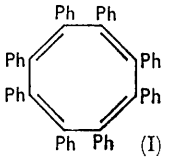
575. *The Crystal and Molecular Structure of Octaphenylcyclo-octatetraene*

By P. J. Wheatley

The crystal structure of octaphenylcyclo-octatetraene has been determined by three-dimensional *X*-ray methods. The crystals are tetragonal, space group $I4_1/a$, with four molecules in the unit cell. The molecule is thus required to have symmetry $\bar{4}$. The cell dimensions are $a = 19{\cdot}388$, $c = 10{\cdot}606$ Å. The final molecular dimensions were obtained from a least-squares analysis of 1229 independent reflexions collected with a Hilger-Watts linear diffractometer. The final *R* factor was 11·7%. The eight-membered ring consists of alternating single and double bonds of length 1·493 and 1·343 Å. There are significant angular distortions in the molecule, but all bond lengths adopt the expected values.

A brief Note indicating that the molecule previously described as "octaphenylcubane" [1] is in reality octaphenylcyclo-octatetraene (I) has recently appeared.[2] Since the Note was submitted, a structure analysis of cubane itself has appeared,[3] and a structure analysis of (I) has been carried out by Professor Lipscomb.[4] His conclusions are essentially the same as mine but, since the analyses were independent and by different techniques, it appears worthwhile to record the full results separately for comparison.



(I)

Experimental

$C_{56}H_{40}$. $M = 712{\cdot}9$. Tetragonal. $a = 19{\cdot}388 \pm 0{\cdot}032$, $c = 10{\cdot}606 \pm 0{\cdot}014$ Å. $U = 3986{\cdot}7$ Å^3. $D_m = 1{\cdot}20$. $Z = 4$. $D_c = 1{\cdot}188$. $F(000) = 1504$. Space group $I4_1/a$ (C_{4h}^6, No. 88).

Excellent crystals (m. p. 425—427°), with [*c*] as the axis of elongation can be obtained from diphenyl ether.[5] The cell dimensions were obtained from oscillation photographs taken with Cu-*K* radiation ($\lambda = 1{\cdot}5418$ Å). The intensities were collected round [*c*] with Mo-*K* radiation on a Hilger-Watts diffractometer equipped with SrO–ZrO_2 balanced filters.[6] One quarter of the reciprocal lattice was covered, so that each independent reflexion and a symmetrically equivalent one was recorded. Moreover four cycles were carried out at each reflecting position, two with each filter in place. An arithmetic mean was then taken of the four corrected counts so obtained. In this way 2557 independent reflexions were obtained, of which 515 (20·1%) were found to be zero. A complete refinement was carried out with these 2557 reflexions but, since the *R* factor was rather high (19·7%), it was decided to reject all planes whose counts were less than twice the standard deviation of the total counts. In this way 1229 independent reflexions were obtained, and the final parameters are based on this smaller number of reflexions. Whether the refinement was carried out with 2557 or with 1229 reflexions, there were no significant differences in the co-ordinates, but it was felt that the temperature factors might be unduly affected by the inclusion of a large number of weak reflexions and, moreover, that the standard deviations obtained for the temperature factors and for the co-ordinates were artificially low.

The structure was solved from a three-dimensional sharpened Patterson synthesis. Since the structure of an apparently isoelectronic and isomorphous compound has already been determined,[7] a search was made for vectors corresponding to the face- and body-diagonals of a cube of side 1·54 Å. No such peaks could be found. Indeed it was very noticeable that a shell of peaks occurred at 1·3—1·4 Å from the origin, but that no other peaks were present until

[1] H. H. Freedman and D. R. Petersen, *J. Amer. Chem. Soc.*, 1962, **84**, 2837; H. H. Freedman and R. S. Gohlke, *Proc. Chem. Soc.*, 1963, 249.
[2] H. P. Throndsen, P. J. Wheatley, and H. Zeiss, *Proc. Chem. Soc.*, 1964, 357; G. S. Pawley, W. N. Lipscomb, H. H. Freedman, *J. Amer. Chem. Soc.*, 1964, **86**, 4725.
[3] E. B. Fleischer, *J. Amer. Chem. Soc.*, 1964, **86**, 3889.
[4] Personal communication from Professor W. N. Lipscomb and Dr. H. H. Freedman.
[5] H. P. Throndsen and H. Zeiss, *J. Organometallic Chem.*, 1964, **1**, 301.
[6] U. Arndt and D. C. Phillips, *Acta Cryst.*, 1961, **14**, 807.
[7] T. R. R. McDonald and W. S. McDonald, *Proc. Chem. Soc.*, 1963, 382.

another shell started at about 2·4 Å. This could only mean that the bonds between carbon atoms enclosed angles of about 120°, and effectively eliminated a cubane structure. Attention was then turned to a model based on cyclo-octatetraene, a structure which had been excluded as a possibility on the basis of the absence of a Raman frequency corresponding to a carbon–carbon double bond.[1] Immediately a satisfactory vector interpretation could be found for the eight-membered ring, and the orientation of the benzene rings rapidly followed. Since the centre of gravity of the molecule must lie at the centre of inversion, a set of trial co-ordinates could be obtained, and three-dimensional refinement started straight away. In all, six refinement cycles were carried out with 2557 reflexions, and three with 1229. All calculations were made on an Elliott 803B computer with the programmes of Daly, Stephens, and Wheatley.[8] Constant weights were employed, and the least-squares programme uses the block diagonal approximation. The origin of the cell was chosen to lie on a centre of symmetry. Hydrogen atoms were ignored. The final R factor was 11·7%.

Results

The final atomic co-ordinates are given in Table 1, and the temperature factors in Table 2. Table 3 lists the observed and calculated structure factors obtained from the parameters given in Tables 1 and 2. Table 4 gives the bond lengths and angles. Figure 1 shows the molecule as it appears when viewed down [c], and the labelling of the atoms. All bond lengths adopt their expected values.[9] The eight-membered ring consists of alternating single and double

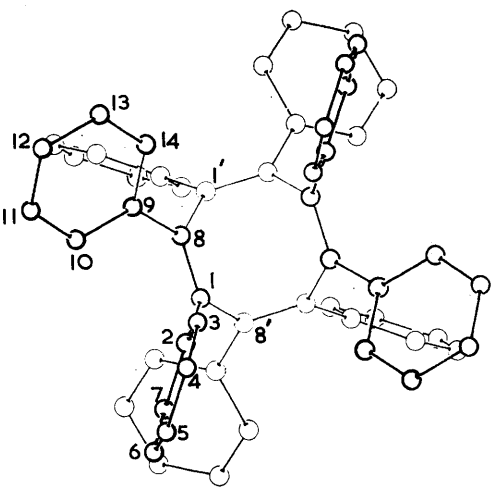


FIGURE 1. The molecule as it appears when viewed down [c], and the labelling of the atoms

TABLE 1

Atomic co-ordinates in Å. Standard deviations are given as units in the last place

Atom	X	Y	Z	Atom	X	Y	Z
C(1)	0·9219(69)	3·6176(65)	1·8883(61)	C(8)	−0·3851(67)	3·3196(64)	1·8350(58)
C(2)	1·8352(71)	3·2204(70)	3·0137(66)	C(9)	−1·0646(69)	2·3926(67)	2·7766(58)
C(3)	1·4185(90)	3·4885(79)	4·3353(67)	C(10)	−0·4982(81)	1·1286(75)	3·0562(76)
C(4)	2·3180(95)	3·1970(87)	5·4042(73)	C(11)	−1·1783(95)	0·2618(87)	3·9223(80)
C(5)	3·5726(88)	2·6449(90)	5·1531(83)	C(12)	−2·4248(99)	0·6224(90)	4·4697(71)
C(6)	3·9721(87)	2·3673(94)	3·8489(88)	C(13)	−2·9988(96)	1·8559(93)	4·1807(77)
C(7)	3·1082(78)	2·6573(85)	2·7589(79)	C(14)	−2·3019(85)	2·7607(79)	3·3144(70)

bonds of length 1·493 and 1·342 Å. The benzene rings are attached to the central ring by bonds, whose mean value is 1·494 Å. The mean length of the twelve bonds in the benzene rings is 1·409 Å. There are no significant departures from either of these mean values. The mean value of the angles within both benzene rings is 120·0°, again with no significant departures. The least-square planes through the benzene rings are defined by the equations:

C(2)–C(7) ..... $0{\cdot}3901X + 0{\cdot}9181Y - 0{\cdot}0703Z = 3{\cdot}4569$
C(9)–C(14) ..... $0{\cdot}4677X + 0{\cdot}3991Y + 0{\cdot}7887Z = 2{\cdot}6394$

[8] J. J. Daly, F. S. Stephens, and P. J. Wheatley, MRSA Final Report, No. 52.
[9] L. E. Sutton *et al.*, "Tables of Interatomic Distances," *Chem. Soc. Special Publ.*, 1958, No. 11.

The departure of the benzene carbon atoms from these planes is very slight, the greatest deviation being −0·012 Å for C(10). On the other hand C(1) lies out of the first plane by +0·091 Å, and C(8) out of the second by −0·047 Å, both of which are significant, so that clearly there is

TABLE 2

Thermal parameters in Å². Standard deviations are given as units in the last place

Atom	U_{11}	U_{22}	U_{33}	$2U_{12}$	$2U_{23}$	$2U_{13}$
C(1)	0·0508(42)	0·0384(37)	0·0231(29)	0·0062(65)	−0·0015(57)	0·0000(60)
C(2)	0·0492(42)	0·0463(40)	0·0314(34)	−0·0110(67)	0·0129(64)	−0·0160(64)
C(3)	0·0907(62)	0·0553(48)	0·0239(33)	−0·0156(85)	0·0083(68)	−0·0177(78)
C(4)	0·0973(68)	0·0691(56)	0·0302(39)	−0·0178(98)	0·0194(79)	−0·0332(86)
C(5)	0·0733(59)	0·0788(61)	0·0510(50)	−0·0389(95)	0·0508(93)	−0·0534(93)
C(6)	0·0605(55)	0·0855(66)	0·0608(53)	−0·0138(82)	0·0551(99)	−0·0344(92)
C(7)	0·0505(46)	0·0737(55)	0·0471(45)	0·0063(63)	0·0318(85)	−0·0273(76)
C(8)	0·0492(40)	0·0384(37)	0·0201(28)	−0·0042(64)	−0·0086(55)	0·0019(59)
C(9)	0·0500(41)	0·0483(40)	0·0174(28)	−0·0280(64)	0·0069(58)	−0·0002(58)
C(10)	0·0663(51)	0·0499(46)	0·0448(43)	−0·0208(78)	0·0185(74)	−0·0367(79)
C(11)	0·0976(71)	0·0641(55)	0·0431(44)	−0·0487(99)	0·0310(83)	−0·0434(94)
C(12)	0·1110(77)	0·0770(62)	0·0240(36)	−0·0756(111)	0·0018(80)	−0·0025(87)
C(13)	0·0891(67)	0·0835(63)	0·0355(40)	−0·0598(105)	−0·0234(86)	0·0418(89)
C(14)	0·0713(55)	0·0621(50)	0·0308(36)	−0·0272(85)	−0·0100(71)	0·0117(75)

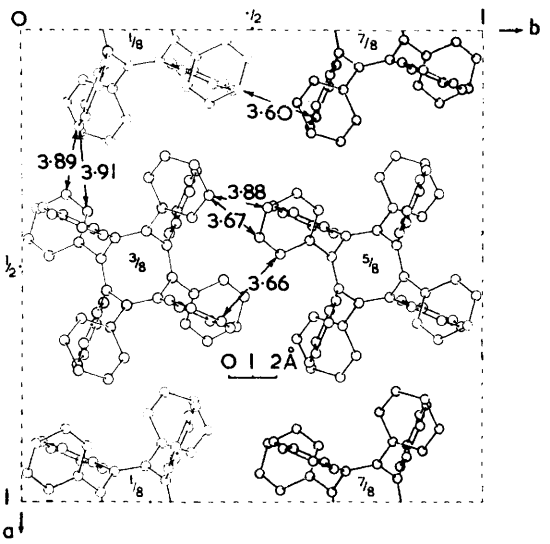
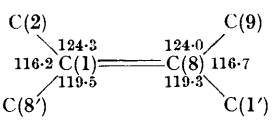


FIGURE 2. The crystal structure as viewed down [*c*], and some van der Waal's distances. (A right-handed set of axes has been chosen, with [*c*] pointing upwards. Figures at the centre of each ring give the heights of the centres of inversion above the plane of the paper.)

some angular distortion to accommodate the benzene rings. The situation is even more marked at the ethylene residue



Apart from the significant (and symmetrical) distortions at C(1) and C(8), the six carbon atoms do not lie in one plane. The equation of the plane through the three atoms C(1′), C(8), and C(9) is

$$-0{\cdot}2137X + 0{\cdot}7688Y + 0{\cdot}6027Z = 3{\cdot}7404,$$

and through C(8′), C(1), and C(2)

$$-0{\cdot}2604X + 0{\cdot}8245Y + 0{\cdot}5024Z = 3{\cdot}6912.$$

TABLE 3

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
2	**0**	0	11791	15193	-3402	9	2	1	-3706	-3840	132	9	16	1	-701	-936	235
4	**0**	0	-26030	-31132	5094	11	2	1	1206	830	376	11	16	1	-2633	-2773	140
6	**0**	0	-16204	-15940	-264	15	2	1	-1162	-1478	316	2	17	1	-2213	-2126	-87
8	**0**	0	-2657	-2963	306	17	2	1	1549	1509	40	6	17	1	1054	1238	-184
10	**0**	0	1393	1609	-216	19	2	1	1302	1667	-365	8	17	1	3090	3287	-197
12	**0**	0	-2500	-1965	-535	2	3	1	8713	8464	249	10	17	1	2733	2538	195
14	**0**	0	1222	1016	206	4	3	1	2426	2520	-92	12	17	1	1613	1683	-70
16	**0**	0	1800	1916	-116	6	3	1	-2432	-2624	192	16	17	1	-1056	-1005	-51
20	**0**	0	-1234	-1194	-40	8	3	1	-510	-91	-419	18	17	1	-917	-698	-219
22	**0**	0	-1104	-1408	304	10	3	1	-6466	-5536	-930	1	18	1	-903	-1178	275
2	2	0	-1754	-2527	773	14	3	1	2215	2102	113	**3**	18	1	-2059	-1914	-145
4	2	0	10706	12946	-1240	16	3	1	1066	1153	-87	7	18	1	961	576	385
6	2	0	5243	5041	202	18	3	1	-1734	-1758	24	9	18	1	745	96	649
8	2	0	12920	12210	710	20	3	1	-1391	-1260	-131	11	18	1	1160	1141	19
10	2	0	-1666	-903	-763	1	4	1	1150	10	1140	2	19	1	-1128	-980	-148
12	2	0	-4219	-3794	-425	3	4	1	-16766	-16184	-582	6	19	1	1553	1589	-36
14	2	0	-1502	-1700	-202	5	4	1	3906	3071	835	8	19	1	1421	1554	-133
16	2	0	739	200	539	7	4	1	-6364	-5742	-622	12	19	1	-945	-366	-579
18	2	0	3172	3412	-240	11	4	1	5836	5563	273	1	20	1	1369	1313	56
20	2	0	1409	1380	29	13	4	1	-1313	-1108	-205	5	20	1	-1022	-1200	178
2	4	0	25286	25240	46	15	4	1	-921	-629	-292	7	20	1	-1152	-1044	-148
4	4	0	9947	9792	155	17	4	1	-901	-558	-343	17	20	1	875	425	450
6	4	0	-8691	-8291	-400	19	4	1	-1014	-1527	513	4	21	1	-847	-989	142
8	4	0	-3082	-2198	-884	2	5	1	-6464	-4978	-1486	6	21	1	-1046	-1133	87
10	4	0	3696	3535	361	4	5	1	-11429	-10557	-872	8	21	1	-903	-1056	153
12	4	0	1724	1445	279	6	5	1	4005	3300	705	5	22	1	-781	-474	-307
14	4	0	-1194	-926	-266	10	5	1	1272	1651	-379	1	26	1	1028	858	170
18	4	0	-1517	-1692	175	14	5	1	-1443	-1472	29	2	0	2	-10463	-9795	-668
20	4	0	-2342	-2169	-173	16	5	1	1218	1079	139	4	0	2	-12719	-12107	-612
22	4	0	777	193	584	18	5	1	2420	2422	-2	6	0	2	-867	-1150	283
26	4	0	875	829	46	20	5	1	1421	1359	62	8	0	2	1084	1463	-379
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4	6	0	-10641	-8521	-2120	3	6	1	11153	9780	1373	12	0	2	-937	-824	-113
6	6	0	-5636	-5729	91	5	6	1	6027	4884	1143	16	0	2	4069	4153	-84
8	6	0	681	20	661	7	6	1	-1256	-1418	162	18	0	2	-1567	-1635	48
10	6	0	3218	3037	181	11	6	1	-3258	-3252	-6	20	0	2	-1302	-1122	-180
12	6	0	2546	2313	233	13	6	1	1310	1560	-241	1	1	2	9253	7892	1361
16	6	0	1266	1430	-164	17	6	1	-2241	-2490	249	3	1	2	-27671	-30903	3232
20	6	0	1116	1217	-101	19	6	1	1066	1076	-10	5	1	2	1455	1231	224
2	8	0	-7004	-5512	-1492	21	6	1	1202	1261	-59	7	1	2	-1331	-1195	-136
4	8	0	2318	1274	1044	2	7	1	-6725	-5920	-805	9	1	2	683	636	47
6	8	0	3959	4012	-53	4	7	1	2954	3210	-256	11	1	2	554	553	37
8	8	0	-6940	-6165	-775	6	7	1	-2233	-2131	-102	13	1	2	2175	2131	44
10	8	0	2526	3530	-1004	8	7	1	-2861	-2463	-398	15	1	2	1349	1600	-251
12	8	0	1367	1061	306	10	7	1	2316	1546	770	2	2	2	-35330	-36826	-1512
16	8	0	2187	2244	-57	14	7	1	-2057	-2149	92	4	2	2	-6926	-4840	-2086
18	8	0	2514	2423	91	18	7	1	1373	1561	-188	6	2	2	1014	961	53
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2	10	0	-2781	-1293	-1488	1	8	1	3090	2796	294	10	2	2	-4621	-3943	-678
4	10	0	10519	10460	59	3	8	1	3640	3153	487	12	2	2	-2903	-2972	69
6	10	0	-2657	-3575	918	5	8	1	-4364	-4331	-33	14	2	2	3266	2869	397
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16	10	0	-735	-918	183	15	8	1	667	687	-20	26	2	2	-935	-52	-883
18	10	0	1122	1280	-158	19	8	1	-805	-571	166	1	3	2	2855	3304	-449
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24	10	0	1098	620	478	2	9	1	10172	9626	546	5	3	2	-6843	-5827	-1016
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12	12	0	2757	2159	598	14	9	1	-1505	-1682	97	23	3	2	-883	-514	-369
16	12	0	-1355	-1406	51	16	9	1	-2161	-2619	458	2	4	2	8121	7546	575
2	14	0	-1389	-1173	-212	18	9	1	-986	-1455	469	4	4	2	-6406	-6259	-147
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6	14	0	961	234	727	1	10	1	-2183	-1874	-315	8	4	2	-3796	-3669	-127
10	14	0	2614	2661	-47	3	10	1	-10930	-10384	-546	10	4	2	661	289	372
12	14	0	805	555	250	5	10	1	-1505	-1725	220	12	4	2	1078	562	516
14	14	0	-1124	-893	-231	7	10	1	5020	4904	116	18	4	2	2127	2201	-74
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4	16	0	6037	6023	14	11	10	1	-2105	-2247	142	3	5	2	-851	-224	-627
6	16	0	-650	-805	155	13	10	1	-2685	-2611	-74	5	5	2	3140	3130	10
8	16	0	-4697	-5155	458	17	10	1	521	660	61	7	5	2	8525	8105	420
10	16	0	-3742	-3236	-446	19	10	1	-753	-745	-8	9	5	2	765	1343	-578
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18	18	0	-1166	-1047	-141	5	12	1	4139	4270	-131	12	6	2	-1597	-1890	293
6	20	0	3132	3337	-145	9	12	1	-1800	-1871	71	14	6	2	-2655	-2272	-383
8	20	0	2510	2401	109	11	12	1	1690	1825	-135	16	6	2	-739	-744	5
10	20	0	-1571	-1664	93	13	12	1	821	33	788	22	6	2	1080	920	160
12	20	0	-827	-655	-172	2	13	1	-2330	-1556	-774	1	7	2	2043	3358	-1315
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17	0	1	801	619	182	13	14	1	1351	1774	-423	4	8	2	3563	2977	586
19	0	1	-1122	-1235	113	17	14	1	-1012	-354	-658	6	8	2	3632	2673	959
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3	**2**	1	6040	6272	-223	14	15	1	-909	-931	22	5	9	2	-3630	-3455	-175
5	**2**	1	3437	3858	-421	3	16	1	-1361	-1638	257	7	9	2	-1459	-1050	-409
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TABLE 3 (*Continued*)

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12	10	2	-1401	-1511	110	5	6	3	460	1128	-668	8	2	4	-7207	-6127	-1080
16	10	2	851	784	67	7	6	3	2279	2287	-8	10	2	4	743	866	-123
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TABLE 3 (*Continued*)

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1	19	4	-1056	-1015	-83	10	0	6	1439	1604	-165	17	0	7	-1194	-909	-285
5	19	4	929	789	140	12	0	6	-4266	-4463	197	2	1	7	370	331	39
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6	20	4	1194	1088	106	20	0	6	-1006	-765	-241	6	1	7	-3154	-3176	22
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13	21	4	1162	853	309	3	1	6	-1525	-1241	-284	10	1	7	2927	2964	-37
6	24	4	-986	-1154	168	5	1	6	-3654	-3073	-581	12	1	7	3044	3113	-69
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3	0	5	-913	-132	-781	9	1	6	630	477	153	1	2	7	2506	3001	-495
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5	4	5	-4546	-4656	108	11	5	6	825	343	482	15	6	7	1589	1838	-249
7	4	5	1323	1223	100	13	5	6	-1950	-2181	231	19	6	7	-1525	-1323	-202
11	4	5	-1142	-1106	-36	2	6	6	1196	1045	151	4	7	7	-3626	-3509	-117
13	4	5	-6139	-6203	64	4	6	6	-799	-6	-793	6	7	7	-3539	-3797	258
15	4	5	-2025	-1996	-29	6	6	6	6268	5931	337	10	7	7	3323	3353	-30
17	4	5	1471	963	488	8	6	6	-1036	-1249	213	12	7	7	1060	1199	-139
19	4	5	982	968	14	10	6	6	-3716	-3662	146	14	7	7	2388	2550	-162
2	5	5	897	933	-36	12	6	6	-1443	-1454	11	16	7	7	-1349	-1206	-143
6	5	5	-705	-652	-53	14	6	6	2151	1907	244	1	8	7	-1692	-2003	111
8	5	5	-2803	-2439	-364	16	6	6	1625	1520	105	3	8	7	1022	1110	-88
10	5	5	-3840	-3495	-345	18	6	6	-1028	-841	-187	5	8	7	-1252	-1543	291
18	5	5	1070	1558	-488	20	6	6	-1034	-1159	125	7	8	7	1106	1179	-73
20	5	5	1022	1180	-158	1	7	6	-893	-638	-255	17	8	7	1166	1093	73
3	6	5	4382	4458	-76	5	7	6	1415	1425	-10	19	8	7	1557	1760	-203
5	6	5	4173	3649	524	7	7	6	2141	1965	176	4	9	7	1601	1667	-66
7	6	5	-5616	-5613	-3	9	7	6	1361	1323	38	8	9	7	-2942	-3073	131
9	6	5	-4366	-3868	-478	11	7	6	1391	1062	329	10	9	7	-3002	-2999	-3
13	6	5	1234	1170	64	13	7	6	2059	2364	-305	1	10	7	1710	1790	-80
15	6	5	1397	1532	-135	17	7	6	-2300	-2552	252	3	10	7	-699	-693	-6
2	7	5	-1032	-738	-294	2	8	6	-3250	-3595	345	5	10	7	-1184	-664	-520
4	7	5	1956	1541	417	4	8	6	2043	1805	238	2	11	7	-2476	-2567	91
8	7	5	-1625	-1485	-140	6	8	6	2344	2481	-137	4	11	7	833	714	119
10	7	5	-737	-803	66	8	8	6	1196	1558	-362	6	11	7	1750	1686	64
16	7	5	-1507	-1389	-118	14	8	6	1028	1260	-232	8	11	7	859	962	-103
1	8	5	-3164	-2680	-484	16	8	6	961	601	360	10	11	7	-907	-426	-481
3	8	5	1409	1134	275	1	9	6	2921	3472	-551	12	11	7	-699	-702	197
5	8	5	4256	4070	186	3	9	6	-637	-975	138	16	11	7	1248	1108	140
11	8	5	787	818	-31	5	9	6	807	699	108	1	12	7	-749	-842	93
13	8	5	1463	1232	231	7	9	6	1144	1401	-257	3	12	7	-2039	-2868	829
15	8	5	-1006	-1108	102	11	9	6	-807	-295	-512	5	12	7	-1395	-1517	122
2	9	5	687	662	25	15	9	6	-1264	-1005	-259	7	12	7	-2077	-1938	-139
6	9	5	-845	-1535	690	2	10	6	-949	-900	-49	11	12	7	2213	2403	-190
8	9	5	-1936	-2206	270	4	10	6	-2853	-3021	168	4	13	7	-2440	-2442	2
10	9	5	1122	1200	-78	6	10	6	-2667	-2635	-32	8	13	7	1343	1215	128
12	9	5	2877	2816	61	8	10	6	1950	2046	-96	10	13	7	905	823	82
1	10	5	3533	3347	186	10	10	6	949	343	606	1	14	7	-1491	-1407	-84
3	10	5	-1485	-1837	348	12	10	6	-829	-761	-68	3	14	7	1256	1308	-52
5	10	5	-1160	-1003	-177	16	10	6	-1349	-1417	68	5	14	7	1712	1391	321
7	10	5	3975	3944	31	1	11	6	-3539	-3564	25	6	15	7	-1995	-1752	-243
11	10	5	-2249	-2536	287	3	11	6	1160	1149	11	9	16	7	-1150	-1482	332
13	10	5	-1510	-1722	-188	5	11	6	1822	1656	166	13	16	7	1114	1568	-454
2	11	5	-1473	-1413	-60	7	11	6	905	1698	-793	4	17	7	1030	503	527
4	11	5	1154	1121	33	13	11	6	-1062	-941	-121	14	17	7	1551	1555	-4
8	11	5	-923	-945	22	15	11	6	1074	1079	-5	3	18	7	1543	1684	-141
10	11	5	-1248	-1065	-183	2	12	6	1032	593	439	5	18	7	1609	1509	100
12	11	5	-1140	-999	-141	4	12	6	-1313	-1396	83	3	20	7	-1712	-1760	48
16	11	5	-1098	-193	-905	10	12	6	-1254	-1417	163	7	20	7	1511	1457	54
1	12	5	2127	2416	-289	1	13	6	-2187	-2245	58	2	0	8	-4073	-3637	-436
7	12	5	-955	-538	-417	7	13	6	905	666	239	4	0	8	-3509	-3224	-285
11	12	5	1160	1247	-87	11	13	6	875	692	183	6	0	8	1365	1524	-159
2	13	5	-2047	-2229	182	2	14	6	1826	1450	376	8	0	8	1479	1265	214
4	13	5	-1826	-1637	-191	4	14	6	2271	2098	173	10	0	8	-1084	-978	-106
6	13	5	1650	1291	359	6	14	6	1826	1786	40	1	1	8	2364	2423	-59
10	13	5	-1268	-1385	117	16	14	6	4112	742	370	3	1	8	-3698	-4008	110
3	14	5	4978	5031	-53	3	15	6	-821	-623	-198	5	1	8	-2207	-2309	102
7	14	5	-855	-491	-364	7	15	6	-1092	-1140	48	7	1	8	-1716	-1614	-102
9	14	5	1525	1681	-156	2	16	6	-1074	-897	-177	9	1	8	2984	2899	85
11	14	5	982	623	359	4	16	6	-1752	-1404	-348	11	1	8	3323	3173	150
2	15	5	1048	1055	-7	8	16	6	961	291	670	13	1	8	-1108	-262	-846
4	15	5	1666	2000	-334	18	16	6	-1108	-1218	110	15	1	8	1633	1900	-267
16	15	5	1032	1060	-28	5	17	6	-859	-664	-235	2	2	8	3927	3552	375
3	16	5	-1262	-1462	200	9	17	6	-1008	-259	-749	4	2	8	3515	3217	298
5	16	5	-921	-979	58	4	20	6	-1349	-1741	392	6	2	8	-717	-895	178
2	17	5	1467	1284	183	1	0	7	3487	3757	-270	8	2	8	-6033	-5468	-565
4	17	5	-1146	-1453	307	3	0	7	-941	-783	-156	10	2	8	-2051	-1539	-512
1	18	5	-1607	-1640	33	5	0	7	-1321	-1712	391	12	2	8	1126	660	466
5	18	5	1222	1290	-68	7	0	7	2921	3044	-123	18	2	8	-1234	-995	-239
2	0	6	-3303	-3244	-59	9	0	7	1820	1722	106	1	3	8	-604	-575	-29
4	0	6	4233	4139	94	11	0	7	-1862	-1866	4						

TABLE 3 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
3	3	6	6240	6167	73	2	3	9	1048	472	576	2	8	10	-2255	-2495	196
5	3	6	2546	2439	107	4	3	9	-2446	-2402	36	10	8	10	1533	1783	-250
7	3	6	-4229	-4384	155	6	3	9	823	1406	-583	1	9	10	-967	-1311	344
9	3	6	-947	-924	-23	8	3	9	3092	3161	-69	3	9	10	990	993	-3
11	3	6	-1240	-1270	30	10	3	9	-1176	-1037	-139	5	9	10	903	582	321
13	3	6	962	977	-15	1	4	9	3146	3757	-611	7	9	10	-927	-1269	342
2	4	6	3600	3606	-206	3	4	9	-1706	-1726	20	11	9	10	2534	2939	-405
4	4	6	2033	1681	352	7	4	9	-1162	-1594	432	13	9	10	1666	1900	-214
6	4	6	-2941	-2926	-15	9	4	9	1140	1303	-163	2	10	10	1858	1775	83
8	4	6	1770	1784	-14	13	4	9	-1034	-548	-486	6	10	10	-1136	-1424	288
10	4	6	2935	2641	94	17	4	9	1503	1315	188	5	11	10	1210	689	521
12	4	6	-1648	-1406	-440	2	5	9	1477	1337	140	7	11	10	-1064	-1363	299
14	4	6	1766	1983	-217	6	5	9	1662	2167	-305	4	16	10	1164	1713	-529
1	5	6	-2590	-2653	263	8	5	9	-2400	-2683	283	1	0	11	1607	1584	23
3	5	6	-755	-570	-185	1	6	9	-5501	-5522	21	3	0	11	3124	3082	42
5	5	6	-2452	-2303	-149	5	6	9	1770	1956	-186	5	0	11	1790	1534	256
7	5	6	-1503	-1805	302	7	6	9	1443	2169	-726	7	0	11	-1638	-1741	97
11	5	6	3329	3195	134	9	6	9	-905	-980	75	9	0	11	-1106	-913	-193
13	5	6	1150	891	259	11	6	9	-1104	-1284	180	2	1	11	534	354	180
15	5	6	-982	-796	-186	2	7	9	-1104	-1148	44	8	1	11	1166	666	498
2	6	6	-2737	-2459	-278	4	7	9	1997	1723	274	10	1	11	-1656	-1589	-67
4	6	6	-1926	-1302	-624	12	7	9	-1656	-2099	243	1	2	11	-1300	-1544	356
6	6	6	-959	-726	-233	1	8	9	1952	1952	0	5	2	11	1692	1640	52
10	6	6	-1078	-1232	154	3	8	9	3868	4020	-152	4	3	11	818	984	-65
12	6	6	1724	2081	-357	5	8	9	-1266	-1402	116	6	3	11	2614	2453	161
1	7	6	-5156	-5126	-30	7	8	9	-1670	-1621	-49	10	3	11	-1327	-1166	-161
3	7	6	-1581	-1663	82	4	9	9	859	1021	-162	3	4	11	759	575	184
5	7	6	1178	1189	-11	6	9	9	1963	2296	-333	5	4	11	-1706	-1762	54
7	7	6	863	637	226	10	9	9	1028	1317	-289	4	5	11	-1866	-1682	-184
9	7	6	-1497	-1642	145	1	10	9	1776	1660	116	6	5	11	-1046	-974	-72
2	8	6	747	603	144	3	10	9	-1625	-1499	-126	10	5	11	1732	1512	220
4	8	6	3712	3674	38	5	10	9	-925	-682	-243	1	6	11	1000	811	189
6	8	6	2251	2173	78	9	10	9	1361	2203	-842	3	6	11	-1256	-1496	242
8	8	6	-4982	-5486	504	11	10	9	1216	1507	-291	5	6	11	1114	1392	-278
10	8	6	-3259	-3238	-61	2	11	9	1367	1776	-409	7	6	11	1439	1643	-204
12	8	6	-1294	-885	-409	1	12	9	-2779	-2959	180	9	6	11	-1507	-1507	0
1	9	6	3036	3161	-125	5	12	9	1856	2026	-170	2	7	11	-2013	-2291	278
3	9	6	2498	2566	-68	9	12	9	-1094	-754	-340	4	7	11	-973	-1049	76
5	9	6	1660	1842	18	15	12	9	1236	319	917	6	7	11	2777	2726	51
7	9	6	-2161	-2280	119	4	13	9	-1343	-1452	109	3	8	11	-1134	-884	-250
9	9	6	-3918	-4021	103	1	14	9	1116	1334	-218	5	8	11	1064	765	299
11	9	6	-951	-745	-206	3	14	9	1533	1674	-141	7	8	11	-1373	-1234	-139
19	9	6	-1323	-1162	-141	2	15	9	-2119	-1521	-198	3	10	11	1194	239	955
2	10	6	1004	883	121	8	15	9	1144	737	407	2	11	11	1638	1499	339
6	10	6	1078	1187	-109	10	15	9	1503	1556	-55	6	11	11	-1361	-1151	-210
8	10	6	1688	1591	97	3	16	9	-1776	-2099	323	3	12	11	1565	1483	82
1	11	6	-849	-690	-159	7	16	9	1503	1728	-225	5	14	11	-1549	-1557	8
3	11	6	-2689	-2782	93	2	17	9	1453	1811	-358	2	0	12	2223	2050	173
5	11	6	-1315	-1637	322	4	17	9	1674	1670	4	4	0	12	-1272	-1508	236
9	11	6	2841	2803	38	2	0	10	-384	-280	-104	6	0	12	-1156	-1093	-63
4	12	6	-1902	-1798	-104	4	0	10	-1876	-1772	-104	1	1	12	-909	-1005	96
6	12	6	1024	520	504	6	0	10	1004	944	60	3	1	12	-1615	-1880	265
8	12	6	2428	2565	-137	8	0	10	3196	3519	-323	5	1	12	761	664	97
1	13	6	-1706	-1717	11	12	0	10	-1234	-1366	132	11	1	12	1260	695	565
7	13	6	1497	1661	-164	1	1	10	4119	4078	41	2	2	12	-2265	-2411	126
11	13	6	-1216	-1592	376	3	1	10	-913	-524	-389	4	2	12	1064	1034	30
12	14	6	-1078	-256	-822	5	1	10	-1355	-1331	-24	6	2	12	1120	831	289
1	15	6	1435	1681	-246	7	1	10	-1323	-1510	187	10	2	12	1138	1134	4
3	15	6	1429	1724	-295	9	1	10	-1363	-1366	-17	3	3	12	1435	1674	-239
7	15	6	-1969	-1742	-227	2	2	10	-833	-655	-178	5	4	12	1365	1442	-77
9	15	6	-1429	-1200	-229	4	2	10	-3259	-3659	360	6	4	12	-2410	-2629	219
2	16	6	-1361	-1352	-29	8	2	10	1236	1175	61	1	5	12	1946	2213	-267
2	18	6	1461	1690	-229	10	2	10	1965	2134	-169	3	5	12	1018	1031	-13
4	18	6	1339	1520	-181	18	2	10	-1403	-1269	-134	5	5	12	-1501	-1541	40
1	0	9	-7503	-7467	-16	1	3	10	-1335	-1558	219	7	5	12	-1345	-1422	77
3	0	9	-990	-1290	300	3	3	10	711	129	582	4	6	12	-1517	-1644	127
5	0	9	-717	-718	1	5	3	10	1004	859	145	6	6	12	1712	1659	53
7	0	9	3535	4128	-593	7	3	10	1702	1733	-31	1	7	12	-1260	-1445	185
9	0	9	3405	3408	-77	15	3	10	1036	1595	501	3	7	12	-1030	-1106	76
11	0	9	-1750	-2097	347	2	4	10	4524	4660	-136	7	7	12	1946	2427	-481
13	0	9	-1922	-1905	-17	4	4	10	1718	1904	-186	2	8	12	-1571	-1725	154
17	0	9	1144	1019	125	6	4	10	-1666	-1675	9	2	10	12	1100	1181	-81
2	1	9	925	891	34	12	4	10	-1074	-590	-484	2	1	13	-1523	-1537	14
4	1	9	-3032	-2654	-378	1	5	10	1702	2353	-651	4	1	13	-1967	-1913	-74
6	1	9	-2442	-2192	-250	5	5	10	-1563	-1550	27	6	1	13	-1236	-1375	137
8	1	9	1503	1364	139	7	5	10	-1920	-2086	166	10	1	13	2259	2127	132
1	2	9	5539	5676	263	9	5	10	1154	1413	-259	7	2	13	1140	130	1010
3	2	9	626	100	526	2	6	10	-1706	-1950	244	4	3	13	1501	1628	-127
5	2	9	-4663	-4839	176	6	6	10	1186	1187	-1	5	4	13	-1373	-1508	135
7	2	9	-3587	-3789	202	8	6	10	994	1117	-123	7	4	13	-1890	-2266	366
9	2	9	-1176	-1192	16	1	7	10	803	759	44	2	5	13	1421	1529	-108
11	2	9	2925	3057	-132	3	7	10	1349	1508	-159	5	6	13	2795	3187	-392
17	2	9	-1515	-1404	-111	15	7	10	-1150	-1278	128	6	7	13	1252	1046	206
												3	10	13	-1421	-2686	1265

The angle between these two planes is 7° 6′. The angle between the normal to the plane defining the benzene ring C(2)–C(7) and the normal to the plane containing C(8′), C(1), and C(2) is 46° 59′. That between the other benzene ring and the plane containing C(1′), C(8), and C(9) is 51° 41′.

All intramolecular non-bonded contacts were calculated up to a limit of 3·10 Å. These distances, which are listed in Table 5, show some interesting correlations with the angular distortions that are found to occur in the molecule. All van der Waals's contacts are between benzene rings. There are thirteen such distances less than 4 Å, the shortest being 3·600 Å. Some of these distances are given in Figure 2, which shows the crystal structure as it appears when viewed down [*c*].

TABLE 4

Bond lengths (Å) and bond angles with their standard deviations

C(1)–C(8)	1·342(9)	C(1)–C(2)	1·503(10)
C(1)–C(8′)	1·493(9)	C(8)–C(9)	1·486(9)
C(2)–C(3)	1·411(11)	C(9)–C(10)	1·413(10)
C(2)–C(7)	1·415(11)	C(9)–C(14)	1·398(10)
C(3)–C(4)	1·427(12)	C(10)–C(11)	1·401(12)
C(4)–C(5)	1·394(12)	C(11)–C(12)	1·408(12)
C(5)–C(6)	1·392(13)	C(12)–C(13)	1·391(13)
C(6)–C(7)	1·421(12)	C(13)–C(14)	1·433(12)
C(8′)C(1)C(8)	119·5(6)	C(2)C(3)C(4)	118·5(7)
C(1)C(8)C(1′)	119·3(6)	C(3)C(4)C(5)	120·9(8)
C(8′)C(1)C(2)	116·2(6)	C(4)C(5)C(6)	120·4(8)
C(1′)C(8)C(9)	116·7(5)	C(5)C(6)C(7)	120·2(8)
C(2)C(1)C(8)	124·3(6)	C(6)C(7)C(2)	119·4(7)
C(9)C(8)C(1)	124·0(6)	C(7)C(2)C(3)	120·7(7)
C(1)C(2)C(3)	118·1(6)	C(9)C(10)C(11)	118·8(7)
C(1)C(2)C(7)	121·1(6)	C(10)C(11)C(12)	120·8(8)
C(8)C(9)C(10)	120·0(6)	C(11)C(12)C(13)	120·8(8)
C(8)C(9)C(14)	119·0(6)	C(12)C(13)C(14)	119·0(8)
		C(13)C(14)C(9)	119·8(7)
		C(14)C(9)C(10)	120·9(6)

TABLE 5

Non-bonded intramolecular distances less than 3·10 Å

C(1)C(3)	2·500	C(2)C(8)	2·516	C(1)C(9′)	2·536
C(1)C(7)	2·542	C(1)C(9)	2·497	C(2)C(8′)	2·542
C(8)C(10)	2·511	C(3)C(8)	3·088	C(1)C(14′)	3·002
C(8)C(14)	2·485	C(1)C(10)	3·095	C(7)C(8′)	3·087
C(2)C(9)	3·025	C(1)C(1″)	3·073	C(1)C(8″)	2·809

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