and the true structure factors. Table 5 shows that all R indices are approximately the same, although the agreement between the two sets of data is very bad ($R_1 = 8{\cdot}1\%$).

It is instructive to see how small is the effect on the parameters of appreciable differences in observed intensities, or, alternatively, how sensitive the calculated F values are to small differences in the parameters.

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The Crystal Structure of Bi(anthracene-9,10-dimethylene) Photo-Isomer

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Bi(anthracene-9,10-dimethylene) exists in three modifications referred to as α and β forms and the photo-isomer. The structure of the photo-isomer has been determined and refined by least-squares with three-dimensional data. The crystals are monoclinic, space group $P2_1/a$, with cell dimensions $a = 8{\cdot}56$, $b = 12{\cdot}99$, $c = 9{\cdot}87$ Å, $\beta = 111°\ 39'$.

The structure of the photo-isomer has been compared with preliminary structural information available for the β form.

Introduction

Bi(anthracene-9,10-dimethylene) exists in three modifications referred to as α and β forms and the photo-isomer (Golden, 1961). The modifications arise as follows: crystallization from solution in chloroform in the dark results in the α or β form. The photo-isomer is obtained from the α or β form by the action of visible light, or by recrystallization from chloroform in the presence of light. The photo-isomer changes back into the β form in the dark. Cell dimensions and space groups of the three modifications were determined by J.R.C. Duke and are given by Golden (1961). The object of this paper is to present a complete structure determination of the photo-isomer and some information about the structures of the α and β forms, which leads to a comparison of the three modifications.

Experimental

Crystal data

Bi(anthracene-9,10-dimethylene) photo-isomer $(C_{16}H_{12})_2$.
M.W. 408·544.
Monoclinic
$a = 8{\cdot}56 \pm 0{\cdot}07$ Å
$b = 12{\cdot}99 \pm 0{\cdot}09$.
$c = 9{\cdot}87 \pm 0{\cdot}08$.
$\beta = 111°\ 39'$.
Density, calculated, 1·333 g.cm^{-3}.
measured, 1·326 g.cm^{-3} (S.T.P.).
Total number of electrons per unit cell, $F(000) = 432$.
Systematic absences: hkl none.
$h0l$ $h = 2n+1$
$0k0$ $k = 2n+1$.
Space group $P2_1/a$.

Description of crystals

Crystals of bi(anthracene-9,10-dimethylene) were supplied by Dr J.H. Golden, Ministry of Aviation, E.R.D.E. They are sparingly soluble in benzene and chloroform and crystals suitable for X-ray work were obtained by recrystallization from chloroform in daylight. The crystals are pale yellow with {010}, {001} and {110} faces. The dimensions of the two crystals used for collecting intensity data were $0{\cdot}45 \times 0{\cdot}42 \times 0{\cdot}32$ mm^3 for the b-axis data and $0{\cdot}42 \times 0{\cdot}30 \times 0{\cdot}20$ mm^3 for the a-axis data. The density was determined by flotation in an aqueous potassium iodide solution at S.T.P.

X-ray data

The unit-cell dimensions were redetermined from oscillation photographs about the b axis, using the layer line separation to determine b, and a number of high order reflexions to refine values for a, c and β. Space group absences were found from Weissenberg photographs. The main data were collected from equi-inclination Weissenberg photographs for $b=0 \rightarrow 11$ and supplemented by data from a crystal mounted about [a] for $a=0 \rightarrow 5$. In both cases the zero layer photographs were retaken in order to obtain an estimate of any change in the crystal during X-ray exposure, exposure to light and room temperature. Film packs were used and 1263 and 556 reflexions were observed in the two cases respectively. The blackening of the spots produced by the $K\alpha$ and $K\beta$ radiations of Cu was estimated by visual comparison with an intensity scale and these values were corrected by the appropriate Lorentz-polarization factors and the Phillips correction, which makes allowance for the extension of spots on upper layer Weissenberg photographs.

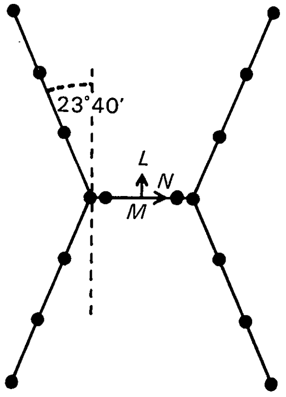

Fig. 1. Projection of molecule on a plane normal to the molecular axis *M*.

Structure analysis

A preliminary set of data, approximately 100 reflexions, was used to establish a trial structure of the photo-isomer. It was assumed in turn that the half-molecules are bent through 2 × 20°, 2 × 25° or 2 × 30° (Fig. 1) and molecular coordinates were generated for various rotations of the molecule about the crystal axes a, b, c^* and the molecular axes L, M, N. This was made possible by the use of a program written by Milledge (1962). The best structure, giving an R index of 30%, was made the basis of a refining process using the data collected as described above. Anisotropic temperature factors were calculated and refined for all carbon atoms and the contributions of the hydrogen atoms were added using isotropic temperature factors.

The instability of the photo-isomer sets a particular difficulty and limits the accuracy. The data from photographs $b=9 \rightarrow 11$ were obtained after a break in tak-

Table 1. *Positional and thermal parameters*

The values of U quoted below are defined by the temperature factor exponent
$[-2\pi^2(h^2a^{*2}U_{11}+\ldots+2klb^*c^*U_{23}+\ldots)]$

	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
C(1)	0·3525	−0·0539	0·2844	0·0805	0·0666	0·0513	−0·0103	0·0030	0·0328
C(2)	0·3537	−0·1337	0·3831	0·1066	0·0820	0·0492	−0·0014	−0·0036	0·0488
C(3)	0·2260	−0·2059	0·3465	0·0881	0·0884	0·0669	0·0025	0·0146	0·0317
C(4)	0·0934	−0·2041	0·2134	0·0626	0·0543	0·0558	0·0089	0·0115	0·0266
C(5)	−0·0226	−0·1467	−0·2770	0·0616	0·0594	0·0503	−0·0138	−0·0049	0·0244
C(6)	0·0617	−0·1164	−0·3729	0·0831	0·1111	0·0513	−0·0062	0·0030	0·0264
C(7)	0·1873	−0·0453	−0·3342	0·0689	0·0924	0·0692	0·0148	0·0148	0·0118
C(8)	0·2367	0·0060	−0·2001	0·0526	0·0535	0·0547	0·0102	0·0122	0·0118
C(9)	0·1988	0·0285	0·0393	0·0505	0·0395	0·0467	−0·0045	0·0003	−0·0181
C(10)	−0·0484	−0·1215	−0·0348	0·0429	0·0542	0·0548	−0·0074	0·0011	−0·0174
C(11)	0·0317	−0·0973	−0·1418	0·0390	0·0241	0·0438	−0·0058	0·0003	0·0042
C(12)	0·1576	−0·0235	−0·1061	0·0328	0·0302	0·0486	0·0022	0·0047	0·0006
C(13)	0·2199	−0·0546	0·1496	0·0460	0·0254	0·0423	−0·0041	−0·0011	0·0077
C(14)	0·0934	−0·1293	0·1138	0·0402	0·0340	0·0445	0·0080	0·0098	0·0055
C(15)	−0·1926	−0·1980	−0·0738	0·0418	0·0427	0·0999	−0·0064	−0·0133	−0·0073
C(16)	0·3248	0·1198	0·0787	0·0558	0·0197	0·1084	−0·0158	−0·0214	−0·0036
H(17)	0·4470	−0·0006	0·3108						
H(18)	0·4452	−0·1359	0·4782						
H(19)	0·2283	−0·2600	0·4169						
H(20)	0·0002	−0·2554	0·1874						
H(21)	−0·1122	−0·2016	−0·3049						
H(22)	0·0280	−0·1489	−0·4679						
H(23)	0·2443	−0·0263	−0·4017						
H(24)	0·3262	0·0611	−0·1717						
H(25)	0·4152	0·1126	0·1756						
H(26)	0·3773	0·1319	0·0064						
H(27)	−0·1530	−0·2521	0·0025						
H(28)	−0·2443	−0·2329	−0·1692						

B (isotropic) for hydrogen atoms = 4·5

The standard deviations calculated for the fractional coordinates of the carbon atoms vary between

0·0006 and 0·0009 for x/a
0·0005 0·0007 y/b
0·0005 0·0008 z/c

ing photographs and the differences between F_{obs} and F_{calc} for data from these photographs stayed systematically higher than for the earlier data. Apparently some changes in the crystal had taken place in the interval. This was confirmed by retaking the zero layer photograph, which showed some changes, although the intensity distribution was still characteristic for the photo-isomer and not for the β form. Therefore only data (1026 reflexions) from the photographs $b=0 \rightarrow 8$ were used for further refinements and this must be borne in mind in assessing the temperature factors.

The final R value was 9·7%. Table 1 gives the positional and thermal parameters and Table 2 the F_{obs} and F_{calc} values using these parameters.

Table 2. *Observed and calculated structure factors*

The values given are $\frac{1}{4}$ the absolute values.

H	K	L	F(OBS)	F(CALC)
2	0	-12	-0.73	-0.58
4	0	-12	1.88	1.69
6	0	-12	1.39	1.19
1	1	-12	-0.60	-1.08
4	1	-12	-0.95	-0.87
5	1	-12	0.86	0.64
6	1	-12	0.79	0.67
7	1	-12	0.82	1.03
3	2	-12	-1.00	-1.03
5	2	-12	0.71	0.86
7	2	-12	0.61	0.58
5	3	-12	-0.88	-1.45
3	4	-12	-0.67	-1.27
4	5	-12	-0.42	-0.69
4	0	-11	1.04	1.34
6	0	-11	0.21	0.38
8	0	-11	0.61	0.18
3	1	-11	2.06	2.05
4	1	-11	1.63	1.22
5	1	-11	-1.24	-1.19
7	1	-11	1.35	0.97
1	2	-11	0.84	0.41
4	2	-11	-1.47	-1.21
5	2	-11	0.61	0.62
6	2	-11	0.47	0.46
8	2	-11	0.84	0.58
1	3	-11	-0.63	-1.04
3	3	-11	-0.49	-0.58
4	3	-11	0.71	0.79
5	3	-11	-1.03	-1.02
7	3	-11	1.22	1.14
8	3	-11	-0.37	-0.55
5	4	-11	-0.94	-1.05
2	5	-11	-0.49	-0.85
6	5	-11	-0.45	-0.30
3	6	-11	-0.48	-0.79
4	6	-11	0.50	0.74
2	7	-11	-0.45	-0.57
2	0	-10	2.64	2.21
4	0	-10	-1.28	-1.46
6	0	-10	-1.09	-0.95
1	1	-10	-1.13	-1.05
3	1	-10	0.64	0.62
4	1	-10	0.75	1.04
8	1	-10	-0.56	-0.32
9	1	-10	-0.81	-0.82
1	2	-10	-1.35	-1.03
2	2	-10	-0.58	-0.61
3	2	-10	1.32	1.67
7	2	-10	-0.64	-0.43
9	2	-10	-1.55	-1.22
2	3	-10	-1.14	-0.99
3	3	-10	-0.81	-1.10
7	3	-10	1.32	1.49
8	3	-10	-0.50	-0.53
1	4	-10	0.32	0.56
2	4	-10	-0.63	-0.77
8	4	-10	0.24	0.31
1	5	-10	0.61	1.01
2	6	-10	-0.60	-0.33
5	7	-10	1.00	1.15
8	7	-10	0.36	0.63
3	8	-10	-0.54	-0.66
4	8	-10	0.54	0.90
2	0	-9	-1.41	-0.37
4	0	-9	-3.79	-3.82
6	0	-9	-0.24	-0.40
8	0	-9	-0.63	-0.79
10	0	-9	0.50	0.61
1	1	-9	2.06	2.39
2	1	-9	4.37	4.51
3	1	-9	-5.46	-4.96
8	1	-9	-0.92	-0.69
9	1	-9	-0.53	-0.50
10	1	-9	-0.57	-0.61
1	2	-9	2.53	2.34
2	2	-9	1.29	1.21
3	2	-9	2.05	2.12
4	2	-9	-1.81	-1.59
6	2	-9	2.48	2.28
8	2	-9	-1.35	-1.10
9	2	-9	-2.09	-1.62
10	2	-9	-0.49	-0.59
1	3	-9	1.36	1.89
2	3	-9	2.38	2.41
5	3	-9	1.88	1.95
6	3	-9	-0.28	-0.52
7	3	-9	1.13	1.26
9	3	-9	-1.20	-1.36
2	4	-9	0.70	0.87
5	4	-9	-0.67	-0.56
6	4	-9	2.23	2.30
7	4	-9	0.61	0.79
9	4	-9	-0.42	-0.53
1	5	-9	1.75	1.97
3	5	-9	-0.68	-0.91
4	5	-9	-2.65	-2.58
5	5	-9	1.11	1.25
8	5	-9	0.52	0.68
9	5	-9	1.00	0.65
3	6	-9	-0.67	-0.61
5	6	-9	-1.59	-1.89
7	6	-9	1.04	1.05
4	7	-9	-1.75	-2.10
8	7	-9	1.04	1.09
7	8	-9	0.71	0.86
2	0	-8	2.88	2.84
4	0	-8	-4.25	-3.94
6	0	-8	2.71	2.71
8	0	-8	1.35	1.21
10	0	-8	-0.64	-0.29
1	1	-8	5.33	5.31
2	1	-8	2.95	2.79
4	1	-8	2.59	2.20
5	1	-8	-1.79	-1.57
6	1	-8	-0.93	-0.68
7	1	-8	1.81	1.70
9	1	-8	-0.39	-0.18
1	2	-8	6.07	5.96
2	2	-8	3.48	3.45
3	2	-8	3.59	3.25
4	2	-8	-4.26	-4.09
6	2	-8	2.33	2.51
8	2	-8	-1.89	-1.89
9	2	-8	-0.60	-0.46
1	3	-8	3.14	3.21
2	3	-8	4.35	4.42
3	3	-8	-2.73	-2.72
4	3	-8	3.42	3.33
5	3	-8	-0.73	-0.79
9	3	-8	-1.33	-1.44
3	4	-8	1.60	1.31
4	4	-8	-2.37	-2.17
5	4	-8	0.70	0.72
6	4	-8	1.43	1.19
8	4	-8	-0.59	-0.56
10	4	-8	-0.31	-0.35
1	5	-8	-1.52	-1.21
3	5	-8	-0.68	-0.61
4	5	-8	-1.44	-1.93
5	5	-8	-1.24	-1.02
7	5	-8	2.03	2.13
1	6	-8	-1.62	-1.74
3	6	-8	-2.80	-3.15
4	6	-8	-1.02	-1.07
5	6	-8	-1.60	-1.76
6	6	-8	1.76	1.90
8	6	-8	0.82	0.90
9	6	-8	1.00	0.77
1	7	-8	0.97	1.20
4	7	-8	-1.99	-2.17
5	7	-8	0.77	0.66
8	7	-8	0.57	0.28
2	8	-8	1.85	1.90
4	8	-8	-0.70	-1.39
5	8	-8	-0.68	-0.85
6	8	-8	0.64	0.36
2	0	-7	6.53	6.48
4	0	-7	-0.82	-0.37
6	0	-7	3.00	2.89
8	0	-7	2.95	3.02
10	0	-7	-0.86	-0.50
1	1	-7	0.99	0.94
2	1	-7	-0.67	-0.91
3	1	-7	2.42	2.53
4	1	-7	-2.83	-2.62
5	1	-7	1.61	1.18
[illegible]	1	-7	2.16	2.15
10	1	-7	0.36	0.40
1	2	-7	1.32	1.28
2	2	-7	1.18	1.13
3	2	-7	-1.09	-0.90
4	2	-7	-1.68	-1.40
5	2	-7	-1.33	-1.38
6	2	-7	-0.61	-0.36
8	2	-7	0.60	0.44
3	3	-7	0.54	0.86
4	3	-7	1.09	0.91
5	3	-7	-3.36	-3.64
7	3	-7	-1.13	-1.12
8	3	-7	-1.91	-1.75
9	3	-7	-0.24	-0.28
10	3	-7	1.85	1.51
1	4	-7	3.09	3.04
4	4	-7	-3.50	-3.59
5	4	-7	3.41	3.18
6	4	-7	-0.68	-0.61
7	4	-7	-1.37	-1.25
8	4	-7	-1.32	-1.17
9	4	-7	0.89	1.05
10	4	-7	-0.69	-0.61
1	5	-7	-0.96	-1.48
2	5	-7	-1.07	-1.03
3	5	-7	0.84	0.96
4	5	-7	2.21	2.14
5	5	-7	-3.51	-3.73
6	5	-7	2.95	2.57
8	5	-7	-0.61	-0.61
9	5	-7	-1.35	-1.14
10	5	-7	1.18	1.26
2	6	-7	1.60	1.65
3	6	-7	-0.99	-1.39
4	6	-7	-2.88	-2.59
5	6	-7	1.83	1.23
8	6	-7	0.61	0.39
9	6	-7	0.71	0.73
2	7	-7	-1.49	-1.70
3	7	-7	-1.13	-1.12
5	7	-7	-0.77	-0.63
6	7	-7	1.57	1.61
7	7	-7	1.96	1.76
8	7	-7	-1.45	-1.58
2	8	-7	2.37	2.54
7	8	-7	-3.22	-3.49
8	8	-7	1.68	1.67
2	0	-6	-1.05	-0.29
4	0	-6	3.26	3.24
6	0	-6	-1.26	-1.24
8	0	-6	2.61	2.33
10	0	-6	-0.64	-0.53
1	1	-6	0.82	0.98
2	1	-6	1.09	0.59
3	1	-6	-0.87	-0.88
4	1	-6	-2.30	-2.23
5	1	-6	0.99	0.79
6	1	-6	1.18	1.40
7	1	-6	1.54	1.61
8	1	-6	-1.73	-1.29
10	1	-6	0.61	0.65
1	2	-6	3.87	3.80
2	2	-6	0.90	0.59
3	2	-6	-4.34	-4.14
4	2	-6	0.79	0.08
5	2	-6	-0.56	-0.54
6	2	-6	-0.74	-0.72
7	2	-6	-0.60	-0.56
8	2	-6	1.77	1.56
9	2	-6	-0.53	-0.22
1	3	-6	-1.62	-1.24
2	3	-6	-1.07	-0.88
3	3	-6	1.46	1.53
4	3	-6	-1.06	-0.74
6	3	-6	-1.88	-1.83
8	3	-6	-1.11	-1.22
9	3	-6	0.27	0.16
10	3	-6	1.42	1.28
2	4	-6	3.26	2.98
3	4	-6	0.89	0.59
6	4	-6	-2.26	-2.04
7	4	-6	-2.30	-2.21
8	4	-6	-0.33	-0.60
9	4	-6	0.96	0.95
10	4	-6	-0.42	-0.25
2	5	-6	-1.09	-0.81
3	5	-6	1.87	1.86
4	5	-6	-0.63	-0.84
5	5	-6	-2.95	-2.92
6	5	-6	2.88	3.14
7	5	-6	-0.99	-1.17
9	5	-6	-0.68	-0.74
10	5	-6	0.39	0.51
1	6	-6	-1.77	-1.60
4	6	-6	-1.19	-1.29
5	6	-6	5.24	5.66
6	6	-6	-2.32	-2.19
10	6	-6	-0.46	-0.29
1	7	-6	-0.74	-0.86
3	7	-6	-1.07	-1.29
5	7	-6	-3.32	-3.46
6	7	-6	2.56	2.61
7	7	-6	1.46	1.61
1	8	-6	-1.03	-0.95
2	8	-6	-1.03	-1.09
5	8	-6	1.69	1.65
6	8	-6	0.71	1.31
7	8	-6	-1.94	-2.06
8	8	-6	0.96	0.69
2	0	-5	4.48	5.64
4	0	-5	5.14	5.52
6	0	-5	-1.88	-1.21
8	0	-5	3.11	3.17
1	1	-5	2.53	2.44
2	1	-5	-3.45	-4.32
3	1	-5	4.27	3.80
4	1	-5	3.12	3.13
5	1	-5	0.99	0.47
6	1	-5	0.50	0.85
7	1	-5	2.49	2.56
8	1	-5	-1.01	-0.88
10	1	-5	0.81	0.48
2	2	-5	-1.42	-1.14
4	2	-5	3.12	3.59
5	2	-5	0.79	0.59
6	2	-5	-1.12	-0.88
7	2	-5	-0.76	-0.69
8	2	-5	0.61	0.45
9	2	-5	0.57	0.70
1	3	-5	2.78	2.53
2	3	-5	-5.43	-4.94
3	3	-5	-2.55	-2.63
5	3	-5	-1.52	-1.57
6	3	-5	-1.73	-1.68
7	3	-5	-2.00	-2.08
9	3	-5	1.11	0.88
10	3	-5	0.86	0.59
1	4	-5	-6.60	-6.14
2	4	-5	-0.95	-0.79
3	4	-5	-3.07	-2.52
4	4	-5	-1.29	-1.55
5	4	-5	0.64	0.23
6	4	-5	-4.13	-3.93
7	4	-5	-1.88	-1.70
8	4	-5	-0.84	-1.00
9	4	-5	0.75	0.68
1	5	-5	0.71	0.99
2	5	-5	-1.14	-1.02
3	5	-5	0.57	0.81
4	5	-5	3.01	2.73
5	5	-5	-5.35	-5.27
6	5	-5	-2.71	-2.71
7	5	-5	-2.30	-1.90
9	5	-5	0.84	0.56
1	6	-5	-2.74	-2.15
2	6	-5	-1.59	-1.40
3	6	-5	-1.07	-1.31
4	6	-5	-1.69	-1.57
5	6	-5	5.98	5.92
7	6	-5	-2.99	-2.61
9	6	-5	-0.53	-0.82
1	7	-5	-1.72	-1.76
3	7	-5	-0.86	-1.21
4	7	-5	5.34	4.79
5	7	-5	4.34	4.03
7	7	-5	-0.76	-0.87
9	7	-5	1.00	0.60
2	8	-5	-1.97	-1.67
3	8	-5	0.85	1.23
4	8	-5	2.73	2.33
5	8	-5	1.87	1.59
6	8	-5	1.31	1.31
9	8	-5	1.21	0.87
2	0	-4	2.78	2.14
4	0	-4	4.42	4.13
6	0	-4	3.82	3.87
10	0	-4	1.13	0.95
1	1	-4	1.06	0.56
2	1	-4	-3.18	-3.62
3	1	-4	2.39	2.21
4	1	-4	-3.54	-3.03
5	1	-4	3.26	2.75
6	1	-4	-2.05	-2.01
7	1	-4	1.43	1.02
8	1	-4	-2.14	-2.10
1	2	-4	-4.00	-3.68
2	2	-4	-6.08	-5.75
3	2	-4	-6.21	-5.99
4	2	-4	5.96	5.55
5	2	-4	-3.46	-2.97
6	2	-4	-1.10	-1.04
7	2	-4	-2.00	-2.23
8	2	-4	-1.43	-1.01
9	2	-4	-0.56	-0.72
10	2	-4	0.54	0.72
1	3	-4	-4.45	-4.65
2	3	-4	-12.31	-12.34
3	3	-4	1.95	2.26
4	3	-4	0.89	0.76
6	3	-4	-2.10	-2.09
7	3	-4	-5.07	-5.38
8	3	-4	-1.51	-1.17
9	3	-4	1.04	1.12
1	4	-4	-3.36	-3.31
3	4	-4	-4.43	-4.60
4	4	-4	-7.45	-7.46
5	4	-4	1.32	1.33
6	4	-4	-1.52	-1.57
7	4	-4	-0.35	-0.73
8	4	-4	-1.41	-1.35
1	5	-4	4.74	4.62
2	5	-4	-6.71	-6.79
3	5	-4	-3.72	-3.33
4	5	-4	7.68	7.46
6	5	-4	-0.67	-0.83
7	5	-4	-2.57	-2.54
9	5	-4	0.59	0.41
1	6	-4	2.30	2.17
2	6	-4	3.84	3.01
3	6	-4	0.82	0.62
5	6	-4	3.41	3.39
6	6	-4	1.35	0.96
7	6	-4	-1.02	-1.05
10	6	-4	0.36	0.60
1	7	-4	2.86	2.93
2	7	-4	-2.84	-2.58
3	7	-4	-0.64	-0.58
4	7	-4	4.88	5.18
5	7	-4	6.17	6.57
6	7	-4	1.39	1.14
7	7	-4	-0.96	-0.80
9	7	-4	0.57	0.25
1	8	-4	-1.07	-1.09
2	8	-4	-1.17	-0.63
4	8	-4	5.54	5.86
5	8	-4	3.72	3.90
9	8	-4	0.79	0.62
2	0	-3	-4.61	-4.47
4	0	-3	-4.04	-3.63
6	0	-3	4.59	4.85
8	0	-3	-4.58	-5.13
1	1	-3	3.96	4.59
2	1	-3	-7.79	-7.74
3	1	-3	-3.37	-3.47
4	1	-3	-3.86	-3.96
5	1	-3	3.22	3.22
6	1	-3	0.84	0.61
7	1	-3	-1.49	-1.89
8	1	-3	-2.51	-2.43
9	1	-3	-2.87	-2.44
1	2	-3	2.42	2.05
2	2	-3	5.95	5.17
3	2	-3	-3.33	-3.31
4	2	-3	-3.22	-3.88
5	2	-3	-4.11	-3.62
6	2	-3	1.54	1.44
7	2	-3	-1.77	-1.86
8	2	-3	-2.65	-2.63
9	2	-3	-0.81	-0.95
10	2	-3	1.52	1.39
1	3	-3	-5.89	-5.71
2	3	-3	-5.11	-4.92
3	3	-3	-4.64	-4.30
4	3	-3	1.38	0.98
5	3	-3	3.06	3.52
7	3	-3	-1.35	-1.33
8	3	-3	-1.60	-1.32
9	3	-3	0.95	0.68
10	3	-3	-2.02	-2.27
1	4	-3	-1.77	-2.04
2	4	-3	0.54	0.64
3	4	-3	8.50	8.30
4	4	-3	-4.33	-4.36
5	4	-3	-2.98	-2.32
6	4	-3	3.23	3.06
9	4	-3	-0.59	-0.88
10	4	-3	1.64	1.73
1	5	-3	-1.10	-0.02
3	5	-3	-7.60	-6.91
4	5	-3	-0.53	-0.64
5	5	-3	4.86	5.25
6	5	-3	0.68	0.79
7	5	-3	0.71	0.68
8	5	-3	0.99	1.01
9	5	-3	0.57	0.43
1	6	-3	2.41	2.08
2	6	-3	1.25	1.08
3	6	-3	-3.26	-3.21
4	6	-3	2.87	2.67
5	6	-3	2.30	2.73
6	6	-3	1.78	1.90
8	6	-3	-1.37	-1.43
9	6	-3	0.57	0.72
10	6	-3	0.35	0.49
1	7	-3	5.07	4.73
2	7	-3	-3.36	-3.39
3	7	-3	5.15	4.93
6	7	-3	0.79	0.99
7	7	-3	-1.16	-1.13
8	7	-3	1.47	1.56
1	8	-3	-3.25	-3.24
2	8	-3	1.00	0.02
3	8	-3	-1.63	-1.35
4	8	-3	4.35	4.64
5	8	-3	2.19	1.85
6	8	-3	-1.59	-0.86
7	8	-3	1.04	1.15
8	8	-3	-1.69	-1.85
2	0	-2	11.45	11.61
4	0	-2	-1.39	-1.17
6	0	-2	2.42	2.50
8	0	-2	-6.08	-5.86
1	1	-2	6.07	5.73
2	1	-2	-12.71	-12.75
3	1	-2	-3.61	-3.32
4	1	-2	1.39	1.28
5	1	-2	1.29	0.93
6	1	-2	2.04	2.16
9	1	-2	-3.79	-3.41
2	2	-2	4.61	3.71
3	2	-2	6.33	6.49
4	2	-2	-2.89	-3.13
5	2	-2	2.99	2.84
6	2	-2	0.82	1.05
7	2	-2	-0.61	-0.85
8	2	-2	-2.14	-2.15
10	2	-2	0.86	0.82
1	3	-2	3.01	2.57
2	3	-2	8.92	8.82
3	3	-2	-7.38	-7.17
4	3	-2	-4.52	-3.93
6	3	-2	1.14	1.19
7	3	-2	1.22	1.20
10	3	-2	-1.19	-1.42
1	4	-2	-0.60	-0.72
2	4	-2	-4.25	-3.46
3	4	-2	5.47	5.65
4	4	-2	-2.02	-1.84
5	4	-2	-2.30	-2.19
6	4	-2	4.16	4.18
8	4	-2	1.00	0.87
9	4	-2	-0.85	-1.24
10	4	-2	0.96	0.93
1	5	-2	-5.54	-5.96
2	5	-2	4.57	4.76
3	5	-2	-1.52	-1.39
4	5	-2	-0.95	-0.77
5	5	-2	3.00	2.68
6	5	-2	-2.54	-2.36
7	5	-2	1.62	1.98
8	5	-2	0.68	0.93
1	6	-2	-1.32	-1.40
2	6	-2	-1.59	-1.69
3	6	-2	-4.04	-4.33
5	6	-2	1.14	1.10
6	6	-2	2.25	2.09
1	7	-2	-1.69	-2.26
2	7	-2	-1.74	-1.60
3	7	-2	3.72	3.15
4	7	-2	2.37	1.61
5	7	-2	-1.05	-0.16
6	7	-2	-0.77	-0.90
7	7	-2	-0.76	-1.22
8	7	-2	1.02	1.09
1	8	-2	-0.83	-1.32
2	8	-2	-1.32	-0.86
4	8	-2	2.80	3.22
6	8	-2	-1.75	-1.58
7	8	-2	1.16	1.11
8	8	-2	-0.76	-0.80
2	0	-1	-9.01	-9.27
6	0	-1	2.32	2.40
8	0	-1	-4.97	-4.93
10	0	-1	0.71	0.58
2	1	-1	9.26	9.23
4	1	-1	4.82	4.49
6	1	-1	0.47	0.69
7	1	-1	-1.42	-1.40
8	1	-1	-0.74	-0.72
9	1	-1	-0.64	-0.51
1	2	-1	0.47	0.47
2	2	-1	-17.84	-17.91
3	2	-1	3.75	4.29
4	2	-1	3.88	3.90
5	2	-1	4.35	4.09
7	2	-1	-0.60	-0.82
8	2	-1	-0.60	-0.35
1	3	-1	-15.95	-16.02
2	3	-1	10.61	10.74
3	3	-1	-2.68	-2.92
4	3	-1	-1.31	-1.60
5	3	-1	2.13	1.85
6	3	-1	0.70	0.57
1	4	-1	9.66	9.14
2	4	-1	-3.66	-4.43
3	4	-1	-6.04	-6.43
4	4	-1	-0.50	-0.54
5	4	-1	-1.05	-1.13
6	4	-1	1.66	1.65
7	4	-1	1.36	1.33
8	4	-1	0.85	0.75
1	5	-1	-1.76	-1.76
2	5	-1	-4.88	-4.26
3	5	-1	-3.63	-3.53
4	5	-1	-1.24	-0.95
5	5	-1	4.76	4.84
1	6	-1	-2.66	-2.97
2	6	-1	-1.77	-1.25
3	6	-1	-3.37	-3.07
4	6	-1	2.17	1.64
7	6	-1	1.36	1.53
8	6	-1	1.14	0.88
1	7	-1	-3.33	-3.66
2	7	-1	-3.21	-2.89
3	7	-1	3.45	3.07
4	7	-1	0.67	1.18
5	7	-1	-1.06	-1.70
7	7	-1	1.11	1.28
1	8	-1	2.54	2.68
2	8	-1	-1.13	-0.95
3	8	-1	-2.30	-2.14
4	8	-1	1.68	1.42
6	8	-1	-1.39	-1.25
2	0	0	-10.46	-10.53
4	0	0	2.31	1.91
6	0	0	2.61	1.74
8	0	0	-2.21	-2.07
2	1	0	4.16	4.95
3	1	0	1.00	0.12
4	1	0	2.76	2.34
5	1	0	5.02	4.77
7	1	0	-2.98	-3.23
8	1	0	-1.04	-1.31
9	1	0	0.43	0.43
1	2	0	11.02	10.95
2	2	0	-9.62	-9.68
3	2	0	5.30	5.37
4	2	0	0.88	0.69
6	2	0	1.53	1.43
7	2	0	-2.34	-2.40
9	2	0	0.71	0.32
1	3	0	-10.22	-10.19
2	3	0	4.10	3.17
3	3	0	-10.84	-10.83
4	3	0	-1.95	-2.01
5	3	0	3.34	3.61
6	3	0	2.04	2.01
1	4	0	5.86	6.34
2	4	0	-16.19	-16.18
3	4	0	-1.10	-0.50
5	4	0	-1.08	-0.89
6	4	0	-0.34	-0.51
7	4	0	1.93	2.42
8	4	0	0.64	0.58
9	4	0	0.50	0.59
1	5	0	-0.44	-1.02
2	5	0	0.71	0.90
3	5	0	-12.32	-12.08
4	5	0	-0.99	-0.86
5	5	0	2.96	3.16
6	5	0	1.86	2.28
1	6	0	5.90	5.42
2	6	0	-4.16	-4.05
4	6	0	1.47	1.06
5	6	0	-0.64	-0.53
7	6	0	0.68	0.74
9	6	0	1.09	0.84
1	7	0	1.81	1.34
2	7	0	-1.80	-2.12
3	7	0	3.77	3.87
6	7	0	-1.50	-1.47
7	7	0	0.93	0.91
1	8	0	1.47	1.22
2	8	0	4.16	4.10
3	8	0	-1.13	-0.88
5	8	0	-3.11	-3.84
2	0	1	0.50	0.90
4	0	1	-1.98	-2.15
6	0	1	-0.48	-0.07
0	1	1	1.42	1.94
1	1	1	6.21	5.99
2	1	1	-4.01	-4.10
3	1	1	-5.39	-5.15
4	1	1	-2.77	-2.90
5	1	1	2.91	2.71
6	1	1	-3.77	-4.25
8	1	1	0.71	0.85
9	1	1	0.56	0.64
0	2	1	8.70	8.75
2	2	1	7.07	5.73
3	2	1	-2.41	-2.00
4	2	1	0.47	0.60
5	2	1	-2.11	-1.63
7	2	1	-3.57	-3.32
8	2	1	0.57	0.82
9	2	1	1.13	1.21
0	3	1	-7.43	-7.42
1	3	1	10.71	10.57
2	3	1	-0.92	-1.22
3	3	1	-2.84	-2.95
4	3	1	-5.65	-5.15
5	3	1	1.99	2.29
6	3	1	-0.94	-0.89
8	3	1	0.67	0.90
1	4	1	-3.11	-2.80
2	4	1	-5.83	-5.56
3	4	1	0.25	0.13
5	4	1	1.92	2.03
9	4	1	0.79	0.74
0	5	1	5.32	4.21
1	5	1	0.79	0.46
2	5	1	-1.43	-1.02
3	5	1	-7.60	-7.90
4	5	1	5.00	5.01
8	5	1	0.59	0.80
9	5	1	-0.39	-0.09
0	6	1	1.54	1.54
1	6	1	2.36	1.99
2	6	1	-4.09	-3.95
3	6	1	7.67	7.44
4	6	1	-2.71	-2.81
8	6	1	-0.99	-0.95
9	6	1	1.07	1.48
0	7	1	3.40	3.04
1	7	1	6.47	5.17
2	7	1	-0.54	-0.63
3	7	1	-2.97	-3.03
4	7	1	3.34	3.81
5	7	1	-0.95	-0.90
6	7	1	-0.96	-1.49
0	8	1	3.40	3.00
1	8	1	-1.20	-1.22
2	8	1	2.46	2.03
3	8	1	2.95	2.97
4	8	1	-1.77	-1.79
5	8	1	-1.39	-1.20
6	8	1	0.89	0.97
7	8	1	-0.62	-0.76
8	8	1	-0.68	-0.77
0	0	2	-7.31	-7.37
2	0	2	-9.93	-9.86
0	1	2	-6.63	-6.64
1	1	2	-3.82	-3.23
3	1	2	-1.45	-1.49
4	1	2	-1.41	-1.29
5	1	2	-2.24	-1.06
6	1	2	-2.87	-3.18
8	1	2	0.31	1.08
9	1	2	1.09	1.09
0	2	2	-2.20	-1.23
2	2	2	4.45	4.53
3	2	2	-5.08	-5.13
4	2	2	0.45	0.40
5	2	2	-0.83	-1.29
6	2	2	-0.89	-1.11
7	2	2	-1.59	-1.32
8	2	2	0.52	0.70
9	2	2	0.57	0.71
0	3	2	1.50	1.15
1	3	2	7.50	6.55
2	3	2	-2.86	-2.02
3	3	2	2.95	2.87
6	3	2	-3.16	-3.38
7	3	2	1.18	0.95
0	4	2	-5.70	-4.62
1	4	2	-3.08	-3.25
2	4	2	4.90	5.43
3	4	2	-3.57	-3.65
4	4	2	2.13	2.31
5	4	2	1.73	2.04
7	4	2	-1.92	-2.05
0	5	2	1.33	0.85
1	5	2	2.81	2.15
2	5	2	-5.49	-5.13
3	5	2	-1.43	-2.14
4	5	2	2.82	2.85
5	5	2	1.57	1.85
6	5	2	-1.79	-1.60
1	6	2	-9.25	-8.38
2	6	2	-0.99	-0.70
3	6	2	4.33	4.28
4	6	2	-1.62	-1.33
5	6	2	0.71	0.73
8	6	2	-0.46	-0.77
0	7	2	1.42	0.96
1	7	2	2.21	2.27
3	7	2	-1.20	-1.10
4	7	2	3.68	4.58
5	7	2	-2.23	-2.42
8	7	2	0.79	0.97
0	8	2	3.96	3.48
1	8	2	1.83	1.51
2	8	2	1.15	1.20
3	8	2	3.20	3.10
4	8	2	-5.15	-5.50
5	8	2	1.69	2.16
6	8	2	1.42	1.26
0	0	3	6.69	6.73
2	0	3	0.35	0.91
4	0	3	0.65	1.11
6	0	3	0.64	0.73
8	0	3	0.63	0.77
0	1	3	-5.82	-5.77
1	1	3	-5.40	-5.43
3	1	3	5.11	4.74
4	1	3	-0.67	-0.97
5	1	3	-0.73	-0.41
6	1	3	-1.08	-1.10
8	1	3	0.57	0.68
0	2	3	-2.40	-2.67
1	2	3	-2.02	-1.86
2	2	3	2.50	1.79
3	2	3	-2.48	-2.21
4	2	3	-3.11	-3.59
5	2	3	-1.98	-2.01
0	3	3	-3.86	-3.70
1	3	3	2.55	2.93
2	3	3	-3.08	-3.06
5	3	3	-3.11	-3.77
6	3	3	-2.40	-2.53
0	4	3	-3.20	-3.58
1	4	3	-1.52	-1.78
2	4	3	-3.29	-2.85
4	4	3	1.63	1.89
5	4	3	-1.51	-1.37
6	4	3	-1.32	-1.03
0	5	3	-6.68	-6.24
2	5	3	-0.78	-0.76
3	5	3	2.46	2.87
4	5	3	2.93	3.10
6	5	3	-1.39	-1.07
0	6	3	1.96	1.76
1	6	3	-2.51	-2.00
2	6	3	2.03	1.94
3	6	3	3.65	3.52
4	6	3	1.52	1.43
8	6	3	0.46	0.49
0	7	3	-2.24	-1.62
1	7	3	-0.98	-0.31
2	7	3	1.71	1.67
3	7	3	1.42	0.97
4	7	3	4.64	3.99
0	8	3	0.56	0.50
1	8	3	1.15	1.21
2	8	3	3.16	3.10
3	8	3	3.90	3.91
4	8	3	-1.98	-2.16
0	0	4	-10.75	-10.67
2	0	4	4.06	3.54
4	0	4	-1.24	-0.69
6	0	4	-1.70	-2.01
0	1	4	-7.34	-7.05
1	1	4	-7.93	-7.25
2	1	4	-3.12	-2.65
3	1	4	1.18	1.31
4	1	4	-1.69	-1.44
5	1	4	-0.92	-0.94
6	1	4	-2.03	-2.08
7	1	4	-0.89	-0.59
0	2	4	-2.76	-2.12
2	2	4	-0.70	-0.09
3	2	4	-2.74	-2.87
4	2	4	-1.38	-1.54
5	2	4	-2.98	-3.15
7	2	4	-0.51	-0.39
0	3	4	-3.32	-3.77
1	3	4	-1.46	-1.19
2	3	4	-3.00	-3.11
3	3	4	2.06	1.79
4	3	4	-1.94	-2.09
6	3	4	-1.64	-1.83
0	4	4	4.55	4.88
1	4	4	-2.46	-2.26
2	4	4	2.06	1.72
3	4	4	2.26	2.47
4	4	4	1.71	1.72
5	4	4	-1.33	-1.15
6	4	4	-0.94	-1.05
0	5	4	-0.50	-0.37
1	5	4	0.79	0.61
3	5	4	5.34	5.64
4	5	4	3.52	3.64
0	6	4	3.09	2.70
1	6	4	-3.18	-3.02
2	6	4	0.79	0.52
3	6	4	8.75	7.83
4	6	4	2.74	2.84
0	7	4	-2.62	-2.61
2	7	4	1.87	1.94
4	7	4	1.81	1.73
0	8	4	-1.28	-1.46
1	8	4	-3.33	-3.28
2	8	4	-2.64	-2.54
3	8	4	1.50	1.37
4	8	4	2.59	1.73
6	8	4	-0.54	-0.44
0	0	5	-3.04	-2.59
2	0	5	-3.47	-2.87
4	0	5	-0.89	-0.66
6	0	5	-3.02	-3.25
0	1	5	-4.58	-4.44
1	1	5	-3.69	-3.52
2	1	5	2.04	1.84
3	1	5	-1.93	-1.79
7	1	5	-2.18	-2.01
0	2	5	-2.19	-1.73
1	2	5	0.50	0.62
2	2	5	-1.26	-1.24
4	2	5	2.04	2.57
6	2	5	-1.13	-1.10
7	2	5	0.86	0.91
2	3	5	-1.03	-1.52
3	3	5	1.25	1.38
5	3	5	1.42	1.71
0	4	5	1.36	1.29
1	4	5	-2.77	-2.88
2	4	5	1.14	0.61
3	4	5	1.00	0.95
4	4	5	3.51	3.62
5	4	5	0.68	0.93
0	5	5	1.99	1.77
2	5	5	3.09	3.41
3	5	5	1.95	2.03
7	5	5	0.36	0.41
0	6	5	0.61	0.53
1	6	5	-2.89	-2.73
2	6	5	-1.84	-1.88
3	6	5	3.02	3.36
4	6	5	1.54	1.85
0	7	5	-1.91	-1.45
1	7	5	-2.99	-3.18
2	7	5	1.99	1.70
3	7	5	1.62	1.79
4	7	5	-1.46	-1.36
1	8	5	-3.86	-4.15
2	8	5	-1.05	-1.27
3	8	5	-1.04	-1.29
6	8	5	-0.42	-0.81
0	0	6	1.36	0.33
2	0	6	-1.93	-2.18
4	0	6	2.67	2.68
6	0	6	-1.10	-1.09
0	1	6	0.64	0.42
1	1	6	1.14	1.06
2	1	6	1.04	0.80
3	1	6	-0.74	-1.09
4	1	6	-0.26	-0.25
5	1	6	1.25	1.47
6	1	6	1.15	1.03
7	1	6	-1.04	-1.30
0	2	6	1.46	1.85
1	2	6	0.82	0.81
2	2	6	-1.89	-1.60
4	2	6	1.60	1.68
5	2	6	1.18	1.17
7	2	6	1.39	1.46
0	3	6	-3.81	-3.65
1	3	6	2.04	1.98
2	3	6	0.59	0.67
3	3	6	-0.58	-0.61
4	3	6	0.59	0.94
6	3	6	0.86	1.19
0	4	6	1.61	1.54
2	4	6	-3.72	-4.16
4	4	6	0.36	0.76
0	5	6	-1.64	-1.44
1	5	6	-3.11	-3.16
2	5	6	2.96	2.56
4	5	6	-0.81	-0.87
0	6	6	-2.38	-2.35
1	6	6	3.34	3.81
3	6	6	-1.44	-1.50
5	6	6	-0.98	-1.34
1	7	6	-1.12	-1.10
2	7	6	0.79	1.43
3	7	6	0.77	0.79
4	7	6	-0.85	-1.48
5	7	6	0.57	0.86
0	8	6	-1.56	-1.68
1	8	6	-1.59	-1.41
2	8	6	2.55	2.58
0	0	7	-1.21	-1.07
4	0	7	1.64	1.57
0	1	7	-0.87	-0.94
2	1	7	-0.92	-1.07
3	1	7	1.28	1.22
0	2	7	2.60	2.47
2	2	7	-1.60	-1.40
3	2	7	-0.61	-0.88
0	3	7	-1.91	-1.70
1	3	7	-2.41	-2.23
4	3	7	0.67	0.86
6	3	7	0.57	0.61
0	4	7	-1.38	-1.90
1	4	7	2.03	1.87
2	4	7	-1.00	-0.98
0	5	7	1.52	1.27
1	5	7	-2.77	-2.90
0	6	7	-2.09	-2.08
1	6	7	0.71	1.23
2	6	7	0.86	0.91
1	7	7	1.81	1.98
4	7	7	-1.13	-1.09
0	8	7	-0.71	-0.90
0	0	8	2.24	1.84
2	0	8	0.90	1.51
4	0	8	0.40	0.50
0	1	8	-1.91	-1.98
1	1	8	-1.73	-1.82
2	1	8	-1.06	-1.12
3	1	8	0.86	1.23
1	2	8	-0.60	-0.90
2	2	8	-0.60	-0.82
4	2	8	0.47	0.75
0	3	8	1.07	1.11
1	3	8	-2.99	-3.59
2	3	8	-1.17	-1.13
0	4	8	-2.98	-2.93
2	4	8	-0.31	-0.88
4	4	8	0.49	0.64
0	5	8	2.48	2.55
1	5	8	-0.99	-1.35
1	6	8	0.68	0.90
2	6	8	-0.62	-0.10
3	6	8	-0.53	-0.96
0	7	8	1.11	1.46
4	7	8	-0.35	-0.79
1	8	8	0.81	0.94
0	0	9	-1.17	-0.80
2	0	9	-1.04	-0.77
4	0	9	0.32	0.35
1	1	9	-0.71	-0.89
3	1	9	-0.38	-0.23
1	2	9	-1.43	-1.26
2	2	9	-0.54	-0.71
3	2	9	-0.21	-0.27
4	2	9	0.39	0.63
0	3	9	-1.03	-1.12
3	3	9	0.52	0.93
4	3	9	-0.33	-0.45
0	4	9	1.55	1.61
1	4	9	-0.31	-0.67
2	5	9	0.54	0.39
1	6	9	1.22	1.53
0	7	9	0.99	0.69
0	0	10	-0.56	-0.17
2	0	10	-0.99	-1.07
[illegible]	1	10	0.36	0.42
1	2	10	0.56	0.98
2	4	10	0.72	1.02
0	5	10	-0.98	-1.35
1	5	10	0.49	0.75
1	6	10	-0.43	-0.50
0	8	10	0.63	1.00
0	0	11	-0.52	-0.15
1	1	11	-0.47	-0.28

Results and discussion

Fig. 2 shows the bond lengths and angles. The calculated standard deviations of the bond lengths vary between 0·009 and 0·014 Å. The molecules lie on centres of symmetry and the packing is shown in Fig. 3. The angle of bending of the half-molecules is 2 × 23° 40′ (Fig. 1), which is almost the same as found in dipara-anthracene (Ehrenberg, 1966). All bonds have normal values within the limits of error, except perhaps C(6)–C(7) = 1·36 Å, which is short. The distance between C(9) and C(10)′ of the centrosymmetrically related part of the dimer is 1·77 Å.

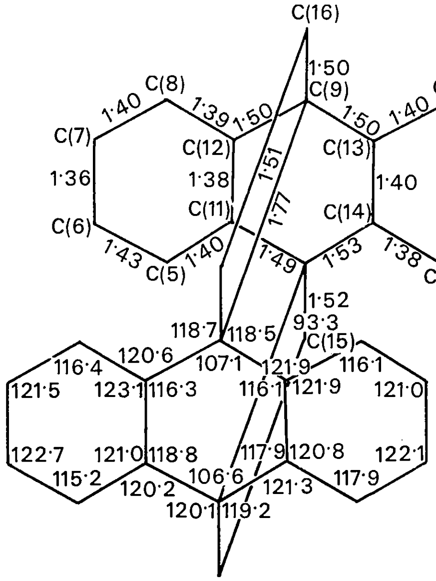

Fig. 2. Bond lengths (Å) and angles (°).

A small number of photographs of the α and β forms, provided by Mr J. R. C. Duke of E.R.D.E., were also examined. Approximate positions of the molecules in these forms were determined, from which the changes introduced by the transition into the photo-isomer could be inferred. The molecules in the α and β forms have the same configuration, but in the β form they are situated on centres of symmetry as in the photo-isomer, whereas in the α form they are in general positions with their centres approximately at $x=\frac{1}{4}$, $y=\frac{1}{2}$, $z=\frac{1}{4}$. Some of these analyses were carried out by Dr H. J. Milledge.

In the β form the distance between the 9 and 10′ positions of anthracene is 2·7 Å, and this is probably also the case in the α form. In dipara-xylylene the corresponding distance is 2·83 Å (Brown, 1953). The reduction of this distance to the value of 1·77 Å in the photo-isomer must imply a very strong interaction between the atoms concerned. This interaction is also suggested by the infrared spectrum of the photo-isomer in the 5 to 6·5 micron region, as shown by Golden (1961). Atoms C(9), C(16), C(10)′, and C(15)′ complete a four-membered ring, if this strong interaction is regarded as a bond. The bond is broken when the photo-isomer changes into the α or β form.

It may be of interest to note that the length of C(6)–C(7) in dipara-anthracene (Ehrenberg, 1966) is also shorter than expected as in the case of the photo-isomer. The molecules of these two substances have

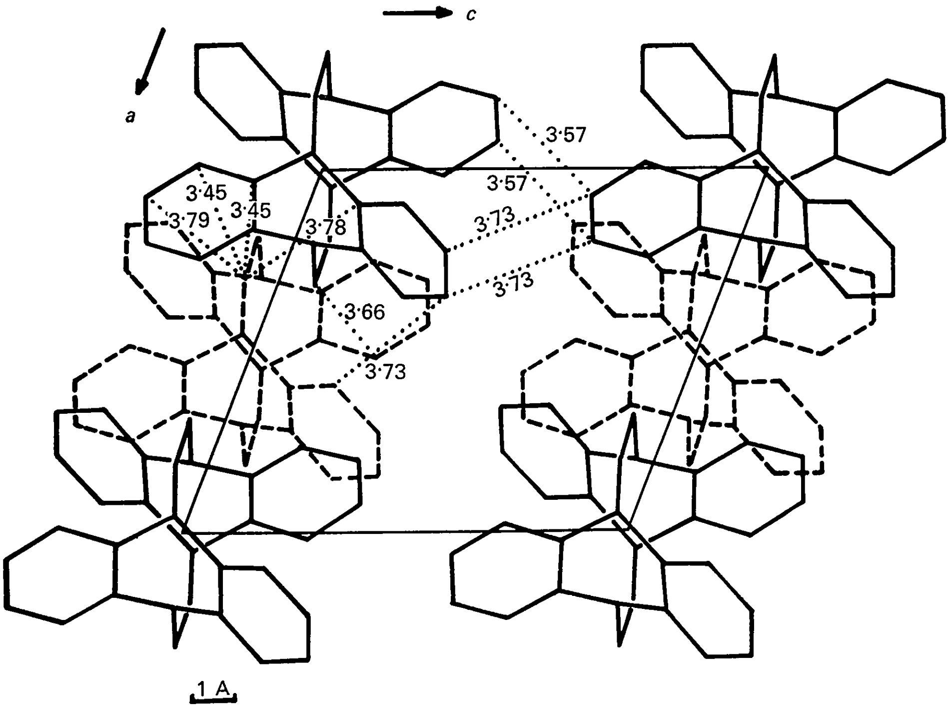

Fig. 3. Projection of structure along [*b*].

similar packing in the unit cell and this bond is involved in a close contact between molecules at (000) and ($\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$) in dipara-anthracene and between molecules at (000) and (001) in the photo-isomer.

I wish to thank Dame Kathleen Lonsdale, F.R.S., for suggesting the problem and for continued encouragement, and the Department of Scientific and Industrial Research for a research grant. I am specially grateful to Dr Golden and Mr Duke for providing the material and some photographs and to Dr Milledge for help and useful discussions.

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The Crystal Structures of Two Sulphur-Nitrogen Compounds with (S–N)$_3$ Rings
I. α-Sulphanuric Chloride, α (NSOCl)$_3$

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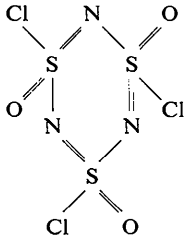
α-Sulphanuric chloride, α(NSOCl)$_3$ is orthorhombic with $a=7{\cdot}552$, $b=11{\cdot}540$, and $c=10{\cdot}078$ Å; the space group is $Pnma$ (D_{2h}^{16}) and there are 4 molecules in the unit cell. Independent three-dimensional investigations have shown that the molecule exists as the chair form with the chlorine atoms in the axial positions. The mean bond lengths, with e.s.d. are: S–N 1·571 (0·004), S–Cl 2·003 (0·003) and S–O 1·407 (0·007) Å; and the bond angles: N–S–N 112·8 (0·4), S–N–S 122·0 (0·4), N–S–O 111·9 (0·3$_5$), N–S–Cl 106·3 (0·3); and O–S–Cl 107·9° (0·3$_5$). The fact that the S–N bonds are all short, and equal, indicates the presence of delocalized p_π–d_π bonds.

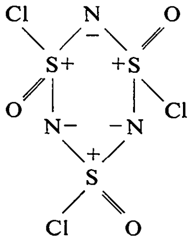
Introduction

The potential aromatic character of the cyclic phosphonitrilic halides and the thiazyl halides has been recognized for some time and has been discussed in detail (Craig, 1959; Dewar, Lucken & Whitehead, 1960; Cruickshank, 1961*a*; Davies, 1962; Craig & Paddock, 1962). Recent X-ray studies on several trimeric and tetrameric phosphonitrilic compounds have shown that in each case the P–N bonds are equal, and short. However, in the case of the thiazyl halides, an X-ray investigation of (NSF)$_4$ showed the molecule to have alternate long and short S–N bonds (Wiegers & Vos, 1962). It therefore seemed worth while to investigate other potentially aromatic (NS$^{\text{IV}}$)$_n$ and (NS$^{\text{VI}}$)$_n$ systems.

Several modifications of sulphanuric chloride, (NSOCl)$_3$, are known. Chemical evidence suggests that both the α and the β forms contain an (NS)$_3$ ring (Kirsanov, 1952; Goehring, 1957). Kirsanov (1952) proposed the structures I and II,



(I)



(II)

and on the basis of their physical properties suggested that the α was the *trans* and the β the *cis* compound.

The structure of the α form has been determined simultaneously in two laboratories, and has been briefly reported by both groups: Banister & Hazell (1962), and Wiegers & Vos (1962). In both cases three-dimensional anisotropic refinements were carried out. Hazell, with 590 visually estimated intensities, refined by the method of least-squares to a discrepancy index of $R=0{\cdot}11$; Wiegers & Vos, with 503 photometrically measured intensities, refined by Fourier methods to $R=0{\cdot}047$. The two structure determinations are described, and results are discussed in terms of the more accurate determination, *i.e.* that of Wiegers & Vos; a compari-

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