Title

Structures of Bicyclo[2.2.1] Systems IV. 6-Endohydroxy-3-Endo-Aminomethylbicyclo[2.2.1] Heptane-2-Endo-Carboxylic Acid Lactam

Authors

Olson, Arthur J
Templeton, David H
Templeton, Lieselotte K

Publication Date

1976-12-01

Submitted to Acta Crystallographica,
Section B

LBL-5761
Preprint c.1

STRUCTURES OF BICYCLO[2.2.1] SYSTEMS IV. 6-*ENDO*-HYDROXY-3-*ENDO*-AMINOMETHYLBICYCLO[2.2.1]HEPTANE-2-*ENDO*-CARBOXYLIC ACID LACTAM

Arthur J. Olson, David H. Templeton, and
Lieselotte K. Templeton

December 1976

Prepared for the U. S. Energy Research and
Development Administration under Contract W-7405-ENG-48

DISCLAIMER

LBL-5761

STRUCTURES OF BICYCLO[2.2.1] SYSTEMS IV. 6-ENDO-HYDROXY-3-ENDO-AMINOMETHYLBICYCLO[2.2.1]HEPTANE-2-ENDO-CARBOXYLIC ACID LACTAM*

By Arthur J. Olson, David H. Templeton and Lieselotte K. Templeton

Materials and Molecular Research Division
Lawrence Berkeley Laboratory

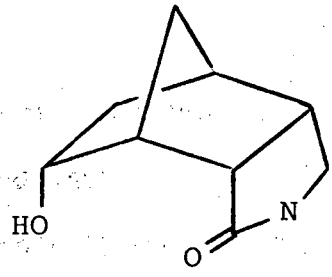
and

Department of Chemistry
University of California
Berkeley, California 94720
U.S.A.

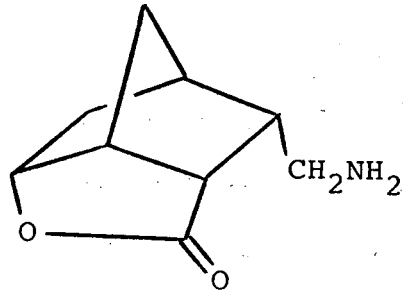
Abstract. $C_9H_{13}NO_2$, monoclinic, $P2_1/c$; at 23°C, a = 10.870(3), b = 7.403(2), c = 10.721(4) Å, β = 107.46(2)°, Z = 4, D_x = 1.350(2), D_m = 1.35(1) g cm^{-3}. For 1169 reflections with I > σ, R = 0.055 and R_w = 0.051. The O(hydroxyl)-C(carbonyl) distance is 2.832 Å, two hydrogen atoms are 2.00 Å from each other, and these distances would be even shorter except for distortion of some of the bond angles. Hydrogen bonds from the hydroxyl and amide groups to the carbonyl oxygen atom link the molecules into chains.

*Work done in part with support from the U.S. Energy Research and Development Administration.

Introduction. To explore effects of orientation on rates of chemical reactions analogous to those catalyzed by enzymes, Koshland and co-workers have measured intramolecular reaction rates for norbornane molecules substituted with a variety of functional groups (Storm & Koshland, 1972). The title compound, a hydroxylactam, was synthesized by Hackney (1975) to serve, in its base catalyzed rearrangement to an aminolactone, as a model for the rate determining step in the hydrolysis of amides by chymotrypsin.



hydroxylactam



aminolactone

We determined the crystal structure of this lactam as part of a program to establish the geometry of substituted norbornane molecules (Chapuis, Zalkin & Templeton, 1973, 197x, 197y). A sample which had been recrystallized from ethyl acetate (m.p. 185°C) was kindly supplied to us by Professor D. E. Koshland and Dr. D. D. Hackney.

A clear colorless crystal 0.18 x 0.12 x 0.15 mm in size was studied by photographic and diffractometer techniques. Laue symmetry 2/m and absent reflections h0ℓ ($\ell \neq 2n$) and 0k0 ($k \neq 2n$) indicate space group $P2_1/c$. Setting angles for 12 reflections with $30° < 2\theta < 40°$ ($MoK\alpha_1$, λ 0.70926 Å) were used for least-squares adjustment of

the cell dimensions. The density was measured by flotation in solutions of CCl_4 and petroleum ether. Intensities were measured with graphite-monochromatized MoKα radiation and θ-2θ scan technique for all the reflections in the half-sphere with ℓ nonnegative and $2\theta < 50°$, many of them twice (a total of 4685 measurements). The scan extended 2° in 2θ with a rate of 1°/min. Background was counted for 10 sec near each end of the scan. After equivalent measurements were averaged there were 1467 unique reflections, of which 1169 had $I > \sigma$. Absorption was small, $\mu = 0.57\ cm^{-1}$, and no correction was made.

The crystal structure was solved by direct methods with the MULTAN program (Germain, Main & Woolfson, 1971). All hydrogen atoms were found in a ΔF map. The structure was refined with Zalkin's full matrix least squares program, modified (Olson, 1975) to use polar scattering factors for hydrogen (Stewart, Davidson & Simpson, 1965) so that the hydrogen coordinates more nearly represent the positions of the protons. For other atoms we used the scattering factors of Doyle & Turner (1968) with dispersion corrections from Cromer & Liberman (1970). Zero weight was assigned to reflections with $I < \sigma$; otherwise, $w = (\sigma(F))^{-2}$; $\sigma(F)$ was derived from $\sigma(I) = [s^2 + (0.058\ I)^2]^{1/2}$ where s^2 is the variance due to counting statistics. In the last cycle no parameter shifted more than 0.003σ. The final residual $R = \Sigma|\Delta F|/\Sigma|F_o|$ was 0.055 for 1169 reflections and 0.078 for 1467 reflections including those of zero weight. The weighted residual minimized by the refinement was $R_w = [\Sigma w(\Delta F)^2/\Sigma w F_o^2]^{1/2}$

= 0.051. Final parameters are listed in Table 1 and 2.*

Discussion. A view of the molecular structure, Fig. 1, shows the numbering of the atoms. The bond distances, Table 3, and most of the bond angles, Table 4, are normal. The angles C(2)-C(1)-C(6) = 111.8° and C(3)-C(4)-C(5) = 110.7° are larger than any of the experimental or theoretical values reported for norbornane (Altona and Sundaralingam, 1972), and they indicate a distortion of the molecule in the direction which partially relieves the crowding of the substituent groups. Angle C(1)-C(6)-O(2) = 115.9° is large for the same reason. The distance O(2)-C(9) = 2.832(3) Å may be compared with 2.783 Å for an analogous distance in the sodium salt of 2-exo-methyl-6-endo-hydroxybicyclo[2.2.1]heptane-2-endo-carboxylic acid (Chapuis, et al., 197x) where the C(2)-C(1)-C(6) angle is 112.2°. In the present case the stress of the lactam ring results in a larger C(1)-C(2)-C(9) angle and thus a longer O(2)-C(9) distance with slightly less strain of the norbornane skeleton than in the salt of the 2,6,2-methylhydroxyacid. The enlargement of the C(3)-C(4)-C(5) angle probably results from the crowding of H(5) and H(10) which are at the abnormally short distance 2.00(4) Å. No other hydrogen atoms in the molecule are closer than 2.26 Å except those which are attached to a common carbon atom. In the methylhydroxyacid salt mentioned above

*A listing of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No.

there was no corresponding crowding at the other end of the molecule, and the angle at C(4) was 107.6°.

For reference in discussion of the rates of conversion to the lactone (Hackney, 1975) in the context of the work reviewed by Bürgi (1975) we include in Table 4 some angles involving the O(2)-C(9) vector.

Figure 2 shows the molecular packing. Hydrogen bonds from the amide and alcohol groups to the carbonyl oxygen atom tie molecules together in strings along the screw axis. Table 5 gives distances and angles descriptive of these hydrogen bonds.

References

Altona, C. & Sundaralingam, M. (1972). Acta Cryst. B 28, 1806-1816.

Bürgi, H. B. (1975). Angew. Chem. internat. Edit. 14, 460-473.

Chapuis, G., Zalkin, A. & Templeton, D. H. (1973). Acta Cryst. B 29, 2642-2644.

Chapuis, G., Zalkin, A. & Templeton, D. H. (197x). Acta Cryst. (in press).

Chapuis, G., Zalkin, A. & Templeton, D. H. (197y). Acta Cryst. (submitted).

Cromer, D. T. & Liberman, D. (1970). J. Chem. Phys. 53, 1891-1898.

Doyle, P. A. & Turner, P. S. (1968). Acta Cryst. A 24, 390-397.

Germain, G., Main, P. & Woolfson, M. M. (1971). Acta Cryst. A 27, 368-376.

Hackney, D. D. (1975). Models for Chymotrypsin and the Interaction of Lysozyme with Urea. Thesis, University of California, Berkeley.

Olson, A. J. (1975). Polar Hydrogen Scattering Factors in X-Ray Diffraction Analysis. Thesis, University of California, Berkeley.

Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). J. Chem. Phys. 42, 3175-3187.

Storm, D. R. & Koshland, D. E. (1972). J. Amer. Chem. Soc. 94, 5815-5825.

Table 1. Parameters for Heavy Atoms. The form of the temperature factor is $\exp[-0.25(h^2a^{*2}B_{11}+2hka^*b^*B_{12}+\ldots)]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
C(1)	.2119(2)	.5819(3)	.1390(2)	2.13(9)	1.9(1)	3.5(1)	.10(8)	.88(8)	.51(9)
C(2)	.1548(2)	.3927(3)	.0960(2)	2.17(9)	2.4(1)	2.6(1)	-.14(8)	.63(9)	.02(8)
C(3)	.2756(2)	.2730(3)	.1080(3)	2.8(1)	2.5(1)	3.6(1)	-.04(8)	1.61(9)	-.3(1)
C(4)	.3876(2)	.4061(3)	.1661(3)	2.04(9)	2.8(1)	4.4(1)	.01(8)	1.45(9)	-.0(1)
C(5)	.3935(2)	.4582(4)	.3050(3)	2.2(1)	3.1(1)	4.0(1)	.17(9)	.54(9)	-.1(1)
C(6)	.2796(2)	.5904(3)	.2863(3)	2.4(1)	2.0(1)	3.7(1)	-.23(8)	.94(9)	-.24(9)
C(7)	.3304(3)	.5780(4)	.0893(3)	2.9(1)	2.9(1)	4.2(1)	-.65(9)	1.4(1)	.3(1)
C(8)	.2605(3)	.1071(4)	.1879(3)	3.4(1)	1.9(1)	5.3(2)	.17(9)	2.1(1)	.0(1)
C(9)	.0790(2)	.2932(3)	.1700(2)	2.37(9)	1.9(1)	3.5(1)	-.27(8)	1.02(8)	-.46(9)
O(1)	-.0292(1)	.3361(2)	.1782(2)	2.15(7)	2.53(8)	5.3(1)	-.16(6)	1.60(7)	-.26(7)
O(2)	.2032(2)	.5427(3)	.3680(2)	3.21(8)	3.23(8)	3.92(9)	.55(7)	1.61(7)	.19(7)
N(1)	.1405(2)	.1408(3)	.2191(2)	2.93(9)	1.95(9)	4.9(1)	.01(7)	2.03(8)	.71(8)

Table 2. Parameters for Hydrogen Atoms. The form of the temperature factor is $\exp(-B\lambda^{-2}\sin^2\theta)$.

	x	y	z	B
H(1)	.147(2)	.690(3)	.105(2)	2.3(5)
H(2)	.098(2)	.396(3)	-.002(2)	1.3(4)
H(3)	.278(2)	.232(4)	.013(3)	3.2(6)
H(4)	.480(2)	.361(3)	.153(2)	2.6(5)
H(5)	.377(2)	.344(4)	.360(2)	3.0(6)
H(6)	.483(3)	.521(4)	.358(3)	4.5(7)
H(7)	.316(2)	.728(3)	.309(2)	2.4(5)
H(8)	.301(2)	.564(3)	-.020(3)	2.5(5)
H(9)	.390(2)	.698(3)	.121(2)	3.1(5)
H(10)	.343(3)	.093(4)	.290(3)	3.7(6)
H(11)	.248(2)	-.010(4)	.130(3)	3.6(6)
H(12)	.103(3)	.051(4)	.268(3)	4.7(7)
H(13)	.139(4)	.635(5)	.361(4)	6.7(10)

Table 3. Bond Lengths (Å)

C(1)-C(2)	1.545(3)	C(1)-H(1)	1.06(2)
C(1)-C(6)	1.530(3)	C(2)-H(2)	1.05(2)
C(1)-C(7)	1.533(3)	C(3)-H(3)	1.08(3)
C(2)-C(3)	1.557(3)	C(4)-H(4)	1.11(2)
C(2)-C(9)	1.499(3)	C(5)-H(5)	1.08(3)
C(3)-C(4)	1.545(3)	C(5)-H(6)	1.07(3)
C(3)-C(8)	1.534(4)	C(6)-H(7)	1.09(3)
C(4)-C(5)	1.521(4)	C(7)-H(8)	1.13(3)
C(4)-C(7)	1.539(4)	C(7)-H(9)	1.09(3)
C(5)-C(6)	1.544(3)	C(8)-H(10)	1.19(3)
O(1)-C(9)	1.246(3)	C(8)-H(11)	1.05(3)
O(2)-C(6)	1.420(3)	N(1)-H(12)	1.00(3)
N(1)-C(8)	1.462(3)	O(2)-H(13)	0.97(4)
N(1)-C(9)	1.336(3)		

Table 4. Bond Angles (°)

C(2)-C(1)-C(6)	111.8(2)	C(1)-C(6)-C(5)	103.1(2)
C(2)-C(1)-C(7)	100.6(2)	C(1)-C(6)-O(2)	115.9(2)
C(6)-C(1)-C(7)	99.4(2)	C(5)-C(6)-O(2)	110.9(2)
C(1)-C(2)-C(3)	103.8(2)	C(1)-C(7)-C(4)	94.5(2)
C(1)-C(2)-C(9)	121.5(2)	C(3)-C(8)-N(1)	104.1(2)
C(3)-C(2)-C(9)	105.1(2)	C(2)-C(9)-N(1)	109.5(2)
C(2)-C(3)-C(4)	102.3(2)	C(2)-C(9)-O(1)	126.3(2)
C(2)-C(3)-C(8)	105.9(2)	O(1)-C(9)-N(1)	124.0(2)
C(4)-C(3)-C(8)	119.3(2)	C(8)-N(1)-C(9)	115.5(2)
C(3)-C(4)-C(5)	110.7(2)	C(6)-O(2)...C(9)	86.3(1)
C(3)-C(4)-C(7)	99.8(2)	C(2)-C(9)...O(2)	82.1(1)
C(5)-C(4)-C(7)	101.7(2)	O(1)-C(9)...O(2)	91.6(2)
C(4)-C(5)-C(6)	103.7(2)	N(1)-C(9)...O(2)	100.7(2)

Table 5. Hydrogen Bonding

Bond (X-H...Y)	d(X...Y)	d(H...Y)	X-H-Y
O(2)-H(13)...O(1^{i})	2.824(2) Å	1.87(4) Å	168(3)°
N(1)-H(12)...O(1^{ii})	2.926(3)	1.95(3)	164(3)

Symmetry Code:

(i) -x, 1/2 + y, 1/2 - z (ii) -x, -1/2 + y, 1/2 - z

Figure Captions

Fig. 1. Perspective view of a molecule with 50% probability thermal ellipsoids, drawn with Johnson's ORTEP. Size of hydrogen atoms is arbitrary.

Fig. 2. Stereoscopic view of molecular packing, viewed along the b axis.

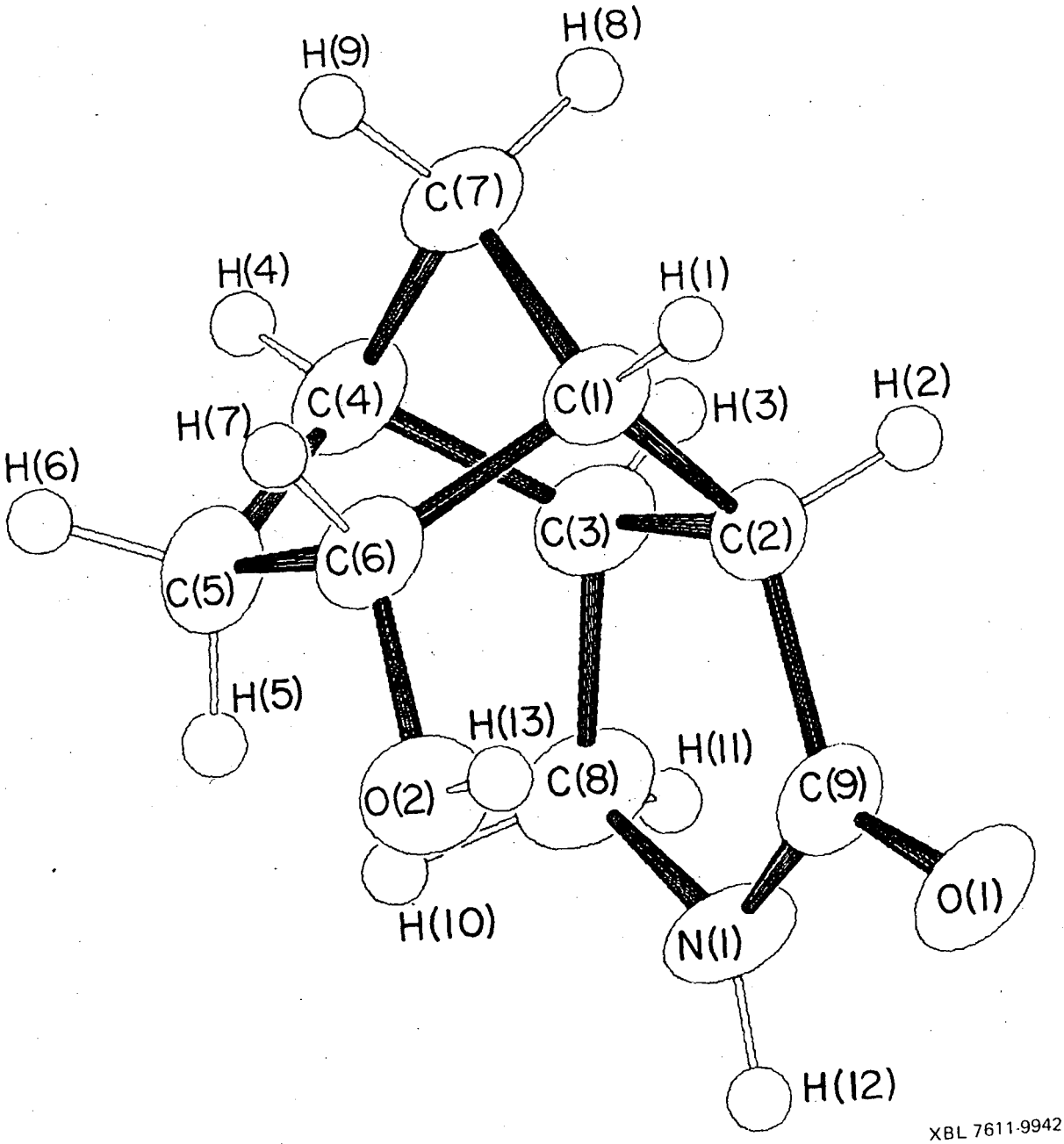
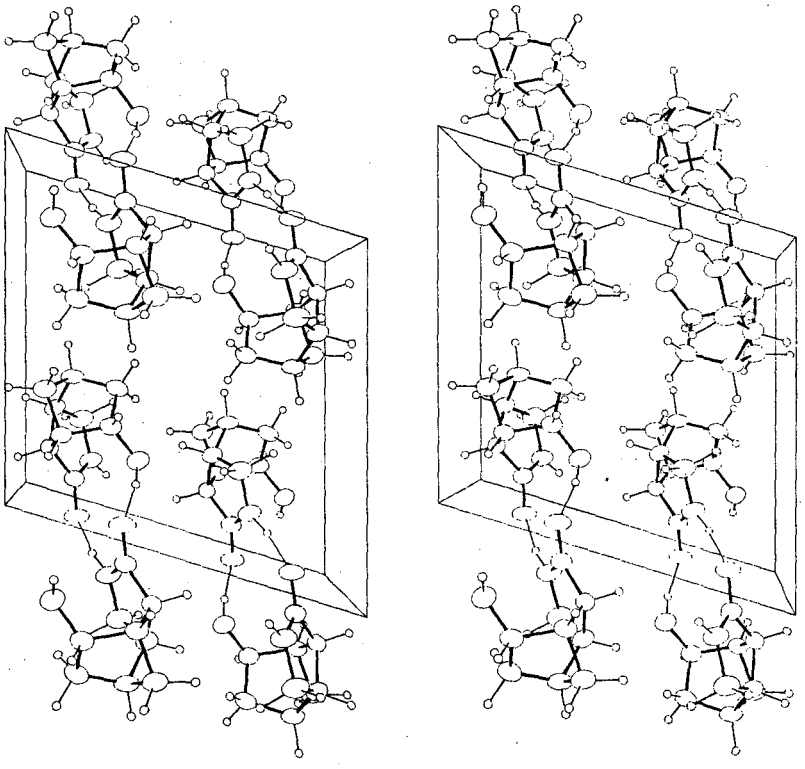


Fig. 1



XBL 762-471

Fig. 2

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X10.0)
C9 H13 N O2 F(0,0,0) = 3601

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

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
K,L=	0,	0		2	363	11	7	K,L=	0,	10		2	389	11	3	5	80	3	-4
1	0305	-313*		3	111	4	3	-10	31	13	16	3	149	5	2	6	67	3	-7
2	815	24	-15	4	161	5	3	-9	18	29	11*	4	103	4	5	7	46	6	3
3	113	5	5	5	150	5	-1	-8	116	5	2	5	23	6	9	8	64	4	1
4	24	9	3	6	48	5	-2	-7	176	6	-0	6	72	3	5	9	58	6	4
5	145	4	-2	7	4	28	-0*	-6	0	20	-6*	7	45	8	-6	10	43	9	1
6	28	3	-1	8	58	4	-2	-5	91	5	5	8	24	17	4	11	42	12	-9
7	65	4	-6	9	45	11	2	-4	15	20	-17*	9	148	5	-2	K,L=	1,		4
8	77	3	6	10	64	9	6	-3	67	4	-2	10	24	26	-13*	-12	6	21	-18*
9	157	5	-2	K,L=	0,		6	-2	37	7	6	11	105	5	-2	-11	20	24	3*
10	45	4	-1	-12	82	4	4	-1	70	4	3	K,L=	1,		2	-10	117	5	0
11	10	20	-7*	-11	36	6	-1	0	98	4	3	-12	73	4	1	-9	22	10	20
12	47	5	-9	-10	158	5	3	1	34	10	-4	-11	9	25	4*	-8	61	6	-3
K,L=	0,	2		-9	47	7	11	2	63	5	9	-10	56	7	-1	-7	88	3	1
-12	0	20	-23*	-8	94	3	5	3	28	10	3	-9	157	5	-4	-6	83	3	-1
-11	125	5	-1	-7	160	5	-4	4	29	11	25	-8	19	16	2	-5	165	5	9
-10	123	4	6	-6	216	7	11	K,L=	0,	12		-7	17	18	-4*	-4	94	3	4
-9	144	5	-3	-5	121	4	6	-7	21	30	-7*	-6	133	4	2	-3	226	7	1
-8	152	5	6	-4	54	5	6	-6	46	6	0	-5	274	8	13	-2	266	8	-9
-7	259	8	6	-3	132	4	7	-5	0	24	-15*	-4	78	4	5	-1	210	6	-22
-6	122	4	5	-2	356	10	-52	-4	29	9	3	-3	260	8	7	0	409	13	-10
-5	250	7	8	-1	49	4	15	-3	0	26	-10*	-2	20	34	-5*	1	176	6	-1
-4	123	4	-2	0	209	6	10	-2	82	5	13	-1	441	13	-36	2	10	21	6*
-3	166	6	9	1	144	5	8	-1	59	4	3	0	704	21	-41	3	109	3	1
-2	24	27	18*	2	18	12	1	0	6	31	5*	1	235	6	-2	4	113	4	-1
-1	469	14	-9	3	68	5	0	K,L=	1,		0	2	35	10	-9	5	0	22	-14*
0	933	28	-12	4	132	5	5	1	384	11	18	3	103	4	-9	6	90	4	1
1	714	21	8	5	149	5	5	2	137	5	-1	4	184	6	6	7	53	7	5
2	44	13	-8	6	120	5	4	3	197	6	-7	5	41	6	-4	8	59	4	-2
3	51	6	4	7	108	4	2	4	38	7	4	6	32	5	1	9	18	24	5*
4	66	3	-1	8	80	5	3	5	108	4	4	7	175	6	-6	10	88	4	7
5	51	4	10	9	28	13	13	6	236	7	2	8	84	4	1	K,L=	1,		5
6	279	8	-7	K,L=	0,		8	7	254	8	-1	9	98	4	0	-12	11	24	-1*
7	54	4	4	-12	67	5	9	8	63	3	-3	10	18	24	8*	-11	73	4	6
8	61	4	-5	-11	83	6	-0	9	14	21	2*	11	72	4	-2	-10	77	6	-4
9	80	4	0	-10	48	10	0	10	157	5	-4	K,L=	1,		3	-9	171	5	3
10	31	14	-3	-9	32	12	3	11	84	4	-3	-12	25	10	14	-8	35	9	9
11	93	6	-3	-8	157	5	5	12	62	4	2	-11	19	28	11*	-7	134	4	4
K,L=	0,	4		-7	212	6	10	K,L=	1,		1	-10	93	3	-3	-6	182	6	5
-12	73	6	-15	-6	158	5	9	-12	32	8	1	-9	24	11	21	-5	205	6	15
-11	55	4	-4	-5	182	6	6	-11	53	5	-2	-8	40	5	-4	-4	382	13	11
-10	0	23	-14*	-4	71	7	-8	-10	118	6	3	-7	228	7	3	-3	34	15	-6
-9	18	18	-0*	-3	154	5	-16	-9	139	4	-7	-6	35	4	2	-2	140	4	-5
-8	274	8	9	-2	261	8	-6	-8	69	3	4	-5	282	8	17	-1	111	3	-5
-7	465	14	9	-1	57	8	6	-7	35	4	-0	-4	99	3	8	0	260	8	3
-6	29	14	5	0	28	13	-1	-6	321	9	10	-3	196	6	0	1	289	9	10
-5	328	10	18	1	63	4	10	-5	149	4	1	-2	52	9	6	2	241	7	7
-4	10	16	-6*	2	45	6	7	-4	435	13	22	-1	305	9	-37	3	18	13	3
-3	103	3	7	3	140	4	11	-3	160	6	-1	0	174	6	-6	4	93	3	4
-2	47	7	-2	4	12	22	-7*	-2	272	8	5	1	497	15	-3	5	20	22	-3*
-1	101	5	-3	5	58	9	-6	-1	649	19	-4	2	517	15	-13	6	85	4	-2
0	588	17	4	6	24	17	12	0	246	8	1	3	75	4	0	7	110	4	1
1	165	5	-0	7	36	8	-9	1	519	15	-3	4	129	4	2	8	86	6	1

STRUCTURE FACTORS CONTINUED FOR
C9 H13 N O2

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
9	23	30	17*	0	25	9	1	-6	41	6	8	-2	70	5	1	6	58	7	-8
K,L=		1,	6	1	36	7	2	-5	23	25	8*	-1	17	29	5*	7	101	4	-5
-12	25	10	-2	2	77	6	-5	-4	52	7	5	0	61	7	-4	8	48	6	-6
-11	16	26	13*	3	54	5	4	-3	0	22	-2*	1	427	13	-6	9	13	21	3*
-10	53	4	0	4	30	7	12	-2	28	12	-10	2	223	7	1	10	24	15	8
-9	124	4	2	5	20	27	4*	-1	26	27	23*	3	32	6	-6	K,L=		2,	5
-8	163	5	3	6	37	8	-7	0	39	16	2	4	52	3	-3	-12	16	22	10*
-7	169	6	6	7	35	7	6	K,L=		2,	0	5	15	20	4*	-11	8	20	1*
-6	22	9	6	K,L=		1,	9	0	298	9	-3	6	44	5	-1	-10	58	9	-3
-5	22	19	4	-11	70	5	10	1	356	10	4	7	93	4	2	-9	243	7	-9
-4	67	3	5	-10	25	27	15*	2	347	10	3	8	38	9	2	-8	111	4	-3
-3	60	3	-0	-9	29	8	5	3	183	6	6	9	13	24	-9*	-7	76	4	3
-2	119	4	-9	-8	84	6	-4	4	86	3	-1	10	121	4	-1	-6	7	17	-8*
-1	79	4	-4	-7	9	22	-6*	5	286	9	6	11	19	23	16*	-5	79	4	-4
0	109	4	-1	-6	115	6	8	6	45	3	0	K,L=		2,	3	-4	14	18	14*
1	61	4	3	-5	44	7	-4	7	116	4	3	-12	27	16	2	-3	174	5	3
2	89	3	2	-4	76	4	-5	8	17	20	10*	-11	23	24	0*	-2	45	3	3
3	69	4	-5	-3	90	4	-9	9	36	6	1	-10	228	7	-5	-1	89	4	-6
4	56	4	4	-2	71	4	-6	10	73	4	-4	-9	267	8	-11	0	130	4	-5
5	20	15	15	-1	21	23	12*	11	55	7	8	-8	47	7	4	1	95	4	-3
6	14	20	4*	0	69	4	7	12	24	11	-11	-7	197	6	1	2	334	10	-4
7	54	10	1	1	21	13	2	K,L=		2,	1	-6	80	4	2	3	161	5	3
8	55	9	5	2	84	5	13	-12	34	8	3	-5	280	8	5	4	181	6	4
K,L=		1,	7	3	47	6	6	-11	20	23	10*	-4	101	3	3	5	64	7	4
-12	110	4	6	4	39	8	10	-10	123	4	-2	-3	176	5	4	6	10	25	8*
-11	45	7	5	5	51	6	-7	-9	67	5	1	-2	271	8	5	7	63	5	5
-10	43	7	1	K,L=		1,	10	-8	26	16	-1	-1	67	6	-13	8	114	4	-6
-9	139	5	6	-10	25	24	15*	-7	18	18	12	0	141	5	-8	9	24	19	5
-8	96	5	3	-9	21	23	4*	-6	57	4	10	1	144	5	-4	K,L=		2,	6
-7	57	6	6	-8	32	15	1	-5	274	8	16	2	19	9	-3	-12	12	29	6*
-6	109	4	4	-7	78	5	-6	-4	12	20	9*	3	147	5	3	-11	25	11	4
-5	62	5	6	-6	64	8	4	-3	228	7	13	4	42	6	2	-10	39	9	2
-4	27	14	-6	-5	36	7	-5	-2	574	17	11	5	53	5	-11	-9	54	7	-1
-3	102	8	-3	-4	37	6	-3	-1	0	28	-3*	6	48	6	-3	-8	58	6	3
-2	102	4	-3	-3	16	21	-0*	0	217	7	-15	7	198	6	-1	-7	103	4	1
-1	123	4	-8	-2	105	4	2	1	5	28	5*	8	90	4	0	-6	25	11	-1
0	80	3	6	-1	91	3	7	2	822	24	3	9	18	20	-4*	-5	150	5	2
1	66	5	3	0	16	20	-9*	3	315	9	5	10	0	25	-26*	-4	9	19	6*
2	80	4	1	1	19	29	12*	4	251	7	9	K,L=		2,	4	-3	164	5	-12
3	60	5	-3	2	25	11	4	5	129	4	4	-12	24	28	2*	-2	43	4	-12
4	9	33	3*	3	35	9	-2	6	56	7	-5	-11	24	14	4	-1	80	4	-3
5	21	30	20*	4	36	10	12	7	85	3	-4	-10	59	6	-10	0	15	21	15*
6	81	4	-2	K,L=		1,	11	8	33	8	-13	-9	185	6	-3	1	123	4	2
7	96	4	7	-9	33	34	12*	9	101	4	-4	-8	10	21	-6*	2	134	4	1
8	30	22	-3	-8	16	24	16*	10	57	5	-9	-7	96	4	-2	3	26	11	1
K,L=		1,	8	-7	36	13	2	11	13	27	-9*	-6	136	5	6	4	24	11	8
-11	41	8	13	-6	74	7	12	K,L=		2,	2	-5	309	9	6	5	22	12	-6
-10	20	24	11*	-5	25	14	23	-12	12	22	1*	-4	15	17	8*	6	15	28	-7*
-9	25	28	8*	-4	19	21	-15*	-11	39	7	3	-3	357	11	-3	7	18	27	4*
-8	137	4	3	-3	41	10	12	-10	62	4	-4	-2	123	4	-7	8	48	5	7
-7	210	6	2	-2	21	29	1*	-9	172	6	1	-1	55	3	-6	K,L=		2,	7
-6	24	13	7	-1	49	6	3	-8	53	7	-4	0	80	4	-4	-12	17	22	13*
-5	35	6	15	0	69	9	2	-7	53	5	7	1	85	3	-2	-11	43	6	4
-4	90	5	-5	1	21	21	10*	-6	140	4	6	2	99	3	-1	-10	37	9	-12
-3	99	4	-8	2	0	24	-9*	-5	167	5	3	3	49	4	3	-9	23	23	22*
-2	131	4	-6	K,L=		1,	12	-4	39	6	-1	4	22	22	14*	-8	16	21	1*
-1	15	19	-5*	-7	39	12	1	-3	40	7	-3	5	81	4	1	-7	64	5	-3

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
-6	30	6	12	-5	27	9	22	4	46	6	7	-12	28	15	25	0	77	4	0
-5	177	6	3	-4	45	6	-2	5	82	3	-2	-11	63	6	4	1	36	10	-4
-4	40	5	1	-3	73	4	2	6	96	4	-3	-10	27	5	-13	2	306	9	-6
-3	13	30	7*	-2	41	12	-10	7	38	6	-5	-9	109	5	-1	3	30	8	5
-2	109	4	-2	-1	57	9	-9	8	60	8	-3	-8	70	4	2	4	149	5	-2
-1	0	18	-11*	0	24	26	22*	9	48	9	6	-7	139	4	3	5	67	6	-3
0	115	4	-4	1	12	25	-16*	10	96	6	-4	-6	76	3	4	6	39	12	4
1	38	11	7	2	19	25	10*	11	59	6	-4	-5	30	6	0	7	23	17	18
2	96	3	3	3	15	24	-3*	K,L=		3,	2	-4	91	3	-1	8	37	16	4
3	159	5	-6	4	43	6	4	-12	51	6	-5	-3	24	14	2	K,L=		3,	7
4	38	31	7	K,L=		2,	11	-11	19	25	9*	-2	89	4	1	-11	44	9	7
5	19	31	9*	-8	19	27	-3*	-10	21	21	7*	-1	87	3	-6	-10	44	7	7
6	18	20	16*	-7	17	27	-8*	-9	47	6	2	0	152	5	2	-9	69	4	-4
7	70	6	3	-6	44	13	5	-8	118	4	4	1	280	8	-1	-8	135	4	-1
K,L=		2,	8	-5	67	4	-4	-7	21	21	-16*	2	230	7	-4	-7	25	16	-8
-11	58	5	12	-4	64	4	1	-6	65	4	4	3	199	6	3	-6	22	10	20
-10	22	25	17*	-3	51	6	-0	-5	49	6	-1	4	112	4	1	-5	58	6	-9
-9	122	5	-1	-2	57	6	-2	-4	64	3	7	5	103	4	-1	-4	31	12	1
-8	18	20	3*	-1	22	17	11	-3	167	5	-0	6	71	3	-2	-3	61	5	-9
-7	162	5	0	0	51	8	13	-2	209	6	-4	7	34	6	-1	-2	24	8	8
-6	19	26	-1*	1	9	24	4*	-1	175	5	1	8	126	5	-4	-1	20	20	-5*
-5	86	3	0	2	57	8	7	0	51	3	-6	9	33	7	4	0	91	4	-7
-4	34	7	-8	K,L=		2,	12	1	68	4	3	K,L=		3,	5	1	80	4	2
-3	181	4	-7	-6	39	17	6	2	162	5	10	-12	51	9	-2	2	61	8	3
-2	23	27	-16*	-5	29	21	-10	3	243	7	6	-11	32	6	-16	3	42	9	-3
-1	124	4	-8	-4	30	33	4*	4	27	7	4	-10	81	4	-11	4	2	33	-15*
0	35	6	1	-3	17	25	-3*	5	165	5	4	-9	26	13	7	5	22	27	20*
1	68	7	1	-2	14	26	-9*	6	20	26	12*	-8	20	27	19*	6	20	27	11*
2	49	8	6	-1	32	15	-2	7	126	5	-3	-7	12	23	6*	7	12	25	11*
3	16	31	-5*	K,L=		3,	0	8	41	7	-4	-6	75	3	4	K,L=		3,	8
4	39	6	1	1	226	7	4	9	103	5	-8	-5	163	5	-4	-11	56	7	-1
5	3	21	-0*	2	57	3	-2	10	55	9	-1	-4	26	13	6	-10	31	13	4
6	26	11	5	3	427	13	18	K,L=		3,	3	-3	107	4	-0	-9	14	28	-4*
K,L=		2,	9	4	189	6	5	-12	25	13	15	-2	236	7	-7	-8	38	12	9
-11	26	27	10*	5	220	7	5	-11	28	10	14	-1	18	22	7*	-7	102	4	2
-10	37	16	-1	6	17	9	1	-10	58	8	-4	0	39	4	-6	-6	65	5	-2
-9	21	25	1*	7	142	4	-4	-9	114	4	-12	1	10	17	7*	-5	64	6	-6
-8	41	12	14	8	168	5	-2	-8	189	6	-2	2	181	6	-2	-4	97	5	3
-7	18	31	10*	9	145	4	-4	-7	56	4	2	3	189	6	-4	-3	22	27	-5*
-6	26	9	9	10	27	20	-2	-6	75	3	-2	4	30	26	3	-2	21	23	12*
-5	203	6	-3	11	34	6	2	-5	233	7	1	5	14	20	2*	-1	25	17	2
-4	9	20	-7*	K,L=		3,	1	-4	96	3	6	6	87	5	6	0	30	9	6
-3	162	6	-12	-11	62	4	-2	-3	26	7	8	7	88	4	-3	1	186	6	-6
-2	38	10	3	-10	69	4	-3	-2	104	3	-1	8	16	27	-6*	2	44	6	-8
-1	78	5	-3	-9	124	4	-4	-1	19	7	9	9	12	22	8*	3	134	5	-3
0	50	5	1	-8	122	5	-0	8	338	10	5	K,L=		3,	6	4	49	6	7
1	35	9	9	-7	92	3	0	1	240	7	5	-11	17	25	15*	5	23	14	22
2	22	13	13	-6	106	4	-3	2	201	6	4	-10	0	22	-6*	6	53	9	11
3	18	20	15*	-5	81	4	-1	3	170	5	1	-9	68	6	7	K,L=		3,	9
4	27	16	11	-4	130	4	3	4	47	4	-7	-8	19	29	14*	-10	24	24	-10*
5	45	6	7	-3	63	4	-2	5	59	6	-6	-7	178	6	-1	-9	55	5	8
K,L=		2,	10	-2	73	4	2	6	67	4	0	-6	44	4	-3	-8	26	13	-5
-10	32	9	2	-1	34	8	-3	7	76	7	-2	-5	138	5	-6	-7	23	24	-5*
-9	22	24	-8*	0	328	10	15	8	50	10	-5	-4	46	6	2	-6	19	28	10*
-8	33	14	-7	1	270	8	4	9	29	12	6	-3	88	3	-4	-5	29	14	-5
-7	38	7	8	2	134	4	6	10	43	8	7	-2	112	4	-6	-4	63	6	-3
-6	19	24	15*	3	13	15	-8*	K,L=		3,	4	-1	43	6	-6	-3	38	5	9

STRUCTURE FACTORS CONTINUED FOR
C9 H13 N O2

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
-2	108	4	-1	-2	28	4	5	9	96	4	-2	1	33	6	-1	K,L=	4,	10	
-1	64	5	1	-1	195	6	4	K,L=	4,	4		2	31	11	-3	-8	44	10	5
0	58	4	13	0	333	10	8	-11	23	27	-1*	3	45	9	1	-7	74	4	-2
1	37	12	1	1	259	8	11	-10	33	7	-0	4	64	4	8	-6	76	4	3
2	13	22	5*	2	226	7	2	-9	45	6	0	5	29	17	-9	-5	42	6	2
3	41	7	-0	3	33	8	-2	-8	19	20	9*	6	20	20	14*	-4	26	16	-8
4	23	28	11*	4	389	11	7	-7	186	6	-2	7	24	17	-7	-3	21	28	16*
K,L=		3,	10	5	36	8	2	-6	27	12	-5	K,L=		4,	7	-2	49	9	-2
-9	25	13	4	6	58	6	1	-5	73	3	-1	-10	59	7	2	-1	26	10	8
-8	40	8	4	7	94	4	5	-4	169	6	3	-9	25	14	5	0	23	25	-1*
-7	18	25	2*	8	146	5	-4	-3	29	5	12	-8	31	13	7	1	45	10	-1
-6	35	7	11	9	12	28	-5*	-2	21	9	12	-7	33	8	0	2	63	5	3
-5	11	23	-6*	10	15	28	8*	-1	47	4	-4	-6	76	6	-1	K,L=		4,	11
-4	74	4	2	K,L=		4,	2	0	50	6	-3	-5	66	4	-10	-6	17	23	-6*
-3	21	27	0*	-11	24	19	18	1	106	4	2	-4	13	26	7*	-5	17	23	14*
-2	80	5	1	-10	55	7	-1	2	140	4	1	-3	15	20	10*	-4	23	15	18
-1	19	20	17*	-9	53	8	9	3	45	6	-1	-2	31	6	13	-3	17	22	-0*
0	26	14	7	-8	104	4	6	4	33	6	2	-1	126	4	-5	-2	23	25	7*
1	37	11	-2	-7	106	4	-1	5	72	4	-2	0	14	21	8*	-1	56	10	4
2	69	5	5	-6	55	6	-2	6	36	7	5	1	118	4	-4	K,L=		5,	0
3	31	10	7	-5	127	4	-2	7	53	5	-1	2	134	5	-4	1	163	5	6
K,L=		3,	11	-4	314	9	3	8	21	30	13*	3	46	8	1	2	133	4	0
-8	51	8	11	-3	13	23	-6*	9	25	26	22*	4	37	8	4	3	156	5	9
-7	72	5	5	-2	135	4	3	K,L=		4,	5	5	11	23	4*	4	143	4	-3
-6	0	34	-9*	-1	133	4	-8	-11	40	10	-2	6	23	30	-7*	5	124	4	-5
-5	15	30	8*	0	197	6	-3	-10	47	5	10	K,L=		4,	8	6	44	4	-6
-4	27	28	7*	1	221	7	4	-9	14	23	10*	-10	30	11	-8	7	56	3	2
-3	21	31	3*	2	57	3	0	-8	99	4	-2	-9	23	11	11	8	112	4	2
-2	19	21	-5*	3	28	7	5	-7	148	5	-1	-8	42	9	-10	9	28	8	-0
-1	18	27	-1*	4	117	5	-7	-6	43	4	3	-7	94	5	2	10	36	7	1
0	48	12	5	5	151	5	-3	-5	47	6	6	-6	42	14	-2	K,L=		5,	1
1	8	30	-29*	6	31	11	-1	-4	34	5	0	-5	84	4	-5	-10	47	10	-4
K,L=		3,	12	7	68	4	-3	-3	54	4	-2	-4	71	5	-0	-9	54	4	5
-4	37	17	-3	8	45	10	-1	-2	17	22	-3*	-3	101	4	-10	-8	29	12	7
K,L=		4,	0	9	35	8	9	-1	125	4	-6	-2	42	10	2	-7	33	7	10
0	356	10	4	10	9	27	-3*	0	152	5	-5	-1	26	16	18	-6	146	5	-5
1	124	4	2	K,L=		4,	3	1	173	5	-3	0	52	5	1	-5	31	14	-2
2	47	2	0	-11	100	4	-4	2	70	4	-1	1	14	22	14*	-4	136	4	-1
3	36	5	6	-10	11	22	1*	3	135	4	7	2	109	4	3	-3	82	4	1
4	66	3	3	-9	26	9	17	4	152	5	-5	3	41	11	0	-2	116	4	1
5	19	20	5*	-8	135	4	-1	5	63	4	5	4	57	7	3	-1	19	10	5
6	95	3	-2	-7	181	6	-7	6	26	27	-11*	5	41	11	-9	0	65	3	-1
7	117	4	2	-6	24	7	0	7	6	25	-4*	K,L=		4,	9	1	81	3	4
8	66	4	-1	-5	97	3	7	8	13	29	-8*	-9	22	23	1*	2	28	8	3
9	34	5	4	-4	11	22	7*	K,L=		4,	6	-8	41	6	-3	3	36	5	-7
10	85	4	4	-3	11	16	-5*	-11	18	22	11*	-7	66	6	-3	4	48	4	-2
11	51	7	-3	-2	119	4	4	-10	22	13	14	-6	43	8	-10	5	120	5	-3
K,L=		4,	1	-1	68	3	-8	-9	42	5	-1	-5	90	4	-5	6	40	5	2
-11	82	4	2	0	127	4	-0	-8	116	4	-6	-4	35	16	6	7	71	5	-7
-10	1	20	-13*	1	44	8	6	-7	97	4	-8	-3	91	6	-2	8	61	5	5
-9	106	4	3	2	88	4	1	-6	149	5	-7	-2	33	7	-8	9	18	26	11*
-8	20	23	-9*	3	18	20	1*	-5	37	5	1	-1	27	28	-2*	K,L=		5,	2
-7	62	4	6	4	39	9	2	-4	121	4	-6	0	22	26	1*	-10	57	5	0
-6	30	7	-0	5	32	13	4	-3	115	4	-2	1	28	31	-0*	-9	35	11	2
-5	71	3	4	6	32	6	-7	-2	18	21	7*	2	70	5	-3	-8	39	6	4
-4	204	6	6	7	11	22	8*	-1	19	28	-5*	3	68	6	5	-7	31	16	27
-3	126	4	2	8	54	6	3	0	23	14	17	4	27	33	11*	-6	55	4	1

STRUCTURE FACTORS CONTINUED FOR
C9 H13 N O2

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
-5	19	27	6*	-9	21	15	-2	-4	137	5	-10	7	42	6	-1	-9	53	8	9
-4	102	4	0	-8	17	20	0*	-3	29	12	26	8	0	28	-20*	-8	23	12	13
-3	28	6	10	-7	20	23	-10*	-2	28	16	5	K,L=	6,	2		-7	19	21	-3*
-2	218	7	-4	-6	125	4	-1	-1	51	5	9	-9	64	4	-0	-6	94	4	-9
-1	90	4	5	-5	79	6	-1	0	37	8	2	-8	0	21	-12*	-5	114	4	-3
0	58	3	4	-4	44	6	1	1	42	9	1	-7	43	6	-4	-4	7	20	-2*
1	15	17	11*	-3	22	13	11	2	33	7	7	-6	167	5	-3	-3	84	4	1
2	30	11	-6	-2	105	4	-5	3	49	8	-3	-5	25	26	-4*	-2	154	5	5
3	145	5	5	-1	81	3	2	4	32	11	11	-4	32	18	-2	-1	23	25	-5*
4	16	18	10*	0	163	5	-2	K,L=	5,	9		-3	16	21	-5*	0	20	13	-2
5	60	6	-5	1	103	4	3	-8	73	7	7	-2	69	4	1	1	8	28	7*
6	143	5	-1	2	35	9	6	-7	113	6	8	-1	240	7	-4	2	72	5	2
7	17	27	-7*	3	31	6	5	-6	43	23	6	0	38	5	16	3	21	22	15*
8	15	27	-11*	4	81	5	-6	-5	37	19	-8	1	66	6	-3	4	23	16	7
9	8	22	6*	5	29	13	10	-4	30	8	-7	2	93	4	1	5	23	16	9
K,L=	5,	3		6	33	13	4	-3	40	11	-10	3	15	18	8*	6	0	29	-2*
-10	18	21	13*	7	30	10	2	-2	39	13	-1	4	37	6	-2	K,L=	6,	6	
-9	18	29	2*	K,L=	5,	6		-1	71	4	5	5	6	23	5*	-8	28	11	-3
-8	36	7	4	-10	53	9	6	0	24	11	21	6	22	27	21*	-7	37	10	6
-7	109	4	-2	-9	0	28	-13*	1	44	6	-1	7	19	22	-1*	-6	35	7	10
-6	62	6	3	-8	76	5	-7	2	32	15	-2	8	33	8	3	-5	74	4	8
-5	274	8	-9	-7	74	4	-1	K,L=	5,	10		K,L=	6,	3		-4	7	24	-13*
-4	51	7	1	-6	39	8	-1	-6	33	10	7	-9	27	24	22	-3	22	23	17*
-3	118	4	-3	-5	28	7	8	-5	13	22	4*	-8	59	5	1	-2	44	7	7
-2	64	3	3	-4	20	14	3	-4	66	6	0	-7	20	27	14*	-1	127	4	-5
-1	203	6	7	-3	68	4	-3	-3	52	5	7	-6	63	7	-6	0	27	15	-2
0	75	4	2	-2	19	20	1*	-2	25	27	22*	-5	20	16	11	1	48	6	-1
1	64	5	1	-1	46	5	-1	-1	18	22	-4*	-4	120	4	1	2	22	15	5
2	39	9	4	0	123	4	1	0	37	9	7	-3	31	11	-6	3	87	4	2
3	24	9	1	1	0	24	-2*	K,L=	6,	0		-2	175	5	-3	4	31	9	2
4	126	4	-2	2	16	22	1*	0	184	6	-3	-1	63	5	-4	5	25	25	9*
5	49	6	-6	3	90	4	3	1	139	4	0	0	150	5	4	K,L=	6,	7	
6	78	3	0	4	47	5	1	2	263	8	-0	1	131	4	-1	-8	21	28	8*
7	15	21	-5*	5	63	4	6	3	23	14	-4	2	83	4	1	-7	69	5	10
8	30	11	5	6	28	11	5	4	28	5	7	3	123	5	7	-6	78	5	-3
K,L=	5,	4		K,L=	5,	7		5	40	4	2	4	12	23	-5*	-5	28	9	24
-10	36	11	-1	-9	13	28	3*	6	64	4	5	5	96	5	-2	-4	21	19	2
-9	34	7	4	-8	70	4	-5	7	11	22	-0*	6	14	23	1*	-3	36	16	1
-8	182	6	-2	-7	7	25	4*	8	20	14	15	7	29	32	6*	-2	3	23	1*
-7	34	10	5	-6	0	20	0*	9	33	8	7	K,L=	6,	4		-1	0	34	-4*
-6	137	5	-3	-5	42	11	-5	K,L=	6,	1		-9	44	7	-13	0	67	5	-7
-5	67	4	3	-4	58	4	6	-9	34	7	8	-8	23	12	-3	1	60	5	-1
-4	116	5	-5	-3	23	26	3*	-8	77	4	-1	-7	39	6	3	2	19	26	12*
-3	68	5	-3	-2	135	5	-6	-7	64	6	-0	-6	158	5	2	3	33	7	4
-2	67	4	-1	-1	47	8	-11	-6	105	4	2	-5	122	5	-4	K,L=	6,	8	
-1	13	29	-11*	0	64	7	-3	-5	171	5	-4	-4	61	6	-1	-7	42	11	-4
0	114	4	1	1	32	15	-6	-4	45	7	-4	-3	14	29	9*	-6	50	5	4
1	91	4	0	2	23	22	17	-3	104	4	0	-2	74	6	2	-5	63	6	2
2	59	4	3	3	20	21	18*	-2	55	5	1	-1	21	23	-7*	-4	22	22	2*
3	21	14	-2	4	59	5	0	-1	33	8	7	0	92	3	-1	-3	21	22	20*
4	68	3	1	5	21	28	19*	0	108	4	-0	1	28	7	5	-2	21	25	5*
5	48	6	-1	K,L=	5,	8		1	73	4	5	2	71	4	2	-1	63	4	3
6	76	5	1	-9	0	42	-1*	2	39	7	3	3	81	5	1	0	25	32	7*
7	61	6	-1	-8	13	22	12*	3	28	9	10	4	18	26	9*	1	21	17	12
8	43	7	16	-7	22	29	-1*	4	13	19	5*	5	32	13	9	2	7	23	2*
K,L=	5,	5		-6	144	7	-8	5	19	30	7*	6	76	4	7	K,L=	6,	9	
-10	22	25	15*	-5	27	18	6	6	86	4	-6	K,L=	6,	5		-5	29	27	28

STRUCTURE FACTORS CONTINUED FOR
C9 H13 N O2

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
-4	17	23	11*	6	23	36	22*	-2	22	13	4								
-3	6	23	-19*	K,L=	7,	4		-1	13	28	-1*								
-2	49	7	2	-7	20	27	-3*	0	29	8	8								
-1	21	27	15*	-6	81	4	0	1	38	8	-3								
K,L=	7,	0		-5	12	20	5*	2	36	12	6								
1	94	4	-1	-4	29	9	9	3	24	16	-0								
2	68	3	-3	-3	51	10	-9	4	70	4	-1								
3	31	5	10	-2	73	4	0	K,L=	8,	2									
4	37	6	2	-1	185	6	3	-5	31	10	6								
5	19	20	16*	0	29	9	2	-4	37	10	20								
6	31	6	8	1	37	9	16	-3	8	30	3*								
7	22	13	-3	2	33	10	-11	-2	56	5	10								
K,L=	7,	1		3	25	15	3	-1	52	6	9								
-7	29	9	1	4	46	6	2	0	29	8	26								
-6	23	33	23*	5	17	29	-3*	1	34	7	5								
-5	24	27	12*	K,L=	7,	5		2	0	27	-14*								
-4	27	12	9	-7	0	22	-5*	3	28	32	-9*								
-3	38	8	7	-6	95	4	2	4	34	15	6								
-2	11	27	9*	-5	54	5	0	K,L=	8,	3									
-1	170	5	-5	-4	81	4	2	-5	26	30	25*								
0	92	5	0	-3	96	7	2	-4	119	5	-3								
1	195	6	4	-2	34	7	-0	-3	132	5	3								
2	93	4	-6	-1	26	22	22	-2	71	8	5								
3	17	19	9*	0	47	9	3	-1	22	15	5								
4	56	7	-5	1	71	5	-2	0	62	7	4								
5	46	14	2	2	65	6	-1	1	27	10	-2								
6	22	14	7	3	64	6	7	2	22	29	3*								
7	17	21	6*	4	60	7	4	3	101	5	12								
K,L=	7,	2		K,L=	7,	6		K,L=	8,	4									
-7	118	4	6	-6	74	8	14	-4	23	13	8								
-6	20	20	6*	-5	23	25	8*	-3	19	23	11*								
-5	25	10	12	-4	11	21	-2*	-2	17	25	3*								
-4	56	6	5	-3	23	16	23	-1	28	10	10								
-3	8	20	8*	-2	20	26	-8*	0	44	5	5								
-2	44	5	0	-1	23	25	-9*	1	47	15	-7								
-1	88	4	-5	0	70	4	3	2	35	9	-4								
0	42	5	2	1	19	23	3*	K,L=	8,	5									
1	61	6	5	2	98	4	13	-3	89	5	6								
2	47	9	-1	K,L=	7,	7		-2	10	22	-6*								
3	22	15	8	-5	40	8	-4	-1	28	31	18*								
4	67	7	-5	-4	63	5	4	0	31	9	25								
5	53	7	1	-3	85	4	1												
6	57	9	3	-2	0	32	-3*												
K,L=	7,	3		-1	36	7	2												
-7	50	8	-6	0	16	23	2*												
-6	72	5	-4	1	26	21	15												
-5	36	9	-2	K,L=	8,	0													
-4	80	4	1	0	30	9	0												
-3	16	23	13*	1	22	21	19												
-2	38	9	12	2	18	20	-8*												
-1	12	20	3*	3	55	4	3												
0	61	6	-6	4	24	11	13												
1	44	6	-1	5	43	7	-1												
2	64	4	-5	K,L=	8,	1													
3	92	4	-1	-5	32	15	15												
4	41	5	2	-4	138	5	-2												
5	25	17	20	-3	144	5	-4												

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720