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Molecular Complexes Exhibiting Polarization Bonding. IV. The Crystal Structure of the Anthracene-*s*-trinitrobenzene Complex

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The crystal structure of the 1:1 complex formed between anthracene and *s*-trinitrobenzene has been determined at room temperature and at low temperature (*ca.* −100 °C). The structure is basically the same at the two temperatures though there are small differences in atomic positions. The crystals are monoclinic with four molecules of complex in a cell of dimensions $a = 11{\cdot}70$, $b = 16{\cdot}20$, $c = 13{\cdot}22$, all $\pm 0{\cdot}02$ Å, $\beta = 132{\cdot}8° \pm 0{\cdot}5°$ at room temperature, and $a = 11{\cdot}35$, $b = 16{\cdot}27$, $c = 13{\cdot}02$, all $\pm 0{\cdot}02$ Å, $\beta = 133{\cdot}2° \pm 0{\cdot}5°$ at low temperature, giving the maximum contraction approximately along the $[10\bar{3}]$ crystal direction. The space group is $C2/c$. The structure has been determined at each temperature by three-dimensional Fourier and least-squares methods. The component molecules are stacked alternately, each in two different orientations, in infinite columns along the *c* axis and the most important intermolecular contacts are approximately along this direction.

Introduction

The complex between anthracene, $C_{14}H_{10}$, and *s*-trinitrobenzene, $C_6H_3(NO_2)_3$, is one of the series of trinitrobenzene complexes discussed briefly in part III (Wallwork, 1961). The conclusion drawn for the series as a whole was that if there are charge transfer forces operating in the crystal lattices, they must be weak. On the other hand the orange colour of the crystals of the anthracene complex and the evidence from spectroscopic studies of the complex in solution (Briegleb & Czekalla, 1955; McGlynn & Boggus, 1958) suggest that there is a certain amount of charge transfer. Since this complex is one of the more highly coloured and one of the more stable of the aromatic hydrocarbon–trinitrobenzene series, it was felt that a detailed crystallographic examination would be of interest.

Experimental

Crystals were deposited slowly as orange needles after warm solutions of the components in ethanol had been mixed and allowed to cool. In polarized light at room temperature, the crystals exhibited pleochroism (with colours ranging from orange to yellow) with the maximum absorption of light when the electric vector was parallel to the needle axis. At the low temperature (*ca.* −100 °C) attained by blowing the vapour from boiling liquid nitrogen over the crystal, its general

colour changed to pale yellow, and in polarized light the pleochroic colours ranged from pale yellow to pale green, but with the direction of maximum absorption still parallel to the needle axis.

X-ray photographs were taken by the multiple-film Weissenberg technique, those at low temperature (*ca.* −100 °C) being obtained by the method described elsewhere (Brown & Wallwork, 1962). At room temperature complete three-dimensional data (327 reflexions) were obtained up to the point of fade-out of the reflexions, but for the low-temperature data the apparatus restricted the observable layer lines to those with $\mu < 20°$ so that 919 independent reflexions were observed corresponding to about a half of those within the copper sphere. The intensities were estimated by a microphotometer method (Wallwork & Standley, 1954) and were converted to $|F_o|^2$ and $|F_o|$ by applying the usual corrections. No corrections were made for either absorption or extinction since each of the crystals used for the more accurate low-temperature measurements had a maximum dimension of only about 0.2 mm. In obtaining the room-temperature data the intensities of ten reflexions were only roughly estimated, since the spots were too large for the aperture of the microphotometer. These ten reflexions were subsequently omitted from the final least-squares analysis.

Crystal data

$C_{14}H_{10}.C_6H_3(NO_2)_3$, $M = 391{\cdot}5$. Monoclinic, $a = 11{\cdot}70$, $b = 16{\cdot}20$, $c = 13{\cdot}22$, all $\pm 0{\cdot}02$ Å, $\beta = 132{\cdot}8° \pm 0{\cdot}5°$, $U = 1838{\cdot}4$ Å^3 (at room temperature). $a = 11{\cdot}35$, $b = 16{\cdot}27$, $c = 13{\cdot}02$, all $\pm 0{\cdot}02$ Å, $\beta = 133{\cdot}0 \pm 0{\cdot}5°$, $U = 1758{\cdot}5$ Å^3 (at approx. −100 °C). $F(000) = 808$, Cu $K\alpha$, $\lambda = 1{\cdot}542$ Å, $\mu = 10{\cdot}6$ cm^{-1}. Absent spectra, hkl when $h+k$ odd, $h0l$ when l odd. Space group $C2/c$ (no. 15) or Cc (no. 9). Negative pyroelectric test indicates $C2/c$ and this is confirmed by refinement of the structure.

Structure analysis

The dichroic effect was interpreted in the light of results obtained by Nakamoto (1952) to indicate stacking of the molecules in a plane-to-plane manner down the needle (c) axis. If the space group is $C2/c$, which has an eightfold general position, the four molecules of each type in the cell must occupy special positions. Of those available, the *s*-trinitrobenzene can only occupy (*e*) $0, y, \frac{1}{4}$; $0, \bar{y}, \frac{3}{4}$; $\frac{1}{2}, \frac{1}{2}+y, \frac{1}{4}$; $\frac{1}{2}, \frac{1}{2}-y, \frac{3}{4}$; implying a twofold symmetry axis in the molecule, because the other fourfold positions require a centre of symmetry. The anthracene molecules were placed in the special positions (*a*) $0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$. A trial structure was obtained with the molecules occurring alternately along the c axis and with the planes of the molecules perpendicular to this direction. The orientation of the aromatic rings in the anthracene molecule was found to be the same as that of the aromatic ring in the trinitrobenzene molecule, by the observation of only six intense areas near the 'benzene circle' in the $hk0$ weighted reciprocal lattice.

The structure at room temperature was refined initially by electron-density projections and three-dimensional sections and lines. Thereafter, refinement was carried out by nine cycles of least-squares analysis with the SFLS (ISO) program written by J. S. Rollett (Mills & Rollett, 1961). This program refines atomic coordinates, individual temperature factors and the scale factor, using the block diagonal approximation of the normal equations matrix. Hydrogen atoms were not included in the calculations. A weighting scheme,

$$\sqrt{w} = 1 \quad \text{if} \quad |F_o| < F_A$$

otherwise

$$\sqrt{w} = F_A/|F_o|$$

was employed, and scattering factors of Berghuis (Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal, 1955) for carbon and of Freeman (1959)

Table 1. *Atomic parameters and their standard deviations (room temperature)*

Atom	x/a	y/b	z/c	B	σ_x	σ_y	σ_z
C(1)	−0·011	0·087	−0·018	5·3 Å^2	0·042 Å	0·029 Å	0·042 Å
C(2)	0·143	0·044	0·097	5·5	0·037	0·026	0·037
C(3)	0·283	0·098	0·182	4·7	0·039	0·031	0·040
C(4)	0·265	0·181	0·156	5·9	0·042	0·031	0·044
C(5)	0·116	0·222	0·053	8·0	0·048	0·036	0·049
C(6)	−0·020	0·172	−0·035	5·2	0·042	0·029	0·042
C(7)	−0·149	0·035	−0·107	2·4	0·035	0·024	0·033
C(8)	0·145	0·123	0·349	2·6	0·035	0·024	0·036
C(9)	0·136	0·041	0·344	4·8	0·042	0·028	0·042
*M*C(1)	0·000	−0·009	0·250	5·3	0·000	0·047	0·000
*M*C(2)	0·000	0·168	0·250	3·7	0·000	0·039	0·000
N(1)	0·317	−0·007	0·467	5·9	0·034	0·026	0·034
*M*N(1)	0·000	0·247	0·250	6·7	0·000	0·039	0·000
O(1)	0·120	0·292	0·330	5·9	0·027	0·021	0·029
O(2)	0·275	−0·075	0·432	9·0	0·034	0·026	0·034
O(3)	0·410	0·041	0·541	8·9	0·034	0·026	0·034

for oxygen and nitrogen were used. The reflexions too weak to be observed as well as the ten roughly estimated intensities referred to above were omitted from the analysis. Convergence was reached with a reliability index of 0·180.

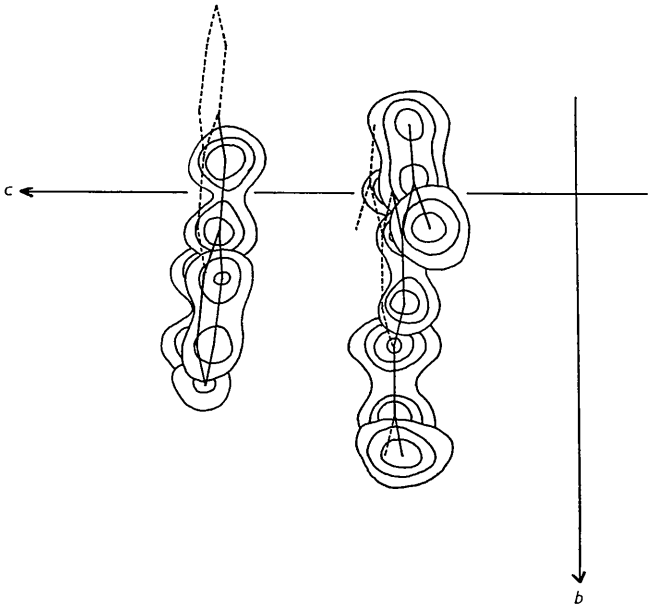

Fig. 1. Composite Fourier diagram of sections parallel to (100) (room temperature). Contours at 2, 3, 4, ... e.Å^{-3}.

The final composite electron-density diagram is shown in Fig. 1 and final coordinates, standard deviations (derived from the least-squares variances) and molecular dimensions are summarized in Tables 1–3. The molecular dimensions and intermolecular approaches less than 3·6 Å were calculated with the use of the distance–angle routine of R. A. Sparks (Mills & Rollett, 1961).

The X-ray photographs at low temperature showed that the structure must undergo very little change on cooling. The low temperature structure was therefore assumed initially to have the same atomic positions as at room temperature and was then refined by

Table 2. *Bond lengths and their standard deviations (room temperature)*

Bond	Length (Å)	σ (Å)	Bond	Length (Å)	σ (Å)
C(1)–C(2)	1·52	0·04	C(8)–C(9)	1·34	0·04
C(1)–C(6)	1·40	0·04	C(8)–*M*C(2)	1·45	0·03
C(1)–C(7)	1·45	0·04	C(9)–*M*C(1)	1·42	0·04
C(2)–C(3)	1·49	0·04	C(9)–N(1)	1·75	0·04
C(2)–C(7′)	1·28	0·04	*M*C(2)–*M*N(1)	1·28	0·05
C(3)–C(4)	1·37	0·04	N(1)–O(2)	1·17	0·04
C(4)–C(5)	1·45	0·05	N(1)–O(3)	1·14	0·04
C(5)–C(6)	1·42	0·05	*M*N(1)–O(1)	1·26	0·03

Table 3. *Bond angles and their standard deviations (room temperature)*

Atoms	Angle	σ	Atoms	Angle	σ
C(2)–C(1)–C(6)	122°	6°	C(9)–C(8)–*M*C(2)	117°	5°
C(2)–C(1)–C(7)	117	3	C(8)–C(9)–*M*C(1)	128	6
C(6)–C(1)–C(7)	121	6	C(8)–C(9)–N(1)	113	5
C(1)–C(2)–C(3)	115	3	*M*C(1)–C(9)–N(1)	119	3
C(1)–C(2)–C(7′)	120	3	C(8)–*M*C(2)–*M*N(1)	120	2
C(3)–C(2)–C(7′)	124	4	C(9)–N(1)–O(2)	97	5
C(2)–C(3)–C(4)	119	6	C(9)–N(1)–O(3)	110	3
C(3)–C(4)–C(5)	125	6	O(2)–N(1)–O(3)	152	6
C(4)–C(5)–C(6)	118	4	*M*C(2)–*M*N(1)–O(1)	125	2
C(1)–C(6)–C(5)	121	6	C(9)–*M*C(1)–C(9′)	111	3
C(1)–C(7)–C(2′)	122	6	C(8)–*M*C(2)–C(8′)	120	2
			O(1)–*M*N(1)–O(1′)	110	6

Table 4. *Atomic parameters and their standard deviations (low temperature)*

Atom	*x/a*	*y/b*	*z/c*	*B*	σ_x	σ_y	σ_z
C(1)	−0·0091	0·0862	−0·0175	0·9 Å^2	0·011 Å	0·010 Å	0·012 Å
C(2)	0·1431	0·0464	0·0915	0·8	0·011	0·010	0·012
C(3)	0·2842	0·0975	0·1833	1·3	0·012	0·010	0·013
C(4)	0·2762	0·1810	0·1655	2·1	0·014	0·011	0·016
C(5)	0·1258	0·2196	0·0547	1·8	0·014	0·010	0·014
C(6)	−0·0143	0·1733	−0·0355	1·6	0·014	0·010	0·014
C(7)	−0·1501	0·0383	−0·1083	1·0	0·011	0·010	0·013
C(8)	0·1466	0·1260	0·3517	1·4	0·014	0·010	0·014
C(9)	0·1400	0·0427	0·3471	1·6	0·014	0·010	0·016
*M*C(1)	0·0000	−0·0041	0·2500	1·7	0·000	0·015	0·000
*M*C(2)	0·0000	0·1660	0·2500	0·9	0·000	0·013	0·000
N(1)	0·2978	−0·0035	0·4524	2·4	0·012	0·010	0·014
*M*N(1)	0·0000	0·2556	0·2500	1·2	0·000	0·011	0·000
O(1)	0·1288	0·2910	0·3388	1·4	0·009	0·007	0·009
O(2)	0·2896	−0·0778	0·4360	2·6	0·010	0·008	0·010
O(3)	0·4129	0·0368	0·5419	2·2	0·010	0·008	0·010

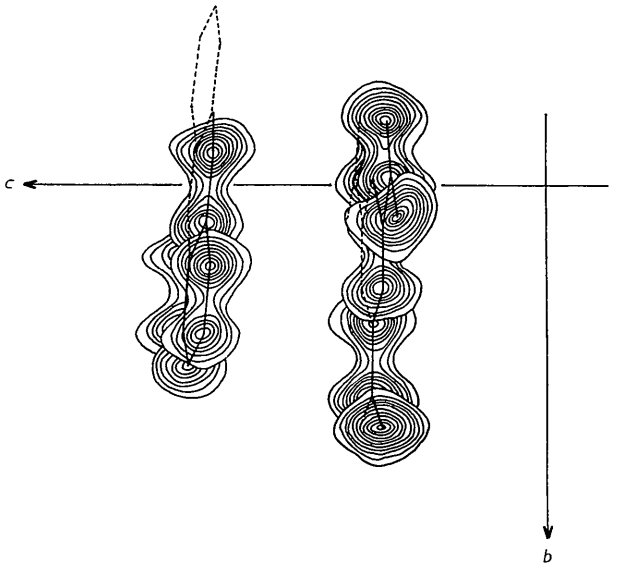

Fig. 2. Composite Fourier diagram of sections parallel to (100) (low temperature). Contours as in Fig. 1.

three-dimensional Fourier sections and by least-squares analysis, using the same scattering factors and weighting scheme as before.

Six cycles of least-squares refinement were carried out, refining positional and isotropic temperature parameters for all atoms except hydrogen. The refinement converged with a reliability index of 0·162.

Table 5. *Bond lengths and their standard deviations (low temperature)*

Bond	Length (Å)	σ (Å)	Bond	Length (Å)	σ (Å)
C(1)–C(2)	1·44	0·01	C(8)–C(9)	1·35	0·01
C(1)–C(6)	1·43	0·01	C(8)–*M*C(2)	1·39	0·01
C(1)–C(7)	1·41	0·01	C(9)–*M*C(1)	1·40	0·01
C(2)–C(3)	1·44	0·01	C(9)–N(1)	1·51	0·01
C(2)–C(7′)	1·39	0·01	*M*C(2)–*M*N(1)	1·46	0·02
C(3)–C(4)	1·37	0·01	N(1)–O(2)	1·22	0·01
C(4)–C(5)	1·42	0·02	N(1)–O(3)	1·19	0·01
C(5)–C(6)	1·39	0·02	*M*N(1)–O(1)	1·22	0·01

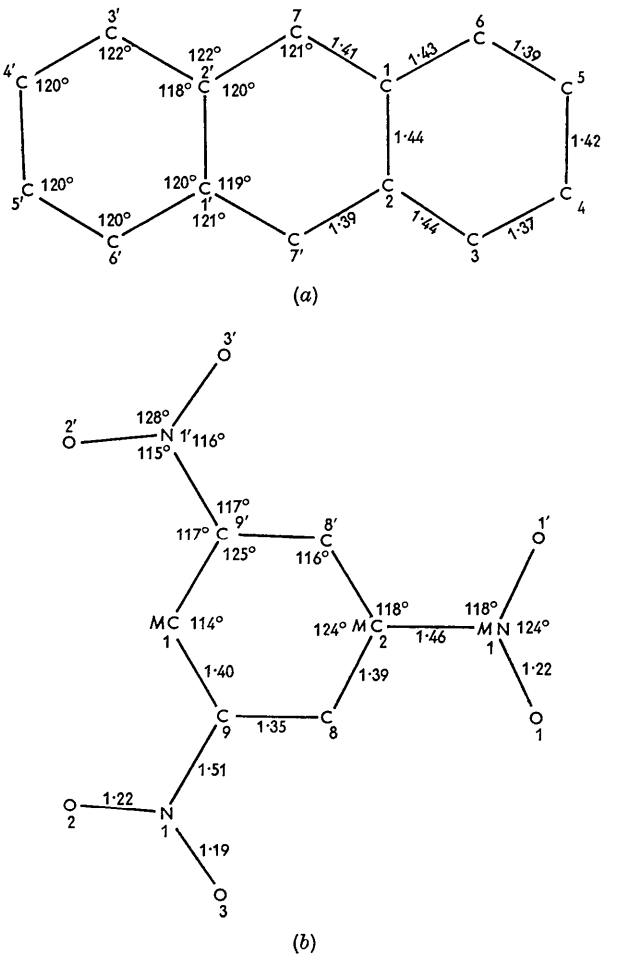

Fig. 3. Molecular dimensions (low temperature).

The final composite electron-density diagram is shown in Fig. 2 with contours drawn at the same intervals as in Fig. 1. Molecular and intermolecular dimensions and standard deviations were calculated in the same way as for the room temperature structure and the results are shown in Figs. 3(*a*) and 3(*b*) and in Tables 4–6.

Table 6. *Bond angles and their standard deviations (low temperature)*

Atoms	Angle	σ	Atoms	Angle	σ
C(2)–C(1)–C(6)	120°	2°	C(9)–C(8)–*M*C(2)	116°	2°
C(2)–C(1)–C(7)	119	1	C(8)–C(9)–*M*C(1)	125	2
C(6)–C(1)–C(7)	121	2	C(8)–C(9)–N(1)	117	2
C(1)–C(2)–C(3)	118	1	*M*C(1)–C(9)–N(1)	117	1
C(1)–C(2)–C(7′)	120	1	C(8)–*M*C(2)–*M*N(1)	118	1
C(3)–C(2)–C(7′)	122	1	C(9)–N(1)–O(2)	115	2
C(2)–C(3)–C(4)	122	2	C(9)–N(1)–O(3)	116	1
C(3)–C(4)–C(5)	120	2	O(2)–N(1)–O(3)	128	2
C(4)–C(5)–C(6)	120	1	*M*C(2)–*M*N(1)–O(1)	118	1
C(1)–C(6)–C(5)	120	2	C(9)–*M*C(1)–C(9′)	114	2
C(1)–C(7)–C(2′)	121	1	C(8)–*M*C(2)–C(8′)	124	2
			O(1)–*M*N(1)–O(1′)	124	2

Table 7. *Observed and calculated structure factors*

(Asterisk line gives h, k)

(a) Room temperature

l	$25F_o$	$25F_c$
* 0 0		
2	1966	2188
6	408	574
* 0 2		
0	2669	3258
1	−1870	−1824
2	2358	2777
3	1734	1469
4	−269	−277
5	1266	1614
6	−442	−448
* 0 4		
0	2350	2191
2	742	664
3	1162	1089
4	496	393
5	1388	1359
6	−878	−637
* 0 6		
0	368	14
1	793	1174
4	218	173
5	−218	−143
* 0 8		
0	−1255	−1002
1	−442	−306
2	−680	−586
4	329	415
5	385	527
* 0 10		
0	425	167
3	−445	−533
6	499	577
7	−337	−284
* 0 12		
4	1000	1043
5	258	360
* 1 1		
0	2411	2476
1	−3071	−2953
2	−1003	−1040
7	405	329
8	558	785
−1	1876	1651
−3	−1346	−1087
−4	−1408	−1024
−6	−431	−568
* 1 3		
0	−949	−922
1	518	314

l	$25F_o$	$25F_c$
* 1 3		
2	−1232	−1072
4	−1527	−1599
3	−431	−420
−1	−994	−941
−2	−2692	−3323
−3	1394	1287
−4	−935	−857
−5	−513	−496
−6	−850	−695
−7	626	523
−8	−626	−582
* 1 5		
0	−439	−286
1	−892	−983
2	−1598	−1673
3	−1439	−1224
−1	300	487
−2	1128	1208
−4	269	322
−5	924	987
−6	−1487	−1387
−7	858	819
* 1 7		
0	603	357
1	431	297
4	−326	−506
−1	300	541
−2	−1944	−2094
* 1 9		
0	−703	−511
1	1258	444
−1	688	1010
−4	−283	−313
4	450	421
−5	218	152
−7	317	384
* 1 11		
4	1198	1317
5	340	70
−7	419	572
−8	391	358
* 1 13		
3	714	656
4	694	730
−7	−272	−386
* 1 15		
0	−382	−400
* 2 0		
0	−952	−504

l	$25F_o$	$25F_c$
* 2 0		
−2	−595	−637
2	983	574
8	657	773
* 2 2		
0	−1507	−1673
−1	−810	−670
1	1451	1167
−2	606	600
2	−1196	−1178
−3	−1527	−1491
−4	−558	−576
−5	1000	841
6	569	467
−7	−229	−327
7	547	677
−8	−493	−346
* 2 4		
0	473	503
−1	1092	835
1	450	476
−2	−898	−776
2	−2099	−1963
3	−1567	−1699
−4	640	450
4	−524	−464
5	329	255
−6	−408	−453
−7	572	489
7	249	66
* 2 6		
0	360	355
−1	−1119	−1283
1	−997	−1099
−2	−501	−279
2	−601	−382
−4	−368	−118
−5	−402	−452
−6	−499	−482
* 2 8		
−1	550	578
−2	−1128	−938
−3	−1213	−1277
−4	−555	−493
−7	215	278
−8	351	260
* 2 10		
0	−575	−416
−4	198	187
−5	−244	−297

l	$25F_o$	$25F_c$
* 2 10		
−6	337	228
−7	473	669
−8	382	481
* 2 12		
0	533	311
4	518	493
−7	−218	−159
−8	785	915
* 3 1		
−7	−275	−286
* 3 1		
0	799	810
−1	1283	1126
1	1349	1377
−2	2278	2162
−6	1873	1474
−7	−881	−714
−8	−646	−477
−9	−584	−643
* 3 3		
0	−1099	−1111
−1	1595	1309
1	1691	1796
−2	1442	1426
−3	499	428
−4	1887	1770
−5	−805	−564
−7	−414	−232
−9	−884	−769
* 3 5		
0	717	640
1	873	702
2	−1133	−848
−5	−232	−97
−6	943	898
−7	−431	−375
−8	487	413
3	405	383
−10	−788	−592
−2	323	138
* 3 7		
1	700	772
−2	−513	−587
−4	266	252
−5	−201	−221
−6	−1091	−915
* 3 9		
0	329	385
−3	329	539

l	$25F_o$	$25F_c$
* 3 9		
−4	−620	−616
−5	558	327
* 3 11		
0	1561	1482
1	606	463
−4	−224	−86
−7	241	140
* 3 13		
0	1116	842
−1	671	595
−8	317	440
* 4 0		
0	−697	−547
−2	−734	−926
4	1360	1522
−4	813	805
* 4 2		
0	−705	−683
−1	−779	−583
1	−839	−647
−2	−1482	−1336
−3	−507	−628
4	425	753
−4	−1587	−1413
−6	−708	−330
−7	−535	−208
−8	−1026	−977
2	394	487
* 4 4		
0	−1618	−1390
−1	−2357	−2231
−2	−2485	−2418
−5	1133	1045
−6	−1091	−906
−7	504	292
1	467	338
−3	−435	−286
−10	−518	−441
−11	629	517
* 4 6		
1	−609	−649
−5	1011	1070
−6	−819	−673
−7	−567	−511

l	$25F_o$	$25F_c$
* 4 10		
0	558	483
−4	−295	−358
−5	856	416
* 4 12		
0	1697	1444
* 5 1		
−1	−788	−847
−3	884	860
3	816	862
4	637	622
−5	507	461
−6	575	534
−9	397	449
−2	365	102
* 5 3		
0	−561	−488
−1	−479	−670
−2	−1065	−1018
−3	1201	1145
−4	−448	−403
−5	329	134
−6	445	467
−8	408	345
2	520	347
* 5 5		
0	448	393
−2	−1649	−1441
−7	−212	−146
* 5 7		
−5	−280	−217
−6	−799	−692
−7	−365	−583
* 5 9		
−4	−453	−279
−6	−246	−223
* 5 11		
−1	−935	−638
−4	422	462
* 5 13		
−4	365	296
* 6 0		
0	939	913
−4	416	417
* 6 2		
−1	589	781
−5	484	522
−6	994	1010
−7	−1147	−930
−8	1434	929

l	$25F_o$	$25F_c$
−9	−572	−410
* 6 4		
−3	1173	1422
−4	−938	−745
−5	−261	−206
−6	−309	−304
−8	518	531
−2	−408	−339
* 6 6		
−4	388	215
−5	300	444
−9	−507	−582
* 6 10		
0	−295	−143
−2	612	442
−4	666	698
−7	227	254
* 6 12		
−4	1374	1480
−5	306	206
* 7 1		
0	1247	1387
−1	935	898
−4	−399	−473
−5	−742	−890
−6	−329	−523
−8	−482	−377
−10	−422	−231
−11	−997	−810
−12	652	269
* 7 3		
−4	−1317	−1172
−5	−1179	−1061
−6	−1269	−1183
−7	127	183
−2	380	438
* 7 5		
−5	−334	−458
−6	−992	−1197
* 7 7		
−5	−252	−288
* 7 9		
0	−374	−167
* 7 11		
−4	717	692
−5	−303	−479
−6	280	390
* 8 0		
0	1045	828
−6	263	490
−12	2125	1341
* 8 2		
−10	703	703
−11	−980	−711
−12	833	482
−2	484	203

l	$25F_o$	$25F_c$
* 8 4		
−6	−686	−667
−7	669	784
* 8 6		
−5	382	384
* 8 10		
−4	−340	−271
* 8 12		
−5	−371	−243
−8	470	611
* 9 1		
−4	776	990
−5	431	470
−11	−456	−304
−12	810	497
−3	−334	−175
* 9 3		
−8	−728	−637
* 9 5		
−7	280	326
* 9 11		
−7	272	232
−8	589	785
* 9 13		
−8	224	473
* 10 0		
−4	1128	1409
−16	589	308
* 10 2		
−9	−501	−502
* 10 4		
−10	−850	−647
* 12 0		
−8	584	981

Estimated intensities.

l	$25F_o$	$25F_c$
* 2 0		
−4	10440	7917
* 3 1		
−3	−3363	−4243
−4	9960	7217
−5	1903	1535
* 4 2		
−5	−1840	−943
* 4 0		
−6	−2760	−1318
−8	2160	1290
* 5 1		
−7	−4060	−2168
−8	−4300	−2348
* 6 0		
−8	3520	3031

Table 7 (*cont.*)

(*b*) Low temperature

l	$25F_o$	$25F_c$
0 0		
2	2442	2423
6	362	384
8	−456	−566
10	−1114	−1319
12	322	469
0 2		
0	2657	3229
1	−1745	−1901
2	2657	2938
3	1825	1748
4	−215	−198
5	2040	1956
6	−832	−867
7	336	410
8	−268	−73
10	362	457
11	564	590
12	−188	−208
0 4		
0	2375	2290
2	805	711
3	1261	1221
4	416	287
5	2107	2017
6	−1181	−1038
10	−322	−418
0 6		
0	−295	−118
1	1409	1368
2	−242	−279
3	497	332
5	−416	−237
7	644	494
10	−429	−509
11	362	116
0 8		
0	−1919	−1461
1	−953	−665
2	−993	−939
3	443	518
4	644	650
5	1060	918
0 10		
0	590	348
1	376	326
3	−1114	−1041
4	376	398
5	−523	−540

l	$25F_o$	$25F_c$
0 12		
0	−188	−294
1	−349	−269
2	242	141
3	698	640
4	2201	1915
5	752	670
0 14		
0	−255	−584
1	309	238
2	403	257
3	845	628
4	443	242
5	228	166
0 16		
0	−550	−582
1	778	766
2	−362	−438
3	228	200
4	188	17
5	−322	−267
0 18		
0	242	148
1	161	12
5	684	566
0 20		
2	−376	−380
3	−121	−146
1 1		
0	2201	2378
1	1409	1595
2	−2429	−2910
5	−389	−396
6	−537	−665
−6	−1852	−1636
−7	1664	1550
−8	282	264
−12	−295	−513
1 7		
0	698	480
−1	1060	942
1	792	644
−2	−3087	−3019
2	−228	−255
−3	336	391
3	−376	−263
−4	349	145
4	−537	−564
−5	255	267
1 9		
0	−980	−832

l	$25F_o$	$25F_c$
1 3		
0	−926	−914
−1	−966	−923
1	403	220
−2	−3087	−3705
2	−1261	−997
−3	1275	1286
3	−644	−522
−4	−805	−927
4	−2080	−1883
−5	−376	−305
5	295	61
6	590	674
7	416	563
8	711	998
9	268	397
−6	−711	−641
−7	752	817
−8	−577	−620
−10	577	940
−11	−497	−668
1 5		
0	−456	−445
−1	483	760
1	−1100	−1113
−2	1503	1375
2	−2094	−1835
−3	429	331
3	−2013	−1673
−4	470	537
−5	1610	1580
5	−389	−396
6	−537	−665
−6	−1852	−1636
−7	1664	1550
−8	282	264
−12	−295	−513
1 7		
0	698	480
−1	1060	942
1	792	644
−2	−3087	−3019
2	−228	−255
−3	336	391
3	−376	−263
−4	349	145
4	−537	−564
−5	255	267
1 9		
0	−980	−832

l	$25F_o$	$25F_c$
1 9		
−1	2026	1818
1	899	778
2	523	447
−3	−416	−240
3	−497	−585
−4	−537	−448
4	926	914
−5	644	685
5	−671	−594
1 11		
0	268	153
−1	953	815
1	631	640
2	684	580
−3	322	343
3	−1100	−1113
−4	−590	−494
4	3060	2946
−5	−456	−573
5	537	79
1 13		
−1	−805	−779
1	228	140
−2	−671	−501
2	1074	983
−3	376	301
3	2040	1723
4	1758	1574
−5	−255	−269
5	−564	−697
1 15		
0	−550	−430
−1	−577	−533
1	−295	−196
−2	−899	−957
2	255	461
3	−470	−422
4	497	545
−4	−376	−296
5	282	131
1 17		
0	322	341
−1	−376	−337
−2	−443	−536
5	309	238
1 19		
−1	−376	−346
1	−188	−229
2	−564	−518

l	$25F_o$	$25F_c$
1 19		
3	−134	−103
−4	215	117
2 0		
0	−1127	−856
−2	−537	−690
2	953	761
−4	6428	8394
4	−282	−374
6	−523	−625
8	2080	2221
10	−322	−328
−8	−295	−354
−12	483	464
2 2		
0	−1651	−1646
−1	−725	−636
1	1423	1318
−2	644	765
2	−1382	−1404
2 4		
−3	−1664	−1649
3	−644	−665
−4	−658	−539
4	215	189
−5	792	847
5	−335	−350
−7	−859	−907
−8	−456	−347
2 6		
−1	−416	−518
−2	376	492
−13	−188	−321
6	1087	1206
7	1221	1244
8	671	606
10	188	280
2 8		
3	−470	−422
0	604	427
−1	1275	1142
1	564	669
−2	−1060	−1109
2	−2348	−2074
−3	−429	−580
3	−2067	−1994
−4	590	513
4	−497	−379
−5	215	197
−6	−456	−473
−7	845	790
−8	−416	−469

l	$25F_o$	$25F_c$
2 4		
0	−698	−667
−1	−309	−358
−12	335	343
7	362	232
8	255	162
2 6		
0	537	444
−1	−1771	−1912
1	−1543	−1546
−2	−819	−586
2	−242	−34
3	282	74
−4	−510	−465
4	295	309
−5	−845	−776
−6	−832	−851
−9	590	634
10	−362	−182
2 8		
−1	617	544
−2	−1839	−1446
2	−859	−811
−3	−2724	−2417
3	−416	−273
−4	−1087	−845
−5	−470	−448
2 10		
0	−939	−824
−1	−1006	−974
1	−778	−612
−2	−389	−307
2	644	691
−3	−752	−641
3	−1006	−736
−4	537	405
4	−523	−554
−5	−819	−794
2 12		
0	416	409
−1	−228	−152
1	604	782
−2	228	278
2	−899	−882
−3	−456	−333
3	−309	−35
4	1087	952
5	−282	−108
2 14		
0	−389	−312

l	$25F_o$	$25F_c$
2 14		
−2	−684	−715
2	−738	−597
−3	429	358
3	309	78
4	−872	−760
2 16		
−1	335	370
1	−376	−177
−2	−631	−707
2	−483	−409
−3	1154	1146
−4	−322	−228
5	−389	−303
2 18		
0	−174	−29
−1	309	389
1	510	502
2	−389	−420
−3	174	178
3	−215	−131
−4	295	242
4	−295	−365
2 20		
0	−121	−162
1	−483	−512
−2	−242	−183
−3	322	428
3 1		
0	1181	1112
−1	1060	976
1	1449	1501
−2	2107	2325
2	−268	−119
−3	−4429	−4883
3	389	498
−4	5502	7475
−5	886	1017
−6	1624	1814
−7	−980	640
−8	−671	−569
−9	−1033	−1118
−10	−362	−324
−13	335	424
−14	−349	−393
6	−295	−80
7	1006	1087
3 3		
0	−1543	−1414
−1	1570	1379

l	$25F_o$	$25F_c$
3 3		
1	2053	2045
−2	1423	1592
2	−389	−389
−3	537	312
3	684	736
−4	1946	2082
−5	−805	−858
5	590	561
6	−389	−428
7	−228	−364
−7	−483	−442
−9	−939	−1169
−11	−953	−67
3 5		
0	644	520
−1	443	466
1	1221	1133
−2	228	47
2	−1637	−1482
−3	−134	−145
3	819	679
−4	−121	−196
−5	−322	−123
−6	1329	1206
−7	−765	−608
−8	805	852
−10	−1074	−968
−11	322	244
−13	−255	−264
3 7		
0	−309	−201
−1	684	614
1	1208	1085
−2	−845	−879
2	832	690
−3	443	458
−4	416	405
4	497	639
−5	−134	−124
5	362	278
3 9		
0	537	521
2	−295	−301
−3	1235	1085
3	309	215
−4	−1315	−1145
4	−443	−360
−5	1221	850
5	−778	−775

l	$25F_o$	$25F_c$
3 11		
0	2751	2864
−1	−497	−457
1	1141	813
−2	322	118
2	939	968
3	−1127	−897
−4	470	192
−5	698	642
3 13		
0	1678	1406
−1	1691	1447
1	−537	−588
−2	845	682
2	295	295
−4	−228	−399
4	−215	−122
−5	−617	−556
5	564	579
3 15		
0	376	326
1	295	150
−2	228	224
−4	−819	−901
4	188	79
−5	−671	−577
5	309	267
3 17		
0	−121	−135
−1	228	55
1	295	123
−2	−268	−267
2	403	313
−3	376	327
−4	268	193
−5	−309	−256
3 19		
−1	−376	−399
−2	−403	−378
−3	−148	−136
−4	−174	−130
−5	−362	−309
4 0		
0	−684	−413
−2	−926	−1054
−4	188	288
4	3213	3316
8	−188	−169
−6	−1798	−2052
−8	980	964

l	$25F_o$	$25F_c$
4 0		
−10	−201	−125
4 2		
0	−389	−349
−1	−1154	−956
1	−1100	−1114
−2	−1664	−1516
2	1074	1145
−3	−497	−740
3	1261	1368
−4	−1718	−1772
4	1127	1148
−5	−1382	−1306
5	255	363
6	738	676
8	−268	−282
−6	−698	−490
−7	−242	−92
−8	−1208	−1293
−9	282	299
−10	−362	−414
−14	322	485
4 4		
0	−1865	−1511
−1	−3006	−2688
1	−349	−36
−2	−2711	−2600
−3	−483	−320
3	−322	−293
−4	−161	−36
4	470	416
−5	1584	1636
5	−577	−570
8	322	486
−6	−1543	−1491
−7	671	577
−8	255	228
−9	456	487
−10	−577	−431
−11	1221	1336
−13	−268	−260
−14	268	299
4 6		
0	174	136
−1	−322	−217
1	−966	−868
−2	−282	−150
−3	−564	−659
3	−550	−267
−4	376	161

l	$25F_o$	$25F_c$
4 6		
4	−201	−148
−5	−1476	−1277
5	698	668
−6	−805	−547
−7	429	549
−9	859	736
−10	−980	−853
−11	590	382
4 8		
0	336	224
−1	−698	−670
−2	−403	−412
2	−644	−562
−3	376	253
3	−309	−396
4	215	161
−4	−255	−159
−5	2080	1874
−8	−832	−853
4 10		
0	913	961
1	376	108
−2	1074	1077
2	335	174
−3	470	443
3	−604	−583
−4	−617	−526
4	−336	−209
−5	711	448
5	−228	−307
4 12		
0	3006	3160
−1	483	300
1	−537	−665
−2	376	303
3	537	621
4	255	39
−4	−255	−75
−5	−201	−127
4 14		
0	−295	−100
2	470	509
−3	−295	−179
3	255	96
−4	−295	−72
4	−268	−332
−5	−590	−535

l	$25F_o$	$25F_c$
4 16		
0	523	520
−3	−188	−112
3	−282	−384
4 18		
0	−174	−175
−1	−470	−360
1	322	372
−2	−309	−259
4 20		
−3	−349	−377
5 1		
−1	−872	−824
1	201	267
−2	174	82
2	335	190
−3	1221	1142
3	1651	1667
−4	134	112
4	1288	1269
−5	604	592
5	−523	−436
6	−282	−174
7	295	350
−6	832	819
−7	−3449	−3422
−8	3422	3330
−9	416	407
−11	−483	−427
−12	−510	−536
−13	−590	−620
5 3		
0	−483	−363
−1	−721	−598
1	−215	−2
−2	−1154	−1069
2	228	98
−3	1570	1479
−4	−537	−402
4	336	155
5	242	150
−6	658	574
−8	550	622
−12	−577	−354
−13	−416	−559
−14	−497	−92
−15	−429	−265
5 5		
0	671	556
−1	322	132

Table 7 (*cont.*)

l	$25F_o$	$25F_c$
• 5 5		
−2	−2107	−1767
−3	215	215
3	389	387
−4	456	471
4	−362	−307
−7	−658	−696
−8	−604	−663
−9	−470	−438
−14	−322	−361
• 5 7		
−1	−282	−298
1	470	398
−2	738	659
2	−765	−982
3	577	715
−4	161	360
4	−255	−31
−5	−631	−579
5	215	215
• 5 9		
0	−577	−591
−1	336	433
1	−497	−390
−2	−926	−783
2	−242	−463
3	349	371
−4	−778	−635
4	−456	−572
−5	−416	−336
5	242	277
• 5 11		
−1	−1409	−1103
−2	456	473
−3	792	834
3	389	392
−4	966	927
−5	−523	−406
• 5 13		
1	−855	−49
−2	−845	−797
2	−293	−426
−3	−604	−341
−4	376	217
4	−322	−831
−5	456	322
• 5 15		
−2	−886	−820
2	−765	−665
3	−429	−369

l	$25F_o$	$25F_c$
• 5 15		
−4	−174	−194
• 5 17		
−2	268	127
−5	537	484
• 5 19		
−2	−738	−891
−3	−148	−77
−5	−215	−58
• 6 0		
0	1396	1598
−2	249	416
2	−456	−416
4	242	76
−4	698	687
−8	3181	3637
−12	−416	−409
6	−242	−338
• 6 2		
0	121	103
−1	1194	1292
1	537	700
−4	201	150
4	−792	−854
−5	429	458
5	335	316
6	−228	−352
−6	1516	1456
−7	−1651	−1440
−8	1584	1193
−9	−1080	−966
−10	523	819
−11	−322	−284
−12	−429	−392
−13	−456	−481
−14	−242	−331
• 6 4		
1	−443	−301
−2	−889	−753
2	−644	−531
−3	2000	1887
−4	−1396	−1161
4	188	311
−5	−456	−260
6	−456	−467
−6	−617	−503
−8	1006	855
−9	725	741
−12	429	546
−14	−537	−274

l	$25F_o$	$25F_c$
• 6 4		
−15	389	523
• 6 6		
0	134	25
−1	631	658
1	684	795
2	−282	−242
−3	282	203
3	−295	−195
−4	349	112
−5	738	760
5	−389	−357
−7	497	490
−9	−1194	−1065
−14	−644	−576
• 6 8		
−1	−349	−433
1	−872	−977
−2	−403	−402
2	−738	−567
−3	805	794
3	497	479
−4	295	190
−5	242	213
5	−389	−398
• 6 10		
0	−443	−451
−1	−295	−260
1	−362	−431
−2	1020	863
−3	1141	861
−4	1436	1347
4	−134	−89
• 6 12		
0	282	258
−1	−215	−354
1	201	162
−2	255	302
2	295	263
−4	3274	3380
−5	939	665
• 6 14		
−1	295	112
1	604	548
−2	738	758
2	−376	−452
−5	389	214
• 6 16		
−1	242	43
1	255	216

l	$25F_o$	$25F_c$
• 6 16		
−2	201	139
−4	590	502
• 6 18		
−2	−268	−191
−3	255	260
−4	−188	−158
−5	−483	−553
• 7 1		
0	2483	2792
−1	1503	1513
1	−832	−749
−2	617	620
2	590	647
3	483	512
−4	−483	−463
4	−161	−74
−5	−1302	−1229
5	362	400
−6	−939	−943
−8	−1154	−1021
−10	−738	−621
−11	−1516	−1538
−12	577	496
• 7 3		
0	510	499
−1	−268	−287
−2	698	610
−3	−966	−1072
−4	−1490	−1234
−5	−1906	−1531
5	456	625
−6	−1946	−1477
−7	362	244
−8	−349	−224
−9	−295	−305
−10	−456	−440
• 7 5		
0	−215	−88
−1	−336	−313
−2	−255	−128
2	523	432
−3	−282	−335
−4	349	432
−5	−725	−545
−6	−1946	−1501
−7	−362	−318
−8	−443	−481
−9	215	222
−10	−617	−327

l	$25F_o$	$25F_c$
• 7 5		
−13	765	219
−14	−604	−585
−15	429	456
• 7 7		
0	−134	−66
−1	−429	−228
−2	−456	−554
2	−684	−730
−3	−322	−268
−4	−215	−144
−5	−819	−806
• 7 9		
0	−671	−575
−1	−242	−260
−2	−268	−370
2	201	266
−3	−349	−288
3	−201	−342
−5	295	272
• 7 11		
0	228	177
−3	577	495
3	−188	−284
−4	1490	1401
−5	−859	−820
• 7 13		
0	−349	−286
−1	188	73
1	215	193
−2	295	204
−3	−1006	−1016
−4	711	776
• 7 15		
0	−510	−642
−1	−282	−334
−2	−362	−227
−3	228	147
−4	228	204
• 7 17		
−2	−242	−209
−3	−295	−256
−4	−201	−206
• 8 0		
0	1610	1617
2	−564	−527
−4	215	150
−6	765	879
−8	765	751
−10	−550	−537

l	$25F_o$	$25F_c$
• 8 0		
−12	2778	2635
• 8 2		
0	−497	−579
−1	416	337
−2	282	20
2	−228	−227
−3	470	481
3	188	213
−6	−295	−319
−7	429	350
−8	268	282
−9	322	260
−10	1651	1607
−11	−1691	−1476
−12	980	1017
−13	−295	−494
• 8 4		
0	228	237
−1	456	382
−2	−389	−339
2	−429	−509
−3	161	123
3	−295	−392
−4	268	193
−5	−255	−201
−6	−1208	−882
−7	1704	1468
−8	−389	−287
−11	−483	−725
• 8 6		
1	255	187
2	−282	−390
−3	631	690
−5	1033	922
−13	−859	−987
−14	−644	−826
• 8 8		
0	−242	−372
−1	913	1024
−2	−792	−947
−3	−456	−468
−5	−510	−431
• 8 10		
−1	268	272
1	282	378
2	201	237
−4	−845	−802
• 8 12		
0	−201	−228

l	$25F_o$	$25F_c$
• 8 12		
−4	201	142
−5	−913	−578
• 8 14		
−2	−684	−760
−3	215	254
−4	−295	−398
−5	−255	−22
• 8 16		
−3	−215	−134
−4	−161	−154
−5	309	332
• 9 1		
0	−389	−376
−1	429	440
1	161	161
−2	282	289
−3	−711	−630
−4	1637	1727
−5	993	894
−9	−349	−247
−10	−416	−68
−11	−550	−693
−13	523	578
−14	362	99
−15	−698	−607
• 9 3		
1	483	564
−1	−309	−133
−2	−564	−573
2	−362	−442
−4	−215	−171
−6	322	229
−8	−1100	−984
−9	−889	−496
−12	1033	907
• 9 5		
1	−376	−442
−2	335	388
2	−510	−583
−6	−617	−641
−7	899	724
−9	362	367
−10	−470	−448
• 9 7		
1	−282	−195
−2	−2047	−2020
−5	−362	−277
• 9 9		
0	−188	−85

l	$25F_o$	$25F_c$
• 9 9		
−3	−497	−570
−4	−456	−218
• 9 11		
−4	336	351
• 9 13		
−3	362	281
−4	161	118
−5	389	154
• 9 15		
−4	−148	−250
• 10 0		
−4	2952	3364
−6	604	612
−8	−671	−749
−12	−268	−246
−16	698	934
• 10 2		
0	−228	−138
−1	295	279
−2	564	592
−3	−577	−584
−4	497	452
−5	389	212
−6	429	312
−7	−429	−438
−8	−604	−446
−9	−1020	−837
−10	−832	−795
−12	−322	−416
• 10 4		
−3	−215	−302
−4	389	417
−9	−859	−824
−10	−1423	−1059
−11	456	372
• 10 6		
−3	268	181
−5	−510	−503
• 10 8		
−3	−174	−167
−4	−416	−503
−5	282	284
• 10 10		
−3	268	267
• 10 12		
−4	−255	−260
• 11 1		
−2	−282	−378
−3	−309	−364

l	$25F_o$	$25F_c$
• 11 1		
−5	309	326
−6	349	222
−7	−336	−275
−8	577	584
−12	443	489
• 11 3		
−2	−523	−641
−3	483	457
−6	−550	−590
−7	416	456
−8	−255	−255
−11	349	240
• 11 5		
−2	−443	−532
−5	322	335
−6	255	223
−7	188	302
−8	322	318
−9	537	467
−10	−698	−773
−11	899	805
−14	322	31
• 11 7		
−4	188	232
−5	282	283
• 11 9		
−4	−268	−440
−5	564	570
• 12 0		
−8	2255	2562
−12	−416	−574
• 12 2		
−3	322	428
−4	−295	−325
−6	416	482
−7	−792	−715
−8	470	294
−9	416	265
−11	−429	−465
−12	−295	−396
−13	−416	−461
• 12 4		
−3	228	231
−11	335	313
• 12 6		
−5	−389	−454
• 12 8		
−5	228	234

l	$25F_o$	$25F_c$
• 13 1		
−5	215	221
−7	−711	−906
−8	1006	1152
−10	403	421
−11	−188	−215
−13	−201	−238
• 13 3		
−8	322	350
−13	−255	−413
• 14 0		
−12	765	1157
• 14 2		
−8	−188	−386
−9	−148	−153
−10	174	276
−11	−376	−362

Description and discussion of the structure

The structure of the complex at the two temperatures is basically the same. The molecules are arranged alternately in infinite columns parallel to the *c* axis and are stacked plane-to-plane. Fig. 4 shows part of one column; there is another identical column related to it by the *C* face centring. When seen edge-on in the *h*0*l* projection, the planes of the aromatic rings of the trinitrobenzene and the anthracene molecules make an angle of 83° with the *c* axis. However, they are not quite parallel since the plane of the aromatic ring of the trinitrobenzene molecule is parallel to the *b* axis, whereas that of the anthracene molecule makes an angle of 8° with this direction.

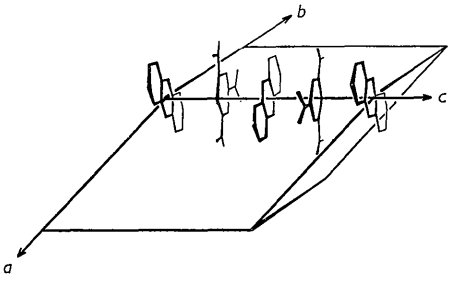

Fig. 4. Part of the cell contents, showing the stacking of molecules along the *c* axis. There is a similar column of molecules related to the one shown by the *C* face centring.

There are no abnormal intermolecular contacts at either temperature between adjacent columns of molecules. The closest low-temperature approaches of this type are C · · · O of 3·22 Å and O · · · O of 3·08 Å (3·32 and 3·23 respectively at room temperature), both between adjacent trinitrobenzene molecules. The C · · · C contacts of this type are all larger than 3·6 Å at either temperature. These are of the same order as generally accepted van der Waals distances and are similar to the intermolecular C · · · O, O · · · O and C · · · C contacts found in *m*-dinitrobenzene (Trotter, 1961). Within any one column of molecules, however, there are some intermolecular contacts which are shorter than the expected van der Waals distances. All the approaches of this type less than 3·4 Å are shown in Fig. 5. At low temperature the closest C–C distance is 3·30 Å between C(7′) and *M*C(1) (see Fig. 3 for numbering) and there are several contacts of approximately 3·35 Å. The corresponding room temperature values are in general slightly higher.

The molecular dimensions were reliably established only in the low-temperature structure determination. They are shown in Figs. 3(*a*) and 3(*b*), and Tables 5 and 6; the approximate dimensions obtained from the room temperature study are given in Tables 2 and 3. The large standard deviations of the room temperature dimensions mean that the differences between these and the low temperature dimensions are unlikely to be significant. The low temperature dimensions of the anthracene molecules in the complex are very similar to those obtained for anthracene alone (Cruickshank, 1956) and those for *s*-trinitrobenzene are consistent with dimensions in other aromatic nitrocompounds, particularly nitrobenzene (Trotter, 1959), *m*-dinitrobenzene (Trotter, 1961) and *p*-dinitrobenzene (Abrahams, 1950). As in these compounds, the nitro groups in *s*-trinitrobenzene deviate from coplanarity with the aromatic ring by varying amounts. The two related nitro groups attached to C(9) and C(9′) are twisted through 18° whereas that attached to *M*C(2) is coplanar with the ring. As a further distortion, the C(9)–N(1) bond is moved out of the plane of the aromatic ring through 2½°. The temperature factors for the atoms of the anthracene molecule show, at each temperature, a general increase with increasing distance of the atoms from the centre line C(7)–C(7′). This may be interpreted in terms of oscillation of the whole molecule about this line. In the trinitrobenzene molecule the *B* values for the carbon atoms are of the same order as those for the atoms in the central ring of the anthracene molecule, but the atoms of the nitro groups show abnormally high values, particularly at room temperature. This is presumably related to the apparent looseness of packing in the region of these groups. Further evidence of the thermal effects in the structure may be obtained from the thermal contraction ellipsoid, calculated from the change in cell dimensions with temperature. The ellipsoid as seen in the *h*0*l* projection is shown in Fig. 6. The direction of maximum contraction is

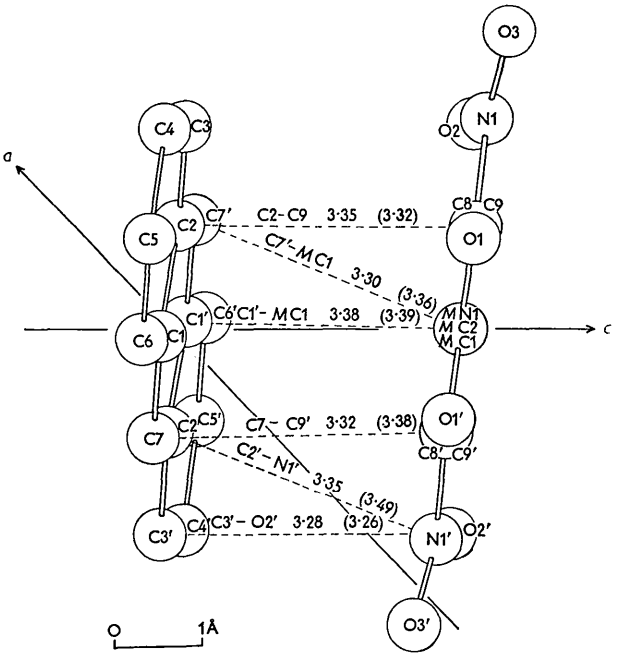

Fig. 5. Closest intermolecular contacts between anthracene and *s*-trinitrobenzene molecules. (Room temperature values in parentheses.)

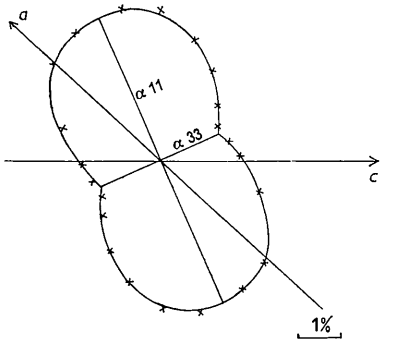

Fig. 6. Projection along the *b* axis of the ellipsoid showing the total percentage contraction from room temperature to *ca.* −100 °C.

approximately at right angles to the stacking direction and represents a total contraction of 3.5% from room temperature to low temperature. The corresponding total contraction along the stacking direction is 1.9%, whilst in a direction parallel to the *b* axis there is a corresponding expansion of 0.4%. The shape and orientation of the ellipsoid indicate that, as the molecular planes within each column move closer together, there is an even greater sideways movement of adjacent columns. This increases the efficiency of packing in the regions of the nitro groups and is accompanied by a large reduction in thermal motion of these groups in particular, as evidenced by the changes in the *B* values. The slight expansion in the direction of the *b* axis presumably allows modification of the packing to take place in the most efficient way consistent with the retention of normal intermolecular distances. It is likely, however, that the change in colour of the complex on cooling is due more to the reduction in the plane-to-plane separations within each column of molecules than to these changes in the environment of each molecule in sideways directions.

The conclusions from this work are that there are no unusual molecular or intermolecular dimensions apart from the rather close contacts between the molecules in directions approximately perpendicular to their planes. The latter would suggest the possibility of a small amount of charge transfer by π–π orbital overlap, as indicated also by spectroscopic studies, even though the relative orientations of the molecules to each other do not seem specially favourable for this (Wallwork, 1961). It seems that the formation of the complex is due primarily to the existence of charge transfer forces, although the crystal structure is a compromise between molecular orientations most favourable to π–π interaction and those which give the most efficient molecular packing.

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