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Crystal Structure of 2,7-Diphenyl-2,3,5,6-octatetraene

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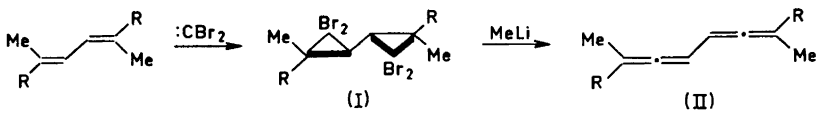
The crystals belong to the monoclinic system with space group $P2_1/c$ and cell dimensions $a = 15.653$ Å, $b = 7.457$ Å, $c = 6.454$ Å, $\beta = 98.20°$. There are two molecules in the unit cell. The phase problem was solved by direct methods, and the R-value arrived at by full-matrix least squares refinement was 6.0 % for 1049 observed reflections. The cumulated double bonds are 1.310 Å and 1.306 Å, respectively, and the single bond length 1.470 Å. The torsion angle about the bond to the phenyl ring (of length 1.491 Å) is 20.6°.

When properly substituted, a diallene can exist in a *meso*-configuration or as a racemic modification. The synthesis and some thermal reactions of conjugated *meso*-diallenes have been described by Kleveland and Skattebøl.[1] The two-step synthesis consists of the addition of dibromocarbene to the conjugated dienes followed by treatment of the diadducts with methyllithium (R = phenyl and *tert*-butyl):



(I) (II)

Structural assignments of intermediates (I) and products (II) were based on spectroscopic evidence and crystallographic space group determinations:

Compound	Space group	Number of molecules in the unit cell
(I)(R = C_6H_5)	*Pbca*	4
(I)(R = $C(CH_3)_3$)	$P2_1/c$	2
(II)(R = C_6H_5)	$P2_1/c$	2
(II)(R = $C(CH_3)_3$)	$P2_1/c$	2

Table 1. Final fractional coordinates and anisotropic temperature factors with estimated standard deviations (multiplied by 10^5 for carbon and 10^4 for hydrogen).

ATOM	X	Y	Z	B	B11	B22	B33	B12	B13	B23
C1	24727(16)	58171(33)	29575(40)		376(12)	1116(58)	1982(74)	158(39)	59(49)	247(108)
C2	31348(19)	58791(40)	42239(49)		402(14)	1845(66)	2233(87)	133(48)	53(58)	-824(132)
C3	39874(18)	58776(41)	37485(58)		367(14)	2171(69)	3866(118)	-7(49)	-16(64)	-117(141)
C4	41558(20)	49835(43)	28154(53)		383(14)	2418(74)	3131(103)	173(56)	961(68)	688(154)
C5	35197(20)	41225(43)	7361(53)		523(16)	2172(72)	2588(97)	78(57)	653(68)	-275(146)
C6	26769(18)	41441(37)	11948(44)		428(14)	1698(58)	2208(98)	-34(47)	188(59)	-194(128)
C7	15743(16)	49915(33)	34765(42)		362(12)	1292(58)	2878(75)	135(42)	33(52)	84(107)
C8	9144(16)	46392(35)	28454(46)		333(11)	1824(64)	2375(88)	-56(44)	334(55)	138(119)
C9	2486(16)	43087(41)	6355(45)		345(13)	1971(70)	2558(94)	-72(45)	198(56)	-411(126)
C10	14384(24)	53869(51)	56922(53)		445(16)	2583(88)	2780(101)	217(61)	421(65)	-744(154)
H2	3814(15)	6582(35)	5228(44)	3,7(,7)						
H3	4468(17)	6491(36)	4896(46)	5,1(,7)						
H4	4738(17)	4926(38)	1655(44)	5,2(,7)						
H5	3613(17)	3473(38)	-424(51)	5,4(,8)						
H6	2228(14)	3484(31)	191(48)	3,5(,6)						
H9	37(16)	3852(41)	358(46)	5,2(,7)						
H101	841(21)	5229(36)	5811(49)	5,3(,8)						
H102	1594(20)	6553(51)	6310(57)	8,4(1,1)						
H103	1838(21)	4582(44)	6869(57)	7,9(,9)						

Under the assumption of an ordered crystal structure, this crystallographic information demands the molecules to be centrosymmetrical, a requirement which is only satisfied by the *meso*-configuration. In order to eliminate the possibility of disorder, a crystal structure determination of (II)(R = C_6H_5) has been carried out.

The crystals belong to the monoclinic system and the systematic absences lead to the space group $P2_1/c$. The cell parameters measured by means of a four circle diffractometer, and their estimated standard deviations, are: $a = 15.653(3)$ Å, $b = 7.457(2)$ Å, $c = 6.454(1)$ Å, $\beta = 98.20(2)°$. Since there are two molecules in the unit cell ($\varrho_{obs} = 1.15$ g cm^{-3}, $\varrho_{calc} = 1.14$ g cm^{-3}), the molecules themselves must be centrosymmetrical.

With $2\theta(\max) = 50°$ and Mo$K\alpha$-radiation, 1445 reflections were measured on an automatic four-circle diffractometer. 1049 were recorded as observed

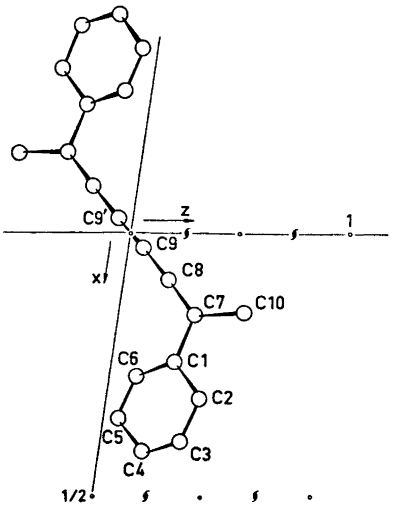


Fig. 1. The molecule viewed along [010].

Table 2. Observed and calculated structure factors on 10 times absolute scale.

L=	0,K=	0	=12	186	202	= 4	16	19	9	36	36	L=	1,K=	8	= 9	38	36	0	81	84	=14	29	30
=16	86	69	=11	23	24	= 3	42	45	10	79	82	= 3	18	22	= 4	15	16	3	84	83	=13	29	31
=17	65	59	=10	38	46	3	40	45	11	101	97	= 2	31	30	= 3	296	282	4	17	8	=11	27	28
=16	86	83	= 9	121	134	4	24	19	13	123	115	= 1	42	43	= 2	19	18	6	17	13	=10	144	148
=15	18	13	= 8	68	72	5	15	11	14	65	63	0	21	20	= 1	84	88	9	81	85	= 9	81	84
=14	43	41	= 6	90	97	8	21	23	15	29	26	1	28	22	0	408	386	L=	2,K=	8	= 8	66	67
=13	44	42	= 5	152	159	9	64	69	16	32	23	2	67	67	1	140	147	= 7	30	26	= 7	49	50
=12	186	178	= 4	160	165	11	30	29	L=	1,K=	4	4	61	65	2	142	138	= 6	16	18	= 6	41	43
=11	58	56	= 3	43	45	L=	0,K=	8	=16	64	66	L=	2,K=	0	3	244	237	= 4	20	17	= 5	89	89
=10	59	57	= 2	92	92	= 7	18	11	=15	40	37	=16	23	26	5	32	36	= 2	19	19	= 4	43	44
= 9	84	83	= 1	39	40	= 6	21	21	=13	84	84	=15	125	126	6	70	67	= 1	46	46	= 3	31	27
= 8	151	141	1	39	40	= 3	47	53	=11	45	43	=14	23	28	7	34	34	0	60	64	= 2	18	20
= 7	297	285	2	95	92	= 2	37	40	=10	64	62	=13	25	32	8	38	42	1	37	40	= 1	100	98
= 6	74	68	3	46	45	0	23	24	= 9	37	39	=12	60	59	9	46	50	2	86	87	0	64	64
= 5	71	73	4	171	166	2	41	40	= 8	34	35	=11	38	43	10	88	80	3	28	24	1	15	8
= 4	282	281	5	162	159	3	48	53	= 7	35	32	=10	49	49	11	21	23	4	22	22	2	18	23
= 3	238	238	6	96	97	L=	1,K=	1	= 6	32	32	= 9	139	148	12	85	78	5	18	16	4	39	36
= 2	314	316	8	75	72	=16	34	30	= 5	45	47	= 8	42	35	13	26	21	L=	3,K=	1	5	80	83
2	308	316	9	137	135	=16	45	46	= 4	100	102	= 7	19	16	14	76	67	=16	26	30	7	108	102
3	231	238	10	46	46	=15	18	20	= 3	61	64	= 6	368	376	15	33	27	=15	88	32	8	68	68
4	277	281	11	27	24	=14	38	44	= 2	67	63	= 5	116	113	16	89	83	=14	37	41	9	21	19
5	67	73	12	207	202	=11	77	74	= 1	112	107	= 4	152	157	L=	2,K=	4	=13	66	68	10	47	43
6	70	68	15	73	69	=10	15	5	0	109	110	= 3	405	426	=15	18	19	=12	83	80	11	26	23
7	253	265	L=	0,K=	4	= 8	178	170	1	333	328	= 2	186	185	=14	16	7	=11	46	43	13	71	66
8	139	141	=15	40	36	= 7	379	370	2	41	35	= 1	118	128	=12	117	117	=10	90	94	L=	3,K=	5
9	78	83	=13	34	36	= 6	96	93	3	58	59	0	80	57	=11	79	77	= 8	120	127	=11	26	30
10	55	57	=12	87	97	= 5	313	309	4	120	114	1	34	38	=10	63	60	= 7	165	186	=10	108	109
11	55	56	=11	23	23	= 4	313	314	5	91	90	2	104	118	= 9	140	141	= 6	246	246	= 9	48	48
12	173	178	=10	53	52	= 3	577	556	6	26	23	3	124	149	= 8	20	20	= 5	122	117	= 7	60	63
13	39	42	= 8	34	36	= 1	778	740	8	112	114	4	116	128	= 7	19	21	= 4	208	198	= 6	28	29
14	39	41	= 7	64	71	1	726	700	9	66	65	5	274	346	= 6	78	73	= 3	119	112	= 5	65	63
15	15	13	= 6	86	89	2	425	419	11	79	76	7	36	48	= 5	16	11	= 2	382	362	= 3	56	56
16	82	83	= 5	33	32	3	193	185	12	17	25	9	48	56	= 3	130	122	= 1	131	133	= 2	31	26
17	59	59	= 4	40	44	4	269	248	14	29	31	10	26	30	= 2	22	20	2	149	143	= 1	110	104
18	79	69	= 3	260	267	5	140	126	L=	1,K=	5	11	24	31	= 1	21	17	3	30	33	0	45	39
L=	0,K=	1	= 1	139	148	6	90	87	=15	22	23	12	235	274	0	232	232	4	124	125	1	207	210
=15	46	44	0	137	138	7	32	34	=13	67	69	13	37	35	1	100	98	5	172	174	2	184	189
=12	125	125	1	142	148	8	28	29	=12	18	26	14	66	70	2	132	130	6	30	31	3	48	46
=11	24	22	2	15	15	9	91	92	=11	124	125	15	72	72	3	171	163	7	125	132	4	125	120
=10	26	27	3	269	268	11	211	204	=10	117	117	17	41	34	4	22	18	9	62	68	6	31	30
= 9	111	114	4	42	44	13	293	286	= 8	68	68	L=	2,K=	1	6	78	74	10	78	83	8	81	80
= 8	63	66	5	40	32	15	46	44	= 7	43	46	=16	24	15	7	20	19	11	96	102	10	43	48
= 7	22	24	6	92	89	16	33	34	= 6	83	83	=14	15	18	8	18	15	12	81	17	12	27	24
= 6	106	113	7	73	71	L=	1,K=	2	= 5	37	41	=13	16	15	9	91	98	13	26	31	L=	3,K=	6
= 5	94	104	8	38	35	=17	24	19	= 4	126	131	=12	30	25	10	32	30	14	33	32	=11	34	34
= 4	125	128	10	63	62	=16	70	66	= 3	40	38	=10	19	22	11	63	59	L=	3,K=	2	=10	26	26
= 3	69	72	12	98	98	=15	32	33	= 2	144	146	= 9	77	80	12	27	26	=17	25	23	= 9	32	33
= 2	70	70	13	36	36	=14	24	24	= 1	42	44	= 8	28	25	14	33	33	=14	29	31	= 8	18	18
2	72	70	15	41	36	=13	90	89	0	78	76	= 6	151	142	15	36	27	=13	46	46	= 7	19	17
3	74	72	L=	0,K=	5	=11	60	60	1	117	117	= 4	25	25	L=	2,K=	8	=11	63	63	= 6	30	31
4	133	128	=15	24	26	=10	108	109	2	36	40	= 3	221	224	=13	24	15	=10	179	180	= 5	32	38
5	106	104	=14	22	18	= 9	46	47	3	29	21	= 1	87	84	=11	17	19	= 9	40	42	= 4	15	14
6	117	113	=13	33	37	= 8	26	20	4	61	61	0	304	301	=10	17	18	= 8	125	127	= 3	20	14
7	27	24	=12	71	81	= 7	55	55	5	42	40	1	103	99	= 9	34	43	= 7	88	88	0	20	22
8	68	66	=10	19	14	= 6	25	28	6	20	19	2	76	76	= 8	27	28	= 6	80	49	3	20	16
9	120	115	= 8	27	32	= 5	40	44	7	28	29	3	187	191	= 7	47	51	= 5	86	87	4	18	7
10	26	27	= 6	31	29	= 4	110	116	8	71	69	4	23	19	= 6	77	75	= 4	75	70	6	38	34
11	23	22	= 5	77	82	= 3	90	91	10	101	96	5	26	17	= 5	35	35	= 3	38	37	7	52	53
12	128	125	= 4	80	80	= 2	212	206	11	34	27	6	72	71	= 4	25	26	= 1	148	135	8	36	34
14	15	11	= 3	29	33	= 1	375	346	14	56	51	8	14	18	= 3	113	111	0	101	93	9	17	13
15	47	44	= 2	25	26	0	152	146	L=	1,K=	6	9	46	40	= 2	67	67	1	61	53	L=	4,K=	7
L=	0,K=	2	= 1	14	13	1	739	702	=13	22	13	10	33	36	= 1	40	37	2	16	19	= 9	36	35
=17	39	37	2	28	26	2	258	236	= 9	18	11	12	49	44	0	99	99	4	76	74	= 7	83	28
=16	63	60	3	32	33	3	73	68	= 8	23	21	14	41	38	1	42	46	6	86	83	= 6	88	81
=15	27	24	4	82	80	4	256	238	= 7	15	7	15	29	24	2	48	51	7	116	108	= 5	24	26
=14	21	21	5	82	82	5	133	124	= 5	22	26	L=	2,K=	2	3	47	51	8	58	52	= 2	19	20
=13	30	33	6	32	29	6	13	5	= 4	36	39	=16	19	26	4	18	23	9	23	20	= 1	37	41
=12	137	150	8	34	32	7	42	39	= 3	38	39	=15	85	85	5	30	32	10	84	82	0	37	40
=11	41	49	11	18	17	8	138	136	= 2	32	29	=13	19	20	7	22	23	11	50	47	1	94	98
=10	88	85	12	82	81	9	67	69	= 1	28	29	=12	15	17	8	33	32	13	98	85	2	108	112
= 9	68	70	13	37	37	10	23	28	0	63	61	= 8	42	36	9	29	30	14	70	56	3	44	47
= 8	89	91	14	20	16	11	101	104	1	55	56	= 7	17	15	10	41	43	L=	3,K=	3	4	47	53
= 7	170	178	15	25	26	12	17	21	2	79	82	= 6	248	237	11	35	34	=15	21	26	6	22	18
= 6	110	120	L=	0,K=	6	14	48	42	3	24	22	= 5	49	44	12	43	38	=12	27	28	L=	5,K=	8
= 5	14	19	=13	23	30	16	16	7	4	36	38	= 4	68	66	L=	2,K=	6	=11	48	46	= 1	22	19
= 4	181	188	=12	51	55	L=	1,K=	3	5	28	28	= 3	299	275	=12	98	99	=10	125	126	2	22	17
= 3	88	88	=10	44	50	=16	27	27	6	23	23	= 1	50	54	=11	74	73	= 9	33	34	L=	4,K=	0
= 2	136	139	= 7	22	19	=15	26	25	8	26	23	0	199	185	=10	87	80	= 8	86	84	=17	25	23
= 1	128	131	= 6	41	50	=13	57	54	9	32	31	2	16	22	= 9	115	116	= 7	125	125	=16	51	44
0	1252	1251	= 5	28	29	=12	15	13	10	32	30	3	51	51	= 8	32	34	= 6	116	112	=14	22	19
1	134	131	= 4	15	11	=11	70	68	12	19	15	4	111	102	= 7	32	28	= 5	33	29	=13	38	38
2	144	139	= 3	164	177	=10	89	91	13	26	22	5	103	96	= 6	15	10	= 4	93	88	=12	22	27
3	93	88	= 2	19	12	= 9	24	22	L=	1,K=	7	6	239	220	= 5	35	29	= 3	99	91	=11	86	87
4	189	189	= 1	39	44	= 8	26	29	=11	79	82	7	38	40	= 4	28	24	= 2	188	142	=10	35	40
5	21	19	0	26	22	= 7	133	130	=10	44	55	8	15	20	= 3	33	41	= 1	66	66	= 9	371	398
6	124	120	1	42	44	= 6	96	94	= 9	26	22	10	35	37	= 2	38	38	0	88	84	= 8	44	49
7	181	179	2	18	12	= 5	97	97	= 8	21	25	11	51	52	= 1	80	86	1	168	161	= 7	36	38
8	98	91	3	172	177	= 4	27	27	= 7	23	28	12	189	178	0	136	138	2	104	98	= 6	66	69
9	72	71	4	18	11	= 3	204	198	= 6	26	28	13	16	14	1	65	66	3	19	16	= 4	34	32
10	66	65	5	33	29	= 2	190	185	= 4	90	93	14	56	53	2	98	99	4	82	83	= 3	101	108
11	49	49	6	44	50	= 1	160	146	= 3	19	16	15	32	30	3	103	108	5	89	49	= 2	179	196
12	153	151	7	16	19	0	104	101	= 2	40	46	L=	2,K=	3	4	97	96	6	33	32	= 1	137	143
13	36	33	10	49	50	1	362	358	= 1	19	17	=14	29	31	5	37	36	7	81	48	0	124	147
14	20	21	12	55	55	2	73	77	0	54	53	=13	28	27	L=	2,K=	7	8	22	24	1	58	63
15	28	24	13	29	30	3	56	60	1	76	79	=12	44	43	= 8	30	27	9	41	41	2	23	27
16	61	60	L=	0,K=	7	4	133	131	2	23	27	=11	22	18	= 7	45	43	10	66	69	3	86	84
17	42	37	=11	25	29	5	116	108	4	21	25	=10	30	32	= 6	29	28	11	38	36	5	17	22
L=	0,K=	3	= 9	86	89	6	60	54	5	17	17	= 9	119	122	= 5	83	11	13	81	47	9	101	120
=15	71	69	= 8	24	23	7	87	84	8	47	45	= 7	30	28	= 4	65	64	14	31	21	11	47	54
=13	16	18	= 6	20	11	8	100	96	10	41	41	= 6	168	168	= 3	48	47	L=	3,K=	4	12	26	19

Table 2. Continued.

L=	4,K=	1	4	67	62	= 4	52	51	8	26	20	0	52	46	= 4	26	28	= 2	32	32	= 1	21	24
=14	29	22	5	19	18	= 6	123	120	L=	4,K=	7	1	62	59	= 1	86	84	0	55	59	1	43	41
=13	32	29	6	84	84	= 5	31	28	= 1	24	17	2	115	117	0	43	40	3	190	222	2	48	41
=12	33	35	7	71	67	= 3	22	20	0	55	51	3	28	28	1	29	27	5	68	61	5	36	28
=11	23	26	8	67	62	= 2	42	39	2	28	29	4	66	66	2	88	88	7	18	17	7	19	19
=10	26	26	9	107	99	= 1	18	7	4	35	33	5	71	69	3	26	24	L=	6,K=	1	L=	6,K=	4
= 9	89	89	10	16	14	0	61	58	L=	5,K=	1	7	26	17	4	39	37	=12	33	30	=10	22	20
= 8	19	20	11	49	46	1	102	98	=14	26	21	7	22	23	5	50	49	= 9	84	83	= 9	37	33
= 5	43	43	L=	4,K=	3	2	72	71	=13	56	58	9	28	17	6	17	16	= 8	19	16	= 3	53	53
= 4	54	51	=14	40	43	3	159	155	=12	74	74	10	22	11	9	26	22	= 7	24	21	0	56	49
= 3	40	47	=13	54	52	4	80	43	=10	163	159	L=	5,K=	3	L=	6,K=	5	= 6	47	44	2	44	39
= 1	21	15	=12	44	41	5	15	12	= 8	166	164	=14	24	21	=11	46	42	1	22	24	3	29	23
0	63	64	=11	42	47	6	41	40	= 7	81	77	=12	41	39	= 9	31	24	2	28	26	L=	6,K=	6
1	21	18	=10	42	39	7	22	20	= 6	43	40	=11	38	38	= 7	60	60	L=	6,K=	2	= 6	55	52
2	16	13	= 9	87	88	9	42	44	= 5	35	34	=10	45	53	= 5	58	58	=12	27	24	1	33	29
3	132	131	= 8	19	10	10	24	23	= 4	46	43	= 9	24	23	= 4	36	35	=11	19	19	2	28	24
6	66	70	= 7	19	11	11	33	32	= 3	41	44	= 8	69	69	= 3	18	14	=10	19	14	L=	7,K=	1
10	16	12	= 6	57	57	L=	4,K=	5	= 2	29	18	= 6	17	15	= 1	22	17	= 9	56	59	= 7	29	22
12	34	35	= 5	55	57	=13	26	27	= 1	42	47	= 5	46	49	1	41	35	= 7	23	15	= 5	43	34
L=	4,K=	2	= 4	69	71	= 6	34	36	0	33	30	= 4	40	40	2	63	61	= 5	29	30	= 4	41	44
=16	41	35	= 3	77	76	= 5	40	39	1	30	32	= 3	26	28	3	16	13	= 4	23	22	= 2	37	35
=15	20	16	= 1	37	33	= 4	49	48	2	196	195	= 1	32	33	5	53	49	= 3	78	73	0	26	24
=14	19	10	0	83	77	= 3	45	41	3	21	18	0	27	22	L=	5,K=	6	= 2	27	23	1	20	13
=13	37	37	1	52	51	= 1	26	22	4	203	227	1	36	35	= 8	30	33	0	28	18	2	68	67
=11	49	48	2	32	27	1	29	26	5	45	64	2	119	116	= 7	30	28	2	33	27	4	54	59
=10	33	34	3	226	218	3	105	96	6	51	53	4	123	115	= 3	21	18	3	158	146	L=	7,K=	2
= 9	264	263	4	26	23	4	47	42	7	19	23	5	73	67	0	25	19	5	61	55	= 8	30	27
= 8	47	53	5	30	24	6	40	41	9	16	22	6	35	29	1	41	35	6	17	16	= 7	27	33
= 7	20	22	6	108	103	L=	4,K=	6	10	33	38	7	39	34	4	25	24	7	21	14	= 5	23	20
= 6	49	49	8	22	22	= 8	24	22	11	70	67	9	21	18	L=	5,K=	0	8	24	21	= 2	32	20
= 5	61	61	9	18	23	= 6	101	104	12	31	35	10	30	23	=13	26	35	L=	6,K=	3	= 1	31	27
= 4	14	10	10	16	16	= 4	25	27	L=	5,K=	2	L=	5,K=	4	=11	31	36	=11	18	8	1	30	21
= 3	74	71	12	68	69	0	55	59	= 9	37	37	=10	22	9	=10	37	39	= 9	88	86	2	19	16
= 2	138	127	L=	4,K=	4	1	74	77	= 8	82	77	= 9	38	37	= 9	70	77	= 8	38	31	3	17	10
= 1	85	84	=13	26	25	2	82	84	= 6	27	33	= 8	80	76	= 7	16	22	= 7	48	39	L=	7,K=	3
0	73	70	=12	43	38	3	116	115	= 5	41	39	= 7	18	14	= 5	30	38	= 6	81	73	= 4	25	28
1	83	80	=11	21	24	4	39	35	= 2	22	17	= 6	27	29	= 4	17	20	= 3	23	24	= 1	83	18
2	46	50	=10	28	28	6	26	22	= 1	116	108	= 5	28	31	= 3	69	78	= 2	82	83	1	41	37
3	104	101	= 9	66	69																		

when an observed-unobserved cutoff at 2.5 $\sigma(I)$ was used. No corrections have been made for absorption or secondary extinction effects.

The structure was solved by direct methods and refined by full-matrix least squares technique. Hydrogen atom positions were calculated; for the methyl group with one H in the plane defined by the three nearest carbon atoms. Anisotropic temperature factors were introduced for the carbons, and weights in least squares were calculated from the standard deviations in intensities, $\sigma(I)$, taken as

$$\sigma(I) = (C_T + (0.02\ C_N)^2)^{\frac{1}{2}}$$

were C_T is the total number of counts and C_N is the net count (peak minus background). The conventional R-value arrived at was 6.0 % (weighted value $R_w = 6.4$ %) for 1049 observed reflections. The form factors used were those of Hanson *et al.*[2] for C-atoms and those of Stewart *et al.*[3] for hydrogens.

Table 3. Interatomic distances and angles with estimated standard deviations.

DISTANCE	(Å)	DISTANCE	(Å)	DISTANCE	(Å)
C1 - C2	1,383(4)	C2 - C3	1,381(4)	C3 - C4	1,378(4)
C4 - C5	1,378(4)	C5 - C6	1,379(4)	C6 - C1	1,388(4)
C1 - C7	1,491(3)	C7 - C18	1,505(4)	C7 - C8	1,318(3)
C8 - C9	1,388(3)	C9 - C9	1,478(6)		

ANGLE	(°)	ANGLE	(°)
C1 - C2 - C3	121,3(3)	C2 - C3 - C4	120,1(3)
C3 - C4 - C5	119,6(3)	C4 - C5 - C6	120,3(3)
C5 - C6 - C1	121,1(3)	C6 - C1 - C2	117,5(3)
C2 - C1 - C7	121,6(2)	C6 - C1 - C7	120,9(2)
C1 - C7 - C18	118,5(2)	C8 - C7 - C18	120,3(3)
C1 - C7 - C8	121,2(2)	C7 - C8 - C9	179,8(3)
C8 - C9 - C9	124,3(3)		

Final fractional coordinates and thermal vibration parameters are given in Table 1. The expression for anisotropic vibration is:

$$\exp\left[-(B_{11}\,h^2 + B_{22}\,k^2 + B_{33}\,l^2 + B_{12}\,hk + B_{13}\,hl + B_{23}\,kl)\right]$$

The maximum r.m.s. amplitudes obtained by thermal analysis range from 0.22 Å to 0.28 Å. Rigid-body analysis of translational and librational motion [4] gave relatively large r.m.s. discrepancy between atomic vibration tensor components calculated from the thermal parameters of Table 1, and those calculated from the rigid-body parameters. By including all atoms, the value obtained was 0.0040 Å^2. This number does not support the assumption of regarding the molecule as an oscillating rigid-body, and the coordinates were therefore not corrected for librational motion.

A comparison between observed and calculated structure factors is presented in Table 2. Bond distances and angles are listed in Table 3. The numbering of atoms is shown in Fig. 1 where the molecule is viewed along [010].

The bond distances C7 = C8, C8 = C9, C9 – C9′, and the angle C8 = C9 – C9′ agree closely with the corresponding values obtained by a recent electron diffraction investigation of the free molecule of 1,2,4,5-hexatetraene:[5] 1.316 Å, 1.313 Å, 1.471 Å, 124.0°. The three carbon atoms C7, C8, C9 are, within error limits, situated on a straight line, and the bond lengths C1 – C7(1.491 Å) and C7 – C10(1.505 Å) indicate some degree of conjugation in this part of the molecule.

The phenyl ring is planar to within 0.007 Å, and the torsion angle of 20.6° about C1 – C7 gives contacts between H2 and two methyl hydrogens of 2.42 Å and 2.67 Å, respectively. The ring angles have normal values except for C2 – C1 – C6 which is about 3° smaller. Owing to the electron donating characteristics of the system attached to C1, the effect is what should be expected.[6]

No short inter-molecular contacts are observed.

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