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The Crystal Structure of 2,2′-*p*-Phenylenebis-(5-phenyloxazole) – ‘POPOP’*

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The crystal structure of the organic scintillator POPOP, 2,2-*p*-phenylenebis-(5-phenyloxazole), has been determined and refined by three-dimensional least-squares methods. The final *R* index for 1370 observable reflections is 0·058, and the standard deviations in the positions of the C, N, and O atoms are about 0·003 Å.

The crystals are monoclinic, space group $P2_1/c$, with $a = 9{\cdot}230$, $b = 5{\cdot}285$, $c = 19{\cdot}322$ Å and $\beta = 92{\cdot}09°$; there are two centrosymmetric molecules per unit cell. The three benzene and two oxazole rings are each planar, but they are twisted slightly with respect to one another to form a propeller-shaped molecule. The bond distances indicate appreciable conjugation between the rings and localization of charges within the oxazole rings. The intermolecular contacts appear to be normal.

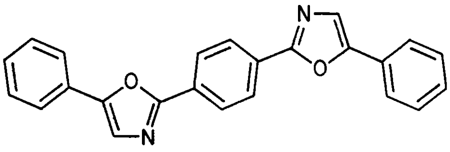
Introduction

POPOP, $C_{24}H_{16}N_2O_2$(I), with the structural names:

(*a*) 2,2′-*p*-phenylenebis-(5-phenyloxazole)

(*b*) 1,4-bis-2-(5-phenyloxazolyl)benzene

is a scintillator, capable of emitting a brief pulse of fluorescent light upon interaction with a high-energy particle or quantum (*e.g.*, Bell & Hayes, 1958).



(I)

An X-ray diffraction study has been completed of the molecular structure of this strong scintillator.

Experimental

Scintillation-grade crystals of POPOP were obtained from Packard Instrument Company. They occur as long, pale yellow needles, with the needle axis parallel to the crystallographic *b* axis. The crystals are soft and have no pronounced cleavage, and as a result all attempts to obtain a specimen suitable for mounting about any axis other than *b* were unsuccessful. The crystal used for collecting intensity data was about 0·07 × 0·07 mm in cross section and about 3 mm in length.

The unit-cell dimensions and other crystal data are given in Table 1. Values for *a*, *c*, and *β* were determined from a least-squares treatment based on 34 high-angle ($\sin\theta > 0{\cdot}81$) *h*0*l* reflections measured on a Straumanis-type rotation photograph about **b**; the value of *b* was obtained from a weighted average of 270 measurements made on precession photographs, taken with Mo and Fe radiation, of the *hk*2*h* zone and calibrated from the previous values of *a*, *c*, and *β*.

Table 1. *Unit cell parameters of POPOP and their estimated standard deviations*

($\lambda_{\text{Cu}\,K\alpha} = 1{\cdot}5418$ Å)

$a = 9{\cdot}2300(3)$ Å	$V = 941{\cdot}9(3)$ Å^3
$b = 5{\cdot}2850(8)$	$Z = 2$
$c = 19{\cdot}3220(7)$	$\varrho_c = 1{\cdot}285(1)$ g.cm^{-3}
$\beta = 92{\cdot}088(2)°$	$\varrho_o = 1{\cdot}306(10)$ g.cm^{-3}

In the least-squares treatment of the *h*0*l* data, weights on an absolute scale were derived from the distribution of discrepancies between repeated measurements; the resulting goodness of fit was 0·8, suggesting that the

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observational errors were somewhat overestimated. The standard deviations of a, c, and β were calculated directly from the diagonal terms of the inverse matrix of the normal equations; the standard deviation of b includes the uncertainties in a, c, and β as well as in the film measurements. The uncertainties listed in Table 1 have been taken as twice the calculated standard deviations to acknowledge possible systematic errors.

The space group $P2_1/c$ was indicated by the absence of $h0l$ reflections with l odd (on Weissenberg films) and $0k0$ reflections with k odd (on precession films). The precession photograph needed to confirm the latter observation with reasonable certainty required 280 hours exposure.

Intensities were estimated visually from multiple-film, equi-inclination Weissenberg photographs prepared with Cu $K\alpha$ radiation for layers 0 through 5 around **b**. Within the effective copper sphere ($\sin\theta \leq 0{\cdot}98$) approximately 2130 independent reflections are permitted by the space group; of these, 1984 were recorded, 1370 having measurable intensity. They were corrected, as usual, for Lorentz and polarization factors; no absorption corrections were applied. Layer lines 0–4 were scaled roughly together on the basis of exposure times; the fifth layer line was recorded on a different camera and was scaled empirically during the course of the refinement.

Determination of structure

The initial attempt of structure determination was a stochastic one based on the (010) projection. With two molecules per unit cell and space group $P2_1/c$, each molecule must have a symmetry center. The molecule was assumed to be planar, the rings regular, and the bond distances normal. The shortness of the b axis required that the molecules be resolved in the (010) projection with the molecular plane making an angle of about 50° with (010), and defined circles in the (010) projection, about 2·5 Å in diameter with centers on the screw axes and symmetry centers, within which no heavy atom can lie. An additional clue was the great strength of the 102 reflection, and accordingly the orientation was initially chosen to be with the long dimension of the molecule in the (102) plane. Successive structure-factor and electron-density calculations based on a number of different models eventually led to a structure with encouraging agreement between observed and calculated structure-factor amplitudes.

Refinement of the parameters

The structure was refined by least-squares methods on a Burroughs 220 computer with the use of a structure-factor least-squares program which accepts three positional and six vibrational parameters for each atom. The normal-equation matrix is block-diagonal; for each atom the cross terms between the temperature parameters and between the x and z coordinates are collected. The function minimized is $\Sigma w(\Delta F^2)^2$. Atomic form factors were averages of the values of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) and Hoerni & Ibers (1954) for oxygen, nitrogen, and carbon, and McWeeny's (1951) values for hydrogen.

The first $h0l$ structure-factor calculation, including only the heavy atoms with fixed isotropic temperature factors ($B=2{\cdot}9$), led to an R index of 0·56. When subsequent refinement using weights inversely proportional to the square of the scattering factor of carbon was unsatisfactory, the refinement was limited to low order reflections ($\sin^2\theta/\lambda^2 \leq 0{\cdot}15$). The R index then fell quickly from 0·40 to 0·20, when full $h0l$ data were again included. The isotropic temperature factors of the heavy atoms were included as parameters and the contributions of the eight hydrogen atoms (at assumed positions and with $B=2{\cdot}5$) were included in the structure-factor calculations. The $h0l$ refinement was stopped at $R=0{\cdot}09$.

Approximate y parameters were calculated through knowledge of the x and z coordinates and assumption of a planar molecule, and were partially refined on the basis of the $h1l$ data. Three-dimensional least-squares refinement based on the complete set of data ($h0l$–$h5l$) was then initiated. Anisotropic temperature parameters for the heavy atoms and the coordinates of the hydrogen atoms were refined, and the layer scale factors were adjusted every few cycles. Apparent convergence was reached at $R=0{\cdot}10$. This value seemed higher than warranted by the quality of the data, and led us to suspect that the atoms in the oxazole ring should be interchanged. However, after a number of refinement cycles and a difference map based on such a model, this thesis was rejected. The trouble was eventually found to be a programming error which caused the first-layer observations to be weighted ten times too high. When this error was corrected, convergence proceeded smoothly.

The weighting scheme used in the last few cycles was taken as the function best representing our estimates of the observational uncertainties; it was

$$\sqrt{w} = 1/\sigma(F_0^2) = 1/(1+0{\cdot}1F^2)\,.$$

Unobserved reflections were included only for the 11 cases where the value of F_c exceeded the threshold value of F_o. The final R index for 1381 observed reflections of non-zero weight was 0·058, and the goodness of fit – here defined as $\{\Sigma w(\Delta F^2)^2/(n-p)\}^{\frac{1}{2}}$ – was 1·1. When refinement was halted the maximum indicated shift in a heavy-atom coordinate was 15% of its estimated standard deviation, in a hydrogen atom coordinate 24% of its e.s.d., and in a heavy-atom temperature parameter 26% of its e.s.d. From the initial structure proposed, with $R=0{\cdot}56$, to the final one, the average shift in the position of a heavy atom was 0·32 Å.

The final parameters and their standard deviations are listed in Table 2. The observed and final calculated structure factors are listed in Table 3. Final electron density maps in the planes of the center phenyl, the oxazole, and the end phenyl rings are shown in Fig. 1; the corresponding difference Fourier syntheses are shown in Fig. 2. For the difference maps the coefficients were taken as the differences between the observed structure factors, with the signs of the final F_c, and the structure factors calculated for only the heavy atoms.

The geometry of the molecule

The bond distances and angles as calculated from the parameters of Table 3 are shown in Fig. 3. Their standard deviations, as calculated from the uncertainties of the final atomic parameters, are 0·003–0·004 Å and 0·3–0·6° for distances and angles involving heavy atoms only and 0·3 Å and 3–4° for those involving hydrogen atoms. Additional uncertainties are undoubtedly introduced by the effects of thermal libration and, to some extent, of systematic errors in the data.

In Fig. 4 are shown the canonical structures we believe to have major contributions to the structure and our estimates of their relative contributions. The predicted bond distances of the resonance hybrid shown in Fig. 4 were obtained from curves drawn through points representing observed bond distances for bond numbers 1·0, 1·5, and 2·0. The values chosen for C–O and C–N distances are those as given in Table 6 of Marsh, Bierstedt & Eichhorn (1962); the C–C distances are from Pauling (1960). This analysis is felt to be at best descriptive, pointing out significant departure from the normal Kekulé-type structures. The observed bond distances in the terminal phenyl ring are significantly

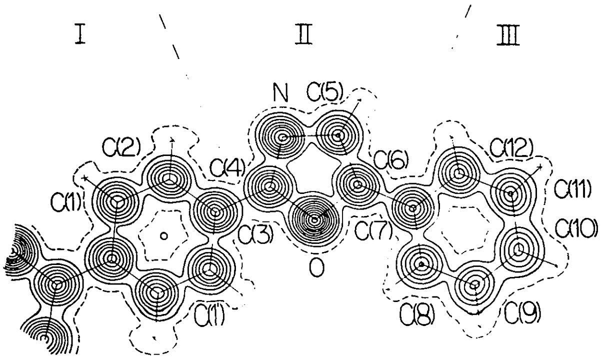

Fig. 1. The electron density in the planes of the three rings. The straight dashed lines set off the regions which are in different planes (see Table 4). Contours are at intervals of 1·0 e.Å^{-3} beginning with the 1·0 e.Å^{-3} level, which is dashed.

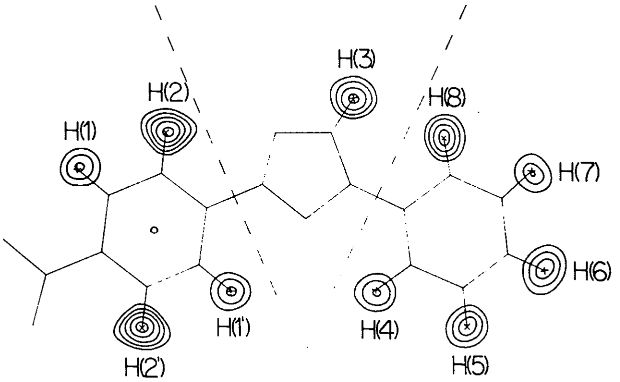

Fig. 2. The difference Fourier map corresponding to Fig. 1. Contours are at intervals of 0·1 e.Å^{-3} beginning with the 0·2 e.Å^{-3} level.

Table 2. *The final parameters and their estimated standard deviations*

All values except the hydrogen temperature factors are multiplied by 10^4. The anisotropic temperature factors are of the form:

$$T_i = \exp\{-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)\}.$$

The values of the temperature factors of the hydrogen atoms were assumed.

Atom	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
C(1)	1126 (2)	−1681 (5)	146 (1)	133 (3)	377 (9)	24 (1)	37 (8)	−3 (2)	−2 (4)
C(2)	791 (2)	145 (5)	623 (1)	127 (3)	419 (10)	22 (1)	7 (8)	−9 (2)	−5 (4)
C(3)	−335 (2)	1859 (4)	482 (1)	117 (3)	339 (9)	22 (1)	−31 (7)	5 (2)	7 (3)
C(4)	−669 (2)	3769 (4)	998 (1)	116 (3)	353 (9)	22 (1)	1 (7)	2 (2)	9 (3)
C(5)	−771 (3)	6166 (5)	1873 (1)	160 (3)	373 (9)	22 (1)	8 (9)	−4 (2)	−21 (4)
C(6)	−1881 (2)	6851 (4)	1441 (1)	136 (3)	331 (9)	21 (1)	−36 (8)	9 (2)	−18 (3)
C(7)	−3026 (2)	8734 (5)	1464 (1)	124 (3)	356 (9)	26 (1)	−30 (8)	12 (2)	8 (4)
C(8)	−4134 (3)	8827 (5)	957 (1)	155 (4)	500 (12)	31 (1)	81 (10)	−4 (3)	−15 (5)
C(9)	−5200 (3)	10657 (6)	995 (2)	162 (4)	610 (15)	38 (1)	104 (12)	−6 (3)	28 (6)
C(10)	−5187 (3)	12383 (6)	1531 (2)	173 (4)	479 (13)	45 (1)	131 (11)	43 (3)	26 (6)
C(11)	−4099 (3)	12291 (5)	2035 (1)	169 (4)	416 (11)	39 (1)	0 (10)	38 (3)	−26 (5)
C(12)	−3016 (3)	10489 (5)	2004 (1)	139 (3)	392 (10)	31 (1)	−43 (9)	16 (2)	−25 (4)
O	−1830 (2)	5305 (3)	868 (1)	122 (2)	356 (6)	21 (0)	0 (5)	−5 (1)	−11 (2)
N	−1 (2)	4205 (4)	1586 (1)	144 (3)	388 (8)	23 (0)	34 (7)	−9 (2)	−14 (3)

Atom	x	y	z	B
H(1)	1985 (29)	−2793 (53)	252 (14)	3·50 Å^2
H(2)	1386 (29)	282 (53)	1073 (14)	3·50
H(3)	−524 (29)	6850 (55)	2345 (14)	3·50
H(4)	−4142 (28)	7490 (55)	572 (14)	3·50
H(5)	−5947 (30)	10704 (58)	652 (15)	4·25
H(6)	−5985 (31)	13575 (61)	1574 (15)	4·25
H(7)	−3990 (31)	13422 (62)	2438 (15)	4·25
H(8)	−2265 (29)	10323 (56)	2332 (15)	3·50

Table 3. *The observed and calculated structure factors*

Within each group are values for l, $10F_o$, $10F_c$, reading from left to right. Reflections indicated by an asterisk were given zero weight in the least-squares calculations and were omitted from the R index.

00l		
0	---	3808
2	78	73
4	701*	-810
6	<17	7
8	238	-255
10	92	94
12	152	160
14	72	80
16	154	-148
18	66	-67
20	176	174
22	<24	23
24	54	-56
10l		
0	410	451
2	747*	1358
4	153	-165
6	45	38
8	398	-405
10	256	-255
12	67	70
14	<26	5
16	146	150
18	76	-81
20	106	-103
22	41	41
24	19	-16
20l		
0	604*	699
2	234	271
4	114	-115
6	259	-270
8	198	-193
10	186	-180
12	55	59
14	84	-91
16	81	-85
18	84	85
20	52	-52
22	37	-35
24	<15	-2
30l		
0	58	-59
2	251	-257
4	92	80
6	299	293
8	394	-382
10	193	-191
12	58	56
14	62	-67
16	67	-72
18	<32	10
20	<29	-17
22	42	-39
40l		
0	73	73
2	100	-97
4	476	-481
6	145	139
8	112	112
10	131	-124
12	96	90
14	83	-90
16	155	-149
18	<31	-0
20	30	28
22	25	22
50l		
0	<21	-1
2	<21	-13
4	105	-100
6	<23	-8
8	29	-20
10	<29	-18
12	143	148
14	<33	-19
16	141	-140
18	<29	-20
20	<20	-4
22	43	41
60l		
0	<24	21
2	127	130
4	<25	5
6	73	73
8	41	39
10	98	-110
12	92	96
14	100	107
16	102	-100
18	32	-38
20	<18	-3
70l		
0	<26	-15
2	45	41
4	104	109
6	129	130
8	77	79
10	28	-22
12	46	-60
14	45	43
16	<23	7
18	<18	-9
80l		
0	142	-142
2	133	131
4	134	138
6	112	123
8	87	45
10	38	-33
12	<29	-6
14	<26	-12
90l		
0	62	-62
2	134	-131
4	111	116
6	130	130
8	89	80
10	27	-20
12	45	-42
14	44	-35
10,0,l		
0	106	103
2	29	-21
4	<24	-13
6	67	60
8	21	14
10	<21	-2
12	17	-13
11,0,l		
0	<22	10
2	<22	2
4	29	-23
6	26	22
8	16	15
$\bar{1}0l$		
2	397	-435
4	472	505
6	175	180
8	76	81
10	81	-79
12	83	78
14	61	-65
16	49	-52
18	173	171
20	107	109
22	<22	-15
24	32	-29
$\bar{2}0l$		
2	65	64
4	196	-208
6	289	273
8	112	-113
10	81	84
12	48	42
14	180	-191
16	54	51
18	165	166
20	141	143
22	<25	2
24	26	-26
$\bar{3}0l$		
2	261	-273
4	279	261
6	109	114
8	57	58
10	117	-117
12	328	-331
14	27	29
16	143	152
18	121	119
20	87	90
22	27	-27
24	<13	-5
$\bar{4}0l$		
2	162	-157
4	36	36
6	82	87
8	116	-113
10	269	-264
12	62	-60
14	71	71
16	<33	6
18	80	71
20	46	47
22	39	-36
$\bar{5}0l$		
2	<21	2
4	69	-65
6	233	-233
8	<24	-4
10	101	-100
12	68	-62
14	43	45
16	<32	-20
18	<30	-0
20	<25	3
$\bar{6}0l$		
2	190	-190
4	296	-310
6	114	106
8	86	88
10	153	-149
12	<28	16
14	<28	-8
16	62	-88
18	<27	-1
20	24	22
$\bar{7}0l$		
2	166	-167
4	54	-62
6	58	54
8	52	-48
10	<28	-18
12	<28	17
14	31	26
16	68	-65
18	<23	-4
20	24	26
$\bar{8}0l$		
2	121	-122
4	33	24
6	32	31
8	58	51
10	42	-44
12	34	34
14	26	-18
16	20	-17
18	82	83
$\bar{9}0l$		
2	147	140
4	<36	-26
6	<27	7
8	36	-23
10	35	-28
12	50	45
14	50	45
16	64	68
$\bar{10},0,l$		
2	32	-38
4	44	-46
6	29	18
8	25	-18
10	<23	2
12	47	47
14	48	68
$\bar{11},0,l$		
2	<19	9
4	22	-13
6	20	-17
8	19	-19
10	13*	-10
01l		
1	---	243
2	175	-143
3	286	284
4	67	66
5	64	70
6	166	-169
7	149	-151
8	95	91
9	79	77
10	66	62
11	147	-152
12	28	29
13	98	-88
14	72	74
15	111	107
16	117	120
17	44	49
18	90	92
19	51	50
20	54	-53
21	<30	-9
22	25	20
23	31	-31
24	18	20
11l		
0	148	-146
1	342	-369
2	154	161
3	227	249
4	31	-34
5	39	44
6	56	55
7	111	114
8	<21	-18
9	19*	1
10	208	210
11	168	-158
12	<21	2
13	123	-124
14	57	-56
15	96	90
16	144	143
17	92	89
18	111	107
19	34	-32
20	<28	-20
21	30	-26
22	27	-23
23	23	-18
24	<16	10
21l		
0	118	116
1	284	-315
2	93	-97
3	19	12
4	31	-32
5	374*	-429
6	84	88
7	186	-193
8	68	-60
9	243	263
10	<25	-18
11	24	30
12	216	202
13	53	-40
14	79	-88
15	72	-77
16	53	-56
17	29	-32
18	138	140
19	<37	19
20	<32	12
21	<29	-10
22	31	-27
23	<21	-4
24	11*	-10
31l		
0	166	178
1	140	-149
2	<16	-12
3	23	-20
4	16	-10
5	77	-80
6	81	-81
7	242	-269
8	22	24
9	25	29
10	28	-29
11	30	-31
12	43	-44
13	30	34
14	50	49
15	124	116
16	43	-40
17	107	-104
18	<34	17
19	66	-66
20	<28	26
21	<27	-13
22	20	-16
23	<17	-1
41l		
0	201	209
1	47	49
2	22	14
3	28	32
4	197	-208
5	119	-116
6	108	-106
7	115	-118
8	64	-62
9	70	73
10	<26	1
11	<27	-9
12	<28	3
13	91	-88
14	71	-67
15	100	96
16	43	-45
17	<34	-6
18	<33	18
19	83	-85
20	26	24
21	<24	5
22	<19	-1
51l		
0	29	28
1	247	-269
2	95	94
3	118	119
4	76	79
5	47	49
6	198	-202
7	42	-29
8	101	-112
9	83	87
10	58	-83
11	<28	-6
12	50	-43
13	99	-102
14	<32	18
15	<36	14
16	<34	-23
17	32	33
18	<33	-20
19	34	-33
20	<24	1
21	<19	-13
22	12*	10
61l		
0	54	53
1	200	-202
2	<23	-20
3	38	-32
4	50	-52
5	115	111
6	58	-59
7	<30	33
8	72	-73
9	119	118
10	<35	-23
11	<36	22
12	61	-60
13	81	-81
14	42	-41
15	33	-30
16	<31	7
17	<29	-1
18	23	12
19	26	22
20	18	16
71l		
0	77	-78
1	<28	2
2	62	62
3	123	-131
4	113	112
5	<24	18
6	131	-135
7	94	91
8	98	-97
9	127	130
10	<36	12
11	64	65
12	<37	-18
13	101	-97
14	<34	-18
15	37	-37
16	<27	6
17	21	-14
18	<21	11
19	<15	8
81l		
0	52	44
1	103	100
2	95	-96
3	89	86
4	61	61
5	47	-47
6	59	56
7	<32	-11
8	87	-93
9	38	39
10	<33	-2
11	73	73
12	<31	13
13	<29	-12
14	<27	-16
15	32	-35
16	<21	4
17	18	-19
91l		
0	43	39
1	<35	13
2	35	36
3	59	60
4	<34	9
5	<30	23
6	32	24
7	<32	1
8	<34	-16
9	<30	13
10	28	-22
11	<27	-6
12	25	22
13	19	-9
14	18	12
15	<13	-13
10,1,l		
0	52	50
1	68	64
2	30	24
3	68	63
4	39	39
5	<31	23
6	<30	17
7	31	-29
8	<25	0
9	24	-19
10	<21	-6
11,1,l		
0	<23	-2
1	<23	-6
2	30	29
3	31	33
4	38	35
5	<20	11
6	18	20
7	<16	12
8	12*	-12
$\bar{1}1l$		
1	337	-362
2	25	-20
3	---	1073
4	---	-913
5	343	372
6	134	138
7	121	-119
8	83	81
9	216	-220
10	114	-119
11	269	-291
12	104	105
13	73	73
14	67	65
15	143	150
16	89	93
17	131	134
18	<32	19
19	<31	-4
20	<33	14
21	77	-74
22	34	35
23	20	24
24	36	-38
$\bar{2}1l$		
1	573*	719
2	---	-1037
3	639*	768
4	64	74
5	347	-379
6	183	189
7	214	-230
8	355	-373
9	160	-142
10	<25	11
11	65	65
12	74	72
13	66	68
14	<30	-5
15	59	64
16	47	50
17	44	48
18	55	55
19	71	-64
20	<32	-14
21	36	34
22	40	-37
23	73	73
24	<15	1
$\bar{3}1l$		
1	313	327
2	169	-174
3	16	19
4	174	-183
5	<18	5
6	177	-186
7	69	-66
8	111	-112
9	56	-52
10	<23	-19
11	<25	6
12	43	45
13	<27	-12
14	36	-36
15	47	45
16	<32	20
17	34	-25
18	<35	13
19	<36	-15
20	38	-34
21	86	82
22	<25	-6
23	46	45
24	12*	-15
$\bar{4}1l$		
1	156	-158
2	373	-398
3	68	-61
4	95	98
5	43	37
6	104	107
7	61	-61
8	183	-184
9	45	43
10	33	34
11	26	27
12	47	-43
13	37	-37
14	52	-50
15	90	-89
16	81	77
17	<35	-15
18	<34	-3
19	51	51
20	55	-55
21	53	48
22	45	-44
23	27	31
$\bar{5}1l$		
1	190	-194
2	<22	4
3	124	126
4	111	112
5	<23	-5
6	95	-95
7	28	-27
8	55	-63
9	<30	21
10	<27	-0
11	<28	13
12	33	31
13	112	-107
14	48	42
15	81	-69
16	<35	3
17	59	58
18	39	-39
19	<30	-7
20	50	-51
21	25	23
22	16	-14
$\bar{6}1l$		
1	<26	-9
2	33	-31
3	25	-17
4	87	54
5	23	23
6	26	21
7	25	15
8	26	-28
9	<28	-4
10	93	92
11	<32	-11
12	<32	1
13	114	-118
14	<35	-6
15	38	31
16	89	89
17	35	30
18	42	-42
19	41	-44
20	39	-39
21	<18	22
$\bar{7}1l$		
1	48	48
2	<28	-9
3	34	35
4	67	48
5	<28	7
6	<29	2
7	135	-130
8	57	55
9	<32	8
10	<32	6
11	34	33
12	32	29
13	<34	15
14	107	110
15	38	36
16	33	-36
17	60	-56
18	49	-50
19	29	-31
20	13*	8
$\bar{8}1l$		
1	36	-35
2	37	-37
3	<23	-17
4	48	41
5	84	-79
6	41	38
7	44	-44
8	<32	2
9	82	83
10	42	38
11	47	48
12	100	99
13	<31	-0
14	<21	-13
15	27	-24
16	28	-26
17	<21	-8
18	<16	12
$\bar{9}1l$		
1	<24	18
2	<28	-19
3	<24	-21
4	42	43
5	61	-59
6	<34	11
7	<33	-17
8	<32	-7
9	46	43
10	66	66
11	59	55
12	30	23
13	<23	-2
14	<23	-1
15	<20	10
$\bar{10},1,l$		
1	44	-43
2	<25	21
3	67	-66
4	32	20
5	30	-8
6	54	-50
7	<28	5
8	35	34
9	59	58
10	34	35
11	<22	13
12	<19	4
13	16	-19
$\bar{11},1,l$		
1	52	-52
2	<23	-1
3	28	23
4	46	-44
5	<21	6
6	<16	15
7	<13	-12
8	16	18
02l		
0	---	105
1	---	-62
2	80	83
3	141	131
4	189	-177
5	198	-177
6	369	-350
7	154	-134
8	152	-149
9	175	163
10	173	158
11	35	-37
12	120	129
13	127	137
14	<30	-15
15	116	119
16	<31	-13
17	69	-63
18	<33	-5
19	37	31
20	<30	-12
21	48	46
22	<23	-13
23	<18	-1
12l		
0	213	222
1	43	44
2	127	-114
3	25	28
4	109	-93
5	122	115
6	85	83
7	111	-115
8	229	-243
9	25	28
10	105	-99
11	84	81
12	164	169
13	61	61
14	131	147
15	123	131
16	<31	27
17	48	-46
18	<33	-2
19	<31	6
20	<29	-25
21	48	48
22	56	-54
23	21	-21
22l		
0	163	-158
1	317	333
2	50	54
3	19	-8
4	77	-69
5	62	-63
6	73	66
7	29	25
8	45	-46
9	61	-60
10	69	-64
11	<24	10
12	139	141
13	119	121
14	84	84
15	86	89
16	54	46
17	88	-83
18	<32	25
19	37	-37
20	32	-27
21	52	54
22	38	-38
23	18	-18
32l		
0	39	40
1	177	164
2	332	-329
3	206	211
4	102	-97
5	55	56
6	123	125
7	<21	-7
8	161	168
9	48	-50
10	50	-48
11	149	-166
12	<29	2
13	<30	15
14	123	125
15	157	159
16	<31	18
17	<33	-7
18	<31	18
19	81	-78
20	<26	-2
21	<23	1
22	42	-44
42l		
0	29	31
1	<19	1
2	115	-119
3	25	-26
4	207	-205
5	<21	12
6	45	42
7	33	-33
8	48	47
9	<25	-4
10	155	169
11	33	-32
12	69	66
13	124	-138
14	46	-40
15	<31	9
16	<33	11
17	48	47
18	<29	-19
19	<27	-14
20	<23	8
21	<19	-8
22	12*	-3
52l		
0	46	-41
1	39	-38
2	25	-21
3	46	-49
4	173	-182
5	82	86
6	51	-63
7	<28	-5
8	123	115
9	187	-187
10	<30	32
11	46	-52
12	124	113
13	<31	0
14	<33	-8
15	<32	-22
16	49	-50
17	<29	10
18	<26	-6
19	<23	-8
20	26	-26
21	12*	-0
62l		
0	55	53
1	28	31
2	68	-59
3	186	-194
4	53	56
5	108	-106
6	82	-81
7	139	145
8	71	-75
9	34	-37
10	55	59
11	117	-118
12	38	66
13	33	-23
14	31	26
15	<30	-20
16	59	-67
17	<25	7
18	<22	-20
19	27	23
72l		
0	<30	-6
1	73	80
2	<30	-17
3	<31	24
4	39	-40
5	94	-96
6	75	84
7	<31	-18
8	28	-30
9	<31	-7
10	59	-61
11	53	-58
12	<31	7
13	<30	4
14	<28	8
15	<26	20
16	<23	-5
82l		
0	39	-43
1	31	33
2	24	-26
3	<31	-18
4	<31	14
5	<31	-19
6	<30	21
7	44	44
8	<32	-4
9	<31	-6
10	58	-59
11	37	-39
12	<27	-14
13	23	-17
14	<22	-6
15	<19	10
16	14*	-5
92l		
0	<32	-6
1	39	41
2	32	-33
3	31	30
4	31	-31
5	37	-38
6	<30	21
7	41	40
8	34	34
9	<26	12
10	29	-29
11	26	-23
12	44	-45
13	15	10
14	12*	-13
10,2,l		
0	<27	15
1	27	24
2	<26	-5
3	35	35
4	<25	-2
5	24	-17
6	23	-20
7	22	14
8	20	-14
9	32	38
10	14*	7
11,2,l		
0	28	30
1	<18	10
2	20	16
3	16*	7
4	14*	-8
5	12*	4
$\bar{1}2l$		
1	65	-56
2	223	-202
3	21	20
4	202	-188
5	321	-316
6	<16	10
7	20	-19
8	23	18
9	32	35
10	<22	-11
11	<23	14
12	52	-45
13	106	104
14	<27	-7
15	27	22
16	37	-44
17	34	-37
18	<30	8
19	67	69
20	<29	18
21	50	49
22	<23	-18
23	29	-26
$\bar{2}2l$		
1	208	-189
2	59	51
3	78	73
4	116	-107
5	114	-110
6	<18	8
7	168	-172
8	196	212
9	<21	-9
10	64	-67
11	32	-37
12	92	-91
13	26	23
14	75	-75
15	65	69
16	28	-22
17	<34	8
18	27	27
19	28	29
20	<29	3
21	23	-22
22	<22	5
23	16	-16
$\bar{3}2l$		
1	245	256
2	<17	-20
3	153	143
4	65	65
5	481*	-552
6	440*	505
7	201	-205
8	74	-78
9	142	149
10	164	-166
11	54	-56
12	47	-45
13	50	53
14	<27	-11
15	31	32
16	<31	-4
17	66	-71
18	<29	-18
19	<27	-8
20	32	30
21	<24	17
22	39	-38
23	12*	8
$\bar{4}2l$		
1	49	52
2	<20	-13
3	175	-170
4	282	306
5	253	-287
6	38	36
7	161	170
8	<24	25
9	<24	5
10	<28	-0
11	148	-142
12	54	-64
13	63	67
14	48	48
15	<31	-0
16	54	-67
17	56	-68
18	<30	5
19	<28	16
20	<25	-6
21	<22	3
22	29	-33
$\bar{5}2l$		
1	109	116
2	133	136
3	83	-80
4	53	57
5	137	-138
6	88	93
7	28	28
8	29	25
9	37	-40
10	50	-60
11	64	64
12	137	139
13	74	81
14	39	-29
15	93	-91
16	60	-68
17	48	-60
18	<28	-4
19	23	27
20	28	-27
21	<17	-0
$\bar{6}2l$		
1	43	-42
2	<25	5
3	55	-57
4	56	-62
5	26	-22
6	42	43
7	86	89
8	71	75
9	99	101
10	144	141
11	28	23
12	<31	-19
13	62	-72
14	53	-54
15	31	-28
16	<29	-16
17	37	39
18	35	-35
19	26	21
20	19	15
$\bar{7}2l$		
1	59	60
2	73	-81
3	<30	22
4	<31	-3
5	<31	-26
6	54	53
7	98	97
8	93	93
9	53	58
10	<34	18
11	<33	-28
12	<32	4
13	<31	20
14	<30	-3
15	<28	21
16	48	-53
17	<23	14
18	<19	1
19	12*	-8
$\bar{8}2l$		
1	34	26
2	34	-23
3	44	-46
4	41	-42
5	<31	4
6	83	57
7	93	101
8	68	73
9	<32	17
10	<31	-13
11	<30	15
12	<29	-22
13	<27	8
14	<25	-13
15	<22	10
16	<19	-5
17	17	24
$\bar{9}2l$		
1	<32	-3
2	32	-23
3	34	-30
4	26	19
5	31	34
6	37	39
7	30	27
8	35	-34
9	<28	18
10	39	-39
11	<25	13
12	27	26
13	<21	-6
14	<17	10
15	19	30
$\bar{10},2,l$		
1	<27	-12
2	<27	15
3	<27	-18
4	<26	-8
5	<26	-10
6	<25	-14
7	24	22
8	27	-27
9	21	22
10	<19	-3
11	14	-16
$\bar{11},2,l$		
1	24	-28
2	<18	4
3	31	-35
4	<16	4
5	<15	14
6	20	-26
03l		
1	---	-104
2	24	26
3	147	-148
4	35	-34
5	21	21
6	56	56
7	45	-38
8	<17	-13
9	29	-28
10	40	-33
11	<23	-16
12	<24	-1
13	34	-38
14	<25	-19
15	37	39
16	36	41
17	37	40
18	<23	9
19	<23	-2
20	46	-49
21	<17	-3
22	<12	-8
13l		
0	107	-120
1	<9	1
2	210	-197
3	330	-317
4	160	156
5	139	-125
6	143	132
7	47	45
8	48	-47
9	73	70
10	<22	-12
11	73	76
12	24	22
13	<24	4
14	82	-84
15	<27	12
16	<27	7
17	30	30
18	64	66
19	<22	9
20	35	-36
21	23	26
22	17	-22
23l		
0	28	26
1	113	90
2	100	-86
3	57	-52
4	180	-170
5	249	-248
6	98	98
7	42	-38
8	98	94
9	102	99
10	50	49
11	156	161
12	<24	11
13	88	90
14	87	-87
15	25	25
16	26	-26
17	<25	17
18	32	35
19	35	-34
20	<19	1
21	15	10
33l		
0	134	-124
1	<15	-1
2	15	-13
3	16	18
4	28	26
5	76	-75
6	30	-28
7	114	-111
8	75	77
9	104	102
10	<24	5
11	165	167
12	52	46
13	108	101
14	38	-40
15	27	24
16	44	-48
17	24	20
18	27	28
19	23	-22
20	24	-24
21	27	-35
43l		
0	67	64
1	46	47
2	58	-66
3	31	31
4	29	31
5	80	73
6	134	-131
7	72	-68
8	30	31
9	73	-83
10	166	168
11	152	160
12	<27	-17
13	125	140
14	52	-55
15	<26	15
16	45	-45
17	26	-20
18	20	16
19	24	-26
20	<13	6
53l		
0	<22	-12
1	41	-43
2	<22	11
3	18	-22
4	82	79
5	18	12
6	35	38
7	156	152
8	133	-141
9	35	-38
10	<25	-1
11	54	-81
12	90	106
13	78	84
14	<25	-8
15	27	26
16	25	-23
17	<20	-8
18	<17	-10
19	21	-23
63l		
0	26	-25
1	44	-44
2	24	-24
3	<24	-19
4	41	44
5	41	-42
6	31	-29
7	<25	14
8	56	53
9	59	60
10	<27	-4
11	38	-41
12	<25	-20
13	<24	-6
14	<23	6
15	<21	6
16	<18	-11
17	22	-23
18	10*	14
73l		
0	<25	16
1	61	-68
2	39	-35
3	<25	-28
4	77	76
5	31	-32
6	<27	1
7	<27	-8
8	55	-57
9	<25	18
10	35	40
11	<24	-12
12	<22	-3
13	41	-42
14	<19	8
15	<16	-7
16	<12	6
83l		
0	30	-28
1	41	-46
2	30	-26
3	<26	-21
4	<26	22
5	31	-34
6	<25	11
7	28	-28
8	<23	-21
9	<22	-16
10	32	33
11	<19	-5
12	<18	5
13	<15	-4
14	23	-27
93l		
0	23	23
1	21	-19
2	31	-26
3	<22	15
4	<22	9
5	<21	-11
6	<21	4
7	34	-33
8	26	-31
9	20	-20
10	<15	9
11	18	-23
10,3,l		
0	<17	-5
1	23	-23
2	<17	5
3	<16	2
4	<15	16
5	23	28
6	12	-15
7	10*	-11
$\bar{1}3l$		
1	<9	-6
2	114	-106
3	21	-17
4	55	51
5	14	11
6	64	53
7	88	-89
8	113	-110
9	81	-79
10	<19	8
11	51	-63
12	112	106
13	<24	9
14	67	-69
15	27	22
16	27	-28
17	26	-24
18	38	39
19	<23	-8
20	45	-38
21	17	-13
22	<12	2
$\bar{2}3l$		
1	59	-50
2	66	-68
3	21	21
4	39	-39
5	21	21
6	148	151
7	60	-59
8	69	-70
9	56	-61
10	<22	14
11	26	23
12	22	19
13	<23	-17
14	94	-99
15	64	-63
16	74	71
17	<26	-9
18	<24	13
19	<22	-12
20	42	-42
21	24	-23
22	10*	5
$\bar{3}3l$		
1	20	20
2	152	-143
3	72	74
4	125	124
5	67	68
6	<18	-2
7	81	-81
8	115	-116
9	48	52
10	129	134
11	114	96
12	38	-42
13	94	-97
14	54	-51
15	42	-44
16	30	27
17	29	-26
18	<23	-3
19	24	-24
20	<18	-6
21	16	-14
$\bar{4}3l$		
1	38	-39
2	95	-90
3	28	28
4	55	58
5	<21	-4
6	120	124
7	112	102
8	75	70
9	263	260
10	137	-141
11	52	-55
12	68	-61
13	109	-114
14	<27	10
15	<26	-18
16	31	35
17	<23	-18
18	29	25
19	<19	-2
20	14	-13
$\bar{5}3l$		
1	69	-67
2	<22	-7
3	32	34
4	144	144
5	103	108
6	87	81
7	234	243
8	204	-228
9	45	46
10	<25	10
11	73	-77
12	63	61
13	<27	3
14	33	-34
15	<25	-1
16	31	32
17	<21	-13
18	<19	-11
$\bar{6}3l$		
1	52	-57
2	40	-43
3	<24	11
4	125	125
5	135	140
6	29	-28
7	115	114
8	42	-45
9	<27	15
10	<27	21
11	<27	10
12	41	-48
13	<25	0
14	24	22
15	<22	-3
16	<20	6
17	<18	-12
$\bar{7}3l$		
1	72	-73
2	47	50
3	69	72
4	33	56
5	81	81
6	57	-58
7	<27	6
8	36	-40
9	<26	12
10	<25	6
11	<25	10
12	29	29
13	22	20
14	<20	-3
15	<18	-0
16	<16	-6
17	<11	1
$\bar{8}3l$		
1	<26	1
2	32	-24
3	24	22
4	<26	-14
5	31	-32
6	<25	6
7	<23	3
8	<24	-9
9	<23	13
10	<22	7
11	<21	13
12	<19	7
13	16	17
14	<15	-5
15	10*	-10
$\bar{9}3l$		
1	21	-16
2	21	-11
3	21	-17
4	28	30
5	20	-17
6	26	-21
7	<21	-2
8	<20	-14
9	<18	-2
10	<20	18
11	15	12
12	<12	-1
$\bar{10},3,l$		
1	<17	3
2	<17	3
3	<17	-7
04l		
0	---	-39
1	---	21
2	8*	7
3	17	-14
4	67	62
5	112	-92
6	77	-70
7	66	61
8	77	-72
9	119	120
10	26	-24
11	78	-81
12	23	-30
13	65	-65
14	60	58
15	<18	-9
16	22	23
17	55	-56
18	<14	1
19	17	-18
20	17	-21
14l		
0	76	-83
1	31	28
2	34	36
3	15	14
4	13	11
5	45	-44
6	61	-59
7	64	-62
8	38	-39
9	52	51
10	32	-30
11	<17	12
12	27	29
13	33	-33
14	37	35
15	22	-27
16	27	28
17	66	-63
18	<14	10
19	29	-32
24l		
0	48	-41
1	25	22
2	29	-24
3	19	-15
4	66	62
5	39	-36
6	16	-17
7	<16	-7
8	32	32
9	<17	-4
10	72	-74
11	29	27
12	<40	-39
13	19	-8
14	119	120
15	24	-25
16	36	40
17	33	-35
18	<13	-6
19	20	-22
34l		
0	119	-112
1	70	-63
2	93	-91
3	55	53
4	38	34
5	35	34
6	<16	2
7	47	47
8	71	70
9	39	-36
10	86	86
11	33	-34
12	86	-81
13	57	65
14	<18	-11
15	<17	3
16	60	63
17	33	-38
18	16	18
44l		
0	16	15
1	17	-13
2	95	-103
3	68	-62
4	<16	-9
5	42	46
6	<17	4
7	87	91
8	46	44
9	71	75
10	64	62
11	35	-37
12	<18	9
13	<18	-9
14	<17	-6
15	34	35
16	13	-12
17	23	-26
18	7*	-8
54l		
0	42	42
1	50	57
2	76	-80
3	19	-12
4	43	-41
5	<19	-3
6	<19	12
7	107	112
8	44	41
9	42	41
10	59	70
11	<18	13
12	23	-23
13	<16	-1
14	20	-22
15	23	24
16	<11	1
64l		
0	30	32
1	<19	-1
2	26	27
3	41	40
4	41	-44
5	45	-46
6	46	-61
7	50	32
8	22	23
9	81	91
10	31	34
11	16	15
12	<15	-3
13	<14	1
14	23	-27
15	11	-12
74l		
0	15	-17
1	18	19
2	33	-30
3	22	21
4	52	49
5	18	16
6	<17	-3
7	<17	-11
8	42	-45
9	18	19
10	30	31
11	21	22
12	<11	-5
13	15	21
84l		
0	<16	6
1	19	13
2	<16	-8
3	<16	-2
4	31	-35
5	<15	1
6	38	39
7	<14	10
8	<13	5
9	14	-13
10	11	-12
94l		
0	<12	-8
1	<12	-5
2	17	16
3	<11	-9
4	<11	-2
5	11	-13
6	12	-15
$\bar{1}4l$		
1	83	76
2	117	129
3	63	58
4	18	-18
5	31	-28
6	175	-159
7	118	105
8	65	64
9	31	25
10	39	-44
11	88	-93
12	19	-23
13	<17	2
14	17	20
15	22	-21
16	<17	-8
17	46	-43
18	<14	-3
19	12	-9
20	15	-16
$\bar{2}4l$		
1	123	110
2	<10	-4
3	26	21
4	47	-43
5	83	80
6	152	143
7	134	126
8	<12	-9
9	42	-41
10	114	-120
11	60	-67
12	<19	-10
13	<19	-10
14	<19	-11
15	22	21
16	<17	-4
17	19	-17
18	14	13
19	<11	-1
$\bar{3}4l$		
1	114	107
2	109	101
3	137	132
4	168	161
5	89	82
6	17	-16
7	68	-65
8	73	-74
9	<17	-2
10	23	-26
11	<18	-7
12	<19	-8
13	38	41
14	<18	-4
15	<17	7
16	<16	8
17	36	-36
18	<12	10
19	17	25
$\bar{4}4l$		
1	54	52
2	127	117
3	129	121
4	15	10
5	43	-43
6	28	29
7	34	36
8	<19	-3
9	23	26
10	21	-21
11	22	-24
12	19	19
13	18	18
14	17	-13
15	22	-23
16	<15	9
17	22	23
18	<10	-12
$\bar{5}4l$		
1	112	120
2	55	64
3	38	35
4	38	32
5	49	-51
6	<19	1
7	<19	6
8	22	-16
9	19	15
10	25	21
11	17	16
12	22	21
13	40	-40
14	19	19
15	<14	7
16	<12	-6
17	<9	9
$\bar{6}4l$		
1	23	22
2	<19	-11
3	36	-35
4	22	-22
5	<19	-10
6	<19	3
7	33	36
8	<18	-7
9	24	24
10	55	59
11	72	-81
12	62	69
13	31	-30
14	39	-41
15	13	19
16	24	-32
$\bar{7}4l$		
1	<18	4
2	18	-19
3	<18	12
4	18	-18
5	18	-18
6	20	-17
7	20	19
8	26	28
9	30	-36
10	86	82
11	36	-60
12	36	-32
13	<11	-3
14	22	-28
$\bar{8}4l$		
1	<16	14
2	35	-36
3	<16	-2
4	<16	-17
5	<15	10
6	<15	-11
7	<14	-6
8	29	26
9	46	-55
10	<11	9
11	19	-25
$\bar{9}4l$		
1	21	23
2	18	-21
3	<12	14
4	20	-21
5	13	-14
6	<10	-2
7	24	-33
05l		
1	---	40
2	86	-84
3	19	17
4	112	112
5	63	73
6	20	-18
7	46	-42
8	53	-68
9	35	-36
10	16	-14
11	<16	1
12	15	11
13	32	-36
14	<14	5
15	<12	4
16	33*	-36
15l		
0	19*	14
1	65	60
2	24	-26
3	55	-57
4	12	13
5	13	14
6	44	43
7	<15	-3
8	65	-66
9	56	-59
10	18	-18
11	50	50
12	21	-21
13	<14	-11
14	13	14
15	56	-56
25l		
0	101	-93
1	96	97
2	56	-56
3	51	-51
4	14	-11
5	25	-19
6	37	33
7	<15	12
8	19	16
9	60	-62
10	<16	-11
11	<15	-8
12	13	-13
13	36	38
14	42	-42
15	24	-23
35l		
0	41	-44
1	84	91
2	47	-49
3	28	-29
4	25	24
5	53	-50
6	19	-16
7	<16	-2
8	<16	3
9	32	-30
10	41	41
11	<15	13
12	<14	3
13	<13	4
14	25*	-12
45l		
0	14	17
1	48	43
2	51	-48
3	31	31
4	13	11
5	22	-24
6	45	42
7	<16	-11
8	18	-18
9	44	-43
10	25	27
11	<14	-2
12	27	28
13	27*	30
55l		
0	14	-9
1	<16	-6
2	29	31
3	<16	7
4	32	30
5	24	26
6	25	26
7	23	22
8	<14	-1
9	22	-23
10	<13	13
11	<11	-10
12	10*	16
65l		
0	17	-19
1	23	-24
2	<15	-0
3	21	23
4	34	40
5	<14	10
6	49	50
7	35	38
8	<12	-3
9	<11	3
10	9*	-9
75l		
0	13	-8
1	31	-31
2	25	-26
3	<12	5
4	21	23
5	41	46
6	38	36
7	26*	26
$\bar{1}5l$		
1	132	121
2	132	128
3	54	55
4	25	28
5	38	-37
6	69	-67
7	33	-32
8	43	-47
9	<16	-3
10	16	14
11	16	-14
12	50	53
13	14	-18
14	14	-16
15	17	19
16	10*	-10
$\bar{2}5l$		
1	85	83
2	<12	1
3	55	-51
4	<14	-6
5	25	24
6	13	-10
7	21	18
8	<16	-2
9	35	-37
10	74	76
11	29	-28
12	<15	-4
13	<14	-5
14	18	-19
15	32	30
$\bar{3}5l$		
1	13	12
2	15	17
3	12	-14
4	19	20
5	<15	4
6	<15	-3
7	25	-25
8	51	48
9	<16	-6
10	<15	4
11	20	-19
12	<14	3
13	13	9
14	12	12
15	10*	-1
$\bar{4}5l$		
1	31	-34
2	<15	1
3	48	-63
4	35	37
5	<16	-2
6	27	30
7	25	22
8	<16	9
9	<15	-9
10	<15	7
11	20	-19
12	13	9
13	17	-14
14	10*	-25
$\bar{5}5l$		
1	59	-60
2	37	40
3	26	-29
4	<16	-8
5	18	20
6	15	15
7	<15	8
8	<15	10
9	14	-11
10	22	-25
11	39	-40
12	11*	-5
$\bar{6}5l$		
1	46	-45
2	15	-16
3	<15	7
4	<14	10
5	<14	-7
6	17	15
7	<13	-6
8	41	-43
9	24	-22
10	11*	-7
11	8*	-12
$\bar{7}5l$		
1	<13	7
2	15	-17
3	14	-16
4	<12	-7
5	23	-24
6	24	-24
7	10*	8
8	8*	-2
$\bar{8}5l$		
1	6*	4
2	7*	1

shorter than predicted, which can probably be attributed to relatively large thermal motion(s) of this part of the molecule. The angles around C(4) and C(6) reflect the extensive double-bond character of the C(4)–N and C(5)–C(6) bonds.

The average apparent C–H distance of 0·98 Å is significantly shorter than the standard internuclear separation of 1·09 Å. This shortening is not an uncommon observation for C–H distances.

The equations for the best planes of various groups within the molecule, with out-of-plane deviations of the atoms, are given in Table 4. The molecule is significantly non-planar, although the center phenyl (I), oxazole (II), and end phenyl (III) groups are each planar within experimental error. The dihedral angle between planes I and II is 3·75°; that between II and III is 6·45°. The sense of the two tilts is the same; *i.e.* the five planes in a molecule are oriented in a screw fashion. The line of intersection of planes II and III is the C(6)–C(7) bond; the I–II intersection passes through C(4) and between C(3) and C(1′), making an angle of 16·7° with the C(3)–C(4) bond.

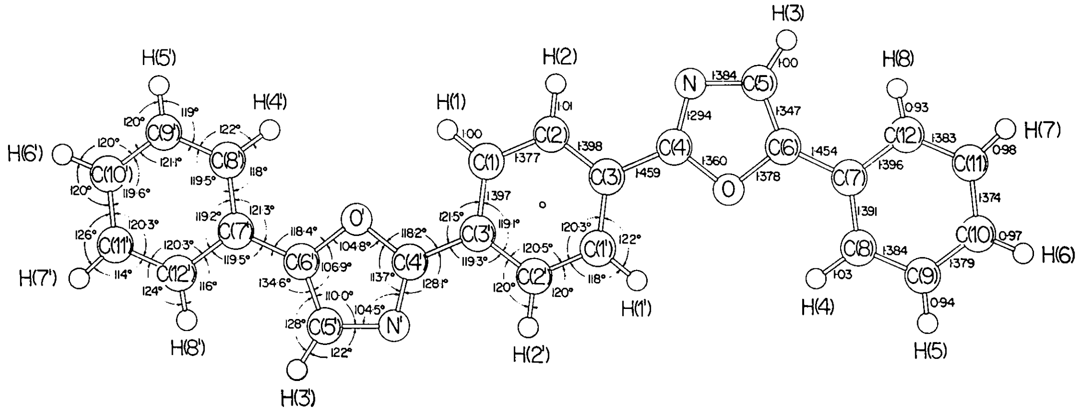

Fig. 3. Bond distances and angles computed from the least-squares parameters of Table 3. The center phenyl contains a center of symmetry.

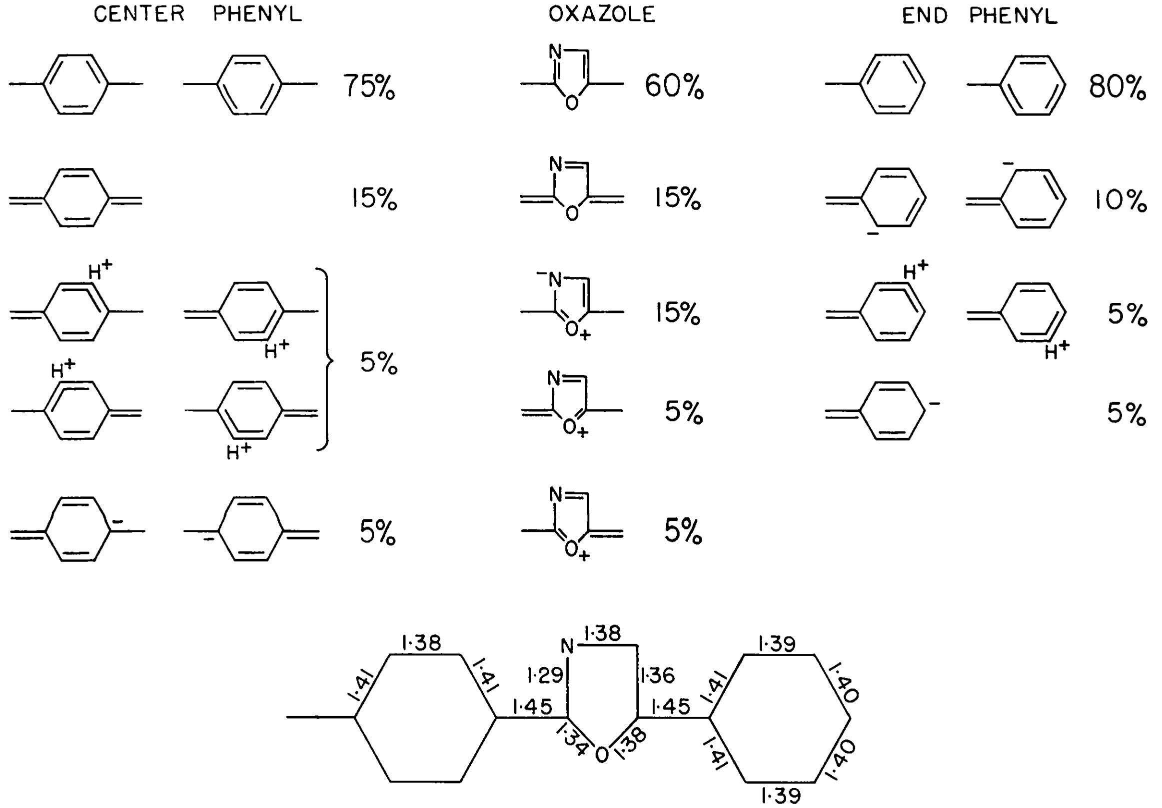

Fig. 4. Canonical structures of the three rings and the bond distances predicted from the indicated relative contributions. The groups were considered separately.

A drawing of the structure of POPOP viewed along the *b* axis is shown in Fig. 5. Closest intermolecular approaches are given in Table 5. Considering the best plane of the whole molecule (plane *A* of Table 4), the interplanar spacing between adjacent molecules along *b* is 3·462 Å.

Table 4. *Least-squares planes*

The direction cosines are relative to *abc**; the origin-to-plane distance is in Å

Plane	Atoms involved	Equation of plane
A	Full molecule: C(1)–C(12), O, N, C(1′)–C(12′), O′, N′	$0{\cdot}5999X+0{\cdot}6550Y-0{\cdot}4595Z=0$
B	Asymmetric unit: C(1)–C(12), O, N	$0{\cdot}5906X+0{\cdot}6461Y-0{\cdot}4836Z=-0{\cdot}0803$
I	Center phenyl: C(1)–C(3), C(1′)–C(3′)	$0{\cdot}6578X+0{\cdot}6271Y-0{\cdot}4172Z=0$
II	Oxazole: C(4)–C(6), O, N	$0{\cdot}6076X+0{\cdot}6613Y-0{\cdot}4398Z=0{\cdot}0535$
III	End phenyl: C(7)–C(12)	$0{\cdot}5669X+0{\cdot}6242Y-0{\cdot}5376Z=-0{\cdot}2805$

Out-of-plane deviations

Atom	*A*	*B*	I	II	III
C(1)	−0·094*	−0·022*	0·002*	−0·140	0·158
C(2)	−0·091*	−0·046*	−0·002*	−0·115	0·071
C(3)	0·010*	0·062*	0·002*	−0·022	0·199
C(4)	0·007*	0·030*	−0·007	−0·001*	0·098
C(5)	−0·034*	−0·062*	−0·020	−0·002*	−0·108
C(6)	−0·009*	−0·011*	−0·099	0·001*	0·003
C(7)	−0·013*	−0·015*	−0·190	−0·004	0·000*
C(8)	−0·122*	−0·092*	−0·399	−0·110	−0·002*
C(9)	−0·116*	−0·086*	−0·473	−0·133	0·002*
C(10)	−0·008*	−0·011*	−0·349	0·000	0·001*
C(11)	0·094*	0·058*	−0·149	0·128	−0·003*
C(12)	0·098*	0·063*	−0·062	0·133	0·002*
O	0·016*	0·047*	−0·092	0·000*	0·137
N	−0·019*	−0·031*	0·190	0·001*	−0·042
H(1)	−0·10	−0·04	0·06	−0·14	0·13
H(2)	−0·13	−0·11	0·02	−0·14	−0·06
H(3)	−0·10	−0·15	−0·05	−0·04	−0·26
H(4)	−0·23	−0·18	−0·52	−0·27	−0·03
H(5)	−0·19	−0·14	−0·62	−0·23	−0·00
H(6)	−0·08	−0·08	−0·48	−0·07	−0·07
H(7)	0·17	0·11	−0·05	0·22	−0·01
H(8)	0·15	0·10	0·06	0·20	−0·01

* These atoms were included, each with weight inversely proportional to the square of the average standard deviation of its coordinates, in the calculation of the plane.

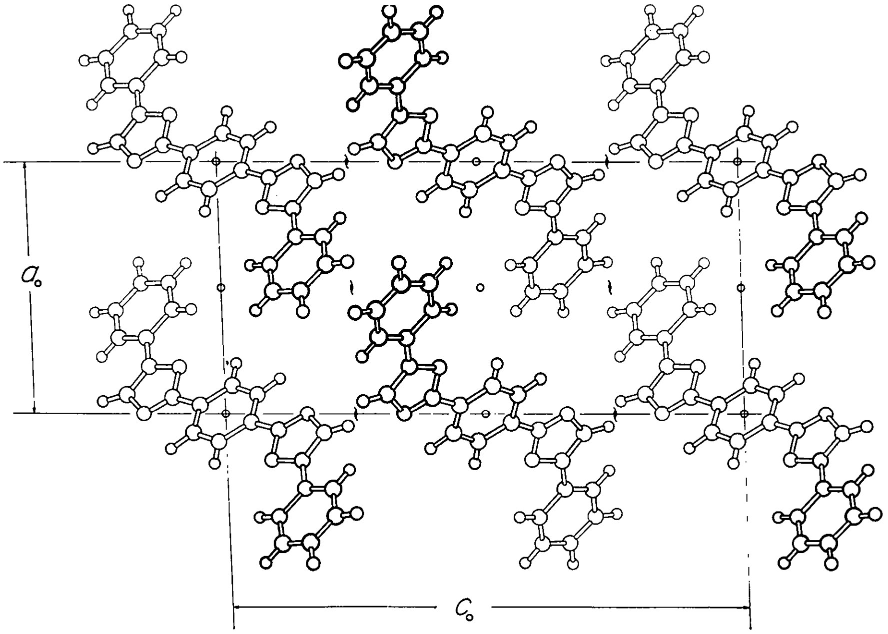

Fig. 5. The structure viewed along the *b* axis.

Table 5. *Closest intermolecular approaches*

All distances less than 3·6 Å between heavy atoms, and 3·0 Å between a hydrogen atom and a heavy atom, are included.

From	To	In unit at	Distance
C(4)	C(1)	$(x, 1+y, z)$	3·381 Å
C(5)	C(2)		3·549
C(6)	C(2)		3·449
C(6)	C(3)		3·559
C(7)	C(3)		3·583
C(7)	C(4)		3·573
C(11)	C(6)		3·389
C(11)	O		3·514
C(12)	C(4)		3·433
C(12)	O		3·559
C(12)	N		3·524
O	C(1)		3·494
O	C(2)		3·564
C(5)[H(3)]	N	$(\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z)$	3·435[2·44]
H(8)	N		2·96
H(3)	C(5)		2·96

The temperature factors

We should emphasize here that, since the scale factors of the various layer lines were adjusted empirically during the course of the refinement, the coupling between these scale factors and the b_{22} terms of the temperature factor is complete and hence these b_{22} terms are, in principle, not determined. In point of fact, however, the adjustments to the scale factors originally derived from the relative exposure times (see *Experimental*) were small, 5% or less for all layers except the fifth, which was recorded with a different camera; moreover, the final values of b_{22} seem very reasonable. Accordingly, we feel justified in discussing briefly the apparent thermal anisotropies.

In Fig. 6 are shown representations of the thermal ellipsoids derived from the anisotropic temperature factors of Table 2. The maximum mean square amplitudes of thermal motion of the various atoms range from 0·103 Å^2 (corresponding to a B value of 8·15) for C(10) to 0·051 Å^2 for C(4); the minimum amplitudes range from 0·058 Å^2 for C(9) to 0·038 Å^2 for C(6). No obvious combination of rigid-body motions seems capable of explaining the thermal motions; rather, the rings appear to be moving independently of one another. The largest motion is an in-plane libration of the end phenyl group; the center of libration is near C(7) and the r.m.s. amplitude is about 5°. This motion is sufficient to explain the apparent shortening of the C–C bonds in this ring.

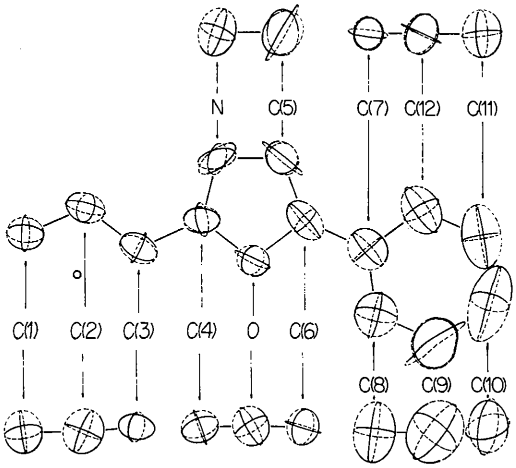

Fig. 6. Ellipsoids representing the thermal motions. The central drawing is a view perpendicular to the best molecular plane (A, Table 4); the top and bottom sets of ellipsoids are viewed parallel to this plane. Lengths of the principal axes are proportional to the mean square displacements $B/8\pi^2$; the scale is arbitrary. An arbitrary pair of eigenvectors is drawn for the degenerate minor axes of C(8).

In a substantial study of organic scintillators, Sangster & Irvine (1956) discuss the fluorescence and scintillation properties of crystalline organic compounds as functions of various structural features of the molecule. The apparent contribution of non-Kekulé-type structures, involving conjugation between the rings and separation of charges, to the over-all structure of POPOP is in good agreement with their conclusions conserning the electronic properties of scintillators.

The work described here was carried out as an undergraduate research project (I.A.).

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