

Lawrence Berkeley National Laboratory

Lawrence Berkeley National Laboratory

Title

SYNTHESIS AND STRUCTURE OF TWO CRYSTALLINE FORMS OF
CYCLOOCTATETRAENETHORIUM (IV) DICHLORIDE BISTETRAHDROFURAN

Permalink

<https://escholarship.org/uc/item/6j27p71t>

Author

Zalkin, Allan

Publication Date

1980-03-01



Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

Materials & Molecular Research Division

Submitted to Inorganic Chemistry

SYNTHESIS AND STRUCTURE OF TWO CRYSTALLINE FORMS
OF CYCLOOCTATETRAENETHORIUM(IV) DICHLORIDE BISTETRAHYDROFURAN

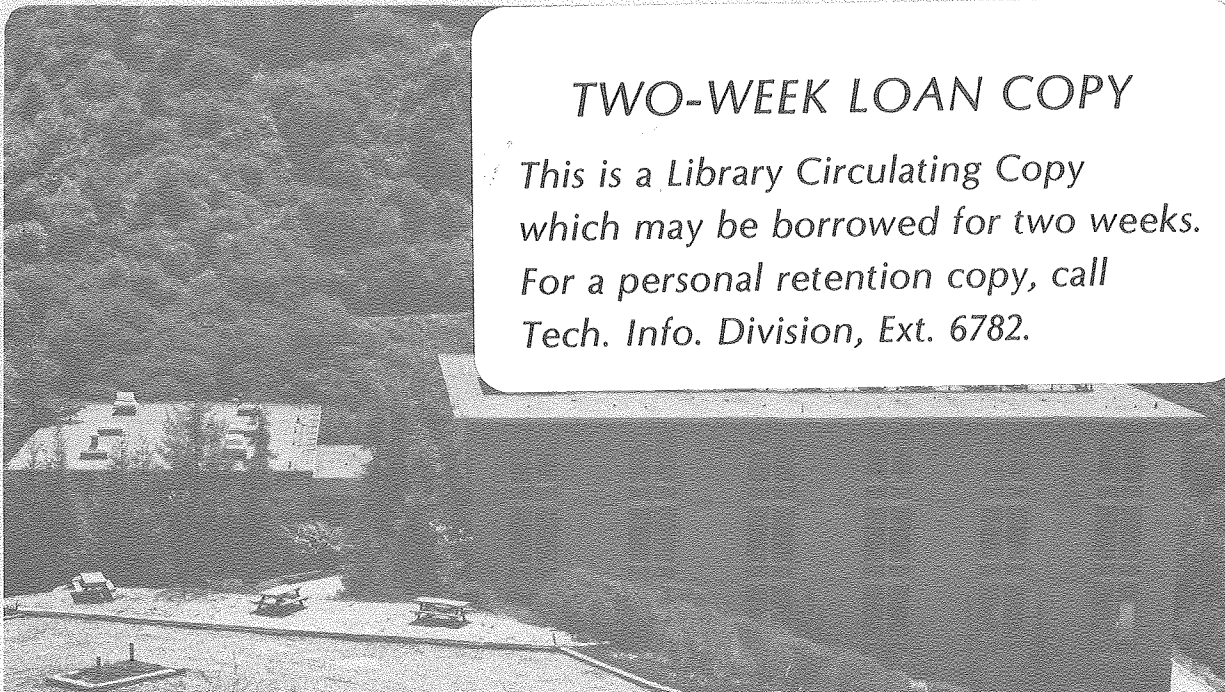
Allan Zalkin, David H. Templeton,
Carole Le Vanda and Andrew Streitwieser, Jr.

March 1980

RECEIVED
LAWRENCE
BERKELEY LABORATORY

APR 25 1980

LIBRARY AND
DOCUMENTS SECTION



TWO-WEEK LOAN COPY

*This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 6782.*

LBL 10537 c.2

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

SYNTHESIS AND STRUCTURE OF TWO CRYSTALLINE
FORMS OF CYCLOOCTATETRAENETHORIUM(IV)
DICHLORIDE BISTETRAHYDROFURAN

by Allan Zalkin,* David H. Templeton, Carole Le Vanda¹
and Andrew Streitwieser Jr.

Materials and Molecular Research Division
Lawrence Berkeley Laboratory and
Department of Chemistry
University of California
Berkeley, California 94720

MARCH 1980

$\text{Th}(\text{C}_8\text{H}_8)\text{Cl}_2(\text{OC}_4\text{H}_8)_2$ crystallizes in two modifications. The α -form, space group $\text{P2}_1/\text{n}$, has dimensions: $a = 8.589(4) \text{ \AA}$, $b = 27.222(10) \text{ \AA}$, $c = 7.950(4) \text{ \AA}$, $\beta = 96.92(5)^\circ$, $Z = 4$ and $d_x = 1.99 \text{ g/cm}^3$. The β -form, space group $\text{P2}_1/\text{c}$, has dimensions: $a = 13.036(6) \text{ \AA}$, $b = 11.601(6) \text{ \AA}$, $c = 24.598(10) \text{ \AA}$, $\beta = 102.90(5)^\circ$, $Z = 8$ and $d_x = 2.02 \text{ g/cm}^3$. The α -form has one molecule in the asymmetric unit whereas the β -form has two which are chemically equivalent but crystallographically different. The study thus yields three independent determinations of the same molecular structure. Thorium is bonded to the cyclooctatetraene ring, to two chlorine atoms, and to two oxygen atoms from the tetrahydrofuran moieties. Significant distances (averaged) are: $\text{Th-Cl} = 2.69 \text{ \AA}$, $\text{Th-O} = 2.57 \text{ \AA}$, and $\text{Th to plane of } \text{C}_8\text{H}_8 = 2.02 \text{ \AA}$.

INTRODUCTION

Since the first synthesis of uranocene, di- π -cyclooctatetraene-uranium(IV),² a large number of related compounds have been prepared.³ The bis-cyclooctatetraene compounds of all the lower actinides are now known, including thoracene, di- π -cyclooctatetraeneethorium(IV).⁴ X-ray crystal structures have been determined at Berkeley for several of these compounds.⁵ All show the central metal atom in the center of two parallel planar eight-member rings.

We recently reported the preparation of mono-cyclooctatetraene-thorium(IV) dichloride and diborohydride.⁶ In this paper we report the crystal structure of the dichloride which was isolated as the bis-tetrahydrofuran compound, $C_8H_8ThCl_2 \cdot 2C_4H_8O$, 1, by the reaction of thoracene with thorium tetrachloride in THF. Compound 1 is more soluble in THF than is thorocene itself.

EXPERIMENTAL

Cyclooctatetraenethorium dichloride bis-tetrahydrofuran. A suspension of 1.3 g (3.0 mmoles) of thoracene and 1.7 g (4.5 mmoles) of thorium tetrachloride in tetrahydrofuran (THF) was stirred at reflux under argon until the yellow color of thoracene disappeared (ca 1 wk). The mixture was degassed, taken into the glove box and the solid was separated by centrifugation. The THF-soluble portions were combined and the solvent was removed by vacuum transfer. Crystals were grown

from hot saturated THF solutions. Anal. Calcd. for $C_{16}H_{24}ThClO_2$: C, 34.86; H, 4.39; Cl, 12.86. Found: C, 34.65; H, 4.38; Cl, 12.22.

X-Ray Diffraction. White crystals of the compounds, because of their extreme sensitivity to the atmosphere, were sealed inside thin-walled quartz capillaries for the X-ray experiments. Weissenberg photography showed the material to be monoclinic, later designated as the β -form. Upon investigating a different crystal on a Picker FACS-I automated diffractometer, which was equipped with a graphite monochromator and a copper X-ray tube, we found it to be monoclinic with different cell dimensions than the first crystal. This new form was designated as the α -form and a set of intensity data was collected from it. A third crystal from the same preparation was investigated and observed to be the β -form, and a set of intensity data was collected from it.

In both cases, setting angles of 12 reflections where $95 < 2\theta < 106^\circ$ ($\lambda_{CuK\alpha_1} = 1.54056 \text{ \AA}$) were used for least-squares adjustment of the cell dimensions. Cell dimensions and other crystal data are given in Table I.

A θ - 2θ scan technique with a scan speed of $2^\circ/\text{min}$ was used to collect the intensities in the range of $4^\circ < 2\theta < 120^\circ$; backgrounds were measured for 4 seconds at the beginning and end of each scan. Omega scans of several low-angle reflections showed widths at half-peak height of 0.13° to 0.15° . Three standard reflections were measured after each 200th scan to monitor for crystal decay, instrumental stability, and crystal alignment. A decay of 5% was observed in the intensities of the standards of both data sets, and the data

were adjusted accordingly. Correction for absorption was made by an analytical integration method.⁷ During refinement, effects of extinction were evident in the data, and an empirical isotropic correction was applied, see Table I. Atomic scattering factors of Cromer and Waber⁸ were used for Th, of Doyle and Turner⁹ for Cl, O and C, and of Stewart, Davidson and Simpson¹⁰ for hydrogen. Anomalous scattering corrections of Cromer and Liberman¹¹ were applied.

Determination of Structures. Three-dimensional Patterson maps indicated the positions of the Th atoms. Subsequent least-squares refinements and difference Fourier maps readily revealed all of the non-hydrogen atoms. All of the atoms, with the exception of the hydrogen atoms, were assigned anisotropic thermal parameters in the final refinements. For the β compound, because the thermal tensor for one of the C_8H_8 carbon atoms was not positive-definite, the thermal parameters of the opposing carbons in the C_8H_8 ring were constrained to be equal. Hydrogen atom parameters were estimated from the geometry at C-H distances of 0.95 Å and included in the least-squares calculations, but not refined. The full-matrix least-squares program minimizes the function $\Sigma w(\Delta F)^2 / \Sigma w F_o^2$. After the last cycle of refinement the largest shift of a parameter was 0.02 and 0.24 of its e.s.d. for the α and the β compound, respectively. R factors and other statistical results of the least-squares refinements are given in Table I.

Positional parameters are given in Table II. Tables of the anisotropic thermal parameters, the calculated hydrogen positions,

and the lists of observed structure factors are in the supplementary material. Distances and angles are given in Tables III and IV, with atoms numbers as in Fig. 1.

DISCUSSION

The Th atom is bonded to the cyclooctatetraene (COT) ring, to two chloride ions and to the oxygen atoms of the two THF molecules; see Fig. 1. The COT ring is centrally located on the Th atom with its plane at a distance of 2.02 Å. The chloride ions and THF molecules are alternatively disposed on the opposite side, with Th-Cl and Th-O distances of 2.686 ± 0.006 Å and 2.57 ± 0.02 Å, respectively. The Cl and the O atoms are very nearly equidistant from the COT plane; see Table V. The comparable Th-to-ring distance in thoracene^{5b} is 2.00 Å, and the Th-Cl distances in these structures are just slightly under the 2.72 Å and 2.90 Å reported for ThCl₄.¹² The Cl-Cl vector is orthogonal to the O-O vector (see Fig. 2) and both are from 4° to 9° from an eclipsed orientation with the COT carbon atoms.

The 3 molecular structures determined in this study are chemically identical with essentially identical bond distances. About the only significant geometrical difference between the α and β forms is the larger Cl-Th-Cl and smaller O-Th-O angles that the α form exhibits, which is probably a packing effect. Nothing in the experiments reported here gives any information concerning what fosters the crystallization of one form rather than the other.

ACKNOWLEDGEMENT

We thank Dr. Jeffrey P. Solar for glove box manipulation of the crystals into the quartz capillaries. This work was supported by the Division of Nuclear Sciences, Office of Basic Energy Sciences, U. S. Department of Energy, under contract No. W-7405-Eng-48.

SUPPLEMENTARY MATERIAL AVAILABLE

A list of anisotropic thermal parameters, a list of estimated hydrogen positional parameters, and a listing of observed structure factors (35 pages). Ordering information is given on any current masthead page.

REFERENCES

1. Fellow of the Miller Institute for Basic Research in Science, 1975-7; NSF Postdoctoral Fellow, 1977-8.
2. Streitwieser, Jr., A; Müller-Westerhoff, U. J. Am. Chem. Soc. 1968, 90, 7364.
3. For recent reviews see various chapters in "Organometallics of the f-Elements", eds., D. Reidel Publishing Co., Dordrecht, Holland, 1979.
4. Streitwieser, Jr., A.; Yoshida, N. J. Am. Chem. Soc. 1979, 91, 7528.
5. (a) Uranocene: Zalkin, A.; Raymond, K. N. J. Am. Chem. Soc. 1969, 91, 5667; (b) Uranocene and thorocene: Avdeef, A.; Raymond, K. N.; Hodgson, K. O.; Zalkin, A. Inorg. Chem. 1972, 11, 1083; (c) bis(1,3,5,7-tetramethylcyclooctatetraene)uranium: Hodgson, K. O.; Raymond, K. N. Inorg. Chem. 1973, 12, 458; (d) bis(1,3,5,7-tetraphenylcyclooctatetraene)uranium: Templeton, L. K.; Templeton, D. H.; Walker, R. Inorg. Chem. 1976, 15, 3000; (e) bis(cyclobutenocyclooctatetraene)uranium: Zalkin, A.; Templeton, D. H.; Berryhill, S. R.; Luke, W. D. Inorg. Chem. 1979, 18, 2287.
6. Le Vanda, C.; Solar, J. P.; Streitwieser, Jr., A. J. Am. Chem. Soc. 1980, 102, in press.
7. Templeton, L. K.; Templeton, D. H. Abstracts, American Crystallographic Association Proceedings, 1973, Series 2, Vol. 1, p. 143.
8. Cromer, D. T.; Waber, J. T. Acta Crystallogr. Sect. A 1965, 18, 104.
9. Doyle, P. A.; Turner, P. S. Acta Crystallogr. Sect. A 1968, 24, 390.

10. Stewart, R. F.; Davidson, E. R.; Simpson, W. T. J. Chem. Phys. 1965, 42, 3175.
11. Cromer, D. T.; Liberman, D. J. Chem. Phys. 1970, 53, 1891.
12. Mucker, K.; Smith, G. S.; Johnson, Q.; Elson, R. E. Acta Crystallogr. 1969, B25, 2362.

Table I. Summary of Crystal Data Intensity Collection and Least-Squares Refinement Statistics

Compound	$\alpha\text{-C}_8\text{H}_8\text{ThCl}_2(\text{OC}_4\text{H}_8)_2$	$\beta\text{-C}_8\text{H}_8\text{ThCl}_2(\text{OC}_4\text{H}_8)_2$
Formula wt	551.31	551.31
a, Å	8.589(3)	13.036(4)
b, Å	27.22(2)	11.601(3)
c, Å	7.950(3)	24.598(8)
β , deg	96.92(4)	102.90(4)
V, Å ³	1845	3626
Space group	P2 ₁ /n	P2 ₁ /c
Z	4	8
Density, calcd, g/cm ³	1.985	2.020
Color	white	white
Crystal size, mm	parallelepiped 0.1 x 0.2 x 0.3	0.15 x 0.15 x 0.3
Crystal vol, mm ³	0.007	0.007
μ , cm ⁻¹	288	293
T, °C	22	21
No. of scans (including standards)	5679	11573
Decay correction range	1.0-1.05	1.0-1.05
No. of unique data	2740	5390
No. data $F^2 > 3\sigma$ used in least-squares	2242	3914
Extinction factor k $F_{\text{corr}} = (1 + kI)F_{\text{obs}}$	5×10^{-7}	7×10^{-7}

Ignorance factor, p, in weighting expression $w = ((\sigma^2 F^2) + (p F^2)^2)^{-1}$	0.04	0.06
No. of variables in least-squares	190	331
$R_w = [\Sigma w (\Delta F)^2 / \Sigma w F_{obs}^2]^{1/2}$	0.045	0.054
$R = \Sigma \Delta F / \Sigma F_{obs} $ $F^2 > 3\sigma$	0.036	0.045
R for all data	0.044	0.064
Goodness of fit	1.24	1.16

Table II. Positional Parameters^a

α -form

ATOM	X	Y	Z
TH	.46399(4)	.13344(1)	.05714(3)
CL(1)	.5612(3)	.08843(9)	-.2128(3)
CL(2)	.2512(3)	.0769(1)	.1868(3)
O(1)	.223(1)	.1350(3)	-.169(1)
O(2)	.6250(3)	.0622(2)	.1857(7)
C(1)	.393(2)	.2010(4)	.292(1)
C(2)	.530(2)	.1810(4)	.360(1)
C(3)	.677(2)	.1714(4)	.305(2)
C(4)	.740(2)	.1799(4)	.156(2)
C(5)	.689(2)	.2004(4)	.000(2)
C(6)	.547(2)	.2202(4)	-.073(2)
C(7)	.400(2)	.2291(4)	-.017(2)
C(8)	.336(2)	.2207(4)	.133(2)
C(9)	.230(2)	.1477(6)	-.344(2)
C(10)	.072(2)	.1397(5)	-.429(2)
C(11)	-.032(3)	.1411(7)	-.293(3)
C(12)	.063(2)	.1387(7)	-.138(2)
C(13)	.603(2)	.0395(4)	.347(1)
C(14)	.758(2)	.0174(5)	.414(2)
C(15)	.838(2)	.0101(6)	.265(2)
C(16)	.768(2)	.0425(5)	.126(2)

Table II. Continued

β -form

ATOM	X	Y	Z
TH(1)	.08705(4)	.17124(4)	.33807(2)
TH(2)	.41202(4)	.26318(4)	.62281(2)
CL(1)	-.0870(3)	.0453(3)	.3322(2)
CL(2)	.2072(3)	.0214(3)	.2963(1)
CL(3)	.2107(3)	.1956(3)	.5916(2)
CL(4)	.4755(3)	.2098(4)	.5290(1)
O(1)	.0054(8)	.1715(7)	.2337(4)
O(2)	.1444(8)	.0169(8)	.4139(4)
O(3)	.4190(3)	.0417(8)	.6268(4)
O(4)	.3192(8)	.4179(8)	.5532(4)
C(1)	-.017(1)	.372(1)	.3352(7)
C(2)	.055(2)	.393(1)	.3044(7)
C(3)	.160(2)	.372(1)	.3073(7)
C(4)	.243(1)	.332(1)	.3487(8)
C(5)	.251(1)	.290(1)	.4002(8)
C(6)	.185(2)	.274(1)	.4368(7)
C(7)	.075(2)	.290(1)	.4316(7)
C(8)	-.005(1)	.331(1)	.3897(8)
C(9)	.383(1)	.309(2)	.7264(6)
C(10)	.454(2)	.217(2)	.7333(7)
C(11)	.549(2)	.198(1)	.7187(7)
C(12)	.612(1)	.253(2)	.6858(7)
C(13)	.606(1)	.362(2)	.6600(6)
C(14)	.533(2)	.454(1)	.6541(6)
C(15)	.441(2)	.477(1)	.6715(7)
C(16)	.380(1)	.416(2)	.7002(7)
C(17)	.067(1)	.187(1)	.1905(6)
C(18)	-.016(2)	.191(2)	.1385(7)
C(19)	-.117(2)	.214(3)	.1500(8)
C(20)	-.107(1)	.196(1)	.2110(6)
C(21)	.252(1)	-.021(1)	.4339(6)
C(22)	.259(1)	-.069(2)	.4895(8)
C(23)	.152(2)	-.100(2)	.4922(7)
C(24)	.085(1)	-.013(1)	.4558(6)
C(25)	.364(2)	-.023(1)	.6620(8)
C(26)	.370(2)	-.144(2)	.6432(9)
C(27)	.467(2)	-.155(2)	.6226(7)
C(28)	.497(1)	-.032(1)	.6138(7)
C(29)	.369(2)	.485(2)	.5167(7)
C(30)	.286(2)	.569(2)	.487(1)
C(31)	.213(2)	.575(2)	.520(1)
C(32)	.221(1)	.471(1)	.5549(7)

^aEstimated standard deviation of the least significant digit is given in parentheses here and in the following tables.

Table III. Interatomic Distances

α			β (molecule 1)		β (molecule 2)	
Atoms	D(Å)		Atoms	D(Å)	Atoms	D(Å)
Th -Cl(1)	2.690(2)		Th(1)-Cl(1)	2.676(4)	Th(2)-Cl(3)	2.681(4)
-Cl(2)	2.688(3)		-Cl(2)	2.692(3)	-Cl(4)	2.691(3)
-O(1)	2.58(1)		-O(1)	2.55(1)	-O(3)	2.57(1)
-O(2)	2.53(1)		-O(2)	2.57(1)	-O(4)	2.59(1)
-C(1)	2.74(1)		-C(1)	2.69(2)	-C(9)	2.71(1)
-C(2)	2.73(1)		-C(2)	2.71(2)	-C(10)	2.70(2)
-C(3)	2.73(1)		-C(3)	2.69(2)	-C(11)	2.73(2)
-C(4)	2.72(1)		-C(4)	2.73(2)	-C(12)	2.72(2)
-C(5)	2.73(1)		-C(5)	2.71(2)	-C(13)	2.74(2)
-C(6)	2.71(1)		-C(6)	2.75(2)	-C(14)	2.73(2)
-C(7)	2.71(1)		-C(7)	2.72(2)	-C(15)	2.75(2)
-C(8)	2.72(1)		-C(8)	2.68(2)	-C(16)	2.70(2)
C(8) -C(1)	1.40(2)		C(8) -C(1)	1.40(2)	C(16)-C(9)	1.40(3)
C(1) -C(2)	1.35(2)		C(1) -C(2)	1.35(2)	C(9) -C(10)	1.40(3)
C(2) -C(3)	1.41(2)		C(2) -C(3)	1.37(3)	C(10)-C(11)	1.38(2)
C(3) -C(4)	1.39(2)		C(3) -C(4)	1.39(3)	C(11)-C(12)	1.43(2)

Table III. (Continued)

C(4) -C(5)	1.38(2)	C(4) -C(5)	1.34(2)	C(12)-C(13)	1.40(2)
C(5) -C(6)	1.39(2)	C(5) -C(6)	1.38(3)	C(13)-C(14)	1.41(2)
C(6) -C(7)	1.41(2)	C(6) -C(7)	1.43(3)	C(14)-C(15)	1.39(2)
C(7) -C(8)	1.39(2)	C(7) -C(8)	1.38(3)	C(15)-C(16)	1.37(2)
C-C(ave)	1.39 ± .02	C-C(ave)	1.38 ± .03	C-C(ave)	1.40 ± .02
O(1) -C(9)	1.44(1)	O(1) -C(17)	1.48(2)	O(3) -C(25)	1.45(2)
-C(12)	1.43(2)	-C(20)	1.47(2)	-C(28)	1.42(2)
O(2) -C(13)	1.46(1)	O(2) -C(21)	1.44(2)	O(4) -C(29)	1.45(2)
-C(16)	1.47(1)	-C(22)	1.46(2)	-C(32)	1.43(2)
C(9) -C(10)	1.46(2)	C(17)-C(18)	1.48(2)	C(25)-C(26)	1.48(3)
C(10)-C(11)	1.48(2)	C(18)-C(19)	1.43(3)	C(26)-C(27)	1.47(3)
C(11)-C(12)	1.40(3)	C(19)-C(20)	1.49(2)	C(27)-C(28)	1.51(3)
C(13)-C(14)	1.50(2)	C(21)-C(22)	1.46(2)	C(29)-C(30)	1.52(3)
C(14)-C(15)	1.45(2)	C(22)-C(23)	1.46(3)	C(30)-C(31)	1.39(3)
C(15)-C(16)	1.49(2)	C(23)-C(24)	1.49(2)	C(31)-C(32)	1.47(2)

Ave of 6 Th-Cl values = 2.686 ± .006 Å

Ave of 6 Th-O values = 2.57 ± .02 Å

Ave of 24 Th-C values = 2.72 ± .02 Å

Ave of 24 C-C values = 1.39 ± .02 Å

Table III. (Continued)

α		$\beta(\text{molecule 1})$		$\beta(\text{molecule 2})$	
Cl(1)-Cl(1)	4.396	Cl(1)-Cl(2)	4.132	Cl(3)-Cl(4)	4.084
O(1) -O(2)	4.635	O(1) -O(2)	4.749	O(3) -O(4)	4.793
Cl(1)-O(1)	3.232	Cl(1)-O(1)	3.280	Cl(3)-O(3)	3.203
Cl(1)-O(2)	3.230	Cl(1)-O(2)	3.248	Cl(3)-O(4)	3.184
Cl(2)-O(1)	3.222	Cl(2)-O(1)	3.241	Cl(4)-O(3)	3.305
Cl(2)-O(2)	3.237	Cl(2)-O(2)	3.177	Cl(4)-O(4)	3.297

Table IV. Selected Angles

α			β (molecule 1)		β (molecule 2)	
Atoms		Angle	Atoms	Angle	Atoms	Angle
Cl(1)-Th	-Cl(2)	109.6(1)	Cl(1)-Th(1)-Cl(2)	100.7(1)	Cl(3)-Th(2)-Cl(4)	99.0(3)
O(1)-Th	-O(2)	130.6(2)	O(1)-Th(1)-O(2)	136.0(3)	O(3)-Th(2)-O(4)	136.5(3)
Cl(1)-Th	-O(1)	75.7(2)	Cl(1)-Th(1)-O(1)	77.7(2)	Cl(3)-Th(2)-O(3)	75.1(3)
Cl(1)-Th	-O(2)	76.4(1)	Cl(1)-Th(1)-O(2)	76.4(2)	Cl(3)-Th(2)-O(4)	74.4(2)
Cl(2)-Th	-O(1)	75.5(2)	Cl(2)-Th(1)-O(1)	76.4(2)	Cl(4)-Th(2)-O(3)	77.8(2)
Cl(2)-Th	-O(2)	76.7(2)	Cl(2)-Th(1)-O(2)	74.2(2)	Cl(4)-Th(2)-O(4)	77.3(2)
Cl(1)-Th	-C(5)	83.1(3)	Cl(1)-Th(1)-C(8)	86.6(4)	Cl(3)-Th(2)-C(9)	89.5(4)
Cl(2)-Th	-C(1)	84.6(2)	Cl(2)-Th(1)-C(4)	89.8(3)	Cl(4)-Th(2)-C(13)	86.9(3)
O(1)-Th	-C(7)	73.0(4)	O(1)-Th(1)-C(2)	71.9(3)	O(3)-Th(2)-C(11)	71.2(4)
O(2)-Th	-C(3)	73.2(3)	O(2)-Th(1)-C(6)	70.2(4)	O(4)-Th(2)-C(15)	70.1(4)
C(8)-C(1)-C(2)		135(1)	C(8)-C(1)-C(2)	131(2)	C(16)-C(9)-C(10)	133(2)
C(1)-C(2)-C(3)		136(1)	C(1)-C(2)-C(3)	138(2)	C(9)-C(10)-C(11)	135(2)
C(2)-C(3)-C(4)		134(1)	C(2)-C(3)-C(4)	135(2)	C(10)-C(11)-C(12)	137(2)
C(3)-C(4)-C(5)		136(1)	C(3)-C(4)-C(5)	134(2)	C(11)-C(12)-C(13)	133(2)
C(4)-C(5)-C(6)		135(1)	C(4)-C(5)-C(6)	137(2)	C(12)-C(13)-C(14)	134(2)

Table IV. Continued

C(5) -C(6)-C(7)	135(1)	C(5) -C(6) -C(7)	133(2)	C(13)-C(14)-C(15)	136(2)
C(6) -C(7)-C(8)	135(1)	C(6) -C(7) -C(8)	134(2)	C(14)-C(15)-C(16)	134(2)
C(7) -C(8)-C(1)	135(1)	C(7) -C(8) -C(1)	138(2)	C(15)-C(16)-C(9)	138(2)

Table V. Least-square Plane and Distances (Å) of Atoms from the Planes.

Plane: C(1) - C(8) in α compound

$$2.367 x + 24.583 y + 2.336 z = 6.542$$

C(1)	.014	C(5)	.015	Th	-2.03
C(2)	.004	C(6)	-.005	Cl(1)	-3.54
C(3)	-.013	C(7)	-.001	Cl(2)	-3.62
C(4)	-.003	C(8)	-.010	O(1)	-3.09
				O(2)	-3.10

Plane: C(1) - C(8) in β compound molecule 1

$$1.334 x + 10.740 y + 8.166 z = 6.739$$

C(1)	-.028	C(5)	-.019	Th(1)	-2.02
C(2)	.045	C(6)	.023	Cl(1)	-3.66
C(3)	-.019	C(7)	.000	Cl(2)	-3.81
C(4)	.003	C(8)	-.004	O(1)	-2.98
				O(2)	-2.98

Table V. (Continued)

Plane: C(9) - C(16) in β compound molecule 2

$$4.408 x + 4.739 y + 18.471 z = 16.586$$

C(9)	-.018	C(13)	-.011	Th(2)	-2.02
C(10)	-.012	C(14)	-.004	Cl(3)	-3.80
C(11)	.044	C(15)	.025	Cl(4)	-3.72
C(12)	-.021	C(16)	-.003	O(3)	-2.96
				O(4)	-2.98

FIGURE CAPTIONS

Fig. 1. ORTEP drawing of the $C_8H_8ThCl_2(OC_4H_8)_2$ molecules: (a) α -form, (b) β -form molecule 1 and (c) β -form molecule 2.

Fig. 2. ORTEP drawing perpendicular to the COT ring showing the orientation of the Cl atoms and THF molecules to the COT ring.

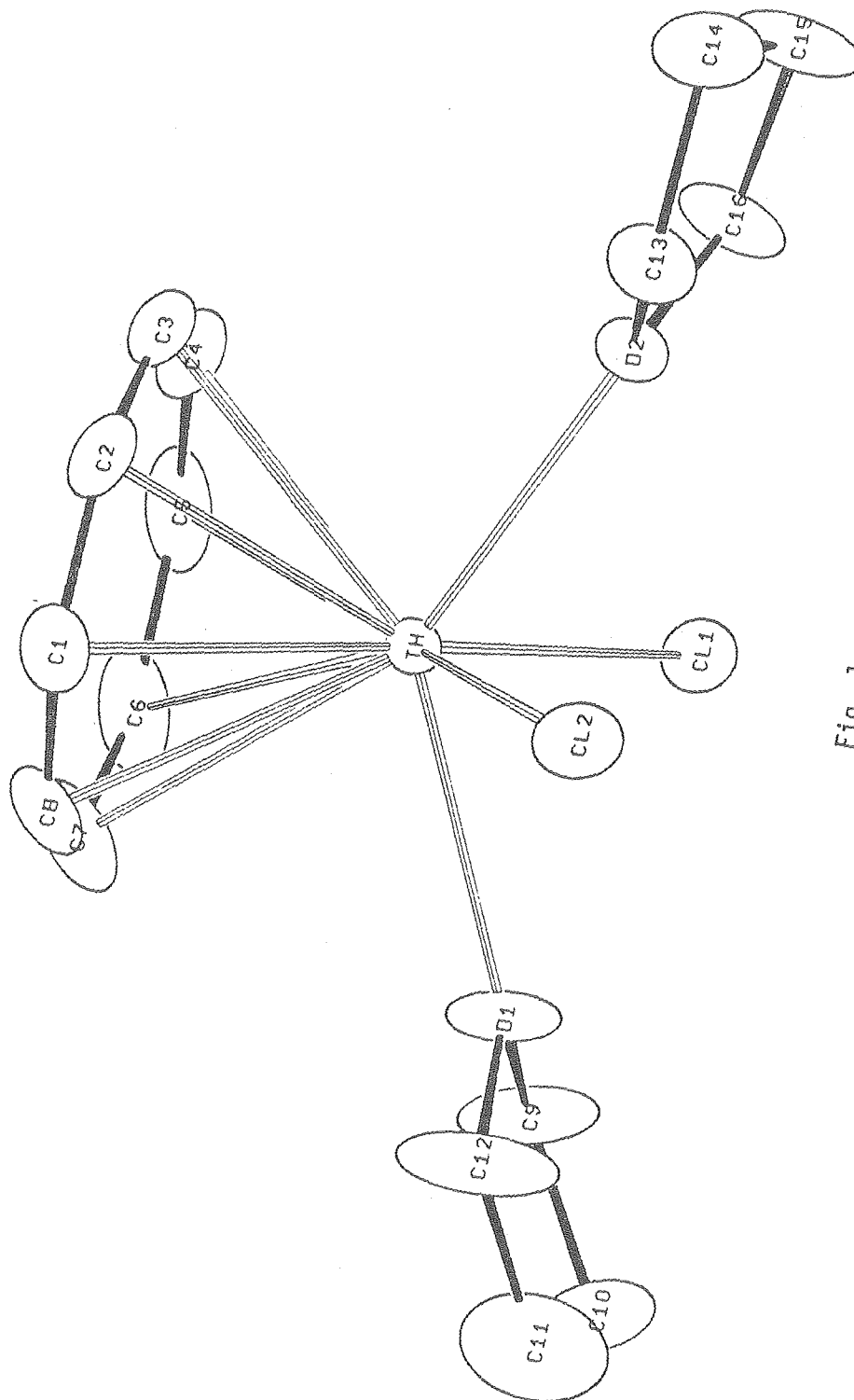
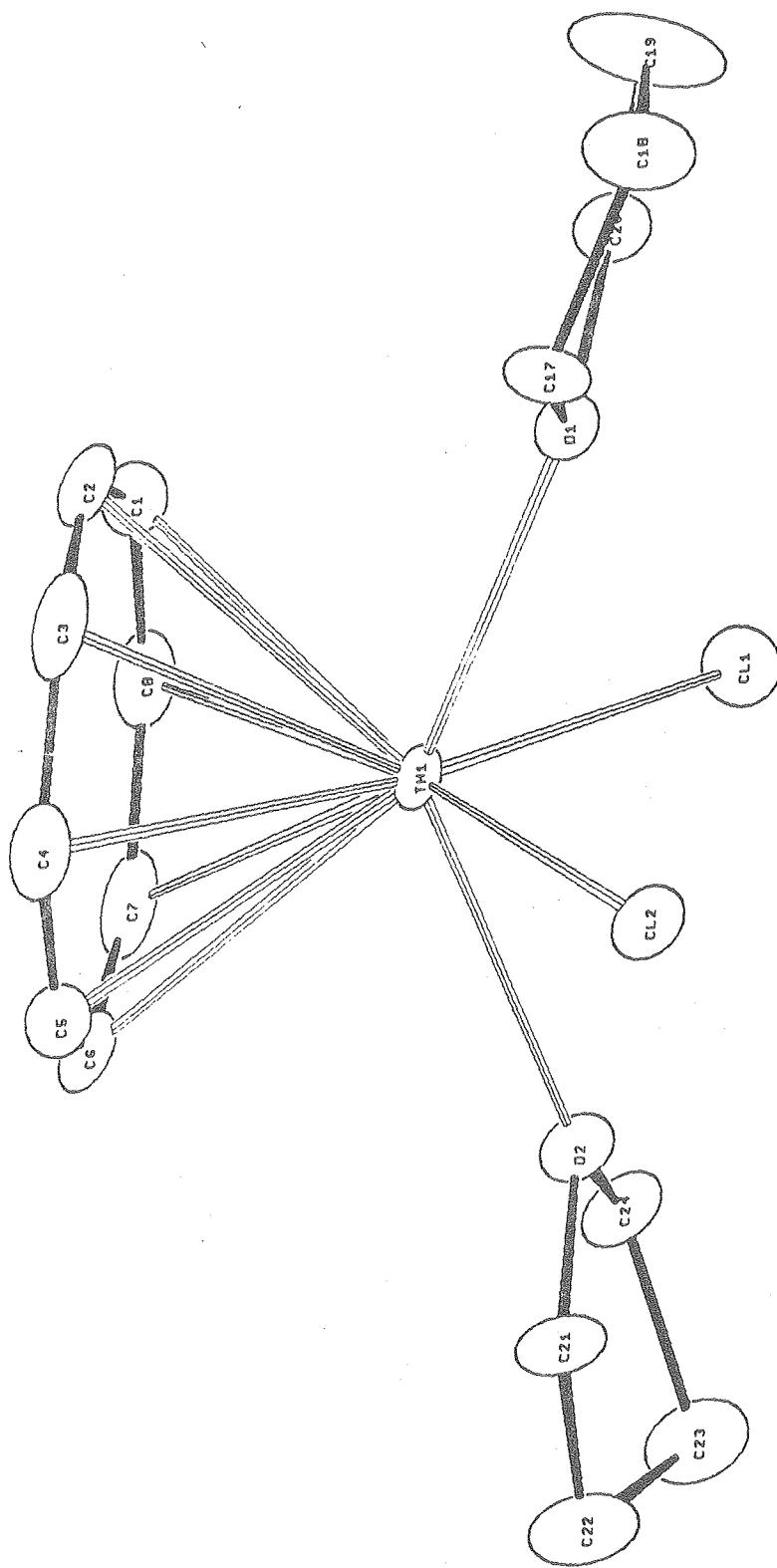


Fig. 1a

XBL 793-8720



XBL 793-8721

Fig. 1b

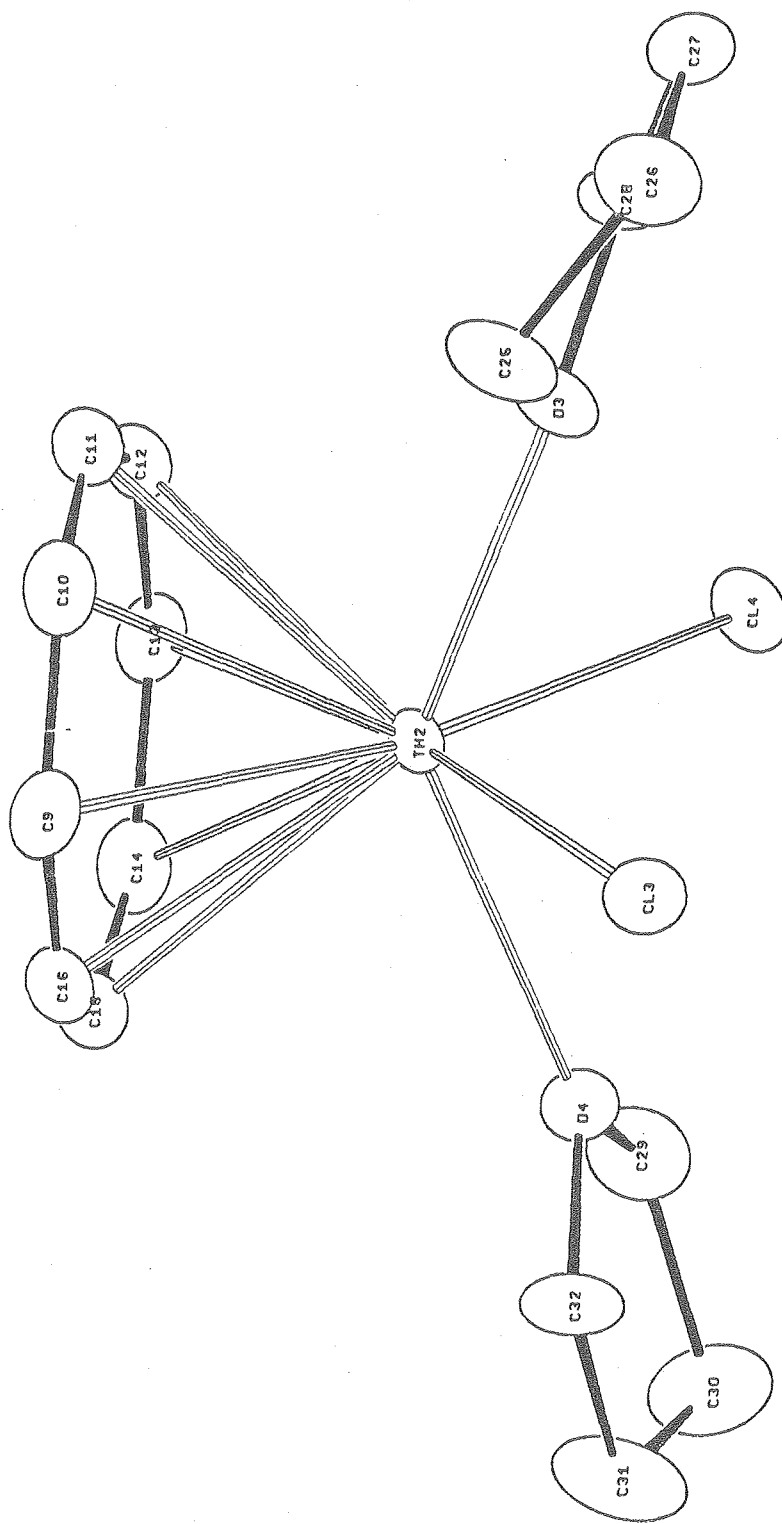


Fig. 1c

XBL 793-8722

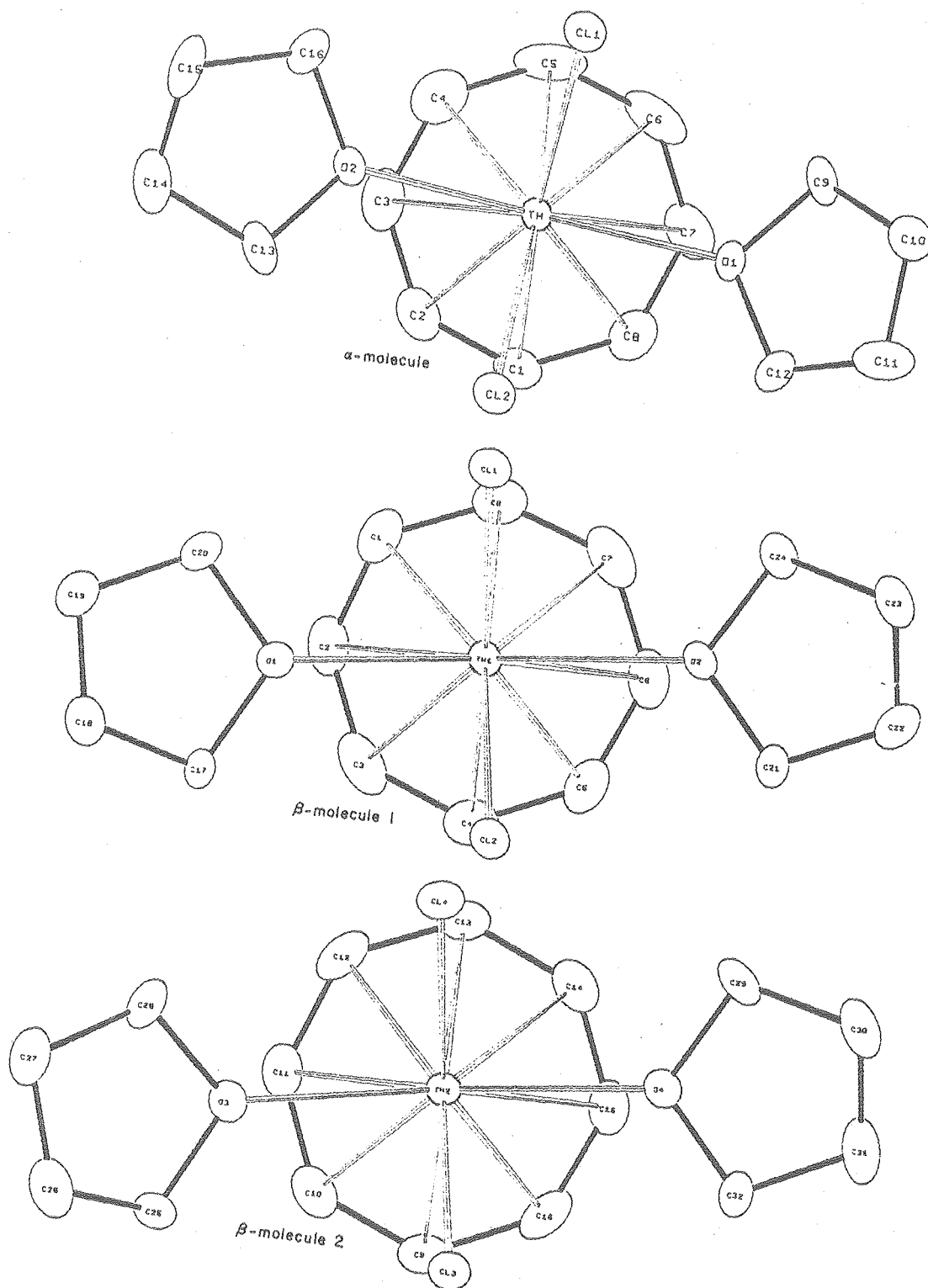


Fig. 2

XBL 734-9430

Supplementary Material for

SYNTHESIS AND STRUCTURE OF TWO CRYSTALLINE FORMS OF
CYCLOOCTATETRAENETHORIUM(IV) DICHLORIDE BISTETRAHYDROFURAN

by Allan Zalkin, David H. Templeton, Carole Le Vanda and
Andrew Streitwieser, Jr.

Anisotropic Thermal Parameters^a

α -form

ATOM	B11	B22	B33	B12	B13	B23
TH	2.99(3)	2.53(2)	2.53(2)	.12(1)	.28(2)	.254(8)
CL(1)	5.2(1)	5.8(1)	3.18(9)	.7(1)	.45(9)	-.94(8)
CL(2)	4.4(1)	5.9(1)	5.2(1)	-1.0(1)	.8(1)	1.8(1)
O(1)	3.0(4)	9.9(5)	4.3(3)	1.1(3)	-.2(3)	2.8(3)
O(2)	4.5(4)	4.0(3)	3.0(2)	.8(2)	.3(2)	.8(2)
C(1)	6.8(8)	4.9(5)	4.0(5)	.6(5)	1.7(5)	-1.1(4)
C(2)	7.3(8)	4.5(5)	3.9(5)	-1.9(5)	-.6(5)	-.6(4)
C(3)	7.2(8)	4.1(5)	6.5(7)	-1.0(6)	-2.5(6)	-.8(5)
C(4)	5.4(8)	5.0(6)	9.2(9)	-2.3(5)	-.1(7)	-2.2(6)
C(5)	8.4(10)	4.0(5)	10.3(10)	-2.3(6)	6.2(9)	-1.7(6)
C(6)	14.3(16)	3.2(5)	5.9(7)	-1.7(6)	4.6(9)	1.0(4)
C(7)	13.2(13)	3.8(5)	6.4(7)	2.8(6)	2.9(8)	1.9(5)
C(8)	7.4(8)	4.2(5)	7.7(8)	2.9(5)	1.2(6)	-.6(5)
C(9)	4.9(5)	15.6(12)	3.9(5)	.4(8)	-1.1(5)	4.2(6)
C(10)	4.5(8)	11.4(9)	4.7(6)	-1.2(6)	-.1(6)	1.7(5)
C(11)	7.9(14)	17.5(16)	9.2(12)	2.4(10)	4.9(12)	3.2(10)
C(12)	4.0(9)	20.4(18)	7.5(9)	4.3(9)	1.5(8)	5.6(10)
C(13)	8.1(9)	5.4(5)	4.1(5)	.9(5)	-.0(5)	2.1(4)
C(14)	8.6(11)	9.4(9)	6.5(7)	1.2(8)	-2.0(7)	2.3(7)
C(15)	6.3(9)	10.1(9)	11.1(10)	3.7(8)	-1.2(8)	4.5(8)
C(16)	5.8(8)	8.8(7)	7.2(7)	4.7(7)	1.3(6)	1.4(6)

Anisotropic Thermal Parameters (Continued)

β -form

ATOM	B11	B22	B33	B12	B13	B23
TH(1)	3.35(3)	1.46(2)	2.60(2)	-.06(2)	.98(2)	.01(1)
TH(2)	3.05(3)	2.60(2)	2.37(2)	-.09(2)	1.05(2)	-.31(2)
CL(1)	3.8(2)	4.6(2)	4.7(2)	-1.0(2)	1.3(2)	.9(2)
CL(2)	4.6(2)	3.0(1)	3.6(2)	.9(1)	1.6(1)	.2(1)
CL(3)	3.6(2)	4.0(2)	4.9(2)	-.2(1)	1.3(2)	.5(1)
CL(4)	5.7(2)	5.0(2)	3.7(2)	.5(2)	2.7(2)	-.5(1)
O(1)	3.1(5)	2.6(4)	3.8(5)	-.1(4)	.9(4)	.5(3)
O(2)	4.1(5)	3.1(4)	3.1(4)	.3(4)	1.5(4)	.9(4)
O(3)	5.9(7)	2.7(4)	5.2(5)	.2(4)	2.7(5)	-.1(4)
O(4)	4.3(6)	3.8(5)	3.7(5)	.2(4)	1.4(4)	.9(4)
C(1)	5.3(8)	2.9(5)	5.7(7)	.3(5)	-.7(6)	-.2(5)
C(2)	8.2(9)	1.6(4)	4.5(6)	.0(5)	.6(6)	.2(4)
C(3)	10.8(12)	2.2(5)	4.7(7)	-1.7(6)	3.0(8)	-.5(5)
C(4)	5.4(7)	2.7(5)	6.7(8)	-.2(5)	1.9(6)	-1.4(5)
C(5)	5.3447	2.9406	5.7256	.2684	-.7065	-.2329
C(6)	8.2166	1.5587	4.4893	.0065	.5826	.1711
C(7)	10.7636	2.1929	4.680	-1.711	3.0429	-.5192
C(8)	5.3857	2.7487	6.6688	-.2008	1.9311	-1.4008
C(9)	4.1(7)	6.6(7)	3.0(5)	-.1(6)	1.0(4)	.0(5)
C(10)	6.8(9)	4.4(6)	3.7(6)	-1.3(6)	.8(6)	.2(5)
C(11)	6.0(8)	3.3(5)	4.5(6)	-.1(5)	-.1(5)	-.4(5)
C(12)	4.4(7)	6.3(7)	4.4(6)	1.7(6)	.3(5)	-2.0(6)
C(13)	4.0633	6.6399	3.0483	-.0681	.9998	.043
C(14)	6.8441	4.4294	3.7487	-1.3428	.7753	.2256
C(15)	5.9746	3.2714	4.4623	-.075	-.0571	-.4318
C(16)	4.356	6.2746	4.4106	1.7455	.2562	-1.9679
C(17)	3.3(8)	5.3(8)	2.5(6)	.6(6)	.1(5)	.7(6)
C(18)	6.0(12)	8.6(12)	3.8(8)	1.1(10)	1.1(8)	1.3(8)
C(19)	4.6(11)	17.9(25)	4.2(9)	2.6(14)	.3(8)	2.1(12)
C(20)	3.2(8)	3.7(7)	4.8(8)	1.0(6)	.5(6)	.1(6)
C(21)	4.6(9)	4.6(8)	3.3(7)	1.8(7)	.9(6)	1.3(6)
C(22)	4.6(11)	7.0(11)	6.5(10)	2.8(9)	1.0(8)	1.7(9)
C(23)	7.6(13)	6.1(10)	4.6(9)	.8(9)	2.4(9)	2.4(8)
C(24)	5.5(10)	3.2(7)	4.7(8)	.1(7)	1.7(7)	2.0(6)
C(25)	6.8(12)	3.5(7)	8.1(11)	.3(8)	5.2(10)	.7(8)
C(26)	9.8(16)	4.4(9)	7.4(12)	.4(10)	2.8(11)	1.3(9)
C(27)	8.1(14)	5.4(10)	4.3(9)	2.8(9)	1.0(9)	1.0(7)
C(28)	4.4(10)	3.9(8)	6.6(10)	1.4(7)	.7(8)	-.3(7)
C(29)	8.3(13)	4.4(8)	6.1(10)	-.4(9)	3.9(9)	1.9(8)
C(30)	8.5(15)	5.6(11)	9.4(14)	.3(11)	2.3(12)	4.0(11)
C(31)	14.9(23)	4.3(10)	10.6(16)	3.2(12)	6.0(16)	2.8(11)
C(32)	5.1(10)	3.5(7)	7.1(10)	1.3(7)	2.0(8)	1.6(7)

Estimated Positional Parameters for Hydrogen

α -form

H(1)	.3177	.2024	.3703
H(2)	.5256	.1707	.4740
H(3)	.7483	.1556	.3887
H(4)	.846	.169	.1615
H(5)	.7677	.2012	-.0734
H(6)	.5493	.2298	-.1873
H(7)	.328	.2445	-.1005
H(8)	.2294	.2302	.1268
H(9)	.3035	.1275	-.3909
H(10)	.2596	.1813	-.3529
H(11)	.0646	.1085	-.4834
H(12)	.0436	.1647	-.5103
H(13)	-.1029	.1146	-.3044
H(14)	-.0885	.1714	-.2988
H(15)	.0477	.1666	-.0722
H(16)	.0348	.1098	-.0789
H(17)	.5242	.0148	.3303
H(18)	.5723	.0635	.4233
H(19)	.743	-.0131	.4681
H(20)	.8151	.039	.4919
H(21)	.8284	-.0231	.2293
H(22)	.9464	.018	.2915
H(23)	.8376	.0685	.1062
H(24)	.7425	.0244	.0241

Assigned Isotropic Thermal Parameters

	Atoms	$B(\text{\AA})^2$
α -form	H(1) -H(8)	8.0
	H(9) -H(24)	10.0
β -form	H(1) -H(16)	7.0
	H(17) -H(48)	9.0

Estimated Positional Parameters for Hydrogen

β -form

H(1)	-.0875	.3857	.315
H(2)	.0257	.436	.2719
H(3)	.1803	.3894	.2735
H(4)	.3074	.3350	.3372
H(5)	.3203	.2646	.4152
H(6)	.2218	.248	.4723
H(7)	.0536	.2674	.4641
H(8)	-.0700	.3327	.401
H(9)	.3248	.2950	.743
H(10)	.4323	.1533	.7524
H(11)	.5806	.1285	.7345
H(12)	.6685	.2082	.6804
H(13)	.664	.3756	.6432
H(14)	.5533	.5150	.6328
H(15)	.4141	.5519	.6601
H(16)	.3203	.4604	.703
H(17)	.1131	.1243	.190
H(18)	.1053	.257	.1957
H(19)	-.0184	.1184	.1198
H(20)	0	.2497	.1148
H(21)	-.1682	.1622	.1294
H(22)	-.1376	.2908	.1401
H(23)	-.1277	.263	.2277
H(24)	-.1487	.1324	.2175
H(25)	.2981	.0432	.436
H(26)	.269	-.0773	.4098
H(27)	.287	-.014	.5175
H(28)	.3028	-.1358	.4946
H(29)	.1423	-.095	.5294
H(30)	.1348	-.1760	.4785
H(31)	.0187	-.0455	.4386
H(32)	.0747	.0526	.4768
H(33)	.2928	.0016	.6562
H(34)	.3977	-.015	.6999
H(35)	.3104	-.1603	.6139
H(36)	.3713	-.1945	.6734
H(37)	.4539	-.1972	.5885
H(38)	.5199	-.1931	.6493
H(39)	.5634	-.015	.6378
H(40)	.5014	-.0208	.5762
H(41)	.3919	.4359	.4906
H(42)	.4286	.5251	.5379
H(43)	.2542	.5407	.451
H(44)	.3167	.6421	.4839
H(45)	.1449	.5813	.4973
H(46)	.228	.641	.5437
H(47)	.2189	.4904	.5919
H(48)	.1644	.420	.5399

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
ALPHA C8H6.THCL2.2(OC4H5) F(0,0,0) = 3076

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		4	419	9	1	26	61	5	1	20	289	12	4	2	14	20	6*
2	92	2	-0	5	391	8	-17	27	128	4	2	21	39	14	5*	3	87	3	5
4	962	20	-133	6	297	6	-10	28	238	7	-2	22	104	5	-1	4	314	15	-4
6	262	5	-15	7	219	5	-7	H,L=	0,	4		23	30	19	-6*	5	54	4	4
8	554	11	-25	8	657	15	-13	0	48	4	5	24	243	6	-1	6	55	5	-3
10	357	7	-13	9	409	9	-16	1	515	37	13	25	72	3	10	7	61	6	3
12	475	10	-29	10	335	7	2	2	23	10	12*	H,L=	0,	6		8	225	5	-6
14	598	12	-3	11	47	3	1	3	409	13	19	0	171	5	-3	9	35	6	4
16	358	8	-8	12	572	12	-8	4	96	3	9	1	279	16	12	10	135	4	-5
18	504	10	-14	13	496	12	-17	5	685	18	17	2	40	10	-1*	11	23	10	-2*
20	315	7	-10	14	263	6	-7	6	74	3	-3	3	249	12	6	12	176	4	-7
22	471	10	2	15	13	23	9*	7	278	6	0	4	228	6	4	13	49	4	-2
24	146	4	7	16	287	6	-5	8	99	4	5	5	370	20	16	H,L=	1,	-8	
26	344	10	4	17	383	8	-4	9	588	14	-19	6	103	4	-1	1	212	5	-3
28	39	9	11*	18	252	5	1	10	80	4	-3	7	124	4	-1	2	47	5	15
30	275	9	13	19	49	7	7	11	197	4	-6	8	281	6	7	3	241	6	-3
H,L=	0,	1		20	164	4	4	12	26	10	15*	9	385	8	15	4	21	24	10*
1	656	13	-19	21	257	6	-1	13	452	9	-12	10	83	5	-0	5	144	5	-2
2	321	7	-11	22	273	6	0	14	47	6	11	11	42	13	7*	6	31	12	6*
3	804	22	-3	23	109	4	5	15	29	9	16*	12	173	4	0	7	263	6	7
4	31	4	10	24	51	4	3	16	34	9	13*	13	365	8	15	8	32	8	-1*
5	412	9	-27	25	164	4	2	17	429	9	-7	14	135	4	4	9	74	3	5
6	209	4	-12	26	240	6	7	18	63	7	0	15	50	6	15	10	17	24	2*
7	407	9	-13	27	141	4	3	19	172	4	0	16	80	6	1	11	275	6	-8
8	190	4	-2	28	34	10	8*	20	30	10	6*	17	318	12	12	12	0	20	-8*
9	322	7	2	29	114	6	-7	21	374	13	9	18	150	5	7	13	14	23	-5*
10	68	3	-7	H,L=	0,	3		22	34	12	-3*	19	36	7	9*	H,L=	1,	-7	
11	730	17	-21	1	63	3	8	23	149	4	-3	20	44	7	5	0	469	17	21
12	124	3	-6	2	728	35	33	24	47	6	1	21	218	5	6	1	140	4	5
13	37	3	4	3	360	7	2	25	288	6	2	22	151	4	0	2	22	19	4*
14	224	5	1	4	43	4	-2	26	36	7	2*	H,L=	0,	7		3	115	4	5
15	594	12	-21	5	111	3	-3	27	143	5	-4	1	258	11	-2	4	399	9	13
16	133	3	-7	6	593	12	-22	H,L=	0,	5		2	262	6	10	5	127	4	11
17	73	3	9	7	455	9	-2	1	71	5	11	3	245	6	-2	6	65	4	15
18	206	5	1	8	247	5	-9	2	512	34	21	4	13	23	5*	7	75	4	4
19	494	10	4	9	147	3	-5	3	131	4	-1	5	223	12	3	8	283	6	3
20	94	4	0	10	466	10	-11	4	179	9	15	6	195	4	10	9	134	4	5
21	134	3	7	11	334	7	1	5	108	4	7	7	219	5	-3	10	141	4	2
22	82	4	6	12	244	5	-7	6	650	13	44	8	71	4	4	11	45	10	-0*
23	369	8	6	13	164	4	1	7	230	5	7	9	86	4	3	12	191	5	3
24	95	4	-3	14	325	7	-11	8	274	6	8	10	135	5	1	13	138	4	-6
25	177	4	1	15	197	4	1	9	32	13	9*	11	201	5	-13	14	221	5	-1
26	13	25	5*	16	319	7	-5	10	479	14	5	12	117	4	6	15	33	8	8*
27	238	6	8	17	11	25	5*	11	176	5	-4	13	21	17	10*	16	154	5	1
28	104	4	1	18	212	5	-4	12	267	6	-0	14	152	4	5	17	101	4	-3
29	172	7	3	19	169	4	0	13	77	5	-2	15	215	5	-4	18	238	6	-7
30	41	6	4	20	377	8	-3	14	338	7	2	16	122	4	-4	19	22	10	13*
H,L=	0,	2		21	83	4	8	15	70	5	4	17	67	4	2	H,L=	1,	-6	
0	259	10	-26	22	127	4	8	16	327	12	-1	18	113	3	0	1	264	14	7
1	403	21	7	23	144	4	4	17	25	27	13*	H,L=	0,	8		2	318	12	10
2	284	6	-4	24	317	7	4	18	214	5	3	0	342	16	-18	3	299	11	13
3	424	9	-9	25	70	4	4	19	26	15	4*	1	80	4	-1	4	61	6	6

STRUCTURE FACTORS CONTINUED FOR
 ALPHA C8H8.THCL2.2(OC4H8)

PAGE 2

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
5	249	6	15	11	163	4	1	9	156	3	-2	3	756	16	-16	27	50	6	-6
6	327	7	23	12	218	5	-1	10	520	13	-11	4	92	2	1	25	41	7	-2
7	291	6	9	13	94	6	-8	11	554	11	-16	5	334	7	-9	29	26	10	-4*
8	175	4	9	14	334	7	-2	12	361	7	1	6	416	8	-18	30	234	14	-13
9	108	4	-1	15	82	4	-3	13	143	3	-8	7	315	6	-5	H,L= 1, 2			
10	278	16	13	16	327	7	-5	14	362	7	-4	8	102	2	-0	1	533	45	46
11	242	6	4	17	56	5	1	15	372	8	1	9	265	5	-6	2	327	20	13
12	184	14	-2	18	225	6	1	16	255	5	-2	10	210	4	6	3	559	11	-4
13	12	23	-5*	19	31	29	18*	17	63	3	3	11	597	14	-32	4	40	9	1*
14	230	5	5	20	391	17	-6	18	266	6	-1	12	277	9	-9	5	244	5	1
15	236	18	-0	21	34	7	7*	19	250	5	0	13	29	4	5	6	373	8	-10
16	175	12	-2	22	159	4	2	20	288	6	2	14	98	11	6	7	648	15	-16
17	88	4	-0	23	0	23	-4*	21	100	4	-1	15	527	13	-34	8	141	12	4
18	187	14	5	24	297	8	1	22	86	4	-1	16	194	4	-8	9	288	8	-2
19	228	19	-4	25	59	5	-8	23	183	5	6	17	79	3	-2	10	307	6	-17
20	140	4	-8	26	93	3	2	24	313	12	1	18	102	3	0	11	623	15	-21
21	78	4	1	27	26	26	18*	25	119	4	-2	19	504	14	-10	12	232	5	-11
22	85	4	4	H,L= 1, -3				26	34	7	4*	20	112	3	-2	13	49	3	4
H,L= 1, -5				0	381	10	7	27	148	4	4	21	165	4	6	14	279	6	1
0	213	5	4	1	526	11	2	28	254	6	-4	22	77	4	4	15	491	13	-12
1	348	15	9	2	65	5	5	29	106	5	0	23	401	15	-6	16	286	6	-9
2	102	4	1	3	500	13	-3	H,L= 1, -1				24	52	6	4	17	41	7	4
3	347	7	25	4	206	4	-1	0	1108	24	1	25	197	5	3	18	144	4	0
4	262	6	20	5	638	16	-12	1	557	12	15	26	25	10	21*	19	421	9	-10
5	492	10	24	6	140	3	2	2	114	2	-3	27	257	7	1	20	158	4	-5
6	206	5	6	7	289	6	-1	3	283	6	-3	28	45	6	3	21	61	8	-0
7	227	5	5	8	173	4	2	4	684	14	1	29	174	7	-1	22	65	4	8
8	239	15	1	9	589	12	-15	5	507	11	-6	30	0	26	-6*	23	309	7	-4
9	470	22	-3	10	87	3	3	6	471	10	-5	H,L= 1, 1				24	116	4	-1
10	158	5	-0	11	109	3	3	7	74	2	4	0	847	67	-43	25	144	4	4
11	73	7	11	12	177	4	0	8	777	16	-7	1	248	5	-3	26	0	23	-19*
12	238	5	-1	13	471	13	-6	9	585	12	-16	2	235	5	1	27	182	5	-5
13	429	17	5	14	57	4	8	10	466	9	-12	3	34	4	27	28	133	8	-3
14	104	5	-4	15	15	19	-12*	11	29	3	3	4	823	32	-16	29	155	9	-3
15	21	33	19*	16	89	3	-3	12	556	13	-8	5	305	6	-5	H,L= 1, 3			
16	108	4	2	17	442	14	-0	13	456	9	-7	6	229	5	-8	0	399	33	16
17	395	16	2	18	151	4	5	14	350	7	1	7	225	5	9	1	543	45	21
18	130	4	-0	19	155	4	-3	15	44	3	2	8	670	19	-28	2	219	18	8
19	54	7	3	20	65	6	1	16	351	10	-2	9	134	3	-11	3	561	25	46
20	39	7	4*	21	372	12	-3	17	336	7	3	10	210	4	-4	4	385	18	10
21	299	14	2	22	108	5	-0	18	287	6	-3	11	46	3	-5	5	506	10	3
22	130	4	-3	23	206	5	-1	19	12	19	-9*	12	493	13	-13	6	300	6	3
23	65	5	-1	24	44	6	-3	20	192	4	-4	13	215	8	-8	7	267	6	-10
24	37	6	13	25	234	6	3	21	239	5	-2	14	567	12	-29	8	444	9	-7
25	191	15	-6	26	63	4	10	22	359	8	1	15	140	3	-2	9	439	9	-7
H,L= 1, -4				27	166	5	4	23	92	4	1	16	279	11	-9	10	224	5	-6
1	46	8	11	28	23	11	3*	24	60	6	3	17	93	3	4	11	61	4	-4
2	713	19	35	H,L= 1, -2				25	135	4	0	18	471	13	-16	12	399	8	-15
3	43	6	-3	1	116	5	-3	26	304	7	-5	19	34	10	8*	13	383	8	-3
4	89	3	2	2	511	15	-16	27	133	4	3	20	266	9	-5	14	198	4	3
5	116	4	-5	3	432	9	-9	28	0	26	-29*	21	24	13	14*	15	92	3	-2
6	572	17	-4	4	108	19	6	29	102	5	1	22	389	8	-3	16	278	6	-1
7	174	4	-9	5	86	2	-2	30	225	9	-7	23	13	22	-16*	17	412	13	-8
8	249	11	3	6	710	14	-10	H,L= 1, 0				24	119	5	-8	18	178	4	1
9	16	19	15*	7	601	13	-7	1	746	25	-39	25	35	7	16*	19	115	4	1
10	444	17	10	8	343	9	-5	2	277	6	3	26	300	8	0	20	161	4	2

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.THCL2.2(OC4H8)

PAGE 4

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
23	182	5	-2	18	363	11	-1	13	226	5	0	11	31	14	3*	15	69	4	3
24	34	6	12	19	13	20	4*	14	398	11	1	12	262	6	9	16	33	8	2*
25	282	15	-0	20	168	10	0	15	20	17	11*	13	335	7	-1	17	293	18	-8
26	102	4	-4	21	169	4	2	16	325	7	-1	14	208	5	4	18	32	8	-1*
27	171	5	1	22	395	8	1	17	136	4	-3	15	87	5	-4	19	35	7	-1*
28	19	20	17*	23	71	4	-1	13	342	7	-2	16	190	5	1	20	22	10	18*
29	207	20	-2	24	87	4	3	19	53	5	5	17	383	8	3	H ₂ L= 2, 7			
H ₂ L= 2, -1				25	107	4	1	20	275	6	-3	18	155	4	-1	1	149	10	-6
1	247	5	6	26	318	8	7	21	15	29	-4*	19	116	4	9	2	254	16	-14
2	341	7	-8	27	57	5	-8	22	374	8	-0	20	94	4	1	3	122	4	-5
3	340	7	-9	28	40	10	-4*	23	49	6	2	21	297	6	0	4	114	11	-6
4	346	7	-0	29	87	4	1	24	133	4	0	22	136	4	4	5	62	4	-2
5	280	9	-3	H ₂ L= 2, 1				25	63	7	-12	23	100	4	5	6	308	24	-16
6	635	19	-5	1	624	55	37	26	273	7	-8	24	35	9	-3*	7	113	4	-2
7	580	14	-2	2	338	7	27	27	61	5	-0	25	196	8	-2	8	164	12	-11
8	428	12	6	3	662	16	-6	28	33	6	27*	26	140	6	-6	9	28	18	5*
9	81	2	1	4	153	3	-3	H ₂ L= 2, 3				H ₂ L= 2, 5				10	287	20	-7
10	627	18	-6	5	418	10	-11	1	474	43	37	1	106	3	1	11	124	3	-0
11	525	12	-14	6	25	6	13*	2	422	32	33	2	556	47	19	12	136	11	-14
12	311	8	-2	7	744	15	-20	3	551	47	53	3	79	4	1	13	0	20	-3*
13	50	3	-3	8	97	3	1	4	108	3	8	4	38	9	12*	14	208	13	-9
14	412	14	-9	9	455	14	-7	5	296	17	34	5	75	5	7	15	102	3	-4
15	351	10	-5	10	50	3	-3	6	402	16	20	6	429	30	17	16	146	4	-9
16	194	8	-1	11	622	14	-21	7	483	13	21	7	79	5	1	H ₂ L= 2, 8			
17	47	4	-1	12	74	2	-4	8	162	4	6	8	146	4	13	0	194	17	-15
18	218	5	-1	13	34	4	5	9	84	4	3	9	36	8	7*	1	120	12	-11
19	303	14	-1	14	103	3	0	10	207	5	4	10	337	21	6	2	27	7	6*
20	282	15	-2	15	530	15	-13	11	562	11	5	11	50	7	-10	3	107	3	-11
21	77	4	1	16	41	5	7	12	164	4	-3	12	278	14	11	4	194	16	-17
22	77	4	1	17	141	4	-4	13	33	8	-2*	13	60	5	11	5	145	11	-14
23	226	11	-4	18	71	4	7	14	178	4	-1	14	318	12	6	6	49	5	0
24	263	15	0	19	445	14	-10	15	458	9	-1	15	28	13	-6*	7	92	4	-13
25	148	5	4	20	69	5	2	16	206	5	2	16	317	12	10	8	173	12	-17
26	20	23	-2*	21	163	5	1	17	24	26	2*	17	22	26	17*	9	122	4	-21
27	174	5	2	22	86	5	1	18	114	5	-3	18	202	5	3	H ₂ L= 3, -8			
28	218	15	-2	23	379	8	5	19	379	8	-2	19	52	6	-5	1	158	4	-0
29	131	5	-2	24	44	6	2	20	235	6	-2	20	255	6	1	2	65	5	-7
H ₂ L= 2, 0				25	176	4	1	21	55	6	8	21	35	8	-1*	3	222	5	-1
0	634	61	35	26	0	25	-19*	22	110	4	2	22	108	4	1	4	85	4	-0
1	158	4	-1	27	267	16	0	23	244	6	-5	23	83	5	1	5	105	4	4
2	208	4	-1	28	0	23	-6*	24	136	5	-3	H ₂ L= 2, 6				6	114	4	-3
3	74	4	1	29	149	7	-6	25	142	6	7	0	125	13	4	7	252	14	-3
4	814	17	-22	H ₂ L= 2, 2				26	36	7	5*	1	317	25	-3	8	89	4	-0
5	268	9	-8	0	996	77	59	27	137	6	-2	2	28	13	-1*	9	87	7	-2
6	159	3	-3	1	52	4	9	H ₂ L= 2, 4				3	217	19	-3	10	111	4	-2
7	172	5	3	2	136	3	12	0	381	33	18	4	76	4	2	11	255	18	3
8	710	18	-22	3	107	3	10	1	439	37	4	5	407	33	10	12	42	7	-2
9	386	12	4	4	810	16	8	2	28	6	11*	6	36	13	4*	H ₂ L= 3, -7			
10	299	8	-6	5	379	12	7	3	454	38	20	7	94	4	5	0	390	8	5
11	141	7	-5	6	241	5	10	4	316	27	24	8	27	12	9*	1	40	15	-3*
12	491	13	-17	7	55	3	5	5	355	24	18	9	459	31	13	2	98	4	2
13	302	13	-2	8	626	13	3	6	72	5	6	10	91	4	4	3	43	8	16*
14	321	11	-4	9	367	8	3	7	253	14	12	11	97	3	1	4	399	19	23
15	0	20	-3*	10	384	8	-1	8	288	15	30	12	58	5	4	5	50	7	8
16	279	11	-3	11	148	3	-6	9	288	6	13	13	393	24	6	6	146	5	-1
17	231	9	-3	12	440	9	-2	10	175	4	7	14	94	4	3	7	27	32	-7*

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.THCL2.2(OC4H8)

PAGE 3

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
21	323	7	-5	20	0	23	-6*	9	70	3	-5	18	252	18	-3	24	7	21	4*
22	212	5	-3	21	249	6	3	10	86	5	-6	19	16	26	13*	25	227	17	-1
23	100	4	-1	22	37	12	3*	11	193	10	-14	20	128	12	1	26	90	4	3
24	70	5	5	23	125	4	4	H ₂ L= 2, -8		21	129	5	4	H ₂ L= 2, -3					
25	212	5	-6	24	41	6	13	0	277	6	-5	22	220	22	0	1	158	4	5
26	188	6	-4	H ₂ L= 1, 6		1	6	1	26	15	2*	H ₂ L= 2, -5		2	885	34	-22		
27	120	4	-3	1	56	6	6	2	59	4	8	1	329	13	18	3	38	4	1
28	16	24	8*	2	339	23	4	3	19	25	8*	2	339	7	31	4	31	4	11
H ₂ L= 1, 4		3	149	4	6	4	6	4	267	6	-0	3	283	6	11	5	40	4	-3
1	151	11	12	4	126	4	7	5	75	4	-5	4	114	4	3	6	767	21	-5
2	753	61	47	5	62	4	7	6	126	4	-2	5	173	4	1	7	72	3	-4
3	252	21	21	6	364	23	8	7	35	9	8*	6	374	20	1	8	154	3	8
4	146	8	4	7	182	11	12	8	277	6	-1	7	274	19	-6	9	0	19	-11*
5	148	4	19	8	238	6	3	9	85	4	4	8	200	5	4	10	400	12	-11
6	661	24	47	9	65	8	-12	10	151	4	-0	9	86	5	1	11	33	5	1
7	265	6	11	10	348	15	12	11	18	20	10*	10	336	15	-2	12	358	13	-3
8	184	4	4	11	178	4	-1	12	252	6	-6	11	286	13	-3	13	23	9	19*
9	136	3	-2	12	201	5	6	13	56	5	-2	12	224	5	-1	14	341	14	-8
10	400	10	2	13	44	6	22	H ₂ L= 2, -7		13	20	24	6*	15	39	6	1		
11	249	5	2	14	333	13	12	1	272	7	6	14	273	15	6	16	436	16	-9
12	260	6	0	15	136	4	-1	2	97	5	3	15	303	14	-2	17	0	22	-7*
13	66	6	-7	16	171	5	2	3	319	7	2	16	187	4	-2	18	280	12	-3
14	291	6	6	17	27	10	10*	4	5	25	-11*	17	50	6	0	19	78	4	-0
15	199	5	3	18	183	4	-0	5	193	5	10	18	205	5	-3	20	408	14	-7
16	380	8	1	19	70	4	5	6	65	5	12	19	219	20	-2	21	0	22	-5*
17	19	24	19*	20	192	5	-11	7	317	7	7	20	184	5	-2	22	147	11	8
18	184	5	-6	21	48	6	1	8	0	26	-4*	21	57	6	2	23	33	11	4*
19	113	4	-2	H ₂ L= 1, 7		9	118	4	5	22	131	7	8	24	326	7	-0		
20	354	8	1	0	320	21	-1	10	103	6	11	23	153	13	-3	25	21	16	5*
21	51	6	-6	1	209	10	3	11	302	26	10	24	169	6	-4	26	93	3	6
22	123	4	-6	2	25	24	-1*	12	0	31	-4*	25	83	3	0	27	18	20	11*
23	89	6	-3	3	181	5	-2	13	55	5	22	H ₂ L= 2, -4		28	269	23	2		
24	272	7	-2	4	295	15	7	14	33	33	-4*	0	57	8	-6	H ₂ L= 2, -2			
25	62	4	5	5	243	16	-0	15	278	27	-4	1	543	20	15	0	234	5	1
26	61	5	-3	6	74	4	-4	16	33	11	19*	2	68	4	12	1	385	19	-27
H ₂ L= 1, 5		7	108	4	10	17	50	5	3	3	486	21	6	2	30	7	-12*		
0	152	12	15	8	210	13	-1	18	8	21	0*	4	96	4	1	3	471	10	-4
1	360	25	12	9	256	6	0	H ₂ L= 2, -6		5	447	21	-5	4	300	6	-3		
2	43	5	1	10	127	4	-1	0	483	10	3	6	100	4	-9	5	674	17	2
3	272	20	14	11	70	7	2	1	172	4	8	7	206	8	-1	6	95	2	3
4	116	10	18	12	156	4	-3	2	30	15	0*	8	107	3	-2	7	366	12	-11
5	509	31	14	13	225	14	1	3	70	7	8	9	453	13	-11	8	245	5	-1
6	61	6	7	14	122	4	-6	4	506	18	35	10	86	3	-1	9	740	24	-14
7	208	5	11	15	30	7	4*	5	278	6	17	11	44	6	3	10	215	5	10
8	0	24	-21*	16	85	4	-2	6	69	7	-2	12	175	4	-2	11	106	6	10
9	506	10	19	17	202	11	-13	7	85	5	8	13	451	16	-7	12	180	4	2
10	21	24	12*	18	146	4	-3	8	332	22	4	14	119	4	-2	13	521	13	-13
11	123	4	16	H ₂ L= 1, 8		9	282	18	3	15	41	6	-5	14	212	5	-1		
12	36	10	8*	1	196	15	-10	10	164	4	-2	16	143	12	-1	15	33	5	20
13	463	10	8	2	184	12	-7	11	87	5	-2	17	472	22	4	16	231	9	2
14	48	6	18	3	202	11	-9	12	216	17	8	18	78	4	-2	17	444	16	-3
15	24	25	15*	4	20	14	14*	13	222	14	6	19	82	4	-7	18	142	4	9
16	14	28	6*	5	145	4	-4	14	249	17	-1	20	32	9	1*	19	102	3	-3
17	377	8	2	6	142	4	-11	15	63	5	6	21	351	21	1	20	122	3	-0
18	26	12	13*	7	203	13	-12	16	164	4	5	22	56	5	-4	21	361	14	3
19	79	4	-9	8	0	19	-8*	17	148	4	3	23	97	4	-2	22	102	4	-1

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.THCL2.2(OC4H8)

PAGE 5

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
8	344	29	12	23	72	4	-5	26	39	6	3	24	57	4	3	19	17	25	-5*
9	70	5	7	24	35	7	-6*	27	140	5	1	25	230	17	1	20	159	17	6
10	147	4	4	H,L= 3, -4				H,L= 3, -2				26	130	4	0	21	145	15	-4
11	26	16	0*	1	238	5	3	1	72	4	-5	27	133	6	-4	22	389	24	-2
12	265	27	10	2	543	13	6	2	919	26	-5	28	7	24	-6*	23	50	6	3
13	43	8	1	3	319	20	-4	3	93	3	-6	29	148	6	-12	24	113	15	-4
14	184	13	-4	4	102	3	-2	4	36	3	-0	H,L= 3, 0				25	81	5	-5
15	15	29	-11*	5	126	3	-0	5	95	2	-1	1	447	26	6	26	301	10	-6
16	166	20	1	6	440	20	-1	6	722	27	3	2	278	6	13	27	41	12	-4*
17	31	8	11*	7	215	12	-2	7	70	2	-2	3	397	8	-3	28	42	6	-2
H,L= 3, -6				8	191	9	-2	8	239	5	1	4	396	8	4	H,L= 3, 2			
1	319	19	19	9	31	10	17*	9	51	4	1	5	354	7	1	1	460	38	33
2	86	10	29	10	399	17	-3	10	467	18	2	6	401	17	-10	2	280	29	33
3	371	14	30	11	283	14	-10	11	124	3	-5	7	568	14	-18	3	685	49	75
4	123	4	1	12	305	15	-3	12	346	14	-6	8	321	12	-7	4	189	9	11
5	248	14	15	13	19	21	14*	13	49	5	-1	9	187	8	-10	5	330	10	28
6	122	5	9	14	341	22	-7	14	329	17	-0	10	500	24	-17	6	41	5	7
7	366	25	8	15	315	19	-5	15	159	4	-1	11	418	11	-15	7	627	13	7
8	23	27	3*	16	283	15	-5	16	420	21	3	12	156	8	-4	8	120	3	-4
9	160	4	2	17	17	25	-2*	17	46	6	1	13	31	5	11	9	132	3	-4
10	135	6	-8	18	229	14	-1	18	250	15	-4	14	339	19	-5	10	60	6	0
11	345	27	1	19	188	13	2	19	73	4	7	15	389	22	-14	11	626	16	-5
12	35	18	23*	20	247	16	5	20	418	23	4	16	160	11	-2	12	27	10	11*
13	24	26	3*	21	38	7	8	21	43	10	1*	17	63	5	-5	13	132	10	-0
14	91	6	8	22	104	4	-3	22	158	4	1	18	174	4	-0	14	81	4	-7
15	304	30	-0	23	102	4	-2	23	21	22	10*	19	368	15	-12	15	434	15	-9
16	0	24	-21*	24	216	17	-5	24	300	22	-2	20	209	15	-3	16	73	4	14
17	45	10	-6*	25	69	6	-1	25	25	19	-2*	21	136	4	0	17	43	10	12*
18	49	9	6*	26	36	6	2	26	93	4	0	22	52	6	0	18	48	6	7
19	244	26	-11	H,L= 3, -3				27	44	5	12	23	286	24	0	19	411	19	-5
20	64	5	3	0	125	4	3	28	248	26	-9	24	194	15	-4	20	41	10	12*
21	97	4	2	1	606	12	2	H,L= 3, -1				25	132	5	1	21	144	4	2
H,L= 3, -5				2	29	7	14*	0	271	18	-7	26	37	7	-2*	22	18	23	-2*
0	467	10	32	3	561	14	-9	1	423	9	-2	27	173	6	-6	23	332	18	-10
1	194	5	4	4	68	3	4	2	100	3	1	28	177	7	-5	24	26	13	19*
2	28	21	19*	5	439	15	3	3	271	6	8	29	134	5	12	25	181	6	1
3	68	5	13	6	66	3	0	4	366	8	-5	H,L= 3, 1				26	27	10	22*
4	346	21	3	7	343	13	3	5	650	19	-4	0	847	70	65	27	196	11	-15
5	327	19	-11	8	99	3	5	6	32	4	0	1	299	33	31	H,L= 3, 3			
6	65	5	-1	9	376	16	-2	7	170	7	-0	2	146	11	7	0	537	41	16
7	82	4	1	10	62	3	0	8	267	11	-10	3	100	4	5	1	168	9	4
8	283	14	5	11	27	7	2*	9	674	23	-4	4	803	23	4	2	23	9	10*
9	415	21	-1	12	93	3	-2	10	267	8	-13	5	177	8	3	3	82	3	1
10	170	5	-10	13	506	22	-10	11	165	8	-4	6	289	6	-0	4	480	38	30
11	106	4	-1	14	71	4	-3	12	215	9	-6	7	43	5	3	5	329	19	18
12	276	18	-2	15	73	3	-1	13	456	17	-8	8	691	14	-12	6	195	12	13
13	304	15	5	16	55	5	9	14	228	8	-14	9	171	11	-4	7	41	10	22*
14	234	15	-8	17	513	27	-10	15	86	4	-3	10	268	6	-1	8	519	20	41
15	47	9	6*	18	86	4	-1	16	217	9	-3	11	45	4	-2	9	312	7	15
16	196	15	-3	19	95	4	-5	17	400	23	-7	12	441	18	-13	10	305	6	18
17	186	14	1	20	37	7	-3*	18	185	5	-1	13	183	12	1	11	73	4	4
18	208	17	0	21	355	24	-0	19	104	4	-2	14	307	13	-6	12	414	9	8
19	23	14	17*	22	54	5	3	20	148	4	-0	15	56	4	1	13	165	5	4
20	116	4	4	23	108	3	-2	21	331	19	0	16	245	14	-13	14	319	7	7
21	144	15	-2	24	38	7	6	22	147	4	-3	17	110	4	-2	15	73	6	4
22	181	15	-2	25	258	22	-0	23	156	11	1	18	385	24	1	16	330	7	8

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.THCL2.2(OC4H8)

PAGE 6

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
17	121	4	5	20	94	13	3	1	227	15	6	18	76	6	-1	23	106	16	-1
18	275	6	-5	21	238	21	-11	2	44	10	-4*	19	236	28	4	24	254	22	1
19	68	6	8	22	101	4	-5	3	294	13	19	20	91	5	4	25	36	12	1*
20	205	5	-1	H,L= 3, 6				4	64	5	11	21	107	4	1	26	68	3	4
21	132	4	2	1	36	8	18*	5	165	13	8	22	46	6	6	H,L= 4, -2			
22	252	8	-2	2	406	32	-20	6	109	4	6	23	212	24	1	0	142	14	6
23	81	6	4	3	52	4	-2	7	258	24	4	H,L= 4, -4				1	539	11	13
24	46	9	-2*	4	86	4	-16	8	112	16	-6	0	397	22	15	2	18	25	14*
25	92	5	-1	5	67	4	-2	9	111	4	4	1	298	6	11	3	486	14	2
26	242	8	11	6	342	26	-2	10	114	5	1	2	99	8	4	4	138	8	7
H,L= 3, 4				7	67	4	-1	11	251	26	-3	3	135	5	2	5	427	14	-6
1	324	28	22	8	191	11	-2	12	73	4	8	4	307	13	1	6	61	3	-6
2	459	32	27	9	60	5	1	13	0	24	-13*	5	347	16	-3	7	257	10	-6
3	313	25	11	10	295	25	0	14	90	4	-2	6	180	4	-8	8	36	4	17
4	27	11	2*	11	31	15	13*	15	245	27	-9	7	115	5	7	9	414	17	-11
5	243	24	12	12	215	15	-4	16	52	4	17	8	307	17	-2	10	16	18	7*
6	396	30	33	13	33	11	18*	H,L= 4, -6				9	389	17	-14	11	98	5	6
7	315	25	23	14	235	19	-5	0	447	21	25	10	188	11	-4	12	63	4	-3
8	109	4	9	15	28	11	6*	1	85	6	-3	11	106	4	4	13	438	23	-11
9	109	4	8	16	227	17	-7	2	35	13	14*	12	302	23	-3	14	32	16	-6*
10	270	14	17	17	20	20	10*	3	18	28	-2*	13	376	23	-9	15	45	5	-6
11	368	27	17	18	162	14	-8	4	384	20	9	14	204	5	-5	16	21	22	3*
12	189	5	16	19	27	13	-12*	5	40	12	-5*	15	74	4	10	17	450	30	-3
13	39	9	25*	H,L= 3, 7				6	69	10	-2	16	220	17	4	18	81	21	5*
14	183	5	10	0	135	13	-1	7	38	11	-6*	17	246	16	6	19	143	13	-3
15	375	19	24	1	164	13	-5	8	344	24	0	18	166	16	-2	20	48	5	0
16	270	6	20	2	0	24	-7*	9	23	24	13*	19	21	20	-3*	21	366	32	-1
17	0	28	-9*	3	110	10	-8	10	152	13	-4	20	119	4	2	22	51	5	6
18	138	4	4	4	84	3	4	11	21	25	-4*	21	187	12	4	23	112	4	4
19	251	15	13	5	262	23	-18	12	258	23	-3	22	167	18	1	24	37	5	10
20	239	6	13	6	24	12	18*	13	28	19	12*	23	98	4	0	25	252	25	-3
21	37	9	1*	7	109	12	-12	14	195	18	-9	24	27	10	-2*	26	21	23	13*
22	74	5	11	8	46	6	6	15	26	13	-7*	25	155	18	-2	27	126	5	-5
23	172	15	-4	9	279	22	-21	16	147	4	-3	H,L= 4, -3				H,L= 4, -1			
24	202	7	2	10	33	6	5	17	42	8	8*	1	209	11	4	1	146	4	0
H,L= 3, 5				11	68	5	-6	18	217	23	-6	2	665	14	-3	2	650	13	5
0	275	26	11	12	33	5	2	19	20	24	12*	3	204	14	-7	3	127	3	2
1	380	30	-5	13	254	23	-20	20	114	12	5	4	135	3	-1	4	111	3	12
2	13	25	2*	14	63	4	-2	H,L= 4, -5				5	97	3	-1	5	54	4	4
3	374	30	9	H,L= 3, 8				1	311	7	14	6	454	18	-11	6	559	21	-13
4	222	25	14	1	104	3	-6	2	163	5	6	7	230	17	-5	7	223	5	-10
5	317	22	7	2	166	17	-29	3	368	19	2	8	194	4	-4	8	223	5	-2
6	23	15	15*	3	118	11	-10	4	88	9	-4	9	61	4	-2	9	17	18	6*
7	198	17	9	4	52	4	-3	5	199	11	-1	10	405	24	-10	10	393	24	-20
8	144	18	-2	H,L= 4, -8				6	194	5	10	11	244	19	0	11	245	10	-10
9	306	19	3	0	211	5	0	7	376	19	-7	12	257	12	-9	12	245	14	-8
10	47	7	10	1	119	4	-5	8	113	4	0	13	16	24	14*	13	62	5	0
11	33	6	10*	2	23	19	-7*	9	123	4	5	14	308	19	-12	14	331	23	-11
12	112	4	1	3	90	4	2	10	256	13	6	15	243	21	20	15	192	5	-9
13	365	24	4	4	211	5	3	11	406	29	-12	16	316	23	-1	16	355	25	-9
14	76	6	-4	5	164	4	-2	12	124	4	5	17	32	14	3*	17	27	11	11*
15	44	13	-8*	6	71	5	-5	13	56	5	11	18	200	11	5	18	270	24	-7
16	91	4	-2	7	57	6	2	14	163	5	-0	19	182	15	0	19	123	5	-2
17	326	22	8	8	195	18	-2	15	292	29	-7	20	275	20	-4	20	361	32	-6
18	117	14	-0	9	148	16	-3	16	87	4	5	21	5	23	-11*	21	23	25	2*
19	84	4	2	H,L= 4, -7				17	34	7	6*	22	110	5	2	22	145	14	-3

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.THCL2.2(OC4H8)

PAGE 7

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
23	80	4	1	22	38	8	3*	22	14	24	0*	5	263	19	-3	12	24	27	1*
24	261	29	2	23	281	20	1	23	221	29	2	6	14	23	-12*	13	13	27	-9*
25	37	9	-3*	24	147	4	1	24	45	7	-4	7	110	14	-9	14	26	19	-5*
26	60	4	3	25	109	6	1	25	168	4	19	8	77	5	-13	15	267	31	-3
27	10	26	-26*	26	35	8	-6*	H ₂ L= 4, 4				9	252	19	-7	16	8	23	-2*
H ₂ L= 4, 0				27	176	7	-8	0	336	30	7	10	0	20	-14*	17	55	5	-1
0	651	60	59	H ₂ L= 4, 2				1	142	11	-2	11	47	6	-8	18	30	7	20*
1	396	43	51	0	660	59	36	2	73	4	3	12	41	5	-1	H ₂ L= 5, -5			
2	21	24	12*	1	69	4	4	3	160	4	3	13	242	21	-15	0	486	36	19
3	203	5	9	2	37	5	6	4	386	30	12	14	64	4	-11	1	84	6	3
4	549	15	26	3	80	3	1	5	232	14	3	15	22	9	5*	2	39	16	-8*
5	547	13	4	4	581	45	58	6	146	19	14	16	44	4	-5	3	80	7	2
6	147	4	-2	5	48	6	-2	7	145	13	3	H ₂ L= 4, 7				4	431	26	2
7	161	4	0	6	221	15	13	8	366	31	10	1	0	21	-7*	5	28	19	-0*
8	342	11	6	7	129	4	1	9	235	10	9	2	227	19	-26	6	104	4	-6
9	497	19	-7	8	532	17	36	10	217	14	8	3	39	8	5*	7	36	10	7*
10	186	8	-2	9	79	4	15	11	22	24	-15*	4	65	3	-1	8	379	37	-8
11	110	4	-1	10	239	5	10	12	332	29	14	5	20	15	13*	9	72	5	-2
12	194	5	-3	11	62	8	5	13	219	12	10	6	237	24	-33	10	172	18	-6
13	448	34	-4	12	409	12	5	14	208	5	2	7	34	5	19	11	16	23	11*
14	242	11	-2	13	67	7	-1	15	27	11	19*	8	103	4	-12	12	256	27	-3
15	56	8	-2	14	271	6	3	16	228	22	9	9	0	19	-4*	13	107	4	-5
16	199	12	2	15	15	29	4*	17	168	5	6	10	204	19	-33	14	197	20	-8
17	371	26	-13	16	272	15	-2	18	188	17	3	H ₂ L= 5, -8				15	17	22	7*
18	282	7	-7	17	73	5	-6	19	73	4	8	1	73	4	-7	16	166	26	5
19	61	9	6	18	330	7	1	20	135	4	-1	2	213	20	-2	17	70	5	-2
20	159	5	1	19	33	13	22*	21	120	4	4	3	112	5	-6	18	215	27	-3
21	246	27	-4	20	141	4	-6	22	182	23	-8	4	19	23	-2*	19	20	21	12*
22	212	15	-2	21	58	6	5	23	94	6	-3	5	59	5	-4	20	129	18	-2
23	95	4	4	22	295	9	-2	H ₂ L= 4, 5				H ₂ L= 5, -7				21	52	5	0
24	56	6	-16	23	57	5	9	1	236	26	-10	0	306	30	13	H ₂ L= 5, -4			
25	183	20	-1	24	70	6	3	2	390	29	5	1	91	5	4	1	201	14	5
26	150	6	-1	25	69	6	6	3	232	20	-13	2	19	26	3*	2	216	14	-1
27	135	9	13	26	288	8	26	4	49	6	-1	3	80	5	8	3	365	33	-13
H ₂ L= 4, 1				H ₂ L= 4, 3				5	160	17	-3	4	255	24	5	4	89	5	5
1	479	43	36	1	298	23	22	6	329	23	5	5	117	4	-1	5	114	4	4
2	403	41	47	2	54	4	15	7	192	21	-13	6	57	9	1	6	179	12	-13
3	559	41	50	3	477	37	38	8	132	4	4	7	27	21	-5*	7	435	35	-22
4	164	14	16	4	53	5	-2	9	88	4	-6	8	199	20	-2	8	124	4	-4
5	418	12	22	5	215	17	12	10	238	14	4	9	132	5	-8	9	164	20	0
6	342	7	10	6	66	4	11	11	189	17	-3	10	130	5	-2	10	200	15	-11
7	400	11	11	7	636	44	51	12	178	12	1	11	30	13	8*	11	388	36	-13
8	208	5	-1	8	130	4	2	13	34	9	14*	12	167	26	-2	12	127	4	-4
9	131	3	-8	9	179	15	17	14	155	16	3	13	127	17	-3	13	82	4	12
10	362	14	-2	10	123	4	9	15	200	15	-2	H ₂ L= 5, -6				14	152	16	-11
11	361	15	-13	11	562	30	39	16	195	17	2	1	341	18	18	15	267	27	-9
12	172	11	-4	12	17	33	-6*	17	30	17	-9*	2	30	19	16*	16	106	4	-3
13	36	6	13	13	67	5	5	18	89	3	1	3	289	26	2	17	30	11	21*
14	260	15	-4	14	93	6	8	19	193	23	-11	4	47	10	3*	18	128	14	4
15	375	20	-12	15	470	17	29	20	196	6	-5	5	245	23	4	19	218	26	-5
16	166	17	-0	16	50	12	-5*	H ₂ L= 4, 6				6	50	7	-7	20	114	5	-3
17	120	4	3	17	14	26	3*	0	146	17	-9	7	257	22	-3	21	76	5	-8
18	128	4	1	18	58	6	8	1	232	22	-9	8	68	5	1	22	60	4	-6
19	372	26	-2	19	299	17	9	2	21	13	13*	9	102	4	3	23	194	29	-1
20	169	21	8	20	57	6	12	3	173	17	-5	10	43	12	-8*	H ₂ L= 5, -3			
21	119	7	-1	21	115	4	10	4	142	11	-11	11	295	31	-3	0	165	14	16

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.THCL2.2(OC4H8)

PAGE 6

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
1	291	16	2	5	580	27	28	6	38	7	11	10	246	20	11	2	220	21	-19
2	111	7	3	6	207	5	-1	7	134	16	5	11	41	8	2*	3	99	11	-18
3	161	4	15	7	251	13	-1	8	263	6	14	12	366	37	10	4	80	3	-2
4	226	15	3	8	109	4	7	9	357	22	23	13	62	5	18	5	106	12	-11
5	349	15	-9	9	485	35	5	10	124	4	8	14	248	21	12	6	231	25	-13
6	146	4	0	10	55	5	-3	11	66	7	14	15	15	23	-1*	7	66	4	-16
7	144	6	2	11	89	17	10*	12	177	4	4	16	332	35	71	8	91	4	-4
8	295	28	-2	12	156	4	4	13	346	23	-5	17	42	7	10	9	55	4	-7
9	343	22	-9	13	440	40	-8	14	267	6	-1	18	233	24	3	10	195	24	-15
10	176	14	6	14	38	8	7*	15	44	12	24*	19	24	26	13*	11	73	15	-17*
11	136	17	1	15	35	15	13*	16	133	57	-31*	20	126	24	-6*	12	107	14	-7
12	269	25	-5	16	34	14	4*	17	296	25	1	21	40	6	4	13	0	18	-4*
13	304	25	-5	17	432	45	-7	18	266	17	1	22	219	9	-11	H ₂ L= 5, 7			
14	153	5	-3	18	13	23	10*	19	46	7	7	23	6	21	4*	0	66	4	-16
15	0	32	-6*	19	73	5	2	20	121	13	1	H ₂ L= 5, 4				1	151	16	-27
16	157	19	-1	20	25	14	4*	21	173	13	-8	1	220	22	1	2	17	13	-6*
17	245	20	-6	21	306	37	-7	22	186	14	2	2	180	12	25	H ₂ L= 6, -7			
18	131	4	1	22	29	9	16*	23	67	5	6	3	346	32	11	1	122	10	-6
19	72	4	-5	23	120	4	5	24	72	4	-3	4	30	8	12*	2	151	10	-28
20	92	3	0	24	0	28	-17*	25	143	26	-8	5	127	14	-7	3	134	7	-25
21	220	22	-7	25	216	34	-9	H ₂ L= 5, 2				6	154	4	7	4	34	20	-5*
22	126	15	-7	26	36	6	13	1	471	49	28	7	463	46	10	5	62	10	-20
23	92	4	-6	H ₂ L= 5, 0				2	224	31	29	8	73	4	8	6	143	23	-3
24	16	22	-12*	1	92	5	2	3	403	38	25	9	114	4	-3	7	185	28	-6
H ₂ L= 5, -2				2	659	73	74	4	68	4	6	10	80	4	13	8	74	4	-1
1	123	4	9	3	259	20	19	5	335	35	29	11	424	44	7	9	57	4	15
2	588	17	24	4	77	4	10	6	245	33	30	12	115	4	-0	H ₂ L= 6, -6			
3	73	5	3	5	67	5	-1	7	370	29	27	13	102	15	5	0	366	39	1
4	152	4	7	6	547	19	17	8	69	4	9	14	69	4	11	1	87	5	-3
5	126	6	4	7	234	5	1	9	134	4	8	15	269	33	-6	2	0	29	-6*
6	527	28	-11	8	242	14	3	10	151	22	16	16	93	4	7	3	48	13	-9*
7	61	6	6	9	51	5	-3	11	372	31	24	17	13	22	8*	4	302	28	-4
8	159	11	-8	10	376	27	4	12	94	4	13	18	37	6	13	5	122	5	-0
9	20	22	9*	11	174	4	-2	13	19	27	-7*	19	230	31	-7	6	42	9	-0*
10	439	34	-16	12	343	25	-1	14	124	4	9	20	64	6	-8	7	46	7	10
11	84	20	5*	13	33	9	7*	15	432	29	21	H ₂ L= 5, 5				8	224	25	-6
12	216	17	1	14	334	34	-6	16	117	12	47	0	286	27	-10	9	108	6	-2
13	71	4	5	15	182	5	-6	17	93	4	13	1	156	14	4	10	131	19	-7
14	294	32	-6	16	332	28	-0	18	60	6	-2	2	55	4	-1	11	13	24	6*
15	118	4	-2	17	17	24	-1*	19	319	28	13	3	131	10	0	12	173	25	-2
16	295	27	-7	18	236	31	-9	20	120	5	0	4	272	30	-7	13	100	17	0
17	25	12	22*	19	155	4	-5	21	102	7	5	5	172	4	-4	14	178	26	-9
18	153	17	-4	20	238	32	-4	22	33	11	-10*	6	116	15	-3	15	16	21	3*
19	127	13	2	21	29	10	-2*	23	224	31	5	7	78	6	4	H ₂ L= 6, -5			
20	313	30	-5	22	105	5	-6	24	113	4	3	8	252	28	-9	1	275	31	-17
21	18	25	10*	23	97	4	-5	H ₂ L= 5, 3				9	182	18	-5	2	37	10	18*
22	108	4	-5	24	200	29	-5	0	393	40	12	10	109	13	0	3	285	30	-12
23	66	4	-2	25	54	16	-14*	1	22	14	4*	11	44	5	6	4	34	12	2*
24	256	29	-8	26	45	5	-1	2	80	5	-5	12	199	21	-9	5	227	27	-11
25	28	13	-5*	H ₂ L= 5, 1				3	20	24	15*	13	131	4	-2	6	50	9	10*
H ₂ L= 5, -1				0	526	54	48	4	468	47	10	14	131	18	-6	7	257	28	-14
0	82	5	12	1	286	38	27	5	47	7	15	15	20	20	1*	8	24	14	24*
1	541	65	73	2	58	8	-0	6	164	13	13	16	128	18	-12	9	113	4	-5
2	133	4	8	3	285	38	29	7	27	13	10*	17	119	4	-7	10	13	23	-4*
3	414	15	25	4	445	39	57	8	412	43	11	H ₂ L= 5, 6				11	239	30	-17
4	29	12	14*	5	289	30	21	9	25	16	-11*	1	123	14	-14	12	0	24	-6*

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.TMCL2.2(OC4H8)

PAGE 9

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
13	29	11	-0*	3	250	6	8	10	50	9	7	17	207	33	-3	10	84	5	2
14	27	32	12*	4	221	6	8	11	71	7	11	18	232	24	5	11	208	26	-25
15	248	38	-9	5	367	15	8	12	112	5	5	19	34	12	1*	12	58	4	0
16	10	23	-7*	6	123	23	1*	13	420	35	-3	20	105	21	-2*	13	46	5	-10
17	34	8	-10*	7	212	17	3	14	30	14	-5*	21	167	8	-10	H ₂ L= 6, 6			
18	18	22	-4*	8	227	23	1	15	41	7	4	22	213	5	22	0	156	21	-36
H ₂ L= 6, -4				9	364	26	-4	16	64	6	0	H ₂ L= 6, 3				1	129	12	-18
0	305	38	0	10	145	7	1	17	311	33	-5	1	322	36	11	2	9	17	-3*
1	95	5	-7	11	116	4	1	18	22	26	10*	2	123	26	-1*	3	90	4	-13
2	71	8	-3	12	183	33	-8	19	44	6	4	3	353	40	18	4	148	23	-30
3	92	5	7	13	303	36	-5	20	22	22	14*	4	25	11	14*	5	155	18	-24
4	343	27	5	14	120	4	-3	21	222	30	-8	5	212	25	12	6	31	5	-1
5	124	4	-2	15	46	6	11	22	41	7	-2	6	130	25	-5*	H ₂ L= 7, -6			
6	96	6	-3	16	143	23	-1	23	96	5	-0	7	347	38	14	1	109	8	-27
7	29	16	-10*	17	261	28	-5	H ₂ L= 6, 1				8	32	8	12*	2	113	11	-29
8	346	39	-2	18	80	4	-6	1	235	28	9	9	76	5	-2	3	158	6	-17
9	117	5	-8	19	96	5	3	2	399	55	27	10	107	15	-6	4	43	10	-3*
10	145	18	3	20	68	6	-4	3	196	19	-2	11	332	39	11	5	84	5	-9
11	0	33	-20*	21	235	33	-4	4	48	5	17	12	23	11	14*	6	101	7	-27
12	246	35	-7	22	113	17	-3	5	187	12	17	13	26	10	13*	7	149	8	-39
13	119	4	4	23	101	4	-4	6	336	49	23	14	37	9	-8*	8	61	11	-13*
14	181	25	-2	H ₂ L= 6, -1				7	238	30	14	15	301	43	-7	9	59	5	-5
15	16	28	16*	1	172	30	17	8	175	20	15	16	61	4	4	10	110	28	-6*
16	146	24	-7	2	544	66	59	9	84	4	5	17	53	4	6	H ₂ L= 7, -5			
17	123	13	-2	3	61	9	12	10	272	35	16	18	43	6	-6	0	306	46	-25
18	195	28	-4	4	145	14	5	11	271	27	15	19	253	40	-10	1	51	18	-6*
19	36	7	10*	5	144	13	11	12	230	29	20	20	77	21	-6*	2	25	30	3*
20	115	16	-6	6	506	22	18	13	0	27	-5*	H ₂ L= 6, 4				3	71	6	10
21	86	4	-6	7	42	9	30*	14	274	33	16	0	304	38	-9	4	294	32	-12
H ₂ L= 6, -3				8	212	5	1	15	232	14	15	1	27	8	5*	5	39	10	14*
1	146	5	9	9	19	37	6*	16	222	21	11	2	48	4	4	6	53	6	2
2	330	17	5	10	360	31	-2	17	52	6	9	3	42	5	8	7	41	17	6*
3	287	7	11	11	64	9	11	18	188	25	10	4	298	36	-11	8	224	30	-13
4	80	5	6	12	238	24	-2	19	144	4	7	5	35	8	11*	9	35	12	5*
5	97	9	17	13	44	7	9	20	193	8	0	6	144	4	-24	10	106	16	-8
6	323	24	-10	14	267	30	-8	21	65	5	5	7	24	13	4*	11	20	23	15*
7	360	34	-7	15	72	5	8	22	103	23	-3*	8	304	32	-17	12	163	29	-8
8	92	6	-10	16	238	19	-3	23	122	8	-1	9	23	12	11*	13	59	5	4
9	129	4	9	17	29	9	24*	H ₂ L= 6, 2				10	177	20	-7	14	155	30	-11*
10	240	21	-6	18	163	20	-7	0	478	54	5	11	20	22	-6*	15	29	10	6*
11	368	39	-5	19	69	5	4	1	223	37	-11	12	248	28	-6	H ₂ L= 7, -4			
12	163	4	-5	20	239	30	-6	2	24	12	14*	13	18	20	12*	1	281	26	0
13	73	5	3	21	14	23	3*	3	203	34	1	14	171	21	-10	2	27	27	15*
14	149	14	-2	22	75	5	-7	4	432	44	16	15	25	9	-0*	3	294	7	3
15	245	35	0	23	59	4	9	5	221	33	-6	16	168	25	-11	4	47	9	7*
16	179	17	-10	H ₂ L= 6, 0				6	40	7	13	17	17	22	-3*	5	212	23	5
17	23	14	14*	0	65	6	8	7	112	4	4	H ₂ L= 6, 5				6	55	9	-14
18	113	4	-1	1	303	33	25	8	255	23	12	1	113	16	-17	7	274	34	-10
19	170	21	0	2	78	6	6	9	181	31	-5	2	152	17	-0	8	57	11	-1*
20	176	21	-6	3	299	38	27	10	161	19	10	3	192	24	-27	9	97	5	0
21	76	5	7	4	38	9	14*	11	41	6	1	4	14	19	6*	10	48	8	-2
22	87	4	-1	5	391	50	45	12	210	27	-0	5	93	3	-8	11	283	46	-10
H ₂ L= 6, -2				6	108	5	7	13	174	26	3	6	126	10	0	12	38	11	-3*
0	272	44	34	7	152	4	4	14	239	25	14	7	224	29	-23	13	39	9	28*
1	356	43	38	8	115	5	-1	15	0	27	-2*	8	30	7	2*	14	59	5	3
2	46	8	12	9	453	31	17	16	157	26	-3	9	82	4	-6	15	257	41	-8

STRUCTURE FACTORS CONTINUED FOR
ALPHA C8H8.THCL2.2(OC4H8)

PAGE 10

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
16	18	23	6*	11	68	5	4	2	311	47	3	6	62	3	-12	13	151	18	5
17	44	7	-4	12	131	16	9	3	210	17	3		H ₂ L=	8,	-5	14	164	26	5
	H ₂ L=	7,	-3	13	276	30	-0	4	65	5	3	1	126	7	-28	15	25	15	13*
0	423	67	54	14	65	5	9	5	109	4	12	2	101	7	-14	16	144	27	-2*
1	96	7	3	15	23	25	16*	6	276	43	7	3	164	6	-37		H ₂ L=	8,	-1
2	48	10	6*	16	59	5	-0	7	206	22	8	4	20	32	7*	1	107	26	6*
3	124	4	0	17	232	31	-5	8	109	19	11	5	90	7	-14	2	354	60	11
4	321	23	16	18	85	15	4*	9	64	4	2	6	79	7	-14	3	132	25	3*
5	100	5	-4	19	66	5	-0	10	197	32	1	7	196	38	-15*	4	24	12	14*
6	117	5	-2	20	30	16	-5*	11	179	22	5	8	56	6	0	5	79	7	3
7	83	5	3	21	216	41	-6*	12	128	17	2	9	76	4	1	6	245	41	8
8	296	34	2		H ₂ L=	7,	0	13	13	21	-2*		H ₂ L=	8,	-4	7	156	29	5
9	137	15	-4	1	32	9	27*	14	159	26	0	0	266	14	-41	8	58	6	-7
10	159	7	-7	2	361	54	22	15	155	6	5	1	60	10	-3	9	88	5	4
11	29	12	24*	3	34	15	4*	16	173	31	-8	2	0	47	-14*	10	166	25	3
12	250	35	-7	4	107	4	8	17	33	7	-6*	3	71	7	-4	11	148	32	7*
13	137	4	-6	5	13	27	0*	18	121	26	-12*	4	247	7	-28	12	138	21	4
14	178	27	-13	6	380	55	20		H ₂ L=	7,	3	5	28	19	24*	13	37	7	11*
15	32	9	17*	7	55	7	11	0	278	38	-24	6	72	7	1	14	132	27	-2*
16	162	32	-5*	8	216	29	15	1	127	17	-4	7	32	15	1*	15	128	30	-2*
17	136	12	-7	9	36	9	13*	2	24	10	-0*	8	221	31	-16	16	189	38	5*
18	170	24	-9	10	384	58	19	3	154	25	-7	9	13	25	2*	17	18	21	-3*
19	22	22	12*	11	76	5	13	4	253	30	-9	10	120	17	-5		H ₂ L=	8,	0
	H ₂ L=	7,	-2	12	194	32	7	5	99	19	-17*	11	37	8	5*	0	71	5	7
1	162	32	18*	13	0	24	-4*	6	82	4	-8	12	179	27	-15	1	262	46	10
2	390	60	39	14	279	44	14	7	101	4	-14	13	28	11	7*	2	38	8	9*
3	275	48	37	15	37	12	18*	8	218	29	-11		H ₂ L=	8,	-3	3	200	35	3
4	28	28	18*	16	186	29	11	9	90	5	-12	1	242	45	26*	4	94	5	1
5	72	12	3	17	20	29	9*	10	98	13	-4	2	54	8	5	5	306	51	11
6	280	18	13	18	145	25	1	11	17	19	7*	3	262	47	23	6	36	7	6*
7	253	23	5	19	34	8	23*	12	155	25	-14	4	30	30	2*	7	129	6	0
8	78	7	5	20	240	7	35	13	109	23	-18*	5	153	21	11	8	108	25	5*
9	66	5	0		H ₂ L=	7,	1	14	167	5	10	6	63	7	-6	9	305	51	1
10	176	19	-4	0	132	5	6	15	31	7	-1*	7	231	24	7	10	15	27	6*
11	253	30	-1	1	280	41	2	16	113	21	-14*	8	90	4	11	11	66	5	4
12	156	20	-1	2	11	22	-6*		H ₂ L=	7,	4	9	62	9	-2	12	59	5	-1
13	59	7	0	3	173	24	-3	1	156	20	-11	10	83	5	5	13	259	45	-2
14	124	5	-2	4	142	12	19	2	35	6	-7	11	242	40	-11	14	38	6	11
15	198	30	-2	5	398	60	21	3	195	26	-18	12	55	6	4	15	0	21	-16*
16	189	25	-1	6	66	12	7*	4	28	8	14*	13	15	27	3*	16	22	18	-2*
17	11	25	2*	7	112	25	4*	5	133	22	-14	14	62	5	-2		H ₂ L=	8,	1
18	106	5	-3	8	138	18	10	6	25	11	-12*	15	234	36	-13	1	22	24	-1*
19	154	23	-1	9	397	59	13	7	214	27	-22		H ₂ L=	8,	-2	2	244	41	-6
20	170	27	-8	10	107	4	3	8	23	8	22*	0	308	64	20*	3	18	21	11*
	H ₂ L=	7,	-1	11	81	5	-6	9	68	5	-9	1	171	27	10	4	137	24	-1
0	166	41	18*	12	132	4	11	10	24	12	10*	2	62	5	14	5	22	14	8*
1	307	45	25	13	333	51	14	11	228	34	-21	3	155	27	2	6	292	46	-5
2	26	24	1*	14	71	5	4	12	14	18	-0*	4	279	59	30*	7	41	6	24
3	258	37	24	15	36	8	6*	13	27	6	6*	5	135	21	9	8	148	27	-6
4	161	37	16*	16	47	7	9		H ₂ L=	7,	5	6	92	6	11	9	0	34	-2*
5	326	44	34	17	255	45	-10	0	201	32	-37	7	66	6	-4	10	264	49	-8*
6	74	28	12*	18	63	10	1	1	50	5	-9	8	205	38	5*	11	40	5	18
7	161	6	11	19	29	20	-5*	2	22	15	-4*	9	114	5	-4	12	139	23	-7
8	151	27	12	20	19	19	-1*	3	58	4	-5	10	128	5	11	13	20	20	6*
9	293	25	3		H ₂ L=	7,	2	4	199	28	-40	11	18	25	11*	14	191	40	-8*
10	75	5	4	1	168	24	-0	5	49	5	2	12	184	27	3	15	29	8	9*

K	FOB	SG	DEL
H,L=	8,	2	10
0	126	15	-5
1	145	26	-20
2	25	12	-5*
3	94	17	-16
4	129	22	1
5	204	42	-26*
6	49	5	-2
7	86	17	-11*
8	116	6	-9
9	223	45	-12*
10	40	5	5
11	66	4	-1
12	66	4	-7
13	202	42	-22*
H,L=	8,	3	1
1	108	5	-4
2	158	32	-26*
3	159	23	-14
4	12	20	-2*
5	94	12	-2
6	132	32	-24*
7	167	24	-15
8	39	5	3
9	72	4	-4
10	98	24	-21*
H,L=	8,	4	0
0	178	30	-30
1	65	4	-19
2	32	5	6
3	81	14	-16
H,L=	9,	-4	5
1	108	8	-32
2	44	11	-38*
3	129	14	-50
4	42	7	32
H,L=	9,	-3	1
0	234	58	1*
1	25	25	8*
2	34	9	0*
3	37	11	0*
4	232	57	-0*
5	36	10	9*
6	91	22	5*
7	29	11	9*
8	216	44	6*
H,L=	9,	-2	1
1	148	34	-8*
2	77	32	-15*
3	201	6	21
4	38	7	3*
5	104	21	2*
6	86	4	-1
7	199	43	7*
8	49	8	-1
9	56	5	-2

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 2.0)
BETA C8H8.THCL2.2(OC4H8) F(0,0,0) = 4102

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

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	0,	0		10	146	5	6	7	76	8	-17	7	32	35	-16*	11	360	14	6
2	319	10	4	11	395	12	-10	8	372	12	-7	8	481	16	26	12	490	17	41
4	1095	34	15	12	210	7	-7	9	317	10	17	9	54	20	5*	13	297	11	19
6	773	24	-15	13	82	6	-8	10	204	7	-5	10	315	11	9	14	33	34	29*
8	252	8	-12	14	140	6	0	11	254	9	-2	11	48	31	-5*	15	263	13	2
10	239	8	-5	15	43	14	-11*	12	530	28	-8	12	644	23	20	16	394	14	23
12	33	11	18*	16	106	7	-9	13	60	12	8*	13	67	30	22*	17	260	13	17
14	108	5	-5	17	286	10	-1	14	76	12	21	14	35	49	16*	18	101	27	-17*
16	13	33	-17*	18	158	8	-5	15	29	45	22*	15	128	10	5	19	21	34	-15*
18	340	12	-4	19	183	8	1	16	398	14	19	16	563	21	20	20	131	21	-14
20	255	11	1	20	302	12	4	17	183	8	12	17	37	38	32*	21	106	22	-22*
22	332	15	-5	21	121	10	-6	18	43	44	-13*	18	161	9	-2	H,K=	0,	9	
24	378	16	-6	22	153	13	2	19	230	12	1	19	136	16	-4	1	321	11	-8
26	102	16	-7	23	220	15	-11	20	271	36	5	20	238	10	29	2	213	8	2
H,K=	0,	1		24	215	16	-3	21	81	11	-5	21	41	20	14*	3	528	21	-7
1	219	10	-5	25	52	22	-19*	22	28	37	25*	22	123	15	-17	4	0	45	-16*
2	218	10	-12	26	100	21	-7*	23	218	16	-5	23	114	20	-20	5	60	14	0*
3	330	17	-13	H,K=	0,	3		24	121	14	-11	H,K=	0,	7		6	299	13	3
4	411	16	-8	1	90	18	12*	25	58	14	8*	1	256	9	17	7	358	15	10
5	39	9	10*	2	685	21	17	H,K=	0,	5		2	723	23	16	8	132	8	8
6	247	8	-6	3	102	10	4	1	206	7	7	3	307	10	22	9	201	15	2
7	139	5	4	4	219	8	-8	2	889	28	35	4	388	14	8	10	131	9	3
8	565	18	0	5	212	8	3	3	221	8	3	5	154	9	15	11	13	46	5*
9	203	7	-1	6	432	13	-7	4	250	8	14	6	445	15	24	12	45	15	7*
10	977	30	0	7	400	13	2	5	328	10	9	7	137	7	8	13	75	14	3*
11	136	5	5	8	119	5	1	6	549	17	12	8	374	12	20	14	119	9	2
12	218	7	-4	9	525	16	-6	7	62	17	27*	9	40	24	11*	15	124	12	2
13	186	6	-1	10	498	16	-1	8	388	13	1	10	24	39	15*	16	85	8	2
14	643	20	-6	11	153	7	-1	9	407	14	12	11	112	8	10	17	134	22	-26
15	175	6	-0	12	162	7	-10	10	211	7	5	12	52	18	10*	18	137	26	-10*
16	90	12	-14	13	390	12	-5	11	172	7	1	13	85	13	9	19	109	23	-28*
17	61	11	-4*	14	316	11	-1	12	54	14	5*	14	53	18	7*	H,K=	0,	10	
18	447	15	-6	15	430	14	-10	13	228	8	3	15	80	20	-10*	0	204	12	-1
19	139	9	3	16	43	26	-13*	14	88	13	-7	16	181	9	-1	1	124	7	2
20	244	10	4	17	98	9	-2	15	283	10	-1	17	128	16	-1	2	73	9	2
21	128	7	4	18	283	10	8	16	179	9	-4	18	51	17	-1*	3	114	10	-2
22	166	7	7	19	234	11	-2	17	194	9	-5	19	22	37	-27*	4	278	12	-4
23	53	14	33*	20	39	40	28*	18	150	11	-7	20	325	12	29	5	112	12	0
24	79	10	19	21	142	8	1	19	188	8	2	21	128	23	-11	6	137	10	1
25	100	14	-1	22	269	12	14	20	243	14	6	22	258	10	22	7	359	21	-12
26	55	17	41*	23	46	18	11*	21	44	22	9*	H,K=	0,	8		8	176	11	1
H,K=	0,	2		24	70	19	-9*	22	265	10	30	0	102	9	11	9	0	34	-8*
0	899	28	32	25	92	13	-7	23	38	25	5*	1	261	10	7	10	101	7	8
1	680	21	22	26	128	30	-21*	24	156	19	9	2	102	9	3	11	398	23	-20
2	223	11	-8	H,K=	0,	4		H,K=	0,	6		3	126	7	10	12	49	26	-15*
3	34	39	15*	0	602	19	15	0	274	10	16	4	107	9	7	13	205	17	-10
4	731	29	-51	1	407	13	22	1	357	11	20	5	120	8	24	14	33	26	3*
5	639	25	-29	2	192	8	8	2	328	11	2	6	243	8	9	15	159	32	-34*
6	31	17	-5*	3	65	10	1	3	46	15	14*	7	432	15	13	16	112	20	-5
7	312	10	-11	4	390	12	16	4	53	10	34*	8	280	10	19	17	242	12	-8
8	550	17	-17	5	543	20	8	5	353	12	6	9	83	12	14	H,K=	0,	11	
9	203	7	-8	6	318	11	5	6	404	13	17	10	198	8	1	1	222	16	-25

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	40	14	1*	H ₂ K=	1,	1	-26	49	18	15*-24	59	13	28*-21	92	12	-5			
3	284	16	-30	-27	116	42	-3*-25	93	10	-6	-23	145	11	9	-20	333	36	4	
4	100	9	-6	-26	356	13	27	-24	133	9	1	-22	259	9	1	-19	158	11	9
5	77	10	-7	-25	60	16	-13*-23	152	11	2	-21	273	12	20	-18	0	42	-22*	
6	70	9	-6	-24	39	42	12*-22	135	9	-7	-20	101	27	-4*-17	321	11	4		
7	192	15	-22	-23	81	10	-5	-21	0	46	-13*-19	58	16	5*-16	297	11	7		
8	190	16	-30	-22	442	18	-13	-20	206	8	-7	-18	350	13	-3	-15	42	45	35*
9	51	37	-19*	-21	176	10	-22	-19	156	10	-15	-17	265	9	1	-14	101	7	9
10	183	14	-25	-20	190	9	3	-18	240	10	-6	-16	34	46	-5*-13	469	25	1	
11	41	14	16*	-19	120	9	-8	-17	348	15	-12	-15	179	7	-1	-12	234	8	2
12	61	18	-11*-18	301	11	1	-16	273	12	-12	-14	336	11	0	-11	224	8	-6	
13	25	30	2*-17	69	11	18	-15	18	45	3*-13	82	7	-4	-10	201	7	4		
14	268	18	-23	-16	222	8	-2	-14	189	7	-11	-12	33	16	10*	-9	236	8	-3
	H ₂ K=	0,	12	-15	205	7	-6	-13	404	13	-15	-11	263	9	-16	-8	224	8	1
0	268	38	-36	-14	87	6	0	-12	709	22	-16	-10	465	15	-26	-7	578	18	0
1	16	36	4*-13	210	7	-11	-11	280	10	-4	-9	524	16	-17	-6	567	18	-9	
2	92	13	-15	-12	69	7	31	-10	160	5	2	-8	326	10	-8	-5	52	28	9*
3	131	12	-13	-11	116	5	-7	-9	52	6	1	-7	250	8	-8	-4	341	11	4
4	199	38	-33*-10	117	5	13	-8	818	25	-29	-6	349	11	-17	-3	373	12	7	
5	38	14	2*	-9	282	9	-4	-7	466	14	-19	-5	309	10	-8	-2	438	17	12
6	189	20	-35	-8	513	16	-28	-6	74	7	5	-4	98	15	4	-1	511	16	28
7	164	20	-41	-7	13	25	-1*	-5	205	7	-5	-3	309	15	5	0	766	24	40
8	45	10	-12*	-6	357	11	-9	-4	307	10	-24	-2	574	18	-2	1	196	8	10
9	61	10	-20	-5	40	7	7	-3	322	17	-19	-1	45	33	37*	2	195	8	-8
10	123	23	-37*	-4	868	31	-18	-2	54	15	-10*	0	483	15	18	3	54	10	10
	H ₂ K=	0,	13	-3	268	8	-6	-1	295	18	3	1	175	9	12	4	586	18	-12
1	86	13	-34	-2	946	29	-37	0	206	7	4	2	185	7	3	5	280	9	-9
2	97	21	-45*	-1	41	4	13	1	246	8	5	3	506	16	-19	6	124	6	-6
	H ₂ K=	1,	0	0	835	26	29	2	259	9	-9	4	478	15	-14	7	377	12	-2
-26	58	14	33*	1	383	17	8	3	51	11	14*	5	464	14	-26	8	518	24	-13
-24	51	17	-0*	21081	49	-68	4	103	9	-11	6	398	12	-8	9	421	20	-8	
-22	217	12	-6	3	163	6	-2	5	254	8	-10	7	537	21	-12	10	124	6	-1
-20	169	12	-10	4	227	8	-8	6	463	14	-11	8	379	16	0	11	478	28	0
-18	459	15	-14	5	329	13	-15	7	197	6	-10	9	65	11	11	12	164	7	0
-16	600	19	-17	6	307	18	-20	8	61	7	-3	10	416	13	-12	13	30	38	20*
-14	290	9	-11	7	335	14	-3	9	290	9	-10	11	149	6	-3	14	150	8	8
-121000	31	-21	8	295	9	-12	10	574	18	-14	12	108	11	-5	15	437	31	-2	
-10	146	5	-4	9	372	12	-3	11	446	14	-2	13	323	10	-5	16	37	54	-18*
-81025	31	-11	10	237	8	0	12	404	13	-5	14	226	8	3	17	230	10	9	
-6	96	4	6	11	107	5	0	13	57	13	12*	15	226	8	7	18	261	12	-2
-4	569	17	7	12	32	36	-1*	14	395	13	-5	16	188	8	-0	19	146	8	-8
-2	346	11	-1	13	138	5	-0	15	346	11	-12	17	84	10	9	20	142	7	5
0	43	6	22	14	88	8	2	16	443	14	-2	18	192	10	5	21	169	9	-1
2	360	11	1	15	141	6	0	17	166	7	-2	19	391	45	13	22	247	14	2
4	213	7	-3	16	252	9	-8	18	90	9	2	20	207	11	-1	23	83	10	-2
6	813	25	-12	17	36	37	8*	19	78	11	25	21	180	10	7	24	100	23	-26*
8	528	16	-10	18	16	37	2*	20	342	12	1	22	159	8	2	25	44	17	-6*
10	699	22	-12	19	173	8	1	21	157	10	9	23	137	9	6	H ₂ K=	1,	5	
12	670	21	-20	20	387	14	-10	22	44	23	-8*	24	163	13	-0	-25	150	8	9
14	408	13	-3	21	39	64	-2*	23	112	16	-4	25	226	9	31	-24	61	17	-17*
16	452	14	-15	22	173	12	-4	24	99	9	-7	H ₂ K=	1,	4	-23	156	17	-17	
18	94	8	5	23	72	10	21	25	63	12	22*-26	36	44	-7*-22	75	15	-10*		
20	429	16	-9	24	345	16	-3	26	76	16	-16*-25	0	41	-41*-21	200	11	-7		
22	0	39	-9*	25	121	9	-3	H ₂ K=	1,	3	-24	222	21	-14	-20	240	15	0	
24	73	13	-17	26	184	21	-22	-26	141	18	-12	-23	94	20	-7*-19	15	54	-3*	
26	0	46	-32*	H ₂ K=	1,	2	-25	185	9	13	-22	34	37	33*-18	278	11	9		

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-17	149	8	4	-11	65	14	22*	-3	102	11	6	8	330	11	14	-15	108	9	-9
-16	347	13	-5	-10	231	10	-1	-2	54	13	6*	9	106	8	18	-14	150	12	6
-15	82	23	5*	-9	49	18	9*	-1	69	16	14*	10	61	22	6*	-13	108	7	0
-14	470	16	5	-8	40	30	23*	0	135	6	11	11	98	9	24	-12	194	10	0
-13	96	10	10	-7	204	8	-0	1	53	12	33*	12	22	47	4*	-11	139	13	-10
-12	299	10	7	-6	477	15	14	2	141	8	-5	13	14	39	-25*	-10	28	38	-10*
-11	84	9	-6	-5	123	6	4	3	71	11	-3	14	54	17	9*	-9	52	27	-5*
-10	704	22	7	-4	325	11	10	4	322	10	-2	15	44	46	-2*	-8	209	8	13
-9	203	8	-3	-3	174	6	6	5	268	9	-2	16	39	20	5*	-7	259	11	4
-8	54	15	17*	-2	651	20	14	6	23	36	17*	17	119	16	-8	-6	27	37	25*
-7	174	6	10	-1	61	11	22	7	48	16	10*	18	204	14	-3	-5	413	14	-3
-6	577	18	11	0	323	26	42	8	574	19	19	19	86	10	-11	-4	151	7	-8
-5	173	6	14	1	115	7	-2	9	326	11	8	20	16	38	4*	-3	76	9	9
-4	118	6	8	2	261	9	13	10	371	13	10	H ₂ K= 1,		9	-2	27	37	-4*	
-3	380	12	20	3	169	6	2	11	50	18	1*	-19	213	9	2	-1	528	19	-24
-2	314	10	12	4	753	24	15	12	400	13	1	-18	118	18	-13	0	98	8	-1
-1	14	36	-29*	5	99	7	5	13	267	10	7	-17	37	20	11*	1	181	11	-3
0	58	11	-0*	6	121	6	13	14	480	18	22	-16	152	11	3	2	86	8	-3
1	409	13	21	7	340	11	-3	15	26	37	3*	-15	395	13	17	3	320	12	-8
2	91	13	5	8	355	12	7	16	151	7	3	-14	178	10	10	4	149	10	3
3	487	15	15	9	33	42	22*	17	221	10	2	-13	188	10	0	5	315	12	-2
4	341	11	8	10	151	7	6	18	299	18	-9	-12	131	10	9	6	166	9	-1
5	253	9	-2	11	199	8	-5	19	27	36	8*	-11	385	13	6	7	98	8	5
6	56	9	7	12	53	20	2*	20	50	14	-4*	-10	262	10	16	8	116	8	-7
7	323	10	-1	13	76	11	20	21	57	11	-11*	-9	427	18	7	9	235	14	-4
8	505	16	-5	14	111	12	16	22	88	13	-4	-8	73	17	35*	10	193	8	7
9	81	8	-3	15	173	8	-6	H ₂ K= 1,		8	-7	118	8	10	11	123	15	-6	
10	352	21	7	16	90	10	-3	-21	61	21	-17*	-6	205	8	4	12	175	12	-1
11	17	36	-20*	17	77	11	19	-20	254	10	22	-5	371	13	12	13	34	37	21*
12	531	36	7	18	208	12	0	-19	246	14	10	-4	5	38	-15*	14	101	10	-1
13	37	34	13*	19	116	10	9	-18	92	9	-7	-3	137	8	9	15	56	10	7*
14	479	44	9	20	0	37	-22*	-17	45	52	4*	-2	144	7	-3	16	161	17	-9
15	121	11	-5	21	41	33	15*	-16	116	10	9	-1	40	21	30*	H ₂ K= 1,		11	
16	205	8	14	22	339	15	33	-15	62	11	6	0	60	12	-5*	-14	4	31	-2*
17	0	52	-49*	23	26	41	-3*	-14	43	23	-2*	1	114	7	9	-13	110	8	-12
18	427	17	15	H ₂ K= 1,		7	-13	27	44	14*	2	157	7	2	-12	29	31	9*	
19	210	26	15	-23	41	17	-14*	-12	90	12	1	3	251	9	3	-11	227	19	-31
20	63	13	37*	-22	34	31	18*	-11	157	7	12	4	54	15	17*	-10	125	11	-10
21	101	13	-16	-21	41	19	18*	-10	220	8	9	5	217	8	0	-9	238	9	-15
22	156	16	2	-20	324	11	19	-9	79	12	8	6	178	8	3	-8	186	7	-13
23	83	15	-10	-19	127	22	-0	-8	39	28	34*	7	272	13	-2	-7	146	8	-10
24	0	35	-3*	-18	240	10	10	-7	139	8	19	8	214	10	9	-6	72	8	-5
H ₂ K= 1,		6	-17	35	38	-29*	-6	423	15	9	9	472	18	5	-5	195	11	-13	
-24	384	16	32	-16	359	15	6	-5	346	11	-3	10	82	12	-0	-4	236	10	-20
-23	23	43	17*	-15	280	12	8	-4	293	11	7	11	68	11	-15	-3	0	33	-3*
-22	71	10	17	-14	543	19	15	-3	111	16	10	12	222	13	-1	-2	202	8	-8
-21	75	20	-18*	-13	70	25	-4*	-2	313	12	-2	13	417	20	-13	-1	43	26	-3*
-20	316	20	6	-12	188	8	15	-1	529	17	8	14	202	9	-3	0	105	6	4
-19	69	13	14*	-11	205	9	11	0	470	15	-1	15	157	15	6	1	72	9	1
-18	211	8	-4	-10	565	19	31	1	203	8	11	16	102	9	-6	2	275	12	-24
-17	248	10	8	-9	127	8	8	2	84	10	15	17	223	22	-22	3	110	8	2
-16	96	10	-2	-8	176	9	4	3	362	12	1	18	144	18	-18	4	38	18	16*
-15	110	9	-3	-7	179	8	10	4	522	16	18	19	188	11	10	5	111	8	-14
-14	68	18	4*	-6	371	12	14	5	326	11	14	H ₂ K= 1,		10	6	267	14	-22	
-13	184	7	4	-5	185	9	16	6	30	38	20*	-17	39	15	-2*	7	193	11	-15
-12	95	10	7	-4	266	9	7	7	67	20	9*	-16	158	18	-13	8	82	10	-9

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 4

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
3	244	14	-26	H,K=	2,	1	-26	165	12	-11	-23	108	9	6	-20	125	8	-9		
10	97	14	-17	-27	71	15	2*-25	200	12	-4	-22	162	8	-9	-19	242	10	10		
11	53	19	-23*	-26	0	40	-10*-24	275	12	-1	-21	272	12	-2	-18	315	11	3		
12	45	14	-19*	-25	27	38	22*-23	53	10	-0	-20	217	8	11	-17	0	41	-6*		
13	280	14	-11	-24	63	12	4*-22	152	7	5	-19	60	14	29*-16	150	8	2			
	H,K=	1,	12	-23	96	14	-12	-21	131	8	-9	-18	178	11	-3	-15	260	9	5	
-10	17	30	3*-22		0	37	-27*-20	376	15	-14	-17	227	9	-10	-14	330	11	-4		
-9	109	13	-19	-21	127	12	-8	-19	272	10	-6	-16	213	9	-6	-13	216	7	2	
-8	196	22	-30	-20	405	14	-16	-18	191	7	4	-15	287	11	-20	-12	311	10	-2	
-7	25	35	5*-19		55	14	2*-17	101	7	-1	-14	197	7	-7	-11	149	6	-3		
-6	160	13	-21	-18	106	7	-10	-16	317	11	-5	-13	216	7	-5	-10	499	15	-1	
-5	188	11	-25	-17	183	7	-0	-15	146	8	1	-12	361	12	-16	-9	238	8	-4	
-4	80	10	-9	-16	582	18	-20	-14	106	5	-4	-11	523	16	-26	-8	464	14	-27	
-3	35	15	9*-15		263	9	-18	-13	347	11	-7	-10	334	10	-18	-7	431	14	7	
-2	134	14	-27	-14	362	13	-8	-12	106	7	-4	-9	447	14	-12	-6	351	11	0	
-1	244	14	-30	-13	57	13	-1*-11	217	7	-11	-8	561	17	-21	-5	250	9	-4		
0	121	15	-15	-12	716	22	-23	-10	332	11	-13	-7	396	12	-26	-4	364	12	-2	
1	60	13	-5*-11		114	5	-4	-9	147	5	-9	-6	217	7	-3	-3	571	18	3	
2	0	38	-15*-10		787	24	-29	-8	136	5	-8	-5	797	33	-19	-2	195	7	-6	
3	203	12	-31	-9	282	9	0	-7	261	8	-4	-4	349	11	1	-1	761	29	38	
4	119	12	-11	-8	597	16	-6	-6	698	21	-28	-3	129	8	12	0	96	7	-1	
5	93	9	-3	-7	69	5	17	-5	312	10	-22	-2	269	9	5	1	0	35	-22*	
6	178	15	-20	-6	489	15	-19	-4	188	6	1	-1	190	9	14	2	464	14	15	
7	82	6	-16	-5	168	6	0	-3	399	21	-15	0	373	12	34	3	762	24	2	
8	32	21	1*	-4	48	14	18*	-2	690	36	-46	1	333	11	18	4	113	6	6	
9	58	7	8	-3	58	8	2	-1	601	32	-6	2	370	12	8	5	229	7	-2	
	H,K=	1,	13	-2	306	9	-4	0	671	21	38	3	260	9	0	6	351	11	0	
-1	22	26	-7*	-1	93	6	6	1	32	40	17*	4	457	17	-23	7	396	12	7	
0	154	19	-32		0	32	34	6*	2	654	36	-13	5	195	7	-8	8	99	10	15
	H,K=	2,	0	1	288	20	1	3	578	18	-21	6	29	23	5*	9	190	7	-5	
-26	257	30	-4	2	156	8	-8	4	203	7	-8	7	608	23	-6	10	455	31	-16	
-24	381	19	-6	3	149	6	-9	5	326	10	-8	8	428	13	-5	11	113	7	-1	
-22	143	10	-4	4	212	9	-7	6	420	13	-6	9	107	7	3	12	131	7	-6	
-20	564	19	-17	5	224	7	-3	7	179	6	-10	10	180	6	-3	13	164	8	-7	
-18	34	34	-4*	6	366	15	-13	8	433	13	-14	11	456	27	-7	14	434	34	11	
-16	157	7	-3	7	265	11	-16	9	256	8	-4	12	428	22	-3	15	241	9	-4	
-14	75	6	-9	8	786	24	-22	10	216	7	-8	13	486	27	14	16	166	8	-4	
-12	72	6	2	9	83	5	2	11	160	6	-5	14	112	7	-6	17	180	9	6	
-10	655	21	-13	10	186	22	-26	12	298	10	-4	15	17	45	-22*	18	247	11	11	
-8	64	6	27	11	209	7	-2	13	67	8	8	16	305	29	12	19	136	9	-7	
-6	827	25	-8	12	727	22	-24	14	84	9	0	17	378	26	11	20	155	12	2	
-4	194	6	2	13	117	7	-4	15	253	8	0	18	158	8	4	21	293	11	25	
-21	960	83	204	14	242	13	-31	16	99	9	-2	19	237	21	9	22	130	8	1	
0	675	21	-20	15	31	34	24*	17	136	7	18	20	244	26	13	23	95	9	-1	
2	729	23	-106	16	428	14	-1	13	265	10	8	21	57	22	18*	24	40	17	18*	
4	781	24	-65	17	73	10	-2	13	90	17	-13*	22	43	25	4*	H,K=	2,	5		
6	73	7	13	18	299	10	-4	20	105	9	4	23	158	15	-16	-25	26	34	21*	
8	609	19	-9	19	0	47	-41*	21	200	10	-0	24	161	13	1	-24	181	16	-11	
10	32	11	24*	20	162	8	4	22	353	44	-1	25	86	9	-2	-23	19	37	-13*	
12	184	6	8	21	32	37	11*	23	58	17	-11*	H,K=	2,	4	-22	330	17	-6		
14	237	8	-5	22	155	8	2	24	37	40	15*-26	78	9	4	-21	166	11	-4		
16	135	9	-8	23	77	11	6	25	104	8	-3	-25	259	19	-17	-20	92	13	1	
18	287	10	2	24	57	17	-13*	H,K=	2,	3	-24	51	25	-21*-19	141	8	4			
20	86	10	-1	25	28	37	-2*-26	131	17	0	-23	67	11	13	-18	293	12	-6		
22	383	18	-5	H,K=	2,	2	-25	51	18	1*-22	218	23	2	-17	184	9	11			
24	64	12	22*-27	13	39	-12*-24	126	11	-3	-21	193	8	6	-16	35	40	10*			

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 5

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-15	322	11	5	-8	561	18	17	1	385	12	18	13	148	9	-2	-10	111	7	3
-14	163	8	17	-7	55	21	16*	2	422	13	0	14	304	17	-7	-9	390	13	-8
-13	64	13	7*	-6	48	12	-0*	3	55	13	1*	15	258	16	-6	-8	67	9	6
-12	27	35	18*	-5	291	9	8	4	472	15	19	16	194	10	-1	-7	239	13	-13
-11	303	10	2	-4	468	15	4	5	338	12	-2	17	50	12	42*	-6	221	10	-2
-10	132	7	6	-3	84	9	8	6	481	15	9	18	153	8	14	-5	159	7	-9
-9	158	6	0	-2	127	7	5	7	61	15	7*	19	119	20	-9	-4	135	7	-6
-8	412	13	10	-1	306	10	18	8	66	10	30	20	109	26	-36*	-3	227	8	-8
-7	235	8	2	0	84	8	12	9	92	11	4	H ₂ K= 2,		9	-2	213	12	-1	
-6	167	6	6	1	39	23	7*	10	127	8	0	-20	89	30	-10*	-1	158	9	0
-5	301	10	12	2	58	10	37	11	23	40	19*	-19	79	13	-27	0	143	7	2
-4	828	33	28	3	335	11	6	12	54	17	10*	-18	98	9	-6	1	78	14	9
-3	111	7	7	4	286	10	3	13	46	25	-8*	-17	188	8	10	2	157	10	-16
-2	231	8	8	5	133	6	7	14	79	11	-1	-16	111	11	3	3	81	7	16
-1	156	6	16	6	450	14	8	15	75	12	33	-15	37	21	27*	4	171	8	-8
0	895	28	43	7	179	7	4	16	83	10	4	-14	112	9	3	5	253	16	-14
1	161	7	6	8	255	8	6	17	33	39	23*	-13	32	33	25*	6	203	9	-5
2	582	18	19	9	167	7	2	18	125	9	-6	-12	75	9	17	7	108	8	-15
3	139	8	12	10	633	37	-5	19	106	15	-13	-11	114	11	0	8	94	8	-0
4	494	15	9	11	31	42	-7*	20	202	23	-14	-10	33	43	16*	9	348	19	-18
5	43	13	12*	12	148	7	5	21	30	31	6*	-9	277	12	12	10	108	7	3
6	579	18	-13	13	118	8	9	H ₂ K= 2,		8	-8	156	10	-5	11	245	9	1	
7	469	15	-4	14	500	44	16	-21	0	33	-19*	-7	114	9	1	12	32	33	6*
8	161	6	-4	15	70	16	-11*	-20	50	14	8*	-6	54	22	13*	13	151	15	-19
9	240	8	4	16	253	14	-7	-19	174	19	-7	-5	395	14	17	14	86	14	-7
10	280	9	-5	17	65	18	-8*	-18	258	16	-6	-4	321	12	7	15	336	18	-5
11	261	9	-1	18	195	10	7	-17	254	14	2	-3	441	14	-5	16	40	18	40*
12	62	21	25*	19	37	39	-14*	-16	92	10	16	-2	151	7	-1	H ₂ K= 2,		11	
13	250	23	-0	20	212	15	1	-15	106	8	-0	-1	234	9	-8	-14	64	9	-13
14	57	19	-6*	21	73	10	-9	-14	326	14	10	0	235	12	-7	-13	40	16	13*
15	29	47	2*	22	31	31	16*	-13	448	17	6	1	510	17	-8	-12	209	18	-22
16	95	12	-7	H ₂ K= 2,		7	-12	284	11	6	2	170	7	-1	-11	9	45	-17*	
17	215	26	11	-23	164	25	-17	-11	87	17	20*	3	95	8	11	-10	196	16	-19
18	193	8	-4	-22	325	13	4	-10	239	9	22	4	207	8	-17	-9	149	10	-13
19	0	43	-11*	-21	48	29	-6*	-9	292	11	7	5	376	17	2	-8	56	9	16
20	266	18	-13	-20	38	22	21*	-8	398	14	14	6	154	7	8	-7	85	10	-10
21	49	38	-8*	-19	112	7	-3	-7	255	10	11	7	216	13	1	-6	252	14	-24
22	34	37	-21*	-18	243	17	-10	-6	49	19	5*	8	194	10	1	-5	244	11	-23
23	76	9	-2	-17	129	9	5	-5	208	8	14	9	87	9	21	-4	32	33	-29*
H ₂ K= 2,		6	-15	146	8	-2	-4	276	10	10	10	10	68	9	5	-3	248	13	-25
-24	49	17	-4*	-15	75	16	-10*	-3	185	8	7	11	106	8	10	-2	59	8	12
-23	19	34	12*	-14	11	40	-14*	-2	47	18	12*	12	56	14	-18*	-1	170	10	-28
-22	105	13	-14	-13	38	40	-10*	-1	91	10	10	13	77	11	7	0	29	31	5*
-21	101	8	7	-12	46	21	17*	0	33	42	8*	14	0	47	-4*	1	316	16	-34
-20	100	8	5	-11	0	39	-22*	1	64	11	19	15	63	19	-8*	2	74	8	-13
-19	95	8	18	-10	218	8	15	2	190	8	-2	16	73	9	-9	3	27	30	21*
-18	467	18	-4	-9	65	12	7*	3	16	43	-12*	17	65	14	5*	4	116	9	-6
-17	7	41	-27*	-9	327	11	15	4	102	8	-1	18	34	35	-18*	5	262	13	-25
-16	132	9	11	-7	169	7	8	5	304	10	1	H ₂ K= 2,		10	6	105	8	-5	
-15	21	40	16*	-6	0	36	-26*	6	298	10	13	-17	189	8	-5	7	156	8	-5
-14	617	20	11	-5	112	7	17	7	156	9	0	-16	52	18	-19*	8	198	11	-4
-13	51	17	21*	-4	529	27	21	8	56	35	-12*	-15	121	12	3	9	45	14	-16*
-12	439	14	14	-3	345	11	3	9	351	16	-3	-14	72	14	-8*	10	67	8	-3
-11	86	9	6	-2	195	7	3	10	411	15	7	-13	368	21	-17	11	81	8	-4
-10	347	11	19	-1	299	10	3	11	334	13	1	-12	44	24	38*	12	217	17	-10
-9	158	6	5	0	642	24	12	12	44	20	20*	-11	63	10	14	13	39	20	-14*

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 6

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
H ₂ K#	2,	12	-20	359	12	-12	-18	420	15	-11	-14	70	7	11	-10	298	10	2		
-10	29	16	9*-13	71	14	2*-17		32	39	17*-13		246	8	-12	-9	582	18	-10		
-9	153	15	-35	-18	222	8	-10	-16	61	10	-24	-12	287	10	-8	-8	220	8	-10	
-8	138	19	-47	-17	190	7	1	-15	302	10	-12	-11	399	13	-13	-7	221	7	-9	
-7	10	29	1*-16	209	7	0	-14	570	18	-23	-10	79	6	4	-6	351	11	0		
-6	173	18	-24	-15	72	7	6	-13	345	11	-19	-9	53	8	12	-5	596	18	23	
-5	132	6	-17	-14	53	8	22	-12	87	5	8	-8	352	11	-15	-4	249	8	6	
-4	30	39	-23*-13	145	5	-1	-11	82	7	3	-7	320	10	-15	-3	438	14	3		
-3	25	35	-8*-12	68	7	11	-10	814	25	-35	-6	214	7	4	-2	716	29	2		
-2	313	24	-48	-11	134	5	-3	-9	426	13	-13	-5	637	26	-21	-1	293	9	12	
-1	44	32	-28*-10	234	12	-1	-8	258	8	-1	-4	438	22	-15	0	172	7	18		
0	120	10	-17	-9	208	7	-1	-7	361	11	-7	-3	96	7	4	1	30	44	7*	
1	24	28	11*	-9	424	13	-5	-6	531	16	-18	-2	16	34	-27*	2	691	26	24	
2	205	27	-32	-7	59	5	1	-5	315	10	-12	-1	882	37	15	3	442	14	13	
3	0	33	-26*	-6	456	14	-19	-4	331	10	-16	0	562	17	35	4	171	8	-9	
4	272	23	-21	-5	140	5	4	-3	348	11	-6	1	613	19	47	5	346	11	-4	
5	110	9	-26	-4	497	15	-11	-2	90	10	5	2	117	7	17	6	442	23	-3	
6	54	20	-12*	-3	7	26	-6*	-1	218	17	-1	3	191	7	2	7	292	19	-11	
7	89	11	-21	-2	177	6	4	0	36	66	5*	4	555	24	-28	8	63	10	6	
8	194	17	-18	-1	293	10	1	1	107	21	18*	5	545	23	-24	9	517	31	-12	
9	125	13	-29	0	951	31	4	2	258	20	6	6	68	12	-5	10	246	22	-8	
H ₂ K#	3,	0		1	145	11	7	3	338	11	3	7	144	6	1	11	109	7	13	
-26	53	15	25*	2	100	25	-12*	4	555	17	-3	8	365	18	-2	12	66	11	38	
-24	42	21	26*	3	89	12	-0	5	25	30	-13*	9	86	7	3	13	290	25	-11	
-22	139	11	-15	4	679	21	-22	6	422	13	-4	10	115	6	4	14	148	8	-4	
-20	173	10	-14	5	195	6	-7	7	312	10	10	11	267	19	2	15	355	37	4	
-18	626	21	-29	6	336	10	-25	8	314	10	-2	12	350	25	1	16	166	10	-1	
-16	238	8	-13	7	146	5	8	9	478	15	-5	13	110	8	-12	17	106	9	7	
-14	797	25	-39	8	351	11	-5	10	573	21	-9	14	114	3	-3	18	166	9	-5	
-12	273	9	-1	9	40	11	8*	11	49	13	39*	15	192	10	9	19	267	35	-4	
-10	776	24	-7	10	225	8	-1	12	162	7	1	16	219	10	2	20	198	12	6	
-8	348	11	-8	11	146	6	-10	13	304	10	-6	17	304	30	15	21	96	7	19	
-6	401	12	-4	12	179	7	-5	14	536	28	-5	18	164	9	8	22	204	19	-13	
-4	212	7	3	13	161	6	8	15	276	9	-3	19	196	11	12	23	56	18	-0*	
-2	107	4	-0	14	212	7	11	16	85	11	12	20	205	11	-6	H ₂ K# 3, 5				
0	183	7	-7	15	64	22	18*	17	33	50	-34*	21	139	8	5	-25	86	9	4	
2	323	11	7	16	96	9	-5	18	338	33	6	22	104	10	5	-24	35	44	2*	
4	292	9	-2	17	109	8	-0	13	224	9	2	23	209	16	-9	-23	172	11	-10	
6	411	13	-5	18	308	11	3	20	102	10	-6	24	207	10	25	-22	121	8	-4	
8	486	15	-17	19	34	44	-4*	21	83	13	-12	H ₂ K# 3,				4	-21	0	38	-17*
10	816	25	-21	20	225	25	-0	22	140	11	7	-26	261	19	-10	-20	305	11	14	
12	277	9	-8	21	33	38	2*	23	79	13	0	-25	90	10	-14	-19	98	13	-2	
14	659	21	-23	22	236	12	2	24	41	21	10*-24	119	8	-12	-18	198	11	7		
16	49	18	13*	23	71	13	-0*	H ₂ K# 3,				3	-23	74	13	-4	-17	257	9	7
18	418	15	3	24	242	22	-18	-26	71	16	8*-22	275	27	9	-16	500	16	20		
20	113	8	1	25	26	36	20*-25	103	16	-5	-21	213	8	5	-15	95	9	10		
22	170	9	-1	H ₂ K# 3,				2	-24	235	11	1	-20	151	8	6	-14	104	9	8
24	26	39	-21*-27	91	9	2	-23	290	12	5	-19	276	10	7	-13	140	11	24		
H ₂ K# 3,				1	-26	90	9	14	-22	119	8	2	-18	275	9	7	-12	713	32	20
-27	21	44	-36*-25	112	9	-3	-21	139	7	6	-17	105	15	9	-11	112	11	-3		
-26	97	9	5	-24	48	23	17*-20	314	13	2	-16	78	16	11*-10	293	10	18			
-25	68	12	17	-23	13	37	-1*-19	188	8	-5	-15	371	12	2	-9	276	9	9		
-24	353	15	-10	-22	170	7	0	-18	91	9	3	-14	212	8	-3	-8	720	22	34	
-23	80	10	-2	-21	183	8	-1	-17	285	9	1	-13	389	12	-12	-7	57	13	11*	
-22	313	11	-3	-20	119	10	-12	-16	319	11	2	-12	51	12	2*	-6	412	13	12	
-21	17	42	-6*-19	225	9	-12	-15	52	21	-10*-11	222	8	6	-5	429	13	29			

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 7

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	277	9	11	3	91	9	2	12	484	21	3	-15	241	10	4	5	41	18	13*
-3	199	7	9	4	188	8	21	13	123	8	-2	-14	46	20	38*	6	134	6	1
-2	230	8	19	5	66	11	-0	14	54	13	20*	-13	272	12	3	7	282	17	-8
-1	537	20	24	6	417	13	0	15	123	10	-11	-12	297	11	4	8	85	9	-10
0	59	14	11*	7	39	24	26*	16	323	19	-5	-11	428	14	12	9	79	13	-10
1	302	10	33	8	366	13	4	17	128	7	5	-10	74	9	13	10	126	10	-11
2	332	11	7	9	206	8	1	18	136	11	6	-9	96	7	15	11	0	33	-36*
3	270	9	5	10	34	39	17*	19	71	22	-1*	-8	345	12	-2	12	46	13	7*
4	143	6	6	11	26	39	14*	20	124	17	-17	-7	397	14	8	13	52	19	-4*
5	353	12	7	12	48	24	3*	H,K= 3,			8	-6	190	7	7	14	138	22	-15
6	400	13	-5	13	108	9	-0	-21	226	11	-6	-5	159	8	2	15	107	28	-7*
7	49	24	-16*	14	74	14	-5*	-20	163	12	-5	-4	222	10	0	H,K= 3,			11
8	478	28	-3	15	72	13	8*	-19	68	18	-18*	-3	186	9	6	-14	47	20	-15*
9	43	24	12*	16	183	32	1	-18	73	10	-7	-2	35	37	11*	-13	208	16	-24
10	276	24	6	17	106	9	1	-17	138	8	-5	-1	116	9	1	-12	0	40	-27*
11	97	13	-4	18	75	10	15	-16	145	9	3	0	74	14	-10	-11	289	16	-26
12	507	48	2	19	28	42	-7*	-15	72	10	-3	1	162	8	-1	-10	90	7	5
13	147	8	14	20	250	9	28	-14	53	28	30*	2	110	10	-14	-9	51	11	-2*
14	63	26	3*	21	99	15	2	-13	44	31	-12*	3	106	8	-9	-8	39	27	11*
15	56	17	19*	22	218	12	18	-12	63	13	17*	4	177	10	-1	-7	240	11	-21
16	467	64	16	H,K= 3,			7	-11	117	8	10	5	134	7	9	-6	148	10	-12
17	100	8	13	-23	19	33	-0*	-10	77	11	28	6	151	7	2	-5	84	8	-9
18	115	10	-5	-22	139	10	-5	-9	83	10	7	7	374	16	-2	-4	230	13	-16
19	160	12	0	-21	57	15	-1*	-8	190	9	9	8	187	10	9	-3	101	7	-4
20	191	17	-11	-20	139	8	-7	-7	285	9	14	9	19	34	15*	-2	116	7	-12
21	47	18	11*	-19	50	13	27*	-6	258	9	6	10	111	7	3	-1	117	8	-14
22	68	26	-16*	-18	174	10	8	-5	146	7	0	11	392	14	21	0	336	16	-4
23	147	8	11	-17	163	7	5	-4	229	9	3	12	151	7	-4	1	73	8	-7
H,K= 3,			6	-16	440	15	11	-3	487	25	22	13	177	8	13	2	44	12	-10*
-24	99	12	-11	-15	204	9	2	-2	520	17	17	14	0	36	-18*	3	81	7	-5
-23	68	10	11	-14	40	40	1*	-1	207	8	14	15	200	24	-22	4	203	12	-13
-22	304	16	4	-13	227	9	14	0	70	12	31	16	178	19	-13	5	116	7	-2
-21	44	27	7*	-12	515	20	42	1	371	12	-6	17	213	33	-33	6	133	8	-19
-20	306	12	0	-11	279	10	15	2	447	15	2	H,K= 3,			10	7	258	19	-41
-19	75	11	5	-10	320	11	14	3	295	10	6	-17	113	18	-10	8	99	17	-7
-18	82	11	5	-9	31	40	15*	4	88	10	-16	-16	50	11	40*	9	43	15	29*
-17	131	9	2	-8	355	12	18	5	100	8	1	-15	117	9	4	10	25	48	-44*
-16	226	11	2	-7	324	10	25	6	319	10	3	-14	186	8	-5	11	299	16	-2
-15	77	13	-3	-6	352	11	18	7	294	12	9	-13	51	20	25*	12	9	31	-6*
-14	96	10	-0	-5	40	23	19*	8	129	9	8	-12	53	11	34*	H,K= 3,			12
-13	208	8	5	-4	188	7	13	9	35	15	13	-11	60	9	28	-10	221	22	-35
-12	137	8	7	-3	168	7	9	10	74	11	-11	-10	220	9	8	-9	16	32	-31*
-11	50	29	7*	-2	123	7	16	11	43	22	31*	-9	190	7	0	-8	201	19	-34
-10	106	7	5	-1	93	13	0	12	71	17	-8*	-8	70	10	9	-7	131	16	-36
-9	91	9	1	0	9	48	-10*	13	39	22	-4*	-7	300	10	6	-6	83	6	-5
-8	277	10	7	1	7	39	-6*	14	14	37	-2*	-6	196	8	1	-5	89	7	-25
-7	61	10	26	2	140	8	-3	15	39	29	-29*	-5	46	16	-7*	-4	194	12	-25
-6	487	15	20	3	113	7	17	16	59	12	-3*	-4	59	11	-0*	-3	141	10	-36
-5	180	10	2	4	43	46	19*	17	98	15	3	-3	465	18	-31	-2	86	13	-23
-4	352	19	18	5	42	35	30*	18	60	13	16*	-2	178	7	-6	-1	93	7	-17
-3	197	7	-1	6	388	14	7	19	69	10	-14	-1	295	10	2	0	48	10	6*
-2	751	32	31	7	299	11	8	H,K= 3,			9	0	41	17	-5*	1	152	12	-21
-1	105	8	4	8	321	11	9	-19	26	33	11*	1	258	15	-22	2	115	13	-21
0	104	9	12	9	44	26	33*	-18	52	10	32*	2	138	7	-8	3	139	7	-13
1	132	9	6	10	278	12	2	-17	242	16	8	3	404	17	-13	4	158	12	-20
2	736	23	6	11	271	10	5	-16	163	7	-3	4	56	20	3*	5	101	6	-12

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 5

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	19	28	-8*	-1	129	6	-11	2	877	69	-9	7	217	8	-10	12	268	26	2
7	141	10	-30	0	187	7	10	3	220	8	8	8	309	17	-6	13	194	8	3
H ₂ K# 4, 0				1	54	20	21*	4	152	6	-4	9	178	7	2	14	241	32	-1
-26	360	17	-10	2	381	12	20	5	202	7	-5	10	198	7	-2	15	90	12	10
-24	77	17	-12*	3	310	32	10	6	492	15	-10	11	384	25	2	16	233	10	2
-22	461	18	-26	4	136	6	9	7	455	14	-13	12	279	24	1	17	50	55	-7*
-20	69	12	-1	5	117	6	-1	8	43	19	-6*	13	83	11	2	18	221	39	-3
-18	406	13	-25	6	639	20	-29	9	112	7	-1	14	211	8	0	19	218	36	-6
-16	133	6	-11	7	92	6	-2	10	215	8	-5	15	291	10	13	20	73	14	-21*
-14	47	9	15*	8	195	7	-5	11	159	7	0	16	163	9	-1	21	134	10	-5
-12	57	6	18	9	297	9	-14	12	174	7	18	17	235	22	6	22	119	9	-15
-10	84	4	5	10	581	13	-25	13	266	9	-9	18	168	11	2	H ₂ K# 4, 5			
-8	452	14	-6	11	198	7	-8	14	59	16	-9*	19	105	16	-9	-25	33	36	17*
-6	135	5	3	12	388	12	-6	15	51	41	-10*	20	121	8	5	-24	365	18	1
-4	548	17	-13	13	60	34	-8*	16	242	9	6	21	158	10	-1	-23	30	52	-12*
-2	521	16	-6	14	433	14	-3	17	102	10	5	22	119	8	5	-22	75	11	2
0	523	16	-14	15	178	7	1	18	0	40	-33*	23	65	13	-3*	-21	101	10	9
21	130	35	28	16	372	13	-3	19	197	8	3	H ₂ K# 4, 4				-20	320	11	8
4	408	13	-25	17	126	13	7	20	232	33	-10	-26	79	12	-16	-19	75	17	-10*
6	846	26	-68	18	54	60	-23*	21	36	20	-7*	-25	201	8	16	-18	137	8	5
8	185	7	-11	19	12	39	-29*	22	60	14	-18*	-24	109	8	12	-17	221	10	12
10	328	11	-19	20	227	33	1	23	100	14	-15	-23	180	9	7	-16	154	11	10
12	35	41	-4*	21	50	19	-14*	H ₂ K# 4, 3				-22	99	10	-5	-15	22	42	-23*
14	78	10	8	22	29	44	12*	-26	50	18	-1*	-21	325	11	13	-14	50	18	29*
16	229	9	2	23	46	22	6*	-25	118	10	-13	-20	252	10	10	-13	467	15	12
18	78	14	10	24	75	11	9	-24	150	11	0	-19	147	8	6	-12	0	46	-37*
20	286	13	-11	H ₂ K# 4, 2				-23	251	10	2	-18	309	11	5	-11	189	8	5
22	80	12	-18	-27	145	7	0	-22	112	8	8	-17	301	10	5	-10	300	10	3
24	332	11	34	-26	329	18	-8	-21	89	20	5*	-16	215	8	-1	-9	233	9	2
H ₂ K# 4, 1				-25	123	8	1	-20	247	9	-8	-15	202	8	5	-8	140	6	-2
-27	42	47	25*-24	5	38	-22*	-19	212	11	-3	-14	415	13	-1	-7	298	10	7	
-26	56	17	24*-23	140	11	-8	-18	173	9	-6	-13	35	51	-19*	-6	582	18	22	
-25	39	38	-3*-22	407	15	-11	-17	307	11	-12	-12	179	7	3	-5	10	33	-8*	
-24	34	38	5*-21	258	9	-1	-16	314	11	-10	-11	47	13	18*	-4	357	11	22	
-23	29	41	8*-20	72	12	-3	-15	63	18	-17*	-10	506	16	-24	-3	168	7	4	
-22	188	8	-11	-19	79	12	-2	-14	155	7	-4	-9	389	13	-4	-2	574	21	30
-21	27	37	26*-18	297	12	-2	-13	554	18	-19	-8	196	7	14	-1	15	36	-6*	
-20	220	8	-8	-17	283	9	-4	-12	357	12	-15	-7	249	3	-2	0	769	24	29
-19	91	17	-11*-16	96	8	-1	-11	329	10	-15	-6	450	22	2	1	114	12	2	
-18	423	15	-27	-15	281	9	-2	-10	132	6	-3	-5	377	12	2	2	209	9	17
-17	95	12	-26	-14	39	21	7*	-9	296	10	-10	-4	0	33	-10*	3	137	7	5
-16	389	13	-14	-13	25	30	7*	-8	427	13	-18	-3	776	24	29	4	625	19	-9
-15	158	7	2	-12	174	6	-2	-7	613	26	-21	-2	270	9	16	5	142	8	-10
-14	443	14	-8	-11	192	6	-12	-6	165	6	-5	-1	45	23	-22*	6	78	9	27
-13	260	8	-9	-10	134	5	-3	-5	171	6	3	0	135	8	-6	7	147	9	-2
-12	720	22	-13	-9	267	8	-18	-4	276	16	-8	1	664	21	46	8	228	9	-6
-11	179	6	-5	-8	270	9	-20	-3	254	14	0	2	201	8	15	9	241	8	5
-10	108	4	6	-7	80	7	-4	-2	140	6	-5	3	379	12	4	10	7	46	-9*
-9	131	5	4	-6	263	8	-10	-1	536	17	18	4	424	13	-12	11	286	37	-8
-8	859	26	-5	-5	382	12	-12	0	365	12	5	5	173	7	7	12	62	14	15*
-7	266	8	4	-4	580	23	7	1	446	14	32	6	188	7	-16	13	68	19	15*
-6	118	4	-1	-3	487	20	-16	2	412	13	3	7	346	26	-10	14	136	11	2
-5	110	5	1	-2	589	18	-15	3	208	21	-6	8	347	27	-5	15	245	30	8
-4	317	10	-7	-1	260	17	8	4	309	21	-7	9	125	7	-1	16	22	37	-8*
-3	95	8	3	0	365	24	-4	5	440	22	-7	10	235	20	-8	17	106	11	-1
-2	123	6	4	1	541	17	29	6	394	16	-7	11	105	10	3	18	228	13	-3

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 9

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
19	118	8	-1	-13	140	7	1	-5	292	10	5	12	65	13	-11*	4	86	12	-12	
20	56	22	-0*	-18	159	8	2	-4	89	10	14	13	18	33	11*	5	160	12	-26	
21	59	13	12*	-17	20	46	-9*	-3	32	36	16*	14	67	8	11	6	155	15	-30	
22	274	10	33	-16	163	9	18	-2	103	11	11	15	66	17	-4*	7	84	7	-12	
H,K=			4,	6	-15	140	7	9	-1	35	37	25*	16	68	11	1	8	67	7	1
-24	18	39	-39*	-14	135	10	-1	0	82	13	11	H,K=			4,	10	9	93	16	-9
-23	93	9	-3	-13	70	13	16*	1	42	29	22*	-17	54	9	13	10	164	7	-13	
-22	0	36	-4*	-12	95	10	-8	2	124	8	3	-16	0	38	-10*	H,K=			4,	12
-21	64	12	10*	-11	85	11	28	3	119	8	8	-15	311	20	-26	-9	89	8	-22	
-20	278	10	8	-10	194	8	21	4	182	8	-5	-14	140	9	-0	-8	164	14	-35	
-19	70	12	-8	-9	166	7	7	5	43	23	10*	-13	153	8	-7	-7	61	8	-14	
-18	204	8	-1	-8	54	15	34*	6	36	37	32*	-12	55	12	1*	-6	0	29	-7*	
-17	139	14	3	-7	69	20	16*	7	220	13	-4	-11	300	13	-9	-5	71	7	-14	
-16	484	16	17	-6	471	15	31	3	322	14	-1	-10	101	8	-1	-4	270	22	-49	
-15	82	12	10	-5	316	10	18	9	296	17	-10	-9	235	9	-16	-3	69	7	-10	
-14	517	17	21	-4	254	9	11	10	131	7	-9	-8	98	7	-5	-2	173	13	-30	
-13	146	7	15	-3	60	21	12*	11	156	12	-8	-7	136	7	-3	-1	29	36	-16*	
-12	226	8	13	-2	561	23	31	12	233	9	8	-6	97	7	-11	0	178	15	-18	
-11	182	8	1	-1	349	23	12	13	323	12	16	-5	316	12	-6	1	86	8	-16	
-10	720	23	37	0	411	13	10	14	273	14	21	-4	191	7	4	2	262	12	-9	
-9	37	45	31*	1	32	43	15*	15	73	22	-4*	-3	97	7	-7	3	16	27	-2*	
-8	141	9	8	2	279	10	6	16	121	12	-3	-2	140	6	3	4	48	8	3	
-7	180	7	9	3	216	10	3	17	160	25	-13	-1	41	24	-8*	5	106	8	-23	
-6	488	15	20	4	503	16	-9	18	255	11	18	0	166	7	1	H,K=			5,	0
-5	60	11	-2*	5	159	9	-4	H,K=			4,	9	1	97	10	-8	-26	27	38	4*
-4	107	9	7	6	79	10	17	-19	213	11	-13	2	144	9	-7	-24	83	9	1	
-3	230	8	9	7	111	10	-3	-18	44	15	29*	3	212	10	-9	-22	56	19	-1*	
-2	29	41	6*	8	349	15	-7	-17	34	36	-4*	4	86	11	-5	-20	367	13	-12	
-1	133	7	2	9	104	9	15	-16	146	7	-3	5	112	10	-11	-18	22	40	18*	
0	48	18	13*	10	208	8	6	-15	121	10	-7	6	179	7	8	-16	619	20	-25	
1	175	7	11	11	56	57	-0*	-14	74	8	22	7	255	9	11	-14	196	7	-3	
2	87	10	-0	12	31	36	10*	-13	66	11	-4	8	29	34	-6*	-12	577	18	-16	
3	57	12	28*	13	29	45	18*	-12	149	7	-2	9	269	19	-19	-10	748	23	-26	
4	266	10	-1	14	21	36	-16*	-11	150	7	5	10	126	14	-4	-8	396	12	-13	
5	152	7	2	15	26	37	-6*	-10	170	10	13	11	69	9	-7	-6	786	24	-3	
6	71	18	-13*	16	80	19	-12*	-9	40	48	8*	12	39	14	22*	-4	90	7	26	
7	72	12	7	17	47	18	-15*	-8	58	16	8*	13	287	13	-2	-2	116	7	-11	
8	530	18	-3	18	183	24	-24	-7	254	11	13	H,K=			4,	11	0	131	8	-4
9	96	10	1	19	88	22	-33*	-6	229	10	7	-14	138	16	-19	2	41	25	11*	
10	261	9	3	H,K=			4,	8	-5	358	12	13	-13	30	34	-12*	4	378	13	-2
11	52	24	20*	-21	77	8	-7	-4	173	10	4	-12	219	19	-24	6	362	11	-20	
12	436	48	-13	-20	169	10	-8	-3	159	9	-0	-11	93	6	-6	8	616	19	-20	
13	0	55	-19*	-19	135	7	-0	-2	251	9	3	-10	29	39	0*	10	177	7	3	
14	384	46	-3	-18	126	7	7	-1	540	18	-13	-9	92	7	-6	12	687	30	-29	
15	41	21	28*	-17	71	9	26	0	298	12	-9	-8	235	11	-14	14	186	8	-12	
16	137	9	-5	-16	183	8	-0	1	128	7	3	-7	156	7	-8	16	421	15	-13	
17	84	11	-11	-15	393	15	5	2	100	17	1	-6	81	7	-1	18	296	12	-7	
18	333	14	41	-14	380	12	16	3	377	15	-13	-5	244	14	-30	20	61	16	-20*	
19	54	30	-15*	-13	106	8	9	4	206	11	-6	-4	124	8	-11	22	142	20	-23	
20	48	14	17*	-12	184	8	4	5	320	13	-16	-3	30	33	-5*	H,K=			5,	1
21	88	26	-22*	-11	412	14	3	6	28	43	-2*	-2	56	22	-13*	-27	0	49	-27*	
H,K=			4,	7	-10	433	15	16	7	133	7	-5	-1	327	17	-36	-26	312	14	-12
-23	103	16	-7	-9	288	10	7	8	93	10	-9	0	90	7	-20	-25	92	10	-6	
-22	33	34	3*	-8	55	21	-3*	9	176	13	-1	1	80	9	-14	-24	266	14	-18	
-21	83	15	-15	-7	175	9	11	10	62	19	-5*	2	70	9	3	-23	45	20	-8*	
-20	282	15	3	-6	341	12	6	11	33	34	1*	3	255	14	-27	-22	191	9	-4	

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 10

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-21	93	9	-10	-17	256	10	-2	-11	219	8	-17	-5	340	16	-2	3	210	8	7	
-20	363	14	-27	-16	485	16	-21	-10	329	18	-19	-4	517	22	6	4	164	8	6	
-19	119	8	-6	-15	274	11	-10	-9	179	6	-15	-3	35	24	21*	5	112	10	-1	
-18	128	7	3	-14	330	11	-5	-8	194	7	-21	-2	179	7	12	6	444	26	-0	
-17	36	27	-1*	-13	158	6	-1	-7	428	23	-13	-1	146	8	9	7	185	8	-8	
-16	238	9	-11	-12	315	10	-13	-6	391	20	-23	0	551	17	19	8	61	24	-12*	
-15	265	9	-11	-11	394	13	-18	-5	82	10	-7	1	279	9	11	9	131	8	3	
-14	93	6	8	-10	453	18	-6	-4	199	7	3	2	316	10	7	10	450	48	-13	
-13	150	6	-4	-9	171	7	7	-3	567	25	-8	3	133	7	9	11	47	56	4*	
-12	83	6	1	-3	433	13	-21	-2	392	24	14	4	381	19	-5	12	91	14	8	
-11	61	6	-2	-7	193	7	-6	-1	472	27	15	5	146	7	-6	13	62	15	-7*	
-10	196	7	1	-6	387	12	-7	0	330	11	7	6	207	8	-14	14	413	64	-4	
-9	229	7	-12	-5	450	14	-16	1	83	10	-8	7	324	20	-6	15	69	13	-10*	
-8	52	6	12	-4	305	10	-7	2	490	15	18	8	188	27	-5	16	166	11	8	
-7	367	11	-8	-3	197	7	3	3	529	46	14	9	272	22	-9	17	159	11	0	
-6	823	25	-8	-2	251	8	-7	4	124	7	2	10	62	14	8*	18	198	15	-13	
-5	22	27	-7*	-1	200	7	4	5	383	20	-3	11	233	8	5	19	43	17	28*	
-4	43	8	13*	0	241	8	-2	6	337	11	-7	12	193	9	-7	20	162	9	10	
-3	272	9	-10	1	413	25	4	7	213	7	1	13	290	31	2	21	194	8	23	
-2	934	33	-12	2	65	12	11	8	44	17	4*	14	24	51	13*	H,K= 5, 6				
-1	289	9	-3	3	66	9	40	9	232	9	1	15	49	31	9*	-24	201	16	-6	
0	473	24	-10	4	492	15	3	10	267	27	-10	16	216	25	11	-23	94	10	-8	
1	148	10	-1	5	222	8	-1	11	65	17	13*	17	224	10	1	-22	314	15	0	
2	866	27	59	6	246	11	1	12	26	41	-16*	18	45	24	8*	-21	50	16	15*	
3	191	9	-0	7	357	12	-3	13	92	10	15	19	19	36	-5*	-20	72	11	10	
4	526	26	-22	8	474	15	-7	14	280	22	4	20	146	16	-12	-19	78	12	-2	
5	129	6	4	9	123	8	-1	15	193	33	-1	21	75	18	-7*	-18	306	11	18	
6	378	12	-4	10	82	13	-3	16	0	41	-17*	H,K= 5, 5				5	-17	47	20	-1*
7	123	8	-9	11	304	20	4	17	132	7	5	-25	183	9	-6	-16	60	15	19*	
8	279	9	-3	12	395	24	-0	18	184	10	-6	-24	50	21	14*	-15	227	10	14	
9	201	7	-8	13	279	10	-5	19	90	9	3	-23	86	9	12	-14	57	19	-5*	
10	19	36	-13*	14	109	13	2	20	0	40	-24*	-22	197	11	3	-13	134	8	20	
11	85	10	0	15	52	59	28*	21	236	10	24	-21	137	8	-6	-12	70	12	21	
12	62	15	9*	16	307	29	10	22	163	11	9	-20	42	39	22*	-11	238	9	8	
13	105	9	-3	17	235	34	-2	H,K= 5, 4				-19	135	8	-3	-10	180	9	10	
14	56	18	-1*	18	117	8	8	-26	150	9	1	-18	452	15	17	-9	75	11	3	
15	175	8	-1	19	109	10	-5	-25	33	41	13*	-17	127	9	12	-8	369	12	11	
16	197	8	9	20	171	11	6	-24	208	15	-2	-16	176	9	-4	-7	99	9	-6	
17	125	13	13	21	66	16	6*	-23	85	11	-6	-15	241	10	16	-6	206	8	17	
18	173	10	-5	22	94	8	2	-22	271	10	14	-14	515	17	16	-5	123	7	13	
19	46	19	17*	H,K= 5, 3				-21	268	11	10	-13	40	41	18*	-4	712	33	50	
20	121	8	-5	-26	175	9	4	-20	152	8	-3	-12	459	15	12	-3	111	9	17	
21	116	12	-10	-25	292	12	-5	-19	121	12	10	-11	192	8	-5	-2	133	9	19	
22	301	15	25	-24	124	11	3	-18	227	10	11	-10	329	11	10	-1	33	45	24*	
23	0	37	-32*	-23	160	8	2	-17	261	9	15	-9	130	7	-4	0	579	28	22	
H,K= 5, 2				-22	144	9	4	-16	177	8	2	-8	436	16	29	1	88	10	27	
-27	122	9	2	-21	226	11	-9	-15	435	15	-1	-7	413	13	21	2	351	11	7	
-26	64	15	6*	-20	176	8	-7	-14	74	10	1	-6	246	8	21	3	0	45	-16*	
-25	15	59	-8*	-19	266	9	-15	-13	73	10	7	-5	193	7	12	4	365	21	6	
-24	68	18	-15*	-18	232	10	-3	-12	263	10	6	-4	302	10	18	5	49	19	12*	
-23	113	9	0	-17	26	39	-18*	-11	438	14	-6	-3	264	9	14	6	445	16	5	
-22	61	15	-17*	-16	126	11	-7	-10	106	9	3	-2	99	8	7	7	119	8	8	
-21	177	8	-10	-15	183	8	-4	-3	73	8	20	-1	400	13	12	8	68	12	42	
-20	310	13	-9	-14	246	9	-6	-8	329	11	-5	0	47	21	27*	9	127	8	3	
-19	0	44	-10*	-13	237	8	-9	-7	257	9	16	1	139	7	7	10	200	13	-3	
-18	152	7	-10	-12	150	6	4	-6	67	8	0	2	146	8	5	11	187	13	-5	

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(C6H8)

PAGE 11

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
12	77	15	9*-16	38	47	31*		2	86	8	-2	-2	263	16	-30	-22	110	8	-5
13	148	8	-3 -15	48	20	-5*		3	152	9	-9	-1	6	36	-11*-21	60	15	1*	
14	84	14	-8 -14	30	36	-3*		4	13	40	-25*	0	75	13	-9 -20	153	12	-4	
15	58	13	-14*-13	89	9	3		5	242	12	-10	1	55	10	-10*-19	140	8	10	
16	84	8	7 -12	75	11	3		6	168	14	-3	2	189	15	-15 -18	437	17	-22	
17	139	12	-0 -11	88	9	30		7	20	37	-28*	3	0	30	-20*-17	98	8	3	
18	128	20	-24 -10	138	8	6		8	64	24	2*	4	232	16	-16 -16	163	7	-18	
19	42	18	3*-9	212	9	5		9	280	18	-15	5	157	15	-28 -15	186	7	-0	
H,K= 5, 7				180	8	9		10	183	16	-16	6	25	30	-8*-14	663	23	-21	
-22	123	8	-4 -7	72	14	-5*		11	200	19	-13	7	36	38	-24*-13	117	6	11	
-21	104	8	-6 -6	196	8	18		12	70	15	6*	8	119	19	-30 -12	121	6	2	
-20	55	14	-6*-5	367	12	11		13	150	11	-16	9	220	8	3 -11	168	6	-3	
-19	100	9	13 -4	432	28	23		14	133	16	-26	H,K= 5, 12				-10	769	24	-16
-18	304	14	-2 -3	366	22	13		15	303	11	26	-7	127	9	-28 -9	264	8	-7	
-17	151	8	-0 -2	60	21	9*		H,K= 5, 10				-6	182	12	-32 -8	404	13	-5	
-16	58	12	32*-1	251	9	4		-16	156	11	-13	-5	104	13	-28 -7	186	6	-1	
-15	103	8	8 0	450	29	-3		-15	7	33	-41*	-4	100	6	-19 -6	559	17	-17	
-14	581	20	28 1	338	13	-8		-14	100	8	-6	-3	156	12	-35 -5	196	6	-5	
-13	296	10	15 2	289	11	-4		-13	23	32	7*	-2	23	27	-2*-4	201	7	-7	
-12	349	12	14 3	54	16	45*-12		229	11	4	-1	76	7	-10 -3	303	9	-12		
-11	0	47	-30*4	218	9	-9		-11	83	8	11	0	85	11	-11 -2	91	11	7	
-10	386	12	27 5	350	13	-4		-10	103	7	5	1	147	14	-26 -1	180	7	-0	
-9	250	9	18 6	335	15	-6		-9	205	8	-4	2	98	16	-22 0	117	8	-2	
-8	517	17	30 7	127	8	6		-8	128	9	1	3	67	6	-1 1	94	10	1	
-7	77	11	11 8	50	19	23*-7		41	15	24*	H,K= 6, 0				2	121	8	16	
-6	10	40	-0*9	155	9	-0		-6	123	8	2	-26	31	39	-5*3	145	9	6	
-5	125	7	14 10	116	11	-10		-5	265	18	-8	-24	372	13	-13 4	328	11	-0	
-4	239	9	9 11	62	12	-5*-4		99	7	23	-22	269	14	-21 5	76	38	-11*		
-3	0	39	-7*12	7	45	-4*-3		277	28	-19	-20	300	13	-10 6	199	7	-8		
-2	174	8	19 13	63	17	-3*-2		91	9	0	-18	362	15	-15 7	73	12	-14		
-1	36	45	20*14	57	10	16		-1	219	12	-17	-16	109	8	2 8	415	13	-24	
0	61	14	12*15	48	17	-11*0		74	10	0	-14	220	7	-4 9	222	12	-9		
1	79	11	-4 16	51	18	-9*1		418	21	-23	-12	48	10	-11*10	360	12	-13		
2	16	39	10*17	46	51	-13*2		0	38	-5*-10	246	8	-1 11	61	17	-12*			
3	59	19	35*H,K= 5, 9			3		34	20	18*-8	251	8	-8 12	210	8	-9			
4	203	9	11 -13	208	17	-18		4	75	11	-4	-6	677	21	-19 13	174	8	-16	
5	77	14	4*-18	184	9	-5		5	331	11	10	-4	814	25	-13 14	521	36	-20	
6	262	23	2 -17	177	14	-13		6	15	32	9*-2	464	14	-8 15	124	12	4		
7	129	9	-1 -16	127	7	9		7	143	11	-15	0	881	33	-80 16	33	38	17*	
8	142	8	-10 -15	177	9	6		8	166	15	-1	2	71	13	11*17	28	38	20*	
9	182	8	1 -14	231	11	5		9	55	10	5*4	711	22	17 18	309	11	14		
10	504	16	37 -13	444	15	-2		10	0	33	-32*6	267	9	-16 19	107	8	6		
11	164	15	-9 -12	166	7	-2		11	48	13	-4*8	156	7	-3 20	85	11	3		
12	38	21	17*-11	33	34	-0*12		160	15	-17	10	185	8	-1 21	65	25	-10*		
13	120	7	-1 -10	226	8	6		H,K= 5, 11				12	29	45	25*H,K= 6, 2				
14	373	25	-25 -9	393	13	8		-13	250	25	-55	14	48	24	28*-26	24	48	-4*	
15	148	18	-6 -8	108	8	1		-12	64	10	-4	16	0	39	-19*-25	91	9	8	
16	232	20	-3 -7	203	8	9		-11	34	19	-4*18	241	11	-5 -24	295	10	-1		
17	33	25	15*-6	151	8	-6		-10	61	14	-15*20	109	14	-30 -23	290	11	2		
18	166	7	18 -5	227	9	5		-9	230	12	-13	22	226	9	17 -22	145	9	1	
H,K= 5, 8				136	9	9		-8	106	8	-13	H,K= 6, 1				-21	87	16	11
-21	94	8	11 -3	258	12	-3		-7	118	9	-12	-27	100	9	14 -20	269	10	11	
-20	66	11	10 -2	113	14	-4		-6	142	6	-6	-26	64	18	17*-19	160	9	-5	
-19	167	7	7 -1	74	9	4		-5	120	8	-8	-25	79	15	18*-18	234	9	0	
-18	214	9	2 0	9	45	-6*-4		68	12	-18	-24	104	10	8 -17	252	10	-9		
-17	145	7	5 1	33	39	4*-3		87	12	-17	-23	36	39	2*-16	192	8	1		

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE12

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-15	51	15	-2*	-9	25	33	22*	0	301	10	12	10	158	9	5	-20	196	10	1
-14	64	11	15	-7	113	6	7	1	353	12	17	11	36	48	17*	-19	50	15	1*
-13	252	9	4	-6	441	21	-22	2	123	10	21	12	35	39	-2*	-18	129	10	15
-12	170	7	5	-5	230	8	-7	3	228	21	-1	13	268	13	-8	-17	124	8	13
-11	299	15	-15	-4	170	7	-10	4	173	7	-4	14	71	30	20*	-16	180	8	4
-10	77	9	31	-3	375	13	-1	5	414	32	-20	15	118	10	2	-15	40	23	24*
-9	88	7	40	-2	390	19	3	6	252	9	-13	16	124	12	17	-14	69	12	-1
-8	476	15	-22	-1	48	45	30*	7	115	8	3	17	75	12	-4	-13	136	8	14
-7	348	11	-7	0	19	39	-19*	8	287	22	-1	18	63	11	-6	-12	89	17	16*
-6	207	7	5	1	173	8	7	9	163	8	-5	19	86	17	-23*	-11	74	16	1*
-5	365	12	-2	2	342	11	5	10	137	9	-5	H,K= 6,		6	-10	62	25	1*	
-4	463	14	-4	3	314	39	3	11	111	11	34	-23	164	7	-3	-9	49	29	14*
-3	48	11	38*	4	117	8	-10	12	339	33	-9	-22	165	13	5	-8	401	13	26
-2	260	8	0	5	115	8	-1	13	86	14	6	-21	102	13	18	-7	153	8	28
-1	379	20	7	6	221	8	-9	14	60	16	-12*	-20	228	8	2	-6	259	10	15
0	589	29	4	7	180	8	-10	15	41	26	14*	-19	96	9	3	-5	0	40	-23*
1	346	23	8	8	109	8	8	16	258	45	-9	-18	225	10	3	-4	423	13	27
2	49	35	34*	9	367	12	-5	17	126	20	-29	-17	51	18	30*	-3	220	11	13
3	108	17	22	10	259	9	-20	19	0	47	-35*	-16	430	14	15	-2	590	19	36
4	653	43	-3	11	66	24	13*	19	117	7	9	-15	138	8	11	-1	146	8	1
5	449	22	-15	12	62	16	10*	20	175	8	13	-14	121	9	11	0	58	22	44*
6	58	13	12*	13	269	11	-11	H,K= 6,		5	-13	52	21	41*	1	208	8	-1	
7	219	9	2	14	248	12	-13	-24	99	9	8	-12	621	19	34	2	501	17	-1
8	190	7	-7	15	186	8	1	-23	58	14	-9*	-11	56	19	48*	3	158	12	-4
9	118	9	9	16	77	11	4	-22	316	11	7	-10	218	8	11	4	210	9	-0
10	67	28	57*	17	72	11	3	-21	14	38	4*	-9	94	16	6	5	110	9	-0
11	158	8	-11	18	151	9	-9	-20	241	9	9	-8	508	16	30	6	308	14	-8
12	133	8	-6	19	140	11	-5	-19	202	9	1	-7	89	11	5	7	141	11	-8
13	122	17	-16	20	78	11	11	-18	221	8	19	-6	369	12	28	8	213	10	-3
14	92	10	15	21	40	18	4*	-17	20	46	7*	-5	164	8	6	9	103	8	-8
15	57	34	-3*	H,K= 6,		4	-16	140	9	5	-4	85	11	-1	10	59	13	-3*	
16	109	12	5	-25	98	18	6	-15	270	12	9	-3	136	8	22	11	65	11	11
17	173	29	-3	-24	112	9	-2	-14	35	43	-8*	-2	161	8	7	12	67	11	-10
18	111	16	-2	-23	307	13	3	-13	227	9	14	-1	222	8	4	13	17	36	-28*
19	105	19	-2	-22	91	10	20	-12	130	8	11	0	51	22	4*	14	80	11	-7
20	92	9	-10	-21	50	20	23*	-11	253	11	8	1	112	11	-3	15	48	14	25*
21	60	28	-25*	-20	257	10	8	-10	171	8	9	2	108	9	13	16	122	30	-26*
H,K= 6,		3	-19	188	8	-2	-9	244	9	-3	3	73	13	17	17	60	14	-10*	
-26	193	13	4	-18	71	17	20*	-8	238	8	13	4	81	16	-5*	H,K= 6,		8	
-25	86	10	-6	-17	187	9	4	-7	151	8	24	5	143	8	-2	-20	140	9	-8
-24	43	47	37*	-16	486	16	7	-6	358	12	33	6	346	14	-15	-19	20	34	12*
-23	26	44	-19*	-15	49	22	40*	-5	270	9	11	7	89	11	29	-18	160	8	-1
-22	197	11	5	-14	27	51	6*	-4	297	10	32	8	319	34	-8	-17	254	10	4
-21	187	8	2	-13	88	9	16	-3	232	9	24	9	114	10	6	-16	344	12	6
-20	37	39	2*	-12	463	15	-1	-2	602	19	38	10	305	42	-23	-15	120	9	-1
-19	305	12	-3	-11	221	9	-4	-1	25	41	17*	11	92	11	-19	-14	35	42	1*
-18	331	12	-1	-10	118	7	20	0	121	9	-7	12	374	18	-12	-13	321	12	7
-17	30	48	8*	-9	142	8	6	1	26	52	-9*	13	12	37	5*	-12	409	14	13
-16	54	21	4*	-8	408	22	-0	2	617	19	20	14	35	10	-2	-11	333	11	6
-15	408	15	-5	-7	224	8	-5	3	61	18	-13*	15	48	57	-12*	-10	91	9	7
-14	360	25	-1	-6	58	18	27*	4	90	10	5	16	378	13	42	-9	164	8	5
-13	370	12	-9	-5	245	8	3	5	131	9	4	17	31	34	-5*	-8	261	12	16
-12	46	17	20*	-4	399	23	10	6	396	28	-15	18	83	14	-11	-7	365	12	8
-11	179	7	-0	-3	161	8	8	7	53	26	3*	H,K= 6,		7	-6	222	8	22	
-10	303	11	-9	-2	34	36	23*	8	146	9	12	-22	261	13	-3	-5	173	7	14
-9	320	10	-2	-1	435	14	24	9	296	12	-15	-21	137	7	-1	-4	134	8	19

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 13

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	116	12	5	-12	67	9	12	0	133	8	-8	18	69	11	30	-21	192	11	-0
-2	153	8	11	-11	303	14	-14	2	170	8	15	19	87	15	-6	-20	98	13	10
-1	65	25	-1*	-10	91	7	7	4	44	51	28*	20	263	11	17	-19	34	39	16*
0	37	40	4*	-9	72	12	-10	6	512	17	-5	H ₂ K= 7,		2	-16	324	13	-1	
1	75	11	-8	-8	83	11	11	8	156	11	-12	-26	25	38	-8*	-17	195	8	16
2	104	9	6	-7	244	12	-19	10	414	16	-25	-25	123	11	5	-16	109	10	-28
3	117	8	-1	-6	89	8	-9	12	286	10	-6	-24	82	11	7	-15	256	10	-5
4	41	24	27*	-5	58	16	-6*	14	297	12	-15	-23	147	10	-1	-14	277	12	-10
5	93	8	-1	-4	165	21	-13	16	339	20	-19	-22	89	16	-2*	-13	69	13	-2*
6	264	17	-9	-3	130	7	-1	18	104	21	-9*	-21	79	11	5	-12	224	10	-2
7	240	16	-18	-2	34	29	-3*	20	203	15	-2	-20	142	7	1	-11	127	11	-8
8	241	14	-18	-1	52	33	-16*	H ₂ K= 7,		1	-19	236	11	-6	-10	231	8	-6	
9	29	34	18*	0	204	14	-17	-26	344	20	-9	-18	259	10	-2	-9	262	9	-3
10	135	45	-14*	1	110	7	-11	-25	113	9	-9	-17	190	12	-15	-8	179	8	-1
11	312	11	17	2	30	32	12*-24	80	11	-11	-16	356	13	-16	-7	128	8	19	
12	325	11	24	3	40	16	18*-23	51	20	-4*-15	48	24	11*	-6	303	10	-3		
13	104	11	2	4	167	13	-15	-22	369	14	-17	-14	363	13	-14	-5	162	8	-5
14	53	11	-1*	5	175	12	-24	-21	142	7	-0	-13	278	9	-12	-4	271	17	3
15	146	23	-29	6	65	9	-6	-20	112	11	-10	-12	473	17	-11	-3	350	22	1
H ₂ K= 6,		9	7	258	9	15	-19	89	10	-6	-11	210	7	-0	-2	214	8	-2	
-18	109	7	-5	8	133	17	-14	-18	391	14	-6	-10	188	7	-3	-1	26	37	15*
-17	131	11	-9	9	38	12	33*-17	58	43	15*	-9	191	7	-3	0	256	9	-8	
-16	29	32	11*	10	37	13	24*-16	78	9	5	-8	500	20	-23	1	518	44	6	
-15	177	9	8	H ₂ K= 6,		11	-15	177	10	-12	-7	332	10	-15	2	234	9	7	
-14	126	8	5	-11	57	10	-2	-14	77	9	4	-6	147	6	-1	3	202	29	7
-13	82	8	9	-10	178	12	-19	-13	28	33	14*	-5	196	7	-1	4	263	23	-5
-12	109	8	-1	-9	52	10	2*-12	204	8	2	-4	354	17	-15	5	299	24	5	
-11	23	45	-14*	-3	100	7	-2	-11	47	19	-23*	-3	244	15	4	6	235	21	-6
-10	117	11	-2	-7	185	11	-24	-10	72	7	3	-2	83	12	-4	7	316	27	-7
-9	164	8	10	-6	87	7	-5	-9	214	8	-9	-1	272	19	1	8	185	6	7
-8	99	12	8	-5	44	11	9*	-8	542	17	-13	0	156	7	5	9	51	23	-8*
-7	284	10	9	-4	120	8	-7	-7	70	8	6	1	174	7	6	10	178	8	1
-6	173	7	10	-3	253	15	-31	-6	196	7	-4	2	58	19	25*	11	98	14	17
-5	32	37	10*	-2	33	21	22*	-5	169	8	-3	3	117	11	5	12	99	13	-9
-4	35	29	20*	-1	134	10	-11	-4	733	23	-38	4	51	39	10*	13	223	9	-3
-3	416	29	-2	0	34	23	-1*	-3	338	11	-12	5	331	24	-1	14	131	11	-1
-2	303	11	2	1	203	15	-32	-2	420	13	1	6	309	10	-7	15	133	11	-6
-1	249	9	-6	2	55	22	-11*	-1	50	15	-7*	7	176	10	9	16	154	12	-4
0	30	40	16*	3	161	14	-21	0	376	27	-23	8	101	10	-5	17	49	21	-22*
1	318	16	-18	4	117	10	-16	1	188	25	-9	9	196	8	-8	18	61	27	-1*
2	255	10	-9	5	76	12	-20	2	632	40	11	10	330	11	-4	19	133	22	-17
3	346	17	-25	6	80	9	-0	3	237	12	15	11	215	8	2	H ₂ K= 7,		4	
4	25	45	4*	H ₂ K= 7,		0	4	189	12	10	12	300	12	-12	-25	84	9	4	
5	41	34	-14*-26	23	39	18*	5	47	34	18*	13	0	42	-13*	-24	241	11	-5	
6	181	12	-11	-24	37	43	-1*	6	413	24	-23	14	264	34	-1	-23	98	9	-3
7	241	19	-10	-22	263	14	-6	7	109	10	-11	15	150	12	-5	-22	97	12	2
8	37	39	6*-20	156	8	-5	8	33	44	25*	16	220	14	-9	-21	34	41	-10*	
9	61	14	6*-18	389	15	-26	9	77	14	11	17	138	13	12	-20	341	12	13	
10	115	16	-1	-16	419	17	-29	10	189	12	7	18	147	24	-12	-19	245	9	3
11	33	21	20*-14	487	16	-16	11	0	46	-20*	19	55	23	11*-16	50	18	24*		
12	25	32	-18*-12	601	20	-32	12	66	18	20*	20	99	37	-23*-17	260	11	14		
13	46	27	-9*-10	189	7	6	13	65	23	-9*	H ₂ K= 7,		3	-16	229	10	-12		
H ₂ K= 6,		10	-8	965	27	-33	14	50	19	48*-25	86	16	-27	-15	58	17	23*		
-15	182	7	-16	-6	113	7	-1	15	70	14	-3*-24	112	10	12	-14	97	10	11	
-14	17	31	14*	-4	210	8	0	16	157	9	-1	-23	207	8	9	-13	403	13	-5
-13	210	10	-12	-2	134	6	-7	17	10	51	-3*-22	207	3	3	-12	100	10	8	

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(C0C4H6)

PAGE 14

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-11	187	8	10	0	64	17	22*	13	54	14	6*	-7	249	10	17	-11	116	8	-14	
-10	222	8	10	1	374	12	17	14	25	35	15*	-6	267	19	7	-10	33	36	-13*	
-9	266	9	-1	2	46	52	12*	15	66	10	0	-5	308	27	15	-9	54	19	-4*	
-8	200	8	7	3	109	16	-2	16	79	10	-3	-4	239	10	16	-8	140	8	8	
-7	375	19	11	4	192	8	-3	17	0	32	-9*	-3	72	15	19*	-7	181	19	-2	
-6	355	23	20	5	122	9	6	H,K= 7,				7	-2	306	26	13	-6	30	31	24*
-5	56	13	44*	6	45	26	35*	-21	37	27	11*	-1	428	35	13	-5	241	26	-10	
-4	313	25	19	7	154	9	-14	-20	285	11	-2	0	321	33	1	-4	125	6	-1	
-3	339	12	10	8	380	45	-14	-19	145	7	13	1	133	8	9	-3	83	8	0	
-2	381	31	11	9	64	17	-16*	-16	125	8	-5	2	185	8	3	-2	29	31	-6*	
-1	111	9	9	10	118	12	-8	-17	48	17	5*	3	282	16	-15	-1	320	16	-30	
0	284	10	18	11	64	13	2*	-16	330	12	7	4	303	14	-9	0	81	9	-5	
1	0	45	-34*	12	330	57	-22	-15	144	11	15	5	164	7	-12	1	29	32	9*	
2	299	10	21	13	59	13	15*	-14	370	13	17	6	32	48	28*	2	89	7	-6	
3	124	11	5	14	242	19	-15	-13	78	10	15	7	75	11	-20	3	306	10	3	
4	391	31	-13	15	87	17	-8*	-12	190	8	14	8	134	11	5	4	35	17	12*	
5	311	31	-13	16	140	15	-6	-11	229	9	15	9	78	13	4	5	166	15	-21	
6	180	8	4	17	29	37	-1*	-10	496	16	34	10	24	33	15*	6	118	13	-12	
7	159	8	11	18	247	9	35	-9	97	11	8	11	16	36	13*	7	84	6	3	
8	262	10	-1	H,K= 7,				6	-8	91	11	7	12	47	12	16*	8	67	19	-8*
9	237	9	-5	-23	0	35	-9*	-7	167	9	11	13	24	31	-4*	H,K= 7, 11				
10	50	24	-10*	-22	44	29	36*	-6	366	12	20	14	48	37	-7*	-9	141	10	-17	
11	302	38	1	-21	140	5	4	-5	184	8	15	H,K= 7,				9	-8	136	30	-7*
12	98	10	-4	-20	295	11	13	-4	288	10	19	-17	106	13	-0	-7	125	10	-25	
13	64	13	3*	-19	50	17	7*	-3	32	42	5*	-16	126	8	5	-6	23	28	8*	
14	89	20	-13*	-13	143	9	4	-2	41	59	6*	-15	342	14	-9	-5	132	8	-23	
15	189	14	-4	-17	150	8	13	-1	67	21	36*	-14	175	7	-6	-4	170	7	4	
16	47	17	15*	-16	129	8	2	0	78	12	53	-13	139	7	-1	-3	17	28	6*	
17	104	18	-1	-15	67	18	20*	1	90	12	-0	-12	92	17	6*	-2	133	10	-9	
18	127	18	-9	-14	81	12	14	2	113	11	-8	-11	331	28	-4	-1	36	17	9*	
19	82	19	-1*	-13	151	8	12	3	91	10	-1	-10	183	8	5	0	161	15	-22	
H,K= 7,				5	-12	85	11	22	4	284	42	-12	-9	250	12	12	1	39	18	24*
-24	70	26	4*	-11	89	14	18	5	151	8	0	-8	68	10	17	2	196	14	-18	
-23	141	9	-1	-10	170	9	18	6	28	40	1*	-7	125	8	-3	3	81	13	-13	
-22	38	42	-6*	-9	169	11	18	7	64	21	-3*	-6	181	7	9	H,K= 8,				
-21	156	7	6	-8	85	12	11	8	340	17	-13	-5	261	10	7	-24	353	13	0	
-20	204	8	10	-7	111	10	0	9	162	7	-7	-4	72	10	7	-22	187	8	-16	
-19	35	49	8*	-6	547	17	39	10	109	15	-5	-3	59	17	1*	-20	386	17	-2	
-18	173	9	17	-5	41	51	8*	11	95	10	10	-2	188	10	-3	-18	0	49	-20*	
-17	110	10	6	-4	215	10	25	12	312	11	31	-1	43	16	20*	-16	233	9	-6	
-16	364	12	23	-3	141	8	18	13	122	14	-8	0	65	10	0	-14	124	8	1	
-15	109	9	8	-2	538	27	54	14	250	9	23	1	67	13	-10*	-12	106	8	-11	
-14	410	13	11	-1	125	9	8	15	25	31	18*	2	65	10	-9	-10	224	8	-4	
-13	53	59	7*	0	514	31	33	H,K= 7,				8	3	177	29	-16	-8	227	8	-5
-12	236	9	17	1	135	9	14	-19	145	12	-5	4	70	12	-9	-6	503	24	-27	
-11	84	12	9	2	277	22	7	-18	78	10	10	5	52	12	4*	-4	173	7	-8	
-10	542	17	26	3	164	14	-6	-17	23	33	1*	6	66	9	9	-2	593	32	-35	
-9	216	8	9	4	468	17	-4	-16	45	23	0*	7	183	15	-7	0	172	9	-9	
-8	87	10	17	5	61	28	-16*	-15	119	7	4	8	200	8	17	2	494	38	20	
-7	116	10	16	6	34	41	24*	-14	36	27	13*	9	262	9	20	4	479	17	25	
-6	442	14	18	7	177	11	2	-13	36	44	13*	10	76	15	-20*	6	257	10	3	
-5	135	8	11	8	240	10	-1	-12	55	13	7*	11	87	10	-2	8	168	11	-1	
-4	55	18	37*	9	38	33	3*	-11	41	48	-13*	H,K= 7,				10	10	95	13	5
-3	465	15	34	10	69	13	-7*	-10	163	9	3	-14	77	3	-7	12	92	14	-0	
-2	219	8	25	11	96	9	-14	-9	115	7	11	-13	85	8	5	14	83	12	-9	
-1	61	19	-1*	12	63	10	37	-8	39	27	33*	-12	177	8	-2	16	90	11	1	

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 15

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL		
18	92	13	-23	-17	96	9	4	-6	151	9	-7	6	241	23	0	-20	105	9	-6		
H ₂ K= 8,				1	-16	256	10	-5	-5	329	25	-13	7	152	8	1	-19	32	36	28*	
-25	17	37	0*	-15	192	9	-9	-4	291	22	7	8	32	43	-25*	-18	341	14	13		
-24	134	8	6	-14	101	13	3	-3	70	22	-3*	9	183	12	-7	-17	0	39	-22*		
-23	72	13	6	-13	195	8	1	-2	33	11	-0	10	300	16	-19	-16	55	15	14*		
-22	81	13	12	-12	88	9	-3	-1	91	12	-10	11	46	39	15*	-15	33	38	2*		
-21	128	8	-11	-11	33	43	4*	0	220	9	1	12	65	12	33	-14	482	17	32		
-20	293	11	-23	-10	131	8	-6	1	241	9	0	13	53	18	-2*	-13	99	9	6		
-19	0	70	-43*	-9	105	8	-4	2	83	11	29	14	241	21	-29	-12	280	10	18		
-18	65	12	34*	-8	97	8	6	3	180	16	-1	15	144	16	-4	-11	72	13	34		
-17	65	20	-3*	-7	273	9	-3	4	222	26	6	16	63	13	-13*	-10	400	14	31		
-16	526	21	-46	-6	377	19	-28	5	269	29	-12	17	56	62	-20*	-9	158	8	19		
-15	98	9	1	-5	27	37	3*	6	54	22	32*	H ₂ K= 8,				5	-8	468	16	32	
-14	170	7	-20	-4	15	36	12*	7	295	27	-7	-23	34	35	5*	-7	122	10	8		
-13	45	49	-4*	-3	202	8	-4	8	307	32	-4	-22	264	9	3	-6	128	10	24		
-12	518	17	-24	-2	439	34	-10	9	32	45	-2*	-21	137	15	1	-5	127	11	-1		
-11	96	7	10	-1	255	9	3	10	27	52	11*	-20	156	9	13	-4	341	26	33		
-10	360	12	-24	0	89	12	-27	11	288	39	-9	-19	67	10	6	-3	130	12	25		
-9	44	25	11*	1	140	9	-2	12	267	13	-9	-18	302	11	21	-2	64	19	1*		
-8	290	9	-18	2	486	62	-1	13	248	15	-16	-17	151	9	4	-1	203	12	25		
-7	121	8	-8	3	314	27	13	14	54	15	6*	-16	44	26	-1*	0	21	46	14*		
-6	451	14	-25	4	230	13	18	15	26	50	12*	-15	212	8	14	1	118	10	18		
-5	148	6	-8	5	156	15	-4	16	163	19	-14	-14	77	18	-2*	2	67	17	11*		
-4	64	10	-0	6	314	12	-18	17	147	28	-20*	-13	39	45	24*	3	121	10	0		
-3	73	11	6	7	77	17	30*	13	41	20	36*	-12	51	20	29*	4	213	10	-11		
-2	81	10	-1	8	194	8	-1	H ₂ K= 8,				4	-11	288	11	9	5	43	52	26*	
-1	100	10	9	9	148	9	6	-24	71	10	-3	-10	142	9	7	6	296	41	-15		
0	62	16	31*	10	105	11	-0	-23	69	12	-3	-9	0	43	-19*	7	46	20	2*		
1	97	15	-6	11	90	11	6	-22	145	9	2	-8	261	9	8	8	121	8	-15		
2	69	18	25*	12	62	16	17*	-21	203	11	-4	-7	261	9	12	9	69	18	-9*		
3	163	9	19	13	45	49	-2*	-20	49	20	4*	-6	139	11	7	10	276	60	-28*		
4	282	10	18	14	50	21	-22*	-19	161	8	0	-5	225	22	16	11	44	25	-13*		
5	0	53	-18*	15	117	8	4	-13	267	9	6	-4	595	40	44	12	25	35	8*		
6	144	12	0	16	79	11	6	-17	29	40	9*	-3	61	22	-4*	13	59	18	4*		
7	147	14	3	17	29	42	-13*	-16	93	9	29	-2	70	17	42*	14	312	12	33		
8	413	35	-27	18	122	37	-31*	-15	300	13	11	-1	53	38	41*	15	34	40	7*		
9	29	57	21*	H ₂ K= 8,				3	-14	459	17	-0	0	555	28	38	H ₂ K= 8,				7
10	57	27	-9*	-25	39	23	36*	-13	196	9	2	1	94	14	5	-20	42	16	19*		
11	91	11	15	-24	167	8	1	-12	201	8	-2	2	246	10	9	-19	85	10	-9		
12	432	19	-38	-23	129	8	10	-11	24	44	11*	3	186	9	1	-18	190	8	11		
13	0	50	-42*	-22	107	9	13	-10	373	25	3	4	382	15	-10	-17	71	14	9*		
14	117	9	1	-21	172	8	-9	-9	168	10	5	5	58	21	3*	-16	72	10	7		
15	39	39	32*	-20	178	10	5	-8	261	11	-3	6	287	13	-9	-15	75	10	10		
16	317	12	11	-19	29	39	24*	-7	303	22	5	7	188	12	-21	-14	48	16	31*		
17	69	14	-14*	-18	155	7	8	-6	251	10	9	8	116	14	-3	-13	27	38	-9*		
18	91	11	-14	-17	297	11	-9	-5	181	10	10	9	14	39	-22*	-12	81	10	10		
19	43	44	10*	-16	338	25	-4	-4	149	8	6	10	154	13	-15	-11	94	10	-3		
H ₂ K= 8,				2	-15	317	12	-2	-3	319	28	19	11	170	13	-13	-10	91	11	-2	
-25	191	8	2	-14	56	28	-15*	-2	225	9	9	12	53	16	16*	-9	102	10	-7		
-24	179	8	3	-13	67	14	-2*	-1	373	21	3	13	118	10	-6	-8	221	9	13		
-23	94	11	-10	-12	292	22	-12	0	71	26	-3*	14	56	13	2*	-7	69	17	15*		
-22	208	10	-4	-11	487	17	-15	1	263	10	23	15	0	36	-37*	-6	161	8	7		
-21	115	11	2	-10	167	7	-6	2	138	11	-6	16	43	19	-20*	-5	180	10	12		
-20	321	12	0	-9	116	8	-10	3	392	32	20	H ₂ K= 8,				6	-4	463	32	33	
-19	184	8	-1	-8	261	21	-16	4	51	23	36*	-22	151	8	0	-3	157	8	15		
-18	181	13	4	-7	277	9	-4	5	128	9	-3	-21	78	10	-20	-2	56	39	25*		

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 16

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	174	8	19	-9	180	8	1	12	161	12	-29	-15	198	11	-3	-2	94	11	-9
0	468	37	22	-7	35	40	-2*	14	300	11	4	-14	455	20	-38	-1	385	42	-0
1	259	9	3	-6	41	21	1*	16	51	35	-10*	-13	224	8	-20	0	298	33	6
2	202	10	2	-5	249	34	-4	H,K# 9, 1				-12	69	12	33	1	219	9	3
3	68	22	-19*	-4	234	26	-3	-24	363	18	-21	-11	154	9	-9	2	58	20	34*
4	239	9	3	-3	241	9	-5	-23	121	12	-5	-10	423	15	-17	3	186	9	9
5	113	8	-4	-2	87	7	6	-22	117	8	-3	-9	230	11	-9	4	279	19	-1
6	199	10	-12	-1	172	8	-9	-21	0	40	-56*	-8	246	9	-9	5	260	15	-7
7	9	39	-12*	0	203	42	-21*	-20	253	10	-13	-7	46	24	-3*	6	56	24	-7*
8	30	36	-3*	1	301	17	-23	-19	44	20	8*	-6	269	11	-20	7	105	11	-10
9	55	30	-2*	2	55	10	19	-18	195	10	-12	-5	144	9	4	8	194	11	-5
10	97	10	0	3	44	25	13*	-17	150	10	-8	-4	89	14	4	9	156	8	1
11	39	44	24*	4	162	15	-10	-16	157	9	-17	-3	177	10	-13	10	73	11	10
12	45	16	7*	5	214	17	-24	-15	44	24	23*	-2	124	9	-6	11	174	14	-17
13	30	33	17*	6	66	14	-21*	-14	51	18	35*	-1	66	18	-0*	12	120	15	-4
H,K# 8, 8				7	77	8	-19	-13	40	33	26*	0	31	46	3*	13	64	16	-14*
-18	205	10	-16	8	84	13	-5	-12	81	14	4	1	137	10	12	14	78	14	-18
-17	170	7	-2	9	73	7	1	-11	49	37	12*	2	110	12	-11	15	57	14	-4*
-16	34	42	-13*	H,K# 8, 10				-10	160	9	-17	3	244	10	10	16	87	28	-19*
-15	91	12	-3	-12	28	35	-5*	-9	57	14	-9*	4	163	11	14	H,K# 9, 4			
-14	288	12	3	-11	21	30	12*	-6	117	8	-13	5	57	59	-19*	-23	38	38	19*
-13	286	10	3	-10	114	7	0	-7	108	8	-4	6	228	16	-13	-22	246	10	0
-12	240	9	8	-9	289	16	-24	-6	287	19	-20	7	158	10	-4	-21	82	16	-7*
-11	23	36	16*	-8	39	25	15*	-5	71	12	-10	8	206	13	-13	-20	28	40	-16*
-10	235	9	12	-7	128	6	-8	-4	458	29	-21	9	130	16	-10	-19	241	9	6
-9	344	23	26	-6	153	26	-3	-3	92	10	14	10	260	18	-27	-18	221	9	-11
-8	252	22	4	-5	96	6	2	-2	200	9	-24	11	23	49	9*	-17	56	13	39*
-7	83	10	-12	-4	54	18	5*	-1	146	9	6	12	156	36	-16*	-16	73	17	-14*
-6	79	12	1	-3	81	9	-17	0	561	67	-29	13	131	17	-21	-15	337	15	1
-5	157	7	11	-2	157	10	-10	1	108	13	-13	14	282	10	17	-14	168	8	3
-4	176	10	18	-1	39	15	-6*	2	49	68	46*	15	95	22	-11*	-13	290	11	-11
-3	146	8	15	0	39	14	-1*	3	63	28	-5*	16	37	32	-3*	-12	50	43	1*
-2	70	10	15	1	30	25	22*	4	548	60	15	17	50	27	2*	-11	217	9	13
-1	46	15	35*	2	155	15	-10	5	155	18	5	H,K# 9, 3				-10	110	12	-6
0	46	23	37*	3	94	8	-15	6	93	47	-10*	-24	214	15	-9	-9	439	41	16
1	94	11	-10	4	46	19	4*	7	73	22	-11*	-23	217	9	-4	-8	162	8	10
2	41	21	-15*	5	179	7	9	8	232	21	-15	-22	0	49	-5*	-7	57	29	12*
3	33	35	-10*	H,K# 9, 0				9	34	59	-18*	-21	47	18	24*	-6	368	36	2
4	139	10	-10	-24	116	10	-3	10	64	21	-9*	-20	207	10	-5	-5	169	31	13
5	190	14	-19	-22	103	11	-9	11	54	25	-9*	-19	209	11	-3	-4	188	8	10
6	162	12	-14	-20	249	11	-11	12	6	43	-5*	-18	47	42	26*	-3	223	34	3
7	69	10	1	-18	357	13	-3	13	21	41	14*	-17	149	13	-12	-2	430	57	8
8	53	33	-5*	-16	206	11	-10	14	28	47	-35*	-16	271	11	-7	-1	82	21	1*
9	150	12	-18	-14	524	22	-41	15	38	41	24*	-15	36	41	17*	0	85	14	11
10	256	9	15	-12	38	29	34*	16	34	37	6*	-14	52	35	-5*	1	76	21	17*
11	119	16	-22	-10	470	25	-26	17	42	48	1*	-13	218	12	-3	2	363	13	13
12	24	32	3*	-8	227	9	-19	H,K# 9, 2				-12	198	9	-4	3	272	11	9
H,K# 8, 9				-6	368	12	-18	-24	76	13	19	-11	186	9	2	4	17	46	10*
-16	50	14	3*	-4	253	9	-10	-23	37	34	30*	-10	61	24	19*	5	65	18	-14*
-15	51	10	14*	-2	179	8	-8	-22	125	10	-14	-9	123	9	1	6	278	13	-14
-14	74	10	7	0	89	14	26	-21	138	7	14	-8	235	27	-5	7	119	10	-8
-13	38	41	11*	2	50	50	7*	-20	115	9	-10	-7	234	10	4	8	42	43	34*
-12	64	11	-4	4	277	13	12	-19	168	8	3	-6	82	15	5*	9	219	40	-9
-11	61	11	4	6	259	13	-7	-13	240	11	-17	-5	408	41	0	10	108	16	-11
-10	37	23	24*	8	307	15	-28	-17	35	40	27*	-4	370	40	-9	11	40	48	4*
-9	206	8	5	10	213	12	-33	-16	183	11	0	-3	34	43	-19*	12	25	38	7*

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.TMCL2.2(OC4H8)

PAGE 17

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
13	185	26	-23	-7	175	12	17	-15	66	8	23	0	36	13	15*	10	343	12	11
14	6	47	-39*	-6	219	9	17	-14	50	18	20*	1	196	18	-37	11	78	22	-2*
15	128	22	-30	-5	82	13	13	-13	40	22	38*	H ₂ K= 10,		0	12	106	29	-34*	
H ₂ K= 9,		5	-4	332	25	31	-12	29	45	4*	-22	326	13	-16	13	0	41	-4*	
-22	113	7	6	-3	73	27	-2*	-11	76	11	-11	-20	49	32	-7*	14	191	10	-10
-21	26	36	1*	-2	450	15	40	-10	73	13	11*	-18	275	10	-14	15	66	12	-15
-20	135	8	3	-1	60	31	-8*	-9	64	20	6*	-16	140	9	-5	H ₂ K= 10,		2	
-19	127	10	-6	0	147	11	-5	-8	166	7	6	-14	110	22	-6*	-23	102	21	-8*
-18	182	8	4	1	67	17	-18*	-7	204	8	14	-12	121	8	-7	-22	231	11	-7
-17	84	12	-7	2	466	34	9	-6	191	8	7	-10	45	46	-16*	-21	208	9	6
-16	367	12	13	3	31	40	17*	-5	46	18	18*	-8	254	9	-12	-20	0	40	-15*
-15	46	21	19*	4	120	9	-3	-4	189	7	12	-6	108	10	-4	-19	29	43	21*
-14	137	8	16	5	59	14	-3*	-3	256	27	17	-4	400	28	-33	-18	199	11	-11
-13	30	40	-15*	6	213	34	-15	-2	245	24	5	-2	232	11	-12	-17	154	11	-4
-12	545	19	19	7	23	38	16*	-1	112	9	0	0	460	46	-28	-16	35	38	29*
-11	37	40	24*	8	142	10	-7	0	115	9	1	2	462	51	0	-15	178	9	-3
-10	82	12	-2	9	53	26	-5*	1	242	46	-13*	4	244	10	10	-14	92	10	-8
-9	181	10	8	10	0	36	-46*	2	252	13	-4	6	326	24	-25	-13	63	13	35*
-8	403	34	13	11	41	47	22*	3	197	14	-15	8	35	44	26*	-12	45	24	2*
-7	127	12	10	12	32	33	6*	4	59	13	42*	10	50	31	-35*	-11	88	12	-23
-6	271	26	20	13	58	16	-21*	5	70	11	11	12	45	48	35*	-10	31	53	16*
-5	286	11	14	H ₂ K= 9,		7	6	144	45	-19*	14	26	46	-16*	-9	228	9	-14	
-4	123	13	4	-19	25	39	-8*	7	135	13	-5	H ₂ K= 10,		1	-8	214	10	-12	
-3	41	46	29*	-18	173	9	4	8	79	7	3	-23	0	42	-37*	-7	20	46	10*
-2	106	11	21	-17	168	7	4	9	38	17	8*	-22	192	12	-5	-6	188	11	-13
-1	326	25	38	-16	332	12	9	H ₂ K= 9,		9	-21	31	41	9*	-5	216	11	3	
0	63	23	45*	-15	127	8	4	-14	46	12	15*	-20	20	42	-1*	-4	409	46	-2
1	186	12	19	-14	35	43	10*	-13	212	10	-12	-19	99	10	0	-3	137	12	12
2	123	10	16	-13	112	11	9	-12	224	10	-10	-18	266	25	-9	-2	303	40	-3
3	96	13	-3	-12	386	24	17	-11	272	12	-6	-17	91	9	-0	-1	100	17	-11
4	93	20	15*	-11	193	8	10	-10	13	35	1*	-16	265	10	-18	0	296	37	-4
5	191	9	7	-10	87	14	7	-9	126	6	4	-15	39	32	17*	1	271	56	-5*
6	205	49	-23*	-9	153	8	10	-8	207	10	5	-14	300	13	-21	2	279	14	-3
7	54	19	-13*	-8	342	22	22	-7	246	10	-5	-13	78	13	-7	3	122	14	9
8	163	31	-15*	-7	168	8	15	-6	21	39	-11*	-12	385	15	-19	4	151	17	3
9	95	9	1	-6	184	8	14	-5	55	13	-11*	-11	44	24	18*	5	122	19	14
10	179	23	-30	-5	50	18	11*	-4	97	7	2	-10	156	7	4	6	188	38	-30*
11	34	37	11*	-4	119	8	10	-3	82	9	4	-9	87	11	-4	7	173	23	-23
12	288	14	20	-3	90	12	11	-2	48	20	14*	-8	449	27	-32	8	92	12	-15
13	0	35	-27*	-2	109	9	9	-1	63	20	-4*	-7	76	12	6	9	50	24	0*
14	44	22	-9*	-1	40	33	10*	0	75	13	-8	-6	68	12	35	10	62	25	-14*
H ₂ K= 9,		6	0	52	18	8*	1	51	16	-20*	-5	0	46	-12*	11	84	16	-5*	
-21	28	44	-21*	1	41	29	11*	2	55	10	5	-4	292	30	-13	12	0	46	-42*
-20	222	11	-0	2	127	9	-5	3	40	15	3*	-3	144	9	-10	13	88	25	-7*
-19	105	8	-10	3	107	8	-6	4	75	11	-5	-2	73	16	44*	14	32	37	16*
-18	111	7	13	4	31	39	4*	5	113	15	-16	-1	61	38	-6*	15	42	32	-8*
-17	77	11	6	5	82	18	24*	6	44	12	-14*	0	0	51	-12*	H ₂ K= 10,		3	
-16	159	8	3	6	204	14	-19	H ₂ K= 9,		10	1	56	31	43*	-22	137	8	-0	
-15	82	10	9	7	108	15	-7	-6	11	37	-11*	2	181	13	10	-21	74	11	4
-14	69	15	65*	8	134	10	-11	-7	205	13	-24	3	137	12	15	-20	175	8	8
-13	152	8	7	9	35	37	21*	-6	102	8	-5	4	49	56	22*	-19	145	8	-5
-12	79	12	8	10	132	29	-28*	-5	19	30	-18*	5	131	21	15	-18	150	7	7
-11	145	12	15	11	102	15	-19	-4	17	29	9*	6	316	27	-14	-17	265	11	-6
-10	80	14	-4	H ₂ K= 9,		8	-3	254	19	-33	7	37	55	25*	-16	212	11	-3	
-9	88	12	11	-17	90	8	-10	-2	84	7	-4	8	0	49	-23*	-15	44	30	0*
-8	317	12	27	-16	107	7	0	-1	126	10	-19	9	92	17	-1*	-14	135	11	-9

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 18

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL		
-13	333	14	-9	5	86	22	-7*	-7	135	10	25	-6	159	23	8	-13	136	7	5		
-12	238	10	-4	6	82	11	-10	-6	275	10	21	-5	123	7	5	-12	0	40	-14*		
-11	139	10	-7	7	162	60	-16*	-5	66	14	20*	-4	46	16	21*	-11	72	14	18*		
-10	125	10	12	8	197	13	-17	-4	90	10	32	-3	25	38	9*	-10	119	8	-13		
-9	294	12	2	9	0	40	-6*	-3	59	18	2*	-2	31	36	-23*	-9	132	14	-6		
-8	232	27	-6	10	87	9	13	-2	93	11	3	-1	68	10	0	-8	163	9	2		
-7	271	27	-2	11	57	25	-16*	-1	78	12	23	0	29	41	17*	-7	104	13	-10		
-6	139	9	6	12	165	26	-32	0	54	24	24*	1	47	13	24*	-6	396	35	-24		
-5	168	9	6	13	56	36	-8*	1	154	11	2	2	25	33	2*	-5	57	19	15*		
-4	188	8	-1	H,K= 10,				5	2	94	10	5	3	77	14	-22	-4	45	38	29*	
-3	124	10	1	-20	218	11	-6	3	0	44	-7*	4	72	8	-12	-3	89	13	7		
-2	222	10	-8	-19	110	8	10	4	163	28	-10	5	37	16	7*	-2	506	80	-20		
-1	232	33	-4	-18	79	11	6	5	78	15	-23*	6	22	34	12*	-1	84	22	-3*		
0	86	16	-8*	-17	225	11	10	6	17	39	-25*	H,K= 10,				9	0	94	14	6	
1	113	11	-1	-16	138	8	0	7	35	44	-2*	-10	89	13	-11	1	75	29	0*		
2	207	33	3	-15	46	22	37*	8	264	10	13	-9	42	12	35*	2	342	60	-15		
3	53	49	-16*	-14	41	30	35*	9	74	11	18	-8	46	18	34*	3	163	11	2		
4	144	14	-9	-13	215	9	13	10	95	15	-9	-7	194	12	-13	4	208	21	-3		
5	164	24	-14	-12	56	18	37*	11	0	44	-3*	-6	171	34	-1*	5	62	22	2*		
6	191	21	-19	-11	62	28	-18*	H,K= 10,				7	-5	184	13	-11	6	163	13	-7	
7	81	13	9	-10	175	10	8	-17	51	13	-6*	-4	99	7	9	7	71	40	-1*		
8	105	17	-12	-9	189	9	9	-16	89	10	-10	-3	112	30	-7*	8	129	21	-24		
9	138	18	-9	-8	42	29	25*	-15	0	43	-11*	-2	115	17	-12	9	98	18	-24*		
10	190	9	15	-7	131	12	3	-14	41	21	26*	-1	263	17	-25	10	0	49	-14*		
11	255	10	26	-6	392	41	19	-13	62	13	6*	0	149	14	-10	11	27	41	-8*		
12	68	42	-8*	-5	0	45	-24*	-12	13	37	3*	1	33	28	-2*	12	41	23	30*		
13	34	40	7*	-4	217	29	17	-11	63	12	22*	2	47	12	-1*	13	50	14	32*		
14	95	26	-17*	-3	104	12	23	-10	132	7	11	H,K= 11,				0	H,K= 11,				2
H,K= 10,				4	-2	361	45	24	-9	153	7	15	-22	88	14	-17	-21	101	17	-12	
-22	89	9	-6	-1	102	10	17	-8	64	12	17*	-20	179	8	-4	-20	213	9	-1		
-21	224	10	0	0	364	31	26	-7	95	12	9	-18	82	10	-9	-19	42	23	32*		
-20	150	12	-1	1	36	51	15*	-6	281	37	12	-16	433	19	-27	-18	72	12	2		
-19	40	40	5*	2	174	8	15	-5	79	12	12	-14	185	9	-9	-17	218	11	-2		
-18	159	8	11	3	53	34	23*	-4	38	40	-3*	-12	466	38	-35	-16	274	12	-17		
-17	158	8	6	4	265	12	-8	-3	30	39	7*	-10	302	15	-20	-15	162	7	1		
-16	227	9	1	5	129	9	-9	-2	332	28	15	-8	253	10	-15	-14	161	8	-7		
-15	170	8	4	6	8	48	-24*	-1	165	10	10	-6	328	13	-32	-13	117	8	2		
-14	288	12	3	7	70	13	8*	0	207	13	-9	-4	178	9	-19	-12	311	13	-10		
-13	34	39	12*	8	123	20	-25	1	32	42	29*	-2	130	10	-4	-11	208	8	-15		
-12	274	11	11	9	75	18	-25*	2	180	36	-12*	0	0	52	-16*	-10	149	10	-14		
-11	118	9	0	10	37	26	33*	3	139	32	-13*	2	161	10	-4	-9	89	15	9		
-10	340	14	2	11	188	8	6	4	272	72	-26*	4	69	20	-6*	-8	237	10	-9		
-9	273	38	10	12	0	34	-13*	5	56	13	-0*	6	207	21	-4	-7	154	9	1		
-8	70	16	-3*	H,K= 10,				6	6	10	35	8*	8	204	33	-51	-6	154	8	1	
-7	142	9	-3	-19	131	7	5	7	48	15	-8*	10	79	46	-24*	-5	196	40	3*		
-6	253	13	1	-18	122	8	8	8	157	58	-17*	12	298	10	0	-4	143	9	-14		
-5	283	33	20	-17	21	39	-20*	9	38	16	8*	H,K= 11,				1	-3	49	27	38*	
-4	47	35	5*	-16	334	23	17	H,K= 10,				8	-22	178	10	-14	-2	21	47	-23*	
-3	255	37	19	-15	69	17	11*	-14	199	10	-3	-21	103	10	-8	-1	194	37	7*		
-2	124	10	10	-14	338	12	26	-13	67	10	-2	-20	238	9	-7	0	127	9	18		
-1	37	46	5*	-13	41	26	30*	-12	179	8	-0	-19	121	9	-1	1	108	12	-16		
0	141	9	9	-12	205	10	12	-11	255	11	15	-18	41	23	2*	2	64	34	-10*		
1	299	36	14	-11	123	16	1	-10	262	30	5	-17	41	22	26*	3	42	47	-7*		
2	77	22	7*	-10	393	14	30	-9	131	7	5	-16	209	11	-9	4	168	19	-12		
3	181	11	9	-9	49	21	10*	-8	44	21	-4*	-15	103	8	12	5	140	10	8		
4	162	15	-24	-8	48	20	34*	-7	160	8	7	-14	53	20	-11*	6	35	46	5*		

STRUCTURE FACTORS CONTINUED FOR
 BETA C8H8.THCL2.2(OC4H8)

PAGE 19

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	113	43	-39*	-6	52	17	48*-10	162	9	20	H,K=	12,	0	-13	144	8	11		
8	148	46	-54*	-5	172	8	7	-9	48	21	36*-20	237	13	-9	-12	154	8	-10	
9	0	59	-14*	-4	376	62	5	-8	190	10	16	-18	210	11	-11	-11	152	9	-8
10	38	39	-2*	-3	39	40	23*	-7	117	9	19	-16	119	11	-0	-10	101	9	4
11	119	33	-38*	-2	56	23	7*	-6	121	9	8	-14	54	17	13*	-9	0	44	-28*
12	187	9	5	-1	120	13	-11	-5	62	17	44*-12	54	13	44*	-8	135	10	-5	
	H,K=	11,	3	0	274	51	-3*	-4	295	33	13	-10	262	11	-16	-7	131	8	8
-21	169	7	10	1	94	26	9*	-3	90	11	15	-8	124	11	-6	-6	170	11	-6
-20	49	19	-13*	2	103	10	-3	-2	31	47	30*	-6	254	10	-10	-5	168	8	8
-19	120	8	-3	3	54	32	-5*	-1	62	15	29*	-4	327	31	-25	-4	200	35	-21
-18	152	8	0	4	143	20	-25	0	377	43	16	-2	170	13	-32	-3	48	28	33*
-17	43	27	24*	5	30	40	-1*	1	71	13	7*	0	349	68	-27*	-2	197	10	7
-16	113	8	15	6	57	17	-1*	2	163	8	4	2	32	46	-17*	-1	189	50	-6*
-15	89	10	-4	7	138	17	-25	3	49	19	1*	4	334	12	31	0	257	65	-6*
-14	233	13	-4	8	123	24	-13*	4	217	51	-10*	6	111	20	-9	1	121	12	-2
-13	140	14	-7	9	29	39	-20*	5	0	36	-7*	8	94	40	-49*	2	80	13	27
-12	105	10	0	10	10	39	-18*	6	172	16	-22	10	41	52	-20*	3	86	14	-13
-11	35	40	23*	11	114	33	-37*	7	96	8	-7	H,K=	12,	1	4	182	31	-37	
-10	216	12	-2	H,K=	11,	5	8	50	12	-8*-20	166	11	1	5	117	23	-24*		
-9	146	10	-3	-19	54	27	-9*	H,K=	11,	7	-19	68	12	2	6	50	63	34*	
-8	91	9	22	-18	290	13	16	-15	96	8	14	-18	234	11	-8	7	32	44	-10*
-7	274	37	3	-17	77	13	24	-14	313	18	-2	-17	66	18	7*	8	99	34	-39*
-6	255	42	-12	-16	91	8	25	-13	122	8	-5	-16	125	8	-0	9	43	34	-17*
-5	50	28	13*-15	51	19	-2*-12	170	11	23	-15	118	9	-13	H,K=	12,	3			
-4	66	23	6*-14	347	12	20	-11.	22	36	15*-14	406	17	-34	-19	180	15	-6		
-3	252	41	16	-13	79	12	6	-10	263	10	14	-13	65	18	-9*-18	179	11	-3	
-2	259	47	-2	-12	138	8	8	-9	160	7	9	-12	71	12	-0	-17	14	43	-0*
-1	245	42	2	-11	14	42	-41*	-8	240	10	16	-11	61	13	10*-16	0	42	-11*	
0	70	15	21*-10	278	31	18	-7	48	49	29*-10	388	44	-20	-15	184	12	-3		
1	0	46	-45*	-3	62	15	7*	-6	68	12	27	-9	156	29	-8*-14	230	31	11	
2	183	46	-1*	-8	243	28	11	-5	94	9	13	-8	99	9	5	-13	98	10	-7
3	244	46	-1*	-7	193	11	9	-4	164	9	9	-7	72	17	-3*-12	55	33	-1*	
4	0	49	-21*	-5	95	12	5	-3	30	37	21*	-6	212	10	-14	-11	129	8	-6
5	66	25	-11*	-5	35	44	10*	-2	35	38	0*	-5	75	13	-7	-10	206	26	-2
6	140	27	-33*	-4	167	8	16	-1	83	11	19	-4	91	21	-13*	-9	240	29	-0
7	96	34	-11*	-3	138	10	13	0	14	37	-2*	-3	76	15	4*	-8	85	12	-10
8	56	25	49*	-2	33	41	3*	1	12	38	-6*	-2	53	25	12*	-7	12	43	-16*
9	85	12	-19	-1	174	8	13	2	35	23	26*	-1	46	52	8*	-6	216	35	2
10	120	41	-37*	0	65	14	36*	3	32	33	15*	0	0	56	-67*	-5	182	55	-2*
11	26	37	16*	1	21	46	-37*	4	128	43	-8*	1	60	20	-4*	-4	78	12	12
12	16	39	15*	2	80	15	4*	5	71	13	-12	2	14	48	-12*	-3	170	43	1*
	H,K=	11,	4	3	211	25	6	H,K=	11,	3	3	94	18	8*	-2	181	45	5*	
-20	126	7	3	4	85	11	-6	-11	68	10	2	4	137	35	-17*	-1	75	12	47
-19	75	12	-13	5	33	47	4*-10	86	9	14	5	0	47	-17*	0	35	50	-27*	
-18	122	8	10	6	153	13	-24	-9	110	10	-8	6	52	63	-43*	1	51	27	-0*
-17	234	10	2	7	76	14	-24*	-8	128	7	9	7	69	77	-20*	2	127	52	-14*
-16	143	8	10	8	45	37	-17*	-7	35	43	15*	8	164	11	4	3	129	54	3*
-15	173	8	6	9	57	12	9*	-6	104	30	5*	9	66	24	-18*	4	55	20	3*
-14	108	8	10	H,K=	11,	6	-5	183	10	9	10	139	43	-46*	5	74	32	-18*	
-13	72	15	13*-17	135	23	11	-4	218	39	-1	H,K=	12,	2	6	131	25	-14*		
-12	157	9	7	-16	48	20	18*	-3	84	8	-9	-19	122	9	-10	7	92	21	-18*
-11	253	12	3	-15	108	9	10	-2	37	26	23*-18	72	12	6	8	45	55	-22*	
-10	40	51	23*-14	23	38	1*	-1	147	11	8	-17	128	8	5	9	110	39	-30*	
-9	54	20	-10*-13	60	15	-4*	0	277	10	26	-16	130	8	-13	H,K=	12,	4		
-8	227	40	6	-12	36	50	-11*	1	204	13	-13	-15	39	57	-1*-18	83	10	18	
-7	152	8	9	-11	149	11	9	2	110	56	-21*-14	66	11	53	-17	69	15	-8*	

STRUCTURE FACTORS CONTINUED FOR
BETA C8H8.THCL2.2(OC4H8)

PAGE 20

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-16	252	10	14	-8	256	11	17	0	207	66	-17*	-14	76	10	0	-3	60	17	11*
-15	55	16	28*	-7	45	47	10*	1	48	59	-10*	-13	196	40	11*	-2	66	17	-10*
-14	65	19	17*	-6	140	8	11	2	178	26	-39	-12	95	9	-5	-1	32	41	17*
-13	118	8	9	-5	130	8	10	3	0	44	-23*	-11	101	9	-4	0	62	14	13*
-12	265	12	3	-4	135	7	28	4	74	18	-25*	-10	126	8	3	1	45	32	-11*
-11	82	11	8	-3	53	28	14*	5	31	49	5*	-9	179	10	12	H,K= 14, 2			
-10	47	52	2*	-2	84	13	9	6	211	10	5	-8	80	11	7	-12	38	41	34*
-9	67	12	31*	-1	99	10	5	H,K= 13, 2				-7	148	8	6	-11	0	39	-6*
-8	232	10	5	0	0	39	-8*	-17	123	10	-5	-6	149	34	-14*	-10	121	12	11
-7	118	10	2	1	62	15	-16*	-16	160	10	-7	-5	71	17	9*	-9	53	21	-20*
-6	41	33	2*	2	84	9	4	-15	35	47	-14*	-4	89	10	7	-8	65	12	6*
-5	164	34	12*	3	77	14	-18	-14	197	9	-1	-3	146	11	32	-7	112	10	-21
-4	188	38	11*	4	27	32	16*	-13	160	10	-4	-2	182	48	-11*	-6	134	50	-14*
-3	0	44	-34*	H,K= 12, 7				-12	189	10	-6	-1	91	15	6	-5	38	43	31*
-2	55	16	52*	-10	36	47	7*	-11	125	8	6	0	127	40	-16*	-4	37	43	1*
-1	235	52	7*	-9	12	35	2*	-10	178	10	-7	1	33	39	14*	-3	123	45	-18*
0	74	15	-12*	-8	204	14	6	-9	120	10	1	2	120	17	-14	-2	205	97	-39*
1	159	44	6*	-7	81	14	1	-8	153	34	-2*	3	57	13	3*	-1	83	12	-2
2	80	26	-11*	-6	139	32	-1*	-7	175	36	5*	H,K= 13, 5				0	38	39	25*
3	130	10	-12	-5	43	30	19*	-6	78	15	13*	-12	181	33	3	H,K= 14, 3			
4	88	25	-26*	-4	171	12	-6	-5	26	43	18*	-11	49	53	1*	-10	38	40	-10*
5	100	49	-37*	-3	99	9	3	-4	170	51	-14*	-10	242	10	6	-9	27	38	-18*
6	71	34	-33*	-2	256	54	-7*	-3	83	14	-15	-9	88	11	-0	-8	150	10	3
7	0	38	-6*	-1	38	42	6*	-2	0	45	-9*	-8	87	12	7	-7	127	13	-9
8	105	35	-26*	0	55	20	-6*	-1	91	14	-17	-7	111	9	7	-6	69	14	12*
H,K= 12, 5				H,K= 13, 0				0	45	56	4*	-6	219	42	17*	-5	85	17	-9*
-16	50	29	-11*	-16	185	8	-12	1	59	38	-3*	-5	109	44	1*	-4	112	14	-12
-15	187	11	21	-14	292	14	-25	2	69	15	-5*	-4	45	26	42*	-3	35	37	26*
-14	81	13	5	-12	327	15	-24	3	65	29	-2*	-3	166	9	14	-2	56	16	-3*
-13	95	9	-2	-10	137	18	-10	4	0	49	-3*	-2	91	15	6	-1	77	13	-22
-12	38	39	2*	-8	277	32	-26	5	97	21	-30*	-1	34	38	16*				
-11	72	14	-5*	-6	48	23	1*	6	161	9	12	0	21	37	17*				
-10	62	34	5*	-4	135	9	-9	H,K= 13, 3				1	147	28	5*				
-9	237	24	9	-2	18	55	-23*	-16	94	9	-1	H,K= 13, 6							
-8	161	10	16	0	48	38	-3*	-15	101	9	10	-6	234	13	8				
-7	54	16	50*	2	74	16	-12*	-14	158	10	7	-5	66	12	6*				
-6	140	11	-5	4	47	32	22*	-13	18	39	-10*	H,K= 14, 0							
-5	94	11	4	6	124	56	-61*	-12	147	8	14	-12	26	38	-8*				
-4	177	30	10	H,K= 13, 1				-11	94	10	6	-10	50	33	-24*				
-3	45	25	4*	-17	57	15	-5*	-10	107	11	-6	-8	121	8	3				
-2	283	60	10*	-16	40	24	22*	-9	94	10	4	-6	187	11	-26				
-1	34	41	15*	-15	65	15	-10*	-8	126	12	3	-4	0	42	-15*				
0	95	12	-13	-14	68	18	-7*	-7	72	12	21	-2	285	12	-7				
1	23	41	5*	-13	0	57	-18*	-6	85	12	-3	0	32	42	-35*				
2	262	45	2	-12	107	13	15	-5	160	9	-12	2	167	43	-61*				
3	54	19	2*	-11	90	19	-5*	-4	133	8	1	H,K= 14, 1							
4	32	52	19*	-10	67	33	3*	-3	164	34	2*	-13	49	17	19*				
5	71	10	-10	-9	106	9	-2	-2	183	14	-3	-12	243	23	-39				
6	127	19	-43	-8	215	14	-21	-1	65	20	-12*	-11	75	16	-10*				
H,K= 12, 6				-7	60	16	14*	0	148	36	-14*	-10	134	14	-17				
-14	82	10	-11	-6	37	48	-17*	1	209	73	-10*	-9	38	44	2*				
-13	41	20	28*	-5	55	31	-6*	2	92	14	-16	-8	140	9	-9				
-12	333	18	6	-4	237	38	-33	3	51	20	-13*	-7	34	40	-17*				
-11	24	36	15*	-3	85	13	-9	4	83	33	-38*	-6	154	9	-18				
-10	76	16	3*	-2	171	13	-8	5	79	46	-21*	-5	0	44	-41*				
-9	88	10	6	-1	27	45	23*	H,K= 13, 4				-4	41	55	-14*				