

## Hacia una síntesis convergente del dodecaedro: Estudios, modelo, preparación de precursores y primeros ensayos de las rutas 10 + 10 y 12 + 8.

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**UNIVERSIDAD DE BARCELONA**  
**Departamento de Farmacología y Química Terapéutica**

**HACIA UNA SÍNTESIS CONVERGENTE DEL DODECAEDRANO: ESTUDIOS**  
**MODELO, PREPARACIÓN DE PRECURSORES Y PRIMEROS ENSAYOS DE**  
**LAS RUTAS 10 + 10 Y 12 + 8**



Santiago Vázquez Cruz

Barcelona, Octubre de 1996

**RAYOS X**



X-ray crystal structure determination of 6,7-Dimethyloctacyclo[10.6.6.1<sup>4</sup>,7.16,9.0<sup>2</sup>,11.0<sup>4</sup>,9.0<sup>13</sup>,18.0<sup>19</sup>,2<sup>4</sup>]hexacos-2(11),13,15,17,19,21,23-heptaene.

A prismatic crystal (0.3 x 0.4 x 0.2 mm) was selected and mounted on a Philips PW-1100 four-circle diffractometer. Unit-cell parameters were determined from automatic centring of 25 reflections ( $8 < \Theta < 12^\circ$ ) and refined by least-squares method. Intensities were collected with graphite monochromatized Mo K $\alpha$  radiation, using  $\omega/2\Theta$  scan technique. 3250 reflections were measured in the range  $2.47 \leq \Theta \leq 30.02$ . 3200 reflections were assumed as observed applying the condition  $I > 2\sigma(I)$ . Three reflections were measured every two hours as orientation and intensity control, significant intensity decay was not observed. Lorentz-polarization, but not absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program<sup>[1]</sup> and refined by full-matrix least-squares on F<sup>2</sup> method, with the SHELX93 computer program<sup>[2]</sup>, using 3200 reflections, (very negative intensities were not assumed). The function minimized was  $\sum w[|F_o|^2 - |F_c|^2]^2$ , where  $w = [\sigma^2(I) + (0.0787P)^2 + 0.6095P]^{-1}$ , and  $P = (|F_o|^2 + 2|F_c|^2)/3$ ,  $f$ ,  $f'$  and  $f''$  were taken from International Tables of X-ray Crystallography<sup>[3]</sup>. The 15 H atoms were located from a difference synthesis and refined with an overall isotropic temperature factor. The final R(on F) factor was 0.0325, wR(on |F|<sup>2</sup>) = 0.0751 and goodness of fit = 0.683 for all observed reflections. Number of refined parameters was 178. Max. shift/esd = 0.06, Mean shift/esd = 0.00. Max. and min. peaks in final difference synthesis was 0.089 and -0.101 e $\text{\AA}^{-3}$ , respectively.

[1]Sheldrick, G.M., *Acta Cryst.*, 1990, A46, 467-473.

[2]Sheldrick, G.M., *SHELX93* (1994, in preparation).

[3] *International Tables of X-ray Crystallography*, 1974, Kynock Press, Birmingham, England, vol. IV, 99-100 and 149.

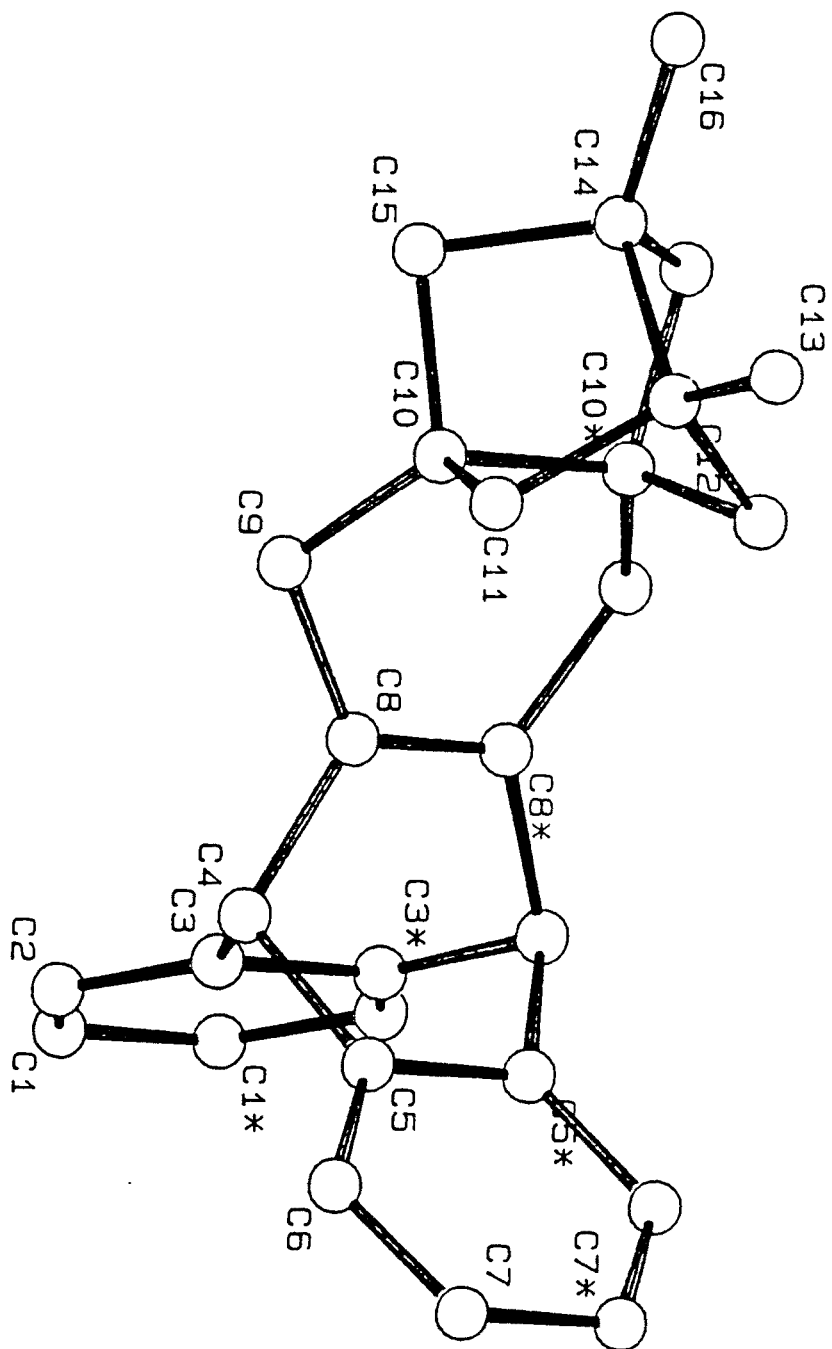


Table 1. Crystal data and structure refinement for 1.

Identification code	far36
Empirical formula	C <sub>28</sub> H <sub>28</sub>
Formula weight	364.53
Temperature	293(2) K
Wavelength	0.71069Å
Crystal system	orthorhombic
Space group	Pnma
Unit cell dimensions	a = 20.586(4)Å    α = 90°. b = 11.435(3)Å    β = 90°. c = 9.006(2)Å    γ = 90°.
Volume	2120.0(8) Å <sup>3</sup>
Z	4
Density (calculated)	1.142 Mg/m <sup>3</sup>
Absorption coefficient	0.691 mm <sup>-1</sup>
F(000)	784
Crystal size	0.3 x 0.4 x 0.2 mm
Theta range for data collection	2.47 to 30.02°.
Index ranges	0<=h<=28, 0<=k<=16, 0<=l<=12
Reflections collected	3250
Independent reflections	3250 [R(int) = 0.0000]
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3200 / 0 / 178
Goodness-of-fit on F <sup>2</sup>	0.683
Final R indices [I>2σ(I)]	R1 = 0.0325, wR2 = 0.0751
R indices (all data)	R1 = 0.1742, wR2 = 0.2810
Extinction coefficient	0.001(2)
Largest diff. peak and hole	0.089 and -0.101 e.Å <sup>-3</sup>



Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
C(1)	4561(1)	1897(2)	7704(2)	65(1)
C(2)	4476(1)	1280(2)	9023(2)	59(1)
C(3)	4392(1)	1887(2)	10333(2)	56(1)
C(4)	4291(1)	1378(2)	11890(2)	66(1)
C(5)	4831(1)	1894(2)	12837(2)	67(1)
C(6)	5309(1)	1291(2)	13630(2)	86(1)
C(7)	5775(2)	1901(2)	14421(2)	105(1)
C(8)	3654(1)	1923(2)	12449(2)	70(1)
C(9)	3060(1)	1213(2)	12844(3)	77(1)
C(10)	2694(1)	1789(2)	14127(2)	62(1)
C(11)	2920(1)	1501(2)	15706(2)	66(1)
C(12)	2541(1)	2500	16443(3)	64(1)
C(13)	2505(2)	2500	18132(4)	92(1)
C(14)	1871(1)	2500	15506(3)	72(1)
C(15)	1972(1)	1490(2)	14390(3)	75(1)
C(16)	1234(2)	2500	16419(5)	103(1)



Table 3. Bond lengths [Å] and angles [°] for 1.

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C(1)-C(1)i	1.378(4)
C(1)-C(2)	1.393(3)
C(2)-C(3)	1.380(2)
C(3)-C(3)i	1.403(4)
C(3)-C(4)	1.532(3)
C(4)-C(5)	1.521(3)
C(4)-C(8)	1.536(3)
C(5)-C(5)i	1.386(4)
C(5)-C(6)	1.399(3)
C(6)-C(7)	1.383(4)
C(7)-C(7)i	1.369(6)
C(8)-C(8)i	1.319(4)
C(8)-C(9)	1.511(3)
C(9)-C(10)	1.528(3)
C(10)-C(11)	1.532(3)
C(10)-C(15)	1.545(3)
C(10)-C(10)i	1.626(4)
C(11)-C(12)	1.535(3)
C(12)-C(13)	1.523(4)
C(12)-C(11)i	1.535(3)
C(12)-C(14)	1.617(4)
C(14)-C(15)	1.545(3)
C(14)-C(15)i	1.545(3)
C(14)-C(16)	1.546(4)

C(1)i-C(1)-C(2)	120.46(12)
C(3)-C(2)-C(1)	119.3(2)
C(2)-C(3)-C(3)i	120.20(12)
C(2)-C(3)-C(4)	127.5(2)
C(3)i-C(3)-C(4)	112.31(10)
C(5)-C(4)-C(3)	105.5(2)
C(5)-C(4)-C(8)	106.4(2)
C(3)-C(4)-C(8)	105.2(2)
C(5)i-C(5)-C(6)	119.5(2)
C(5)i-C(5)-C(4)	112.83(11)
C(6)-C(5)-C(4)	127.6(2)
C(7)-C(6)-C(5)	120.1(3)
C(7)i-C(7)-C(6)	120.3(2)
C(8)i-C(8)-C(9)	122.51(12)
C(8)i-C(8)-C(4)	113.95(10)
C(9)-C(8)-C(4)	123.4(2)
C(8)-C(9)-C(10)	110.2(2)
C(9)-C(10)-C(11)	117.3(2)
C(9)-C(10)-C(15)	119.7(2)
C(11)-C(10)-C(15)	95.9(2)
C(9)-C(10)-C(10)i	115.54(11)
C(11)-C(10)-C(10)i	102.43(11)
C(15)-C(10)-C(10)i	102.79(12)
C(10)-C(11)-C(12)	95.0(2)
C(13)-C(12)-C(11)	117.2(2)
C(13)-C(12)-C(11)i	117.2(2)
C(11)-C(12)-C(11)i	96.2(2)
C(13)-C(12)-C(14)	118.7(3)

C(11)-C(12)-C(14)	102.1(2)
C(11)i-C(12)-C(14)	102.1(2)
C(15)-C(14)-C(15)i	96.7(2)
C(15)-C(14)-C(16)	117.4(2)
C(15)i-C(14)-C(16)	117.4(2)
C(15)-C(14)-C(12)	103.0(2)
C(15)i-C(14)-C(12)	103.0(2)
C(16)-C(14)-C(12)	116.5(3)
C(10)-C(15)-C(14)	93.7(2)

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Symmetry transformations used to generate equivalent atoms:

i x, -y+1/2, z

Table 4. Bond lengths [Å] and angles [deg] for 1.

---

C(1)-H(1)	0.99(2)
C(2)-H(2)	1.06(2)
C(4)-H(4)	0.98(2)
C(6)-H(6)	1.01(2)
C(7)-H(7)	1.07(2)
C(9)-H(9)	1.03(2)
C(9)-H(9A)	1.02(2)
C(11)-H(11)	1.06(2)
C(11)-H(11A)	0.98(2)
C(13)-H(13)	0.99(2)
C(13)-H(13A)	1.11(3)
C(15)-H(15)	1.03(2)
C(15)-H(15A)	1.06(2)
C(16)-H(16)	0.96(3)
C(16)-H(16A)	1.10(4)

C(1) <i>i</i> -C(1)-H(1)	119.5(12)
C(2)-C(1)-H(1)	119.9(12)
C(3)-C(2)-H(2)	120.0(11)
C(1)-C(2)-H(2)	120.6(11)
C(5)-C(4)-H(4)	112.9(13)
C(3)-C(4)-H(4)	111.2(12)
C(8)-C(4)-H(4)	115.0(12)
C(7)-C(6)-H(6)	125.2(12)
C(5)-C(6)-H(6)	114.6(12)
C(7) <i>i</i> -C(7)-H(7)	114.5(11)
C(6)-C(7)-H(7)	125.0(11)
C(8)-C(9)-H(9)	110.7(12)
C(10)-C(9)-H(9)	113.0(11)
C(8)-C(9)-H(9A)	105.0(12)
C(10)-C(9)-H(9A)	113.3(12)
H(9)-C(9)-H(9A)	104(2)
C(10)-C(11)-H(11)	110.4(11)
C(12)-C(11)-H(11)	119.0(11)
C(10)-C(11)-H(11A)	117.0(12)
C(12)-C(11)-H(11A)	108.0(12)
H(11)-C(11)-H(11A)	108(2)
C(12)-C(13)-H(13)	113.8(13)
C(12)-C(13)-H(13A)	108(2)
H(13)-C(13)-H(13A)	109(2)
C(10)-C(15)-H(15)	110.8(12)
C(14)-C(15)-H(15)	120.6(12)
C(10)-C(15)-H(15A)	112.8(11)
C(14)-C(15)-H(15A)	114.3(11)
H(15)-C(15)-H(15A)	105(2)
C(14)-C(16)-H(16)	100(2)
C(14)-C(16)-H(16A)	117(2)
H(16)-C(16)-H(16A)	109(3)

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Symmetry transformations used to generate equivalent atoms:  
*i* x, -y+1/2, z

Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  
 The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C(1)	61(1)	85(1)	50(1)	-7(1)	-7(1)	2(1)
C(2)	51(1)	69(1)	56(1)	-7(1)	3(1)	2(1)
C(3)	51(1)	64(1)	54(1)	-1(1)	14(1)	2(1)
C(4)	78(1)	54(1)	64(1)	-4(1)	28(1)	6(1)
C(5)	93(2)	66(1)	41(1)	0(1)	22(1)	7(1)
C(6)	129(2)	83(2)	44(1)	4(1)	17(1)	18(2)
C(7)	135(2)	134(2)	46(1)	-2(1)	-13(1)	17(2)
C(8)	80(1)	53(1)	75(1)	0(1)	39(1)	-1(1)
C(9)	87(2)	60(1)	83(2)	-10(1)	37(1)	-16(1)
C(10)	54(1)	67(1)	65(1)	0(1)	15(1)	-8(1)
C(11)	51(1)	65(1)	81(2)	4(1)	6(1)	-5(1)
C(12)	48(2)	82(2)	63(2)	0	5(1)	0
C(13)	94(3)	112(3)	68(2)	0	1(2)	0
C(14)	45(2)	101(2)	70(2)	0	14(1)	0
C(15)	54(1)	98(2)	74(1)	-3(1)	4(1)	-16(1)
C(16)	50(2)	165(4)	94(3)	0	19(2)	0

Table 6. Hydrogen coordinates (  $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

	x	y	z	U(eq)
H(1)	4589(10)	1469(17)	6745(24)	88(2)
H(2)	4466(9)	352(19)	9023(22)	88(2)
H(4)	4297(10)	523(19)	11870(22)	88(2)
H(6)	5269(10)	409(20)	13594(22)	88(2)
H(7)	6175(10)	1514(17)	14992(25)	88(2)
H(9)	3183(10)	361(20)	13057(22)	88(2)
H(9A)	2796(10)	1172(18)	11890(23)	88(2)
H(11)	2801(10)	627(19)	15979(22)	88(2)
H(11A)	3382(11)	1613(17)	15926(22)	88(2)
H(13)	2266(10)	1820(18)	18551(23)	88(2)
H(13A)	3009(16)	2500	18580(33)	88(2)
H(16)	922(16)	2500	15623(35)	88(2)
H(16A)	1145(20)	1740(36)	17144(47)	88(2)
H(15)	1920(10)	629(19)	14723(22)	88(2)
H(15A)	1687(10)	1558(18)	13410(24)	88(2)









h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
21	1	4	0	23	1	3	5	4	167	166	3	17	8	4	31	5	18	4	13	4	0	20	1	10	2	5	25	28	13
22	1	4	33	33	16	4	5	4	8	2	8	18	8	4	13	4	12	5	13	4	29	38	29	11	2	5	107	109	4
23	1	4	0	3	1	5	5	4	293	299	2	19	8	4	44	34	11	6	13	4	10	10	10	12	2	5	36	39	8
24	1	4	15	6	15	6	5	4	110	113	3	20	8	4	0	6	1	7	13	4	0	5	1	13	2	5	60	59	5
25	1	4	22	14	21	7	5	4	32	23	7	21	8	4	37	34	16	8	13	4	0	8	1	14	2	5	5	5	4
26	1	4	0	9	1	8	5	4	83	84	4	22	8	4	6	3	6	9	13	4	41	36	14	15	2	5	23	18	22
27	1	4	31	40	31	9	5	4	74	79	4	23	8	4	0	11	1	10	13	4	0	14	1	16	2	5	0	6	1
0	2	4	241	238	2	10	5	4	8	11	7	1	9	4	112	114	4	11	13	4	0	2	1	17	2	5	0	20	1
1	2	4	126	125	2	11	5	4	99	102	4	2	9	4	90	98	4	12	13	4	0	1	1	18	2	5	72	66	6
2	2	4	438	434	2	12	5	4	51	47	6	3	9	4	149	149	4	13	13	4	24	9	24	19	2	5	0	2	1
3	2	4	280	272	2	13	5	4	169	170	3	4	9	4	81	81	5	14	13	4	20	8	19	20	2	5	7	7	6
4	2	4	65	60	3	14	5	4	10	1	10	5	9	4	74	78	5	0	14	4	15	19	15	21	2	5	18	24	17
5	2	4	254	256	2	15	5	4	66	65	6	6	9	4	12	9	11	1	14	4	21	2	20	22	2	5	47	46	11
6	2	4	144	137	2	16	5	4	38	30	10	7	9	4	25	1	18	2	14	4	26	25	25	23	2	5	0	1	1
7	2	4	147	145	2	17	5	4	77	76	6	8	9	4	67	61	6	3	14	4	51	39	12	24	2	5	0	19	1
8	2	4	137	134	3	18	5	4	19	1	19	9	9	4	101	101	5	4	14	4	0	10	1	25	2	5	0	9	1
9	2	4	78	78	3	19	5	4	29	22	18	10	9	4	0	9	1	5	14	4	17	14	16	26	2	5	17	22	17
10	2	4	68	68	4	20	5	4	0	12	1	11	9	4	17	6	17	6	14	4	24	9	23	0	3	5	295	291	2
11	2	4	0	8	1	21	5	4	27	23	26	12	9	4	40	38	10	7	14	4	0	22	1	1	3	5	148	148	3
12	2	4	96	101	3	22	5	4	0	2	1	13	9	4	22	14	22	8	14	4	18	14	17	2	3	5	115	111	3
13	2	4	11	9	10	23	5	4	26	28	25	14	9	4	36	40	13	9	14	4	28	12	27	3	3	5	22	25	11
14	2	4	47	54	6	24	5	4	19	7	19	15	9	4	25	12	25	10	14	4	14	2	14	4	3	5	27	29	8
15	2	4	29	30	13	25	5	4	32	17	28	16	9	4	0	6	1	11	14	4	0	12	1	5	3	5	113	109	3
16	2	4	0	5	1	0	6	4	144	149	3	17	9	4	81	67	7	1	15	4	15	16	15	6	3	5	137	136	3
17	2	4	31	23	12	1	6	4	77	77	3	18	9	4	15	7	14	2	15	4	34	20	19	7	3	5	81	78	4
18	2	4	0	4	1	2	6	4	125	128	3	19	9	4	28	4	28	3	15	4	0	18	1	8	3	5	164	168	3
19	2	4	10	9	10	3	6	4	147	148	3	20	9	4	23	1	22	4	15	4	0	4	1	9	3	5	71	68	4
20	2	4	0	7	1	4	6	4	36	34	7	21	9	4	25	4	25	5	15	4	0	7	1	10	3	5	120	120	3
21	2	4	50	39	8	5	6	4	55	56	4	22	9	4	0	7	1	1	0	5	69	68	3	11	3	5	43	47	7
22	2	4	24	25	23	6	6	4	0	10	1	0	10	4	144	145	4	2	0	5	18	12	18	12	3	5	45	40	7
23	2	4	0	5	1	7	6	4	37	34	7	1	10	4	9	5	9	3	0	5	64	63	3	13	3	5	28	20	12
24	2	4	29	21	28	8	6	4	60	58	5	2	10	4	54	54	6	4	0	5	12	15	12	14	3	5	26	22	18
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26	2	4	11	14	11	10	6	4	69	68	5	4	10	4	0	3	1	6	0	5	20	4	16	16	3	5	25	19	17
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26																													

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24	0	7	27	26	27	18	4	7	0	16	1	0	9	7	15	16	14	3	1	8	111	109	4	5	5	8	0	13	1
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16	1	7	0	39	-1	11	5	7	100	103	5	17	9	7	35	15	20</												

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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6	11	8	0	5	1	17	3	9	0	12	1	1	9	9	16	15	16	12	3	10	0	15	1	9	0	11	0	2	1
7	11	8	0	15	1	18	3	9	7	7	7	2																	

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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4	3	11	0	25	1	11	4	11	22	10	22	7	6	11	0	10	1	1	1	12	72	68	9	3	3	12	21	1	21
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6	3	11	0	10	1	0	5	11	10	2	9	9	6	11	0	0	1	3	1	12	41	44	18	5	3	12	0	6	1
7	3	11	0	6	1	1	5	11	0	16	1	0	7	11	0	1	1	4	1	12	0	8	1	6	3	12	30	12	29
8	3	11	19	10	18	2	5	11	0	8	1	1	7	11	42	36	16	5	1	12	14	12	13	7	3	12	26	15	25
9	3	11	38	32	17	3	5	11	0	14	1	2	7	11	0	26	1	6	1	12	31	0	30	0	4	12	7	6	6
10	3	11	19	0	18	4	5	11	18	6	17	3	7	11	17	1	17	7	1	12	0	20	1	1	4	12	0	15	1
11	3	11	21	23	21	5	5	11	26	16	26	4	7	11	0	23	1	8	1	12	0	14	1	2	4	12	0	11	1
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13	3	11	47	42	14	7	5	11	15	1	14	6	7	11	0	9	1	0	2	12	20	21	20	4	4	12	0	4	1
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3	4	11	38	26	16	10	5	11	0	1	1	2	0	12	54	54	11	3	2	12	25	22	25	2	5	12	0	4	1



ESPECTRO DE DIFRACCIÓN DE RAYOS-X DE 4,5,10,11-TETRAMETILPENTACICLO[8.2.1.1<sup>2,5</sup>.1<sup>4,7</sup>.1<sup>8,11</sup>]HEXADECA-1,7-DIENO, 142.

Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a Enraf-Nonius CAD4 four-circle diffractometer. Unit-cell parameters were determined from automatic centering of 25 reflections ( $12 < \theta < 21^\circ$ ) and refined by least-squares method. Intensities were collected with graphite monochromatized MoK $\alpha$  radiation, using  $\omega/2\theta$  scan-technique. 2271 reflections were measured in the range  $2.73 \leq \theta \leq 29.97$ . 1065 reflections were assumed as observed applying the condition  $I > 2\sigma(I)$ . Three reflections were measured every two hours as orientation and intensity control, significant intensity decay was not observed. Lorentz-polarization but no absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program (Sheldrick, G.M., (1990), Acta Cryst., A46, 467-473) and refined by full-matrix least-squares method with SHELX93 computer program (Sheldrick, G.M., (1994), in preparation), using 2000 reflections, (very negative intensities were not assumed). The function minimized was  $\sum w | |F_o|^2 - |F_c|^2 |^2$ , where  $w = [\sigma^2(I) + (0.3215 P)^2]^{-1}$ , and  $P = (|F_o|^2 + 2 |F_c|^2)/3$ ,  $f$ ,  $f'$  and  $f''$  were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). The extinction coefficient was 0.0(3). All H atoms were computed and refined with an overall isotropic temperature factor using a riding model. The final R(on F) factor was 0.047, wR(on  $|F|^2$ ) = 0.112 and goodness of fit = 0.327 for all observed reflections. Number of refined parameters was 93. Max. shift/esd = 2.5, Mean shift/esd = 0.06. Max. and min. peaks in final difference synthesis was 0.268 and -0.220 eÅ<sup>-3</sup>, respectively.

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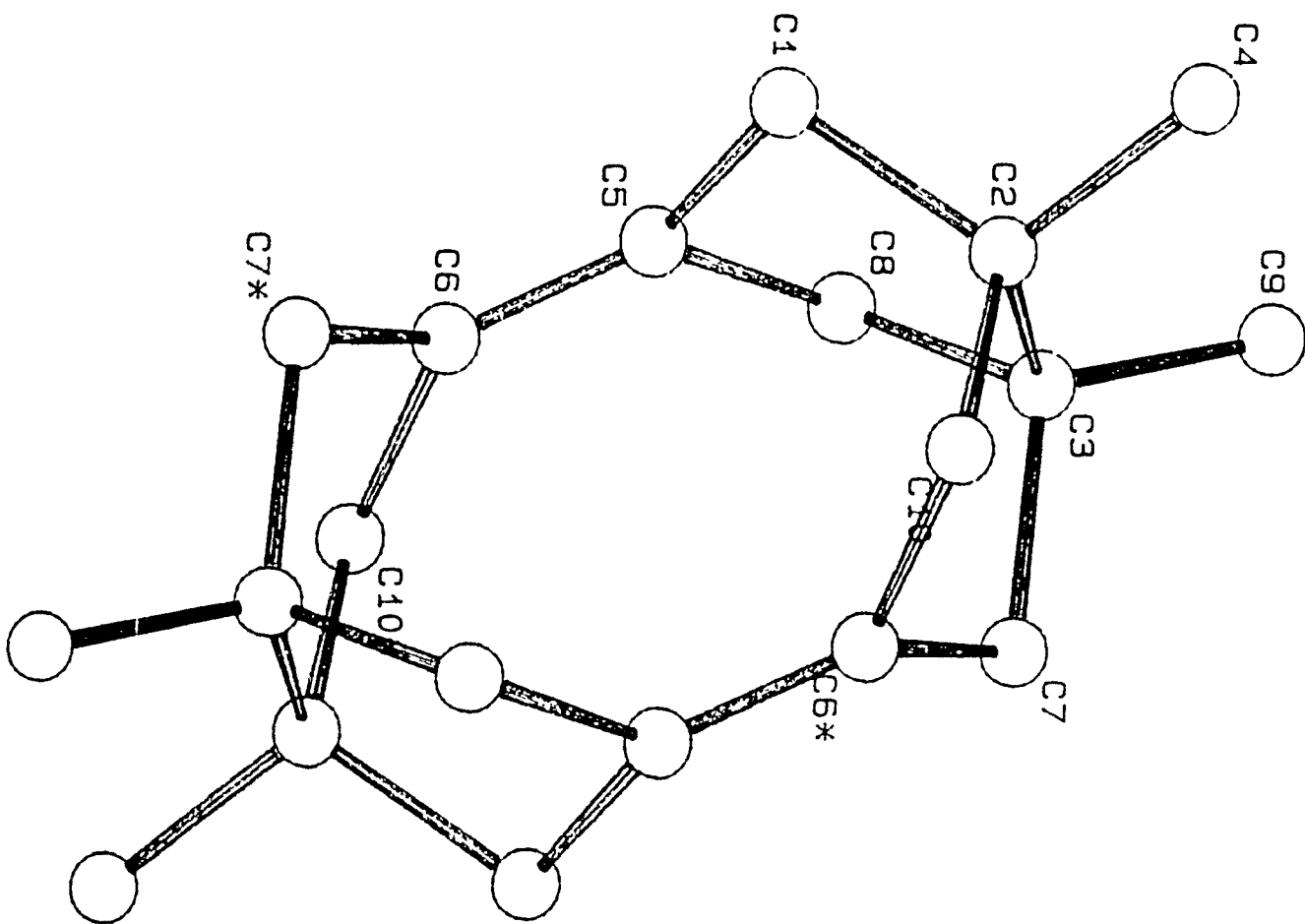




Table 1. Crystal data and structure refinement for 1.

Identification code	qf11
Empirical formula	C <sub>20</sub> H <sub>28</sub>
Formula weight	268.42
Temperature	293(2) K
Wavelength	0.71069Å
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
Unit cell dimensions	a = 6.837(8)Å    α = 90°. b = 11.882(8)Å    β = 94.93(7)°. c = 9.648(6)Å    γ = 90°.
Volume	780.9(12) Å <sup>3</sup>
Z	2
Density (calculated)	1.142 Mg/m <sup>3</sup>
Absorption coefficient	0.063 mm <sup>-1</sup>
F(000)	296
Crystal size	0.1 x 0.1 x 0.2 mm
Theta range for data collection	2.73 to 29.97°.
Index ranges	-9<=h<=9, 0<=k<=16, 0<=l<=13
Reflections collected	2271
Independent reflections	2271 [R(int) = 0.0000]
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2000 / 0 / 93
Goodness-of-fit on F <sup>2</sup>	0.927
Final R indices [I>2σ(I)]	R1 = 0.0471, wR2 = 0.1126
R indices (all data)	R1 = 0.1404, wR2 = 0.3730
Extinction coefficient	0.0(3)
Largest diff. peak and hole	0.268 and -0.220 e.Å <sup>-3</sup>

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{1j}$  tensor.

	x	y	z	$U(\text{eq})$
C(1)	2613(3)	3846(2)	923(2)	28(1)
C(2)	1967(3)	4464(2)	2212(2)	24(1)
C(3)	-284(3)	4060(2)	2312(2)	28(1)
C(4)	3344(4)	4198(3)	3514(3)	38(1)
C(5)	682(3)	3692(2)	19(2)	27(1)
C(6)	-231(3)	5893(2)	1256(2)	29(1)
C(7)	-1476(4)	5201(2)	2079(2)	32(1)
C(8)	-733(4)	3303(2)	1070(3)	31(1)
C(9)	-727(4)	3479(3)	3673(3)	38(1)
C(10)	1850(4)	5724(2)	1950(3)	32(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

---

C(1)-C(5)	1.529(4)
C(1)-C(2)	1.541(3)
C(2)-C(10)	1.520(4)
C(2)-C(4)	1.537(4)
C(2)-C(3)	1.622(4)
C(3)-C(8)	1.509(4)
C(3)-C(9)	1.538(4)
C(3)-C(7)	1.588(4)
C(5)-C(6)#1	1.336(3)
C(5)-C(8)	1.532(4)
C(6)-C(5)#1	1.336(3)
C(6)-C(7)	1.466(4)
C(6)-C(10)	1.533(4)
C(5)-C(1)-C(2)	102.9(2)
C(10)-C(2)-C(4)	111.0(2)
C(10)-C(2)-C(1)	110.5(2)
C(4)-C(2)-C(1)	111.4(2)
C(10)-C(2)-C(3)	105.3(2)
C(4)-C(2)-C(3)	114.1(2)
C(1)-C(2)-C(3)	104.3(2)
C(8)-C(3)-C(9)	111.6(2)
C(8)-C(3)-C(7)	109.3(2)
C(9)-C(3)-C(7)	111.6(2)
C(8)-C(3)-C(2)	105.0(2)
C(9)-C(3)-C(2)	116.2(2)
C(7)-C(3)-C(2)	102.6(2)
C(6)#1-C(5)-C(1)	126.9(2)
C(6)#1-C(5)-C(8)	127.7(2)
C(1)-C(5)-C(8)	102.8(2)
C(5)#1-C(6)-C(7)	127.4(2)
C(5)#1-C(6)-C(10)	125.7(2)
C(7)-C(6)-C(10)	104.5(2)
C(6)-C(7)-C(3)	103.9(2)
C(3)-C(8)-C(5)	104.4(2)
C(2)-C(10)-C(6)	103.6(2)

---

Symmetry transformations used to generate equivalent atoms:  
 #1 -x, -y+1, -z

Table 4. Hydrogen bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 1.

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C(1)-H(1)	0.97
C(1)-H(1A)	0.97
C(4)-H(4)	0.96
C(4)-H(4A)	0.96
C(4)-H(4B)	0.96
C(7)-H(7)	0.97
C(7)-H(7A)	0.97
C(8)-H(8)	0.97
C(8)-H(8A)	0.97
C(9)-H(9)	0.96
C(9)-H(9A)	0.96
C(9)-H(9B)	0.96
C(10)-H(10)	0.97
C(10)-H(10A)	0.97
<hr/>	
C(5)-C(1)-H(1)	111.18(14)
C(2)-C(1)-H(1)	111.17(14)
C(5)-C(1)-H(1A)	111.17(14)
C(2)-C(1)-H(1A)	111.18(13)
H(1)-C(1)-H(1A)	109.1
C(2)-C(4)-H(4)	109.5(2)
C(2)-C(4)-H(4A)	109.5(2)
H(4)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5(2)
H(4)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(6)-C(7)-H(7)	110.98(14)
C(3)-C(7)-H(7)	110.98(13)
C(6)-C(7)-H(7A)	110.98(14)
C(3)-C(7)-H(7A)	110.98(12)
H(7)-C(7)-H(7A)	109.0
C(3)-C(8)-H(8)	110.89(14)
C(5)-C(8)-H(8)	110.88(14)
C(3)-C(8)-H(8A)	110.88(14)
C(5)-C(8)-H(8A)	110.87(14)
H(8)-C(8)-H(8A)	108.9
C(3)-C(9)-H(9)	109.5(2)
C(3)-C(9)-H(9A)	109.5(2)
H(9)-C(9)-H(9A)	109.5
C(3)-C(9)-H(9B)	109.5(2)
H(9)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(2)-C(10)-H(10)	111.04(13)
C(6)-C(10)-H(10)	111.0(2)
C(2)-C(10)-H(10A)	111.04(12)
C(6)-C(10)-H(10A)	111.1(2)
H(10)-C(10)-H(10A)	109.0

---

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  
 The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C(1)	23(1)	33(1)	28(1)	2(1)	1(1)	3(1)
C(2)	19(1)	30(1)	24(1)	-2(1)	-1(1)	2(1)
C(3)	22(1)	34(1)	27(1)	2(1)	0(1)	-1(1)
C(4)	30(1)	46(2)	37(1)	1(1)	-3(1)	3(1)
C(5)	23(1)	31(1)	27(1)	0(1)	0(1)	-1(1)
C(6)	23(1)	34(1)	27(1)	1(1)	-2(1)	1(1)
C(7)	28(1)	38(1)	29(1)	0(1)	0(1)	1(1)
C(8)	29(1)	32(1)	31(1)	1(1)	-2(1)	-2(1)
C(9)	35(1)	44(2)	33(1)	2(1)	2(1)	0(1)
C(10)	27(1)	37(1)	31(1)	2(1)	-4(1)	-3(1)

Table 6. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

	x	y	z	U(eq)
H(1)	3534(3)	4296(2)	449(2)	130(9)
H(1A)	3210(3)	3126(2)	1175(2)	130(9)
H(4)	3395(4)	3399(3)	3658(3)	130(9)
H(4A)	2859(4)	4556(3)	4309(3)	130(9)
H(4B)	4637(4)	4474(3)	3390(3)	130(9)
H(7)	-2746(4)	5068(2)	1578(2)	130(9)
H(7A)	-1670(4)	5559(2)	2960(2)	130(9)
H(8)	-2086(4)	3389(2)	694(3)	130(9)
H(8A)	-503(4)	2520(2)	1321(3)	130(9)
H(9)	-426(4)	3982(3)	4440(3)	130(9)
H(9A)	59(4)	2812(3)	3804(3)	130(9)
H(9B)	-2092(4)	3279(3)	3627(3)	130(9)
H(10)	2828(4)	5963(2)	1341(3)	130(9)
H(10A)	2038(4)	6141(2)	2816(3)	130(9)

Table 7. Observed and calculated structure factors for 1

				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s													
2	0	0	54	5	-1	5	10	0	55	55	55	-3	3	1	102	92	-2	-3	8	1	61	60	1	2	14	1	45	37	4
4	0	0	93	89	-6	6	10	0	51	46	50	-2	3	1	64	70	-2	-2	8	1	18	16	11	3	14	1	32	30	7
6	0	0	33	30	5	7	10	0	16	15	16	-1	3	1	170	176	-3	-1	8	1	122	119	3	4	14	1	28	24	8
8	0	0	97	95	4	1	11	0	42	37	12	0	3	1	225	193	-4	0	8	1	16	14	7	5	14	1	35	32	7
1	1	0	1380	820****		2	11	0	115	107	114	1	3	1	36	29	-3	1	8	1	117	105	6	-4	15	1	0	1	1
2	1	0	356	296-355		3	11	0	93	87	93	2	3	1	176	148	-5	2	8	1	39	34	3	-3	15	1	14	13	14
3	1	0	54	53	-54	4	11	0	19	20	19	3	3	1	252	214	-7	3	8	1	17	17	17	-2	15	1	38	32	6
4	1	0	21	15	-2	5	11	0	23	17	22	4	3	1	135	112	-6	4	8	1	6	4	6	-1	15	1	0	1	1
5	1	0	80	76	12	6	11	0	17	14	17	5	3	1	120	105	7	5	8	1	134	122	7	0	15	1	5	1	5
6	1	0	32	30	10	7	11	0	46	45	46	6	3	1	30	27	6	6	8	1	46	44	4	1	15	1	49	42	5
7	1	0	42	41	8	0	12	0	81	70	4	7	3	1	71	64	6	7	8	1	66	59	5	2	15	1	51	42	5
8	1	0	0	9	1	1	12	0	37	34	2	8	3	1	61	58	5	8	8	1	66	59	5	3	15	1	90	76	4
9	1	0	34	30	19	2	12	0	77	69	29	9	3	1	36	36	8	-8	9	1	10	10	9	4	15	1	0	8	1
0	2	0	889	631	-31	3	12	0	13	11	12	-9	4	1	17	17	16	-7	9	1	25	25	9	-2	16	1	14	11	13
1	2	0	309	250-308		4	12	0	11	12	10	-8	4	1	0	23	1	-6	9	1	69	68	3	-1	16	1	49	42	5
2	2	0	311	263-310		5	12	0	19	14	19	-7	4	1	48	46	4	-5	9	1	0	19	1	0	16	1	64	53	5
3	2	0	213	176-212		6	12	0	51	47	51	-6	4	1	27	27	5	-4	9	1	128	128	2	1	16	1	40	31	6
4	2	0	9	7	-9	1	13	0	42	35	9	-5	4	1	127	126	4	-3	9	1	75	76	2	2	16	1	52	45	5
5	2	0	25	22	24	2	13	0	42	37	42	-4	4	1	45	42	3	-2	9	1	50	47	2	-8	0	2	0	4	1
6	2	0	164	151	127	3	13	0	0	17	1	-3	4	1	69	72	-2	-1	9	1	67	65	2	-6	0	2	217	197	8
7	2	0	14	11	14	4	13	0	42	35	41	-2	4	1	167	155	-3	0	9	1	60	56	2	-4	0	2	156	146	-5
8	2	0	6	6	6	5	13	0	9	7	9	-1	4	1	325	314	-5	1	9	1	118	104	6	-2	0	2	307	255	-6
9	2	0	34	32	11	6	13	0	48	46	5	0	4	1	113	118	-4	2	9	1	23	20	4	0	0	2	439	456	-3
1	3	0	434	356-434		0	14	0	12	10	12	1	4	1	33	14	-3	3	9	1	14	11	14	2	0	2	84	81	-4
2	3	0	89	85	-88	1	14	0	46	40	15	2	4	1	23	2	-2	4	9	1	61	56	3	4	0	2	188	164	-6
3	3	0	308	253-307		2	14	0	9	6	8	3	4	1	247	204	-7	5	9	1	43	39	5	6	0	2	166	162	6
4	3	0	101	97-100		3	14	0	14	14	14	4	4	1	70	60	6	6	9	1	35	33	7	8	0	2	32	31	6
5	3	0	136	128	136	4	14	0	28	28	28	5	4	1	120	104	7	7	9	1	20	19	19	-9	1	2	52	53	5
6	3	0	7	7	7	5	14	0	68	60	60	6	4	1	49	44	4	-7	10	1	0	30	1	-8	1	2	0	8	1
7	3	0	95	89	95	1	15	0	29	25	6	7	4	1	27	24	8	-6	10	1	17	19	16	-7	1	2	85	82	4
8	3	0	23	21	23	2	15	0	25	22	14	8	4	1	30	27	8	-5	10	1	0	4	1	-6	1	2	114	110	5
9	3	0	34	34	23	3	15	0	40	34	40	9	4	1	44	40	7	-4	10	1	8	5	7	-5	1	2	98	96	4
0	4	0	841	623	-37	4	15	0	18	15	18	-9	5	1	26	26	10	-3	10	1	39	41	3	-4	1	2	43	44	-3
1	4	0	367	315-366		0	16	0	14	9	14	-8	5	1	0	18	1	-2	10	1	74	74	2	-3	1	2	33	25	-6
2	4	0	203	172-203		1	16	0	0	10	1	-7	5	1	19	20	11	-1	10	1	0	5	1	-2	1	2	203	184	-6
3	4	0	97	89	-96	2	16	0	61	49	31	-6	5	1	89	91	4	0	10	1	51	49	3	-1	1	2	150	153	-3
4	4	0	151	136	150	-9	0	1	126	126	4	-5	5	1	92	93	4	1	10	1	59	54	2	0	1	2	88	107	-1
5	4	0	15	13	15	-7	0	1	6	2	6	-4	5	1	40	40	2	2	10	1	26	20	6	1	1	2	239	235	-3
6	4	0	99	92	99	-5	0	1	111	104	6	-3	5	1	59	61	-2	3	10	1	16	15	15	2	1	2	9	7	-7
7	4	0	0	13	1	-3	0	1	595	454	-10	-2	5	1	67	70	-1	4	10	1	123	112	6	3	1	2	445	339	-9
8	4	0	32	32	23	-1	0	1	1206	775	-40	-1	5	1	78	78	-1	5	10	1	10	7	10	4	1	2	126	110	-6
9	4	0	16	16	15	1	0	1	204	153	-4	0	5	1	160	144	-4	6	10	1	7	5	6	5	1	2	209	194	7
1	5	0	160	142-145		3	0	1	595	439	-10	1	5	1	346	290	-7	7	10	1	90	79	5	6	1	2	43	44	4
2	5	0	113	107-113		5	0	1	164	148	6	2	5	1	27	22	-4	-7	11	1	0	24	1	7	1	2	33	33	5
3	5	0	241	213-240		7	0	1	0	5	1	3	5	1	16	16	-6	-6	11	1	39	40	10	8	1	2	39	38	5
4	5	0	34	29	15	9	0	1	27	30	8	4	5	1	212	179	7	-5	11	1	0	15	1	9	1	2	36	35	7
5	5	0	81	75	80	-9	1	1	20	19	19	5	5	1	18	15	10	-4	11	1	18	17	9	-9	2	2	45	47	6
6	5	0	24	24	6	-8	1	1	86	85	4	6	5	1	34	33	6	-3	11	1	25	23	12	-8	2	2	11	12	10
7	5	0	5	1	5	-7	1	1	37	35	5	7	5	1	13	12	12	-2	11	1	24	22	5	-7	2	2	12	11	11
8	5	0	34	32	34	-6	1	1	15	17	14	8	5	1	56	52	5	-1	11	1	102	98	3	-6	2	2	51	50	3
9	5	0	5	3	5	-5	1	1	162	152	6	9	5	1	46	44	7	0	11	1	11	8	11	-5	2	2	166	160	6
0	6	0	209	183	-6	-4	1	1	90	82	-5	-8	6	1	29	30	8	1	11	1	37	34	4	-4	2	2	37	36	-3
1	6	0	34	36	-33	-3	1	1	133	125	-5	-7	6	1	33	36	7	2	11	1	104	94	4	-3	2	2	232	192	-6
2	6	0	69	59	-12	-2	1	1	269	255	-5	-6	6	1	34	37	6	3	11	1	4	2	4	-2	2	2	176	179	-5
3	6	0	23	21	22	-1	1	1	91	96	-3	-5	6	1	25	25	6	4	11	1	23	19	9	-1	2	2	189	204	-2
4	6	0	153	142	153	0	1	1	637	464	-25	-4	6	1	111	112	3	5	11	1	44	41	5	0	2	2	444	480	-1
5	6	0	99	96	99	1	1	1	364	283	-5	-3	6	1	8	9	8	6	11	1	73	66	5	1	2	2	8	4	-7
6	6	0	153	146	153	2	1	1	370	278	-7	-2	6	1	49	52	-2	7	11	1	0	10	1	2	2	2	30	22	-1
7	6	0	48	45	47	3	1	1	181	160	-6	-1	6	1	338	329	-5	-6	12	1	7	3	6	3	2	2	22	10	-5
8	6	0	11	9	11	4	1	1	320	261	-8	0	6	1	95	83	-2	-5	12	1	39	40	4	4	2	2	105	92	-6
1	7	0	64	62	-23	5	1	1	37	34	3	1	6	1	254	220	-6	-4	12	1	65	62	3	5</					

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-3	4	2	96	101	-1	0	9	2	59	58	1	3	0	3	347	299	-7	3	5	3	73	68	2	-3	11	3	51	51	5
-2	4	2	0	29	-1	1	9	2	16	15	6	5	0	3	147	142	5	4	5	3	238	215	7	-2	11	3	82	82	1
-1	4	2	0	15	-1	2	9	2	73	73	1	7	0	3	40	39	5	5	5	3	42	36	5	-1	11	3	0	22	1
0	4	2	167	184	-1	3	9	2	37	36	4	9	0	3	86	86	4	6	5	3	30	29	6	0	11	3	70	71	2
1	4	2	125	120	-1	4	9	2	117	106	6	-9	1	3	0	8	1	7	5	3	63	59	5	1	11	3	72	71	2
2	4	2	130	125	-4	5	9	2	13	8	13	-8	1	3	33	34	17	8	5	3	16	16	15	2	11	3	92	88	2
3	4	2	58	51	-5	6	9	2	50	44	5	-7	1	3	0	60	-1	-8	6	3	8	8	8	3	11	3	0	5	1
4	4	2	23	22	5	7	9	2	8	5	8	-6	1	3	155	163	2	-7	6	3	0	13	1	4	11	3	0	4	1
5	4	2	52	47	4	-7	10	2	0	29	1	-5	1	3	89	93	1	-6	6	3	0	69	-1	5	11	3	61	56	4
6	4	2	6	6	5	-6	10	2	0	45	1	-4	1	3	0	3	-1	-5	6	3	0	12	1	6	11	3	0	8	1
7	4	2	18	16	18	-5	10	2	0	29	1	-3	1	3	71	78	-1	-4	6	3	46	45	1	-6	12	3	18	16	18
8	4	2	27	25	11	-4	10	2	0	14	1	-2	1	3	62	70	-1	-3	6	3	89	90	2	-5	12	3	0	42	1
9	4	2	0	11	1	-3	10	2	0	26	1	-1	1	3	0	21	-1	-2	6	3	179	185	-1	-4	12	3	0	23	1
-9	5	2	36	36	11	-2	10	2	128	127	1	0	1	3	168	169	-1	-1	6	3	137	142	-1	-3	12	3	0	17	1
-8	5	2	0	27	1	-1	10	2	22	25	10	1	1	3	113	136	-1	0	6	3	0	47	-1	-2	12	3	54	53	5
-7	5	2	49	53	3	0	10	2	14	13	13	2	1	3	214	227	-4	1	6	3	162	166	-3	-1	12	3	97	96	1
-6	5	2	10	9	10	1	10	2	33	35	2	3	1	3	36	36	-4	2	6	3	43	40	2	0	12	3	0	13	1
-5	5	2	52	54	1	2	10	2	44	40	2	4	1	3	152	136	7	3	6	3	63	57	2	1	12	3	50	49	2
-4	5	2	6	5	6	3	10	2	64	60	2	5	1	3	114	109	6	4	6	3	65	59	5	2	12	3	82	77	2
-3	5	2	123	123	-1	4	10	2	21	20	8	6	1	3	10	7	9	5	6	3	176	163	7	3	12	3	0	12	1
-2	5	2	142	156	-1	5	10	2	88	79	5	7	1	3	0	16	1	6	6	3	44	42	6	4	12	3	0	2	1
-1	5	2	71	83	-1	6	10	2	43	39	6	8	1	3	66	67	4	7	6	3	32	29	8	5	12	3	25	23	8
0	5	2	156	166	-1	7	10	2	14	11	13	9	1	3	43	46	6	8	6	3	0	7	1	6	12	3	0	0	1
1	5	2	123	136	-1	-7	11	2	33	33	6	-9	2	3	47	50	6	-8	7	3	0	30	1	-5	13	3	15	15	15
2	5	2	47	43	4	-6	11	2	27	25	6	-8	2	3	0	20	-1	-7	7	3	25	27	15	-4	13	3	0	24	1
3	5	2	0	2	-1	-5	11	2	17	18	13	-7	2	3	0	40	1	-6	7	3	0	25	-1	-3	13	3	33	32	4
4	5	2	15	11	8	-4	11	2	0	7	1	-6	2	3	127	133	1	-5	7	3	0	30	1	-2	13	3	38	35	8
5	5	2	102	90	8	-3	11	2	99	96	1	-5	2	3	63	67	1	-4	7	3	56	60	1	-1	13	3	0	5	1
6	5	2	50	45	4	-2	11	2	0	16	1	-4	2	3	129	140	-1	-3	7	3	80	83	1	0	13	3	6	3	6
7	5	2	78	71	5	-1	11	2	112	111	1	-3	2	3	237	247	-1	-2	7	3	112	115	1	1	13	3	0	15	1
8	5	2	0	6	1	0	11	2	61	58	1	-2	2	3	161	175	-1	-1	7	3	222	230	1	2	13	3	0	10	1
-8	6	2	0	42	1	1	11	2	2	0	2	-1	2	3	163	165	-1	0	7	3	129	132	1	3	13	3	87	77	3
-7	6	2	0	15	1	2	11	2	65	63	2	0	2	3	209	264	-1	1	7	3	78	76	1	4	13	3	7	3	6
-6	6	2	57	62	2	3	11	2	13	10	13	1	2	3	231	264	-1	2	7	3	31	28	3	5	13	3	24	21	11
-5	6	2	53	55	4	4	11	2	79	73	3	2	2	3	195	223	-1	3	7	3	39	37	3	-4	14	3	29	27	6
-4	6	2	153	157	1	5	11	2	54	51	4	3	2	3	17	16	-3	4	7	3	170	156	7	-3	14	3	53	52	3
-3	6	2	57	62	1	6	11	2	0	14	1	4	2	3	7	4	7	5	7	3	27	26	6	-2	14	3	0	3	1
-2	6	2	61	64	-1	-6	12	2	0	13	1	5	2	3	78	76	4	6	7	3	42	38	6	-1	14	3	0	6	1
-1	6	2	202	217	-1	-5	12	2	50	46	7	6	2	3	86	85	4	7	7	3	18	17	17	0	14	3	0	12	1
0	6	2	161	169	-1	-4	12	2	66	62	2	7	2	3	4	2	4	8	7	3	71	65	5	1	14	3	44	41	8
1	6	2	112	117	-1	-3	12	2	46	45	3	8	2	3	39	43	5	-8	8	3	10	6	10	2	14	3	65	60	3
2	6	2	131	127	-3	-2	12	2	0	28	-1	9	2	3	0	11	1	-7	8	3	42	44	4	3	14	3	14	12	13
3	6	2	28	26	3	-1	12	2	0	13	1	-9	3	3	6	2	6	-6	8	3	4	1	4	4	14	3	78	68	4
4	6	2	64	60	3	0	12	2	62	62	2	-8	3	3	26	30	9	-5	8	3	0	57	-1	-3	15	3	14	12	13
5	6	2	38	34	4	1	12	2	0	0	1	-7	3	3	26	28	17	-4	8	3	0	18	1	-2	15	3	36	35	5
6	6	2	0	1	1	2	12	2	31	28	4	-6	3	3	5	1	4	-3	8	3	74	76	1	-1	15	3	0	17	1
7	6	2	64	57	5	3	12	2	13	10	12	-5	3	3	61	66	1	-2	8	3	182	185	1	0	15	3	33	31	13
8	6	2	48	46	6	4	12	2	49	46	4	-4	3	3	133	134	1	-1	8	3	233	237	1	1	15	3	11	8	10
-8	7	2	0	9	1	5	12	2	0	4	1	-3	3	3	106	116	-1	0	8	3	121	126	1	2	15	3	42	38	5
-7	7	2	51	52	3	6	12	2	23	22	11	-2	3	3	147	178	-1	1	8	3	0	22	1	3	15	3	84	75	4
-6	7	2	68	72	2	-5	13	2	0	11	1	-1	3	3	300	334	-1	2	8	3	147	137	5	-1	16	3	20	17	12
-5	7	2	91	96	1	-4	13	2	0	12	1	0	3	3	245	274	-1	3	8	3	6	1	5	0	16	3	0	1	1
-4	7	2	0	10	1	-3	13	2	20	19	9	1	3	3	72	69	-1	4	8	3	30	26	5	1	16	3	0	27	1
-3	7	2	51	52	3	-2	13	2	0	34	1	2	3	3	159	152	-4	5	8	3	5	4	5	-8	0	4	22	21	21
-2	7	2	207	218	1	-1	13	2	41	42	6	3	3	3	63	61	-3	6	8	3	7	7	7	-6	0	4	24	25	5
-1	7	2	113	113	-1	0	13	2	0	9	1	4	3	3	31	31	3	7	8	3	65	60	5	-4	0	4	84	81	2
0	7	2	24	26	-5	1	13	2	18	15	18	5	3	3	173	148	8	-7	9	3	50	50	3	-2	0	4	182	169	-5
1	7	2	82	94	-1	2	13	2	13	12	13	6	3	3	25	24	7	-6	9	3	0	25	1	0	0	4	165	208	-1
2	7	2	36	37	2	3	13	2	32	30	5	7	3	3	43	41	5	-5	9	3	56	54	5	2	0	4	84	96	-1
3	7	2	44	42	3	4	13	2	35	32	6	8	3	3	45	43	5	-4	9	3	0	7	1	4	0	4	140	136	6
4	7	2	21	21	6	5	13	2	17	14	17	-9	4	3	0	6	1	-3	9	3	0	14	1	6	0	4	134	127	6
5	7	2	4	3	4																								



h k l			10Fo	10Fc	10s	h k l			10Fo	10Fc	10s	h k l			10Fo	10Fc	10s	h k l			10Fo	10Fc	10s						
1	2	4	10	5	-9	4	7	4	5	3	4	1	14	4	0	1	1	-8	5	5	50	52	4	5	10	5	8	8	7
2	2	4	0	0	-1	5	7	4	8	6	8	2	14	4	0	10	1	-7	5	5	0	12	1	6	10	5	0	7	1
3	2	4	145	147	-4	6	7	4	58	55	4	3	14	4	42	37	5	-6	5	5	0	26	1	-6	11	5	0	10	1
4	2	4	106	107	3	7	7	4	7	0	6	4	14	4	14	13	14	-5	5	5	70	71	1	-5	11	5	19	16	9
5	2	4	0	16	1	-8	8	4	7	6	7	-3	15	4	0	10	1	-4	5	5	71	77	1	-4	11	5	7	10	7
6	2	4	37	36	4	-7	8	4	38	37	6	-2	15	4	14	11	13	-3	5	5	64	68	1	-3	11	5	8	8	7
7	2	4	50	50	4	-6	8	4	12	12	11	-1	15	4	0	16	1	-2	5	5	102	110	1	-2	11	5	0	37	1
8	2	4	52	53	5	-5	8	4	90	86	3	0	15	4	27	24	6	-1	5	5	74	78	1	-1	11	5	0	4	1
-9	3	4	8	3	8	-4	8	4	107	104	3	1	15	4	54	50	3	0	5	5	5	3	5	0	11	5	69	69	2
-8	3	4	60	59	6	-3	8	4	103	98	2	2	15	4	0	15	1	1	5	5	131	135	1	1	11	5	0	9	1
-7	3	4	18	17	18	-2	8	4	198	192	5	-9	0	5	56	51	6	2	5	5	35	38	2	2	11	5	30	27	6
-6	3	4	38	33	5	-1	8	4	69	69	1	-7	0	5	72	71	4	3	5	5	119	119	3	3	11	5	77	73	3
-5	3	4	60	58	3	0	8	4	45	45	2	-5	0	5	174	162	7	4	5	5	17	16	7	4	11	5	0	3	1
-4	3	4	73	71	2	1	8	4	206	202	4	-3	0	5	176	159	-6	5	5	5	0	12	1	5	11	5	78	70	4
-3	3	4	64	65	-3	2	8	4	0	8	1	-1	0	5	167	177	-2	6	5	5	0	5	1	-5	12	5	0	24	1
-2	3	4	263	234	-6	3	8	4	105	99	3	1	0	5	126	135	-1	7	5	5	50	48	5	-4	12	5	0	36	1
-1	3	4	138	130	-5	4	8	4	0	11	1	3	0	5	179	186	2	8	5	5	87	84	5	-3	12	5	0	5	1
0	3	4	151	143	-4	5	8	4	55	53	4	5	0	5	13	12	12	-8	6	5	50	54	8	-2	12	5	0	17	1
1	3	4	131	127	-4	6	8	4	33	31	7	7	0	5	0	12	1	-7	6	5	64	65	2	-1	12	5	80	78	2
2	3	4	25	24	-3	7	8	4	72	68	5	-9	1	5	43	42	7	-6	6	5	8	4	7	0	12	5	0	23	1
3	3	4	159	147	5	-7	9	4	15	16	15	-8	1	5	75	73	5	-5	6	5	0	25	1	1	12	5	18	19	11
4	3	4	134	131	6	-6	9	4	68	66	2	-7	1	5	41	40	5	-4	6	5	21	21	4	2	12	5	67	65	3
5	3	4	18	19	8	-5	9	4	0	30	1	-6	1	5	99	94	3	-3	6	5	84	86	1	3	12	5	42	39	5
6	3	4	0	7	1	-4	9	4	83	85	1	-5	1	5	82	80	3	-2	6	5	44	48	1	4	12	5	0	7	1
7	3	4	14	14	14	-3	9	4	0	21	1	-4	1	5	128	121	6	-1	6	5	0	38	-1	5	12	5	10	4	10
8	3	4	52	55	4	-2	9	4	0	34	1	-3	1	5	110	108	-4	0	6	5	5	3	4	-5	13	5	0	37	1
-9	4	4	0	21	1	-1	9	4	182	186	1	-2	1	5	52	55	-1	1	6	5	58	62	1	-4	13	5	0	20	1
-8	4	4	24	24	13	0	9	4	0	2	1	-1	1	5	55	55	-1	2	6	5	11	13	11	-3	13	5	0	38	1
-7	4	4	67	65	5	1	9	4	32	36	3	0	1	5	200	211	-1	3	6	5	19	17	5	-2	13	5	15	14	15
-6	4	4	18	18	12	2	9	4	101	101	1	1	1	5	11	13	-5	4	6	5	52	52	3	-1	13	5	0	20	1
-5	4	4	94	89	4	3	9	4	64	63	2	2	1	5	124	131	-1	5	6	5	36	36	4	0	13	5	0	24	1
-4	4	4	48	47	3	4	9	4	94	89	4	3	1	5	92	97	1	6	6	5	18	19	13	1	13	5	0	23	1
-3	4	4	128	123	5	5	9	4	81	77	4	4	1	5	55	56	2	7	6	5	32	32	7	2	13	5	67	62	3
-2	4	4	0	2	-1	6	9	4	39	35	5	5	1	5	66	67	3	-8	7	5	0	5	1	3	13	5	43	42	5
-1	4	4	25	5	-3	7	9	4	47	45	6	6	1	5	51	48	4	-7	7	5	33	33	5	4	13	5	5	3	5
0	4	4	147	141	-3	-7	10	4	0	8	1	7	1	5	32	30	6	-6	7	5	0	22	1	-4	14	5	0	32	1
1	4	4	150	145	-4	-6	10	4	4	3	4	8	1	5	64	66	5	-5	7	5	32	33	8	-3	14	5	0	6	1
2	4	4	190	180	-5	-5	10	4	10	9	10	-9	2	5	0	23	1	-4	7	5	41	43	2	-2	14	5	0	52	1
3	4	4	194	182	6	-4	10	4	31	32	4	-8	2	5	86	86	5	-3	7	5	35	36	2	-1	14	5	16	17	16
4	4	4	49	51	3	-3	10	4	50	52	5	-7	2	5	0	13	1	-2	7	5	85	88	1	0	14	5	0	16	1
5	4	4	98	92	6	-2	10	4	0	95	-1	-6	2	5	32	31	5	-1	7	5	210	215	1	1	14	5	0	35	1
6	4	4	22	20	9	-1	10	4	13	13	13	-5	2	5	53	53	3	0	7	5	11	8	10	2	14	5	29	28	7
7	4	4	10	10	9	0	10	4	0	18	1	-4	2	5	95	95	3	1	7	5	27	29	3	3	14	5	20	18	19
8	4	4	19	19	19	1	10	4	23	22	4	-3	2	5	192	193	4	2	7	5	123	121	3	-2	15	5	9	9	9
-8	5	4	0	13	1	2	10	4	0	23	1	-2	2	5	14	16	-5	3	7	5	62	63	2	-1	15	5	12	11	12
-7	5	4	69	71	4	3	10	4	33	33	4	-1	2	5	66	74	-2	4	7	5	107	104	3	0	15	5	50	48	4
-6	5	4	98	99	2	4	10	4	21	22	8	0	2	5	36	41	-3	5	7	5	28	24	6	1	15	5	0	8	1
-5	5	4	77	81	2	5	10	4	31	28	6	1	2	5	116	121	-1	6	7	5	27	27	8	-8	0	6	88	85	4
-4	5	4	140	140	3	6	10	4	42	40	5	2	2	5	96	102	-1	7	7	5	9	7	8	-6	0	6	120	110	5
-3	5	4	0	27	-1	-6	11	4	0	0	1	3	2	5	73	74	1	-7	8	5	0	23	1	-4	0	6	160	146	6
-2	5	4	62	69	-1	-5	11	4	7	4	7	4	2	5	147	148	5	-6	8	5	0	17	1	-2	0	6	15	15	-5
-1	5	4	98	106	-1	-4	11	4	31	28	10	5	2	5	25	25	5	-5	8	5	69	68	2	0	0	6	21	22	-3
0	5	4	16	20	-4	-3	11	4	0	22	1	6	2	5	29	28	4	-4	8	5	51	50	2	2	0	6	36	38	2
1	5	4	89	90	-2	-2	11	4	0	0	1	7	2	5	8	5	8	-3	8	5	54	56	2	4	0	6	62	65	2
2	5	4	97	91	3	-1	11	4	0	16	1	8	2	5	37	37	6	-2	8	5	195	197	1	6	0	6	59	59	3
3	5	4	21	19	5	0	11	4	6	5	6	-9	3	5	29	30	10	-1	8	5	74	79	1	8	0	6	0	6	1
4	5	4	262	241	8	1	11	4	59	59	2	-8	3	5	19	20	19	0	8	5	86	89	1	-8	1	6	0	7	1
5	5	4	86	82	4	2	11	4	56	55	2	-7	3	5	41	39	5	1	8	5	60	62	2	-7	1	6	26	22	6
6	5	4	21	21	10	3	11	4	10	10	10	-6	3	5	35	32	5	2	8	5	9	11	9	-6	1	6	11	8	10
7	5	4	36	36	6	4	11	4	0	8	1	-5	3	5	168	160	7	3	8	5	56	53	3	-5	1	6	45	40	4
8	5	4	25	23	16	5	11	4	10	9	9	-4	3	5	70	64	2	4	8	5	32	32	4	-4	1	6	66	60	3
-8	6	4	0	54	1	6	11	4	0	20	1	-3	3	5	0	30	-1	5	8	5	62								

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-8	3	6	0	7	1	3	8	6	71	72	2	7	1	7	45	47	5	3	7	7	30	32	4	3	1	8	16	17	10
-7	3	6	34	33	5	4	8	6	51	51	3	-8	2	7	0	6	1	4	7	7	22	23	7	4	1	8	48	50	3
-6	3	6	0	9	1	5	8	6	0	6	1	-7	2	7	23	21	8	5	7	7	9	6	8	5	1	8	30	31	5
-5	3	6	41	40	4	6	8	6	14	12	13	-6	2	7	21	20	9	6	7	7	38	39	6	6	1	8	35	35	5
-4	3	6	51	48	3	-7	9	6	0	51	-1	-5	2	7	43	40	4	-7	8	7	52	51	5	7	1	8	23	22	9
-3	3	6	34	34	3	-6	9	6	45	43	8	-4	2	7	118	112	5	-6	8	7	0	33	1	-8	2	8	56	52	5
-2	3	6	134	131	3	-5	9	6	5	2	4	-3	2	7	59	56	3	-5	8	7	0	4	1	-7	2	8	0	10	1
-1	3	6	10	7	9	-4	9	6	0	5	1	-2	2	7	98	96	3	-4	8	7	30	31	12	-6	2	8	27	25	7
0	3	6	127	139	1	-3	9	6	5	0	5	-1	2	7	42	41	2	-3	8	7	0	5	1	-5	2	8	22	20	8
1	3	6	35	39	1	-2	9	6	71	69	1	0	2	7	154	153	3	-2	8	7	0	16	1	-4	2	8	39	37	4
2	3	6	78	81	1	-1	9	6	60	59	1	1	2	7	15	14	6	-1	8	7	31	30	3	-3	2	8	53	50	3
3	3	6	53	56	2	0	9	6	0	49	-1	2	2	7	158	159	5	0	8	7	33	33	3	-2	2	8	35	35	3
4	3	6	157	165	3	1	9	6	99	103	1	3	2	7	88	90	2	1	8	7	74	75	1	-1	2	8	88	87	2
5	3	6	37	38	3	2	9	6	5	4	4	4	2	7	62	64	2	2	8	7	84	87	2	0	2	8	42	43	3
6	3	6	54	56	3	3	9	6	41	39	3	5	2	7	29	29	5	3	8	7	20	18	20	1	2	8	21	21	5
7	3	6	0	16	1	4	9	6	33	33	5	6	2	7	104	107	3	4	8	7	77	77	3	2	2	8	19	19	6
8	3	6	13	12	13	5	9	6	9	11	9	7	2	7	22	22	10	5	8	7	40	40	4	3	2	8	82	84	2
-8	4	6	33	33	7	6	9	6	44	45	5	-8	3	7	29	28	8	6	8	7	17	17	17	4	2	8	40	42	4
-7	4	6	36	35	6	-6	10	6	0	5	1	-7	3	7	0	28	1	-6	9	7	0	15	1	5	2	8	6	4	5
-6	4	6	13	14	12	-5	10	6	0	4	1	-6	3	7	63	63	3	-5	9	7	0	1	1	6	2	8	47	49	4
-5	4	6	52	51	4	-4	10	6	21	20	21	-5	3	7	98	100	1	-4	9	7	36	34	4	7	2	8	58	60	4
-4	4	6	104	98	5	-3	10	6	51	48	2	-4	3	7	10	8	9	-3	9	7	45	44	3	-8	3	8	6	6	6
-3	4	6	87	80	2	-2	10	6	47	45	5	-3	3	7	46	48	4	-2	9	7	0	24	1	-7	3	8	13	12	12
-2	4	6	68	70	1	-1	10	6	12	13	12	-2	3	7	55	60	1	-1	9	7	15	15	14	-6	3	8	47	43	5
-1	4	6	85	87	1	0	10	6	35	34	3	-1	3	7	0	40	-1	0	9	7	46	46	3	-5	3	8	0	1	1
0	4	6	5	5	4	1	10	6	0	28	1	0	3	7	59	60	1	1	9	7	0	9	1	-4	3	8	60	58	3
1	4	6	0	0	1	2	10	6	8	6	8	1	3	7	85	91	1	2	9	7	23	26	6	-3	3	8	57	53	3
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7	4	6	14	12	13	-5	11	6	26	25	16	7	3	7	27	29	7	-4	10	7	0	58	-1	3	3	8	41	42	3
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-8	6	6	12	9	11	1	12	6	0	7	1	-8	5	7	28	25	9	2	11	7	0	43	-1	5	4	8	31	29	6
-7	6	6	0	23	1	2	12	6	0	68	-1	-7	5	7	0	7	1	3	11	7	0	19	1	6	4	8	61	63	3
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-5	6	6	0	20	1	4	12	6	0	16	1	-5	5	7	55	55	2	-4	12	7	0	1	1	-6	5	8	64	61	4
-4	6	6	91	92	2	-4	13	6	46	45	4	-4	5	7	43	42	2	-3	12	7	8	4	7	-5	5	8	38	36	6
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-2	6	6	21	24	4	-2	13	6	0	26	1	-2	5	7	82	84	1	-1	12	7	31	27	10	-3	5	8	97	93	2
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0	6	6	3	1	3	0	13	6	19	21	19	0	5	7	0	17	1	1	12	7	61	59	2	-1	5	8	32	31	3
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3	6	6	72	73	2	3	13	6	0	11	1	3	5	7	5	4	4	4	12	7	0	15	1	2	5	8	47	48	3
4	6	6	0	8	1	-3	14	6	86	79	2	4	5	7	0	19	1	-3	13	7	14	11							

h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s											
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5	7	8	18	17	17	6	2	9	44	46	6	-2	10	9	0	6	1	1	6	10	25	23	7	-3	5	11	37	37	4
6	7	8	6	6	6	-7	3	9	32	32	17	-1	10	9	20	19	8	2	6	10	28	27	6	-2	5	11	23	22	7
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-5	8	8	3	2	2	-5	3	9	5	3	4	1	10	9	11	11	10	4	6	10	67	67	4	0	5	11	0	7	1
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0	8	8	21	21	21	0	3	9	30	30	4	-1	11	9	10	11	9	-1	7	10	9	6	8	-5	6	11	0	14	1
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2	8	8	19	17	8	2	3	9	84	87	2	1	11	9	0	12	1	1	7	10	26	25	6	-3	6	11	0	15	1
3	8	8	6	7	6	3	3	9	31	32	4	2	11	9	51	47	4	2	7	10	35	33	5	-2	6	11	39	38	4
4	8	8	43	43	5	4	3	9	34	35	4	-2	12	9	0	22	1	3	7	10	5	4	4	-1	6	11	0	41	1
5	8	8	0	2	1	5	3	9	11	10	11	-1	12	9	23	22	8	4	7	10	0	22	1	0	6	11	0	14	1
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-3	9	8	0	2	1	-5	4	9	43	43	9	-4	0	10	46	41	4	-2	8	10	0	7	1	-4	7	11	56	51	4
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-1	9	8	0	10	1	-3	4	9	73	72	2	0	0	10	113	112	2	0	8	10	28	28	6	-2	7	11	0	3	1
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3	9	8	15	14	14	1	4	9	116	120	1	-6	1	10	15	13	14	-4	9	10	0	0	1	2	7	11	82	82	3
4	9	8	9	8	9	2	4	9	0	10	1	-5	1	10	17	15	17	-3	9	10	0	20	1	3	7	11	23	24	23
5	9	8	67	66	4	3	4	9	77	80	2	-4	1	10	24	22	8	-2	9	10	30	30	5	-2	8	11	17	14	17
-5	10	8	51	47	5	4	4	9	44	45	3	-3	1	10	105	96	4	-1	9	10	49	46	3	-3	8	11	35	35	5
-4	10	8	0	4	1	5	4	9	21	21	10	-2	1	10	21	20	7	0	9	10	19	20	11	-1	8	11	9	7	8
-3	10	8	32	33	5	6	4	9	57	60	4	-1	1	10	55	53	3	1	9	10	23	23	23	0	8	11	43	42	4
-2	10	8	39	35	5	-7	5	9	6	6	6	0	1	10	0	5	1	2	9	10	37	38	5	1	8	11	39	38	5
-1	10	8	57	54	3	-6	5	9	0	2	1	1	1	10	65	66	3	3	9	10	0	0	1	2	8	11	11	10	10
0	10	8	6	1	6	-5	5	9	47	48	4	2	1	10	0	9	1	-3	10	10	0	5	1	-2	9	11	54	51	3
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-1	11	8	0	30	1	3	5	9	42	43	4	-2	2	10	47	46	4	0	11	10	20	20	12	-5	1	12	34	30	7
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1	11	8	10	9	10	5	5	9	0	17	1	0	2	10	24	25	5	-3	0	11	48	44	4	-3	1	12	28	26	8
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-3	12	8	38	39	4	-4	6	9	78	79	3	4	2	10	20	18	10	-6	1	11	31	30	10	1	1	12	57	58	4
-2	12	8	62	57	3	-3	6	9	56	56	3	5	2	10	84	86	4	-5	1	11	40	37	6	2	1	12	20	21	13
-1	12	8	25	23	16	-2	6	9	56	56	2	-6	3	10	19	18	18	-4	1	11	65	59	4	3	1	12	40	41	5
0	12	8	22	20	7	-1	6	9	18	18	7	-5	3	10	46	42	5	-3	1	11	0	10	1	-5	2	12	89	82	5
1	12	8	23	23	23	0	6	9	38	39	3	-4	3	10	33	30	6	-2	1	11	35	34	5	-4	2	12	41	37	6
2	12	8	4	4	4	1	6	9	41	41	3	-3	3	10	77	74	4	-1	1	11	0	5	1	-3	2	12	0	14	1
3	12	8	34	32	7	2	6	9	42	43	3	-2	3	10	58	56	3	0	1	11	0	14	1	-2	2	12	16	16	16
-2	13	8	0	6	1	3	6	9	38	40	4	-1	3	10	7	5	6	1	1	11	18	17	11	-1	2	12	47	45	4
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0	13	8	0	2	1	5	6	9	59	60	4	1	3	10	24	22	6	3	1	11	20	20	11	1	2	12	18	20	18
1	13	8	0	1	1	-6	7	9	22	22	10	2	3	10	16	15	12	4	1	11	14	15	14	2	2	12	0	9	1
-7	0	9	35	31	5	-5	7	9	31	30	7	3	3	10	15	14	14	-6	2	11	33	30	8	3	2	12	40	41	5
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-3	0	9	46	44	3	-3	7	9	0	14	1	5	3	10	16	16	15	-4	2	11	56	54	4	-3	3	12	63	60	4
-1	0	9	114	106	5	-2	7	9	52	50	2	-6	4	10	84	76	5	-3	2	11	5	4	5	-2	3	12	10	8	10
1	0	9	196	193	5	-1	7	9	0	13	1	-5	4	10	4	1	4												

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s						
1	7	12	34	31	6	-2	1	13	29	28	8	-2	2	13	37	36	5	-1	3	13	6	5	5	0	4	13	0	8	1
-3	0	13	17	16	16	-1	1	13	0	11	1	-1	2	13	7	7	6	0	3	13	0	13	1						
-1	0	13	35	35	6	0	1	13	0	2	1	0	2	13	24	25	24	1	3	13	37	36	6						
1	0	13	4	2	4	1	1	13	29	28	8	1	2	13	8	6	8	-2	4	13	0	7	1						
-3	1	13	0	3	1	-3	2	13	0	13	1	-2	3	13	2	1	1	-1	4	13	38	35	5						

ESPECTRO DE DIFRACCIÓN DE RAYOS-X DE 4,5,10,11-TETRAMETILHEPTACICLO[8.2.1.1<sup>2,5</sup>.1<sup>4,7</sup>.1<sup>8,11</sup>.0<sup>1,8</sup>.0<sup>2,7</sup>]HEXADECANO, 141.

Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a Enraf-Nonius CAD4 four-circle diffractometer. Unit-cell parameters were determined from automatic centering of 25 reflections ( $12 < \Theta < 21^\circ$ ) and refined by least-squares method. Intensities were collected with graphite monochromatized MoK $\alpha$  radiation, using  $\omega/2\Theta$  scan-technique. 2221 reflections were measured in the range  $2.02 \leq \Theta \leq 30.08$ . 1001 reflections were assumed as observed applying the condition  $I > 2\sigma(I)$ . Three reflections were measured every two hours as orientation and intensity control, significant intensity decay was not observed. Lorentz-polarization but no absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program (Sheldrick, G.M., (1990), Acta Cryst., A46, 467-473) and refined by full-matrix least-squares method with SHELX93 computer program (Sheldrick, G.M., (1994), in preparation), using 2171 reflections, (very negative intensities were not assumed). The function minimized was  $\sum w ||F_o|^2 - |F_c|^2|^2$ , where  $w = [\sigma^2(I) + (0.2958P)^2 + 0.0476P]^{-1}$ , and  $P = (|F_o|^4 + 2 |F_c|^4) / 3$ ,  $f$ ,  $f'$  and  $f''$  were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). The extinction coefficient was 0.00621(1). 8 H atoms were located from a difference synthesis and refined with an overall and 6 H atoms were computed and refined with an overall isotropic temperature factor using a riding model. The final R(on F) factor was 0.069,  $wR(\text{on } |F|^2) = 0.188$  and goodness of fit = 0.590 for all observed reflections. Number of refined parameters was 101. Max. shift/esd = 0.27, Mean shift/esd = 0.02. Max. and min. peaks in final difference synthesis was 0.463 and -0.271 e $\text{\AA}^{-3}$ , respectively.

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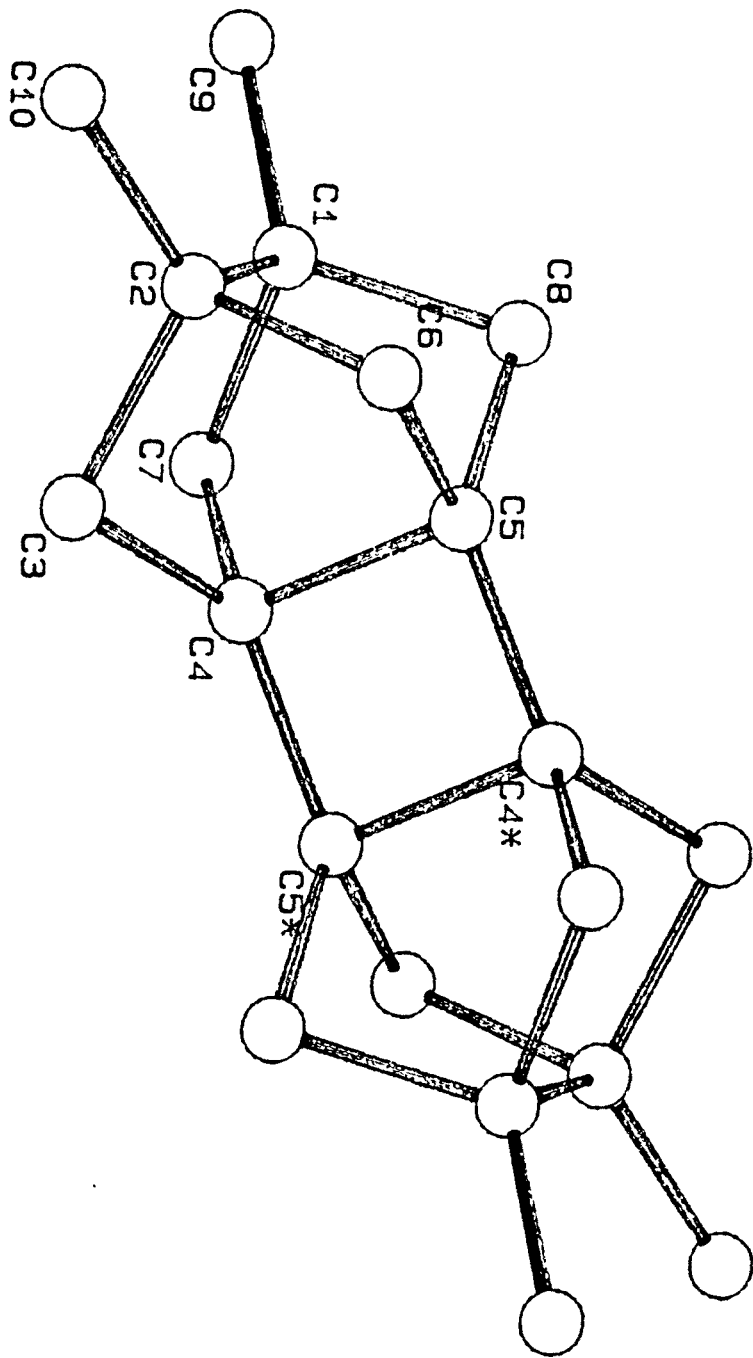


Table 1. Crystal data and structure refinement for 1.

Identification code	qfs1
Empirical formula	C <sub>40</sub> H <sub>56</sub>
Formula weight	536.85
Temperature	243(2) K
Wavelength	0.71069Å
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /a
Unit cell dimensions	a = 6.105(4)Å $\alpha$ = 90°. b = 12.322(2)Å $\beta$ = 92.13(2)°. c = 10.0950(9)Å $\gamma$ = 90°.
Volume	758.9(5) Å <sup>3</sup>
Z	2
Density (calculated)	2.349 Mg/m <sup>3</sup>
Absorption coefficient	0.130 mm <sup>-1</sup>
F(000)	592
Crystal size	0.1 x 0.1 x 0.2 mm
Theta range for data collection	2.02 to 30.08°.
Index ranges	-8<=h<=8, 0<=k<=17, 0<=l<=14
Reflections collected	2221
Independent reflections	2221 [R(int) = 0.0000]
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2171 / 0 / 101
Goodness-of-fit on F <sup>2</sup>	0.712
Final R indices [I>2σ(I)]	R1 = 0.0699, wR2 = 0.1881
R indices (all data)	R1 = 0.1820, wR2 = 0.3666
Extinction coefficient	0.006(12)
Largest diff. peak and hole	0.463 and -0.271 e.Å <sup>-3</sup>

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
C(1)	-1477(5)	9270(2)	2490(3)	42(1)
C(2)	-1952(5)	10586(2)	2541(3)	43(1)
C(3)	-3122(5)	10697(3)	3876(3)	45(1)
C(4)	-1664(5)	9863(2)	4578(3)	39(1)
C(5)	684(5)	10097(2)	4000(3)	38(1)
C(6)	256(5)	11045(3)	3050(3)	45(1)
C(7)	-2447(6)	8868(3)	3799(3)	47(1)
C(8)	938(5)	9210(3)	2962(3)	44(1)
C(9)	-2178(6)	8679(3)	1230(3)	60(1)
C(10)	-3062(7)	11092(3)	1329(3)	59(1)



Table 3. Bond lengths [Å] and angles [°] for 1.

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C(1)-C(9)	1.514(4)
C(1)-C(8)	1.534(4)
C(1)-C(7)	1.550(4)
C(1)-C(2)	1.649(4)
C(2)-C(10)	1.511(4)
C(2)-C(6)	1.533(4)
C(2)-C(3)	1.555(4)
C(3)-C(4)	1.518(4)
C(4)-C(7)	1.525(4)
C(4)-C(5)#1	1.535(4)
C(4)-C(5)	1.594(4)
C(5)-C(8)	1.527(4)
C(5)-C(6)	1.527(4)
C(5)-C(4)#1	1.535(4)
C(9)-C(1)-C(8)	118.4(3)
C(9)-C(1)-C(7)	117.2(3)
C(8)-C(1)-C(7)	96.5(2)
C(9)-C(1)-C(2)	117.0(3)
C(8)-C(1)-C(2)	101.9(2)
C(7)-C(1)-C(2)	102.4(2)
C(10)-C(2)-C(6)	118.8(3)
C(10)-C(2)-C(3)	117.3(3)
C(6)-C(2)-C(3)	95.9(2)
C(10)-C(2)-C(1)	117.0(3)
C(6)-C(2)-C(1)	102.7(2)
C(3)-C(2)-C(1)	101.6(2)
C(4)-C(3)-C(2)	93.8(2)
C(3)-C(4)-C(7)	97.8(3)
C(3)-C(4)-C(5)#1	128.1(2)
C(7)-C(4)-C(5)#1	127.7(2)
C(3)-C(4)-C(5)	103.1(2)
C(7)-C(4)-C(5)	103.0(2)
C(5)#1-C(4)-C(5)	90.7(2)
C(8)-C(5)-C(6)	97.8(2)
C(8)-C(5)-C(4)#1	128.2(2)
C(6)-C(5)-C(4)#1	127.9(2)
C(8)-C(5)-C(4)	103.8(2)
C(6)-C(5)-C(4)	103.5(2)
C(4)#1-C(5)-C(4)	89.3(2)
C(5)-C(6)-C(2)	93.3(2)
C(4)-C(7)-C(1)	93.4(2)
C(5)-C(8)-C(1)	93.3(2)

---

Symmetry transformations used to generate equivalent atoms:  
 #1 -x, -y+2, -z+1

Table 4. Hydrogens lengths [Å] and angles [°] for 1.

---

C(3)-H(3)	0.97
C(3)-H(3A)	0.97
C(6)-H(6)	0.97
C(6)-H(6A)	0.97
C(7)-H(7)	0.97
C(7)-H(7A)	0.97
C(8)-H(8)	0.97
C(8)-H(8A)	0.97
C(9)-H(9)	0.96
C(9)-H(9A)	0.96
C(9)-H(9B)	0.96
C(10)-H(10)	0.96
C(10)-H(10A)	0.96
C(10)-H(10B)	0.96
C(4)-C(3)-H(3)	113.0(2)
C(2)-C(3)-H(3)	113.0(2)
C(4)-C(3)-H(3A)	113.0(2)
C(2)-C(3)-H(3A)	113.0(2)
H(3)-C(3)-H(3A)	110.4
C(5)-C(6)-H(6)	113.1(2)
C(2)-C(6)-H(6)	113.1(2)
C(5)-C(6)-H(6A)	113.1(2)
C(2)-C(6)-H(6A)	113.1(2)
H(6)-C(6)-H(6A)	110.4
C(4)-C(7)-H(7)	113.0(2)
C(1)-C(7)-H(7)	113.0(2)
C(4)-C(7)-H(7A)	113.0(2)
C(1)-C(7)-H(7A)	113.0(2)
H(7)-C(7)-H(7A)	110.4
C(5)-C(8)-H(8)	113.1(2)
C(1)-C(8)-H(8)	113.1(2)
C(5)-C(8)-H(8A)	113.1(2)
C(1)-C(8)-H(8A)	113.1(2)
H(8)-C(8)-H(8A)	110.4
C(1)-C(9)-H(9)	109.5(2)
C(1)-C(9)-H(9A)	109.5(2)
H(9)-C(9)-H(9A)	109.5
C(1)-C(9)-H(9B)	109.5(2)
H(9)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(2)-C(10)-H(10)	109.5(2)
C(2)-C(10)-H(10A)	109.5(2)
H(10)-C(10)-H(10A)	109.5
C(2)-C(10)-H(10B)	109.5(2)
H(10)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5

---

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  
 The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C(1)	34(2)	48(2)	45(2)	-3(1)	7(1)	-1(1)
C(2)	34(1)	49(2)	46(2)	3(1)	11(1)	6(1)
C(3)	35(2)	55(2)	46(2)	0(1)	9(1)	10(1)
C(4)	31(1)	45(2)	42(2)	0(1)	12(1)	-1(1)
C(5)	30(1)	38(1)	46(2)	0(1)	10(1)	0(1)
C(6)	38(2)	47(2)	50(2)	7(1)	9(1)	-4(1)
C(7)	43(2)	49(2)	49(2)	-1(1)	8(1)	-11(1)
C(8)	32(1)	50(2)	50(2)	-4(1)	9(1)	5(1)
C(9)	56(2)	74(3)	50(2)	-14(2)	5(2)	-7(2)
C(10)	56(2)	69(2)	52(2)	7(2)	3(2)	13(2)

Table 6. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

	x	y	z	U(eq)
H(3)	-2982(5)	11416(3)	4260(3)	50(9)
H(3A)	-4650(5)	10480(3)	3812(3)	86(6)
H(6)	1325(5)	11095(3)	2366(3)	84(13)
H(6A)	120(5)	11735(3)	3501(3)	86(6)
H(7)	-4031(6)	8800(3)	3745(3)	161(26)
H(7A)	-1783(6)	8198(3)	4123(3)	86(6)
H(8)	1339(5)	8512(3)	3345(3)	60(10)
H(8A)	1941(5)	9407(3)	2278(3)	54(9)
H(9)	-3719(6)	8787(3)	1055(3)	136(23)
H(9A)	-1883(6)	7918(3)	1332(3)	167(29)
H(9B)	-1377(6)	8958(3)	504(3)	86(6)
H(10)	-4420(7)	10723(3)	1128(3)	113(18)
H(10A)	-2125(7)	11029(3)	590(3)	86(6)
H(10B)	-3348(7)	11844(3)	1498(3)	86(6)

h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s											
2	0	0	352	477	-1	6	11	0	28	28	6	-6	4	1	43	38	4	4	9	1	66	68	3	4	0	2	132	116	2
4	0	0	0	14	1	0	12	0	50	50	3	-5	4	1	87	78	2	5	9	1	19	18	12	6	0	2	44	36	3
6	0	0	35	38	3	1	12	0	75	69	1	-4	4	1	78	68	2	6	9	1	0	15	1	8	0	2	35	25	7
8	0	0	42	49	5	2	12	0	45	42	2	-3	4	1	94	84	1	-	9	1	0	27	1	-8	1	2	38	36	8
1	1	0	472	660	-1	3	12	0	14	8	14	-2	-4	1	35	21	-2	-	10	1	35	22	7	-7	1	2	0	15	1
2	1	0	138	198	-1	4	12	0	62	54	5	-1	4	1	100	99	1	-6	10	1	63	53	4	-6	1	2	49	36	-3
3	1	0	82	116	-1	5	12	0	25	22	2	0	4	1	249	254	2	-5	10	1	46	39	4	-5	1	2	105	91	2
4	1	0	2	102	-1	6	12	0	8	3	7	2	4	1	126	121	2	-4	10	1	10	6	10	-4	1	2	18	11	5
5	1	0	0	20	1	1	13	0	39	37	3	2	4	1	129	116	2	-3	10	1	0	2	1	-3	1	2	159	131	2
6	1	0	0	49	-1	2	13	0	39	33	3	3	4	1	98	97	1	-2	10	1	41	45	3	-2	1	2	115	101	2
8	1	0	0	10	1	3	13	0	34	31	8	4	4	1	46	43	2	-1	10	1	144	142	2	-1	1	2	321	295	2
8	1	0	0	18	1	4	13	0	10	5	9	5	4	1	31	41	9	0	10	1	67	64	2	0	1	2	3	2	3
0	2	0	960	1048	1	5	13	0	31	29	5	6	4	1	12	10	11	1	10	1	0	-	1	1	1	2	227	222	2
1	1	0	0	2	1	0	14	0	43	39	4	4	4	1	20	22	15	2	10	1	66	69	2	2	1	2	50	47	1
2	2	0	60	86	-1	1	14	0	21	24	17	8	4	1	0	41	1	3	10	1	0	10	1	3	1	2	255	223	3
3	2	0	22	30	-2	2	14	0	0	10	1	-8	5	1	32	23	8	4	10	1	14	16	14	4	1	2	42	38	2
4	2	0	52	74	-2	3	14	0	0	12	1	-7	5	1	0	16	1	5	10	1	36	36	5	5	1	2	56	49	2
5	2	0	44	62	-2	4	14	0	46	43	5	-6	5	1	28	28	5	6	10	1	23	21	10	6	1	2	29	21	5
6	2	0	0	33	1	5	14	0	0	11	1	-5	5	1	17	20	9	-6	11	1	0	-	1	1	1	2	0	6	1
7	2	0	0	16	1	1	15	0	12	15	11	-4	5	1	24	21	4	-5	11	1	41	36	5	8	1	2	13	12	12
8	2	0	0	46	-1	2	15	0	23	21	6	-3	5	1	43	41	2	-4	11	1	0	4	1	-8	2	2	0	8	1
1	3	0	114	141	17	3	15	0	38	31	14	-2	5	1	40	37	1	-3	11	1	36	35	4	-	2	2	0	21	1
2	3	0	131	185	-1	4	15	0	0	14	1	-1	5	1	126	130	1	-2	11	1	99	95	2	-6	2	2	0	20	1
3	3	0	0	117	-1	0	16	0	41	37	5	0	5	1	83	84	1	-1	11	1	13	17	13	-5	2	2	77	67	2
4	3	0	0	106	-1	1	16	0	0	13	1	1	5	1	310	301	2	0	11	1	35	34	3	-4	2	2	103	82	2
5	3	0	0	20	1	2	16	0	32	23	4	2	5	1	226	211	2	1	11	1	86	81	2	-3	2	2	30	24	-2
6	3	0	0	45	-1	3	16	0	10	6	9	3	3	1	203	190	3	2	11	1	55	49	2	-2	2	2	102	89	1
8	3	0	0	13	1	1	17	0	18	6	17	3	5	1	134	130	2	3	11	1	8	5	8	-1	2	2	181	176	2
0	3	0	35	48	-5	-8	0	1	0	8	1	5	5	1	5	4	4	4	11	1	53	56	6	0	2	2	126	133	1
1	4	0	411	506	1	-6	0	1	28	24	5	6	6	1	0	22	1	5	11	1	32	31	6	1	2	2	17	17	2
1	4	0	166	199	110	-4	0	1	273	216	3	5	5	1	0	0	1	6	11	1	0	3	1	2	2	2	139	129	2
2	4	0	148	203	-2	-2	0	1	118	111	-2	8	5	1	29	32	11	-6	12	1	23	20	12	3	2	2	62	54	1
3	4	0	44	62	-2	0	0	1	653	552	1	-8	6	1	27	31	26	-5	12	1	0	10	1	4	2	2	87	79	2
4	4	0	91	127	-1	2	0	1	254	224	-2	-8	6	1	56	43	4	-4	12	1	35	28	5	5	2	2	47	43	3
5	4	0	0	3	7	4	0	1	205	168	3	-6	6	1	41	32	4	-3	12	1	17	18	15	6	2	2	36	31	5
6	4	0	0	16	1	6	0	1	33	30	4	-5	6	1	0	18	1	-2	12	1	24	24	6	8	2	2	13	11	13
8	4	0	24	34	9	8	0	1	40	37	7	-4	6	1	30	28	3	-1	12	1	132	127	2	-	2	2	0	22	1
1	5	0	31	31	9	-8	1	1	0	12	1	-3	6	1	20	20	4	0	12	1	56	53	3	-8	3	2	74	68	5
2	5	0	16	20	3	-	1	1	44	38	5	-2	6	1	52	50	1	1	12	1	33	31	4	-7	3	2	55	47	4
3	5	0	61	86	-1	-6	1	1	63	52	3	-1	6	1	81	78	1	2	12	1	20	18	6	-6	3	2	90	73	2
4	5	0	14	17	5	-5	1	1	152	130	2	0	6	1	82	79	-1	3	12	1	22	24	8	-5	3	2	77	67	2
5	5	0	0	28	1	-4	1	1	80	62	2	1	6	1	44	42	-2	4	12	1	0	9	1	-4	3	2	0	6	1
6	5	0	0	42	-1	-3	1	1	408	321	3	2	6	1	14	5	5	5	12	1	0	12	1	-3	3	2	86	74	1
8	5	0	0	27	1	-2	1	1	92	77	1	3	6	1	100	99	1	6	12	1	0	16	1	-2	3	2	145	140	2
0	6	0	0	44	-1	-1	1	1	1324	904	-2	4	6	1	56	58	2	-5	13	1	58	51	4	-1	3	2	257	253	2
1	6	0	222	276	1	0	1	1	40	44	1	5	6	1	52	49	3	-4	13	1	20	12	12	0	3	2	0	55	1
2	6	0	128	145	89	1	1	1	348	313	1	6	6	1	15	9	15	-2	13	1	55	53	3	2	3	2	14	15	4
3	6	0	66	81	32	3	1	1	354	294	3	8	6	1	0	2	1	-1	13	1	0	3	1	4	3	2	111	99	1
4	6	0	87	89	12	4	1	1	47	34	-2	-	7	1	64	51	4	0	13	1	0	10	1	4	3	2	43	46	2
5	6	0	60	61	21	5	1	1	76	68	2	-6	7	1	50	39	4	1	13	1	25	21	6	5	3	2	60	57	3
6	6	0	17	21	7	6	1	1	53	44	3	-5	7	1	77	69	2	2	13	1	11	12	11	6	3	2	19	22	13
7	6	0	0	5	1	7	1	1	51	41	5	-4	-	1	39	37	3	3	13	1	9	6	9	7	3	2	18	19	18
8	6	0	0	11	1	8	1	1	40	30	7	-3	-	1	58	56	2	4	13	1	9	3	9	8	3	2	0	21	1
9	6	0	0	13	1	-8	2	1	0	13	1	-2	-	1	10	9	9	5	13	1	0	9	1	-8	4	2	17	4	16
2	7	0	0	10	6	10	2	1	23	11	-7	-1	-	1	9	13	9	-5	14	1	13	10	12	-7	4	2	20	0	12
3	7	0	0	1	1	-6	2	1	0	3	1	0	7	1	32	31	2	-4	14	1	50	37	4	-6	4	2	33	27	4
4	7	0	0	1	1	-5	2	1	57	54	2	1	7	1	142	141	2	-3	14	1	34	31	5	-5	4	2	21	13	-5
5	7	0	53	45	3	-4	2	1	185	154	3	2	7	1	157	150	2	-2	14	1	12	9	12	-4	4	2	91	82	2
6	7	0	53	46	10	-3	2	1	292	241	3	3	7	1	48	46	2	-1	14	1	0	18	1	-3	4	2	62	60	1
7	7	0	53	47	12	-2	2	1	80	68	1	4	7	1	33	29	4	0	14	1	26	22	6	-2	4	2	85	81	1
0	8	0	55	26	22	-1	2	1	92	87	1	5	7	1	17	22	16	1	14	1	25	20	6	-1	4	2	52	53	1
1	8	0	47	47	3	0	2	1	504	482	1	6	7	1	42	48	5	2	14	1	18	11							

h k l			10Fo			10Fc			10s			h k l			10Fo			10Fc			10s			h k l			10Fo			10Fc			10s		
-6	6	2	34	27	5	-1	12	2	59	55	3	-8	3	3	37	35	7	3	8	3	74	77	2	2	16	3	25	20	9						
-5	6	2	59	52	3	0	12	2	12	10	11	-7	3	3	46	35	5	4	8	3	80	88	3	-8	0	4	34	34	8						
-4	6	2	115	110	2	1	12	2	32	34	4	-6	3	3	0	11	1	5	8	3	14	11	13	-6	0	4	67	62	3						
-3	6	2	60	58	2	2	12	2	0	16	1	-5	3	3	50	45	3	6	8	3	0	1	1	-4	0	4	118	115	2						
-2	6	2	30	30	2	3	12	2	0	2	1	-4	3	3	159	154	2	-	8	3	28	28	10	-2	0	4	236	236	2						
-1	6	2	19	20	3	4	12	2	30	34	6	-3	3	3	50	44	2	-7	9	3	23	19	12	0	0	4	266	289	1						
0	6	2	326	327	2	5	12	2	27	29	8	-2	3	3	120	115	2	-6	9	3	-	4	6	2	0	4	45	50	1						
1	6	2	145	147	2	6	12	2	19	18	18	-1	3	3	126	122	2	-5	9	3	43	37	4	4	0	4	160	153	2						
2	6	2	27	28	2	-5	13	2	0	8	1	0	3	3	83	88	1	-4	9	3	16	10	16	6	0	4	73	69	4						
3	6	2	63	60	2	-4	13	2	0	9	1	1	3	3	291	293	2	-3	9	3	98	97	2	8	0	4	0	0	1						
4	6	2	17	17	2	-3	13	2	15	-	14	2	3	3	37	40	1	-2	9	3	67	67	2	-8	1	4	0	20	1						
5	6	2	62	68	3	-2	13	2	61	56	3	3	3	3	58	61	1	-1	9	3	62	59	2	-7	1	4	55	52	5						
6	6	2	22	28	22	-1	13	2	13	10	13	4	3	3	91	94	2	0	9	3	92	96	1	-6	1	4	86	82	3						
7	6	2	0	0	21	1	0	13	2	15	20	14	5	3	107	107	3	1	9	3	132	140	1	-5	1	4	65	63	2						
8	6	2	19	21	18	1	13	2	11	11	10	6	3	3	36	34	5	2	9	3	58	61	2	-4	1	4	32	30	3						
9	6	2	0	0	7	1	13	2	35	39	5	7	3	3	0	10	1	3	9	3	49	51	2	-3	1	4	232	226	3						
10	6	2	15	15	15	3	13	2	37	44	5	8	3	3	0	13	1	4	9	3	60	64	3	-2	1	4	134	137	2						
11	6	2	23	21	15	4	13	2	0	1	1	-8	4	3	44	39	7	5	9	3	12	12	11	-1	1	4	332	346	2						
12	6	2	106	108	1	5	13	2	0	31	1	-7	4	3	0	18	1	6	9	3	0	31	1	0	1	4	11	10	5						
13	6	2	0	4	1	-5	14	2	0	10	1	-6	4	3	20	17	9	-	9	3	0	2	1	1	1	4	34	29	1						
14	6	2	82	83	1	-4	14	2	38	31	6	-5	4	3	157	146	2	-6	10	3	32	31	7	2	1	4	38	40	1						
15	6	2	84	87	3	-3	14	2	34	30	5	-4	4	3	111	106	1	-4	10	3	0	13	1	3	1	4	253	243	3						
16	6	2	220	226	3	-2	14	2	17	11	1	-3	4	3	70	71	1	-3	10	3	80	76	3	4	1	4	121	113	3						
17	6	2	128	127	1	-1	14	2	0	9	1	-2	4	3	42	39	1	-4	10	3	0	21	1	5	1	4	105	98	2						
18	6	2	138	138	2	0	14	2	0	11	1	-1	4	3	53	53	1	-2	10	3	19	16	6	6	1	4	33	30	6						
19	6	2	27	27	15	1	14	2	8	9	8	0	4	3	113	116	1	-1	10	3	52	53	2	7	1	4	0	-	1						
20	6	2	34	36	4	4	14	2	43	43	4	1	4	3	32	33	2	0	10	3	29	29	3	8	1	4	21	25	21						
21	6	2	47	54	5	3	14	2	0	7	1	2	4	3	70	72	1	1	10	3	0	8	1	-8	2	4	26	29	12						
22	6	2	0	0	1	4	14	2	0	13	1	3	4	3	9	6	9	2	10	3	51	51	3	-	2	4	33	29	6						
23	6	2	0	0	1	-4	15	2	29	26	9	4	4	3	101	102	2	3	10	3	40	40	3	-6	2	4	34	30	5						
24	6	2	0	0	3	-3	15	2	0	22	1	5	4	3	64	68	3	4	10	3	16	3	15	-5	2	4	205	191	3						
25	6	2	53	46	3	-2	15	2	0	2	1	6	4	3	41	42	6	5	10	3	25	27	8	-4	2	4	73	71	2						
26	6	2	139	135	2	-1	15	2	0	2	1	7	4	3	0	24	1	6	10	3	0	17	1	-3	2	4	75	74	1						
27	6	2	0	0	1	0	15	2	16	16	15	8	4	3	13	9	13	-6	11	3	12	13	11	-2	2	4	51	43	-1						
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29	6	2	42	46	2	2	15	2	22	24	12	-7	5	3	33	35	-	-4	11	3	43	40	4	0	2	4	81	81	1						
30	6	2	165	175	2	3	15	2	23	29	22	-6	5	3	46	42	4	-3	11	3	25	31	6	1	2	4	95	9	-						
31	6	2	56	58	2	4	15	2	12	3	11	-5	5	3	108	102	2	-2	11	3	37	36	4	2	2	4	130	126	1						
32	6	2	85	83	1	-3	16	2	27	27	11	-4	5	3	10	12	10	-1	11	3	18	22	17	3	2	4	95	97	-						
33	6	2	0	0	1	-2	16	2	17	5	17	-3	5	3	39	35	2	0	11	3	73	73	2	4	2	4	19	9	6						
34	6	2	20	19	6	-1	16	2	15	4	15	-2	5	3	0	0	1	1	11	3	42	46	3	5	2	4	12	13	11						
35	6	2	0	0	1	0	16	2	0	4	1	-1	5	3	28	18	-2	2	11	3	21	25	6	6	2	4	50	51	6						
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37	6	2	37	46	8	2	16	2	22	20	12	1	5	3	259	268	2	4	11	3	50	51	4	8	2	4	10	1	9						
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40	6	2	41	36	5	1	17	2	8	5	-	4	5	3	58	60	2	-6	12	3	24	8	10	-6	3	4	138	134	2						
41	6	2	39	38	3	-8	0	3	11	11	11	5	5	3	112	122	3	-5	12	3	17	13	16	-5	3	4	1	-	-						
42	6	2	147	149	2	-6	0	3	19	18	11	6	5	3	0	8	1	-4	12	3	9	9	8	-4	3	4	23	26	4						
43	6	2	51	52	2	-4	0	3	61	39	3	7	5	3	0	4	1	-3	12	3	0	0	1	-3	3	4	149	147	2						
44	6	2	6	6	1	-2	0	3	449	414	8	-	6	3	20	13	12	-2	12	3	0	23	1	-2	3	4	135	141	1						
45	6	2	28	30	3	0	0	3	165	177	1	-6	6	3	18	14	16	-1	12	3	43	43	3	-1	3	4	26	13	3						
46	6	2	74	75	2	2	0	3	64	63	1	-5	6	3	0	19	1	0	12	3	25	24	5	0	3	4	31	31	1						
47	6	2	18	8	6	4	0	3	97	98	1	-4	6	3	195	188	3	1	12	3	30	31	4	1	3	4	22	5	-3						
48	6	2	59	61	2	6	0	3	81	74	3	-3	6	3	22	21	4	2	12	3	12	12	12	2	3	4	56	56	1						
49	6	2	0	0	1	8	0	3	0	4	1	-2	6	3	48	50	1	3	12	3	16	4	15	2	3	4	67	64	1						
50	6	2	0	23	1	-8	1	3	24	27	14	-1	6	3	131	133	2	4	12	3	19	2	10	4	3	4	141	141	2						
51	6	2	29	27	7	-	1	3	0	19	1	0	6	3	157	164	2	5	12	3	20	26	20	5	3	4	103	102	3						
52	6	2	0	0	21	-6	1	3	0	6	1	1	6	3	45	44	2	-5	13	3	36	20	7	6	3	4	38	37	6						
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54	6	2	28	24	6	-4	1	3	127	124	2	3	6	3	37	37	2	-3	13	3	0	9	1	8	3	4	0	38	1	1					
55	6	2	92	89	2	-3	1	3	243	22																									

Table with 21 columns: h, k, l, 10Fo, 10Fc, 10s (repeated 3 times). Each row contains numerical values for these parameters, representing observed and calculated structure factors.

h	k	l	IOFo	IOFc	IOs	h	k	l	IOFo	IOFc	IOs	h	k	l	IOFo	IOFc	IOs	h	k	l	IOFo	IOFc	IOs	h	k	l	IOFo	IOFc	IOs	
-2	8	6	21	17	7	0	1	7	31	33	2	3	7	7	39	37	4	4	1	8	30	24	4	1	8	8	0	10	1	
-1	8	6	6	4	2	1	1	7	67	75	1	4	7	7	0	13	1	5	1	8	15	13	15	2	8	8	0	22	1	
0	8	6	5	5	2	2	1	7	14	10	7	5	7	7	0	20	1	6	1	8	19	13	15	3	8	8	19	20	13	
1	8	6	40	43	3	3	1	7	77	77	2	6	7	7	0	13	1	-7	2	8	64	71	4	4	8	8	0	21	1	
2	8	6	65	66	2	4	1	7	5	3	5	-6	8	7	30	28	8	-6	2	8	22	23	12	5	8	8	0	1	1	
3	8	6	13	5	13	5	1	7	0	7	1	-5	8	7	0	25	1	-5	2	8	7	3	6	-5	9	8	27	28	8	
4	8	6	29	32	5	6	1	7	0	10	1	-4	8	7	15	14	14	-4	2	8	10	9	10	-4	9	8	37	33	5	
5	8	6	6	7	1	1	1	7	0	11	1	-3	8	7	28	28	2	-3	2	8	35	35	3	-3	9	8	31	33	6	
-6	9	6	36	46	8	-7	2	7	0	11	1	-2	8	7	65	71	5	-2	2	8	47	45	2	-2	9	8	44	42	4	
-5	9	6	13	14	13	-6	2	7	0	25	1	-1	8	7	88	90	2	-1	2	8	42	41	2	-1	9	8	10	4	10	
-4	9	6	31	33	6	-5	2	7	44	48	4	0	8	7	21	25	6	0	2	8	52	58	2	0	9	8	31	26	5	
-3	9	6	0	4	1	-4	2	7	19	23	8	1	8	7	0	3	1	1	2	8	18	18	5	1	9	8	51	49	3	
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-1	9	6	40	45	3	-2	2	7	97	103	1	3	8	7	0	18	1	3	2	8	23	18	5	3	9	8	0	4	1	
0	9	6	19	24	19	-1	2	7	50	52	1	4	8	7	0	20	1	4	2	8	10	10	10	4	9	8	0	21	10	
1	9	6	31	34	4	1	2	7	0	2	1	5	8	7	0	4	1	5	2	8	20	12	10	-5	10	8	35	29	6	
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6	9	6	0	6	1	5	6	7	0	0	9	-2	9	7	53	55	3	-3	3	8	56	61	3	0	10	8	34	29	5	
-6	10	6	18	10	17	-7	7	7	20	20	19	-1	9	7	28	28	5	-2	3	8	95	98	2	1	10	8	40	38	4	
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5	11	6	27	29	9	-1	4	7	50	53	2	-1	11	7	0	0	1	6	4	8	0	1	1	-3	13	8	0	15	1	
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-3	12	6	59	56	4	2	4	7	73	80	2	2	11	7	14	10	14	-4	5	8	33	32	4	-4	13	8	0	0	1	
-2	12	6	7	4	7	3	4	7	21	22	5	3	11	7	18	3	12	-3	5	8	39	41	4	2	13	8	0	4	1	
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2	12	6	19	13	9	-7	4	7	27	29	11	-2	12	7	0	1	1	1	5	8	0	9	1	-6	0	9	18	19	18	
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h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s													
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0	3	9	11	13	11	-4	11	9	0	16	1	-2	6	10	10	12	9	3	3	11	0	7	1	2	3	12	0	4	-1
1	3	9	16	2	7	-3	11	9	39	37	6	-1	6	10	25	28	7	4	3	11	0	3	1	3	3	12	13	8	13
2	3	9	10	12	9	-2	11	9	18	14	18	0	6	10	14	14	13	-5	4	11	12	7	12	4	3	12	13	15	12
3	3	9	0	2	1	-1	11	9	26	20	7	1	6	10	17	15	13	-4	4	11	12	0	12	-4	4	12	21	18	13
4	3	9	0	7	1	0	11	9	30	27	6	2	6	10	14	6	14	-3	4	11	43	41	4	-3	4	12	50	44	4
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6	3	9	0	13	1	2	11	9	0	4	1	-1	4	11	0	7	1	-1	4	11	23	19	7	-1	4	12	17	9	12
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