	01	74	64
12	14	02	11•	7
12	14	03	100	110
12	14	04	28	32•
12	15	04•	9•	5•
12	15	03•	9•	1•
12	15	02•	11•	4
12	15	01•	94	78•
12	15	00•	13•	4
12	15	01	76	78
12	15	02	85	78
12	15	03	50	52
12	16	03•	8•	11
12	16	02•	9•	4
12	16	01•	63	48•
12	16	00•	13•	5
12	16	01	11•	17
12	16	02	31	34
12	16	03	37	38
12	17	03•	7•	11•
12	17	02•	8•	12
12	17	01•	53	44
12	17	00•	11•	4•
12	17	01	28	36•
12	17	02	8•	5•
12	18	01•	56	48
12	18	00•	11•	14
12	18	01	22	10
12	18	02	8•	4•
12	19	01•	18	14
12	19	00•	22	32•
12	19	01	7•	8
13	01	05•	17	12•
13	01	04•	233	232•
13	01	03•	73	108
13	01	02•	58	46•
13	01	01•	170	140•
13	01	00•	128	104•
13	01	01	14•	1•
13	01	02	65	52
13	01	03	11•	8
13	01	04	13•	15
13	01	05	12•	6•
13	02	06•	13•	10
13	02	05•	27	10•
13	02	04•	77	70•
13	02	03•	207	190
13	02	02•	18•	19•
13	02	01•	17•	2
13	02	00•	103	78
13	02	01	37	38•
13	02	02	34	40
13	02	03	11•	13
13	02	04	18	28
13	02	05	60	54•
13	03	06•	36	30
13	03	05•	32	32•
13	03	04•	70	62•
13	03	03•	50	46
13	03	02•	13•	17
13	03	01•	16•	27
13	03	00•	36	24•
13	03	01	21	18
13	03	02	125	100•
13	03	03	11•	12•
13	03	04	13•	15•
13	03	05	11•	1•
13	04	06•	8•	45
13	04	05•	12•	8•
13	04	04•	20	36•
13	04	03•	11•	11
13	04	02•	13•	22
13	04	01•	59	45
13	04	00•	14•	11•
13	04	01	14•	31•
13	04	02	54	48
13	04	03	50	56
13	04	04	12•	31
13	04	05	50	48•
13	05	05•	12•	10•
13	05	04•	13•	23
13	05	03•	11•	1•
13	05	02•	13•	25
13	05	01•	14•	13•
13	05	00•	38	24
13	05	01	14•	6
13	05	02	76	58•
13	05	03	101	118
13	05	04	16	12•
13	05	05	30	46•
13	06	05•	12•	4•
13	06	04•	13•	9
13	06	03•	69	56•
13	06	02•	148	116•
13	06	01•	48	34•
13	06	00•	109	86
13	06	01	81	64
13	06	02	31	24
13	06	03	11•	3•
13	06	04	12•	24
13	06	05	20	32
13	07	05•	32	34
13	07	04•	13•	36
13	07	03•	80	54•
13	07	02•	177	166•
13	07	01•	30	20
13	07	00•	22	32
13	07	01	105	96
13	07	02	95	78
13	07	03	10•	7•
13	07	04	72	62
13	07	05	13	8
13	08	05•	30	38•
13	08	04•	44	36•
13	08	03•	31	36•
13	08	02•	73	48•
13	08	01•	93	72
13	08	00•	22	12•
13	08	01	83	86
13	08	02	28	24
13	08	03	17	16•
13	08	04	11•	12
13	09	05•	11•	7
13	09	04•	26	12•
13	09	03•	11•	23
13	09	02•	13•	1
13	09	01•	104	86
13	09	00•	129	132•
13	09	01	14•	8•
13	09	02	12•	3
13	09	03	16	28
13	09	04	12•	6•
13	10	05•	19	22•
13	10	04•	38	36•
13	10	03•	77	84
13	10	02•	116	102•
13	10	01•	119	134•
13	10	00•	129	148
13	10	01	14•	13
13	10	02	12•	8•
13	10	03	10•	10
13	10	04	26	30
13	11	05•	19	22•
13	11	04•	66	54•
13	11	03•	10•	2
13	11	02•	104	92
13	11	01•	152	148
13	11	00•	140	154•
13	11	01	12•	3
13	11	02	11•	11•
13	11	03	31	32•
13	11	04	28	28•
13	12	05•	8•	15
13	12	04•	12•	8
13	12	03•	10•	20•
13	12	02•	38	40•
13	12	01•	30	56•
13	12	00•	100	114
13	12	01	12•	22•
13	12	02	11•	10•
13	12	03	37	42
13	12	04	8•	8
13	13	04•	11•	13
13	13	03•	9•	14
13	13	02•	11•	4•
13	13	01•	19	4•
13	13	00•	20	34•
13	13	01	11•	12•
13	13	02	56	44
13	13	03	9•	18•
13	13	04	6•	12•
13	14	04•	9•	3•
13	14	03•	9•	2
13	14	02•	11•	22
13	14	01•	11•	14•
13	14	00•	13•	16•
13	14	01	11•	16
13	14	02	74	74
13	14	03	8•	24
13	15	04•	6•	6•
13	15	03•	8•	9
13	15	02•	9•	10
13	15	01•	11•	17
13	15	00•	49	38•
13	15	01	11•	12•
13	15	02	113	110
13	15	03	10	22
13	16	03•	7•	17•
13	16	02•	9•	4
13	16	01•	146	104
13	16	00•	54	56•
13	16	01	11•	9•
13	16	02	25	38
13	17	03•	6•	55
13	17	02•	40	25•
13	17	01•	95	86
13	17	00•	27	12•
13	17	01	9•	12•
13	17	02	4•	5•
13	18	01•	32	32
13	18	00•	42	42•
13	18	01	32	48•
14	00	06•	30	46
14	00	05•	52	30•
14	00	04•	156	128•
14	00	03•	52	32
14	00	02•	164	114•
14	00	01•	262	240•
14	00	01	55	66
14	00	02	215	176
14	00	03	141	142
14	00	04	20	36•
14	00	05	21	22•
14	01	05•	12•	4
14	01	04•	64	56
14	01	03•	16•	13•
14	01	02•	85	54
14	01	01•	148	136
14	01	00•	59	32•
14	01	01	14•	5•
14	01	02	124	112•
14	01	03	31	52•
14	01	04	12•	11•
14	01	05	11•	16
14	02	05•	19	10
14	02	04•	42	42
14	02	03•	116	104•
14	02	02•	18•	39
14	02	01•	94	86•
14	02	00•	36	34
14	02	01	21	22•
14	02	02	74	42
14	02	03	53	60•
14	02	04	28	26
14	02	05	11	24
14	03	06•	42	46•
14	03	05•	13	20
14	03	04•	64	40
14	03	03•	85	84•
14	03	02•	18•	1•
14	03	01•	42	32
14	03	00•	14•	3
14	03	01	21	26•
14	03	02	53	44•
14	03	03	64	78
14	03	04	26	20•
14	03	05	8•	12•
14	04	06•	34	18•
14	04	05•	32	30
14	04	04•	14•	13•
14	04	03•	16•	20
14	04	02•	13•	23•
14	04	01•	16•	9•
14	04	00•	14•	1
14	04	01	21	30
14	04	02	68	50
14	04	03	85	80•
14	04	04	36	32
14	04	05	52	56
14	05	05•	11•	13
14	05	04•	16•	13
14	05	03•	31	30
14	05	02•	13•	10•
14	05	01•	14•	7•
14	05	00•	39	26
14	05	01	14•	6
14	05	02	40	32
14	05	03	85	100•
14	05	04	36	40
14	05	05	8•	26
14	06	05•	11•	13
14	06	04•	13•	10
14	06	03•	11•	11
14	06	02•	13•	3•
14	06	01•	12•	5
14	06	00•	14•	12
14	06	01	34	26
14	06	02	124	112
14	06	03	78	84•
14	06	04	46	52
14	07	05•	40	30•
14	07	04•	12•	13•
14	07	03•	67	26•
14	07	02•	13•	18
14	07	01•	14•	1
14	07	00•	40	32
14	07	01	34	36
14	07	02	92	76
14	07	03	10•	10
14	07	04	66	60
14	08	05•	38	36
14	08	04•	12•	22
14	08	03•	10•	28
14	08	02•	174	172•
14	08	01•	60	68•
14	08	00•	91	110
14	08	01	52	58
14	08	02	12•	2•
14	08	03	16	26
14	08	04	22	32
14	09	05•	76	92•
14	09	04•	12•	2
14	09	03•	83	70
14	09	02•	204	202
14	09	01•	14•	44
14	09	00•	63	90•
14	09	01	41	56
14	09	02	11•	14•
14	09	03	9•	3
14	09	04	9•	12
14	10	05•	25	20•
14	10	04•	58	46
14	10	03•	9•	17
14	10	02•	50	38
14	10	01•	41	52•
14	10	00•	129	124
14	10	01	118	140•
14	10	02	18	26•
14	10	03	9•	9•
14	10	04	36	38•
14	11	05•	7•	21•
14	11	04•	66	50
14	11	03•	10•	16•
14	11	02•	11•	25•
14	11	01•	12•	8•
14	11	00•	36	52•
14	11	01	78	100
14	11	02	11•	22
14	11	03	9•	2•
14	11	04	26	38
14	12	04•	22	18
14	12	03•	56	50•
14	12	02•	18	8•
14	12	01•	19	16
14	12	00•	38	4
14	12	01	11•	7•
14	12	02	11•	32•
14	12	03	8•	4•
14	13	04•	9•	7•
14	13	03•	9•	1•
14	13	02•	11•	8
14	13	01•	11•	24
14	13	00•	31	4•
14	13	01	11•	29•
14	13	02	9•	7•
14	13	03	27	22
14	14	04•	6•	8
14	14	03•	12•	11•
14	14	02•	14•	1•
14	14	01•	11•	6
14	14	00•	12•	13
14	14	01	11•	4•
14	14	02	13	22
14	14	03	4•	20•
14	15	02•	9•	15•
14	15	01•	11•	12•
14	15	00•	11•	19
14	15	01	11•	5
14	15	02	8•	13
14	16	02•	32	26
14	16	01•	9•	25
14	16	00•	11•	27
14	16	01	9•	19•
14	17	01•	28	24•
14	17	00•	52	46
14	17	01	58	50•
15	01	05•	13	12
15	01	04•	13•	2
15	01	03•	130	112•
15	01	02•	113	90
15	01	01•	44	24•
15	01	00•	272	234•
15	01	01	157	126
15	01	02	225	210
15	01	03	100	92
15	01	04	46	36•
15	02	05•	49	36
15	02	04•	65	58
15	02	03•	87	98•
15	02	02•	47	54
15	02	01•	50	42
15	02	00•	58	56
15	02	01	84	68•
15	02	02	98	92•
15	02	03	57	64•
15	02	04	30	28
15	03	05•	17	18
15	03	04•	13•	19
15	03	03•	27	14•
15	03	02•	18•	11•
15	03	01•	18•	2•
15	03	00•	14•	2
15	03	01	14•	22
15	03	02	12•	4
15	03	03	16	12
15	03	04	11•	2•
15	04	05•	19	26•
15	04	04•	12•	12•
15	04	03•	35	16
15	04	02•	16•	7
15	04	01•	16•	17•
15	04	00•	14•	17•
15	04	01	14•	18•
15	04	02	12•	21•
15	04	03	17	22
15	04	04	11•	9•
15	05	05•	52	40•
15	05	04•	13•	3•
15	05	03•	14•	7•
15	05	02•	18•	44
15	05	01•	18•	5
15	05	00•	14•	24•
15	05	01	14•	14•
15	05	02	12•	31•
15	05	03	56	52
15	05	04	11•	6
15	06	05•	10•	12
15	06	04•	13•	7
15	06	03•	14•	28
15	06	02•	18•	29•
15	06	01•	18•	11
15	06	00•	14•	5
15	06	01	21	30
15	06	02	80	66•
15	06	03	112	106
15	06	04	9•	1
15	07	05•	10•	7
15	07	04•	13•	21
15	07	03•	81	96•
15	07	02•	18•	12•
15	07	01•	21	22•
15	07	00•	96	92
15	07	01	19	
15	07	02	93	86•
15	07	03	123	124
15	07	04	9•	7
15	08	05•	65	56•
15	08	04•	12•	14•
15	08	03•	185	182
15	08	02•	141	106
15	08	01•	12•	25
15	08	00•	75	64
15	08	01	67	90•
15	08	02	45	38•
15	08	03	69	66
15	08	04	8•	7
15	09	05•	7•	1
15	09	04•	69	48
15	09	03•	27	18
15	09	02•	11•	1•
15	09	01•	42	54•
15	09	00•	36	26•
15	09	01	12•	32
15	09	02	11•	18•
15	09	03	9•	5•
15	09	04	8•	13
15	10	04•	22	18
15	10	03•	137	128
15	10	02•	131	110
15	10	01•	39	34•
15	10	00•	52	46•
15	10	01	11•	2
15	10	02	11•	20
15	10	03	7•	15•
15	11	04•	11•	21•
15	11	03•	52	42
15	11	02•	17•	7
15	11	01•	32	26
15	11	00•	34	14
15	11	01	49	54•
15	11	02	9•	2
15	11	03	7•	15
15	12	04•	9•	16•
15	12	03•	50	32
15	12	02•	11•	0•
15	12	01•	11•	21•
15	12	00•	13•	2
15	12	01	11•	23
15	12	02	9•	3•
15	12	03	17	30•
15	13	04•	6•	13•
15	13	03•	37	28
15	13	02•	14•	4
15	13	01•	11•	6
15	13	00•	12•	6
15	13	01	11•	13•
15	13	02	8•	19•
15	14	03•	9•	18•
15	14	02•	12•	10•
15	14	01•	11•	7
15	14	00•	11•	10•
15	14	01	11•	1
15	15	02•	11•	4•
15	15	01•	9•	17
15	15	00•	9•	6
15	15	01	8•	20•
15	16	01•	11•	27
15	16	00•	8•	16
15	16	01	26	28•
16	00	05•	57	38
16	00	04•	30	24
16	00	03•	14•	14
16	00	02•	18•	27•
16	00	01•	83	92•
16	00	01	83	76
16	00	02	236	218
16	00	03	72	80
16	00	04	52	44•
16	01	05•	13	20
16	01	04•	48	28
16	01	03•	98	94
16	01	02•	88	76•
16	01	01•	56	56
16	01	00•	114	108
16	01	01	88	74•
16	01	02	104	94•
16	01	03	37	50•
16	01	04	22	14
16	02	05•	10•	26
16	02	04•	30	14
16	02	03•	137	132
16	02	02•	94	88•
16	02	01•	17•	20
16	02	00•	38	32
16	02	01	19	22
16	02	02	28	26
16	02	03	39	34
16	02	04	36	40•
16	03	05•	10•	17•
16	03	04•	13•	19•
16	03	03•	96	104
16	03	02•	96	94•
16	03	01•	18•	12
16	03	00•	14•	24
16	03	01	12•	14
16	03	02	11•	15•
16	03	03	45	52•
16	03	04	42	44
16	04	05•	13	10
16	04	04•	12•	9•
16	04	03•	14•	3•
16	04	02•	42	34•
16	04	01•	39	30•
16	04	00•	14•	1•
16	04	01	12•	20
16	04	02	46	44
16	04	03	9•	13
16	04	04	26	32•
16	05	05•	8•	15•
16	05	04•	12•	18
16	05	03•	14•	17
16	05	02•	18•	14
16	05	01•	18•	37•
16	05	00•	13•	1•
16	05	01	12•	15•
16	05	02	11•	6
16	05	03	9•	0•
16	05	04	10	10
16	06	05•	8•	11
16	06	04•	12•	30•
16	06	03•	14•	31
16	06	02•	18•	46•
16	06	01•	18•	43
16	06	00•	13•	6•
16	06	01	12•	15•
16	06	02	11•	25•
16	06	03	9•	12•
16	06	04	16	8
16	07	05•	7•	5•
16	07	04•	11•	6
16	07	03•	49	32
16	07	02•	96	88
16	07	01•	17•	29•
16	07	00•	66	64•
16	07	01	11•	9
16	07	02	25	28
16	07	03	7•	27•
16	08	05•	0•	0
16	08	04•	44	24
16	08	03•	12•	18•
16	08	02•	60	64•
16	08	01•	52	40•
16	08	00•	29	26•
16	08	01	74	74
16	08	02	46	52
16	08	03	59	50•
16	09	04•	11•	22

Table 1 (*cont.*)

h	k	l	$10\lvert F_o\rvert$	$10F_c$
16	09	03•	195	166
16	09	02•	165	150
16	09	01•	16•	18
16	09	00•	149	120•
16	09	01	67	76•
16	09	02	9•	10
16	09	03	57	44•
16	10	03•	147	98
16	10	02•	36	24
16	10	01•	16•	9•
16	10	00•	126	130•
16	10	01	88	110
16	10	02	9•	22•
16	10	03	35	36•
16	11	04•	8•	5•
16	11	03•	62	48
16	11	02•	14•	11
16	11	01•	14•	14•
16	11	00•	20	6•
16	11	01	32	44•
16	11	02	8•	12
16	11	03	6•	36
16	12	03•	13	4•
16	12	02•	13•	12•
16	12	01•	14•	5
16	12	00•	11•	18
16	12	01	9•	17
16	12	02	8•	9
16	13	02•	12•	1•
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16	13	01	9•	3•
16	14	01•	11•	2•
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17	01	03•	14•	6
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17	01	01•	54	42
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17	02	01	35	22•
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17	03	02•	98	74
17	03	01•	16•	39
17	03	00•	13•	4•
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17	03	02	11•	14•
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17	04	02•	69	66
17	04	01•	14•	5•
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17	05	01•	17•	6•
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17	11	00•	29	26
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17	12	01	8•	2
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18	02	00•	31	32•
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18	02	02	83	62•
18	02	03	7•	4•
18	03	04•	9•	5
18	03	03•	19	24
18	03	02•	45	30
18	03	01•	14•	24
18	03	00•	13•	8•
18	03	01	18	26•
18	03	02	9•	2•
18	03	03	6•	8•
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18	04	03•	39	26
18	04	02•	58	34•
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18	04	00•	12•	8
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19	01	03•	10•	3•
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19	03	01	74	66•
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19	04	03•	8•	6
19	04	02•	41	38•
19	04	01•	11•	13
19	04	00•	11•	15
19	04	01	9•	21•
19	04	02	8•	2
19	05	03•	75	82
19	05	02•	12•	17•
19	05	01•	12•	9
19	05	00•	11•	28•
19	05	01	9•	10
19	06	03•	74	36•
19	06	02•	12•	10•
19	06	01•	11•	10•
19	06	00•	11•	28
19	06	01	8•	26
19	07	02•	11•	12
19	07	01•	11•	12
19	07	00•	9•	1•
19	07	01	8•	21•
19	08	02•	25	4•
19	08	01•	11•	15
19	08	00•	8•	9•
19	09	01•	11•	29•
19	10	01•	8•	7
20	00	03•	18•	1•
20	00	02•	25•	0
20	00	01•	18	18
20	00	01	58	68•
20	01	01•	24	24
20	01	00•	11•	5•
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20	02	02•	11•	12
20	02	01•	11•	19
20	02	00•	27	34•
20	02	01	52	54•
20	03	02•	53	52
20	03	01•	9•	25•
20	03	00•	29	30•
20	03	01	7•	4•
20	04	02•	75	64
20	04	01•	88	90•
20	04	00•	8•	1
20	04	01	19	30
20	05	01•	11•	1•
20	06	01•	9•	24•
20	06	00•	46	42•
20	06	01	0•	0
20	07	01•	8•	16
20	07	00•	34	16
21	01	00•	6•	3•

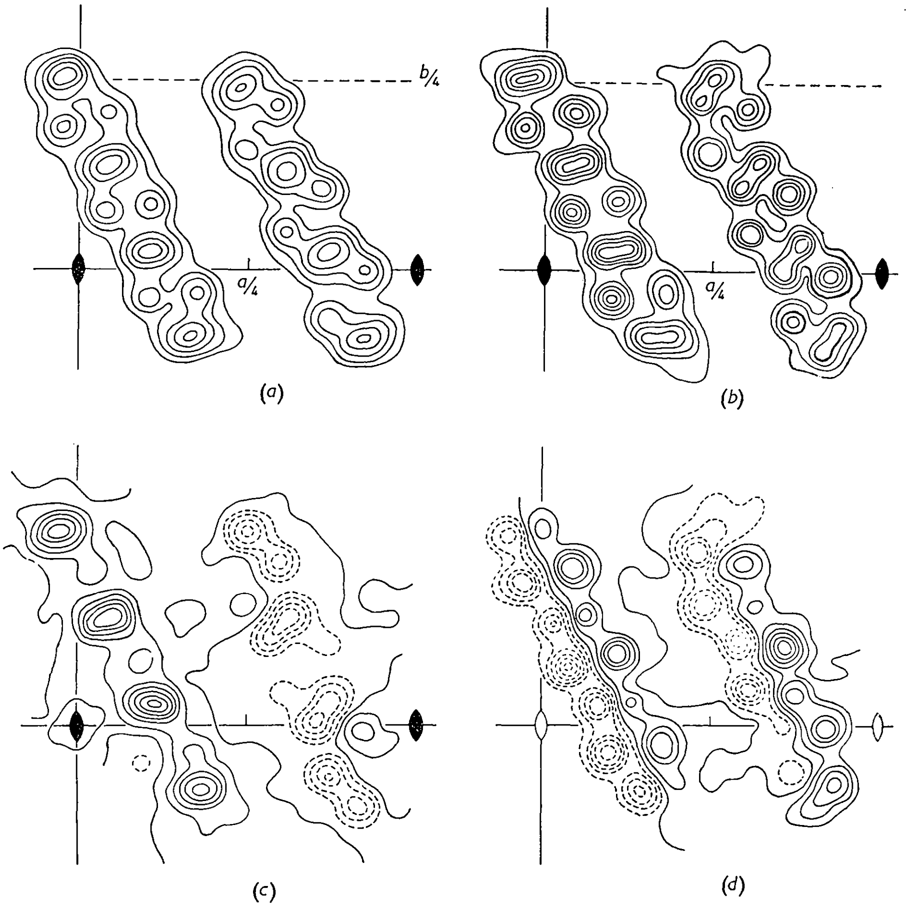

Fig. 2. Generalized projections on (001): (*a*) $\varrho(xy)$; (*b*) $\sigma_1(xy)$; (*c*) $C_1(xy)$; (*d*) $S_1(xy)$.

factory agreement was soon found. All the $F(hkl)$ were then calculated and their signs were used with the observed amplitudes in the calculation of a generalized projection (Cochran & Dyer, 1952) of the electron density on (001). This comprised calculation of $C_1(XY)$, $S_1(XY)$ and $\sigma_1(XY)$ where

$$\sigma_1(XY) = c\int_0^1 \varrho(XYZ)\,.\exp 2\pi iZ\,.dZ = C_1(XY)+iS_1(XY)\,.$$

These projections showed the atoms clearly resolved and a single stage of refinement of the z parameters (from the peak heights in the various syntheses) gave the maps shown in Fig. 2. The z-coordinates were further refined by calculation of the $hk2$ structure factors and generalized projections.

Refinement of the structure

The structure has been refined in three cycles using the full three-dimensional data. The atomic coordinates were refined by the differential synthesis method and the best isotropic temperature factors were estimated by comparison of the 'observed' and 'calculated' peak heights and curvatures. The necessary computations were carried out on FERUT, the electronic digital computor at the University of Toronto, now known as TRANSFER at the Structures Laboratory of the National Research Council, Ottawa, using programmes which are readily applicable to all space groups and which take advantage of the symmetry elements of the space group under consideration (Ahmed & Barnes, 1958).

The first set of three-dimensional structure factors was calculated treating all the atoms, excluding hydrogen, as carbon and using the McWeeny (1951) carbon scattering-factor curve with $B=3{\cdot}93$ Å for them all. The residual error index, R, at this stage was 0·25. As a result of the first differential synthesis using the observed structure amplitudes the atomic coordinates changed by an average of 0·033 Å and a maximum of 0·109 Å. The observed peak heights of the atoms at positions 5 and 19 were 7·76 and 7·45 e.Å^{-3} respectively while the heights at positions 10 and 24 were 9·70 and 9·33 e.Å^{-3}. From this stage, therefore, the latter two were taken to be the nitrogen positions and the McWeeny nitrogen f-curve was used for them.

The second set of structure factors was calculated with the atomic coordinates derived from the first observed differential synthesis and with five different isotropic temperature factors which varied from 3·60 to 4·40 Å depending on the distances of the atoms from their molecular centres. The two molecules were assumed to have the same thermal motion. The R-index was reduced by these calculations to $0{\cdot}17_5$ and the signs of 120 structure factors were changed. A second observed differential synthesis then gave an average shift of 0·005 Å (maximum 0·021 Å) in the atomic positions. A differential synthesis calculated from the calculated structure factors at this stage showed that the average error in an atomic coordinate due to termination of the series errors was 0·005 Å with a maximum 0·015 Å. Refinement of the isotropic temperature factors, from comparison of peak heights and curvatures in the 'observed' and 'calculated' syntheses, confirmed that the atoms further from the centre of each molecule have the higher thermal motion and indicated also that molecule B (atoms 15–28) as a whole is subject to more intense apparent thermal motion than is molecule A.

The atomic coordinates were corrected for finite summation errors by Booth's (1946) back-shift method and a third set of structure factors was calculated using different isotropic temperature factors for the individual atoms as shown in Table 2. The resultant R-index was 0·16.

The contributions to the structure factors of the 18 hydrogen atoms in the asymmetric unit, assumed to be situated 1·08 Å diagonally from the carbon positions with $B=4{\cdot}52$ Å^2 were next calculated, and added to the third set of calculated structure factors. Consequently R was reduced to $0{\cdot}14_6$, 14 reflexions changed sign and the signs of 52 reflexions became doubtful. Corrections were then made to the second observed differential synthesis which took account of the changed contributions of the 14 reflexions which had changed sign and eliminated the contributions of

Table 2. *Final atomic co-ordinates and isotropic temperature factors*

	x/a	y/b	z/c	B (Å^2)
Molecule A				
C_1	−0·0262	0·1895	−0·2235	4·23
C_4	0·0422	0·2083	0·2126	
C_6	0·1743	−0·0279	0·1610	
C_9	0·0993	−0·0369	−0·2748	
C_2	−0·0419	0·2488	−0·1107	4·83
C_3	−0·0069	0·2588	0·1113	
C_7	0·1864	−0·0863	0·0316	
C_8	0·1480	−0·0903	−0·1866	
C_{11}	0·0257	0·1347	−0·1244	3·52
C_{12}	0·0597	0·1443	0·0990	
C_{13}	0·1239	0·0295	0·0727	
C_{14}	0·0867	0·0248	−0·1488	
C_5	0·1091	0·0896	0·1961	3·66
N_{10}	0·0386	0·0769	−0·2447	3·70
Molecule B				
C_{15}	0·2948	0·2139	0·3765	4·52
C_{18}	0·2421	0·1594	0·7718	
C_{20}	0·3745	−0·0686	0·5982	
C_{23}	0·4217	−0·0049	0·2120	
C_{16}	0·2490	0·2542	0·5071	4·99
C_{17}	0·2232	0·2265	0·7082	
C_{21}	0·4156	−0·1065	0·4548	
C_{22}	0·4404	−0·0742	0·2569	
C_{25}	0·3155	0·1421	0·4360	3·76
C_{26}	0·2891	0·1152	0·6393	
C_{27}	0·3528	0·0044	0·5561	
C_{28}	0·3767	0·0362	0·3571	
C_{19}	0·3082	0·0454	0·6956	3·97
N_{24}	0·3589	0·1038	0·3004	3·97

Table 3. *Final observed and calculated peak heights and curvatures*

	Heights (e.Å^{-3})		Curvatures (e.Å^{-5})					
	ϱ_o	ϱ_c	$-A^o_{hh}$	$-A^c_{hh}$	$-A^o_{kk}$	$-A^c_{kk}$	$-A^o_{ll}$	$-A^c_{ll}$
Molecule *A*								
C_1	7·21	7·38	61·2	60·3	54·0	55·9	53·7	58·6
C_4	6·96	7·17	58·6	57·2	48·9	54·1	52·7	56·2
C_6	7·15	7·31	63·8	59·9	50·6	55·3	54·6	58·3
C_9	7·54	7·51	65·8	62·3	59·3	59·6	58·5	60·6
C_2	6·49	6·58	52·1	48·3	50·7	49·7	40·9	47·1
C_3	6·26	6·63	48·9	50·0	46·9	49·7	40·5	48·2
C_7	6·40	6·64	54·2	52·3	48·5	50·7	36·6	45·1
C_8	6·70	6·84	56·6	54·6	52·8	51·4	44·2	51·9
C_{11}	8·46	8·32	77·4	72·6	67·5	67·7	68·9	69·6
C_{12}	8·20	8·21	75·9	71·5	63·5	68·1	65·2	64·8
C_{13}	8·41	8·37	80·4	75·0	64·7	67·9	67·0	69·2
C_{14}	8·42	8·38	79·7	74·3	67·0	68·7	68·1	69·9
C_5	7·90	7·93	71·0	67·2	53·5	59·6	68·8	68·0
N_{10}	9·92	9·89	84·7	81·4	75·9	78·3	83·6	81·2
Molecule *B*								
C_{15}	7·10	7·23	57·6	56·5	59·0	57·5	54·9	58·4
C_{18}	6·91	6·95	56·4	54·0	48·3	50·2	55·5	56·2
C_{20}	6·61	7·06	46·8	52·5	54·3	54·8	49·0	56·1
C_{23}	6·95	7·01	58·1	56·2	53·8	52·9	51·0	53·5
C_{16}	6·39	6·48	50·9	48·8	49·2	46·6	42·0	46·1
C_{17}	6·32	6·57	50·6	49·6	45·7	49·2	43·1	48·4
C_{21}	6·07	6·42	45·5	48·6	49·0	48·5	35·0	43·3
C_{22}	6·23	6·46	48·1	49·1	48·2	47·4	39·4	45·7
C_{25}	7·99	8·03	72·7	69·2	62·9	62·3	65·7	67·3
C_{26}	7·99	7·99	69·9	67·2	62·8	63·5	64·1	66·3
C_{27}	7·74	7·89	66·5	65·9	60·0	61·7	60·9	63·7
C_{28}	8·01	7·99	71·5	68·1	68·1	66·2	60·5	61·7
C_{19}	7·65	7·78	63·4	63·9	61·5	63·3	63·8	64·3
N_{24}	9·47	9·45	78·7	76·5	75·0	75·0	74·1	74·1

the 52 reflexions whose signs were now doubtfully determined. The mean change in the observed coordinates which resulted was 0·001 Å with maximum 0·004 Å. A second 'calculated' differential synthesis (including the *H*-contributions and eliminating the 52 reflexions of doubtful sign) was then computed to give final corrections for finite summation errors. These differed by an average of $0{\cdot}001_6$ Å from those indicated by the first 'calculated' differential synthesis. No attempt has been made to locate the hydrogen atoms in the structure more accurately.

The final atomic coordinates for the carbon and nitrogen atoms, after correction for finite summation errors, are given in Table 2 together with the individual temperature factors. The final observed and calculated peak heights and curvatures are given in Table 3. In these two tables those atoms which have been assigned the same isotropic temperature factors have been grouped together.

Molecular thermal motion

Comparison of the observed and calculated peak heights and curvatures shown in Table 3 suggests that the chosen isotropic temperature factors are not far from their best values and further that the chosen absolute scale of the measurements is very nearly correct. Detailed consideration of the ratios of the principal curvatures along x, y and z separately shows, however, that more serious corrections to the temperature factors are required in order to allow for the anisotropic thermal motion of the individual atoms. These corrections have not been made in the present refinement but the nature of the thermal motion is nevertheless apparent in the results which have been obtained.

Higgs (1955) has shown that the mean-square amplitude of vibration in a molecular crystal is very largely determined by the rigid-body vibrations of the molecule as a whole and that the effects of these rigid-body vibrations can be resolved into components which arise from translation and restricted rotation (libration) of the molecule. Thus it appears that

$$\overline{u_i^2} \simeq P + QR_i^2\,,$$

where R_i is the distance of the atom from the molecular centre. Values of $\overline{u_i^2} = 3B_i/8\pi^2$ for the different atomic groups in the two molecules of acridine II are plotted in Fig. 3 against R_i^2/L^2 on the assumption that the molecules are formed from regular hexagons of side L. Corresponding results for acridine III and anthracene (cf. Part II) are plotted for comparison. It is clear that the apparent molecular thermal motions in the three structures are of the same type but that the translational components of the mean-square amplitudes of vibration appear to be higher in the acridines than in anthracene. This result is consistent

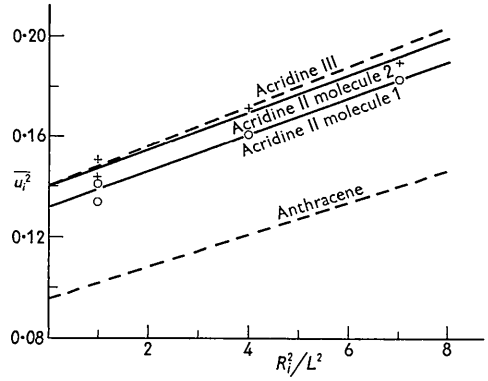

Fig. 3. Graphs of $\overline{u_i^2}$ against R_i^2/L for atomic groups in acridine II, acridine III and anthracene.

with the lower melting-points of the acridines but it may be due in part at least to different systematic errors in the intensity data from which the structures have been determined and to a greater degree of static disorder in the acridines. In acridine II it appears that molecule B is subject to greater translational thermal motion (or disorder) than molecule A but that the librational motions of the two are very closely the same.

Description of the structure

Arrangement of molecules

Fig. 4(a) and (b) show the arrangement of the molecules in the unit cell. As in acridine III the molecules are arranged in anti-parallel pairs about the centres of symmetry but in this structure with its two molecules per asymmetric unit the arrangement is more complex. Molecule A and its symmetry-related fellows are arranged in pairs about the centres of symmetry at $0, 0, 0$ and $\frac{1}{2}, \frac{1}{2}, 0$ while the molecules B are arranged about the centres at $\frac{1}{2}, 0, \frac{1}{2}$ and $0, \frac{1}{2}, \frac{1}{2}$. The structure thus may be described as being built up on (001) from layers of molecules in alternately the A and B orientations with the molecules in each layer fitting into the spaces in the layer below in a form of close-packing.

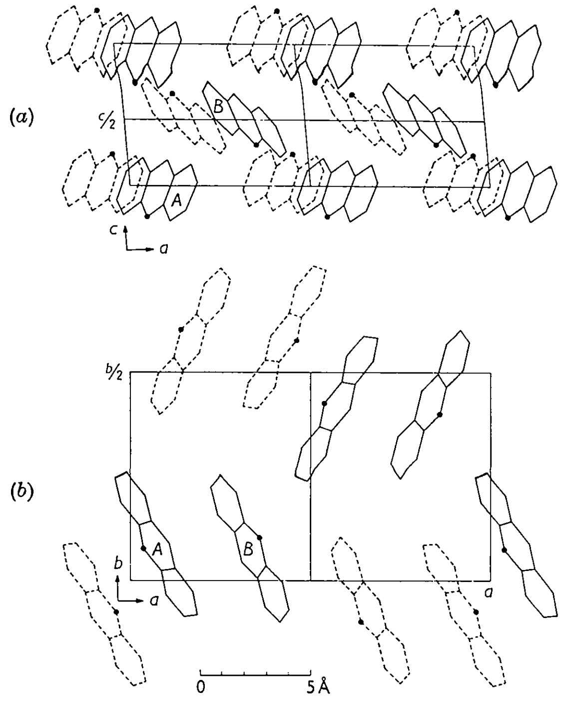

Fig. 4. Projections of the structure on (010) and (001). The two independent molecules in the asymmetric unit are labelled A and B. Nitrogen atoms are shown as full circles.

The packing units, each composed of two molecules, are not all equivalent. The anti-parallel molecules in orientation A are 3·49 Å apart with minimum distance between atoms in adjacent molecules, C_1–C_7' and C_{12}–C_9', equal to 3·53 Å. (The hydrogen atoms have not been considered.) In normal projection one on the other the molecules in these pairs do not overlap exactly but are staggered in a very similar way to that found in acridine III and shown in Fig. 6(a) of Part II. The molecules in orientation B, on the other hand, are further apart than those in orientation A, interplanar spacing 3·61 Å, and in normal projection one on the other only the terminal rings overlap. The shortest distance between atoms in adjacent molecules in these pairs is 3·69 Å between C_{20} and C_{25}'.

These differences in the packing of the two molecules in the asymmetric unit are consistent with the observed differences in their apparent thermal motions. The fact that molecules A which are the more intimately related in pairs appear to be subject to less intense thermal motion than molecules B may indicate that molecules A have the greater tendency to vibrate as two-fold molecular units. It must be remembered, however, that the observations could be explained also by a greater degree of disorder in the packing of molecules B.

The close packing of the two-fold molecular groups depends principally on intermolecular contacts of the kind usually found between benzene rings: all the intermolecular C–C distances concerned are larger than 3·6 Å. The N–C_5 distance between molecules related by the c-axis unit-cell translation is 3·69 Å for molecules A and 3·85 Å for molecules B.

A preliminary analysis of this packing in relation to that found in anthracene has been given by Miasnikova & Kitaigorodskii (1958) in discussion of their investigation of mixed crystals of the acridine–anthracene system. They have shown that the addition of only 7% anthracene prevents the growth of mixed crystals of the acridine II type and, making use of the results presented here which were communicated to them privately, they have shown that this effect arises from the fact that the acridine molecules in this structure pack together more closely than anthracene molecules are able to do. A more detailed comparison of the structures of acridine II, acridine III and anthracene, in relation to the polymorphism of acridine, will be given elsewhere.

Molecular dimensions and accuracy

Bond lengths and angles within the individual molecules, calculated from the final atomic coordinates, are shown in Fig. 5(*a*), (*b*), (*c*) and (*d*).

The factors affecting the accuracy of structure determinations such as this in which the refinement is incomplete were discussed in detail in Part II. They must be taken into account in assessing the accuracy of the present results. Here again the standard deviation of the atomic coordinates have been calculated using the residuals $\Delta F = F_o - F_c$ as estimates of $\sigma(F)$. Their root-mean-square values vary between 0·0037 Å for N_{10} and 0·0072 Å for C_{21}. The standard deviations of the bond lengths and angles, estimated by the use of Ahmed & Cruickshank's (1952) formulae, vary between 0·006 and 0·011 Å for lengths and 20′ and 32′ for angles.

The differences $\Delta(l)$ and $\Delta(\theta)$ between chemically equivalent bonds and angles within the two molecules are shown in Fig. 5(*e*) and (*f*). Estimation of the Student's distribution, $t_0 = (l_1 - l_2)/(S_1^2 - S_2^2)^{\frac{1}{2}}$ (Cruickshank & Robertson, 1953) for these differences indicates that:

(i) for both molecules the differences in the bond lengths are not significant, even for the largest difference 0·021 Å between the bonds C_3–C_4 and C_6–C_7 for which $t_0 = 1{\cdot}81$ and $P > 0{\cdot}05$;

(ii) for molecule *A* the differences in the angles are not significant except for the pair of angles C_1–C_{11}–C_{12} and C_9–C_{14}–C_{13} for which the difference of 62′ is possibly significant ($t_0 = 2{\cdot}09$; $0{\cdot}05 > P > 0{\cdot}01$);

(iii) for molecule *B* the differences in the angles are not significant for 6 pairs, possibly significant for two pairs with $\Delta(\theta) = 75'$ and 78′, and significant for the pair C_{18}–C_{26}–C_{25} and C_{20}–C_{27}–C_{28} for which $\Delta(\theta) = 101'$, $t_0 = 2{\cdot}97$, $0{\cdot}01 > P > 0{\cdot}001$.

Thus there are indications that the chemically equivalent halves of the two molecules may be slightly different in the crystal structure and it is worth remarking that the most significant differences are between bond-angles which may be more readily affected by molecular interactions than bond lengths. The differences are not well established, however, and in view of the uncertainty with which the standard deviations are estimated and the presence of systematic effects not taken into account in the F_c they may be a better indication of the errors remaining in the results than of real differences within the molecules. The weighted means of chemically equivalent bond lengths

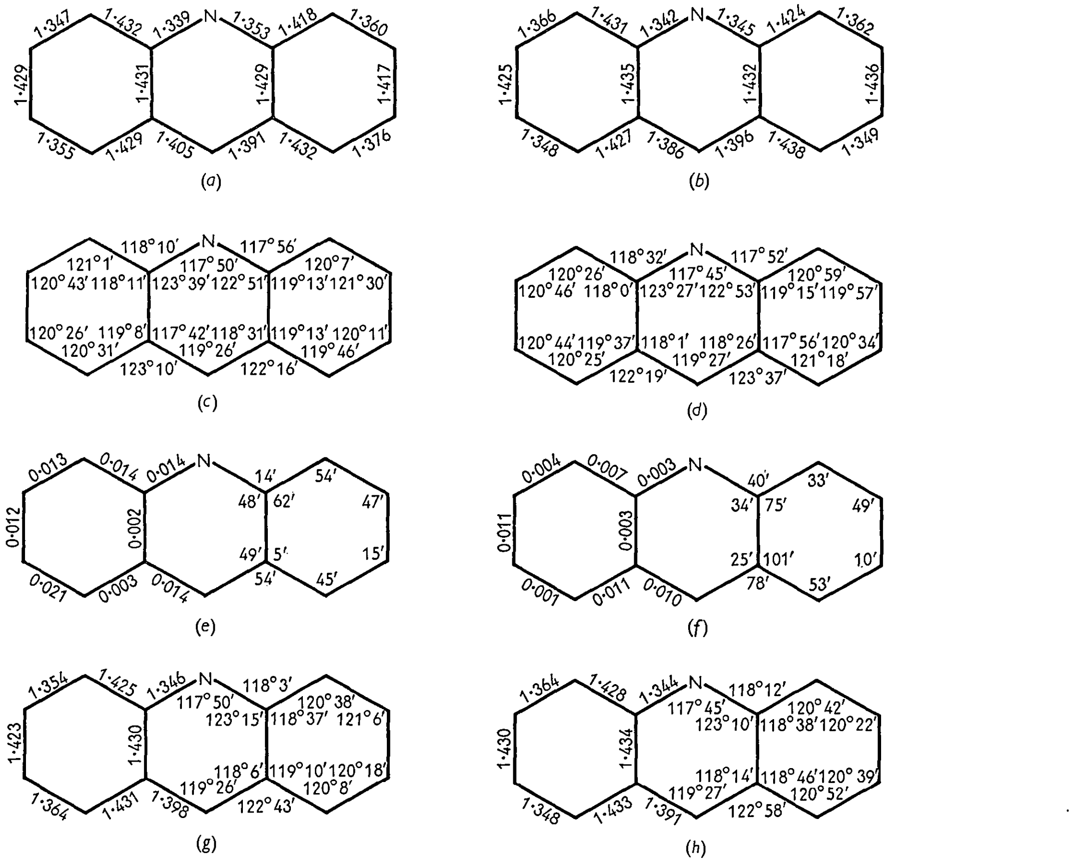

Fig. 5. Bond lengths (Å) and angles in the two molecules *A* and *B*. (*a*, *b*) observed bond lengths; (*c*, *d*) observed bond angles; (*e*, *f*) differences between chemically equivalent bond lengths and angles; (*g*, *h*) weighted mean bond lengths and angles.

Table 4. *Mean bond lengths in acridine II and III, anthracene and phenazine*

						With correction for librations	
Bond	Acridine II	$\sigma(l)$	Acridine III	Anthracene	Phenazine	Acridine II	Anthracene
C_1–C_2	1·358	0·004	1·372	1·364	1·375	1·360	1·366
C_3–C_4	1·357	0·004	1·370	1·364	1·375	1·359	1·366
C_1–C_{11}	1·427	0·003	1·431	1·431	1·408	1·429	1·433
C_4–C_{12}	1·432	0·004	1·425	1·431	1·408	1·434	1·433
C_2–C_3	1·426	0·005	1·417	1·417	1·412	1·428	1·419
C_{11}–C_{12}	1·432	0·003	1·432	1·434	1·433	1·434	1·436
C_5–C_{12}	1·395	0·004	1·389	1·396	—	1·398	1·399
C_{11}–N_{10}	1·345	0·003	1·344	—	1·345	1·348	—

and angles within the two molecules separately have therefore been calculated for comparison of the two molecules on the assumption that the observed differences are not real. These bond lengths and angles are shown in Fig. 5(*g*) and (*h*).

The differences in bond lengths between the two molecules are all not significant, including the difference of 0·016 Å between C_3–C_4 and C_{17}–C_{18} for which $t_0 = 1{\cdot}41$, $P > 0{\cdot}05$. It seems reasonable to assume, therefore, at least for the bond lengths, that there are no real differences between the two molecules and that the four observed values for each bond can be averaged for comparison with similar measurements in acridine III and anthracene. These values are shown in Table 4 together with their standard deviations estimated on the assumption that each mean value is derived from four independent measurements of the same quantity. Corresponding results for acridine III, anthracene and phenazine (Herbstein & Schmidt, 1955) are also shown.

These bond lengths are subject to systematic errors due to the librations of the molecules (Cox, Cruickshank & Smith, 1955). Corrections for these errors have been applied in the latest refinement of the structure of anthracene (Cruickshank, 1956) and in view of the fact that the librational motion of the molecules in the acridines has been shown to be closely similar to that in anthracene it is reasonable to suppose that the corrections required here are the same. The bond angles are not much affected by these errors but intramolecular bond lengths are too short by 0·002 or 0·003 Å. The corrected bond lengths are shown in the last columns of Table 4.

Molecular planarity

The molecules are not strictly planar. The best planes through the two molecules *A* and *B* are given by

$$0{\cdot}8359x' + 0{\cdot}4340y - 0{\cdot}3359z' = 1{\cdot}7465 \qquad (1)$$

and

$$0{\cdot}8144x' + 0{\cdot}3056y + 0{\cdot}4933z' = 6{\cdot}0994 \qquad (2)$$

respectively, where $x' = x + z \cos \beta$, $z' = z \sin \beta$ are the atomic coordinates measured in Ångström units in the orthogonal coordinate system *a*, *b*, *c**. The perpendicular distances of the atoms of each molecule from the mean plane of that molecule are shown in Fig. 6(*a*) and (*b*). Application of the χ^2 test shows that for molecule *A* as a whole $\chi^2 = 53$, $\nu = 11$, $P < 0{\cdot}0001$ and for molecule *B*, $\chi^2 = 272$, $\nu = 11$, $P < 0{\cdot}0001$. The deviations of both molecules from planarity thus are 'highly significant'.

In the search for systematic features in these deviations from planarity it is illuminating to consider the deviations of the atoms from the best planes through the central pyridine rings alone. These planes for the molecules *A* and *B* are

$$0{\cdot}8392x' + 0{\cdot}4338y - 0{\cdot}3280z' = 1{\cdot}7526 \qquad (3)$$

and

$$0{\cdot}8153x' + 0{\cdot}3057y + 0{\cdot}4916z' = 6{\cdot}1211 \qquad (4)$$

respectively, and the perpendicular distances of the atoms from them are shown in Figs. 6(*c*) and (*d*). For the central ring of molecule *A*, $\chi^2 = 4{\cdot}6$, $\nu = 3$, $P > 0{\cdot}05$ and for the central ring of molecule *B*, $\chi^2 = 6{\cdot}7$, $\nu = 3$, $P > 0{\cdot}05$. The central rings of the two molecules thus do not deviate significantly from planarity. Inspection of the deviations shown in Figs. 6(*c*) and (*d*) suggests, however, that the distortion of molecule *A* may be due to a tendency of the central ring to take up a 'chair' configuration to allow for inclusion of the nitrogen atom without upsetting the planar and symmetrical configuration of bonds at the carbon atoms. This is suggested by the fact that the bonds C_{11}–C_1 and C_{14}–C_9 appear to be directed down below the plane of the diagram (and towards the centre of symmetry at 0, 0, 0 and the symmetry related molecule) while the bonds C_{12}–C_4 and C_{13}–C_6 appear to be directed above the plane of the diagram. The best planes of the two outer rings are roughly parallel to one another but are rotated about the length of the molecule with respect to the best plane of the central ring. In molecule *B* on the other hand the central ring appears to have taken up a 'boat' configuration so that the bonds C_{25}–C_{15}, C_{26}–C_{18}, C_{27}–C_{20} and C_{28}–C_{23} are all directed down below the plane of the diagram and away from the centre of symmetry at $\frac{1}{2}$, 0, $\frac{1}{2}$.

Even when uncertainties in estimation of the standard deviations are taken into account it seems certain that molecule *B* is not planar. The distortion is described fairly well by bending across the line N–C_{19} through about 2° and it is particularly interest-

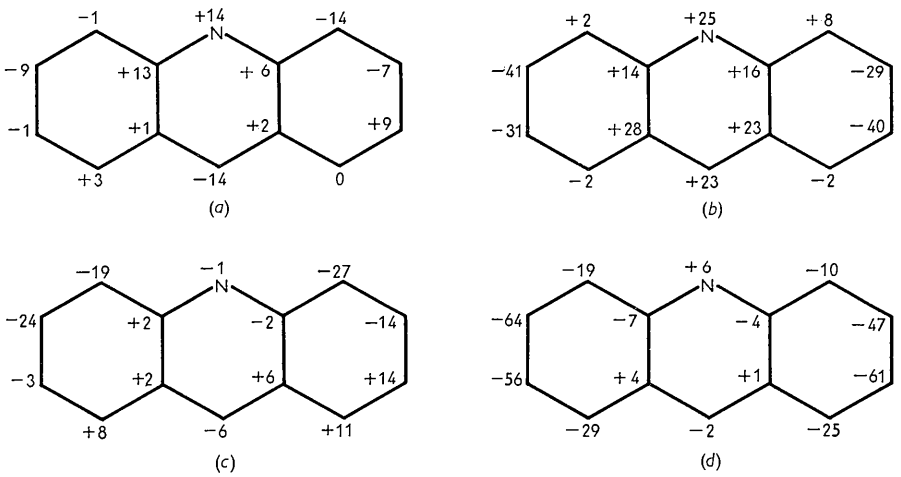

Fig. 6. Perpendicular distances of atoms from possible molecular planes: (*a*) molecule *A* and plane 1; (*b*) molecule *B* and plane 2; (*c*) molecule *A* and plane 3; (*d*) molecule *B* and plane 4. All distances are in Å × 10^3 and positive signs indicate increased distance from the origin.

ing that this result should be so similar to that obtained in acridine III. The deviations from planarity of molecule *A* are not so certainly significant, but interpreted in the way outlined above they too appear to be systematic and meaningful.

Discussion

The results of this investigation are in good agreement with the results obtained earlier by a study of acridine III. In particular the two independent structure determinations have given consistent estimations of the molecular dimensions and also consistent indications that molecules of acridine in the crystalline state are distorted from the ideally planar form. The implications of these results have been discussed already in Part II and are not considered further here.

It is evident that closer investigation of the effects of molecular interactions in acridine II depends first on the collection of more accurate intensity data and then on complete refinement of the structure to fit those data. The results presented here show that such an investigation may give interesting results.

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