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The Crystal Structure of α-2-Ethyl-5-methyl-3,3-diphenyltetrahydrofuran

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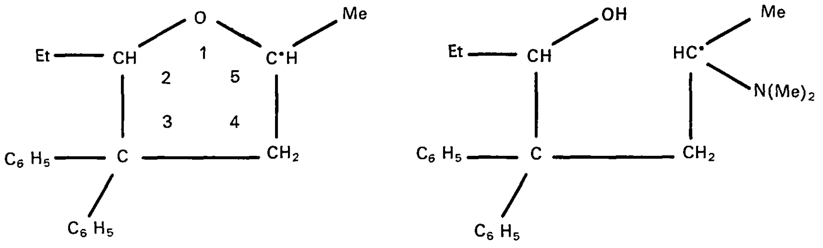
The crystal structure of α-2-ethyl-5-methyl-3,3-diphenyltetrahydrofuran, $C_{19}H_{22}O$, has been determined from X-ray data by the direct method of symbolic addition and has been refined by least-squares to an R index of 0·044 for the 2796 observed reflexions. The unit cell is triclinic, space group $P\bar{1}$, with dimensions $a=9·235$, $b=10·318$, $c=8·911$ Å, $\alpha=93°28'$, $\beta=114°42'$, $\gamma=90°11'$. The saturated five-membered tetrahydrofuran ring is non-planar and its atoms are within $+0·23$ and $-0·25$ Å of their mean plane. The two C–O bonds in the ring are equal, their mean being 1·445 Å, but the three C–C bonds are of lengths 1·556, 1·543, and 1·517 Å ($\sigma=0·004$ Å for each) which are significantly different from each other. The internal valence angles are 110·8° at O, 103·5° to 105·2° at three of the carbon atoms, and only 99·4° ($\sigma=0·2°$) at the C atom where the phenyl groups are substituted. The ethyl group is axial and the methyl group is equatorial, and they are *cis* relative to the furan ring. The axial phenyl ring is nearly normal to the furan ring and is rotated by 83° round the C–C bond joining them, while the equatorial phenyl ring makes a dihedral angle of 40° with the furan ring and is rotated by 32° round the bond joining them. The dihedral angle between the two phenyl rings is about 80°.

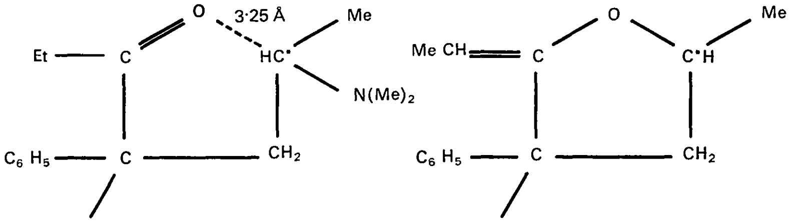
Introduction

The biochemical interest in the structure of 2-ethyl-5-methyl-3,3-diphenyltetrahydrofuran (I, *a*) arises from its close relation to α-methadol (I, *b*) and methadone (I, *c*), which are used as narcotics in pharmaceutical experiments. Methadone has been shown by Harper, Jones & Simmonds (1966) to be readily cyclized to 2-ethylidene-5-methyl-3,3-diphenyltetrahydrofuran (I,*d*). Also, from the X-ray results of Hanson & Ahmed (1958), the O···C* distance in methadone is only 3·25 Å, which shows that the atoms are in positions favourable for forming the tetrahydrofuran ring.

The objective of the present X-ray structure analysis is to determine the dimensions and planarity of the highly saturated five-membered tetrahydrofuran ring, and the *cis*/*trans* orientations of the substituents. It is hoped that this information will contribute to a better understanding of the biological properties of the tetrahydrofuran derivative and the related compound α-methadol. Also, the problem has been considered suit-



(*a*) Tetrahydrofuran (*b*) α-Methadol



(*c*) Methadone (*d*) Tetrahydrofuran

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able for acquiring further experience with the automatic application of the direct method of phase determination. Based on this experience, several modifications have been made to the computer program for symbolic addition procedure which was written in this laboratory by S. R. Hall as part of the NRC set of crystallographic programs for the IBM 360 computer by Ahmed, Hall, Pippy & Huber (1966).

Crystal data

Crystals of α-2-ethyl-5-methyl-diphenyltetrahydrofuran, $C_{19}H_{22}O$, are colourless transparent plates. The unit cell is triclinic, space group $P\bar{1}$, with dimensions

$a = 9{\cdot}235$ Å $\alpha = 93°28'$
$b = 10{\cdot}318$ $\beta = 114\ 42$
$c = 8{\cdot}911$ $\gamma = 90\ 11$
$(\sigma = 0{\cdot}003$ Å$)$ $(\sigma = 5')$.

The unit-cell volume = 769·62 Å^3, F.W. 266·38, $F(000) = 288$ electrons, $\mu(\mathrm{Cu}) = 5{\cdot}36\ \mathrm{cm}^{-1}$. The density, $d_m = 1{\cdot}157\ \mathrm{g.cm}^{-3}$ (by flotation in aqueous potassium iodide solution at 20 °C), and $D_x = 1{\cdot}149\ \mathrm{g.cm}^{-3}$ for $Z = 2$.

Data collection

The unit-cell dimensions and most of the intensity data were measured on the 4-circle Picker automatic diffractometer for a crystal with dimensions 0·14, 0·27, 0·34 mm with Cu radiation [$\lambda(K\alpha_1) = 1{\cdot}54051$, $\lambda(K\alpha_2) = 1{\cdot}54433$ Å] and Ni filters. The reflexions in the range $130° \le 2\theta < 165°$ which were not accessible on this instrument were measured on the General Electric XRD–5 manual diffractometer. The unit-cell constants were calculated from the angular settings of the high-order axial reflexions $(70° \le 2\theta < 130°)$ which were measured at a take-off angle of 1·5° and with a narrow slit inserted before the counter window. The integrated intensities were recorded by the θ, 2θ scan method at a 2θ-scan speed of 2° per minute and a take-off angle of 4°. The 2θ-scan range was 2·5° when $2\theta < 90°$, 3·0° when $90° \le 2\theta < 130°$, and as much as 6·0° when $155° \le 2\theta < 165°$. A 20-second background count was taken both at the start and at the end of the scan range of each reflexion. The very strong reflexions were measured at a low current setting. One of the two standard reflexions, 005 or 006, was measured at intervals of 40 to 60 minutes, and accordingly the intensity data were reduced to the same relative scale. The absorption corrections were considered to be small and were not applied. Of 3391 non-equivalent reflexions within $2\theta < 165°$ there were 2796 (82·3%) observed reflexions with significant net counts.

Structure determination by symbolic addition

As shown in Table 1, the distribution statistics of the normalized structure factor amplitudes, $|E|$, of this structure are considerably closer to the theoretical values of a centrosymmetric structure than to those of a noncentrosymmetric structure as calculated by Karle, Hauptman, Karle & Wing (1958). Based on these statistics, the space group is probably $P\bar{1}$.

Table 1. *Distribution statistics of the $|E|$ amplitudes*

	. . . Tetrahydrofuran	$P\bar{1}$	$P1$
$\langle\lvert E\rvert\rangle$	0·786	0·798	0·886
$\langle\lvert E^2\rvert\rangle$	1·000	1·000	1·000
$\langle\lvert E^2-1\rvert\rangle$	1·001	0·968	0·736
$\lvert E\rvert > 3$	0·4%	0·3%	0·01%
$\lvert E\rvert > 2$	4·8%	5%	1·8%
$\lvert E\rvert > 1$	29·9%	32%	37%

The symbolic addition procedure of phase determination for centrosymmetric structures which was first applied by Karle & Karle (1963), and later described in more detail by Karle & Karle (1966) was carried out on this structure with a modified version of Hall's existing program mentioned earlier. The modification examines the probability of the newly determined signs and restricts their acceptance as tentative signs, in the early stages of the application of the Σ_2 relationships, to those with relatively high probability. For this test, only the sums

$$\sum_{\mathbf{k}} \sigma_3\sigma_2^{-3/2}\,|E_{\mathbf{h}}|E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}} \tag{1}$$

are evaluated instead of the full probability expression

$$P_+(\mathbf{h}) \simeq \tfrac{1}{2} + \tfrac{1}{2}\tanh(\sigma_3\sigma_2^{-3/2}|E_{\mathbf{h}}| \sum_{\mathbf{k}} E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}) \tag{2}$$

given by Woolfson (1954) and Cochran & Woolfson (1955). In this automated procedure, the probability limit is set relatively high to start with, the search for new signs is continued until no more new signs can be accepted, then the probability limit is reduced in steps and the search is repeated.

For this structure $\sigma_3\sigma_2^{-3/2} = 0{\cdot}157$. The first step of the phase determination was restricted to the 162 re-

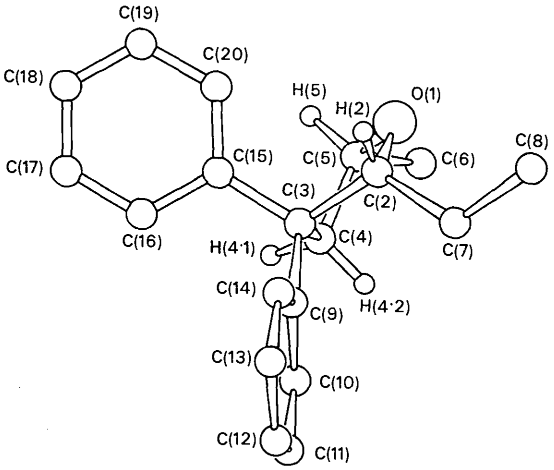

Fig. 1. Perspective view of the molecule excluding the non-furan hydrogen atoms.

flexions with $|E| \geq 2{\cdot}0$. The three origin-defining reflexions $1\bar{4}6$, 810, and 207 which were selected automatically by the computer program were the 1st, 6th, and 11th reflexions, respectively, in the list of descending $|E|$'s. Their signs were assumed to be positive. The successful automatic phase determination proceeded as described herewith. The limit on the sums given in expression (1) was first set to 8·0, the search for new signs was carried out until exhausted, then that limit was reduced to 7·5 and later to 7·0. Thus, before the first symbol (A) was introduced, no new signs were accepted unless their probability was about 1·000. After assuming the symbol A, the process was repeated with the limits set to 6·5, 6·0, and 5·5. The second symbol (B) was then introduced and the limits were reduced to 5·0, 4·5, and 4·0. Similarly, symbol C was then introduced with the limits set to 3·5, 3·0, and 2·5, and finally symbol D was introduced with the limits set to 2·4, 2·2, and 2·0, where this minimum limit of 2·0 corresponds to a probability of 0·98. From the accumulated information about the signs of the 162 reflexions, it was obvious that two of the assumed symbols were probably positive and the two remaining symbols were probably not positive, *i.e.* negative. This procedure produced the signs of the 162 reflexions without giving any contradictions whatever in the Σ_2 relationships between them. The second step in the phasing process was then applied with similar success to the 264 reflexions with $2{\cdot}0 > |E| \geq 1{\cdot}50$. The E map computed with these 426 reflexions gave the complete structure (excluding the H atoms)

Table 2. *Fractional coordinates, vibration tensor components* (Å^2) *for the expression* $T = \exp\,[-2\pi^2(U_{11}a^{*2}h^2 + \ldots + 2U_{23}b^*c^*kl + \ldots)]$, and *their e.s.d.'s* (*all quantities* × 10^4)

	x	y	z	U_{11}	U_{22}	U_{33}	$2U_{23}$	$2U_{13}$	$2U_{12}$
O(1)	−2922 (2)	2230 (2)	−1078 (2)	456 (11)	676 (14)	342 (10)	56 (19)	158 (17)	−126 (20)
C(2)	−1615 (3)	2837 (3)	350 (3)	353 (13)	519 (17)	334 (14)	75 (24)	238 (22)	7 (24)
C(3)	−1674 (3)	2176 (3)	1849 (3)	323 (13)	406 (14)	321 (13)	37 (22)	231 (21)	39 (21)
C(4)	−2203 (3)	788 (3)	1049 (3)	457 (16)	428 (16)	419 (15)	−49 (25)	293 (25)	5 (25)
C(5)	−3412 (3)	1007 (3)	−691 (3)	378 (15)	524 (17)	444 (16)	−148 (27)	252 (25)	−66 (25)
C(6)	−3505 (4)	−51 (4)	−1983 (4)	656 (22)	799 (26)	557 (20)	−511 (37)	206 (35)	86 (39)
C(7)	−61 (3)	2658 (3)	151 (4)	411 (15)	841 (24)	407 (16)	68 (30)	395 (26)	−70 (31)
C(8)	−148 (5)	3194 (5)	−1444 (4)	675 (25)	1630 (45)	523 (21)	324 (49)	684 (39)	−268 (53)
C(9)	−72 (3)	2290 (3)	3358 (3)	327 (13)	475 (15)	315 (12)	55 (22)	290 (21)	45 (22)
C(10)	802 (3)	1228 (3)	4061 (4)	432 (15)	524 (18)	438 (16)	174 (27)	273 (26)	105 (27)
C(11)	2265 (4)	1392 (3)	5431 (4)	460 (17)	762 (23)	480 (18)	408 (33)	232 (28)	267 (32)
C(12)	2861 (3)	2607 (4)	6128 (4)	355 (15)	903 (25)	391 (16)	112 (31)	156 (25)	−25 (31)
C(13)	1993 (3)	3677 (3)	5454 (4)	400 (15)	677 (21)	471 (17)	−190 (30)	318 (27)	−189 (28)
C(14)	543 (3)	3522 (3)	4086 (3)	370 (14)	515 (17)	424 (15)	−28 (26)	304 (24)	6 (25)
C(15)	−2977 (3)	2740 (3)	2328 (3)	311 (12)	412 (14)	362 (13)	−67 (23)	253 (22)	−71 (21)
C(16)	−2941 (3)	2512 (3)	3873 (3)	410 (15)	556 (18)	404 (15)	4 (26)	350 (25)	−52 (26)
C(17)	−4105 (4)	2968 (4)	4344 (4)	498 (18)	747 (23)	517 (18)	−139 (33)	584 (30)	−164 (31)
C(18)	−5343 (4)	3657 (4)	3286 (4)	450 (17)	707 (22)	742 (23)	−257 (36)	710 (33)	−60 (31)
C(19)	−5413 (3)	3882 (3)	1754 (4)	380 (15)	640 (21)	697 (21)	87 (33)	424 (30)	190 (29)
C(20)	−4243 (3)	3428 (3)	1274 (4)	381 (15)	557 (18)	461 (16)	85 (27)	323 (25)	107 (26)

Table 3. *Fractional coordinates* (× 10^3) *and isotropic temperature factors* (Å^2) *of the hydrogen atoms and their e.s.d.'s*

The first subscript in the atom number refers to the serial number of the nearest carbon atom.

	x	y	z	B
H(2)	−186 (3)	379 (2)	39 (3)	3·0 (0·5)
H(4,1)	−266 (3)	24 (3)	167 (4)	4·7 (0·7)
H(4,2)	−124 (3)	34 (3)	101 (3)	3·7 (0·6)
H(5)	−452 (3)	114 (3)	−73 (3)	3·2 (0·5)
H(6,1)	−383 (5)	−85 (4)	−173 (5)	8·6 (1·1)
H(6,2)	−423 (4)	17 (3)	−308 (4)	6·4 (0·9)
H(6,3)	−242 (4)	−15 (3)	−197 (4)	5·9 (0·8)
H(7,1)	8 (4)	158 (4)	16 (4)	6·7 (0·9)
H(7,2)	80 (4)	310 (3)	105 (4)	5·0 (0·7)
H(8,1)	−90 (4)	271 (4)	−227 (5)	7·9 (1·0)
H(8,2)	90 (4)	306 (4)	−147 (5)	7·4 (1·0)
H(8,3)	−58 (6)	412 (5)	−158 (6)	12·9 (1·6)
H(10)	42 (3)	37 (3)	357 (4)	4·5 (0·7)
H(11)	285 (4)	64 (3)	586 (4)	5·4 (0·8)
H(12)	391 (3)	274 (3)	704 (4)	4·5 (0·7)
H(13)	240 (3)	451 (3)	589 (4)	4·9 (0·7)
H(14)	−6 (3)	427 (3)	363 (3)	4·1 (0·6)
H(16)	−207 (3)	203 (3)	461 (3)	4·2 (0·6)
H(17)	−405 (4)	280 (3)	543 (4)	5·6 (0·8)
H(18)	−618 (4)	398 (3)	358 (4)	5·1 (0·7)
H(19)	−627 (4)	436 (3)	98 (4)	5·1 (0·7)
H(20)	−431 (3)	358 (3)	19 (3)	4·2 (0·6)

Table 4. *Observed structure amplitudes and calculated structure factors* (×10)

* Indicates unobserved reflexion and $|F_{th}|$ in place of $|F_o|$.

K	FO	FC
H=	0, L=	0
1	39	39
2	789	-792
3	463	452
4	57	57
5	53	-53
6	143	-139
7	57	-52
8	149	144
9	35	35
10	11*	-7
11	29	28
12	14	-16
13	8*	0
H=	0, L=	1
0	86	83
1	301	-293
2	206	201
3	12	8
4	57	56
5	51	-48
6	153	-147
7	17	12
8	49	-47
9	24	-20
10	58	57
11	17	14
12	10	8
13	7*	17
-1	552	563
-2	137	-131
-3	105	104
-4	185	186
-5	9	-11
-6	8*	13
-7	90	-81
-8	70	-75
-9	32	31
-10	37	42
-11	21	17
-12	15	13
-13	10*	-5
H=	0, L=	2
0	223	226
1	176	180
2	103	-104
3	182	-174
4	201	-185
5	195	-190
6	29	-30
7	19	-26
8	56	-58
9	15	12
10	37	36
11	20	17
12	7*	-2
-1	171	-170
-2	173	-175
-3	75	71
-4	101	-94
-5	160	-154
-6	9*	-5
-7	71	74
-8	62	65
-9	38	-36
-10	58	-59
-11	10*	3
-12	8*	-4
-13	5*	-9
H=	0, L=	3
0	137	-134
1	39	-30
2	7*	-5
3	116	-114
4	53	-52
5	25	-28
6	44	-44
7	16	-17
8	19	21
9	23	-19
10	15	-21
11	32	31
12	6*	4
-1	50	-57
-2	203	-203
-3	18	15
-4	231	225
-5	123	-114
-6	124	-122
-7	73	74
-8	24	26
-9	23	-27
-10	27	-26
-11	9*	-6
-12	9	10
H=	0, L=	4
0	295	-294
1	27	27
2	146	148
3	20	-21
4	29	28
5	10*	-6
6	21	25
7	94	95
8	28	-28
9	75	-77
10	50	50
11	33	42
-1	26	-27
-2	8*	1
-3	21	-18
-4	44	47
-5	41	-41
-6	24	20
-7	130	131
-8	20	22
-9	50	-52
-10	10*	-6
-11	9*	-3
-12	22	-23
H=	0, L=	5
0	128	124
1	9*	-12
2	31	-27
3	204	208
4	26	25
5	59	-54
6	95	99
7	49	48
8	16	-16
9	9*	9
10	18	18
11	7	4
-1	43	-37
-2	135	-134
-3	77	-84
-4	143	145
-5	44	45
-6	101	-99
-7	108	108
-8	113	110
-9	53	-50
-10	32	-35
-11	15	16
H=	0, L=	6
0	40	-41
1	182	-183
2	17	18
3	91	93
4	69	69
5	67	68
6	11*	6
7	14	16
8	12	-15
9	28	-29
10	5*	-1
-1	91	92
-2	16	-15
-3	54	-56
-4	11*	-2
-5	96	101
-6	18	18
-7	48	-50
-8	16	21
-9	25	28
-10	12	13
-11	6*	-2
H=	0, L=	7
0	24	22
1	96	-99
2	14	-16
3	138	137
4	11*	8
5	81	-79
6	10*	1
7	9*	0
8	15	-14
9	5*	-1
-1	11*	-5
-2	45	-48
-3	71	-71
-4	101	-100
-5	52	50
-6	90	92
-7	10*	-4
-8	9*	-9
-9	20	-20
-10	7*	-2
H=	0, L=	8
0	11*	-3
1	62	-62
2	38	-35
3	10*	-1
4	39	37
5	9*	6
6	18	-17
7	14	14
-1	32	30
-2	37	-38
-3	26	22
-4	32	32
-5	58	-59
-6	32	-31
-7	13	-13
-8	7*	3
-9	5*	10
H=	0, L=	9
0	37	36
1	9*	5
2	16	-15
3	35	35
4	7*	-2
5	15	-15
-1	9*	-3
-2	22	-24
-3	24	-25
-4	21	19
-5	39	38
-6	7*	-12
-7	15	-17
H=	0, L=	10
0	21	19
1	21	-22
2	12	12
-1	67	63
-2	13	-12
-3	17	-15
-4	52	51
H=	1, L=	0
0	81	78
1	453	456
2	82	-82
3	481	-485
4	165	167
5	201	195
6	12	-14
7	44	-44
8	51	-57
9	32	-35
10	30	-28
11	21	-19
12	12	-8
13	5*	0
-1	286	-310
-2	349	-357
-3	174	181
-4	26	-16
-5	283	-293
-6	28	-31
-7	39	34
-8	45	46
-9	79	85
-10	14	-10
-11	21	-26
-12	14	-14
-13	5*	-1
H=	1, L=	1
0	166	165
1	367	361
2	686	-684
3	327	321
4	437	436
5	291	-293
6	90	-83
7	38	37
8	54	-57
9	81	-85
10	52	-51
11	25	26
12	19	14
-1	637	-658
-2	250	-246
-3	130	-121
-4	167	163
-5	36	-43
-6	127	-122
-7	118	116
-8	43	-49
-9	106	-111
-10	33	35
-11	15	15
-12	13	-12
-13	8*	12
H=	1, L=	-1
0	230	-235
1	447	450
2	569	575
3	114	114
4	99	100
5	92	88
6	56	56
7	9*	-5
8	128	-127
9	13	-15
10	63	61
11	10*	7
12	9	-5
13	9*	-10
-1	455	-459
-2	412	-421
-3	63	64
-4	147	151
-5	56	-54
-6	36	34
-7	145	151
-8	61	63
-9	29	-30
-10	11*	3
-11	11	-10
-12	8*	-2
-13	27	29
H=	1, L=	2
0	46	-47
1	26	24
2	62	59
3	226	218
4	89	-87
5	50	-51
6	62	65
7	18	18
8	27	-29
9	52	-49
10	10	15
11	21	20
12	7*	-6
-1	123	-123
-2	297	297
-3	92	95
-4	261	-256
-5	19	-14
-6	51	49
-7	10*	-6
-8	21	16
-9	39	-42
-10	22	-18
-11	35	34
-12	13	-10
H=	1, L=	-2
0	492	481
1	260	-253
2	22	-19
3	8	-5
4	137	136
5	196	196
6	75	-73
7	56	60
8	116	118
9	99	-98
10	51	-51
11	34	56
12	8*	0
13	9*	3
-1	175	169
-2	286	-287
-3	139	138
-4	41	42
-5	44	-39
-6	11	7
-7	71	68
-8	87	84
-9	42	41
-10	13	15
-11	9*	4
-12	7*	2
H=	1, L=	3
0	244	238
1	123	-116
2	127	-128
3	158	155
4	94	90
5	59	-56
6	39	-35
7	82	82
8	62	65
9	31	-28
10	21	-24
11	8*	3
12	5*	12
-1	158	149
-2	105	99
-3	96	95
-4	65	61
-5	50	52
-6	14	11
-7	12	8
-8	28	-30
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10	70	-71
11	24	24
12	6*	7
-1	35	-34
-2	101	103
-3	112	114
-4	31	-30
-5	51	-54
-6	11*	4
-7	19	17
-8	34	35
-9	10	9
-10	8*	-5
-11	34	34
H=	3, L=	6
0	90	-91
1	53	56
2	94	91
3	10*	-6
4	17	-19
5	13	-13
6	11	11
7	13	-10
8	35	-34
-1	11*	-4
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-4	26	-28
-5	13	14
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-8	14	-9
-9	17	-14
H=	3, L=	-6
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1	61	60
2	14	-16
3	11	-11
4	111	107
5	27	24
6	11*	2
7	11*	0
8	38	-35
9	31	30
10	9*	-2
11	31	-36
-1	56	-57
-2	101	-100
-3	74	79
-4	82	84
-5	48	-45
-6	11*	5
-7	31	33
-8	23	24
-9	9*	-2
-10	18	-17
H=	3, L=	7
0	10*	-9
1	11	12
2	63	-65
3	16	-15
4	33	33
5	40	-37
6	33	-32
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-2	26	26
-3	33	29
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-5	32	-31
-6	8*	-3
-7	7*	-6
-8	26	-24
H=	3, L=	-7
0	37	-36
1	25	-26
2	10*	4
3	11*	-1
4	23	-23
5	65	64
6	68	69
7	15	-7
8	25	-24
9	9*	6
10	7*	5
-1	88	-86
-2	15	-14
-3	25	24
-4	59	-58
-5	39	39
-6	49	47
-7	42	-40
-8	13	-9
-9	7*	-1
H=	3, L=	8
0	30	30
1	17	-13
2	72	-69
3	6*	-2
4	16	17
-1	22	-23
-2	8*	-1
-3	19	14
-4	15	11
-5	10	9
H=	3, L=	-8
0	87	92
1	101	-106
2	110	-116
3	42	44
4	33	37
5	11*	7
6	11	12
7	10*	-2
8	8*	5
9	16	17
-1	11*	9
-2	99	-99
-3	54	-54
-4	43	41
-5	66	67
-6	49	-49
-7	27	-26
-8	48	48
H=	3, L=	-9
0	10*	-2
1	25	26
2	39	-45
3	14	-13
4	53	56
5	11	12
6	13	-13
7	8*	-5
8	13	-10
H=	3, L=	-9
-1	33	-33
-2	62	-63
-3	35	-33
-4	92	92
-5	34	32
-6	24	-26
-7	40	39
H=	3, L=	-10
0	9*	-9
1	21	-21
2	15	15
3	21	-25
4	23	-21
5	32	31
6	12	12
H=	3, L=	-10
-1	18	15
-2	8*	7
-3	39	39
-4	15	13
-5	14	-17
H=	3, L=	-11
0	16	-15
1	13	6
2	11	9
3	25	26
H=	3, L=	-11
-1	11	12
H=	4, L=	0
0	227	227
1	48	-45
2	176	-181
3	15	-15
4	71	-76
5	71	72
6	19	-18
7	123	-126
8	45	51
9	12	10
10	52	-56
11	8*	3
12	9*	12
-1	65	-70
-2	128	-128
-3	17	-17
-4	117	119
-5	9*	7
-6	103	-106
-7	30	27
-8	11*	5
-9	43	-41
-10	17	-15
-11	13	-9
-12	16	13
H=	4, L=	1
0	159	-154
1	68	-64
2	49	47
3	23	-23
4	40	41
5	28	-27
6	104	-100
7	76	81
8	12	-6
9	84	-87
10	34	34
11	30	30
-1	96	-100
-2	80	-74
-3	77	73
-4	64	70
-5	16	-8
-6	19	-21
-7	25	27
-8	11*	1
-9	67	-67
-10	30	-27
-11	8*	-6
-12	5*	1
H=	4, L=	-1
0	53	55
1	110	105
2	47	48
3	17	6
4	16	-20
5	22	22
6	41	38
7	94	-97
8	63	-62
9	41	42
10	23	26
11	12	-12
12	8*	3
-1	64	62
-2	65	-60
-3	18	-16
-4	22	-8
-5	76	-73
-6	39	37
-7	10*	6
-8	41	-40
-9	54	53
-10	21	22
-11	21	-22
-12	6*	-3
H=	4, L=	2
0	127	-124
1	9*	-7
2	124	127
3	81	-80
4	186	-191
5	18	20
6	171	174
7	59	61
8	57	-56
9	9*	3
10	24	39
11	5*	-6
-1	9	10
-2	100	103
-3	47	46
-4	11	-14
-5	10*	0
-6	21	-28
-7	31	29
-8	79	86
-9	37	-34
-10	56	-60
-11	7*	2
H=	4, L=	-2
0	228	230
1	75	-69
2	84	84
3	137	134
4	143	138
5	27	27
6	83	-84
7	87	-86
8	11*	-6
9	25	23
10	17	-17
11	8*	-4
12	19	19
-1	325	325
-2	347	-352
-3	222	-219
-4	216	220
-5	90	89
-6	17	-20
-7	44	-47
-8	18	16
-9	68	63
-10	20	-19
-11	8*	-2
-12	34	34
H=	4, L=	3
0	158	-157
1	69	61
2	10*	-4
3	91	-90
4	147	149
5	84	84
6	17	-16
7	31	31
8	10*	3
9	23	21
10	11	3
-1	53	-43
-2	16	9
-3	31	26
-4	168	172
-5	90	92
-6	24	-22
-7	25	-29
-8	17	17
-9	9*	5
-10	34	-35
-11	16	-14
H=	4, L=	-3
0	426	428
1	168	-169
2	58	-56
3	122	119
4	25	-26
5	9*	8
6	54	50
7	46	-46
8	47	-50
9	11*	7
10	10*	3
11	11	-13
12	12	-13
-1	125	128
-2	270	-262
-3	69	62
-4	31	-34
-5	61	-59
-6	57	-59
-7	58	-59
-8	123	121
-9	55	57
-10	23	-23
-11	40	37
-12	5*	-6
H=	4, L=	4
0	18	-13
1	51	-55
2	25	-29
3	41	40
4	20	-23
5	11	-12

Table 4 (*cont.*)

K	FO	FC
H=	4, L=	4
6	52	51
7	22	23
8	40	38
9	22	19
-1	35	38
-2	77	80
-3	43	-44
-4	114	-115
-5	45	45
-6	88	94
-7	10*	-8
-8	10*	-2
-9	19	22
-10	9	8
H=	4, L=	-4
0	186	-185
1	219	219
2	114	112
3	26	26
4	126	126
5	126	-123
6	100	-99
7	55	56
8	41	-41
9	26	-29
10	16	14
11	8	8
12	12*	17
-1	166	-164
-2	8*	3
-3	145	-147
-4	106	-106
-5	10*	-16
-6	18	-19
-7	72	71
-8	24	22
-9	57	-59
-10	12	8
-11	16	18
H=	4, L=	5
0	67	-73
1	64	-70
2	31	-29
3	16	16
4	39	40
5	10*	-8
6	11	-13
7	16	18
8	15	15
-1	20	18
-2	11*	8
-3	19	-19
-4	33	35
-5	10*	-7
-6	10*	7
-7	9*	2
-8	43	-43
-9	6*	-8
H=	4, L=	-5
0	85	84
1	222	-229
2	57	-56
3	73	76
4	10*	7
5	10*	-1
6	55	-51
7	61	64
8	66	66
9	65	-63
10	42	-43
11	7*	-3
-1	48	48
-2	10	-7
-3	33	35
-4	111	-110
-5	69	-69
-6	11*	8
-7	16	15
-8	17	11
-9	16	-14
-10	21	17
-11	40	38
H=	4, L=	6
0	75	74
1	56	-53
2	71	-69
3	56	55
4	10	11
5	31	-31
6	19	-17
7	5*	-1
-1	10*	4
-2	33	-32
-3	32	-30
-4	33	-30
-5	9*	10
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-7	7	-6
-8	23	19
H=	4, L=	-6
0	47	-49
1	94	98
2	23	-22
3	67	69
4	14	16
5	95	-97
6	11*	7
7	25	29
8	10*	1
9	37	37
10	30	31
11	14	-17
-1	57	-60
-2	127	132
-3	82	-80
-4	63	-60
-5	84	84
-6	17	15
-7	25	23
-8	10	11
-9	9*	-4
-10	27	25
H=	4, L=	7
0	9*	-5
1	15	-20
2	57	52
3	12	9
4	56	-49
-1	39	39
-2	31	27
-3	9	-10
-4	49	-40
-5	7*	7
-6	22	20
H=	4, L=	-7
0	31	35
1	24	-23
2	47	-51
3	14	-13
4	11*	-3
5	11*	1
6	38	34
7	44	43
8	10*	1
9	21	-19
10	22	19
-1	51	52
-2	27	-27
-3	27	28
-4	136	137
-5	28	-25
-6	59	-58
-7	60	54
-8	18	18
-9	19	-21
H=	4, L=	8
0	5*	30
1	50	48
-1	5*	-2
-2	19	-18
-3	38	35
H=	4, L=	-8
0	69	73
1	13	-13
2	39	-44
3	31	-33
4	18	-13
5	25	-24
6	10*	-2
7	31	30
8	13	14
9	7*	3
-1	11*	3
-2	69	-70
-3	112	112
-4	74	72
-5	87	-84
-6	9*	1
-7	18	18
-8	20	-22
H=	4, L=	-9
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1	32	35
2	10*	2
3	59	-61
4	50	-52
5	28	32
6	12	8
7	25	-26
8	6*	3
H=	4, L=	-9
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-2	17	-17
-3	44	45
-4	18	18
-5	17	-15
-6	32	-27
-7	10	-12
H=	4, L=	-10
0	19	20
1	23	-23
2	17	-17
3	23	-21
4	8*	-11
5	20	15
6	6*	-2
7	5*	-3
H=	4, L=	-10
-1	12	-11
-2	26	-24
-3	75	69
-4	30	25
-5	60	-57
H=	4, L=	-11
0	12	13
1	6	8
2	11	-13
3	23	18
4	5*	4
H=	4, L=	-11
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-2	29	27
H=	5, L=	0
0	74	72
1	162	-158
2	18	18
3	11	12
4	46	-49
5	33	35
6	45	46
7	18	16
8	37	-35
9	12	-12
10	11	11
11	29	-26
-1	84	87
-2	9*	2
-3	112	117
-4	58	-64
-5	63	-61
-6	44	41
-7	70	-77
-8	33	-33
-9	26	29
-10	9*	0
-11	22	18
H=	5, L=	1
0	13	-10
1	82	79
2	19	-21
3	100	103
4	101	98
5	176	-180
6	44	-47
7	56	54
8	22	24
9	44	43
10	32	-33
11	5*	0
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-2	82	80
-3	52	-56
-4	21	21
-5	10*	3
-6	17	13
-7	32	30
-8	34	-33
-9	48	-51
-10	9*	-3
-11	42	39
H=	5, L=	-1
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1	8*	-3
2	26	-26
3	54	55
4	61	-64
5	27	-27
6	47	49
7	11*	7
8	55	-54
9	10*	-7
10	15	16
11	17	-20
-1	155	-160
-2	125	-125
-3	38	35
-4	10	-13
-5	9*	2
-6	94	-100
-7	53	-56
-8	97	100
-9	30	-29
-10	46	-45
-11	40	34
-12	4*	4
H=	5, L=	2
0	92	94
1	93	-96
2	38	-38
3	63	59
4	102	-107
5	42	-42
6	39	39
7	35	34
8	48	50
9	42	-41
10	7	-9
-1	82	85
-2	121	121
-3	146	151
-4	58	-54
-5	107	-108
-6	11*	-2
-7	11*	-4
-8	12	-10
-9	9*	2
-10	8*	-10
-11	37	32
H=	5, L=	-2
0	121	112
1	38	-41
2	166	-167
3	72	68
4	42	37
5	27	-24
6	56	58
7	44	43
8	60	-59
9	60	-58
10	15	14
11	7*	-2
-1	190	-191
-2	188	-188
-3	43	-40
-4	134	138
-5	21	18
-6	137	-142
-7	108	110
-8	65	64
-9	88	-88
-10	9*	10
-11	8*	8
H=	5, L=	3
0	11	-9
1	53	-54
2	18	17
3	11*	-5
4	43	-43
5	54	-55
6	25	-26
7	9*	-4
8	20	-17
9	6*	19
-1	95	98
-2	50	-55
-3	101	-102
-4	128	135
-5	56	56
-6	73	-76
-7	11	14
-8	10*	-8
-9	27	-28
-10	26	-23
H=	5, L=	-3
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1	63	62
2	8*	2
3	111	-114
4	73	78
5	169	166
6	10*	12
7	11*	13
8	19	19
9	47	-45
10	9*	-5
11	7*	-1
-1	95	-91
-2	60	-61
-3	104	107
-4	151	157
-5	43	-46
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-7	59	62
-8	11	9
-9	27	28
-10	9*	8
-11	10	-11
H=	5, L=	4
0	60	66
1	63	-68
2	68	-71
3	45	-44
4	24	-22
5	10*	3
6	44	-41
7	18	-15
8	36	35
-1	70	76
-2	25	-26
-3	48	-46
-4	11*	-2
-5	25	28
-6	57	-56
-7	51	-52
-8	29	30
-9	31	26
H=	5, L=	-4
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1	127	130
2	75	-76
3	33	30
4	87	85
5	10*	5
6	15	13
7	11*	6
8	42	39
9	13	14
10	18	-20
11	7*	1
-1	62	-61
-2	88	-86
-3	40	-37
-4	121	123
-5	36	35
-6	11*	8
-7	138	136
-8	53	52
-9	58	-59
-10	12	-13
-11	6*	1
H=	5, L=	5
0	10*	-12
1	10*	-11
2	23	22
3	30	-27
4	28	-22
5	33	31
6	13	10
7	25	-22
-1	19	21
-2	22	-16
-3	32	-32
-4	17	11
-5	36	36
-6	10	12
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-8	13	-13
H=	5, L=	-5
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1	166	-167
2	42	-46
3	15	8
4	133	131
5	38	30
6	39	-39
7	31	30
8	19	17
9	25	-23
10	8*	-6
11	8*	2
-1	104	105
-2	25	-24
-3	10*	-4
-4	40	37
-5	24	24
-6	89	87
-7	21	-17
-8	78	-76
-9	21	22
-10	16	17
-11	14	-16
H=	5, L=	6
0	42	42
1	22	20
2	16	-19
3	8*	-8
4	79	69
5	17	16
-1	13	15
-2	62	-56
-3	23	-18
-4	42	39
-5	19	15
-6	22	-21
H=	5, L=	-6
0	177	183
1	10*	3
2	159	-161
3	13	13
4	75	77
5	68	-67
6	70	-71
7	11*	5
8	36	38
9	37	37
10	8*	-6
11	14*	-10
-1	18	19
-2	155	-157
-3	74	-73
-4	29	29
-5	22	22
-6	13	-15
-7	15	-13
-8	16	16
-9	8*	-8
-10	26	-24
H=	5, L=	7
0	16	11
1	6*	4
2	5*	-2
-1	6*	1
-2	6*	1
-3	18	-14
-4	21	-19
H=	5, L=	-7
0	128	131
1	29	-29
2	87	-88
3	25	23
4	54	58
5	11*	0
6	60	-59
7	10*	-1
8	9*	1
9	40	-38
10	10*	13
-1	111	-113
-2	107	-105
-3	155	158
-4	11*	0
-5	86	-85
-6	18	11
-7	18	17
-8	10	-11
-9	33	-31
H=	5, L=	-8
0	11*	8
1	54	52
2	19	13
3	44	42
4	58	-59
5	65	-62
6	22	20
7	9*	-5
8	8*	6
9	7*	6
H=	5, L=	-8
-1	38	-39
-2	106	107
-3	11*	9
-4	91	-94
-5	10*	3
-6	24	20
-7	9	8
-8	10	-11
H=	5, L=	-9
0	48	46
1	47	50
2	10*	-6
3	22	19
4	25	24
5	30	-28
6	27	-27
7	8*	2
8	6*	-5
H=	5, L=	-9
-1	13	-9
-2	10*	-5
-3	20	18
-4	9*	12
-5	43	-39
-6	20	-20
-7	34	31
H=	5, L=	-10
0	42	-41
1	33	34
2	46	48
3	11	-11
4	8*	-5
5	7*	-3
6	6*	-6
H=	5, L=	-10
-1	9*	-5
-2	30	28
-3	13	13
-4	22	-21
-5	44	-42
H=	5, L=	-11
0	23	23
1	23	23
2	27	-25
3	14	-13
4	24	23
H=	5, L=	-11
-1	6*	-2
-2	6	-3
H=	6, L=	0
0	64	67
1	55	-56
2	70	-73
3	62	60
4	113	113
5	42	39
6	55	-57
7	16	-14
8	21	19
9	31	-31
10	8	7
-1	72	70
-2	58	-57
-3	64	-69
-4	97	97
-5	37	40
-6	69	-73
-7	11*	-1
-8	14	13
-9	35	38
-10	39	38
-11	5*	-4
H=	6, L=	1
0	110	110
1	18	15
2	56	-59
3	110	111
4	34	32
5	109	-111
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-7	46	-42
-8	10	-9
H=	9, L=	-4
0	36	-36
1	84	90
2	16	-11
3	77	-79
4	39	-37
5	10	8
6	64	60
7	8*	-2
8	23	-19
H=	9, L=	-4
-1	48	-50
-2	33	39
-3	16	-15
-4	11	-9
-5	10*	8
-6	50	-45
-7	11	-7
-8	60	54
H=	9, L=	-5
0	72	-74
1	48	-48
2	33	36
3	19	-19
4	10*	8
5	9*	3
6	9*	11
7	51	45
8	20	-18
H=	9, L=	-5
-1	45	51
-2	11*	6
-3	16	-21
-4	48	46
-5	21	23
-6	11	-8
-7	15	13
-8	8	6
H=	9, L=	-6
0	47	47
1	16	-13
2	66	-66
3	53	-52
4	61	59
5	40	42
6	54	-54
7	22	21
8	54	52
H=	9, L=	-6

Table 4 (*cont.*)

K	FO	FC
H= 9, L= -6		
-1	10*	-6
-2	39	-40
-3	59	61
-4	55	55
-5	11	4
-6	8*	6
-7	6*	-1
H= 9, L= -7		
0	14	11
1	26	-28
2	29	-28
3	13	10
4	25	-32
5	14	14
6	21	20
7	18	-15
H= 9, L= -7		
-1	11	-14
-2	44	43
-3	9*	8
-4	17	-22
-5	32	31
-6	7*	5
-7	16	12
H= 9, L= -8		
0	16	-15
1	42	-45
2	24	-21
3	24	23
4	21	19
5	8	-6
6	13	-13
H= 9, L= -8		
-1	30	28
-2	14	-14
-3	25	-21
-4	32	31
-5	21	19
-6	23	21
H= 9, L= -9		
0	54	53
1	19	-14
2	30	-29
3	10	7
4	25	-21
5	6*	5
H= 9, L= -9		
-1	17	11
-2	44	-38
-3	7*	6
-4	35	30
H= 9, L= -10		
0	19	-22
1	6*	3
2	49	50
3	27	26
H= 9, L= -10		
-1	19	-19
-2	10	-9
H= 10, L= 0		
0	33	31
1	20	22
2	82	-76
3	28	26
4	83	77
-1	28	-27
-2	38	-32
-3	44	-39
-4	19	16
-5	5	3
H= 10, L= 1		
0	12	-11
1	16	-19
2	7	6
-1	6*	3
-2	34	30
-3	34	-31
H= 10, L= -1		
0	50	-49
1	12	-9
2	28	29
3	8*	-5
4	46	45
5	22	22
-1	15	14
-2	41	-35
-3	26	-22
-4	16	15
-5	6*	-4
-6	34	32
H= 10, L= -2		
0	25	22
1	27	-24
2	9*	2
3	33	32
4	8*	6
5	7*	4
6	11	11
H= 10, L= -2		
-1	20	19
-2	9*	-2
-3	39	-38
-4	47	-47
-5	41	38
-6	16	18
H= 10, L= -3		
0	17	-20
1	9*	-2
2	50	49
3	11	-10
4	20	18
5	39	39
6	27	-28
H= 10, L= -3		
-1	10*	-2
-2	68	-67
-3	18	-15
-4	78	75
-5	22	19
-6	30	-27
-7	24	21
H= 10, L= -4		
0	10*	-9
1	36	-36
2	36	37
3	29	28
4	86	-85
5	29	-27
6	63	57
H= 10, L= -4		
-1	13	11
-2	24	20
-3	20	13
-4	12	-16
-5	47	-39
-6	21	-17
-7	49	43
H= 10, L= -5		
0	10*	7
1	10*	0
2	9*	-4
3	12	9
4	16	11
5	31	-28
6	63	-60
H= 10, L= -5		
-1	17	-18
-2	14	-14
-3	14	11
-4	9	-7
-5	29	-22
-6	14	11
H= 10, L= -6		
0	35	36
1	34	35
2	54	-54
3	22	-19
4	11	-9
5	9	-10
6	18	17
H= 10, L= -6		
-1	9*	-4
-2	11	13
-3	10	4
-4	15	13
-5	23	-14
-6	21	-19
H= 10, L= -7		
0	24	24
1	29	32
2	8*	5
3	22	-20
4	7*	-5
5	25	-26
6	7	5
H= 10, L= -7		
-1	14	16
-2	8*	8
-3	30	26
-4	11	-10
-5	19	-17
H= 10, L= -8		
0	80	72
1	8*	-2
2	35	-30
3	10	9
4	20	17
5	8	-7
H= 10, L= -8		
-1	14	15
-2	51	-43
-3	12	6
-4	36	31
H= 10, L= -9		
0	51	50
1	18	14
2	43	-42
3	5*	2
H= 10, L= -9		
-1	38	-32
-2	5*	-3
H= 11, L= -1		
0	5*	0
1	19	-21
H= 11, L= -1		
-1	20	-17
-2	6	-3
H= 11, L= -2		
0	35	31
1	33	-29
2	69	-64
3	5*	1
H= 11, L= -2		
-1	7*	1
-2	32	-26
-3	8	5
-4	47	42
H= 11, L= -3		
0	12	9
1	20	-20
2	14	-11
3	6*	6
4	5*	1
H= 11, L= -3		
-1	7*	7
-2	63	-54
-3	16	12
-4	66	61
H= 11, L= -4		
0	12	11
1	12	-10
2	46	-41
3	21	18
4	19	16
H= 11, L= -4		
-1	33	-29
-2	44	42
-3	71	65
-4	33	-30
H= 11, L= -5		
0	13	-16
1	17	15
2	10	7
3	7*	-6
4	57	54
H= 11, L= -5		
-1	39	36
-2	7*	-4
-3	45	-43
-4	8	9
H= 11, L= -6		
0	31	29
1	17	-21
2	7*	-7
3	21	19
4	5	5
H= 11, L= -6		
-1	20	-16
-2	10	-13
-3	17	15
-4	20	-15
H= 11, L= -7		
0	21	18
1	51	49
2	18	-14
3	8	7
H= 11, L= -7		
-1	44	-41
-2	17	-14
-3	15	-10
H= 11, L= -8		
0	5*	6
1	31	25
2	7	-5
H= 11, L= -8		
-1	5*	-23

unambiguously. The R index for this first trial model, assuming $B=3\cdot8$ Å^2 for all atoms, was 0·29.

Structure refinement

Refinement of the atomic parameters was carried out by block-diagonal least-squares to minimize the quantity $\Sigma w(|F_o|-|F_c|)^2$, using blocks of 4×4 for the isotropic refinement or 9×9 for the anisotropic refinement and 2×2 for the scale. After two isotropic cycles, the R index was reduced to 0·17, and after two anisotropic cycles it was reduced further to 0·11. The hydrogen atoms were located from the difference map which was evaluated at this stage. Their peak heights varied between 0·3 and 0·6 e.Å^{-3}. The refinement was continued, anisotropically for the O and C atoms and isotropically for the H atoms, until the parameters' shifts were within 0·2 of the corresponding estimated standard deviations. The R index for the last three cycles was 0·044. The weighting function employed in these calculations was

$$w=1\div\left[1+\left(\frac{|F_o|-p_2}{p_1}\right)^4\right], \qquad (3)$$

where $|F_o|=0\cdot5$ to 78·9 electrons, $p_1=21$ and $p_2=23$. The weights evaluated with this function are nearly equal for the medium structure amplitudes, and very small for the very weak and very strong reflexions.

As a final check on the refined parameters, the last four cycles of refinement were repeated (a) with $w=1$ for all reflexions, (b) with $w=1\div[p_1+|F_o|+p_2|F_o|^2]$ where $p_1=2F_{\min}$ and $p_2=2/F_{\max}$; two differential syntheses were evaluated also. The mean and maximum changes in the non-hydrogen bond lengths and angles from those of the original refinement with weighting scheme (3) were as follows: 0·001, 0·002 Å and 0·06 and 0·12° for trial (a); 0·002, 0·008 Å and 0·10, 0·26° for trial (b); 0·003, 0·006 Å and 0·13, 0·31° for the differential syntheses. Compared with the calculated e.s.d.'s of 0·002 to 0·003 Å for the bond lengths and 0·1 to 0·2° for the angles, all the discrepancies were within the non-significant level. However, to be on the safe side the calculated e.s.d.'s were incremented by 80%.

The scattering-factor curves employed in all the calculations were those given by Hanson, Herman, Lea & Skillman (1964), except that the H curve was modified by an artificial temperature factor of $-2\cdot5$ Å^2 in order to bring it closer to the correct curve as proposed by Jensen (1965).

Results

The final parameters of the refinement with weighting function (3) are given in Tables 2 and 3. The e.s.d.'s in these Tables are 1·8 times those calculated from the least-squares matrices. The structure factors are listed

Table 5. *Agreement summary*

2796 observed reflexions ($0\cdot5\le|F_o|\le78\cdot9$)

$R=0\cdot044$

Category	Limits			Number
1	$\|\Delta F\|\le1\cdot0\|F_{th}\|$	or	$\|\Delta F\|/\|F_o\|\le0\cdot08$	2741
2	$1\cdot0\|F_{th}\|<\|\Delta F\|\le2\cdot0\|F_{th}\|$	or	$0\cdot08<\|\Delta F\|/\|F_o\|\le0\cdot12$	53
3	$2\cdot0\|F_{th}\|<\|\Delta F\|\le3\cdot0\|F_{th}\|$	or	$0\cdot12<\|\Delta F\|/\|F_o\|\le0\cdot16$	1
4	$3\cdot0\|F_{th}\|<\|\Delta F\|$	or	$0\cdot16<\|\Delta F\|/\|F_o\|$	1
	595 unobserved reflexions ($\|F_{c\max}\|=3\cdot0$)			
1	$\|F_c\|\le1\cdot0\|F_{th}\|$			519
2	$1\cdot0\|F_{th}\|<\|F_c\|\le1\cdot5\|F_{th}\|$			52
3	$1\cdot5\|F_{th}\|<\|F_c\|\le2\cdot0\|F_{th}\|$			7
4	$2\cdot0\|F_{th}\|<\|F_c\|$			17

$|F_{th}|=$ threshold amplitude $=0\cdot2$ to 1·1.

in Table 4, and the corresponding agreement summary is given in Table 5. The individual agreement in the observed data is good except for the two reflexions $32\bar{1}$ ($|F_o|=6{\cdot}5$, $|F_c|=4{\cdot}4$) and $33\bar{1}$ ($|F_o|=3{\cdot}9$, $|F_c|=2{\cdot}3$) which may be affected by double diffraction. The unobserved data include 24 reflexions (those in categories 3 and 4) which were obscured by high background and could not be measured accurately.

A perspective view of the molecule showing the shape of the tetrahydrofuran ring and the orientations of the substituents, but excluding the hydrogen atoms of the methyl, ethyl and phenyl groups, is given in Fig. 1. The bond lengths and angles, not corrected for thermal vibration, are presented in Fig. 2. The C–H bond lengths vary from 0·89 to 1·13 Å and their mean is 0·98 Å. The tetrahydrofuran external angles which have been excluded from Fig. 2 for clarity, are listed in Table 6.

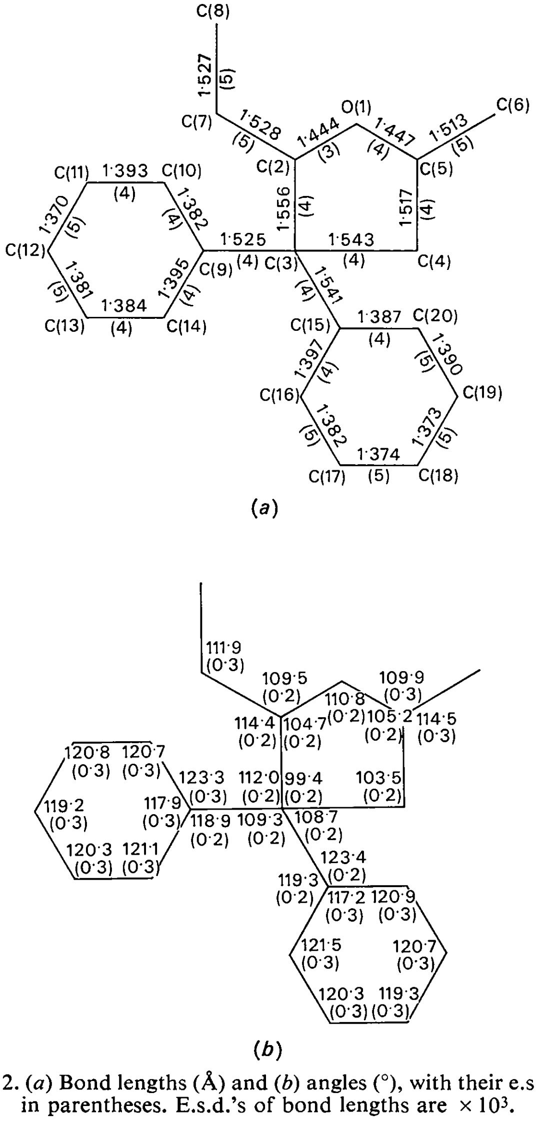

Fig. 2. (*a*) Bond lengths (Å) and (*b*) angles (°), with their e.s.d.'s in parentheses. E.s.d.'s of bond lengths are × 10^3.

Table 6. *The tetrahydrofuran external angles* (°) *which are omitted from Fig. 2, and their e.s.d.'s*

O(1) —C(2)-H(2)	106·4 (1·5)
C(3) —C(2)-H(2)	111·2 (1·6)
C(7) —C(2)-H(2)	110·2 (1·6)
C(2) —C(3)-C(15)	111·8 (0·2)
C(4) —C(3)-C(9)	115·3 (0·2)
C(3) —C(4)-H(4,1)	113·7 (1·8)
C(3) —C(4)-H(4,2)	108·1 (1·6)
C(5) —C(4)-H(4,1)	112·6 (1·8)
C(5) —C(4)-H(4,2)	110·1 (1·6)
H(4,1)-C(4)-H(4,2)	108·6 (2·4)
C(4) —C(5)-H(5)	111·3 (1·5)
O(1) —C(5)-H(5)	105·9 (1·5)
C(6) —C(5)-H(5)	109·6 (1·5)

Discussion

The tetrahydrofuran ring

In the highly saturated five-membered tetrahydrofuran ring, the two C–O bonds are very nearly equal (their weighted mean is 1·445 Å and $\sigma_{\rm wm}=0{\cdot}003$ Å), but the three C–C single bonds are significantly different in length from each other, indicating that they are probably affected by the size of the substituents. Thus the bond between atoms C(2) and C(3) to which the ethyl and the bulky phenyl rings are attached seems to be stretched to 1·556 Å, and this has been compensated for by a contraction of the opposite C(4)–C(5) bond to 1·517 Å, while the intermediate bond has remained at 1·543 Å, which is about the normal length for a C–C single bond. The mean of these three C–C bonds is 1·539 Å. Equivalent valence angles at atoms C(2) and C(5) are equal within the estimated accuracy, but this is not the case for the angles at atoms C(3) and C(4) where the substituents are considerably different in size. As an example, the internal valency angle C(2)–C(3)–C(4) is 99·4° while C(3)–C(4)–C(5) is 103·5°.

The five atoms of the ring are significantly nonplanar as can be seen from the side view shown in Fig. 1. The equation of the mean plane through them, referred to the orthogonal set of axes X' along the a axis, Y' in the $a\ b$ plane, and Z' along the c^* axis is

$$0{\cdot}9062X'-0{\cdot}3964Y'-0{\cdot}1469Z'+2{\cdot}8529=0, \qquad (4)$$

and the maximum deviations of these five atoms from the mean plane are −0·25 Å for C(3) and +0·23 Å for C(4). A projection of the molecule along the normal to this plane is presented in Fig. 3, where the perpendicular distances of the atoms from (plane 4) are given.

Orientation of the substituents

The projection in Fig. 3 shows that the ethyl group on C(2) is axial and the methyl group on C(5) is equatorial, and both are on the same side of the mean plane of the tetrahydrofuran ring. This confirms the configuration deduced by Casy & Hassan (1967) from the proton magnetic resonance spectrum. As is to be expected the axial substituents (and similarly the equatorial substituents) on atoms C(2), C(3), C(4) and C(5), respec-

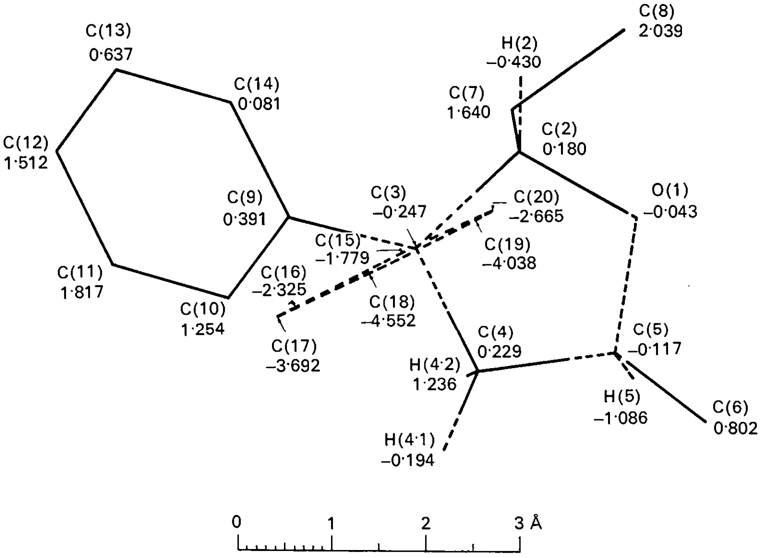

Fig. 3. Projection of the molecule along the normal to the mean plane of the tetrahydrofuran ring, and the perpendicular distances (Å) of the atoms from it.

tively, lie alternately above and below the plane of the tetrahydrofuran ring.

The equations of the mean planes of the phenyl rings through atoms C(9) to C(14) and C(15) to C(20) are

$$0{\cdot}7926X'+0{\cdot}0930Y'-0{\cdot}6026Z'+2{\cdot}4880=0 \qquad (5)$$

and

$$0{\cdot}4081X'+0{\cdot}8287Y'+0{\cdot}3830Z'-1{\cdot}4719=0 \qquad (6)$$

respectively. Each phenyl ring is planar to within the accuracy of this determination. The corresponding χ^2 values are 10·6 and 7·1 respectively, and each of their carbon atoms is within 0·006 Å from the corresponding mean plane. The dihedral angle between the two phenyl rings is 80·2 °.

The orientation of each of the phenyl rings relative to the tetrahydrofuran ring can be described as equatorial or axial, by the angle of rotation round the joining bond, and by the dihedral angle between their mean planes, as follows:

	Orientation	Rotation angle	Dihedral angle
C(9) to C(14)	equatorial	31·9 °	39·7 °
C(15) to C(20)	axial	83·0	89·2

Intermolecular distances

There are no particularly short intermolecular distances in the structure. The shortest observed van der Waals contacts for the different types of atoms, and the corresponding values calculated from the atomic radii given by Pauling (1960), shown in parentheses, are: C...C 3·58 (3·4) Å; C...O 3·68(3·1) Å; H...C 2·86(2·9) Å; H...O 2·77(2·6) Å; H...H 2·51(2·4) Å.

Final difference map

The residual electron density in the final difference map is within ±0·20 e.Å^{-3}, while the calculated $\sigma(\varrho_0)$ is 0·06 e.Å^{-3}. The three strongest positive peaks of heights 0·15 to 0·20 e.Å^{-3} occur on the C(3)–C(2), C(3)–C(9), and C(3)–C(15) bonds about halfway between the pairs of atoms forming the bonds.

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