Title

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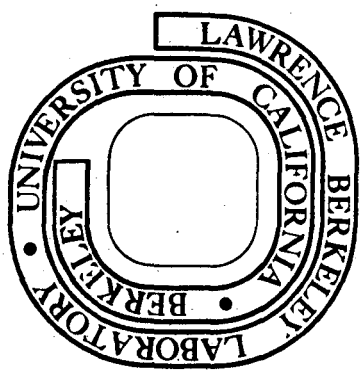

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Structure of 5-Hydroxy-2,3-Norbornane Dicarboxylic Acid γ-Lactone, $C_9H_{10}O_4$*

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May 1973

Abstract

Crystals of this norbornane derivative, $C_9H_{10}O_4$ are monoclinic, space group $P2_1/n$; a = 22.421(8), b = 6.685(2), c = 10.914(4) Å, β = 94.34(5)°, Z = 8, D_x = 1.483 g.cm^{-3}. The two molecules of the asymmetric unit are hydrogen bonded to each other through their carboxyl groups, and form a pseudocentric dimer. The dimensions of two molecules are identical within the statistical accuracy.

*Work done in part under the auspices of the U. S. Atomic Energy Commission.

Introduction

Recently Koshland and coworkers (1971) stressed the importance of orientation factors to chemical reaction velocities with special reference to the catalytic power of enzymes. To explore this hypothesis, they studied the relative velocities of some intramolecular lactonization, using norbornane derivatives which provides a rigid geometrical frame (Storm & Koshland, 1972). This crystallographic study was undertaken for one of these compounds to obtain an accurate description of its molecular geometry. The crystals were kindly supplied to us by Prof. D. E. Koshland and D. Hackney.

A preliminary photographic study of a crystal with dimensions $0.2 \times 0.5 \times 0.7$ mm showed the Laue symmetry 2/m and the diffracting conditions $h + \ell = 2n$ for $(h0\ell)$ and $k = 2n$ for $(0k0)$ reflections, leading to space group $P2_1/n$. Lattice parameters were determined by a least-squares refinement procedure using the setting angles of 12 reflections within the range $40° \leqslant 2\theta \leqslant 44°$, the temperature was $\approx 23°$. The intensities were measured with an automatic PICKER FACS I diffractometer using graphite monochromatized Mo K_α radiation ($\lambda = 0.70926$ Å) and a θ-2θ scan technique. One half of the reciprocal sphere was measured in the range $3° \leqslant 2\theta \leqslant 45°$. A total of 2143 unique reflections were obtained, of which 1667 with $I > \sigma(I)$ were used for the least-squares refinements. Absorption was small, $\mu_{Mo\ K\alpha} = 0.73\ cm^{-1}$, and no correction was necessary. The crystal structure was solved by direct methods using the MULTAN program (Germain, Main & Woolfson, 1971) and refined by our full-matrix least-squares. The final residual values obtained were $R_1 = \Sigma|\Delta F|/\Sigma|F_o| = 0.042$ and $R_2 = [\Sigma w|\Delta F|^2/\Sigma w|F_o|^2]^{1/2} = 0.042$ where $w = 1/\sigma^2(F)$

for all data with $I > \sigma(I)$, otherwise $w = 0$; for all the data $R_1 = 0.065$. The scattering factor used for oxygen and carbon atoms are those tabulated by Doyle and Turner (1968). In the last stage of refinement the polar hydrogen model (Templeton et al., 1972) has been used in connection with the hydrogen scattering factor given by Stewart, Davidson & Simpson (1965). A list of the structure factor is given in Table 4.

Results and Discussion

The final parameters are given in Table 1. The numbering of the atoms is given on the schematic diagram in Fig. 1. The two molecules in the asymetric unit may be related by a non-crystallographic center of symmetry lying approximately at (0.25, 0.30, 0.50). The weak intensities of the reflections (h0ℓ) for which $h \neq 2n$ and $\ell \neq 2n$ are a measure of the departure from a true center of symmetry. This center was also evident by the hypercentric-like distribution of the Wilson plot (Lipson & Woolfson, 1952).

Tables 2 and 3 give the bond distances and angles. The crystal consists of hydrogen bonded dimers where one molecule is related to the other by the non-crystallographic center of symmetry. Due to the strains in the norbornane molecules, the C-C bonds and angles departs significantly from the average values. The short C-C bonds C(2)-C(8), C(3)-C(9), C(11)-C(17), C(12)-C(18) are due to a delocalization of unsaturation from the carbonyl groups. The bond angles (C(1)-C(7)-C(4) [C(10)-C(13)-C(16) for the second molecule] and C(3)-C(4)-C(5) [C(12)-C(13)-C(14)] are characteristic for norbornane derivatives

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* This table has been deposited in the National Lending Library, England. Copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

and agree with the previously known norbornane derivatives (Filippini et al., 1972; Flippen, 1972). Figures 2 and 3 show the molecular conformation and packing. A statistical comparison of the interatomic distances of the two molecules by a probability plot (Hamilton & Abrahams, 1972) yielded a slope of 1.0 which indicates that the two molecules have identical dimensions within the accuracy of the determination.

Acknowledgments

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References

DOYLE, P. A. & TURNER, P. S. (1968). Acta Cryst. A24, 390-397.

FILIPPINI, G., GRAMACCIOLI, C. M., ROVERE, C., & SIMONETTA, M. (1972) Acta Cryst. B26, 2869-2874.

FLIPPEN, J. L. (1972). Acta Cryst. B28, 2046-2048.

GERMAIN, G., MAIN, P., & WOOLFSON, M. M.,(1971). Acta Cryst. A27, 368-376.

HAMILTON, W. C. & ABRAHAMS, S. C. (1972). Acta Cryst. A28, 215-218.

KOSHLAND, D. E., JR, CARRAWAY, K. W., DAFFORN, G. A., GASS, J. D., & STORM, D. R. Cold Spring Harbor Symposia on Quantitative Biology, Volume XXXVI, 1971.

LIPSON, H. & WOOLFSON, M. M. (1952). Acta Cryst. 5, 680-682.

STEWART, R. F., DAVIDSON, E. R., & SIMPSON, W. T. (1965). J. Phys. Chem. 42, 3175-3187. Table II.

STORM, D. R. & KOSHLAND, D. E. (1972). J.A.C.S. 94, 5805-5814.

TEMPLETON, D. H., OLSON, A. J., ZALKIN, A., & TEMPLETON, L. K. (1972) Acta Cryst. A28, Part S4, S252.

Table Caption

Atomic parameters. Estimated standard deviations of the least significant digits are indicated in parentheses. The thermal parameters are in units of $Å^2$. The temperature factor is exp(-T), where

$T = -1/4 \sum h_i h_j B_{ij} a_i^* a_j^*$ for the anisotropic case and

$T = -B\sin^2\theta/\lambda^2$ for the isotropic case.

Table 1

ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23
C(1)	.3341(1)	.2473(4)	.1160(2)	2.6(1)	3.4(1)	3.6(1)	-.4(1)	.6(1)	.3(1)
C(2)	.3444(1)	.4689(4)	.1521(2)	2.7(1)	3.7(1)	2.1(1)	.4(1)	.64(9)	.1(1)
C(3)	.4130(1)	.4954(4)	.1365(2)	2.6(1)	3.0(1)	2.2(1)	-.04(9)	.03(9)	-.17(9)
C(4)	.4335(1)	.2774(4)	.1255(2)	2.2(1)	3.6(1)	2.8(1)	.5(1)	-.12(9)	.29(9)
C(5)	.4164(1)	.2503(4)	-.0114(2)	3.3(1)	2.8(1)	2.8(1)	.5(1)	.5(1)	-.0(1)
C(6)	.3491(1)	.2076(5)	-.0160(2)	3.3(1)	3.4(1)	3.5(1)	-.3(1)	-.3(1)	-.4(1)
C(7)	.3880(1)	.1516(5)	.1871(3)	4.1(2)	3.5(2)	2.9(1)	.3(1)	.5(1)	.5(1)
C(8)	.3041(1)	.6165(4)	.0848(2)	2.2(1)	3.3(1)	3.0(1)	.08(9)	.5(1)	-.2(1)
C(9)	.4256(1)	.5873(4)	.0162(2)	2.0(1)	3.1(1)	3.2(1)	.6(1)	.35(9)	.2(1)
C(10)	.1628(1)	.3509(4)	.8748(2)	2.9(1)	3.8(2)	3.6(1)	-.2(1)	.8(1)	.3(1)
C(11)	.1511(1)	.1274(4)	.8453(2)	2.9(1)	3.9(1)	2.0(1)	.3(1)	.47(9)	-.2(1)
C(12)	.0836(1)	.1046(4)	.8694(2)	2.2(1)	3.4(1)	2.7(1)	-.1(1)	-.47(9)	-.4(1)
C(13)	.0637(1)	.3230(4)	.8791(2)	2.5(1)	3.5(1)	2.7(1)	.7(1)	-.10(9)	.1(1)
C(14)	.0854(1)	.3583(4)	1.0130(2)	3.4(1)	3.2(1)	2.7(1)	.6(1)	.46(9)	-.0(1)
C(15)	.1521(1)	.3997(5)	1.0081(2)	3.4(2)	3.1(1)	3.8(1)	-.2(1)	-.4(1)	-.4(1)
C(16)	.1071(1)	.4424(5)	.8079(3)	4.5(2)	3.3(2)	3.4(1)	.5(1)	.5(1)	.5(1)
C(17)	.1935(1)	-.0154(4)	.9124(2)	2.2(1)	3.5(1)	3.0(1)	-.0(1)	.6(1)	-.5(1)
C(18)	.0743(1)	.0205(5)	.9941(2)	2.0(1)	3.6(1)	3.8(1)	-.1(1)	.08(9)	.6(1)
O(1)	.27270(9)	.7245(3)	.1568(2)	4.4(1)	5.5(1)	3.27(9)	2.19(9)	.71(8)	-.30(8)
O(2)	.29959(8)	.6370(3)	-.0263(2)	4.1(1)	5.7(1)	2.91(9)	2.29(8)	.64(7)	.39(7)
O(3)	.42876(7)	.4420(3)	-.0690(1)	3.52(9)	3.40(9)	2.56(7)	.25(7)	.75(6)	.36(7)
O(4)	.43294(9)	.7602(3)	-.0088(2)	3.9(1)	3.2(1)	5.6(1)	.19(8)	.95(7)	.91(8)
O(5)	.22501(9)	.8777(3)	.8408(2)	4.7(1)	5.4(1)	3.27(9)	2.36(9)	.78(8)	-.23(8)
O(6)	.19862(8)	-.0322(3)	1.0233(2)	4.2(1)	5.4(1)	3.03(9)	2.27(8)	.27(7)	-.15(7)
O(7)	.07498(8)	.1702(3)	1.0762(1)	3.46(9)	4.7(1)	2.70(8)	.24(8)	.72(6)	.43(8)
O(8)	.06579(9)	-.1500(3)	1.0223(2)	4.1(1)	4.0(1)	6.5(1)	-.48(9)	.45(8)	1.85(9)
H(1)	.291(1)	.194(3)	.142(2)	3.1(5)					
H(2)	.338(1)	.479(3)	.246(2)	2.4(5)					
H(3)	.433(1)	.581(3)	.209(2)	2.5(5)					
H(4)	.477(1)	.250(3)	.150(2)	2.6(6)					
H(5)	.441(1)	.144(3)	-.057(2)	2.1(5)					
H(6)	.342(1)	.053(4)	-.037(2)	3.4(6)					
H(7)	.325(1)	.296(4)	-.085(2)	4.3(6)					
H(8)	.392(1)	-.002(4)	.169(2)	4.1(7)					
H(9)	.388(1)	.178(3)	.281(2)	2.7(5)					
H(10)	.243(2)	.814(5)	.100(3)	6.2(8)					
H(11)	.205(1)	.398(4)	.845(2)	4.0(6)					
H(12)	.1555(9)	.105(3)	.754(2)	2.0(5)					
H(13)	.062(1)	.017(3)	.801(2)	2.2(5)					
H(14)	.018(1)	.342(3)	.858(2)	3.1(6)					
H(15)	.062(1)	.470(4)	1.060(2)	3.0(5)					
H(16)	.180(1)	.318(4)	1.078(2)	3.3(5)					
H(17)	.158(1)	.554(5)	1.024(2)	4.6(7)					
H(18)	.103(1)	.406(4)	.710(2)	3.7(6)					
H(19)	.105(1)	.600(4)	.825(2)	2.8(6)					
H(20)	.252(1)	.784(4)	.897(3)	5.9(8)					

Table 2. Bond Length (in Å).

ATOMS	MOLECULE 1	ATOMS	MOLECULE 2
C(1) - C(2)	1.546(4)	C(10) - C(11)	1.547(3)
C(1) - C(6)	1.528(3)	C(10) - C(15)	1.528(3)
C(1) - C(7)	1.528(4)	C(10) - C(16)	1.528(4)
C(2) - C(3)	1.569(3)	C(11) - C(12)	1.564(3)
C(2) - C(8)	1.493(3)	C(11) - C(17)	1.498(3)
C(3) - C(4)	1.537(3)	C(12) - C(13)	1.533(3)
C(3) - C(9)	1.496(3)	C(12) - C(18)	1.501(3)
C(4) - C(5)	1.525(3)	C(13) - C(14)	1.524(3)
C(4) - C(7)	1.519(4)	C(13) - C(16)	1.518(4)
C(5) - C(6)	1.533(4)	C(14) - C(15)	1.525(4)
O(1) - C(8)	1.311(3)	O(5) - C(17)	1.305(3)
O(2) - C(8)	1.217(2)	O(6) - C(17)	1.213(3)
O(3) - C(5)	1.463(3)	O(7) - C(14)	1.462(3)
O(3) - C(9)	1.350(3)	O(7) - C(18)	1.342(3)
O(4) - C(9)	1.202(3)	O(8) - C(18)	1.200(3)
C(1) - H(1)	1.09(2)	C(10) - H(11)	1.06(3)
C(2) - H(2)	1.05(2)	C(11) - H(12)	1.02(2)
C(3) - H(3)	1.05(2)	C(12) - H(13)	1.03(2)
C(4) - H(4)	1.01(2)	C(13) - H(14)	1.03(2)
C(5) - H(5)	1.05(2)	C(14) - H(15)	1.06(2)
C(6) - H(6)	1.07(3)	C(15) - H(16)	1.10(2)
C(6) - H(7)	1.07(2)	C(15) - H(17)	1.05(3)
C(7) - H(8)	1.05(3)	C(16) - H(18)	1.09(2)
C(7) - H(9)	1.04(2)	C(16) - H(19)	1.07(2)
O(1) - H(10)	1.06(3)	O(5) - H(20)	1.04(3)
O(1)...O(6)	2.676(3)		
O(2)...O(5)	2.669(3)		
O(2)...H(20)	1.63(3)		
O(6)...H(10)	1.62(3)		

Table 3. Bond Angles (In Degrees).

Molecule 1		Molecule 2	
C(2) - C(1) - C(6)	111.6(2)	C(11) - C(10) - C(15)	111.6(2)
C(2) - C(1) - C(7)	100.0(2)	C(11) - C(10) - C(16)	99.6(2)
C(6) - C(1) - C(7)	100.6(2)	C(15) - C(10) - C(16)	100.8(2)
C(1) - C(2) - C(3)	102.1(2)	C(10) - C(11) - C(12)	102.2(2)
C(1) - C(2) - C(8)	115.7(2)	C(10) - C(11) - C(17)	115.0(2)
C(3) - C(2) - C(8)	115.7(2)	C(12) - C(11) - C(17)	116.3(2)
C(2) - C(3) - C(4)	101.8(2)	C(11) - C(12) - C(13)	102.1(2)
C(2) - C(3) - C(9)	113.2(2)	C(11) - C(12) - C(18)	113.0(2)
C(4) - C(3) - C(9)	104.1(2)	C(13) - C(12) - C(18)	103.5(2)
C(3) - C(4) - C(5)	97.7(2)	C(12) - C(13) - C(14)	98.1(2)
C(3) - C(4) - C(7)	105.9(2)	C(12) - C(13) - C(16)	105.3(2)
C(5) - C(4) - C(7)	103.9(2)	C(14) - C(13) - C(16)	103.8(2)
C(4) - C(5) - C(6)	103.2(2)	C(13) - C(14) - C(15)	103.8(2)
C(4) - C(5) - O(3)	106.0(2)	C(13) - C(14) - O(7)	105.5(2)
C(6) - C(5) - O(3)	111.5(2)	C(15) - C(14) - O(7)	111.4(2)
C(1) - C(6) - C(5)	102.9(2)	C(10) - C(15) - C(14)	102.7(2)
C(1) - C(7) - C(4)	94.3(2)	C(10) - C(16) - C(13)	94.5(2)
C(2) - C(8) - O(1)	113.6(2)	C(11) - C(17) - O(5)	114.1(2)
C(2) - C(8) - O(2)	124.5(2)	C(11) - C(17) - O(6)	123.7(2)
O(1) - C(8) - O(2)	121.9(2)	O(5) - C(17) - O(6)	122.2(2)
C(3) - C(9) - O(3)	109.4(2)	C(12) - C(18) - O(7)	109.3(2)
C(3) - C(9) - O(4)	129.2(2)	C(12) - C(18) - O(8)	128.6(2)
O(3) - C(9) - O(4)	121.4(2)	O(7) - C(18) - O(8)	122.1(2)

Table 4

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X10.0) FOR THE NORBORNANE-LACTONE COMPOUND F(0,0,0) = 7680

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
H,L=		0,	0	2	179	6	0	2	88	4	-0	H,L=		1,	1	5	0	53	-17*
2	188	5	-3	3	73	7	-3	3	180	6	-3	0	0109		-11*	H,L=		1,	8
4	56	4	4	4	78	10	-3	4	99	6	-5	1	291	8	2	1	81	4	3
6	10	27	9*	5	105	5	-1	5	12	26	1*	2	636	16	-20	2	176	6	-11
H,L=		0,	1	H,L=		0,	8	6	61	8	-12	3	172	5	1	3	33	13	-3
1	195	8	-22	0	420	11	17	H,L=		1,	-5	4	743	19	13	4	125	5	3
2	505	14	-21	1	83	4	-4	0	50	6	-5	5	43	8	4	5	11	28	4*
3	45	5	-5	2	188	5	3	1	652	17	18	6	240	7	1	H,L=		1,	9
4	120	5	2	3	150	5	4	2	508	13	-6	7	0	28	-9*	0	16	24	-21*
5	221	6	2	4	103	9	-1	3	60	5	1	H,L=		1,	2	1	0	25	-8*
6	33	39	18*	5	56	12	5	4	334	9	1	1	915	23	-54	2	58	6	16
7	42	7	-6	H,L=		0,	9	5	30	16	-6	2	32	5	8	3	110	10	5
H,L=		0,	2	1	25	27	1*	6	51	7	5	3	128	4	-2	4	253	8	6
0	2060	52	-7	2	352	10	3	H,L=		1,	-4	4	250	7	-6	H,L=		1,	10
1	148	6	-10	3	201	6	-9	1	96	6	2	5	13	25	-9*	1	154	6	-1
2	163	5	3	4	48	7	1	2	110	4	-2	6	102	7	-5	2	0	33	-19*
3	333	9	10	H,L=		0,	10	3	93	4	-5	7	21	28	-13*	3	62	11	-6
4	49	8	1	0	64	5	0	4	194	7	2	H,L=		1,	3	H,L=		1,	11
5	27	9	-5	1	51	13	2	5	47	12	40	0	92	5	-0	0	0	41	-29*
6	47	12	6	2	49	16	-9	6	97	9	-0	1	115	3	7	1	96	5	7
7	35	20	15	3	32	18	-8	H,L=		1,	-3	2	401	10	-10	2	22	28	4*
H,L=		0,	3	H,L=		0,	11	0	0	26	-6*	3	34	9	4	H,L=		2,	-11
1	119	4	5	1	54	7	3	1	144	5	2	4	16	21	4*	1	58	7	6
2	132	6	-10	2	123	4	8	2	217	7	-1	5	68	18	18	2	150	5	5
3	338	9	-5	H,L=		1,	-11	3	426	11	0	6	229	6	0	H,L=		2,	-10
4	23	9	3	0	32	34	11*	4	74	7	4	H,L=		1,	4	0	131	5	3
5	466	13	-5	1	85	9	-6	5	0	25	-14*	1	342	9	11	1	68	8	-1
6	33	8	7	2	156	7	0	6	125	5	1	2	33	6	7	2	74	6	-4
H,L=		0,	4	H,L=		1,	-10	H,L=		1,	-2	3	118	4	3	3	105	9	-3
0	107	8	8	1	56	10	4	1	142	6	-0	4	295	8	-0	H,L=		2,	-9
1	39	4	0	2	0	28	-15*	2	57	3	-4	5	34	11	14	1	115	4	0
2	96	6	-3	3	51	7	28	3	69	4	5	6	23	39	15*	2	139	5	-2
3	258	7	0	H,L=		1,	-9	4	212	6	4	H,L=		1,	5	3	134	5	-6
4	0	22	-7*	0	39	8	0	5	27	20	20	0	43	5	-5	4	63	11	9
5	33	10	9	1	267	8	-13	6	112	5	2	1	234	6	1	H,L=		2,	-8
6	77	5	5	2	342	9	-0	7	24	28	23*	2	226	7	-3	0	91	4	-11
H,L=		0,	5	3	35	13	3	H,L=		1,	-1	3	188	5	-2	1	96	4	0
1	104	3	0	4	124	5	2	0	0101		-20*	4	329	9	-1	2	153	5	-2
2	174	5	-4	H,L=		1,	-8	1	784	20	-53	5	0	33	-28*	3	331	9	-12
3	40	10	5	1	21	29	5*	2	72	4	-9	6	0	36	-10*	4	63	7	13
4	201	6	2	2	41	8	8	3	64	4	2	H,L=		1,	6	5	192	7	-2
5	163	5	-3	3	221	6	3	4	157	6	0	1	346	9	8	H,L=		2,	-7
6	51	6	-2	4	77	7	1	5	26	12	12	2	254	7	-4	1	0	21	-8*
H,L=		0,	6	5	28	24	24	6	243	7	-4	3	56	5	-4	2	221	6	3
0	917	24	4	H,L=		1,	-7	7	16	30	-2*	4	0	31	-20*	3	317	9	-1
1	61	4	3	0	48	6	-1	H,L=		1,	0	5	43	9	32	4	0	38	-5*
2	114	4	4	1	96	4	4	1	932	24	-38	6	0	30	-30*	5	31	32	14*
3	48	5	5	2	313	8	-2	2	44	7	-9	H,L=		1,	7	H,L=		2,	-6
4	32	16	20	3	126	9	2	3	276	7	-2	0	0	30	-1*	0	723	19	28
5	280	8	4	4	220	6	-7	4	259	8	-5	1	88	4	-0	1	76	4	2
6	48	10	15	5	43	10	1	5	0	24	-4*	2	56	5	2	2	126	4	-2
H,L=		0,	7	H,L=		1,	-6	6	81	6	-6	3	34	10	3	3	170	5	-4
1	21	22	13*	1	269	7	6	7	19	35	-11*	4	250	8	-4	4	101	4	-6

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

K	FOB	SG	DEL
5	91	7	10
6	24	42	9*
H,L=	2,	-5	
1	77	4	7
2	760	20	4
3	186	5	3
4	42	6	7
5	31	35	21*
6	9	29	-15*
H,L=	2,	-4	
0	1619	41	-9
1	20	31	1*
2	180	5	-5
3	28	7	15
4	54	6	4
5	215	6	-2
6	0	31	-21*
H,L=	2,	-3	
1	156	5	-5
2	446	11	-0
3	564	15	-0
4	57	5	-7
5	74	11	-6
6	40	9	29
H,L=	2,	-2	
0	943	24	-50
1	73	12	-10
2	432	11	1
3	414	11	-7
4	0	25	-1*
5	153	7	8
6	77	5	9
7	0	35	-25*
H,L=	2,	-1	
1	36	43	-3*
2	512	13	-25
3	267	7	-2
4	61	7	2
5	70	4	-3
6	81	8	1
7	0	29	-13*
H,L=	2,	0	
0	104	35	10
1	339	9	-15
2	141	4	6
3	455	12	6
4	84	4	3
5	246	7	1
6	40	18	33
7	90	9	7
H,L=	2,	1	
1	364	9	-14
2	791	20	-32
3	510	13	-7
4	169	5	5
5	171	5	-5
6	147	5	-3
7	77	12	1
H,L=	2,	2	
0	1782	45	-8
1	256	7	-11
2	244	6	10
3	200	5	1
4	66	4	1
5	160	6	-4
6	0	43	-12*
7	58	9	-2
H,L=	2,	3	
1	141	4	-1
2	412	10	-6
3	70	4	4
4	41	7	-11
5	103	4	-4
6	110	5	-4
H,L=	2,	4	
0	852	22	30
1	116	4	-1
2	252	7	-2
3	101	5	-2
4	115	6	4
5	123	6	-1
6	85	6	7
H,L=	2,	5	
1	138	4	-2
2	156	4	1
3	239	7	2
4	31	11	19
5	249	7	4
6	0	32	-30*
H,L=	2,	6	
0	969	25	21
1	72	7	8
2	143	7	-4
3	108	4	-4
4	45	10	-6
5	90	5	0
6	0	46	-21*
H,L=	2,	7	
1	33	35	27*
2	104	9	-2
3	65	7	-6
4	182	8	8
5	34	13	16
H,L=	2,	8	
0	39	10	13
1	0	23	-4*
2	18	27	4*
3	73	8	-11
4	25	29	6*
5	30	18	18
H,L=	2,	9	
1	39	9	0
2	155	5	5
3	74	11	-8
4	47	13	-5
H,L=	2,	10	
0	100	8	-8
1	98	6	3
2	61	15	-0
3	113	5	-5
H,L=	2,	11	
1	31	33	-13*
2	54	18	-0
H,L=	3,-11		
0	0	28	-0*
1	0	48	-13*
2	79	6	8
H,L=	3,-10		
1	195	7	-1
2	41	20	11
3	0	39	-24*
H,L=	3,	-9	
0	31	11	1
1	69	17	-7
2	93	5	10
3	158	6	-3
4	81	6	3
H,L=	3,	-8	
1	233	7	1
2	0	25	-13*
3	103	6	-7
4	195	6	-16
5	36	38	9*
H,L=	3,	-7	
0	0	22	-21*
1	130	4	7
2	37	28	10
3	222	7	-4
4	139	5	-1
5	42	29	41
H,L=	3,	-6	
1	77	4	1
2	78	4	-1
3	54	5	6
4	179	5	-10
5	30	25	15
6	34	13	16
H,L=	3,	-5	
0	28	24	-3
1	165	5	0
2	302	8	6
3	77	6	2
4	196	6	-9
5	35	38	21*
6	134	5	-7
H,L=	3,	-4	
1	231	6	-6
2	208	6	-2
3	25	11	4
4	31	25	14
5	13	24	-3*
6	146	5	-4
H,L=	3,	-3	
0	19	40	-16*
1	661	17	-2
2	234	6	3
3	60	4	2
4	264	7	4
5	0	29	-9*
6	136	9	-7
H,L=	3,	-2	
1	260	7	-3
2	401	10	-6
3	443	11	-4
4	263	7	8
5	0	33	-16*
6	182	6	-6
7	25	31	-24*
H,L=	3,	-1	
0	10	43	-18*
1	878	22	-25
2	472	12	-7
3	126	4	2
4	3	28	-29*
5	30	10	11
6	140	8	2
7	22	38	-12*
H,L=	3,	0	
1	378	10	-13
2	90	4	3
3	213	6	-4
4	105	4	-5
5	15	24	-10*
6	80	5	-5
7	92	6	15
H,L=	3,	1	
0	18	36	4*
1	1217	31	-50
2	488	12	-14
3	459	12	1
4	28	10	-4
5	37	9	4
6	89	7	9
7	78	6	2
H,L=	3,	2	
1	280	8	-11
2	358	9	4
3	207	6	-1
4	0	22	-0*
5	37	8	6
6	100	5	5
7	48	16	19
H,L=	3,	3	
0	82	3	-2
1	668	17	-4
2	166	5	2
3	28	8	6
4	246	7	3
5	38	12	5
6	42	11	39
H,L=	3,	4	
1	194	5	5
2	254	7	-6
3	63	9	-7
4	126	4	-0
5	48	7	0
6	183	6	4
H,L=	3,	5	
0	110	4	2
1	246	7	3
2	207	6	2
3	16	26	5*
4	214	8	1
5	35	13	20
6	96	6	3
H,L=	3,	6	
1	68	7	-14
2	23	15	10
3	40	7	-8
4	257	8	-7
5	39	9	26
6	43	16	-2
H,L=	3,	7	
0	89	4	1
1	86	6	6
2	0	27	-8*
3	82	5	-0
4	481	13	4
5	9	28	-19*
H,L=	3,	8	
1	203	6	-4
2	133	5	2
3	25	35	8*
4	286	8	3
5	25	35	19*
H,L=	3,	9	
0	34	15	-4
1	26	17	8
2	208	8	3
3	53	8	-2
4	64	6	16
H,L=	3,	10	
1	365	10	-13
2	115	6	1
3	54	11	-2
H,L=	3,	11	
0	0	29	-17*
1	14	35	-19*
2	57	8	5
H,L=	4,-11		
1	25	30	6*
2	84	12	-3
H,L=	4,-10		
0	448	12	-16
1	0	26	-3*

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
2	27	35	-3*	6	58	13	5	H,L=	4,	6		3	32	12	26	H,L=	5,	1	
3	14	50	2*	7	61	8	1	0	157	6	2	4	0	26	-5*	0	45	18	2
H,L=	4,	-9		H,L=	4,	-1		1	0	23	-25*	5	0	40	-5*	1	201	6	4
1	33	10	13	1	398	10	-19	2	14	21	11*	H,L=	5,	-6		2	585	15	15
2	188	6	3	2	406	10	-11	3	124	4	-0	1	216	6	-1	3	156	9	-1
3	171	5	3	3	75	3	-0	4	15	25	14*	2	170	6	-10	4	384	10	13
4	25	26	1*	4	82	5	-3	5	234	7	-7	3	275	8	7	5	0	28	-1*
H,L=	4,	-8		5	27	32	12*	6	30	31	6*	4	319	9	2	6	76	6	-19
0	284	8	-5	6	139	7	2	H,L=	4,	7		5	27	18	20	7	87	6	-3
1	28	11	16	7	50	9	11	1	87	6	-1	6	93	8	7	H,L=	5,	2	
2	152	6	3	H,L=	4,	0		2	64	7	12	H,L=	5,	-5		1	178	5	1
3	55	6	4	01400		36	-7	3	154	6	-2	0	113	4	3	2	225	6	4
4	14	33	-21*	1	65	11	-4	4	91	5	6	1	50	5	-2	3	13	17	0*
5	111	8	0	2	199	5	-4	5	191	6	8	2	194	6	3	4	251	7	-6
H,L=	4,	-7		3	29	7	2	H,L=	4,	8		3	41	8	2	5	28	12	26
1	92	4	-4	4	37	11	-1	0	43	7	11	4	127	5	-2	6	183	6	-0
2	130	4	-10	5	190	6	-5	1	123	6	-2	5	18	48	-3*	H,L=	5,	3	
3	153	5	2	6	28	38	28*	2	201	8	3	6	56	7	1	0	51	4	2
4	32	19	-8	7	89	8	7	3	110	5	-4	H,L=	5,	-4		1	197	6	1
5	221	7	3	H,L=	4,	1		4	0	43	-4*	1	520	13	21	2	69	4	-5
H,L=	4,	-6		1	198	6	-1	5	32	15	25	2	111	6	1	3	84	5	3
0	220	6	6	2	638	16	-1	H,L=	4,	9		3	212	8	5	4	355	9	6
1	62	8	0	3	385	10	12	1	14	25	13*	4	22	26	-11*	5	13	25	-3*
2	233	7	-3	4	106	4	4	2	109	5	-4	5	35	42	-3*	6	305	8	-9
3	304	9	-4	5	144	6	-2	3	33	13	12	6	101	8	-9	H,L=	5,	4	
4	33	40	1*	6	96	5	-3	4	22	35	9*	H,L=	5,	-3		1	83	6	-9
5	29	15	5	7	38	11	32	H,L=	4,	10		0	64	4	-1	2	51	3	-1
6	23	27	16*	H,L=	4,	2		0	219	6	-5	1	164	5	-3	3	87	3	-2
H,L=	4,	-5		0	856	22	11	1	125	5	0	2	217	8	4	4	274	7	-3
1	18	16	14	1	71	6	-1	2	199	7	0	3	208	6	2	5	27	29	25*
2	55	6	6	2	375	10	14	3	51	9	22	4	263	7	-2	6	34	34	-9*
3	119	4	5	3	81	4	2	H,L=	4,	11		5	28	15	2	H,L=	5,	5	
4	20	28	1*	4	43	6	7	1	9	42	-14*	6	142	8	3	0	44	5	-2
5	180	5	3	5	71	7	6	H,L=	5,	-11		H,L=	5,	-2		1	751	19	0
6	74	5	7	6	82	14	5	0	9	34	4*	1	76	12	4	2	274	7	7
H,L=	4,	-4		H,L=	4,	3		1	53	8	9	2	198	5	4	3	220	7	-0
0	112	3	4	1	59	3	-1	2	64	7	-1	3	100	6	2	4	66	18	3
1	45	4	2	2	71	3	3	H,L=	5,	-10		4	15	27	6*	5	0	30	-4*
2	309	8	2	3	69	7	-3	1	0	27	-1*	5	35	9	7	6	121	6	-8
3	106	4	-2	4	125	4	-0	2	46	9	-8	6	14	33	-8*	H,L=	5,	6	
4	3	32	-5*	5	255	8	-4	3	0	28	-15*	H,L=	5,	-1		1	27	11	2
5	112	5	-3	6	121	6	-3	H,L=	5,	-9		0	16	19	-1*	2	9	18	4*
6	81	6	6	H,L=	4,	4		0	43	12	-2	1	948	24	-0	3	89	4	0
H,L=	4,	-3		0	540	14	-5	1	76	5	-9	2	103	3	-3	4	128	5	2
1	107	4	-2	1	35	9	-7	2	95	13	6	3	43	8	-9	5	29	31	22*
2	127	4	4	2	163	5	5	3	113	5	-7	4	373	10	4	H,L=	5,	7	
3	405	11	10	3	139	4	-3	4	41	13	-15	5	33	34	3*	0	0	25	-4*
4	103	7	6	4	17	27	5*	H,L=	5,	-8		6	57	7	8	1	313	8	5
5	93	4	-1	5	176	6	4	1	128	4	-4	7	124	5	7	2	64	5	4
6	135	5	4	6	51	9	1	2	199	6	-0	H,L=	5,	0		3	192	7	1
H,L=	4,	-2		H,L=	4,	5		3	0	26	-16*	1	425	13	-2	4	61	7	0
0	358	9	12	1	156	5	-1	4	251	7	7	2	247	6	-0	5	38	11	15
1	140	5	-7	2	471	12	2	5	33	40	24*	3	145	4	-0	H,L=	5,	8	
2	255	7	-0	3	230	6	-4	H,L=	5,	-7		4	224	6	-4	1	101	4	-1
3	527	14	9	4	65	5	5	0	116	4	-2	5	25	32	4*	2	223	7	-7
4	105	5	0	5	41	44	6*	1	293	8	-3	6	7	27	3*	3	56	6	-0
5	195	6	5	6	66	9	7	2	129	5	-4	7	60	8	4	4	134	5	-3

OBSERVED STRUCTURES FACTORS (CONT) FOR
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K	FOB	SG	DEL
H,L=	5,	9	
0	70	5	-7
1	28	29	-12*
2	16	46	1*
3	83	6	-5
4	116	5	-7
H,L=	5,	10	
1	149	5	2
2	144	6	10
3	14	28	-21*
H,L=	5,	11	
0	12	28	1*
1	93	9	10
H,L=	6,	-11	
1	52	14	7
2	45	12	-7
H,L=	6,	-10	
0	0	27	-27*
1	0	28	-22*
2	70	6	10
3	0	30	-8*
H,L=	6,	-9	
1	44	7	6
2	19	31	4*
3	80	6	-7
4	23	27	-8*
H,L=	6,	-8	
0	117	5	-6
1	45	12	1
2	200	7	2
3	34	11	-2
4	98	8	2
5	84	6	1
H,L=	6,	-7	
1	103	4	-3
2	26	26	-3*
3	86	6	-8
4	59	7	-5
5	76	9	-7
H,L=	6,	-6	
0	206	6	-7
1	58	4	-1
2	53	8	-6
3	273	7	11
4	114	7	-0
5	133	5	9
6	69	9	14
H,L=	6,	-5	
1	28	9	4
2	37	6	2
3	105	4	-4
4	36	10	-11
5	150	5	-3
6	48	9	-3
H,L=	6,	-4	
0	11	16	-3*
1	134	4	-1
2	21	28	-16*
3	243	12	12
4	54	6	3
5	43	7	16
6	0	45	-7*
H,L=	6,	-3	
1	53	4	2
2	32	5	1
3	125	4	1
4	56	3	3
5	183	5	1
6	73	7	-16
H,L=	6,	-2	
0	689	23	-2
1	221	6	-10
2	443	11	11
3	62	3	-2
4	120	5	-2
5	234	8	0
6	46	52	17*
H,L=	6,	-1	
1	145	6	-1
2	112	4	1
3	8	19	-3*
4	31	10	18
5	68	6	-6
6	152	5	11
H,L=	6,	0	
01388		41	4
1	369	10	-5
2	168	5	-6
3	316	8	6
4	48	7	3
5	65	5	-4
6	30	35	8*
H,L=	6,	1	
1	69	3	2
2	716	18	9
3	547	15	2
4	44	10	-2
5	37	7	11
6	34	14	-0
H,L=	6,	2	
0	312	11	1
1	150	4	2
2	163	6	8
3	38	13	-5
4	21	25	19*
5	193	6	-4
6	19	28	2*
H,L=	6,	3	
1	28	8	2
2	30	7	-10
3	134	5	3
4	55	6	6
5	99	6	-6
6	58	7	7
H,L=	6,	4	
0	310	10	19
1	83	4	-2
2	208	6	-1
3	86	3	4
4	60	5	4
5	28	16	12
6	47	38	8
H,L=	6,	5	
1	102	4	2
2	47	9	-3
3	243	7	9
4	35	16	-4
5	46	10	-5
6	0	29	-17*
H,L=	6,	6	
0	630	20	4
1	22	24	10*
2	120	4	0
3	34	10	-5
4	71	6	-3
5	91	9	15
H,L=	6,	7	
1	103	4	2
2	295	8	2
3	236	7	0
4	68	6	5
5	61	7	-3
H,L=	6,	8	
0	154	5	4
1	18	26	-7*
2	100	5	-1
3	0	46	-15*
4	62	18	4
H,L=	6,	9	
1	69	6	-1
2	87	5	5
3	145	5	2
4	40	12	1
H,L=	6,	10	
0	37	14	-34
1	121	7	6
2	50	10	-1
3	18	30	-22*
H,L=	6,	11	
1	52	9	-4
H,L=	7,	-11	
0	13	35	-18*
1	288	8	6
2	28	23	2
H,L=	7,	-10	
1	98	6	-5
2	65	7	-3
3	79	6	1
H,L=	7,	-9	
0	46	10	11
1	155	5	3
2	0	30	-2*
3	78	6	1
4	40	10	5
H,L=	7,	-8	
1	136	4	3
2	46	7	11
3	84	5	1
4	22	26	1*
5	33	41	31*
H,L=	7,	-7	
0	52	5	2
1	145	4	-5
2	72	5	4
3	14	25	-23*
4	129	9	0
5	0	44	-12*
H,L=	7,	-6	
1	144	4	4
2	103	6	-0
3	64	10	2
4	17	26	12*
5	10	48	-2*
H,L=	7,	-5	
0	86	4	-1
1	428	14	2
2	260	7	-9
3	96	6	-1
4	23	18	7
5	26	38	-7*
6	80	6	4
H,L=	7,	-4	
1	116	4	-0
2	66	4	-2
3	61	4	-0
4	262	7	4
5	0	25	-5*
6	58	8	2
H,L=	7,	-3	
0	0	19	-3*
1	361	10	9
2	133	5	-3
3	214	6	4
4	143	4	-0
5	40	8	12
6	273	9	-3
H,L=	7,	-2	
1	945	27	4
2	98	5	1
3	130	5	-5
4	431	11	5
5	22	25	-2*
6	89	6	4
H,L=	7,	-1	
0	23	7	7
1	379	12	14
2	75	6	-3
3	55	3	-1
4	60	5	1
5	0	25	-23*
6	425	11	4
H,L=	7,	0	
11432		40	47
2	120	5	10
3	173	5	-1
4	71	3	-3
5	13	23	12*
6	81	9	8
H,L=	7,	1	
0	57	3	-0
1	353	9	13
2	359	10	7
3	320	8	-3
4	33	6	13
5	18	35	-3*
6	145	5	5
H,L=	7,	2	
1	814	23	25
2	10	21	-3*
3	113	4	-5
4	65	4	6
5	23	24	12*
6	32	37	-1*
H,L=	7,	3	
0	88	4	-2
1	499	14	4
2	96	6	5
3	25	15	-9
4	85	4	4
5	11	33	-29*
6	105	6	-9
H,L=	7,	4	
1	311	8	12
2	289	7	9
3	56	6	3
4	7	46	-23*
5	38	9	14
6	46	9	15
H,L=	7,	5	
0	14	19	-11*
1	115	3	1
2	224	6	-4
3	51	9	15
4	27	13	17
5	44	9	-1
6	152	6	-6
H,L=	7,	6	
1	26	17	23
2	58	6	10
3	41	18	8
4	10	26	-11*
5	0	36	-2*
H,L=	7,	7	
0	44	18	-8
1	81	4	6

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
2	366	10	-5	1	6	16	-4*	6	105	7	11	2	128	5	2	3	162	5	1
3	42	9	-3	2	51	6	-2	H,L=		8,	4	3	59	14	-3	4	74	4	-2
4	19	26	9*	3	318	9	1	0	179	8	0	4	144	5	-4	5	42	20	18
5	0	28	-5*	4	10	23	-1*	1	54	3	3	H,L=		9,	-7	6	131	6	-13
H,L=		7,	8	5	68	6	6	2	125	9	7	0	19	24	-14*	H,L=		9,	1
1	204	6	7	6	44	17	12	3	6	20	3*	1	180	5	6	0	9	32	-15*
2	46	16	-12	H,L=		8,	-3	4	27	13	3	2	175	5	-3	1	458	13	13
3	10	32	-20*	1	104	3	-1	5	226	8	-0	3	58	7	-2	2	88	4	-0
4	90	6	1	2	53	5	-1	6	0	29	-21*	4	78	6	7	3	35	9	9
H,L=		7,	9	3	57	4	-3	H,L=		8,	5	5	0	33	-20*	4	217	6	2
0	0	45	-14*	4	30	11	9	1	51	5	-4	H,L=		9,	-6	5	18	26	-1*
1	124	7	-6	5	153	5	-4	2	188	5	4	1	219	6	-9	6	124	6	2
2	52	7	9	6	56	48	12	3	103	4	-1	2	77	4	-4	H,L=		9,	2
3	0	28	-14*	H,L=		8,	-2	4	64	6	6	3	70	15	2	1	130	5	7
H,L=		7,	10	01457		47	51	5	116	5	-1	4	228	6	2	2	128	7	5
1	209	9	-13	1	238	8	-2	H,L=		8,	6	5	19	26	0*	3	121	4	2
2	60	8	-3	2	69	5	-0	0	156	7	9	H,L=		9,	-5	4	201	6	-7
H,L=		8,	-11	3	398	10	-1	1	60	13	4	0	21	25	10*	5	40	42	19*
1	61	8	-10	4	23	32	2*	2	117	4	-2	1	713	23	7	6	0	29	-21*
H,L=		8,	-10	5	248	7	-3	3	23	19	1	2	58	6	2	H,L=		9,	3
0	185	6	-3	6	56	7	24	4	76	5	15	3	95	7	6	0	114	4	0
1	33	13	11	H,L=		8,	-1	5	10	27	-2*	4	88	5	-2	1	512	13	3
2	103	5	2	1	79	8	-3	H,L=		8,	7	5	32	23	0	2	399	14	5
3	96	8	2	2	86	4	-5	1	0	25	-21*	6	0	28	-5*	3	23	25	1*
H,L=		8,	-9	3	253	7	-3	2	256	7	-7	H,L=		9,	-4	4	0	23	-17*
1	20	35	1*	4	49	5	-1	3	41	8	17	1	142	4	-6	5	0	27	-3*
2	262	7	0	5	177	7	-1	4	52	8	-1	2	52	9	11	6	64	7	4
3	219	9	6	6	75	8	-1	5	0	28	-4*	3	208	6	3	H,L=		9,	4
4	20	33	17*	H,L=		8,	0	H,L=		8,	8	4	48	7	-2	1	16	23	8*
H,L=		8,	-8	01911		55	40	0	251	7	-14	5	28	22	1	2	76	4	-2
0	237	7	7	1	263	20	-12	1	48	10	-0	6	32	21	0	3	51	8	-9
1	0	24	-5*	2	30	4	8	2	176	5	-5	H,L=		9,	-3	4	36	19	3
2	29	14	12	3	140	5	-0	3	0	27	-20*	0	65	4	2	5	58	8	14
3	68	6	-0	4	91	3	0	4	69	14	0	1	59	3	2	6	21	28	15*
4	46	9	15	5	145	5	2	H,L=		8,	9	2	171	5	5	H,L=		9,	5
H,L=		8,	-7	6	23	43	-3*	1	75	14	1	3	205	7	2	0	55	5	1
1	18	23	-10*	H,L=		8,	1	2	5	26	-7*	4	169	5	-5	1	126	7	2
2	124	4	0	1	103	8	5	3	18	27	15*	5	34	45	-4*	2	39	5	-2
3	146	5	-4	2	155	6	-1	H,L=		8,	10	6	0	28	-4*	3	37	8	4
4	9	27	-22*	3	134	4	2	0	55	8	-9	H,L=		9,	-2	4	79	5	2
5	61	10	7	4	45	7	7	1	37	25	8	1	100	4	5	5	30	41	1*
H,L=		8,	-6	5	85	4	-2	2	47	9	19	2	66	3	3	H,L=		9,	6
0	36	4	3	6	53	18	1	H,L=		9,	-11	3	194	7	-0	1	220	9	7
1	6	18	-3*	H,L=		8,	2	0	0	28	-4*	4	237	6	5	2	214	6	2
2	26	7	5	01611		58	57	1	30	31	21*	5	23	26	16*	3	42	8	-3
3	28	28	5*	1	260	13	8	H,L=		9,	-10	6	157	7	3	4	171	6	7
4	94	6	-1	2	97	6	3	1	11	27	-14*	H,L=		9,	-1	5	0	29	-25*
5	202	6	3	3	264	8	-10	2	0	29	-9*	0	36	14	1	H,L=		9,	7
H,L=		8,	-5	4	0	19	-8*	3	42	10	21	1	292	8	11	0	0	24	-1*
1	227	6	-0	5	83	5	-5	H,L=		9,	-9	2	67	6	-1	1	49	6	11
2	339	11	4	6	29	17	17	0	44	11	0	3	307	8	2	2	31	14	8
3	0	19	-0*	H,L=		8,	3	1	204	7	-2	4	304	9	-5	3	57	14	9
4	47	9	-9	1	268	11	-2	2	318	9	-3	5	17	41	-5*	4	22	40	8*
5	32	13	22	2	368	11	6	3	35	13	21	6	165	6	0	H,L=		9,	8
6	4	27	-13*	3	22	26	8*	4	0	28	-1*	H,L=		9,	0	1	244	7	3
H,L=		8,	-4	4	25	16	-8	H,L=		9,	-8	1	292	8	11	2	69	9	-4
0	687	21	-3	5	37	11	6	1	35	14	14	2	107	3	-4	3	77	5	5

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
4	156	6	4	H,L=	10,	-2		5	125	8	-4	5	0	40	-5*	3	101	4	1
H,L=	9,	9		0	114	4	-2	H,L=	10,	6		H,L=	11,	-4		4	12	23	4*
0	22	28	-18*	1	181	5	-3	0	307	8	1	1	335	15	3	5	21	33	-11*
1	160	5	10	2	285	8	-2	1	79	13	-2	2	23	28	-11*	6	138	5	5
2	0	29	-10*	3	64	5	0	2	78	8	-1	3	7	23	1*	H,L=	11,	4	
3	31	40	-8*	4	86	8	-10	3	166	5	-1	4	61	6	1	1	278	7	-2
H,L=	9,	10		5	146	6	6	4	45	8	15	5	0	29	-10*	2	16	19	15*
1	44	9	-0	6	59	11	-3	5	48	9	10	6	79	7	-6	3	106	6	7
2	28	30	-13*	H,L=	10,	-1		H,L=	10,	7		H,L=	11,	-3		4	77	5	-11
H,L=	10,	-10		1	63	6	4	1	61	5	2	0	33	12	5	5	0	29	-3*
0	368	10	-5	2	183	6	6	2	114	5	4	1	89	6	-3	H,L=	11,	5	
1	74	10	-0	3	465	12	-6	3	22	27	17*	2	317	11	3	0	27	7	7
2	79	15	-6	4	104	4	-3	4	61	7	6	3	194	7	-3	1	463	14	11
H,L=	10,	-9		5	33	35	1*	H,L=	10,	8		4	103	4	3	2	68	5	-4
1	78	5	3	6	118	5	9	0	48	8	-2	5	0	27	-0*	3	22	23	1*
2	299	9	13	H,L=	10,	0		1	114	5	3	6	34	38	-17*	4	216	6	-3
3	103	5	-1	0	14	25	3*	2	39	11	4	H,L=	11,	-2		5	0	29	-8*
H,L=	10,	-8		1	195	6	0	3	141	6	1	1	404	10	24	H,L=	11,	6	
0	308	9	7	2	395	10	-3	4	38	13	11	2	331	11	-4	1	204	6	0
1	123	5	2	3	248	7	-2	H,L=	10,	9		3	101	4	-3	2	9	25	-11*
2	242	7	-7	4	33	37	9*	1	98	7	-5	4	61	9	7	3	142	5	-1
3	182	6	-3	5	285	8	-3	2	16	32	-19*	5	35	37	31*	4	95	5	-5
4	20	44	1*	6	70	6	18	3	54	20	-1	6	139	6	-8	5	26	28	17*
H,L=	10,	-7		H,L=	10,	1		H,L=	10,	10		H,L=	11,	-1		H,L=	11,	7	
1	0	23	-9*	1	193	108	-41	0	141	5	2	0	24	28	1*	0	8	25	-13*
2	63	6	5	2	126	6	2	1	27	51	18*	1	336	9	15	1	121	7	-6
3	0	38	-2*	3	112	5	-8	H,L=	11,	-10		2	47	12	1	2	36	10	20
4	15	33	-10*	4	9	24	4*	1	204	6	6	3	206	8	-1	3	16	25	11*
5	67	5	4	5	80	9	-6	2	72	13	-10	4	132	4	-2	4	221	6	-1
H,L=	10,	-6		6	90	6	-6	H,L=	11,	-9		5	19	26	17*	H,L=	11,	8	
0	550	20	11	H,L=	10,	2		0	0	30	-12*	6	84	6	2	1	173	6	-2
1	92	6	-2	0	100	4	-3	1	14	47	1*	H,L=	11,	0		2	28	17	20
2	86	7	0	1	25	27	-6*	2	52	16	-11	1	220	9	6	3	44	10	-12
3	166	5	-6	2	84	3	-1	3	89	6	8	2	277	8	-3	H,L=	11,	9	
4	0	27	-7*	3	65	4	-2	H,L=	11,	-8		3	173	5	-6	0	33	12	11
5	12	29	6*	4	90	6	5	1	388	11	-2	4	136	5	5	1	115	6	-16
H,L=	10,	-5		5	183	6	-2	2	97	5	-0	5	54	8	-9	2	73	6	7
1	73	8	5	6	45	9	11	3	36	18	-10	6	82	6	14	H,L=	12,	-10	
2	155	4	-5	H,L=	10,	3		4	77	11	-6	H,L=	11,	1		0	177	6	-7
3	208	6	6	1	14	25	-8*	H,L=	11,	-7		0	41	6	3	1	53	9	-8
4	65	7	-8	2	298	8	3	0	55	6	-4	1	677	24	28	2	49	38	-11
5	0	27	-10*	3	135	4	-1	1	24	19	23	2	62	43	-12	H,L=	12,	-9	
H,L=	10,	-4		4	15	24	8*	2	97	11	-2	3	195	6	-8	1	18	28	-6*
0	81	4	6	5	51	8	-14	3	26	44	12*	4	204	8	1	2	79	6	-1
1	22	16	-7	6	60	8	-2	4	186	6	-11	5	57	7	-1	3	112	7	13
2	106	4	5	H,L=	10,	4		H,L=	11,	-6		6	35	13	-1	H,L=	12,	-8	
3	123	5	6	0	212	6	-1	1	6	24	-9*	H,L=	11,	2		0	578	15	7
4	31	10	15	1	54	4	0	2	35	10	5	1	208	8	3	1	103	6	-6
5	260	8	-0	2	37	23	0	3	56	7	-8	2	76	3	4	2	43	10	-5
6	23	33	17*	3	172	5	2	4	129	5	0	3	129	4	1	3	121	5	6
H,L=	10,	-3		4	0	32	-3*	5	0	28	-18*	4	81	5	6	4	28	33	18*
1	15	21	0*	5	110	5	-6	H,L=	11,	-5		5	38	17	18	H,L=	12,	-7	
2	476	14	4	H,L=	10,	5		0	13	23	-6*	6	47	16	8	1	24	25	5*
3	555	16	3	1	181	8	3	1	98	5	-2	H,L=	11,	3		2	191	6	1
4	26	15	7	2	75	4	3	2	138	5	-2	0	48	6	-3	3	144	5	4
5	132	5	-1	3	15	27	-1*	3	32	12	8	1	171	5	1	4	78	6	-8
6	24	30	-19*	4	19	47	-15*	4	308	9	3	2	10	24	4*	H,L=	12,	-6	

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
0	198	6	-1	0	234	6	2	0	27	32	3*	3	0	26	-6*	H,L=	14,		-7
1	38	8	-2	1	56	4	-2	1	142	5	3	4	480	13	-14	1	0	26	-5*
2	196	6	2	2	37	13	0	2	169	6	3	5	17	42	9*	2	15	26	8*
3	92	4	10	3	246	7	1	3	65	7	-13	6	80	8	-13	3	37	17	-7
4	51	14	1	4	0	57	-14*	4	247	7	-1	H,L=	13,		2	4	35	38	14*
5	33	13	9	5	55	7	2	H,L=	13,		-6	1	157	6	-1	H,L=	14,		-6
H,L=	12,		-5	6	44	18	6	1	156	5	3	2	38	12	7	0	386	10	6
1	45	5	2	H,L=	12,		3	2	102	7	-4	3	177	8	2	1	52	12	-4
2	81	4	9	1	69	8	-1	3	134	5	2	4	66	6	4	2	86	5	-2
3	219	7	2	2	154	5	-2	4	51	8	3	5	35	10	13	3	75	5	14
4	77	10	9	3	133	4	1	5	28	21	16	H,L=	13,		3	4	66	15	1
5	156	5	1	4	14	36	9*	H,L=	13,		-5	0	86	8	-3	H,L=	14,		-5
H,L=	12,		-4	5	217	7	-13	0	61	4	-1	1	91	4	-7	1	31	12	14
0	513	17	13	H,L=	12,		4	1	8	22	-17*	2	73	4	-1	2	151	7	2
1	36	8	0	0	227	7	-5	2	100	4	-2	3	44	10	-1	3	17	29	17*
2	60	11	-5	1	115	4	3	3	134	5	4	4	49	13	-9	4	76	25	-5
3	51	28	-3	2	91	5	2	4	33	25	18	5	0	29	-13*	5	29	31	-19*
4	9	26	-8*	3	129	6	5	5	48	6	27	H,L=	13,		4	H,L=	14,		-4
5	56	7	19	4	25	29	20*	H,L=	13,		-4	1	34	9	-9	0	406	15	9
H,L=	12,		-3	5	259	7	2	1	349	12	3	2	110	5	3	1	135	5	-5
1	0	23	-2*	H,L=	12,		5	2	46	8	5	3	54	6	-1	2	0	28	-11*
2	37	16	-5	1	0	25	-26*	3	150	5	1	4	63	6	5	3	259	8	11
3	71	10	-3	2	226	7	4	4	99	5	1	5	29	25	11	4	60	9	-4
4	60	6	-1	3	25	26	24*	5	24	27	13*	H,L=	13,		5	5	117	6	9
5	50	15	15	4	71	6	-0	H,L=	13,		-3	0	16	24	16*	H,L=	14,		-3
6	61	7	3	5	49	8	31	0	15	23	8*	1	308	8	-3	1	41	10	2
H,L=	12,		-2	H,L=	12,		6	1	144	6	4	2	168	6	6	2	94	7	1
0	512	17	20	0	370	10	4	2	128	4	4	3	94	5	1	3	91	8	-13
1	99	3	-2	1	104	5	-2	3	62	6	0	4	25	41	11*	4	62	6	5
2	436	11	-2	2	82	5	1	4	175	6	12	5	0	31	-12*	5	297	8	-4
3	120	5	-1	3	32	38	-3*	5	47	10	-6	H,L=	13,		6	H,L=	14,		-2
4	28	14	8	4	8	27	-6*	H,L=	13,		-2	1	146	6	2	0	338	9	-6
5	285	8	3	H,L=	12,		7	1	342	9	20	2	73	6	-1	1	70	7	-5
6	73	7	9	1	122	10	-4	2	111	7	-1	3	23	25	-4*	2	18	28	-6*
H,L=	12,		-1	2	155	8	9	3	57	12	6	4	58	9	-8	3	270	7	7
1	115	4	4	3	31	39	0*	4	151	5	3	H,L=	13,		7	4	0	35	-2*
2	56	16	3	4	70	6	9	5	44	20	20	0	0	26	-4*	5	42	17	31
3	63	5	-1	H,L=	12,		8	6	92	5	6	1	299	9	-9	H,L=	14,		-1
4	79	8	3	0	35	37	-18*	H,L=	13,		-1	2	170	6	7	1	0	23	-27*
5	177	7	-8	1	105	6	-6	0	32	16	1	3	69	7	-6	2	180	8	2
6	92	6	3	2	101	9	6	1	237	7	13	H,L=	13,		8	3	25	15	21
H,L=	12,		0	3	108	5	6	2	17	21	-5*	1	0	38	-27*	4	109	5	-3
0	826	23	46	H,L=	12,		9	3	0	23	-17*	2	85	5	8	5	234	9	-4
1	107	11	2	1	44	20	20	4	454	12	-2	3	132	5	0	H,L=	14,		0
2	113	8	4	2	60	7	11	5	24	28	3*	H,L=	13,		9	0	949	26	22
3	129	5	-4	H,L=	13,		-10	6	196	7	-4	0	11	28	-2*	1	0	68	-20*
4	76	7	2	1	196	6	-7	H,L=	13,		0	1	0	30	-6*	2	91	3	3
5	17	30	-14*	H,L=	13,		-9	1	363	14	11	H,L=	14,		-10	3	161	5	1
6	66	7	9	0	0	28	-17*	2	10	28	-3*	0	161	6	-15	4	0	29	-0*
H,L=	12,		1	1	47	12	-9	3	28	11	13	H,L=	14,		-9	5	88	11	-1
1	170	554	-62*	2	115	6	2	4	81	6	6	1	26	32	11*	H,L=	14,		1
2	105	8	-6	3	34	20	18	5	0	27	-8*	2	38	12	10	1	42322		-21*
3	261	7	4	H,L=	13,		-8	6	50	10	-5	H,L=	14,		-8	2	51	13	-4
4	157	7	-2	1	136	5	-2	H,L=	13,		1	0	124	5	6	3	190	8	-14
5	138	5	1	2	121	5	1	0	52	13	3	1	27	42	-14*	4	40	48	-8*
6	57	8	4	3	114	6	1	1	251	305	-93*	2	145	5	-7	5	25	41	6*
H,L=	12,		2	H,L=	13,		-7	2	39	47	-16*	3	125	12	8	H,L=	14,		2

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
0	931	25	23	H,L=	15,		-5	5	36	13	4	H,L=	16,		-2	H,L=	16,		8
1	148	18	-13	0	38	9	-2	H,L=	15,		4	0	475	16	8	0	145	5	-5
2	38	8	-2	1	44	8	-5	1	16	40	-1*	1	48	7	-7	1	38	50	2*
3	139	5	3	2	36	14	-7	2	61	15	-5	2	81	5	1	H,L=	17,		-8
4	0	31	-8*	3	101	6	1	3	19	37	-0*	3	168	9	-7	1	78	9	0
5	33	23	28	4	239	7	3	4	39	23	17	4	33	15	17	2	46	10	16
H,L=	14,		3	H,L=	15,		-4	H,L=	15,		5	5	26	27	2*	H,L=	17,		-7
1	50	7	7	1	441	11	8	0	48	7	-8	H,L=	16,		-1	0	0	30	-22*
2	80	5	3	2	0	39	-11*	1	82	5	-1	1	92	10	2	1	92	5	17
3	80	5	5	3	17	27	-12*	2	103	5	-2	2	91	5	-6	2	113	9	5
4	25	26	-1*	4	89	6	2	3	84	14	1	3	81	6	2	3	39	14	-5
5	127	7	5	5	32	15	27	4	177	6	-3	4	74	6	0	H,L=	17,		-6
H,L=	14,		4	H,L=	15,		-3	H,L=	15,		6	5	36	12	6	1	38	10	17
0	55	6	4	0	44	6	1	1	56	8	0	H,L=	16,		0	2	130	7	-6
1	31	11	-3	1	190	6	3	2	63	9	4	0	4	21	-3*	3	148	5	1
2	37	9	10	2	143	14	-7	3	50	8	14	1	168	44	-30	H,L=	17,		-5
3	58	6	-1	3	165	7	-6	H,L=	15,		7	2	0	55	-22*	0	30	11	10
4	41	17	-3	4	0	27	-18*	0	74	12	12	3	181	7	2	1	21	24	2*
5	77	7	9	5	25	45	9*	1	22	41	8*	4	39	21	10	2	79	7	-3
H,L=	14,		5	H,L=	15,		-2	2	52	8	5	5	144	5	-4	3	0	27	-7*
1	103	5	-1	1	221	6	13	3	0	28	-25*	H,L=	16,		1	4	56	9	-2
2	30	36	6*	2	91	7	-1	H,L=	15,		8	1	0	365	-134*	H,L=	17,		-4
3	175	6	1	3	21	26	-10*	1	138	9	-2	2	27	32	0*	1	164	5	-3
4	63	7	15	4	182	6	2	2	12	28	-16*	3	130	5	2	2	35	12	13
H,L=	14,		6	5	0	57	-12*	H,L=	16,		-9	4	47	13	10	3	88	6	-13
0	101	5	2	H,L=	15,		-1	1	64	20	-2	5	0	43	-6*	4	78	5	10
1	35	13	6	0	33	9	-2	H,L=	16,		-8	H,L=	16,		2	H,L=	17,		-3
2	0	32	-20*	1	309	9	22	0	0	27	-3*	0	111	4	9	0	35	11	-4
3	79	6	-13	2	141	6	-7	1	59	10	3	1	78	153	-37*	1	83	7	-5
4	44	10	10	3	33	10	8	2	101	6	7	2	146	46	-13	2	307	9	-4
H,L=	14,		7	4	370	10	-2	H,L=	16,		-7	3	19	36	10*	3	65	7	8
1	73	20	8	5	0	34	-8*	1	96	5	-1	4	10	27	2*	4	207	8	4
2	128	5	-3	H,L=	15,		0	2	40	9	22	5	29	31	2*	H,L=	17,		-2
3	102	6	-4	1	479	17	2	3	121	11	-6	H,L=	16,		3	1	46	13	-2
H,L=	14,		8	2	0	48	-35*	H,L=	16,		-6	1	67	13	-14	2	60	8	-8
0	424	11	-11	3	25	29	-10*	0	50	7	-6	2	223	6	0	3	133	5	0
1	38	15	-16	4	0	33	-16*	1	35	43	34*	3	134	5	1	4	48	9	8
2	83	13	10	5	35	14	-2	2	0	26	-3*	4	53	8	2	5	0	28	-9*
H,L=	15,		-9	H,L=	15,		1	3	260	7	0	H,L=	16,		4	H,L=	17,		-1
0	0	51	-13*	0	21	34	1*	4	21	28	17*	0	54	7	-5	0	0	31	-14*
1	241	8	-4	1	237	66	-24	H,L=	16,		-5	1	57	8	4	1	88	5	4
2	121	7	5	2	32	9	19	1	70	6	-8	2	92	5	-1	2	43	7	16
H,L=	15,		-8	3	170	9	-8	2	125	5	-5	3	0	25	-35*	3	148	7	-3
1	256	7	8	4	49	25	8	3	144	5	-7	4	0	43	-2*	4	129	5	1
2	33	34	-3*	5	37	15	1	4	50	10	4	H,L=	16,		5	5	38	25	26
3	31	22	2	H,L=	15,		2	H,L=	16,		-4	1	75	6	-4	H,L=	17,		0
H,L=	15,		-7	1	555	14	17	0	225	6	-4	2	90	5	-10	1	169	15	-22
0	14	33	-6*	2	0	110	-19*	1	52	32	-6	3	0	27	-14*	2	126	15	-7
1	207	6	7	3	33	19	0	2	0	24	-6*	4	37	12	34	3	90	15	-9
2	150	6	1	4	199	6	-5	3	110	5	1	H,L=	16,		6	4	52	9	-7
3	54	41	-3	5	27	27	-3*	4	19	35	-6*	0	435	12	9	5	42	10	26
4	31	22	-6	H,L=	15,		3	H,L=	16,		-3	1	42	10	7	H,L=	17,		1
H,L=	15,		-6	0	81	5	-2	1	69	5	5	2	98	6	10	0	28	17	-10
1	15	25	9*	1	198	6	3	2	404	11	3	3	77	15	17	1	0	170	-110*
2	18	25	4*	2	157	5	7	3	191	6	-10	H,L=	16,		7	2	0	109	-1*
3	74	8	-5	3	16	26	-5*	4	53	8	-3	1	33	15	-12	3	0	27	-16*
4	93	5	-2	4	79	5	-7	5	63	8	2	2	57	8	2	4	107	7	-8

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
5	0	31	-12*	H,L=	18,		-2	0	49	9	11	1	65	11	1	0	0	36	-9*
H,L=	17,		2	0	300	8	9	1	266	8	6	H,L=	20,		-6	1	31	24	-14
1	0	30	-31*	1	0	30	-16*	2	13	27	0*	0	34	14	-17	2	23	30	-15*
2	0	122	-110*	2	56	6	-8	3	76	6	3	1	0	41	-17*	H,L=	21,		-4
3	34	22	-14	3	168	5	-1	H,L=	19,		-4	2	87	6	7	1	160	7	-13
4	15	28	-13*	4	28	18	10	1	77	15	4	H,L=	20,		-5	2	51	7	16
H,L=	17,		3	H,L=	18,		-1	2	98	8	-6	1	56	14	-11	H,L=	21,		-3
0	42	9	2	1	73	5	-0	3	93	6	-7	2	14	43	-5*	0	44	12	22
1	203	6	-5	2	60	37	-5	H,L=	19,		-3	3	68	8	8	1	282	9	7
2	114	6	8	3	254	7	-4	0	21	25	10*	H,L=	20,		-4	2	56	10	-11
3	97	8	1	4	0	47	-29*	1	38	14	17	0	156	5	-5	3	50	13	-10
4	30	37	-5*	H,L=	18,		0	2	60	9	-1	1	74	7	-14	H,L=	21,		-2
H,L=	17,		4	0	141	6	4	3	128	5	-1	2	16	27	-8*	1	32	15	-7
1	106	4	3	1	0	59	-15*	4	75	8	-4	3	158	6	-4	2	80	6	6
2	58	8	-2	2	211	7	-7	H,L=	19,		-2	H,L=	20,		-3	3	0	39	-19*
3	41	12	18	3	173	5	1	1	94	9	3	1	66	17	-7	H,L=	21,		-1
4	17	28	6*	4	12	27	4*	2	97	13	-4	2	143	8	-3	0	25	26	2*
H,L=	17,		5	H,L=	18,		1	3	22	37	-6*	3	20	30	4*	1	98	8	1
0	39	12	-2	1	0	159	-23*	4	53	10	0	H,L=	20,		-2	2	58	8	8
1	175	6	1	2	164	24	-13	H,L=	19,		-1	0	116	5	-4	3	11	45	-11*
2	25	28	-5*	3	41	11	-9	0	21	25	-3*	1	89	5	-5	H,L=	21,		0
3	108	7	6	4	0	32	-20*	1	120	6	7	2	148	6	-7	1	0	28	-25*
H,L=	17,		6	H,L=	18,		2	2	111	5	-6	3	67	10	-1	2	28	38	4*
1	57	11	10	0	413	11	-9	3	106	17	-3	H,L=	20,		-1	3	0	28	-12*
2	93	6	-4	1	0	217	-89*	4	37	26	5	1	0	28	-27*	H,L=	21,		1
3	57	8	6	2	107	39	-39	H,L=	19,		0	2	59	7	13	0	67	9	4
H,L=	17,		7	3	26	35	13*	1	245	7	-1	3	56	23	-2	1	9	37	-46*
0	37	20	-11	4	41	45	3*	2	174	8	-6	4	34	14	12	2	0	66	-10*
1	0	28	-8*	H,L=	18,		3	3	31	44	-24*	H,L=	20,		0	3	46	12	-3
2	43	11	8	1	16	28	-25*	4	104	5	-6	0	88	7	0	H,L=	21,		2
H,L=	18,		-8	2	104	5	0	H,L=	19,		1	1	45	67	-22*	1	141	9	-26
0	116	11	9	3	0	28	-6*	0	51	7	-5	2	129	21	-6	2	0	180	-94*
1	14	40	-7*	4	17	23	9*	1	119	31	-25	3	37	11	22	3	40	46	-21*
H,L=	18,		-7	H,L=	18,		4	2	68	76	-38*	4	51	11	-6	H,L=	21,		3
1	0	28	-22*	0	162	5	-2	3	0	28	-1*	H,L=	20,		1	0	7	29	1*
2	178	6	9	1	11	26	-5*	4	34	16	-6	1	0	93	-66*	1	127	13	5
H,L=	18,		-6	2	184	9	6	H,L=	19,		2	2	84	15	-16	2	0	93	-8*
0	71	6	18	3	92	5	13	1	233	38	-34	3	71	16	-1	H,L=	21,		4
1	46	14	11	H,L=	18,		5	2	0	129	-51*	H,L=	20,		2	1	108	6	-9
2	78	13	-12	1	0	31	-24*	3	33	17	19	0	0	46	-24*	2	51	24	2
3	0	37	-14*	2	111	7	-3	4	128	5	-6	1	0	448	-33*	H,L=	21,		5
H,L=	18,		-5	3	161	6	9	H,L=	19,		3	2	136	54	-46	0	40	10	20
1	82	16	-4	H,L=	18,		6	0	10	37	4*	3	0	62	-36*	H,L=	22,		-5
2	91	10	-8	0	32	32	-1*	1	189	7	-2	H,L=	20,		3	1	46	33	-6
3	132	5	8	1	0	28	-23*	2	74	23	-15	1	0	48	-8*	H,L=	22,		-4
4	0	28	-3*	2	73	7	-12	3	93	12	-10	2	0	95	-11*	0	68	13	-5
H,L=	18,		-4	H,L=	18,		7	H,L=	19,		4	3	104	11	-18	1	37	16	-22
0	162	5	-11	1	0	29	-0*	1	48	9	4	H,L=	20,		4	2	69	8	-9
1	78	5	2	H,L=	19,		-7	2	153	10	-2	0	53	11	3	H,L=	22,		-3
2	89	6	-4	0	62	9	8	3	40	10	21	1	33	34	-12*	1	40	56	-30*
3	0	29	-23*	1	129	6	-5	H,L=	19,		5	2	132	6	-7	2	34	13	19
4	32	40	-7*	2	153	6	6	0	12	59	-39*	H,L=	20,		5	H,L=	22,		-2
H,L=	18,		-3	H,L=	19,		-6	1	203	6	1	1	0	44	-5*	0	270	7	4
1	12	24	-0*	1	69	13	2	2	31	40	-9*	2	19	34	10*	1	0	32	-10*
2	149	6	-4	2	24	32	5*	H,L=	19,		6	H,L=	21,		-6	2	44	11	-17
3	267	11	-2	3	58	6	4	1	61	9	1	1	0	29	-13*	H,L=	22,		-1
4	45	10	-1	H,L=	19,		-5	H,L=	20,		-7	H,L=	21,		-5	1	0	47	-51*

OBSERVED STRUCTURES FACTORS (CONT) FOR
THE NORBORNANE-LACTONE COMPOUND

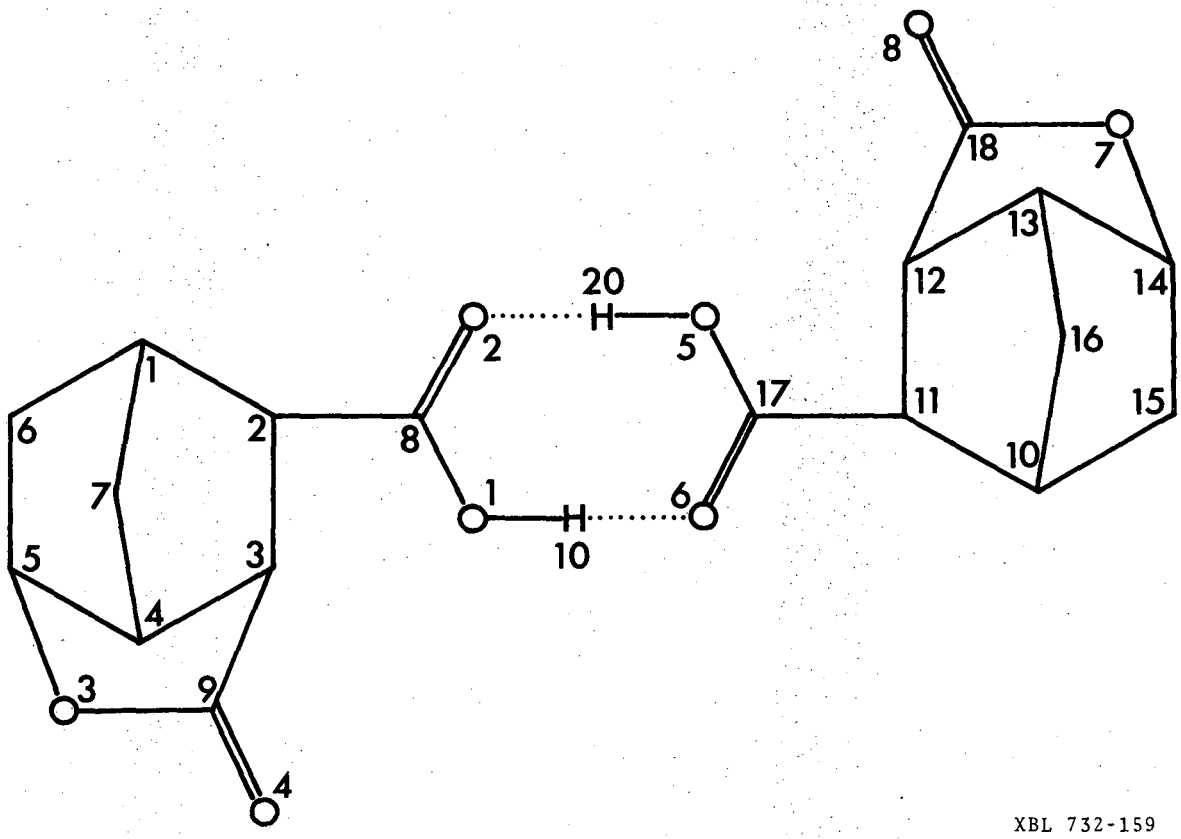
K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
2	72	11	-2																
H,L=	22,	0																	
0	355	10	-10																
1	33	15	13																
2	16	32	8*																
H,L=	22,	1																	
1	0	30	-15*																
2	129	12	-19																
H,L=	22,	2																	
0	122	5	6																
1	0218		-60*																
2	0	93	-12*																
H,L=	22,	3																	
1	0	84	-60*																
H,L=	22,	4																	
0	50	9	6																
H,L=	23,	-4																	
1	63	8	-6																
H,L=	23,	-3																	
0	0	31	-7*																
1	101	5	2																
H,L=	23,	-2																	
1	164	6	-7																
2	49	19	-6																
H,L=	23,	-1																	
0	48	50	19*																
1	169	6	8																
2	80	7	-8																
H,L=	23,	0																	
1	91	6	1																
2	66	8	-6																
H,L=	23,	1																	
0	46	12	-3																
1	35	24	23																
H,L=	23,	2																	
0	61		-45*																
H,L=	24,	-2																	
0	95	6	-3																
H,L=	24,	0																	
0	60	30	-14																

Figure Captions

Fig. 1. Schematic diagram of the two asymmetric molecules of the norbornane derivative.

Fig. 2. Perspective view of one molecule with 50% probability thermal ellipsoids. For hydrogen atoms an arbitrary temperature parameter of 1.0$Å^2$ was given.

Fig. 3. Stereoscopic pair of a unit cell. The view direction is along the monoclinic b axis.



XBL 732-159

Fig. 1

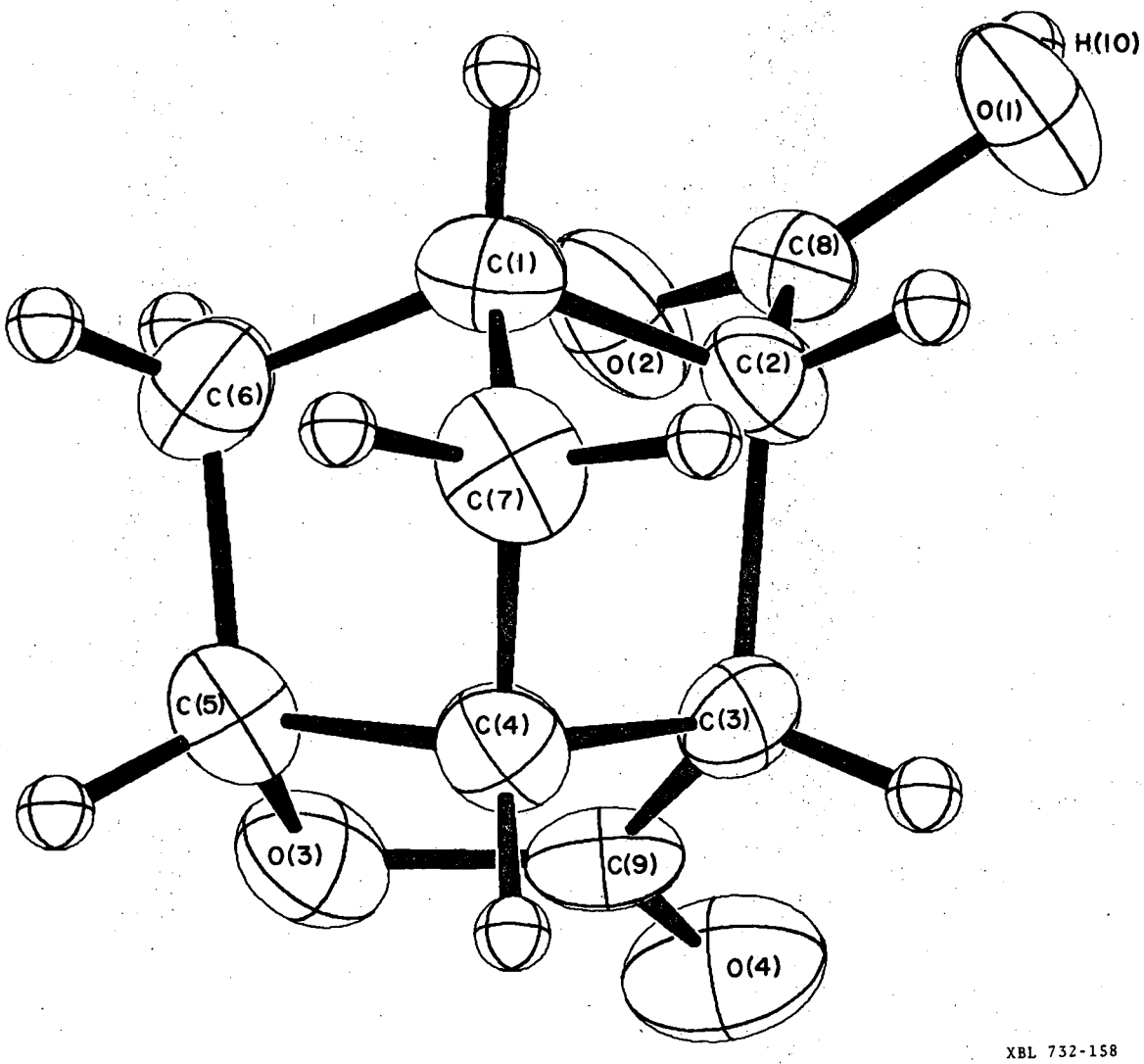


Fig. 2

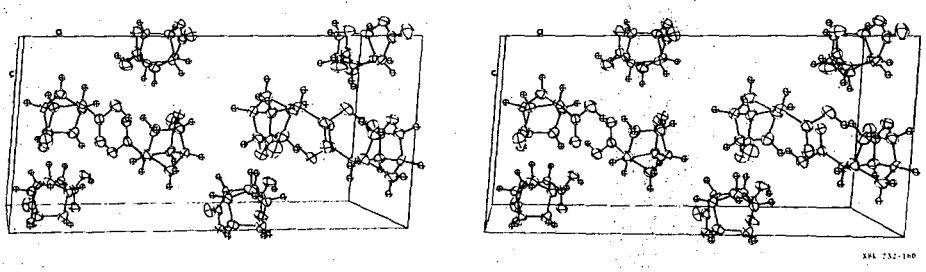


Fig. 3

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