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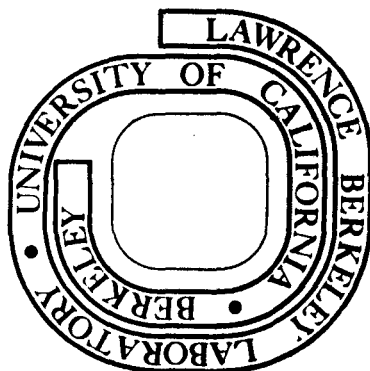
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BOROHYDRIDE DIETHYLETHERATE

Richard R. Rietz, Allan Zalkin, David H. Templeton,
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PREPARATION AND MOLECULAR AND CRYSTAL STRUCTURES
OF URANIUM(IV) BOROHYDRIDE DIMETHYLETHERATE
AND URANIUM(IV) BOROHYDRIDE DIETHYLETHERATE¹

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ABSTRACT

Uranium(IV) borohydride reacts with dimethyl ether and diethyl ether to form $U(BH_4)_4 \cdot O(CH_3)_2$ and $U(BH_4)_4 \cdot O(C_2H_5)_2$, respectively. The yields are > 90%. The latter compound can also be prepared by reacting UF_4 and $LiBH_4$ in diethyl ether for one week. Both compounds are green crystalline solids that can be sublimed in bulk at 50° and 10^{-5} mm. Single crystal x-ray diffractometry has shown both of these materials to be mono-ether complexes in the solid state. $U(BH_4)_4 \cdot O(CH_3)_2$ is orthorhombic, Pnma, with $a = 11.423(5)$ Å, $b = 10.120(4)$ Å, $c = 9.915(4)$ Å, and $Z = 4$. $U(BH_4)_4 \cdot O(C_2H_5)_2$ is monoclinic, $P2_1$, with $a = 7.95(1)$ Å, $b = 15.24(1)$ Å, $c = 5.74(1)$ Å, $\beta = 106.0(1)^\circ$, and $Z = 2$. The structure of each complex consists of infinite linear chains of alternating uranium and boron atoms joined by double hydrogen bridge bonds. The remaining borohydrides are attached to the uranium atom by triple hydrogen bridge bonds. The ether moieties are associated to the uranium by

the oxygen atoms. In the dimethyl ether adduct successive ether molecules along the chain are trans whereas in the diethyl ether compound they are all cis. The total coordination about the uranium atom is fourteen, i.e., one oxygen and 13 hydrogen atoms. The average U-B distances for the triple bridge and double bridge bonds are 2.53(2) and 2.89(1) Å respectively. The average U-O bond length is 2.46(3) Å. A refinement of the anomalous dispersion term f'' for uranium in the ethyl compound shows that the crystal was twinned, containing unequal fractions of the enantiomeric configurations.

INTRODUCTION

Uranium(IV) borohydride, a volatile dark-green crystalline compound obtained by treating UF_4 with $Al(BH_4)_3$ at room temperature, was first synthesized by Schlesinger and Brown during the Manhattan project, and reported in 1953.^{2,3} In an attempt to prepare $U(BH_4)_4$ by another route, they treated UF_4 with $LiBH_4$ in the presence of ether to form a green, ether-soluble product, but were unable to completely separate this material from the solvent. $U(BH_4)_4$ formed a 1:1 complex with ethyl ether which was stable at $-80^\circ C$ but pure $U(BH_4)_4$ could not be recovered by high vacuum fractional distillation.

Recently, Russian workers⁴ have published a new synthesis of $U(BH_4)_4$ by the reaction of finely powdered UCl_4 and $LiBH_4$ (in a vacuum vibration ball mill). This synthesis parallels the well-known method for producing $Hf(BH_4)_4$ and $Zr(BH_4)_4$ ⁵ and avoids the use of $Al(BH_4)_3$, a liquid explosive to oxygen or water.

Hoekstra and Katz⁶ have reported the synthesis of the isomorphic but much less volatile actinide compound, $Th(BH_4)_4$, by treating ThF_4 with $Al(BH_4)_3$. Subsequently, Ehemann and Nöth⁷ synthesized $Th(BH_4)_4$ by the reaction of $ThCl_4$ with $LiBH_4$ in diethyl ether. Here, an etherate complex was formed as an intermediate, but the solvent could be completely removed by vacuum distillation. Consistent with this synthesis was the isolation by Hoekstra and Katz⁶ of $Th(BH_4)_4 \cdot 2(C_2H_5)_2O$ by dissolution of $Th(BH_4)_4$ in diethyl ether with partial recovery of the $Th(BH_4)_4$ after heating in vacuum. Ehemann and Nöth⁷ also treated $Th(BH_4)_4$ with $LiBH_4$ in diethyl ether and reported the synthesis of the

salts $\text{LiTh}(\text{BH}_4)_5$ and $\text{Li}_2\text{Th}(\text{BH}_4)_6$. Etherates were again formed as intermediates but the diethyl ether was easily removed.

In our search for new volatile actinide compounds, we have prepared a number of Lewis base adducts of uranium(IV) borohydride by direct combination of $\text{U}(\text{BH}_4)_4$ and the Lewis base.⁸ Many of these materials are volatile, among them $\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{CH}_3)_2$ and $\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{C}_2\text{H}_5)_2$. We have also repeated the work of Schlesinger and Brown² and have shown their "etherate unstable at room temperature" is actually the stable compound $\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{C}_2\text{H}_5)_2$.

EXPERIMENTAL

Materials and Chemical Techniques. $\text{U}(\text{BH}_4)_4$ was prepared by the method of Schlesinger and Brown² and purified by sublimation at 30-40°C and 10^{-5} mm. UF_4 (Alfa) was vacuum dried at 300° for 3 days. Dimethyl ether (Matheson) was purified by passage through a -78° trap until its v.p. = 283 mm.⁹ Diethyl ether (Mallinckrodt) was doubly distilled from Na/benzophenone under argon. All manipulations were performed in mercury, oil, and grease free Pyrex high vacuum lines or in argon filled dry boxes.⁹

Preparation of $\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{CH}_3)_2$. A 250 ml flask was loaded with 0.29 g $\text{U}(\text{BH}_4)_4$ (0.975 mmole) in a dry box. The flask was fitted with a vacuum line adapter, sealed, removed to the vacuum line, cooled to -196°, and evacuated. Dimethyl ether (3.58 mmole) was condensed onto the flask walls. The vessel was warmed to room temperature.

-3-

No reaction was noted between the gaseous $(\text{CH}_3)_2\text{O}$ and the solid $\text{U}(\text{BH}_4)_4$. The vessel was cooled to -196° and an additional 40 mmoles of $(\text{CH}_3)_2\text{O}$ was condensed in. The vessel was slowly warmed to -78° . No reaction was noted. When the vessel was warmed to -30° the $\text{U}(\text{BH}_4)_4$ first turned white and then went into solution. Green crystals could be forced out of solution by cooling to -78° , but rewarming to -30° only produced the green solution. The white intermediate stage was only seen upon the first dissolution. This phenomenon was observed in every preparation of $\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{CH}_3)_2$ and $\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{C}_2\text{H}_5)_2$. After 30 min at -30° , the flask was cooled to -78° and the excess $(\text{CH}_3)_2\text{O}$ was stripped off. The product was pumped at 20° into a tared trap at -78° . 0.317g green crystals (m.p. 93° , sealed capillary) were recovered. Based on the empirical formula, this is 0.924 mmole (95% yield).

$\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{CH}_3)_2$ hydrolyzes slowly in air and inflames upon contact with water. It can be sublimed in bulk at 50°C . It has been kept under argon or vacuum for several months with little decomposition. Its physical and spectroscopic properties will appear in a subsequent publication.⁸

Direct Preparation of $\text{U}(\text{BH}_4)_4 \cdot \text{O}(\text{C}_2\text{H}_5)_2$. In a typical preparation, 0.396g $\text{U}(\text{BH}_4)_4$ (1.33 mmoles) was sublimed into a 100 ml trap. Diethyl ether (6.54g) was condensed on top of the $\text{U}(\text{BH}_4)_4$ at -196° . The trap was sealed, removed from the vacuum line, and slowly warmed to room temperature with shaking. At $\sim -30^\circ$ the $\text{U}(\text{BH}_4)_4$ turned white and then quickly dissolved to form a deep green solution. Green crystals could be obtained by cooling the solution. This phenomenon is described above.

After 30 min at room temperature, the trap was cooled to -78° , reattached to the vacuum line, and the excess $(C_2H_5)_2O$ removed by pumping for 4 h. The product was pumped at 20° to another tared trap at -78° . 0.464g green crystals (m.p. 66° , sealed capillary) were recovered. Based on the empirical formula, this is 1.25 mmole (94% yield).

$U(BH_4)_4 \cdot O(C_2H_5)_2$ hydrolyzes slowly in air and inflames, often with an explosion, upon contact with water. It can be sublimed in bulk at $50^{\circ}C$. It has been kept for six months in vacuum or under argon without decomposition. Its physical and spectroscopic properties will appear in a subsequent publication.⁸

Preparation of $U(BH_4)_4 \cdot O(C_2H_5)_2$ from UF_4 and $LiBH_4$ in Diethyl Ether.

10.0g of finely ground UF_4 (31.85 mmoles) was loaded into a 250 ml Schlenk flask containing a Teflon stirring egg. The flask was moved into the dry box where 2.8g finely ground $LiBH_4$ (128.6 mmoles) was added. The flask was fitted with a vacuum adapter, sealed, and moved to the vacuum line. After thorough evacuation to remove trapped argon (1 h), ~125 ml diethyl ether was condensed in at -196° . The flask was sealed, removed from the vacuum line, and warmed to room temperature with stirring (~1 h). The stirrer was shut off occasionally to observe the ether solution. At 2 h it was colorless, also at 6 h. At 1 day, it was faint green. At 8 days, the solution was dark green and a grey-white ppt. had formed.

At this point, the flask was filled with argon and the contents Schlenk filtered under argon through a medium frit. The green filtrate was concentrated by pumping at -78° under high vacuum. When the bulk

of the ether had distilled off, the product was pumped at 20° to a tared trap at -78°. ¹⁰ Yield: 4.45g, 38% based on UF₄. No attempt was made to recover the unused UF₄. Identification of the product as U(BH₄)₄·O(C₂H₅)₂ was made by its melting point, infrared spectrum, and x-ray powder patterns. ⁸

A non-volatile, ether-soluble, greenish-white, uranium-containing material was left after removing the U(BH₄)₄·O(C₂H₅)₂ from the filtrate. Absorption bands for uranium-borohydride units appeared in the infrared spectrum of this material. The compound hydrolyzed quickly in air, sometimes catching fire. It often exploded on contact with water. We believe it is a mixture of UF_x(BH₄)_{4-x} species, possibly with associated ethers. No attempts were made to recycle this material.

Crystal Growth. The only method which gave crystals suitable for x-ray diffraction was as follows. Several crystals were ground in an agate mortar and pestle and poured into a capillary drawn from a 14/35 quartz joint. An adapter containing a stopcock to trap argon over the sample was placed over the loaded joint. This assembly was removed from the dry box and connected to a high vacuum line. The capillary was cooled to -78°C, evacuated, and sealed. Crystals were grown inside the capillary by slow sublimation (6-24 h) using a microscope lamp focused on a colored card beneath the capillary as the heat source.

X-Ray Diffraction. A Picker FACS-I automated diffractometer equipped with a graphite monochromator and molybdenum tube was used

for the unit cell measurements and data collection; the details of which are shown in Table I.

For the $U(BH_4)_4 \cdot O(CH_3)_2$ experiments, the only suitable crystal found was an irregularly shaped one that had grown into the tip of the capillary. Omega scans of several low angle reflections showed widths at half-peak height of 0.13° to 0.22° with the latter along the c^* axis. Cell dimensions were obtained by a least-squares refinement procedure of the angular settings of 12 manually centered reflections for which 2θ was between 35° and 40° . A total of 3277 scans were measured and later averaged to give a set of 1402 unique reflections. Three standard reflections were measured after each 200th scan to monitor for crystal decay, instrumental stability, and crystal alignment. After 6 days of data-taking the standards exhibited about 9% decay in their intensities, and the data were corrected accordingly; the crystal color had changed to brown. As the crystal had assumed the shape and distortions of the capillary tip, we were unable to describe the crystal shape in a manner suitable for our absorption program, and therefore no absorption correction was made.

For the $U(BH_4)_4 \cdot O(C_2H_5)_2$ experiment, a crystal, $\sim .3$ mm in size, was found in one of the capillaries. Omega scans of several low angle reflections showed widths at half-peak height of $.17^\circ$ to $.27^\circ$ with the latter along c^* ; the peaks were somewhat unsymmetrical, but adequate for data collection. Cell dimensions were obtained from the angle settings of the (8,0,0), (0,0,5) and (0,16,0) reflections. A total of 4563 scans were measured and later averaged to give a set of 3902

unique reflections according to point group 2, or 2020 for point group 2/m. Three standard reflections were measured after each 200th scan; after 8 days of data-taking each standard exhibited about 8% decay in its intensity, and the data were corrected accordingly. The crystal color had changed to a deep red-brown color. An absorption correction by an analytical integration¹¹ was made, and its validity tested on a set of intensity data at various azimuthal angles for several reflections in a diverse region of reciprocal space. The data were processed, averaged, and given estimated standard deviations using formulas presented in the Supplementary Material. The factor $p = 0.06$ and 0.025 was used in the calculations of $\sigma(F^2)$ for the methyl and ethyl ether complexes respectively.

The Patterson functions revealed the uranium atom positions, and in the case of the methyl ether adduct, most of the light atom positions. Subsequent least-squares and difference Fourier maps gave the positions of all the atoms except hydrogen. The structures were refined by full-matrix least squares where the function $\sum w(\Delta F)^2 / \sum w F_o^2$ was minimized. For the ethyl compound, the four strongest reflections (two Bijvoet pairs) were observed a few percent weaker than calculated, and they were deleted from the data set. Otherwise, no correction for extinction was indicated and none was made for either crystal. The scattering factors used were those of Doyle and Turner¹² for neutral boron, carbon and oxygen and those of Cromer and Waber¹³ for the neutral uranium atom corrected for dispersion according to Cromer and Liberman.¹⁴ The uranium atoms were given anisotropic thermal parameters in both cases.

In the methyl ether complex, all the light atoms were assigned isotropic thermal parameters as attempts at anisotropic refinement resulted in little improvement in the R factors and in widely divergent thermal parameters. This behavior we attribute to errors from the uncorrected absorption effects. Attempts to locate hydrogen atoms in the difference maps failed and these atoms were not included in the calculations. The largest peak in the difference Fourier map was $1.5 \text{ e}/\text{\AA}^3$ and was less than $.4 \text{ \AA}$ from B(1). The final R factor, $\Sigma|\Delta F|/\Sigma|F_o|$, was 0.036 for 851 data where $F^2 > 3\sigma$, and 0.076 for all 1402 data. The weighted R_w factor, $(\Sigma w(\Delta F)^2/\Sigma w F_o^2)^{1/2}$, was 0.045. The standard deviation of an observation of unit weight was 1.03.

In the ethyl ether compound the non-hydrogen atoms were found by Fourier methods and refined by least squares, first using the data averaged according to 2/m. Then the members of each Bijvoet pair were treated as independent observations (data averaged according to point group 2). The absolute configuration which is described by the tables and figures is the one which gave the better agreement after both alternatives had been tested.

A model for the hydrogen positions was derived, starting with the boron and oxygen positions and using the known structure¹⁵ of $U(\text{BH}_4)_4$ for guidance as to how the hydrogen atoms might pack around the uranium atom. A ΔF Fourier map, calculated after anisotropic refinement of the other atoms, showed positive densities in the anticipated locations with peak heights of 0.4 to $1.6 \text{ e}/\text{\AA}^3$. Attempts to locate the hydrogen atoms in the ethyl ether moiety failed, and

these atoms were not included in the calculations. Because the borohydride hydrogen atoms were poorly resolved, and because the map showed spurious peaks elsewhere of similar magnitude, we imposed restraints on the geometry of the borohydride groups in the following manner.¹⁶ Interatomic distances between selected atoms are introduced into the least-squares calculations and treated as observations; estimated standard deviations of these distances are also introduced and used to calculate the weights. Except that the derivatives of these distances with respect to the positional parameters are calculated by a special patch and that these "observations" are not included in the R values reported here, these terms are included in the least-squares calculation in the same manner as the observed structure factors. This procedure allows the structure to adjust to the electron density with a flexibility governed by the weighting. All the hydrogen distances were restrained to the following values: U-H to $2.4 \pm .2 \text{ \AA}$, B-H to $1.19 \pm .05 \text{ \AA}$, H-H to $1.94 \pm .05 \text{ \AA}$. These distances impose tetrahedral geometry on the BH_4^- ions, but leave each one free to rotate about the U-B axis. One common isotropic thermal parameter was used for all sixteen hydrogen atoms. The structure with these restraints was refined to convergence; R was 0.023 for 3210 data where $F^2 > 3\sigma$, and 0.036 for all 3902 data; R_w was 0.026.

Because we are interested in the experimental determination of the anomalous dispersion corrections, we modified our least-squares program to include f'' for uranium (the imaginary part of the dispersion correction) as one of the variables to be refined. The other variables,

and the restraints on some of them, were the same as before. Refinement changed f'' from 9.654 (Cromer and Liberman¹⁴) to 3.9(4) electrons. This discrepancy is far outside the error estimated for either value, and we attribute it to twinning of a mixture of right and left handed crystal domains, with the crystal containing about 70% of one enantiomer and 30% of the other. To a good approximation, because the dispersion effects are a small perturbation, a calculation with a weighted mean value of f'' is equivalent to a calculation of each twin component separately, followed by averaging of the intensities, which is the proper method for a twinned specimen.

The final R was 0.022 for 3206 reflections included in the refinement, and 0.035 for 3898 data including those of zero weight, and the standard deviation of an observation of unit weight was 1.02.

Final positional and thermal parameters are given in Tables II and III. Tables of observed structure factor amplitudes are given in the Supplementary Material. Distances and angles are listed in Tables IV and V. The atom numbering is seen in Figure 1.

DISCUSSION

The molecular structures of both these etherates of uranium borohydride are related to that of uranium borohydride itself. In uranium borohydride¹⁵ the boron atoms are connected to uranium by a combination of triple and double hydrogen bridge bonds. These two types of bridging bonds can be identified by the U-B interatomic

distances of 2.5 Å and 2.9 Å for the triple and double hydrogen bridge bonds respectively. The double bridge bonds tie pairs of uranium atoms together, and in the case of uranium borohydride lead to a three dimensional molecular network with a coordination of fourteen hydrogen atoms about each uranium atom. In both the methyl and ethyl ether compounds the structures consist of infinite linear chains of uranium and boron atoms hooked together by double hydrogen bridge bonds, as shown in Figures 1 through 3. Each uranium atom has thirteen hydrogens and one oxygen atom in its coordination sphere yielding a total of 14, the same as in uranium borohydride. In the methyl complex the ethers are alternately on one side or the other of the chain whereas in the ethyl ether complex they are all on the same side. The ether moieties are coordinated to the uranium atom by their oxygen atoms at 2.44 and 2.49 Å respectively for the methyl and ethyl ether. Because of the lack of an absorption correction for the methyl compound, we doubt that this difference is significant.

In both compounds the boron and oxygen atoms are arranged around uranium in an octahedral manner, but O-U-B and B-U-B angles deviate by as much as 26° from the regular values of 90° and 180°. Corresponding angles for the two compounds agree within about 3° or better (Table V). It seems clear that this distortion is the result of the packing requirements for the hydrogen atoms around the uranium. Bernstein et al.¹⁵ gave a similar interpretation to the structure of crystalline $U(BH_4)_4$, where the situation is analogous.

We refined the hydrogen coordinates only for the ethyl compound, but because of the similarity of the angles noted above we assume that in the methyl compound the hydrogen configuration is the same. In the ethyl compound the oxygen atom and 13 hydrogen atoms, which surround one uranium atom, can be described by the corners of a polyhedron with 14 triangular and 5 quadrilateral faces (Fig. 4), if one overlooks slight deviations from planarity of the atoms at the corners of each quadrilateral face. This solid is topologically distinct from the one which corresponds to the 14 hydrogen neighbors of uranium in $U(BH_4)_4$, described as approximately a bicapped hexagonal antiprism,¹⁵ but some fragments of the two solids are similar. The oxygen atom has 5 hydrogen neighbors with O-U-H angles between 68° and 72° . Each of the 13 hydrogen atoms in the coordination sphere has either 4 or 5 neighbors (O + 3H, 4H, or 5H). The H-U-H angles are 46° to 53° when the hydrogen atoms are in the same borohydride ion, and otherwise they range from 50° to 67° .

Absolute Configuration and Anomalous Dispersion. In discussions of absolute configuration the possibility of twinning of enantiomers is often disregarded. This is appropriate if it is known that the crystal consists of pure enantiomeric molecules, as is often true with materials of biological origin. However, the present case may serve as a reminder that twinning is always possible when the asymmetry exists in the crystal structure but not in its component molecules. This possibility of twinning seriously undermines the validity of a statistical probability test applied to the binary choice of one configuration or the other. In the

present case one configuration fits the data significantly better than does the other, but the twinning model fits still better.

The configuration of a particular specimen in a case like this is not intrinsically of general significance. It is important, however, in connection with the "polar dispersion error" which involves serious errors in atomic coordinates when structures are refined in polar space groups with data sets which are incomplete in the Bijvoet sense and with a model which is incorrect with respect to configuration or anomalous dispersion terms or both.^{17,18} In our case, because complete data were used in the refinement, the interatomic distances differ by trivial amounts regardless of which assumption was made about configuration. However, thermal parameters are strongly correlated with f'' , and vary by several standard deviations among the different models.

Supplementary Material Available: Formulas used in data reduction and listings of the structure factors (22 pages). Ordering information is given on any current masthead page.

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10. In larger preparations, it was found expedient to attach the flask containing the crude filtrate directly to a large sublimator. As the ether was pumped off, the solution cooled sufficiently to prevent transfer of the product. When the filtrate had reached the consistency of a thick paste, the sublimator cold finger was cooled to -78° . The product was then collected by heating the flask very slowly to 50°C . A second sublimation at $30-40^{\circ}$ was needed to purify the product as considerable splattering accompanied the first sublimation.

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Table I. Summary of Crystal Data and Intensity Collection

Compound	$U(BH_4)_4 \cdot O(CH_3)_2$	$U(BH_4)_4 \cdot O(C_2H_5)_2$
Formula Weight	343.47	371.52
\underline{a} , Å	11.423(5)	7.945(10)
\underline{b} , Å	10.120(4)	15.244(10)
\underline{c} , Å	9.915(4)	5.740(10)
β , deg.	90.0	106.04(10)
V , Å ³	1146	668
Z	4	2
Density, g/cc, calcd.	1.99	1.85
Space Group	Pnma	P2 ₁
Crystal Shape and Size, mm	Irregular Shape Dimensions - .10 x .15 x .30	Five sided plate of 7 faces; 001, 00 $\bar{1}$, 110, $\bar{1}00$, $\bar{1}40$, $1\bar{4}0$, $\bar{1}10$. Dimensions - 0.1 x 0.3 x 0.3
Crystal Volume, mm ³	.004	.0083
Temperature, deg. C	23	21
Radiation, Å	MoK α ($\lambda = 0.70926$ and 0.71354) monochromated from (002) face of mosaic graphite	
Transmission Factor	---	.08 - .43
μ , cm ⁻¹	135	116
Data Collection Method	θ -2 θ scan (1°/min along 2 θ)	
Scan Range	1° below K α_1 to 1° above K α_2	
Background Counts, sec.	10	10
2 θ Limits, deg.	3 - 55	3 - 60
Unique Data Used $F_o^2 > 3\sigma(F_o^2)$	851	3206 (includes Friedel pairs)
Final No. of Variables	24	140

Table II. Positional and Thermal Parameters for $U(BH_4)_4 \cdot O(CH_3)_2$ ^a

Atom	x	y	z	B(Å ²)
U	0.11737(4)	0.25	0.21009(6)	*
O	0.1483(9)	0.25	0.453(1)	4.5(2)
B(1)	-0.133(2)	0.25	0.240(3)	6.5(6)
B(2)	0.073(2)	0.494(2)	0.220(2)	7.0(4)
B(3)	0.184(3)	0.25	-0.029(4)	7.7(7)
C	0.180(3)	0.368(3)	0.534(4)	17.9(10)

*B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
1.69(2)	5.32(3)	3.22(2)	0	-0.08(3)	0

^aThe anisotropic temperature factor has the form $\exp(-0.25(B_{11}h^2a^{*2} + 2B_{12}hka^*b^* + \dots))$. The isotropic temperature factor has the form $\exp(-B(\sin\theta/\lambda)^2)$.

Table III. Positional and Thermal Parameters for $U(BH_4)_4 \cdot O(C_2H_5)_2^a$

Atom	x	y	z
U	.26472(2)	0	.12412(3)
B(1)	.287(1)	-.0189(6)	.632(1)
B(2)	.577(1)	.0501(6)	.157(2)
B(3)	.156(1)	.1501(5)	.193(2)
B(4)	-.037(1)	-.0621(7)	-.080(2)
O	.3723(6)	-.1508(3)	.2466(8)
C(1)	.5516(9)	-.1645(5)	.397(2)
C(2)	.662(2)	-.2037(8)	.249(3)
C(3)	.271(1)	-.2325(6)	.197(2)
C(4)	.202(2)	-.259(1)	.405(3)
H(1)	.416(5)	-.009(5)	.578(8)
H(2)	.173(6)	-.039(3)	.467(8)
H(3)	.265(8)	.043(3)	.75(1)
H(4)	.318(8)	-.078(3)	.784(9)
H(5)	.706(5)	.076(4)	.16(1)
H(6)	.532(7)	-.021(2)	.10(1)
H(7)	.455(6)	.090(4)	.02(1)
H(8)	.553(7)	.059(4)	.359(7)
H(9)	.106(7)	.214(3)	.24(1)
H(10)	.072(7)	.090(3)	.23(1)
H(11)	.309(5)	.136(4)	.31(1)
H(12)	.168(8)	.144(4)	-.005(7)
H(13)	-.179(5)	-.081(4)	-.19(1)

Table III. Positional and Thermal Parameters for $U(BH_4)_4 \cdot O(C_2H_5)_2$ ^a
(Continued)

Atom	x	y	z
H(14)	-.015(7)	-.061(4)	.130(6)
H(15)	-.008(6)	.011(3)	-.14(1)
H(16)	.072(6)	-.107(3)	-.13(1)

Atom	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
U	2.837(7)	2.708(6)	1.471(5)	-.28(3)	.683(4)	-.10(4)
B(1)	4.6(3)	6.0(8)	2.1(2)	.1(3)	1.3(2)	-.6(3)
B(2)	3.8(3)	5.3(4)	4.5(4)	-.9(3)	1.3(3)	-.2(3)
B(3)	5.7(4)	3.9(3)	4.4(4)	.7(3)	1.2(3)	-.9(3)
B(4)	4.1(3)	6.6(5)	3.8(4)	-1.2(3)	.1(3)	-.6(3)
O	4.4(2)	3.2(2)	3.6(2)	.0(1)	.8(2)	.3(1)
C(1)	4.2(3)	5.2(3)	5.0(4)	1.4(3)	.7(3)	1.0(3)
C(2)	7.9(6)	7.7(6)	10.7(9)	3.5(5)	4.5(6)	1.6(6)
C(3)	7.7(6)	4.3(4)	7.9(6)	-1.6(3)	-.7(5)	.3(4)
C(4)	10.1(8)	8.7(7)	12.0(12)	-3.4(6)	3.0(8)	2.7(7)

^a The estimated standard deviations for the hydrogen atoms are the result of least-squares refinement on a model in which the hydrogen distances were restrained as described in the text. One isotropic thermal parameter was applied to all the hydrogens and it refined to 4.5(4) Å².

Table IV. Distances (Å) in $U(BH_4)_4 \cdot O(CH_3)_2$ and $U(BH_4)_4 \cdot O(C_2H_5)_2$.

	<u>Methyl cpd.</u>	<u>Ethyl cpd.</u>
U-O	2.44(1)	2.485(5)
U-B(1)	2.87(2)	2.89(1)
U-B(1) ⁱ	2.90(2)	2.89(1)
U-B(2)	2.53(2)	2.55(1)
U-B(4)	(2.53)	2.55(1)
U-B(3)	2.49(4)	2.52(1)
O-C(1)	1.48(4)	1.46(1)
O-C(3)	(1.48)	1.47(1)
C(1)-C(2)	--	1.51(1)
C(3)-C(4)	--	1.50(2)

Ethyl Compound

U-H(1)	2.55(5)	B(1)-H(1)	1.16(3)
-H(2)	2.36(5)	-H(2)	1.15(3)
-H(3)	2.26(6)	-H(3)	1.20(3)
-H(4)	2.42(6)	-H(4)	1.23(3)
		B(2)-H(5)	1.10(3)
-H(6)	2.19(6)	-H(6)	1.16(3)
-H(7)	2.25(6)	-H(7)	1.24(3)
-H(8)	2.48(6)	-H(8)	1.24(3)
		B(3)-H(9)	1.12(3)
-H(10)	2.27(6)	-H(10)	1.19(3)
-H(11)	2.32(6)	-H(11)	1.24(3)

Table IV. (Continued)

-H(12)	2.38(6)	-H(12)	1.17(3)
		B(4)-H(13)	1.17(3)
-H(14)	2.42(6)	-H(14)	1.17(3)
-H(15)	2.29(6)	-H(15)	1.21(4)
-H(16)	2.44(6)	-H(16)	1.21(3)

ⁱSymmetry operations in Tables IV and V

Methyl compound: $1/2 + x, 1/4, 1/2 - z$

Ethyl compound: $x, y, z - 1$

Table V. Angles in $U(BH_4)_4 \cdot O(CH_3)_2$ and $U(BH_4)_4 \cdot O(C_2H_5)_2$.

			<u>Methyl cpd.</u>	<u>Ethyl cpd.</u>
O	-U	-B(1)	92.4(6)	94.3(2)
		-B(1')	71.8(6)	72.6(2)
		-B(2)	89.4(5)	90.2(3)
		-B(4)	(89.4)	89.6(3)
		-B(3)	153.9(8)	154.6(3)
B(1)-U		-B(1) ⁱ	164.24(4)	166.7(4)
		-B(2)	78.4(5)	77.3(3)
		-B(4)	(78.4)	79.5(3)
		-B(3)	113.7(9)	111.2(3)
B(1) ⁱ -U		-B(2)	100.9(5)	99.6(3)
		-B(4)	(100.9)	102.5(3)
		-B(3)	82.1(9)	82.0(3)
B(2)-U		-B(4)	(157(1))	156.8(3)
		-B(3)	95.7(5)	94.9(3)
B(3)-U		-B(4)	(95.7)	95.2(3)
U	-O	-C(1)	125(2)	120.2(4)
		-C(3)	(125)	127.1(5)
C(1)-O		-C(3)	107(3)	112.6(6)
O	-C(1)-C(2)		--	110.4(8)
O	-C(3)-C(4)		--	112(1)
U		-B(1) ⁱ -U ⁱ	176(1)	166.7(4)

FIGURE CAPTIONS

- Figure 1. Stereogram (drawn with C.K. Johnson's ORTEP) of one unit of the ethyl ether complex, showing hydrogen positions and the atomic numbering. The methyl compound is numbered in an analogous manner, except that in it B(2) corresponds to both B(2) and B(4).
- Figure 2. Stereogram showing the chain structure in $U(BH_4)_4 \cdot O(CH_3)_2$.
- Figure 3. Stereogram showing the chain structure in $U(BH_4)_4 \cdot O(C_2H_5)_2$.
- Figure 4. Coordination polyhedron of uranium in the ethyl complex. The numbers identify the hydrogen atoms, and O indicates oxygen.

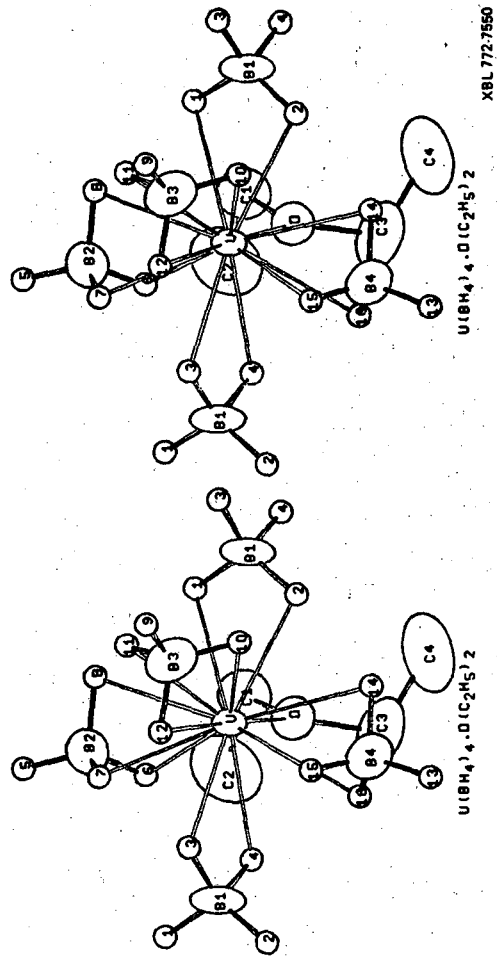
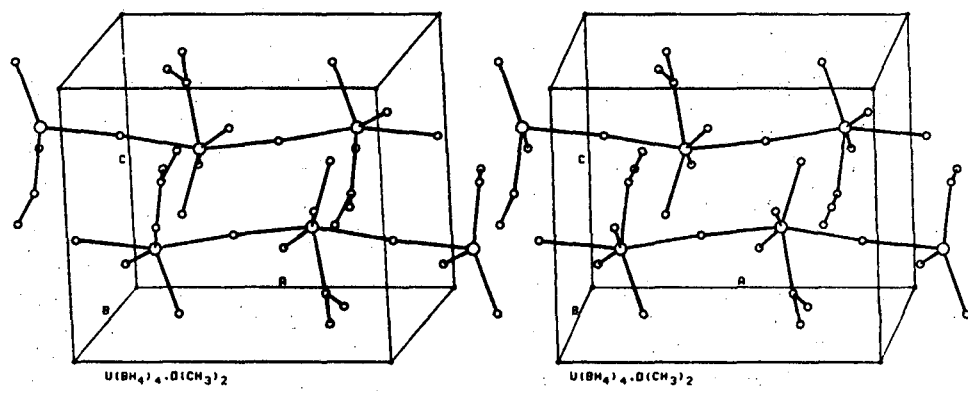
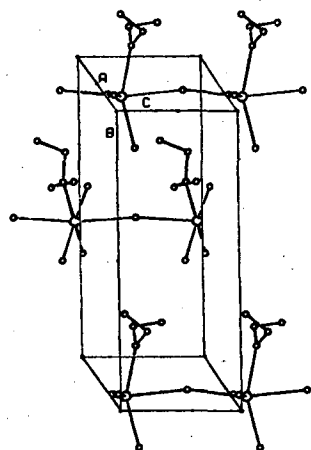


Fig. 1

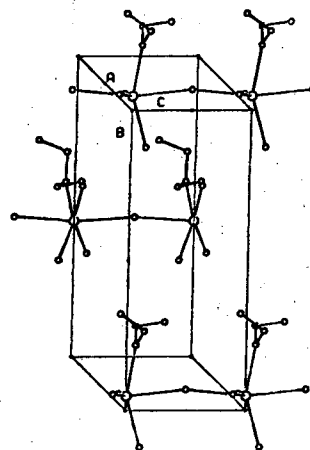


XBL 7612-11427

Fig. 2



$U(BH_4)_4 \cdot 0.5(C_2H_5)_2$



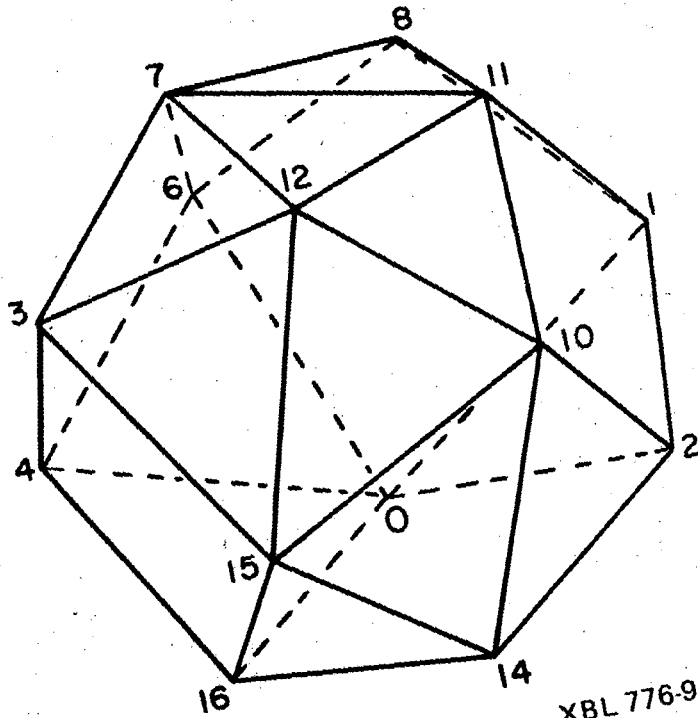
$U(BH_4)_4 \cdot 0.5(C_2H_5)_2$

XBL 7738136

Fig. 3

0 0 0 0 4 8 0 5 3 2 5

-27-



XBL 776-9357

Fig. 4

DATA PROCESSING FORMULAE

$$I = C - (t_c/2t_b)(B_1+B_2)$$

$$\sigma(B) = \text{Max}[(t_c/2t_b)(B_1+B_2)^{\frac{1}{2}}, (t_c/2t_b)|B_1-B_2|]$$

$$\sigma(I) = [C + \sigma^2(B)]^{\frac{1}{2}}$$

$$F^2 = (D \cdot A/L_p)I$$

$$\sigma(F^2) = (D \cdot A/L_p)\sigma(I)$$

$$F_a^2 = \Sigma F^2/n$$

$$\sigma(F_a^2) = [\Sigma \sigma^2(F^2)/n]^{\frac{1}{2}} \quad \text{When } S(F_a^2) > 4\sigma(F_a^2), \sigma(F_a^2) \text{ is replaced by } S(F_a^2).$$

$$S(F_a^2) = [\Sigma |F^2 - F_a^2|^2/n(n-1)]^{\frac{1}{2}}$$

$$\sigma(F_o^2) = [\sigma^2(F_a^2) + (pF_a^2)^2 + q^2]^{\frac{1}{2}}$$

$$F_o = (F_a^2)^{\frac{1}{2}}$$

$$\sigma(F) = F_o - [F_a^2 - \sigma(F_o^2)]^{\frac{1}{2}} \text{ when } \sigma(F_o^2) \leq F_a^2 \text{ or } [\sigma(F_a^2)]^{\frac{1}{2}} \text{ when } \sigma(F_a^2) > F_a^2$$

$$L_p = [\cos^2 2\theta_m + \cos^2 2\theta] / [\sin 2\theta (1 + \cos^2 2\theta_m)]$$

$$\text{wtg} = 1/\sigma^2(F)$$

C = counts recorded during a scan

θ_m = monochromater angle

I = individual raw intensity,
background removed.

θ = crystal diffraction angle

t_c = scan count time

S = scatter

t_b = background count time

a = average

B_1 = individual background count

q = additional uncertainty that
affects the weak intensities

$\sigma(B)$ = estimated standard deviation of the total background count

p = estimate of non-statistical errors

F = structure factor

wtg = weighting factors in least squares

D = decay correction; an empirically applied correction obtained from the fluctuations of the standard reflections.

A = absorption correction

L_p = Lorentz and polarization corrections

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 4.0)
 U(BH4)4.0(CH3)2. F(0,0,0) = 1948

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

H	FCB	SG	DEL	H	FCB	SG	DEL	H	FCB	SG	DEL	H	FCB	SG	DEL	H	FCB	SG	DEL				
	K,L= 0,	0		14	158	20	-17	7	178	12	7	3	26	59	4*	10	180	8	-3				
2	52	22	30*		K,L= 0,	0	4	8	42	46	33*	4	199	11	17	11	290	10	-0				
4	1166	36	-12	0	770	24	98	9	341	11	4	5	38	62	32*	12	260	10	15				
6	229	8	27	1	586	22	9	10	75	21	12*		K,L= 1,	0		13	78	23	26*				
8	634	21	-15	2	20	36	-12*	11	92	18	21*	21	370	42	21	14	138	13	-6				
10	250	10		3	631	20	-2	12	62	62	47*	4	90	7	10		K,L= 1,	4					
12	378	13	9	4	498	16	18		K,L= 0,	8		6	792	25	-27	1	595	18	-15				
14	202	10	-1	5	377	13	23	0	220	11	9	8	237	8	1	2	538	17	35				
	K,L= 0,	2		6	91	9	-12	1	304	11	-12	10	479	15	-8	3	504	16	21				
1	144	5	-3	7	465	15	-15	2	39	58	26*	12	232	9	-2	4	59	9	4				
2	1180	36	-2	8	283	10	-0	3	354	12	3	14	258	10	-1	5	535	17	-6				
3	58	71	23*	9	162	12	1	4	194	13	6		K,L= 1,	1		6	338	12	-4				
4	292	10	17	10	130	9	14	5	209	10	11	0	1181	71	-78	7	277	10	16				
5	191	7	-24	11	325	11	-8	6	67	22	32*	1	73	11	-0	8	134	12	19				
6	770	25	-14	12	172	10	7	7	287	11	-9	2	118	9	4	9	386	12	-16				
7	39	26	-3*	13	96	32	46*	8	124	11	-11	3	166	13	-21	10	207	8	-6				
8	259	10	-7	14	98	22	1*	9	107	16	15	4	1016	31	1	11	109	12	10				
9	147	10	-8		K,L= 0,	0	5	10	68	25	23*	5	66	7	11	12	118	17	6				
10	456	14	-11	1	629	20	27	11	208	11	-9	6	204	7	-20	13	274	10	9				
11	44	46	22*	2	270	9	4		K,L= 0,	9		7	165	9	-10	14	89	49	-26*				
12	229	9	2	3	447	15	19	1	243	10	-6	8	635	21	-5		K,L= 1,	5					
13	106	15	5	4	75	12	5	2	271	9	22	9	42	42	11*	0	271	9	-21				
14	254	10	1	5	569	18	8	3	187	8	1	10	235	11	-4	1	511	16	10				
	K,L= 0,	2		6	195	8	-1	4	66	19	27*	11	127	11	-1	2	33	38	4*				
0	1020	31	87	7	235	9	13	5	249	10	11	12	362	14	7	3	583	18	22				
1	422	14	51	8	52	67	-7*	6	191	9	-7	13	25	57	12*	4	266	9	4				
2	285	13	23	9	409	13	-10	7	95	15	-7	14	183	11	-14	5	322	11	-0				
3	448	14	37	10	102	12	-9	8	93	15	29		K,L= 1,	2		6	44	30	-1*				
4	868	27	37	11	96	14	4	9	184	11	-0	1	432	16	51	7	474	15	-6				
5	171	6	-13	12	51	52	-4*	10	137	13	3	2	715	22	-34	8	181	16	15				
6	263	9	-32	13	287	12	7		K,L= 0,	10		3	271	9	4	9	158	8	7				
7	333	12	3		K,L= 0,	0	6	0	241	12	-4	4	254	8	-11	10	54	55	2*				
8	549	18	-1	0	65	22	-8*	1	126	10	3	5	375	12	12	11	338	11	-8				
9	83	20	-6*	1	474	15	34	2	59	31	30*	6	666	21	9	12	91	19	6*				
10	222	8	-6	2	35	38	16*	3	150	11	-2	7	130	7	-10	13	64	34	18*				
11	224	10	-2	3	542	18	10	4	217	10	-6	8	232	8	-18		K,L= 1,	6					
12	321	11	7	4	73	24	15*	5	98	14	23	9	288	10	11	1	487	16	5				
13	0	52	-31*	5	255	9	-4	6	57	33	-9*	10	406	13	-8	2	52	13	22*				
14	172	12	-5	6	27	44	6*	7	120	13	-15	11	80	19	22*	3	360	12	9				
	K,L= 0,	3		7	466	15	4	8	186	11	16	12	214	9	6	4	45	23	26*				
1	673	26	48	8	72	15	42*	9	62	62	26*	13	171	10	-6	5	498	16	1				
2	817	25	78	9	140	9	10		K,L= 0,	11		14	220	10	-0	6	36	52	7*				
3	474	15	16	10	33	48	19*	1	17	54	-54*		K,L= 1,	3		7	200	13	-1				
4	208	7	40	11	316	11	-13	2	236	10	4	0	855	46	63	8	40	58	21*				
5	508	16	1	12	34	55	21*	3	75	20	29*	1	549	20	27	9	397	13	2				
6	495	16	11	13	80	52	38*	4	41	52	-2*	2	46	25	-9*	10	43	66	27*				
7	223	9	-2		K,L= 0,	0	7	5	100	17	24	3	534	16	2	11	62	29	-21*				
8	213	8	6	1	431	14	-7	6	206	11	16	4	652	20	25	12	26	54	10*				
9	360	11	1	2	114	11	-9	7	10	65	-12*	5	319	10	-5	13	257	11	-5				
10	300	10	-12	3	327	11	16		K,L= 0,	12		6	169	8	-1		K,L= 1,	7					
11	108	19	18	4	29	45	21*	0	209	14	5	7	422	14	-2	0	101	9	-5				
12	175	12	6	5	433	14	-1	1	66	54	50*	8	423	13	4	1	354	11	-7				
13	234	11	2	6	109	19	3	2	74	57	56*	9	142	16	-8	2	25	44	15*				

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.0(CH3)2.

H	F0B	SG	DEL	H	F0B	SG	DEL	H	F0B	SG	DEL	H	F0B	SG	DEL	H	F0B	SG	DEL
3	420	13	-3	4	0	57	-31*	K,L= 2,	4	0	188	8	-12	0	957	32	-78		
4	105	13	2	5	75	28	54*	0	515	27	15	1	287	10	4	1	178	9	3
5	241	10	5	K,L= 2,	0	1	508	16	-18	2	22	58	9*	2	82	14	9		
6	20	56	7*	01239	39	-41	2	17	31	10*	3	306	11	4	3	145	5	7	
7	377	13	-4	2	65	38	32*	3	538	17	17	4	186	9	9	4	878	27	21
8	67	22	-7*	41050	32	21	4	442	14	14	5	202	8	1	5	62	9	-10	
9	132	11	16	6	153	6	15	5	375	13	10	6	77	16	42*	6	199	8	14
10	0	56	-14*	8	645	21	-4	6	55	17	-13*	7	276	10	-0	7	146	8	6
11	281	11	2	10	228	9	-2	7	432	15	-10	8	119	12	-7	8	564	18	5
12	82	22	35*	12	370	13	14	8	296	10	9	9	93	18	-1	9	31	52	5*
K,L= 1,	8	14	167	11	-10	9	163	11	-1	10	0	56	-42*	10	206	11	-5		
1	330	11	-4	K,L= 2,	1	10	80	18	-30*	11	201	11	-8	11	119	15	7		
2	231	10	13	1	151	5	4	11	315	11	-6	K,L= 2,	9	12	316	11	2		
3	279	11	14	2	881	28	-53	12	168	10	9	1	214	8	0	13	71	22	60*
4	18	57	-5*	3	130	8	20	13	74	34	28*	2	232	9	2	14	175	16	-0
5	324	10	3	4	108	6	-11	K,L= 2,	5	3	178	8	0	K,L= 3,	2				
6	172	11	3	5	157	7	-3	1	515	21	11	4	18	44	-18*	1	288	9	-9
7	153	9	5	6	762	24	11	2	234	8	9	5	211	10	-3	2	706	22	4
8	45	54	6*	7	76	13	26	3	416	13	1	6	185	9	-1	3	193	6	-8
9	251	11	-6	8	228	8	2	4	43	33	21*	7	91	20	-16*	4	166	6	-3
10	96	35	-13*	9	157	10	11	5	501	16	7	8	83	21	23*	5	325	11	4
11	28	57	-28*	10	452	14	-9	6	183	8	-6	9	175	15	-2	6	562	19	1
K,L= 1,	5	11	26	47	5*	7	238	9	1	10	105	18	-22	7	114	8	-9		
0	245	10	4	12	220	9	-1	8	68	36	21*	K,L= 2,	10	8	223	9	8		
1	205	9	-6	13	113	16	16	9	398	14	-3	0	207	9	-19	9	248	11	4
2	24	47	3*	14	243	10	4	10	102	15	-10	1	101	16	-9	10	349	11	-14
3	241	9	6	K,L= 2,	2	11	79	19	-11*	12	57	23	33*	11	58	43	6*		
4	216	9	1	0	693	30	-68	12	59	62	4*	3	127	10	-3	12	191	9	6
5	126	11	-15	1	275	12	7	13	254	15	-13	4	213	13	4	13	151	11	-6
6	25	54	-31*	2	89	19	2*	K,L= 2,	6	5	84	15	6	14	195	11	1		
7	196	11	-12	3	345	11	12	0	50	20	5*	6	66	25	7*	K,L= 3,	3		
8	149	11	-10	4	767	24	23	1	387	13	10	7	122	14	-6	0	606	23	0
9	100	24	32*	5	179	6	-9	2	38	27	37*	8	162	19	2	1	375	12	-11
10	85	33	19*	6	186	7	-13	3	464	15	10	9	38	58	1*	2	59	8	-10
K,L= 1,	10	7	314	11	5	4	48	19	-1*	K,L= 2,	11	3	460	15	2				
1	125	11	-12	8	543	17	2	5	249	9	-16	1	71	17	11*	4	539	17	7
2	235	10	-6	9	95	21	1*	6	54	56	48*	2	210	9	-5	5	276	10	7
3	103	11	1	10	215	8	-2	7	438	14	7	3	63	20	18*	6	153	9	1
4	77	18	29*	11	217	9	-1	8	57	24	22*	4	31	49	-6*	7	380	12	5
5	124	16	-20	12	302	11	-0	9	125	14	-9	5	80	31	13*	8	377	12	7
6	201	12	1	13	0	52	-28*	10	14	49	1*	6	186	13	6	9	135	12	1
7	58	34	-0*	14	162	12	-10	11	314	11	-2	7	0	58	-25*	10	149	11	-12
8	71	28	2*	K,L= 2,	3	12	0	55	-14*	K,L= 2,	12	11	256	9	-0				
9	106	25	-12*	1	471	19	-6	K,L= 2,	7	0	205	13	17	12	214	10	-3		
K,L= 1,	11	2	597	18	34	1	368	12	-4	1	67	28	53*	13	46	69	7*		
0	231	9	3	3	402	13	5	2	138	7	11	2	27	56	13*	14	127	14	-0
1	51	55	-4*	4	119	5	21	3	298	10	1	3	50	77	33*	K,L= 3,	4		
2	65	30	43*	5	458	15	1	4	62	15	50*	4	158	13	-13	1	530	17	2
3	26	53	-44*	6	472	15	-1	5	391	13	3	K,L= 3,	0	2	419	13	14		
4	213	9	5	7	234	8	0	6	97	21	1*	2	983	30	-19	3	440	14	5
5	66	30	33*	8	191	8	13	7	181	10	3	4	115	6	-14	4	70	14	10*
6	80	24	25*	9	347	11	2	8	49	38	39*	6	730	23	11	5	461	15	3
7	85	25	17*	10	300	12	-11	9	317	11	-6	8	203	10	-4	6	302	10	-0
K,L= 1,	12	11	77	18	-11*	10	88	17	31*	10	414	13	-17	7	229	9	-0		
1	18	55	-1*	12	167	12	2	11	69	27	0*	12	211	10	5	8	93	30	-8*
2	214	10	13	13	223	11	2	12	57	49	44*	14	218	10	-11	9	354	11	2
3	52	71	35*	14	161	12	-5	K,L= 2,	8	K,L= 3,	1	10	175	9	-14				

STRUCTURE FACTORS CONTINUED FOR
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H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL		
11	81	20	-5*	K,L= 3,	9	13	70	32	-10*	11	64	42	-9*	6	53	56	2*				
12	93	16	-6	0	203	10	-8	14	202	12	4	12	45	58	2*	7	115	16	9		
13	237	13	2	1	176	8	-8	K,L= 4,	2	K,L= 4,	6	8	149	13	17	8	149	13	17		
	K,L= 3,	5		2	58	19	40*	0	748	23	-8	0	18	44	-40*	K,L= 4,	11				
0	267	9	-4	3	200	8	-6	1	200	6	-16	1	303	10	-16	1	58	24	2*		
1	442	14	1	4	189	8	0	2	90	5	-12	2	41	32	31*	2	190	9	8		
2	46	14	36*	5	124	11	-2	3	292	9	-8	3	400	13	-5	3	59	65	23*		
3	492	16	12	6	25	57	-25*	4	620	19	5	4	32	41	-12*	4	0	56	-34*		
4	235	8	8	7	176	12	-8	5	135	10	4	5	196	10	-1	5	76	32	17*		
5	277	9	-8	8	131	12	-11	6	204	8	7	6	67	29	52*	6	153	17	4		
6	19	45	-15*	9	66	32	6*	7	250	9	-4	7	350	11	-8	K,L= 4,	12				
7	409	13	-10	10	34	61	-25*	8	414	13	-0	8	42	57	19*	0	151	17	-9		
8	132	14	-13	K,L= 3,	10	9	59	64	-11*	9	112	12	11	1	22	60	9*				
9	133	10	-1	1	103	12	-18	10	180	8	3	10	0	56	-11*	2	33	57	19*		
10	69	19	23*	2	203	10	-9	11	177	9	1	11	252	10	-6	3	22	65	5*		
11	311	11	5	3	89	14	-1	12	256	10	11	12	37	56	27*	K,L= 5,	0				
12	61	67	-15*	4	61	30	19*	13	61	36	37*	K,L= 4,	7	2	712	22	-23				
13	55	56	15*	5	125	11	-3	K,L= 4,	3	1	320	10	-13	4	94	8	-11				
	K,L= 3,	6		6	187	14	10	1	389	12	-20	2	113	14	14	6	536	17	-2		
1	401	13	-9	7	0	61	-52*	2	497	16	-1	3	246	9	8	8	149	12	-13		
2	43	21	15*	8	60	41	-1*	3	299	9	10	4	41	56	39*	10	337	11	5		
3	291	9	-8	K,L= 3,	11	4	137	7	-6	5	338	11	4	12	169	10	9				
4	39	36	25*	0	190	10	-11	5	395	13	2	6	90	13	10	K,L= 5,	1				
5	438	14	2	1	72	17	24*	6	378	12	5	7	128	10	-4	0	735	23	-10		
6	26	63	0*	2	54	43	34*	7	180	8	10	8	0	62	-7*	1	133	5	17		
7	172	12	-7	3	53	31	-8*	8	157	19	-2	9	250	10	-12	2	78	7	16		
8	21	46	6*	4	185	11	1	9	275	9	-3	10	63	67	14*	3	116	6	8		
9	352	12	2	5	0	57	-29*	10	232	9	-11	11	75	25	20*	4	628	20	-2		
10	39	63	24*	6	62	40	13*	11	78	18	7*	K,L= 4,	8	5	61	11	8				
11	77	35	3*	7	23	59	-37*	12	145	12	13	0	157	15	-4	6	152	7	7		
12	48	56	34*	K,L= 3,	12	13	171	11	-11	13	171	11	-11	1	246	9	2	7	105	10	-3
	K,L= 3,	7		1	59	57	42*	K,L= 4,	4	2	16	53	6*	8	426	14	2				
0	102	14	2	2	160	12	-13	0	399	12	-35	3	263	9	-6	9	31	49	11*		
1	302	10	-12	3	20	79	9*	1	458	14	6	4	149	8	4	10	165	13	3		
2	22	46	17*	4	30	59	3*	2	58	15	15*	5	158	8	4	11	70	20	-17*		
3	373	12	6	K,L= 4,	0	3	465	15	8	6	60	60	32*	12	239	10	-5				
4	94	19	3*	0	952	25	-73	4	371	12	20	7	231	10	1	13	24	62	15*		
5	212	10	4	2	111	7	8	5	278	9	5	8	72	25	-34*	K,L= 5,	2				
6	0	50	-10*	4	836	26	15	6	54	26	-31*	9	0	73	-72*	1	208	7	-15		
7	340	11	5	6	186	7	8	7	357	12	-4	10	32	57	-3*	2	542	17	15		
8	49	42	-15*	8	504	16	1	8	233	11	12	K,L= 4,	9	3	141	9	-12				
9	90	20	-13*	10	178	10	-10	9	112	14	-12	1	181	8	-11	4	123	7	-9		
10	32	58	20*	12	283	10	-5	10	96	13	6	2	181	8	-10	5	238	8	-2		
11	245	11	-2	14	139	17	-21	11	258	13	-1	3	131	9	-12	6	413	13	-11		
12	0	58	-37*	K,L= 4,	1	12	124	13	-4	4	64	18	32*	7	107	10	14				
	K,L= 3,	8		1	166	6	7	13	34	56	-5*	5	182	9	-2	8	167	14	1		
1	293	10	0	2	835	26	-1	K,L= 4,	5	6	138	23	-16	9	184	9	-3				
2	198	11	8	3	124	6	6	1	435	14	-15	7	99	16	19	10	270	12	-9		
3	236	9	2	4	156	6	-15	2	231	8	16	8	65	39	15*	11	42	49	2*		
4	21	42	0*	5	138	6	14	3	333	11	2	9	132	21	-12	12	143	13	-1		
5	270	9	-10	6	588	19	5	4	0	40	-37*	K,L= 4,	10	13	141	18	18				
6	146	9	-3	7	55	17	22*	5	417	13	-3	0	184	11	-6	K,L= 5,	3				
7	135	11	3	8	215	8	14	6	149	11	3	1	77	16	-18*	0	414	13	-40		
8	0	57	-35*	9	115	10	-1	7	155	14	-19	2	0	46	-22*	1	277	9	-14		
9	220	11	-7	10	342	11	-19	8	51	52	7*	3	118	14	0	2	60	10	5		
10	92	19	-4*	11	52	82	36*	9	328	11	3	4	186	9	12	3	344	11	2		
11	74	76	23*	12	180	20	3	10	89	15	4	5	33	55	-26*	4	397	13	-3		

STRUCTURE FACTORS CONTINUED FOR
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H	FOB	SG	DEL	H	FCB	SG	DEL	H	FCB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
5	212	8	12	8	31	65	-19*	8	133	14	-0	9	237	11	-5	2	134	15	2
6	93	11	-25	9	81	23	1*	9	104	14	18	10	79	31	11*	3	58	47	30*
7	286	11	0	10	21	62	12*	10	277	24	1	11	42	59	-13*	K,L= 7, 0			
8	282	11	-2	11	193	11	-1	11	59	27	46*	K,L= 6, 6				2	454	15	-23
9	113	10	11	K,L= 5, 8				12	106	16	-28	0	44	58	17*	4	56	18	2*
10	99	13	-28	1	220	8	-7	13	48	56	-11*	1	196	11	-25	6	367	12	7
11	196	9	-3	2	144	8	-2	K,L= 6, 2				2	35	47	34*	8	110	13	3
12	181	10	12	3	190	8	9	0	435	14	-1	3	268	9	1	10	245	9	15
13	68	29	38*	4	45	31	29*	1	133	6	-18	4	0	41	-28*	12	114	18	3
K,L= 5, 4				5	221	8	2	2	47	17	2*	5	161	8	5	K,L= 7, 1			
1	392	13	-1	6	114	14	-2	3	183	7	-4	6	30	48	26*	0	443	14	-18
2	303	11	-3	7	118	15	17	4	409	13	-7	7	252	10	-7	1	65	11	7
3	327	11	8	8	0	52	-27*	5	116	10	10	8	58	27	37*	2	49	17	13*
4	54	21	3*	9	157	12	-10	6	130	8	17	9	83	26	2*	3	81	10	8
5	342	11	-8	10	69	32	-7*	7	186	8	7	10	40	54	31*	4	408	13	-2
6	243	9	13	K,L= 5, 9				8	312	10	-4	11	194	12	1	5	45	34	11*
7	153	10	-20	0	156	9	-7	9	69	25	13*	K,L= 6, 7				6	108	22	14*
8	28	49	-51*	1	141	12	-3	10	148	9	18	1	219	8	-2	7	74	23	-1*
9	273	11	1	2	13	44	-2*	11	143	10	12	2	78	12	3	8	293	11	3
10	147	12	:	3	160	8	-1	12	178	11	-6	3	180	9	5	9	38	47	23*
11	55	58	-13*	4	144	9	-3	13	0	67	-17*	4	41	48	35*	10	118	12	6
12	98	19	21*	5	90	13	-6	K,L= 6, 3				5	238	9	6	11	62	27	2*
K,L= 5, 5				6	56	33	17*	1	253	9	-8	6	72	19	15*	12	164	12	-5
0	203	8	-1	7	132	13	-12	2	313	11	-7	7	100	24	-7*	K,L= 7, 2			
1	326	10	-7	8	100	15	-11	3	211	8	-4	8	34	50	28*	1	144	7	-2
2	37	31	27*	9	17	61	-29*	4	68	15	8*	9	205	12	9	2	336	11	4
3	357	11	-11	K,L= 5, 10				5	259	9	-2	10	27	57	-8*	3	113	8	6
4	165	8	-7	1	82	14	-13	6	280	11	5	K,L= 6, 8				4	94	9	10
5	212	8	-3	2	165	10	-0	7	133	10	-1	0	110	18	-8	5	157	9	0
6	41	55	12*	3	62	21	-8*	8	111	10	6	1	180	8	11	6	291	12	3
7	313	11	-10	4	52	32	19*	9	211	9	5	2	37	45	29*	7	39	52	-25*
8	109	16	-1	5	69	28	-31*	10	191	16	4	3	180	8	-1	8	136	13	26
9	112	17	9	6	138	13	-1	11	17	52	-36*	4	98	13	-8	9	135	18	7
10	23	50	-13*	7	75	26	35*	12	102	27	2*	5	135	13	15	10	209	10	15
11	252	12	13	K,L= 5, 11				K,L= 6, 4				6	35	58	14*	11	0	54	-28*
12	65	77	6*	0	164	16	6	0	252	9	-19	7	157	14	-11	12	90	21	-11*
K,L= 5, 8				1	66	39	28*	1	298	10	7	8	110	19	33	K,L= 7, 3			
1	293	10	-23	2	42	59	26*	2	30	37	22*	9	82	23	24*	0	284	11	-13
2	48	20	25*	3	38	56	-11*	3	298	10	2	K,L= 6, 9				1	184	8	-13
3	210	9	-15	4	141	13	-4	4	251	8	10	1	136	9	7	2	32	42	4*
4	35	62	24*	5	15	59	-7*	5	200	9	-7	2	140	10	1	3	216	8	-3
5	336	11	-0	K,L= 6, 0				6	22	66	-21*	3	101	14	-6	4	266	9	1
6	36	46	17*	0	578	19	-53	7	271	9	10	4	45	55	23*	5	132	11	-6
7	127	10	-5	2	42	15	25*	8	172	10	2	5	122	12	-8	6	48	54	-26*
8	55	27	43*	4	545	17	-7	9	81	16	-16*	6	118	14	4	7	197	9	6
9	263	10	-8	6	91	11	2	10	37	50	-30*	7	76	31	11*	8	199	9	5
10	51	46	40*	8	396	14	16	11	192	10	-2	8	48	58	11*	9	83	20	13*
11	84	32	27*	10	147	10	9	12	122	14	24	K,L= 6, 10				10	88	16	2
K,L= 5, 7				12	214	10	-2	K,L= 6, 5				0	132	12	-5	11	126	22	-12
0	84	37	8*	K,L= 6, 1				1	272	11	-17	1	66	20	-1*	12	126	14	8
1	241	10	-2	1	92	7	7	2	147	7	16	2	40	56	25*	K,L= 7, 4			
2	36	63	33*	2	512	16	-5	3	233	9	-4	3	67	28	-13*	1	243	8	-8
3	288	12	2	3	71	15	6*	4	42	56	29*	4	127	14	-0	2	203	8	1
4	58	23	-11*	4	68	10	-5	5	285	10	-5	5	81	22	33*	3	201	8	-6
5	160	8	0	5	161	11	10	6	107	17	-3	6	0	70	-36*	4	28	49	1*
6	0	48	-7*	6	425	13	-2	7	139	9	-1	K,L= 6, 11				5	243	8	8
7	261	11	1	7	0	57	-30*	8	63	24	34*	1	45	56	8*	6	154	11	-3

STRUCTURE FACTORS CONTINUED FOR

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H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
7	116	11	-3	7	106	18	6	5	111	9	-11	2	279	9	-3	6	0	50	-12*
8	39	48	-13*		K,L= 7,	10		6	0	55	-37*	4	36	44	-3*	7	153	11	18
9	191	9	3	1	72	26	7*	7	180	15	11	6	204	9	-10	8	64	73	18*
10	106	14	4	2	120	14	6	8	101	19	-3*	8	46	50	-20*	9	0	66	-44*
11	38	55	-10*	3	64	32	15*	9	63	34	4*	10	126	18	-13		K,L= 9,	6	
	K,L= 7,	5		4	0	57	-23*	10	71	28	28*		K,L= 9,	1		1	135	10	6
0	118	17	-8	5	84	23	15*		K,L= 8,	5		0	269	9	-6	2	32	46	22*
1	202	13	-15		K,L= 8,	0		1	189	8	-7	1	49	23	14*	3	103	11	8
2	40	52	32*	0	409	13	-15	2	92	13	1	2	49	20	24*	4	44	52	39*
3	232	9	-11	2	24	39	-5*	3	147	8	0	3	20	48	-25*	5	140	9	2
4	99	10	-14	4	347	11	-3	4	39	46	21*	4	248	9	5	6	0	53	-8*
5	140	9	-7	6	65	20	-10*	5	198	8	5	5	18	41	-2*	7	82	21	26*
6	0	53	-18*	8	235	9	4	6	45	49	-23*	6	56	26	-4*	8	49	73	44*
7	225	11	4	10	83	18	-6*	7	84	17	2*	7	44	49	-1*		K,L= 9,	7	
8	72	20	-5*		K,L= 8,	1		8	59	34	38*	8	172	16	-1	0	39	50	8*
9	97	15	25	1	49	20	-8*	9	171	12	16	9	0	53	-9*	1	93	13	-7
10	0	67	-25*	2	349	11	5	10	0	78	-41*	10	88	23	20*	2	0	52	-1*
11	173	11	7	3	42	43	6*		K,L= 8,	6			K,L= 9,	2		3	124	16	5
	K,L= 7,	6		4	70	26	-2*	0	33	46	9*	1	76	18	-12*	4	31	52	2*
1	212	8	1	5	64	20	2*	1	149	10	0	2	212	8	9	5	9	65	-58*
2	52	26	38*	6	264	9	1	2	46	46	41*	3	67	15	3*	6	35	55	32*
3	145	9	-13	7	32	46	15*	3	191	10	8	4	54	31	1*	7	135	20	25
4	35	43	29*	8	109	12	17	4	43	50	23*	5	92	14	-2		K,L= 9,	8	
5	232	8	5	9	69	20	14*	5	103	11	10	6	180	9	9	1	97	18	3
6	27	48	13*	10	181	11	19	6	49	67	42*	7	61	26	23*	2	53	62	-8*
7	83	18	-12*	11	40	68	32*	7	167	13	-1	8	87	16	19	3	69	28	-6*
8	46	50	38*		K,L= 8,	2		8	31	56	20*	9	85	21	7*	4	65	46	58*
9	203	14	15	0	292	10	-6	9	42	56	-7*	10	121	15	3	5	80	31	-13*
10	43	56	34*	1	107	9	5		K,L= 8,	7			K,L= 9,	3			K,L= 9,	9	
	K,L= 7,	7		2	53	61	7*	1	162	8	10	0	182	8	2	0	75	42	6*
0	65	20	14*	3	123	11	-3	2	43	54	-2*	1	119	9	2	1	65	33	4*
1	166	8	2	4	271	9	4	3	114	10	3	2	14	40	-5*	2	0	56	-6*
2	29	45	26*	5	55	21	-7*	4	0	56	-1*	3	132	8	-1	3	90	21	22*
3	189	11	-3	6	121	10	32	5	156	10	0	4	154	9	-5		K,L= 10,	0	
4	55	33	7*	7	115	11	1	6	38	52	-0*	5	99	12	18	0	200	9	-15
5	123	9	12	8	198	12	5	7	65	45	2*	6	32	51	-15*	2	24	41	16*
6	0	50	-6*	9	53	55	20*	8	68	29	65*	7	126	13	11	4	185	9	-7
7	195	9	16	10	82	34	-3*		K,L= 8,	8		8	118	13	2	6	19	49	-15*
8	59	34	25*	11	93	23	9*	0	70	21	-6*	9	41	54	-1*	8	145	12	7
9	61	66	5*		K,L= 8,	3		1	122	10	9	10	79	23	26*		K,L= 10,	1	
	K,L= 7,	8		1	176	12	-1	2	50	54	45*		K,L= 9,	4		1	57	18	27*
1	154	9	1	2	232	9	11	3	128	10	2	1	148	9	-4	2	172	9	-7
2	73	27	-27*	3	138	16	5	4	83	15	14	2	129	9	7	3	53	21	31*
3	130	9	7	4	39	40	-16*	5	59	62	-14*	3	112	10	-10	4	16	45	-11*
4	33	52	22*	5	174	7	3	6	34	56	21*	4	42	56	22*	5	38	44	4*
5	151	11	1	6	169	11	-2	7	125	14	14	5	135	11	-8	6	159	10	6
6	103	19	23*	7	102	12	23		K,L= 8,	9		6	71	33	-23*	7	0	57	-11*
7	70	27	-1*	8	79	17	6*	1	111	14	21	7	61	26	-9*	8	5	54	-44*
8	26	62	7*	9	138	12	8	2	104	16	14	8	61	30	29*	9	22	58	-11*
	K,L= 7,	5		10	113	16	-3	3	66	35	-3*	9	115	15	0		K,L= 10,	2	
0	112	13	1	11	8	64	-26*	4	13	61	-3*		K,L= 9,	5		0	159	9	6
1	90	15	-5		K,L= 8,	4		5	109	17	21	0	48	42	-30*	1	69	17	14*
2	27	46	17*	0	187	11	-2		K,L= 8,	10		1	125	9	-6	2	0	44	-16*
3	104	17	-6	1	179	8	-7	0	102	38	11*	2	20	53	14*	3	71	20	5*
4	125	13	24	2	45	24	31*	1	99	18	53	3	158	8	9	4	144	9	-3
5	80	29	12*	3	201	8	-1	2	78	47	67*	4	65	20	-4*	5	61	19	22*
6	0	57	-27*	4	161	8	5		K,L= 9,	0		5	88	14	1	6	50	54	9*

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 8.0)
L(BH4)4.0(C2H5)2. F(0,0,0) = 2390

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

K	FOB	SG	DEL	K	FCB	SG	DEL	K	FCB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
	H,L=	0,		12	364	5	2	-19	118	9	-11	-5	54	28	26*	12	220	6	4
-20	187	8	-9	13	371	6	4	-18	138	12	-11	-4	700	13	4	13	181	8	-5
-18	244	6	-10	14	315	5	6	-17	182	6	1	-3	24	44	-9*	14	190	7	7
-16	315	5	4	15	249	4	-1	-16	184	6	-2	-2	726	14	-11	15	150	9	-6
-14	456	6	-1	16	229	5	-4	-15	210	6	-6	-1	47	21	18*	16	153	13	2
-12	563	10	-1	17	187	7	-1	-14	251	5	2	0	706	11	-10	H,L=	0,		6
-10	588	10	20	18	176	7	3	-13	257	4	-4	1	59	15	29*	-13	226	11	4
-8	826	14	9	19	160	7	2	-12	295	6	-5	2	738	13	0	-12	47	67	21*
-6	1020	14	14	20	137	7	5	-11	359	5	-9	3	46	31	14*	-11	269	7	-6
-4	1169	15	16	21	109	14	-7	-10	339	5	-2	4	701	13	8	-10	44	54	26*
	41172	15	8	H,L=	0,	2		-9	404	6	-1	5	44	52	15*	-9	326	7	1
	61014	13	13	-20	18	49	12*	-8	429	7	1	6	599	22	10	-8	66	25	52*
	8	822	12	-19	203	10	4	-7	464	8	-3	7	43	74	28*	-7	354	6	-7
	10	588	10	-18	19	41	12*	-6	468	9	-4	8	514	19	-0	-6	49	32	28*
	12	569	8	-17	262	5	-2	-5	531	9	10	9	40	45	7*	-5	393	6	-10
	14	457	6	-16	0	38	-22*	-4	557	10	6	10	452	6	-3	-4	63	24	56*
	16	314	10	-15	342	5	2	-3	630	11	-0	11	24	54	-4*	-3	439	6	-9
	18	265	6	-14	40	21	15*	-2	595	10	16	12	378	6	3	-2	59	25	34*
	20	200	7	-13	446	6	-1	-1	562	10	5	13	0	46	-17*	-1	434	7	-13
	H,L=	0,	1	-12	22	48	11*	0	644	10	-0	14	286	6	-2	0	51	14	25*
-21	132	8	15	-11	522	8	-1	1	577	9	16	15	0	43	-13*	1	438	7	-10
-20	137	7	6	-10	62	10	19	2	605	10	24	16	240	6	-4	2	43	33	21*
-19	162	9	3	-9	692	11	4	3	634	11	0	17	0	66	-10*	3	442	6	-5
-18	178	6	0	-8	13	29	9*	4	558	9	6	18	182	8	-6	4	35	44	25*
-17	188	6	1	-7	777	13	4	5	534	9	12	H,L=	0,	5	5	398	7	-4	
-16	240	5	8	-6	36	15	4*	6	473	8	-1	-16	156	15	4	6	56	24	35*
-15	249	4	-3	-5	930	14	-5	7	474	7	4	-15	160	8	6	7	357	7	-2
-14	312	5	5	-4	99	4	-1	8	433	7	-1	-14	182	8	1	8	69	22	58*
-13	369	6	1	-3	1026	14	-8	9	409	7	2	-13	190	7	5	9	333	7	9
-12	361	6	2	-2	97	5	-5	10	337	6	-3	-12	216	6	1	10	75	22	56*
-11	368	6	6	-1	1084	14	16	11	369	5	0	-11	231	8	-4	11	266	9	-8
-10	455	7	1	0	182	7	9	12	302	5	1	-10	268	7	-8	12	82	23	55*
-9	465	7	6	1	1100	28	22	13	260	4	1	-9	253	6	-10	13	229	9	7
-8	538	8	16	2	94	12	-8	14	256	5	7	-8	292	8	-7	H,L=	0,		7
-7	652	9	19	3	1030	26	-9	15	210	7	-8	-7	289	6	3	-9	176	9	-2
-6	601	8	2	4	95	4	-3	16	183	7	-4	-6	336	6	5	-8	179	8	2
-5	754	10	-2	5	931	14	-2	17	182	6	1	-5	328	6	-7	-7	199	9	-10
-4	707	9	4	6	54	7	22	18	150	8	1	-4	379	7	-4	-6	194	8	-1
-3	554	8	24	7	781	12	6	19	122	13	-6	-3	367	7	-18	-5	228	6	6
-2	900	15	-9	8	0	35	-3*	H,L=	0,	4	-2	408	7	-7	-4	210	10	0	
-1	994	31	-1	9	691	10	5	-18	180	7	-9	-1	366	5	-9	-3	224	6	-2
0	855	12	-16	10	44	13	2*	-17	0	64	-10*	0	374	5	-1	-2	217	6	-2
1	976	37	-3	11	520	7	3	-16	236	6	-8	1	376	5	-2	-1	241	6	-3
2	906	21	-8	12	29	41	20*	-15	0	51	-14*	2	412	6	-3	0	214	5	-3
3	589	8	25	13	450	6	5	-14	280	6	-8	3	388	6	1	1	237	6	-5
4	703	11	5	14	21	36	-6*	-13	50	26	34*	4	385	8	4	2	222	11	2
5	764	10	1	15	340	5	2	-12	372	6	-6	5	335	9	2	3	230	6	4
6	602	8	6	16	30	38	8*	-11	54	32	25*	6	337	7	6	4	200	6	-13
7	654	9	20	17	259	5	-4	-10	447	7	-9	7	295	7	6	5	221	7	-3
8	547	8	16	18	33	41	27*	-9	44	24	10*	8	294	9	-6	6	192	10	-4
9	461	7	6	19	203	6	4	-8	505	8	-9	9	263	6	-4	7	211	7	3
10	456	7	3	20	0	56	-7*	-7	37	68	21*	10	275	6	-1	8	179	10	1
11	373	5	7	H,L=	0,	3		-6	591	9	1	11	232	6	-3	9	158	10	-20

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
	H,L=	1,	-7	-12	205	20	3	9	518	15	0	-14	401	6	-3	0	915	12	-32
-10	161	16	-24	-11	272	7	-9	10	57	47	-12*	-13	0	66	-4*	1	984	48	-8
-9	172	25	8	-10	240	8	-2	11	439	7	3	-12	497	7	0	2	602	24	12
-8	215	11	-2	-9	313	6	-16	12	41	30	5*	-11	83	9	4	3	677	18	5
-7	165	12	-3	-8	257	7	-2	13	331	5	3	-10	576	9	0	4	565	10	5
-6	236	9	-4	-7	343	6	-10	14	0	42	-27*	-9	88	7	-7	5	804	15	-6
-5	204	12	12	-6	291	9	-9	15	275	5	4	-8	717	11	-1	6	622	8	5
-4	256	8	-3	-5	400	10	-2	16	50	54	14*	-7	34	20	15*	7	673	9	12
-3	210	8	-6	-4	343	10	3	17	216	6	-1	-6	876	12	-24	8	549	8	11
-2	281	9	-0	-3	468	7	9	18	23	61	-2*	-5	116	5	3	9	522	8	8
-1	202	8	-0	-2	356	6	8		H,L=	1,	-3	-4	923	13	-16	10	357	5	14
0	292	5	4	-1	439	7	0	-19	117	19	1	-3	267	6	-2	11	437	6	8
1	200	6	-3	0	358	5	7	-18	178	8	10	-21	604	13	-38	12	370	5	-2
2	280	6	3	1	444	6	2	-17	150	9	3	-1	132	14	12	13	391	6	6
3	216	6	-1	2	354	6	6	-16	227	8	-5	0	1150	20	-28	14	290	5	2
4	259	6	-1	3	469	7	3	-15	188	7	-4	1	133	10	12	15	272	5	0
5	210	6	19	4	348	6	9	-14	262	8	-1	21	023	52	-4	16	190	5	-2
6	254	6	11	5	410	7	-0	-13	261	5	-6	3	278	4	9	17	222	5	2
7	172	8	2	6	298	5	-1	-12	317	5	-11	4	945	24	4	18	156	6	-1
8	200	8	-17	7	355	6	1	-11	292	5	-2	5	118	6	10	19	166	6	-3
9	163	9	-3	8	262	6	1	-10	436	6	2	6	891	13	-14	20	109	9	-11
10	200	8	13	9	332	6	2	-9	377	6	-8	7	339	12	10*	21	134	12	12
	H,L=	1,	-6	10	250	6	6	-8	457	9	-10	8	726	11	10		H,L=	1,	0
-14	203	11	-4	11	275	6	-7	-7	441	7	-6	9	100	6	4	-21	159	12	-1
-13	0	61	-32*	12	198	10	-5	-6	484	10	-16	10	580	8	7	-20	61	26	40*
-12	251	13	-4	13	218	7	5	-5	500	7	-4	11	76	11	-1	-19	219	11	7
-11	74	30	43*	14	147	10	-11	-4	677	12	-14	12	502	7	2	-18	0	52	-26*
-10	318	8	-8	15	180	9	-4	-3	461	7	1	13	40	18	32*	-17	264	6	-9
-9	47	67	4*	16	152	8	20	-2	660	12	-9	14	405	6	4	-16	0	75	-27*
-8	340	10	-11		H,L=	1,	-4	-1	522	10	10	15	45	19	-7*	-15	355	5	-2
-7	84	26	29*	-18	26	55	1*	0	642	12	21	16	299	5	4	-14	26	77	-34*
-6	385	7	-4	-17	201	15	-17	1	514	9	8	17	40	41	1*	-13	511	7	1
-5	71	41	20*	-16	64	25	26*	2	680	12	6	18	243	5	11	-12	0	78	-54*
-4	454	7	-4	-15	264	6	-7	3	478	9	14	19	10	43	-9*	-11	564	10	6
-3	43	53	-16*	-14	36	48	9*	4	700	12	9	20	182	8	7	-10	0	94	-42*
-2	483	7	-0	-13	318	6	-12	5	515	10	12		H,L=	1,	-1	-9	742	13	10
-1	74	20	11*	-12	26	46	-13*	6	499	8	-3	-21	120	13	-2	-8	0	119	-97*
0	459	6	-5	-11	423	6	-16	7	449	7	-1	-20	133	17	14	-7	979	15	10
1	97	9	33	-10	64	18	-4*	8	477	7	6	-19	171	8	2	-6	175	40	-18*
2	488	7	3	-9	504	7	-15	9	381	6	-2	-18	165	7	7	-5	1023	14	-2
3	93	10	34	-8	0	89	-43*	10	442	10	5	-17	216	6	-2	-4	265	8	16
4	457	7	1	-7	560	9	-14	11	293	5	-2	-16	184	6	-5	-3	1098	14	9
5	73	16	20*	-6	77	34	6*	12	324	5	-3	-15	273	6	-2	-2	137	7	9
6	387	6	-0	-5	656	13	-13	13	271	4	3	-14	292	5	4	0	297	4	31
7	42	49	-14*	-4	68	21	-18*	14	271	6	6	-13	384	6	-1	2	126	8	7
8	343	6	-7	-3	726	15	-6	15	193	6	1	-12	360	8	-7	3	1107	18	12
9	23	65	-20*	-2	143	19	25	16	231	5	-1	-11	431	7	7	4	274	7	15
10	320	12	3	-1	705	16	1	17	140	7	-8	-10	350	7	11	5	1005	13	-7
11	75	20	43*	0	80	8	24	18	167	9	-2	-9	517	8	4	6	205	4	9
12	255	7	1	1	710	13	7	19	109	11	-8	-8	546	9	5	7	980	13	8
13	48	51	16*	2	127	7	6		H,L=	1,	-2	-7	668	10	5	8	75	17	-16*
14	201	8	-6	3	738	12	5	-20	179	9	4	-6	616	9	-3	9	739	10	16
	H,L=	1,	-5	4	79	12	-10	-19	0	50	-18*	-5	784	10	-8	10	13	54	-26*
-16	115	16	-16	5	674	12	6	-18	240	10	9	-4	568	7	-3	11	566	8	6
-15	175	10	-8	6	74	20	1*	-17	45	46	5*	-3	666	9	-6	12	37	53	-19*
-14	152	11	-5	7	578	17	4	-16	287	6	-10	-2	591	8	-11	13	516	7	8
-13	201	8	-13	8	26	64	-17*	-15	55	37	3*	-1	957	13	-46	14	0	57	-56*

STRUCTURE FACTORS CONTINUED FCF
U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
15	355	5	-2	-15	46	33	11*	1	626	11	13	-14	182	16	7	-7	174	11	-16
16	12	45	-12*	-14	366	6	-5	2	519	9	12	-13	178	11	3	-6	174	11	-6
17	277	5	5	-13	57	58	1*	3	566	12	13	-12	203	13	-11	-5	182	10	-21
18	33	40	5*	-12	486	7	2	4	494	10	-3	-11	212	9	3	-4	179	24	-12
19	212	6	1	-11	44	57	40*	5	528	9	-2	-10	274	7	4	-3	207	8	-2
20	0	44	-21*	-10	599	12	6	6	412	7	-0	-9	249	9	10	-2	197	8	-1
21	162	7	2	-9	59	13	-5*	7	451	7	-2	-8	294	7	-8	-1	220	8	-4
	H,L=	1,	1	-8	696	15	-0	8	372	6	1	-7	292	9	9	0	199	5	1
-21	113	13	16	-7	77	8	5	9	398	5	-2	-6	318	11	-6	1	220	6	-3
-20	128	12	-13	-6	821	17	-9	10	348	5	-3	-5	296	11	-4	2	193	7	-4
-19	110	14	-18	-5	66	9	6	11	344	7	1	-4	354	7	-8	3	219	6	11
-18	181	7	2	-4	992	18	7	12	264	4	-2	-3	302	9	-16	4	189	7	-3
-17	177	7	1	-3	112	5	6	13	292	7	-2	-2	345	6	-16	5	192	7	-12
-16	228	6	-1	-2	984	18	13	14	212	6	0	-1	319	6	-18	6	188	13	7
-15	222	5	-4	-1	174	5	5	15	216	5	-4	0	337	5	-8	7	181	8	-9
-14	325	5	4	0	991	14	39	16	170	6	-8	1	333	6	-1	H,L=	2,	-8	
-13	296	5	-0	1	172	5	3	17	185	6	3	2	359	6	-8	-2	284	8	4
-12	403	6	6	21	000	14	23	18	115	10	-14	3	312	6	-3	-1	99	18	27*
-11	376	8	-2	3	103	5	-2	19	134	10	3	4	360	6	-1	0	278	6	-3
-10	439	8	6	4	889	13	-1	F,L=	1,	4	5	297	7	-5	1	94	18	23*	
-9	498	10	14	5	58	16	-0*	-17	210	9	11	6	324	6	1	2	286	7	6
-8	653	12	1	6	814	12	-9	-16	71	74	57*	7	287	6	6	H,L=	2,	-7	
-7	513	10	-5	7	73	7	-2	-15	251	7	-8	8	311	6	4	-10	135	41	-6*
-6	645	11	13	8	700	11	2	-14	42	52	18*	9	234	7	-4	-9	229	11	0
-5	602	9	12	9	65	8	5	-13	306	6	-1	10	278	6	8	-8	148	16	0
-4	764	11	3	10	595	9	5	-12	60	61	14*	11	203	7	-8	-7	256	11	2
-3	635	8	-13	11	51	21	42*	-11	400	6	-1	12	215	7	3	-6	150	38	-11*
-2	680	9	4	12	480	7	-1	-10	75	39	41*	13	180	7	3	-5	282	10	6
-1	595	8	18	13	66	13	9*	-9	477	10	6	14	176	13	-1	-4	207	9	19
0	884	11	24	14	371	5	1	-8	27	75	-12*	15	149	9	9	-3	299	10	3
1	628	9	27	15	54	18	25*	-7	509	7	-6	H,L=	1,	6	-2	186	10	-4	
2	695	10	9	16	289	5	2	-6	63	76	32*	-12	242	10	8	-1	306	7	7
3	637	8	-9	17	0	40	-22*	-5	612	9	17	-11	0	68	-28*	0	195	6	14
4	764	10	3	18	230	8	9	-4	100	22	40*	-10	272	9	-3	1	306	7	5
5	594	8	13	19	0	48	-19*	-3	668	17	4	-9	72	38	48*	2	192	12	2
6	653	9	16	20	161	7	-0	-2	72	21	33*	-8	310	15	-15	3	312	7	15
7	516	7	-7	H,L=	1,	3	-1	622	15	-24	-7	21	58	-0*	4	197	9	9	
8	654	9	1	-19	134	19	0	0	78	11	17	-6	359	11	-11	5	280	8	5
9	505	7	16	-18	133	12	3	1	643	11	-6	-5	63	47	25*	6	154	13	-6
10	434	6	4	-17	174	9	-7	2	71	19	28*	-4	358	7	-19	7	279	8	24
11	374	6	0	-16	182	8	5	3	668	12	6	-3	42	68	10*	8	138	16	-11
12	404	5	2	-15	210	10	-6	4	81	18	20*	-2	383	7	-15	9	219	12	-11
13	298	4	1	-14	203	7	-4	5	600	9	15	-1	44	50	17*	10	118	21	-24
14	318	5	-1	-13	299	6	5	6	0	72	-50*	0	396	6	-12	H,L=	2,	-6	
15	232	5	1	-12	271	5	3	7	508	22	-5	1	57	18	28*	-14	18	61	-31*
16	231	4	1	-11	339	6	-3	8	0	42	-41*	2	388	7	-8	-13	227	19	-3
17	174	5	-2	-10	341	6	-9	9	465	7	-7	3	66	17	34*	-12	111	42	54*
18	186	5	6	-9	399	6	3	10	74	16	41*	4	368	6	-10	-11	286	8	-11
19	129	7	2	-8	370	7	1	11	395	7	-2	5	73	16	38*	-10	85	37	14*
20	146	7	4	-7	454	11	2	12	27	46	-17*	6	369	6	-1	-9	341	7	-7
21	84	21	-14*	-6	423	10	6	13	306	5	-2	7	0	53	-22*	-8	98	19	13*
	H,L=	1,	2	-5	541	12	6	14	0	47	-23*	8	322	7	0	-7	377	10	-4
-20	158	16	-3	-4	508	13	6	15	264	5	4	9	0	53	-24*	-6	126	20	33
-19	14	51	-5*	-3	564	15	10	16	22	50	7*	10	271	8	-4	-5	436	8	4
-18	223	7	-1	-2	516	13	11	17	193	7	-4	11	37	55	10*	-4	102	17	5
-17	0	47	-22*	-1	630	15	18	F,L=	1,	5	12	238	8	3	-3	471	7	7	
-16	284	6	-0	0	479	8	-8	-15	144	33	4*	H,L=	1,	7	-2	141	26	40	

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.O(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-1	458	9	-1	-12	368	8	-8	6	417	7	-2	-21	78	32	-10*	-8	799	14	8
0	118	8	14	-11	92	12	-6	7	533	9	-7	-20	142	13	-3	-7	214	4	8
1	461	7	2	-10	468	7	-9	8	351	5	-5	-19	97	17	-16	-6	838	12	1
2	110	13	8	-9	119	25	3*	9	474	6	-6	-18	198	7	4	-5	136	12	-3
3	472	9	9	-8	535	7	-13	10	246	10	-2	-17	148	8	-1	-4	1058	15	-7
4	112	15	15	-7	84	36	-7*	11	417	8	-5	-16	238	6	-7	-3	283	4	5
5	447	7	17	-6	581	9	-12	12	272	6	-2	-15	189	6	-13	-2	895	11	-24
6	120	27	26*	-5	152	7	12	13	315	5	-5	-14	336	5	1	-1	171	24	-34
7	365	7	-13	-4	683	11	-7	14	186	6	-11	-13	260	6	2	0	1146	15	-5
8	113	33	27*	-3	191	6	9	15	265	6	-2	-12	433	6	-2	1	166	21	-33
9	338	12	-5	-2	703	16	-6	16	134	9	-10	-11	292	5	-8	2	892	12	-33
10	104	17	33	-1	164	9	20	17	201	7	-4	-10	496	7	4	3	276	4	9
11	290	7	-6	0	680	13	16	18	121	11	2	-9	410	9	-4	4	1049	14	-14
12	84	47	28*	1	169	8	20	19	175	11	25	-8	657	11	-1	5	138	3	-5
13	220	12	-8	2	695	16	-13	H,L=	2,	-2	-7	452	8	-4	6	828	12	-3	
14	0	74	-49*	3	183	6	4	-20	10	52	-21*	-6	784	12	-9	7	212	5	8
	H,L=	2,	-5	4	674	12	-13	-19	188	8	-3	-5	544	7	0	8	800	13	5
-16	162	14	-18	5	136	8	0	-18	55	29	13*	-4	666	9	-5	9	133	4	-9
-15	120	14	-7	6	579	11	-12	-17	251	6	-3	-3	527	7	-15	10	612	10	3
-14	220	8	6	7	81	26	-8*	-16	69	16	6*	-2	783	10	-8	11	111	6	2
-13	137	11	-20	8	532	7	-12	-15	320	5	4	-1	570	8	-11	12	496	9	5
-12	260	7	-9	9	115	11	-4	-14	55	58	-6*	0	668	9	-29	13	101	10	-2
-11	184	9	-18	10	465	6	-11	-13	461	7	3	1	573	8	-10	14	393	6	1
-10	332	6	-12	11	100	10	5	-12	107	18	0	2	777	10	-2	15	26	64	-44*
-9	233	7	-10	12	368	6	-8	-11	500	7	-8	3	541	7	-10	16	299	5	2
-8	367	6	-3	13	76	15	18*	-10	127	6	-2	4	675	9	-7	17	0	56	-49*
-7	252	7	-5	14	294	6	-4	-9	619	10	-0	5	536	7	2	18	218	9	-5
-6	402	8	-11	15	91	14	24	-8	184	4	-1	6	791	11	-10	19	58	33	24*
-5	276	8	-5	16	233	7	-8	-7	806	13	-3	7	457	7	-5	20	168	6	-2
-4	459	7	-2	17	50	52	0*	-6	170	6	-2	8	655	10	3	21	25	46	-7*
-3	311	11	1	18	185	9	4	-5	850	12	-19	9	419	8	2	H,L=	2,	1	
-2	492	7	19	H,L=	2,	-3	-4	205	4	-1	10	498	9	6	-20	84	46	-9*	
-1	299	17	9	-19	156	24	7	-3	854	11	-26	11	292	5	-4	-19	146	10	-12
0	459	6	8	-18	106	14	-12	-2	158	43	-16*	12	443	6	-0	-18	138	12	4
1	301	6	11	-17	207	7	2	-11	1034	14	-39	13	260	5	0	-17	208	7	-8
2	494	7	19	-16	133	9	-10	0	107	8	-13	14	334	5	2	-16	160	7	-6
3	323	7	12	-15	270	6	3	11	1017	13	-44	15	207	7	4	-15	279	5	5
4	460	7	-2	-14	194	6	-5	2	171	30	1	16	242	7	-4	-14	219	6	8
5	278	6	-5	-13	315	7	-3	3	847	12	-21	17	157	7	7	-13	357	6	-5
6	402	6	-11	-12	269	5	0	4	207	6	0	18	210	8	14	-12	265	7	-5
7	243	6	-16	-11	412	6	-5	5	855	13	-20	19	103	13	-9	-11	425	6	-2
8	367	7	-4	-10	238	7	-10	6	179	4	3	20	147	9	1	-15	348	9	-2
9	222	7	-19	-9	481	8	0	7	802	13	-2	21	89	12	1	-9	534	11	0
10	339	6	-7	-8	364	5	3	8	180	5	2	H,L=	2,	0	-8	369	9	5	
11	202	7	0	-7	526	8	-10	9	615	10	4	-21	0	92	-33*	-7	599	11	5
12	263	6	-6	-6	414	6	-2	10	135	5	5	-20	169	9	-1	-6	477	8	4
13	145	10	-13	-5	586	10	-7	11	512	8	-3	-19	24	64	-8*	-5	710	12	-7
14	216	8	1	-4	398	6	-5	12	107	12	1	-18	215	6	-9	-4	533	8	-3
15	124	16	-2	-3	703	11	-14	13	463	6	5	-17	0	51	-49*	-3	715	11	1
16	189	9	7	-2	442	8	0	14	64	17	3*	-16	294	5	-4	-2	509	7	-13
	H,L=	2,	-4	-1	666	12	-8	15	312	11	-1	-15	68	15	-4*	-1	801	11	2
-18	188	18	8	0	546	9	1	16	84	14	22	-14	388	7	-4	0	628	8	17
-17	22	53	-28*	1	657	12	-14	17	256	6	1	-13	92	43	-8*	1	797	10	13
-16	242	12	0	2	433	6	2	18	62	22	19*	-12	493	7	1	2	523	7	-8
-15	73	19	7*	3	700	12	-14	19	198	7	6	-11	104	25	1*	3	725	10	6
-14	296	6	-2	4	404	7	-5	20	19	51	-11*	-10	615	11	1	4	544	8	3
-13	30	61	-27*	5	585	10	-6	H,L=	2,	-1	-9	143	16	-5	5	708	12	0	

STRUCTURE FACTORS CONTINUED FOR
 U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
6	476	8	8	H,L= 2,	1	82	18	6*	-2	67	26	8*	-14	198	13	-2			
7	603	10	7	-18	150	19	-1	2	601	10	24	-1	356	7	-15	-13	68	34	-7*
8	379	7	6	-17	115	13	-4	3	129	26	12*	0	74	25	2*	-12	236	9	-12
9	537	8	5	-16	205	11	8	4	559	9	19	1	365	8	-6	-11	121	15	27
10	348	8	-2	-15	162	8	-5	5	118	26	0*	2	62	69	5*	-10	311	11	6
11	435	7	3	-14	243	6	-1	6	519	9	15	3	341	7	-2	-9	82	24	-22*
12	266	5	2	-13	185	9	-7	7	88	14	19	4	26	55	-26*	-8	346	7	-5
13	368	6	4	-12	313	6	7	8	469	9	14	5	331	7	3	-7	128	14	5
14	209	5	-3	-11	228	6	-3	9	86	37	-17*	6	49	58	-8*	-6	386	7	0
15	275	6	-1	-10	391	7	-6	10	380	6	3	7	303	8	2	-5	141	28	6*
16	168	7	0	-9	271	5	-3	11	83	16	12*	8	33	71	-13*	-4	453	8	18
17	218	6	1	-8	426	6	-0	12	317	6	4	9	263	17	13	-3	158	19	19
18	120	16	-13	-7	310	5	-8	13	0	62	-44*	10	107	21	71*	-2	464	7	9
19	157	11	-1	-6	465	9	4	14	251	8	-8	11	238	10	17	-1	155	10	8
20	89	12	-4	-5	339	10	-4	15	0	55	-38*	H,L= 2,	7	0	449	7	6		
	H,L= 2,	2	-4	544	12	-7	16	205	8	8	-5	153	12	8	1	166	13	18	
-20	80	32	53*	-3	437	12	3	17	0	57	-35*	-4	177	10	-18	2	475	7	19
-19	176	9	-0	-2	551	14	16	H,L= 2,	5	-3	142	13	-20	3	166	10	28		
-18	62	26	23*	-1	443	12	5	-14	137	28	12*	-2	207	9	-3	4	456	8	22
-17	236	7	-6	0	525	10	-9	-13	198	10	4	-1	157	11	-8	5	117	26	-14*
-16	0	47	-44*	1	457	11	14	-12	156	12	0	0	210	7	-7	6	389	7	4
-15	298	6	-2	2	566	15	24	-11	230	8	5	1	158	15	-7	7	73	27	-49*
-14	66	17	-1*	3	446	10	13	-10	176	10	5	2	217	14	8	8	357	7	7
-13	380	6	-3	4	557	11	8	-9	253	8	-10	3	171	14	9	9	119	14	14
-12	75	21	-17*	5	344	9	4	-8	206	15	-3	4	201	9	6	10	302	7	-2
-11	479	7	-1	6	471	8	15	-7	314	7	2	5	145	13	-0	11	128	13	34
-10	101	20	3*	7	322	8	0	-6	263	11	6	H,L= 3,	-8	12	234	18	-13		
-9	572	10	-9	8	431	6	-4	-5	328	7	-2	-3	274	8	2	13	43	58	-32*
-8	124	7	-5	9	276	5	-0	-4	225	8	-12	-2	92	34	4*	14	190	15	-9
-7	623	14	4	10	401	7	3	-3	333	9	-6	-1	285	8	9	H,L= 3,	3	-5	
-6	145	7	2	11	232	6	2	-2	256	7	-7	0	91	14	-0	-16	113	17	18
-5	795	17	-2	12	305	6	0	-1	342	7	-20	1	281	10	5	-15	200	10	-8
-4	160	4	3	13	191	7	-2	0	270	6	-9	2	95	20	7*	-14	120	16	-0
-3	854	14	20	14	251	9	4	1	371	9	8	3	278	8	8	-13	242	7	-6
-2	141	6	6	15	161	8	-7	2	253	11	-10	H,L= 3,	-7	-12	126	11	-16		
-1	886	18	-3	16	211	7	11	3	351	10	11	-10	243	10	19	-11	304	6	-2
0	236	6	12	17	108	14	-10	4	258	7	16	-9	128	19	6	-10	171	13	-1
1	909	16	18	18	144	11	-6	5	345	7	16	-8	264	10	9	-9	358	6	-6
2	126	5	2	H,L= 2,	6	272	8	12	-7	129	19	-3	-8	196	7	-1			
3	866	14	30	-17	0	58	-35*	7	318	7	5	-6	282	9	-0	-7	382	6	-9
4	162	3	3	-16	201	9	3	8	191	9	-15	-5	169	12	20	-6	222	7	-1
5	796	15	6	-15	71	25	35*	9	277	7	12	-4	307	8	6	-5	431	7	-6
6	148	5	8	-14	256	7	-3	10	191	9	19	-3	168	11	5	-4	248	11	0
7	629	11	13	-13	79	19	34*	11	235	14	9	-2	317	11	7	-3	510	7	4
8	126	6	-2	-12	310	7	-5	12	165	11	9	-1	169	10	8	-2	282	7	14
9	584	10	-2	-11	81	21	7*	13	213	9	18	0	329	6	17	-1	505	9	16
10	116	10	18	-10	382	6	4	14	110	18	-13	1	167	10	6	0	282	8	12
11	480	7	5	-9	129	10	28	H,L= 2,	6	2	312	9	1	1	518	8	26		
12	83	11	-11	-8	455	7	1	-11	209	21	-11	3	149	12	-16	2	265	9	-1
13	387	6	5	-7	86	20	18*	-10	55	65	19*	4	304	7	3	3	505	10	1
14	48	53	-17*	-6	506	9	3	-9	253	24	1	5	160	12	10	4	261	6	9
15	301	6	-2	-5	118	11	-5	-8	65	49	19*	6	302	8	19	5	424	7	-10
16	36	46	-9*	-4	542	10	1	-7	285	10	-18	7	161	13	28	6	218	8	-9
17	236	6	-6	-3	116	42	2*	-6	94	20	35*	8	271	10	14	7	382	6	-10
18	48	50	10*	-2	573	9	0	-5	313	11	-13	9	146	15	23	8	187	7	-9
19	177	8	3	-1	98	29	26*	-4	97	17	42	10	223	12	-3	9	355	10	-12
20	0	45	-26*	0	567	8	-14	-3	324	7	-19	H,L= 3,	-6	10	165	8	-7		

STRUCTURE FACTORS CONTINUED FCF
U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
11	301	9	-6	-7	276	12	-3	9	153	5	-3	-18	67	21	11*	-3	500	10	7
12	138	10	-5	-6	606	10	-2	10	521	8	-1	-17	251	6	-3	-2	705	13	11
13	243	7	-6	-5	356	5	-7	11	155	12	-4	-16	67	18	-18*	-1	441	8	-4
14	107	14	-11	-4	616	10	-11	12	415	6	-3	-15	310	5	8	0	811	12	3
15	206	9	-4	-3	336	5	-6	13	130	7	8	-14	115	14	-0	1	455	8	0
16	104	19	9*	-2	671	11	7	14	340	6	2	-13	390	6	1	2	703	12	12
	H,L=	3,	-4	-1	451	7	2	15	92	12	2	-12	108	15	-6	3	498	8	7
-18	0	63	-51*	0	743	12	-18	16	267	8	3	-11	477	8	5	4	770	14	9
-17	207	8	9	1	430	7	-10	17	48	58	-15*	-10	171	5	6	5	373	7	7
-16	63	28	-10*	2	660	12	1	18	209	8	7	-9	578	11	5	6	562	11	9
-15	248	8	-8	3	339	6	-7	19	41	58	-14*	-8	179	4	1	7	304	9	-3
-14	78	17	-10*	4	621	9	-15	20	155	18	-0	-7	663	12	12	8	525	9	-1
-13	319	6	-0	5	355	6	-11		H,L=	3,	-1	-6	220	5	1	9	276	5	-3
-12	96	12	-12	6	607	10	-9	-20	83	19	7*	-5	842	13	6	10	447	7	3
-11	384	6	-1	7	265	7	-16	-19	161	11	-4	-4	247	6	1	11	222	6	-2
-10	151	14	-4	8	525	7	4	-18	134	9	21	-3	940	15	-1	12	379	6	1
-9	443	6	-3	9	240	5	-2	-17	219	6	-5	-2	313	4	-1	13	184	7	1
-8	168	16	3	10	428	7	-2	-16	129	8	-8	-11	1005	14	17	14	281	5	-4
-7	530	8	-4	11	204	5	2	-15	292	5	0	0	336	4	4	15	163	11	5
-6	164	26	-11	12	378	6	-1	-14	175	6	2	1	989	14	9	16	247	11	5
-5	595	9	-2	13	182	6	-1	-13	359	5	-4	2	303	4	-0	17	130	9	6
-4	196	15	-9	14	239	6	-2	-12	212	6	2	3	940	14	-8	18	185	7	-4
-3	655	12	-0	15	138	8	1	-11	422	6	3	4	250	4	-0	19	86	19	0*
-2	249	13	12	16	234	11	6	-10	285	6	-4	5	829	13	-0	20	126	12	-2
-1	718	16	3	17	105	12	-7	-9	557	9	-3	6	222	4	4		H,L=	3,	2
0	158	7	9	18	175	8	-4	-8	342	6	4	7	662	11	7	-19	0	54	-42*
1	696	16	-15	19	48	55	-39*	-7	602	10	14	8	183	4	7	-18	194	8	12
2	238	6	-4		H,L=	3,	-2	-6	357	6	-5	9	580	9	6	-17	75	20	7*
3	640	13	-12	-20	144	11	-11	-5	744	11	-1	10	162	5	-2	-16	251	6	9
4	196	16	-2	-19	26	52	-28*	-4	465	6	5	11	475	8	3	-15	84	17	19*
5	591	10	-10	-18	201	7	-1	-3	767	11	-1	12	125	16	5	-14	300	6	2
6	164	30	-7	-17	37	48	-26*	-2	450	6	4	13	388	6	1	-13	55	38	-35*
7	524	7	-7	-16	273	6	6	-1	822	11	-16	14	110	8	-4	-12	361	7	-1
8	159	14	-7	-15	89	14	-3	0	420	6	-10	15	302	5	1	-11	120	9	-2
9	436	6	-6	-14	348	6	6	1	814	11	-17	16	94	23	11*	-10	458	7	-8
10	155	16	1	-13	126	7	3	2	456	6	0	17	256	8	3	-9	159	7	-7
11	384	6	-4	-12	425	6	8	3	765	11	-4	18	45	48	-12*	-8	526	10	-6
12	112	9	7	-11	161	6	7	4	459	7	-4	19	177	11	-2	-7	128	20	-0
13	318	6	-0	-10	533	8	5	5	751	10	-1	20	0	51	-47*	-6	583	11	4
14	82	15	-7*	-9	166	5	4	6	356	6	-5		H,L=	3,	1	-5	196	8	-10
15	256	6	4	-8	636	10	-3	7	597	10	8	-20	133	27	5*	-4	711	16	3
16	72	21	-1*	-7	255	4	4	8	349	7	3	-19	91	21	3*	-3	241	7	10
17	202	8	4	-6	726	12	-3	9	555	9	-6	-18	189	8	-1	-2	773	17	8
18	0	57	-50*	-5	233	7	1	10	287	6	1	-17	117	11	-8	-1	178	7	-6
	H,L=	3,	-3	-4	831	14	-8	11	426	6	4	-16	228	9	-13	0	685	12	14
-19	76	22	-10*	-3	201	4	-3	12	209	6	2	-15	145	8	-10	1	178	8	-2
-18	192	8	15	-2	822	13	-36	13	366	5	-1	-14	284	5	-3	2	791	15	18
-17	117	12	5	-1	308	4	7	14	167	6	-5	-13	182	7	-2	3	247	7	10
-16	234	6	6	0	965	13	-9	15	284	7	-6	-12	382	6	6	4	712	13	9
-15	152	13	12	1	296	4	5	16	129	13	-9	-11	225	8	-2	5	198	7	-6
-14	290	6	-3	2	816	12	-36	17	223	6	-1	-10	445	8	2	6	589	10	10
-13	184	6	1	3	197	3	-4	18	121	10	9	-9	268	8	-7	7	127	6	-4
-12	373	6	-3	4	842	13	-7	19	175	8	8	-8	520	11	-0	8	541	9	3
-11	196	5	-4	5	242	4	5	20	72	22	-4*	-7	301	7	-2	9	161	10	-3
-10	428	7	3	6	722	12	-6		H,L=	3,	0	-6	565	11	12	10	463	7	0
-9	245	5	-0	7	250	7	4	-20	0	70	-47*	-5	377	8	2	11	116	8	-4
-8	530	8	4	8	636	10	-3	-19	171	9	-10	-4	763	15	6	12	362	6	5

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
13	65	17	-22*	-5	456	11	6	-3	65	33	-7*	1	447	10	20	-10	378	6	4
14	298	7	0	-4	145	10	-4	-2	291	7	-14	2	208	9	15	-9	166	13	1
15	61	21	-3*	-3	451	8	-3	-1	119	13	35	3	430	7	20	-8	439	6	-14
16	242	6	0	-2	158	10	7	0	296	6	-18	4	189	11	13	-7	206	7	-11
17	94	25	25*	-1	518	8	-1	1	121	13	37	5	385	7	11	-6	524	7	-8
18	185	8	9	0	142	7	-4	2	306	9	3	6	156	10	7	-5	242	7	1
19	59	32	19*	1	541	9	23	3	66	48	14*	7	328	7	-6	-4	534	8	-14
	H,L=	3,	3	2	152	10	-1	4	282	8	4	8	136	12	-1	-3	228	6	4
-18	92	19	11*	3	461	8	7	5	80	25	7*	9	287	7	-7	-2	586	12	2
-17	183	9	19	4	149	9	2	6	258	9	-6	10	114	17	-5	-1	283	8	8
-16	107	14	8	5	465	11	11	7	73	35	3*	11	260	7	12	0	636	11	-4
-15	216	7	8	6	98	22	2*	8	234	10	1	12	79	36	-18*	1	281	6	5
-14	139	10	-5	7	434	7	8	9	73	39	17*	13	216	9	9	2	576	11	-3
-13	237	6	-16	8	98	15	1		F,L=	4,	-8	14	40	60	-40*	3	226	5	-1
-12	166	8	-9	9	325	8	-5	-2	275	10	17		H,L=	4,	-5	4	543	9	-10
-11	304	6	-4	10	87	16	1*	-1	127	20	10	-16	175	10	-5	5	244	11	-0
-10	186	6	2	11	295	6	2	0	274	6	13	-15	100	16	17	6	526	7	-8
-9	384	10	-5	12	40	54	-28*	1	121	15	3	-14	227	12	1	7	214	6	-2
-8	239	6	-2	13	250	15	-1	2	265	14	6	-13	104	14	-7	8	446	6	-1
-7	409	6	2	14	90	18	31*		F,L=	4,	-7	-12	261	15	-10	9	155	7	-11
-6	301	6	-5	15	196	9	1	-10	84	32	-7*	-11	121	16	-1	10	380	6	7
-5	465	7	-5	16	42	67	-10*	-9	241	10	7	-10	308	6	-10	11	141	22	1
-4	255	6	1		H,L=	3,	5	-8	124	53	19*	-9	134	15	-2	12	319	7	0
-3	545	12	5	-13	67	82	-33*	-7	261	10	-4	-8	366	6	-3	13	122	9	1
-2	304	8	1	-12	189	12	-6	-6	138	17	26	-7	164	16	-3	14	266	10	5
-1	494	13	-4	-11	107	19	-18	-5	308	8	16	-6	416	6	-7	15	89	15	-4
0	349	7	3	-10	226	9	12	-4	110	20	-14	-5	190	10	4	16	192	8	-4
1	518	12	12	-9	166	11	23	-3	334	8	19	-4	453	7	-2	17	65	27	-6*
2	304	8	2	-8	265	8	12	-2	101	21	-26*	-3	188	8	6	18	161	10	4
3	558	11	15	-7	178	11	2	-1	328	7	6	-2	492	7	6		H,L=	4,	-3
4	258	6	1	-6	300	9	3	0	132	9	6	-1	235	7	8	-19	145	11	-8
5	467	8	-3	-5	166	18	-19	1	337	9	12	0	521	7	18	-18	74	22	3*
6	315	5	6	-4	304	8	2	2	155	25	27	1	232	7	10	-17	197	8	8
7	419	6	6	-3	200	9	6	3	333	16	16	2	484	8	-3	-16	91	16	-9
8	246	5	4	-2	317	7	-19	4	158	12	34	3	179	7	-0	-15	254	6	-4
9	394	7	1	-1	208	8	-1	5	302	10	10	4	458	9	1	-14	119	9	6
10	187	6	1	0	359	6	-9	6	110	21	-3*	5	185	7	-5	-13	313	7	-4
11	307	8	1	1	210	8	1	7	269	9	3	6	415	8	-8	-12	166	6	14
12	181	7	7	2	329	7	-6	8	107	29	1*	7	165	9	1	-11	373	6	-1
13	260	6	7	3	197	11	4	9	237	10	-0	8	360	6	-12	-10	189	5	-4
14	143	9	-1	4	323	10	20	10	123	42	32*	9	134	9	-1	-9	442	9	-0
15	213	8	4	5	195	9	10		H,L=	4,	-6	10	324	7	4	-8	245	5	1
16	89	38	-5*	6	307	8	9	-14	115	17	35	11	95	22	-30*	-7	536	8	-3
17	169	9	1	7	194	9	19	-13	200	10	-8	12	257	6	-14	-6	211	6	7
18	68	28	-15*	8	250	8	-3	-12	52	69	-47*	13	104	13	-8	-5	577	8	-4
	H,L=	3,	4	9	139	13	-4	-11	251	8	2	14	211	20	-16	-4	290	5	-3
-16	0	59	-52*	10	229	9	13	-10	118	15	-1	15	67	27	-15*	-3	595	10	-5
-15	203	10	7	11	129	30	4*	-9	287	8	-8	16	176	10	-5	-2	266	5	1
-14	54	56	-6*	12	197	18	1	-8	149	11	14		H,L=	4,	-4	-1	679	14	-10
-13	242	8	-11	13	122	35	15*	-7	344	7	10	-18	151	11	-4	0	237	6	7
-12	0	54	-68*		H,L=	3,	6	-6	147	16	-4	-17	76	23	4*	1	670	14	-15
-11	288	7	-5	-9	61	67	5*	-5	379	9	4	-16	189	8	-8	2	261	4	-6
-10	90	43	3*	-8	218	12	-16	-4	188	10	10	-15	89	16	-4*	3	596	11	-7
-9	335	6	3	-7	75	34	5*	-3	427	9	16	-14	265	6	1	4	291	6	-1
-8	118	11	23	-6	258	11	-6	-2	200	12	10	-13	107	24	-16*	5	587	9	-2
-7	425	12	-3	-5	102	19	30*	-1	442	7	15	-12	315	6	-3	6	202	5	-5
-6	104	14	5	-4	262	14	-17	0	183	6	1	-11	151	18	7	7	540	9	-1

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.C(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
8	246	5	3	-16	245	6	0	0	732	11	-1	17	217	6	12	-2	468	7	4
9	446	6	4	-15	92	12	-20	1	332	7	7	18	58	28	-13*	-1	235	14	5
10	192	6	2	-14	305	5	0	2	779	14	11	19	144	18	9	0	487	7	1
11	379	6	2	-13	150	12	4	3	287	6	-1		H,L=	4,	2	1	241	14	12
12	155	6	1	-12	378	6	0	4	767	13	10	-18	82	20	17*	2	466	7	6
13	319	5	1	-11	206	8	-2	5	278	5	6	-17	161	9	-11	3	185	7	13
14	114	9	1	-10	446	7	5	6	572	9	3	-16	77	21	-14*	4	435	8	-2
15	263	6	7	-9	228	6	2	7	241	5	5	-15	230	7	4	5	217	7	4
16	105	11	5	-8	531	9	0	8	537	8	6	-14	91	13	7	6	405	8	2
17	205	13	15	-7	225	4	-7	9	202	4	8	-13	279	9	-6	7	220	8	4
18	84	17	13*	-6	596	9	1	10	485	8	3	-12	95	28	-14*	8	356	6	8
19	138	14	-15	-5	289	6	6	11	156	7	2	-11	346	6	-4	9	154	7	9
	H,L=	4,	-2	-4	685	13	-7	12	381	6	1	-10	164	8	2	10	310	6	2
-19	168	9	17	-3	327	5	-8	13	146	6	4	-9	429	8	-2	11	130	9	-6
-18	11	51	-57*	-2	774	14	-5	14	293	6	6	-8	159	10	-7	12	259	6	-3
-17	224	7	9	-1	294	5	-0	15	86	13	-8	-7	477	7	-7	13	129	10	10
-16	109	11	8	0	752	11	-3	16	255	6	5	-6	135	7	-9	14	210	12	-6
-15	264	6	0	1	302	5	5	17	110	11	21	-5	537	9	-7	15	93	16	6
-14	142	7	8	2	777	13	-1	18	186	7	1	-4	283	8	-5	16	174	14	4
-13	339	5	-2	3	326	6	-7	19	58	59	-3*	-3	559	11	3	17	51	57	-12*
-12	147	6	3	4	695	12	-0		H,L=	4,	1	-2	250	8	-3		H,L=	4,	4
-11	404	6	-1	5	282	6	4	-19	146	10	11	-1	573	13	9	-15	46	59	-16*
-10	149	8	-4	6	607	10	9	-18	68	23	-2*	0	198	5	2	-14	182	10	-11
-9	526	9	-1	7	229	8	1	-17	202	7	-4	1	580	12	15	-13	79	24	-1*
-8	220	5	-7	8	534	9	4	-16	86	15	-12	2	264	5	7	-12	233	8	4
-7	559	8	3	9	228	7	0	-15	239	6	-2	3	565	10	8	-11	113	14	20
-6	244	5	-2	10	451	6	10	-14	115	10	-22	4	235	7	-1	-10	241	9	-19
-5	636	11	-8	11	204	5	-2	-13	288	7	0	5	546	9	1	-9	121	12	13
-4	296	5	-2	12	387	6	4	-12	165	10	11	6	140	8	-0	-8	298	7	-11
-3	754	13	-8	13	149	6	3	-11	391	6	-1	7	485	7	2	-7	133	11	15
-2	304	5	-3	14	301	5	-1	-10	196	6	-12	8	165	9	-4	-6	359	7	0
-1	742	12	-20	15	105	10	-10	-9	480	8	-3	9	438	6	9	-5	145	12	4
0	394	6	-3	16	246	6	-0	-8	228	6	2	10	162	6	3	-4	366	7	1
1	744	12	-19	17	98	12	-5	-7	471	9	-2	11	354	6	6	-3	152	12	8
2	301	7	-2	18	198	7	9	-6	243	5	1	12	109	10	2	-2	404	10	5
3	757	13	-3	19	48	58	-14*	-5	577	11	-0	13	284	8	-1	-1	163	11	0
4	302	5	5	20	128	13	-7	-4	287	9	3	14	79	15	-4*	0	419	7	-9
5	637	11	-4		H,L=	4,	0	-3	695	13	5	15	228	8	2	1	162	10	1
6	245	5	-2	-19	83	18	22*	-2	298	4	4	16	105	13	13	2	413	8	17
7	562	9	5	-18	175	13	-12	-1	585	14	3	17	169	9	-4	3	148	10	4
8	222	6	-2	-17	96	13	8	0	285	4	-3	18	87	39	24*	4	370	7	9
9	524	8	3	-16	233	6	-16	1	595	11	11		H,L=	4,	3	5	150	14	8
10	143	9	-10	-15	98	11	-1	2	295	8	3	-17	81	23	20*	6	366	8	9
11	407	6	0	-14	285	6	-1	3	706	14	10	-16	167	14	-3	7	118	12	2
12	149	6	4	-13	139	9	-7	4	285	8	7	-15	94	17	6	8	309	7	1
13	344	6	4	-12	380	6	-2	5	574	11	2	-14	207	8	-9	9	101	15	-6
14	124	8	-10	-11	152	8	-4	6	237	4	0	-13	100	14	-20	10	272	12	11
15	265	5	2	-10	482	8	-0	7	487	9	6	-12	264	7	3	11	111	14	18
16	102	11	4	-9	194	5	-3	8	223	5	-5	-11	123	10	-12	12	221	10	-8
17	212	8	-3	-8	536	11	7	9	489	7	5	-10	297	6	-10	13	61	36	-18*
18	61	25	-4*	-7	238	6	2	10	209	7	3	-9	149	10	3	14	198	9	4
19	149	19	-2	-6	574	10	1	11	397	6	6	-8	343	8	-5	15	15	58	-46*
	H,L=	4,	-1	-5	267	7	4	12	153	6	0	-7	222	6	2		H,L=	4,	5
-20	117	49	-17*	-4	767	13	5	13	291	8	5	-6	400	8	-4	-12	98	29	12*
-19	60	30	-4*	-3	284	5	-4	14	125	8	-14	-5	211	6	-0	-11	194	11	7
-18	184	8	-5	-2	770	14	5	15	244	6	1	-4	430	7	-6	-10	108	23	12*
-17	106	13	-2	-1	332	7	6	16	86	14	-11	-3	164	18	-10	-9	235	9	15

STRUCTURE FACTORS CONTINUED FCF
U(BH4)4.C(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-8	120	42	7*	-12	211	9	1	15	187	17	-2	1	163	5	-6	19	63	51	-7*
-7	248	9	-7	-11	125	14	-3		H,L= 5,	-4		2	587	10	7		H,L= 5,		-1
-6	137	14	8	-10	231	8	-5	-17	133	13	-17	3	188	6	-6	-19	124	18	-12
-5	260	10	-7	-9	128	42	-15*	-16	95	17	8	4	524	10	-3	-18	86	25	28*
-4	109	19	-23	-8	289	7	1	-15	197	8	-2	5	175	5	-5	-17	206	7	9
-3	279	8	2	-7	162	10	-2	-14	120	14	-7	6	498	7	-3	-16	81	16	1*
-2	156	14	6	-6	327	9	-3	-13	252	6	0	7	142	7	3	-15	229	6	-7
-1	286	7	-9	-5	188	9	1	-12	158	13	5	8	463	6	1	-14	90	12	-2
0	147	8	-4	-4	334	7	1	-11	306	6	5	9	155	6	2	-13	304	7	-1
1	302	7	7	-3	189	10	-12	-10	158	10	-0	10	375	6	0	-12	92	10	-5
2	165	16	16	-2	363	9	8	-9	371	6	1	11	122	8	-4	-11	396	6	-1
3	273	8	-5	-1	206	10	7	-8	213	6	5	12	334	6	6	-13	168	5	-7
4	138	14	9	0	393	6	17	-7	424	8	-11	13	82	20	0*	-9	468	6	-4
5	269	8	1	1	209	10	9	-6	249	5	-8	14	267	9	-6	-8	139	7	-6
6	113	18	-15	2	365	8	13	-5	451	7	3	15	94	13	18	-7	497	10	5
7	258	8	3	3	190	9	-12	-4	235	8	5	16	208	8	1	-6	164	7	13
8	115	19	3	4	332	8	-0	-3	485	7	-2	17	61	45	-3*	-5	585	11	-3
9	216	9	-5	5	197	8	11	-2	277	5	-1	18	149	10	-6	-4	248	4	4
10	101	20	5*	6	327	7	2	-1	491	8	1		H,L= 5,		-2	-3	588	10	-4
11	207	19	19	7	179	9	15	0	305	5	-1	-19	70	78	-0*	-2	219	4	-5
12	93	23	7*	8	293	7	3	1	488	8	-3	-18	171	8	17	-1	607	12	0
	H,L= 4,		6	9	144	11	-3	2	272	6	-4	-17	101	14	18	0	175	3	-3
-6	99	25	17*	10	232	11	-5	3	481	7	-3	-16	204	9	-5	1	616	11	4
-5	222	10	-1	11	137	12	11	4	230	9	2	-15	121	10	-1	2	226	4	1
-4	113	25	32*	12	210	9	1	5	441	6	-7	-14	240	8	-6	3	593	11	-2
-3	216	9	-14	13	112	22	14*	6	251	10	-5	-13	165	9	2	4	246	6	5
-2	76	27	-11*		H,L= 5,		-5	7	430	7	-4	-12	329	5	5	5	586	10	-3
-1	238	8	-4	-15	184	9	-4	8	200	9	-5	-11	176	6	-5	6	150	7	5
0	96	13	5	-14	56	63	-14*	9	372	6	5	-10	395	6	1	7	501	7	10
1	251	9	3	-13	245	7	-2	10	161	7	4	-9	211	8	-2	8	140	7	-10
2	60	43	-27*	-12	96	15	12	11	298	6	-3	-8	446	6	2	9	476	6	2
3	232	9	3	-11	290	6	8	12	157	7	4	-7	290	5	-8	10	167	5	-7
4	73	31	-8*	-10	95	14	-1	13	247	8	-5	-6	495	9	-4	11	390	6	-2
5	224	10	0	-9	325	6	-2	14	129	10	3	-5	260	4	-3	12	103	8	4
6	44	63	-38*	-8	116	21	-6	15	202	11	3	-4	581	9	-11	13	308	11	3
	H,L= 5,		-7	-7	391	6	-10	16	94	15	7	-3	286	7	-11	14	92	11	-2
-9	105	22	36*	-6	138	9	6	17	154	13	4	-2	587	11	-2	15	239	6	0
-8	235	10	-8	-5	418	6	2		H,L= 5,		-3	-1	322	5	-4	16	70	18	-9*
-7	102	23	18*	-4	145	9	16	-18	136	19	-18	0	628	10	-6	17	208	7	10
-6	281	9	12	-3	409	8	-3	-17	0	52	-64*	1	320	6	-6	18	34	50	-24*
-5	69	49	-16*	-2	165	8	24	-16	199	10	-7	2	580	12	-5	19	145	10	9
-4	317	19	22	-1	458	8	2	-15	65	22	-10*	3	290	6	-6		H,L= 5,		0
-3	120	18	34	0	153	8	18	-14	264	9	-7	4	583	10	-8	-19	107	15	-17
-2	323	10	16	1	447	10	-8	-13	61	21	-21*	5	263	4	-0	-18	91	22	14*
-1	103	26	6*	2	143	9	4	-12	323	6	-2	6	490	9	-3	-17	179	8	4
0	317	6	9	3	412	6	-0	-11	115	15	-11	7	295	5	-2	-16	106	13	2
1	91	32	-5*	4	143	8	15	-10	374	6	2	8	446	6	4	-15	228	6	6
2	315	8	6	5	420	6	2	-9	158	8	4	9	214	10	7	-14	121	14	4
3	79	36	-6*	6	136	9	4	-8	462	6	-1	10	394	6	-2	-13	263	6	3
4	312	12	18	7	397	6	-4	-7	135	24	-4	11	189	5	6	-12	160	6	2
5	117	18	33	8	115	16	-5	-6	499	7	-0	12	327	7	2	-11	353	7	-2
6	276	15	7	9	315	13	-12	-5	187	5	4	13	161	6	-0	-10	216	5	-4
7	0	75	-83*	10	108	11	11	-4	527	8	-4	14	244	5	-2	-9	455	7	-5
8	251	11	6	11	279	7	-5	-3	193	5	1	15	109	14	-12	-8	219	6	-3
9	42	62	-25*	12	89	16	4	-2	577	10	-3	16	220	6	9	-7	430	8	-3
	H,L= 5,		-6	13	250	8	2	-1	180	5	8	17	67	74	-15*	-6	253	4	-2
-13	94	45	-6*	14	8	53	-63*	0	572	9	-10	18	155	9	2	-5	536	10	-1

STRUCTURE FACTORS CONTINUED FC*

U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FCB	SG	DEL	K	FCB	SG	DEL	K	FCB	SG	DEL	K	FOB	SG	DEL
-4	285	7	-9	14	241	6	0	0	170	6	8	3	128	16	36	-10	262	11	-7
-3	606	13	1	15	54	27	-10*	1	405	7	8	4	246	9	13	-9	71	21	-1*
-2	282	6	-7	16	193	7	-5	2	172	8	6	5	95	39	5*	-8	317	6	-9
-1	535	10	3	17	50	50	-7*	3	377	6	3	6	234	13	3	-7	100	25	28*
0	263	6	-5	18	169	20	21	4	115	10	-10	7	74	32	-10*	-6	361	6	-7
1	535	10	3	H,L=	5,	2	5	5	364	6	1	8	210	10	4	-5	109	20	22*
2	285	5	-5	-17	73	84	-3*	6	143	8	11	9	136	14	68	-4	373	6	0
3	612	11	3	-16	158	10	0	7	334	6	6	H,L=	6,	-8	-3	104	13	9	
4	297	7	3	-15	75	21	-15*	8	82	15	-24*	0	214	10	10	-2	396	8	-4
5	533	9	0	-14	200	7	-8	9	288	6	-2	H,L=	6,	-7	-1	101	15	7	
6	248	7	-2	-13	118	11	5	10	81	25	-6*	-8	51	63	4*	0	424	8	0
7	438	7	2	-12	255	6	-3	11	253	6	2	-7	266	13	21	1	105	16	10
8	229	6	7	-11	138	8	-3	12	101	13	22	-6	0	69	-58*	2	393	6	-7
9	457	7	-4	-10	294	6	1	13	216	7	4	-5	253	13	-12	3	108	23	12*
10	218	6	-1	-9	177	7	-4	14	64	28	-11*	-4	53	66	3*	4	373	8	1
11	353	5	1	-8	343	6	-7	15	151	11	-14	-3	286	14	11	5	77	17	-10*
12	142	7	-14	-7	154	7	-10	H,L=	5,	4	-2	-2	90	28	30*	6	361	6	-7
13	252	5	-10	-6	406	7	-11	-13	178	13	12	-1	279	9	-3	7	70	18	-2*
14	115	9	-2	-5	214	5	-9	-12	59	52	-27*	0	108	16	34	8	319	6	-8
15	227	6	4	-4	422	6	-2	-11	190	10	-4	2	41	63	-18*	9	73	18	2*
16	98	12	-8	-3	232	7	-9	-10	108	25	-6*	3	294	9	18	10	267	6	-3
17	172	8	-3	-2	462	7	0	-9	210	9	-18	4	89	34	38*	11	63	26	16*
18	60	28	-15*	-1	230	6	-1	-8	120	14	-11	5	262	9	-3	12	241	7	-0
19	105	25	-18*	0	494	7	6	-7	270	7	1	6	63	50	5*	13	0	52	-43*
H,L=	5,	1	1	1	229	6	2	-6	126	13	-10	7	259	9	3	14	198	17	-1
-18	141	20	-7	2	468	7	12	-5	281	8	0	8	63	48	17*	H,L=	6,	-4	-4
-17	47	52	-9*	3	244	8	4	-4	158	10	11	H,L=	6,	-6	-16	156	10	10	10
-16	205	11	8	4	427	6	1	-3	308	7	5	-12	98	21	-25*	-15	95	17	-13
-15	42	48	-24*	5	216	7	-2	-2	154	11	12	-11	183	12	-3	-14	194	8	5
-14	242	6	4	6	423	6	7	-1	313	8	-5	-10	123	16	-18	-13	129	11	-15
-13	83	14	-18	7	168	7	6	0	156	9	16	-9	208	9	-9	-12	213	7	-5
-12	281	5	-9	8	346	5	-1	1	329	7	11	-8	177	10	12	-11	163	14	2
-11	110	9	-2	9	184	6	4	2	148	11	7	-7	279	7	12	-10	259	6	-7
-10	384	6	-4	10	296	5	1	3	307	10	5	-6	188	9	-2	-9	190	12	-3
-9	128	7	1	11	140	8	-2	4	153	10	5	-5	278	7	-2	-8	304	11	-3
-8	424	7	-3	12	257	6	-4	5	290	8	8	-4	198	9	3	-7	244	7	2
-7	185	7	1	13	116	10	2	6	127	14	-9	-3	280	14	-4	-6	356	6	0
-6	433	7	1	14	216	6	9	7	275	7	5	-2	214	12	9	-5	249	5	-0
-5	171	6	-16	15	100	22	9*	8	124	17	-6	-1	328	11	16	-4	374	6	-13
-4	550	12	-13	16	156	9	-2	9	228	8	0	0	221	12	11	-3	247	6	-10
-3	168	5	7	17	76	21	-0*	10	80	61	-32*	1	318	7	6	-2	414	7	1
-2	519	10	-1	H,L=	5,	3	11	11	185	10	-9	2	228	8	24	-1	282	6	1
-1	206	5	2	-15	160	11	-5	12	91	24	5*	3	282	7	-3	0	432	6	-4
0	516	9	1	-14	78	22	4*	13	159	12	-8	4	183	9	-10	1	283	5	2
1	202	5	2	-13	222	14	11	H,L=	5,	5	5	5	275	7	-6	2	414	6	1
2	531	11	11	-12	65	27	-13*	-9	0	63	-68*	6	196	8	8	3	251	5	-1
3	161	9	-1	-11	247	11	-1	-8	202	20	-4	7	269	7	3	4	381	6	-5
4	558	11	-4	-10	87	22	1*	-7	81	42	-2*	8	163	13	0	5	239	5	-9
5	188	10	-4	-9	284	6	-6	-6	228	10	-2	9	207	8	-9	6	355	6	1
6	433	6	5	-8	82	16	-24*	-5	47	66	-43*	10	135	12	-5	7	245	5	5
7	185	5	2	-7	324	8	-5	-4	217	11	-15	11	174	10	-12	8	309	5	0
8	435	6	5	-6	119	11	-13	-3	78	83	-13*	12	119	15	-3	9	201	6	8
9	116	14	-8	-5	354	12	-8	-2	229	10	-15	H,L=	6,	-5	10	267	6	1	
10	390	6	3	-4	121	10	-7	-1	41	67	-57*	-14	199	9	1	11	169	14	9
11	98	16	-15	-3	378	7	2	0	241	7	-8	-13	27	59	-16*	12	203	7	-14
12	296	5	3	-2	168	8	2	1	81	33	-18*	-12	236	7	-4	13	146	9	1
13	100	10	-1	-1	403	11	3	2	249	9	5	-11	10	72	-39*	14	188	8	-1

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FCB	SG	DEL	K	FCB	SG	DEL	K	FCB	SG	DEL	K	FOB	SG	DEL
15	117	23	8*	1	469	9	-3	-16	136	10	-19	5	409	9	2	-2	326	6	3
16	119	13	-27	2	267	4	-1	-15	114	11	3	6	113	8	-1	-1	115	14	21
	H,L=	6,	-3	3	490	7	-3	-14	192	10	-2	7	362	5	3	0	329	6	7
-17	166	13	8	4	277	5	-4	-13	118	20	-16	8	74	13	3	1	96	25	1*
-16	55	61	4*	5	440	6	6	-12	226	6	-11	9	308	5	-5	2	326	6	3
-15	212	7	3	6	285	6	-7	-11	164	6	2	10	78	13	11	3	82	28	-2*
-14	0	49	-45*	7	357	5	0	-10	283	7	-2	11	285	6	9	4	308	6	-2
-13	261	6	2	8	241	5	-1	-9	219	5	-0	12	48	33	-20*	5	72	21	-5*
-12	0	46	-58*	9	351	5	-4	-8	337	5	-1	13	252	6	18	6	291	7	2
-11	313	6	3	10	199	6	2	-7	192	5	-6	14	51	33	0*	7	75	18	1*
-10	74	14	-3*	11	275	6	0	-6	377	6	3	15	183	8	3	8	263	6	2
-9	359	6	3	12	173	8	0	-5	262	5	-6	16	44	56	2*	9	69	22	10*
-8	100	9	19	13	211	6	-8	-4	428	6	-4	17	158	20	7	10	226	8	3
-7	418	6	-9	14	138	8	6	-3	300	6	-13		H,L=	6,	2	11	38	52	-18*
-6	62	30	-13*	15	170	7	-13	-2	452	8	-6	-15	161	23	13	12	191	8	7
-5	471	7	2	16	104	12	6	-1	280	9	-1	-14	102	15	6	13	53	54	5*
-4	131	9	-11	17	154	18	4	0	458	7	6	-13	165	9	-14		H,L=	6,	4
-3	466	6	-6		H,L=	6,	-1	1	287	10	2	-12	130	10	4	-11	74	38	-9*
-2	135	7	8	-18	152	10	7	2	470	8	12	-11	206	7	-5	-10	149	13	-12
-1	507	8	-12	-17	73	30	27*	3	309	5	-3	-10	137	11	-7	-9	81	26	-26*
0	140	11	3	-16	193	15	0	4	437	6	2	-9	240	13	-5	-8	182	10	-5
1	514	8	-3	-15	0	48	-47*	5	254	5	-6	-8	180	7	4	-7	96	20	-25*
2	134	15	7	-14	234	6	6	6	377	5	-1	-7	277	6	-4	-6	211	10	-6
3	471	6	-3	-13	54	38	-7*	7	207	6	8	-6	191	9	1	-5	140	19	9
4	141	11	-0	-12	273	6	-4	8	336	6	0	-5	307	6	-7	-4	222	9	2
5	472	6	1	-11	51	23	-28*	9	225	5	3	-4	212	9	-2	-3	147	27	4
6	71	12	-3	-10	362	6	-3	10	283	5	-1	-3	349	6	3	-2	238	9	4
7	426	6	-1	-9	86	10	-15	11	159	6	-1	-2	203	6	-2	-1	151	27	-1
8	80	12	-3	-8	411	6	-3	12	235	5	-3	-1	370	6	-1	0	239	9	-1
9	364	6	5	-7	80	18	-18*	13	134	8	-0	0	228	5	2	1	164	30	13
10	67	15	-10*	-6	430	6	3	14	194	10	2	1	381	6	11	2	237	8	3
11	311	5	0	-5	102	16	-12	15	102	12	-10	2	198	6	-6	3	130	14	-13
12	43	44	-14*	-4	529	9	-4	16	161	8	6	3	351	9	6	4	221	8	-0
13	266	6	6	-3	149	7	-8	17	101	14	10	4	225	5	10	5	140	12	8
14	52	30	7*	-2	513	10	-9		H,L=	6,	1	5	313	8	-4	6	212	9	-5
15	205	10	-4	-1	122	6	0	-17	150	11	-0	6	192	6	2	7	139	12	19
16	47	50	-4*	0	487	8	-3	-16	89	17	47*	7	280	6	-0	8	186	11	-0
17	158	9	0	1	120	9	-5	-15	182	15	1	8	181	10	6	9	106	17	1
	H,L=	6,	-2	2	529	8	1	-14	59	26	7*	9	234	6	-10	10	153	25	-9
-17	144	13	-7	3	159	8	1	-13	233	8	-1	10	147	8	3	11	99	19	16*
-16	106	34	7*	4	535	9	2	-12	31	75	-37*	11	217	6	4		H,L=	6,	5
-15	186	7	3	5	115	9	-3	-11	262	8	-10	12	119	11	-7	-5	196	18	6
-14	117	11	-16	6	432	6	7	-10	40	55	-26*	13	180	10	1	-4	41108	-16*	
-13	214	11	-7	7	97	22	-4*	-9	313	5	-0	14	68	24	-25*	-3	219	14	18
-12	188	6	13	8	422	6	2	-8	88	11	13	15	139	11	-8	-2	60	80	2*
-11	271	5	-5	9	101	9	1	-7	352	7	-5		H,L=	6,	3	-1	215	11	0
-10	190	6	-7	10	366	5	3	-6	108	9	-5	-13	47	56	-2*	0	30	51	-20*
-9	345	5	-5	11	68	14	-3*	-5	400	6	-6	-12	181	9	-1	1	206	12	-8
-8	241	5	-3	12	281	6	5	-4	103	10	-1	-11	61	33	5*	2	98	23	37*
-7	353	5	1	13	80	13	19	-3	442	6	-4	-10	225	7	1	3	204	12	3
-6	292	6	-1	14	237	8	8	-2	135	24	7	-9	36	52	-23*	4	82	30	25*
-5	437	6	-0	15	42	46	-2*	-1	476	7	-1	-8	256	12	-4	5	200	11	9
-4	273	5	-8	16	197	7	3	0	149	9	1	-7	76	20	1*		H,L=	7,	-7
-3	486	7	-3	17	69	28	23*	1	477	7	4	-6	278	7	-8	-6	249	10	19
-2	265	5	-6	18	139	10	-5	2	128	13	4	-5	93	15	17	-5	0	65	-28*
-1	463	12	-7		H,L=	6,	0	3	455	8	9	-4	306	7	-0	-4	238	14	-2
0	327	6	-9	-17	100	26	8*	4	116	7	9	-3	79	37	-5*	-3	73	40	48*

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-2	235	11	-19	12	85	17	59*	6	377	6	4	-5	368	6	-16	-15	64	28	31*
-1	33	67	2*	13	189	9	-3	7	25	42	-22*	-4	42	48	-14*	-14	176	12	4
0	265	7	0		H,L=	7,	-4	8	329	5	-3	-3	426	8	-10	-13	0	51	-43*
1	0	65	-32*	-15	142	11	12	9	62	17	8*	-2	53	25	-5*	-12	210	7	2
2	257	11	4	-14	124	39	4*	10	278	5	-4	-1	437	6	-5	-11	0	51	-43*
3	0	74	-26*	-13	166	12	-0	11	33	46	-8*	0	48	53	-25*	-10	236	7	-10
4	252	11	5	-12	140	10	-4	12	247	7	7	1	445	7	0	-9	42	46	-7*
5	0	62	-28*	-11	183	8	-14	13	0	48	-26*	2	74	25	22*	-8	281	6	-1
6	220	10	-12	-10	162	11	-3	14	193	10	-3	3	441	7	4	-7	39	58	-5*
	H,L=	7,	-8	-9	229	6	5	15	0	50	-34*	4	55	15	-4*	-6	316	7	-1
-10	183	11	23	-8	200	12	-1	16	156	9	-1	5	379	6	-3	-5	45	36	-4*
-9	160	27	17	-7	264	6	4		H,L=	7,	-2	6	93	9	16	-4	335	6	-5
-8	188	13	-4	-6	232	6	-4	-16	139	11	5	7	346	5	7	-3	64	17	0*
-7	181	21	13	-5	285	6	-0	-15	109	19	-3	8	45	26	2*	-2	338	7	-9
-6	218	15	3	-4	236	6	-6	-14	154	9	-2	9	308	5	0	-1	76	14	17*
-5	196	17	8	-3	320	6	8	-13	135	9	-1	10	41	43	-8*	0	372	6	-4
-4	231	8	1	-2	257	6	-1	-12	198	7	3	11	261	7	5	1	47	26	-9*
-3	197	10	-2	-1	322	6	-7	-11	165	7	-2	12	0	56	-45*	2	346	6	-1
-2	234	14	-11	0	274	5	-9	-10	243	6	5	13	215	6	-4	3	78	12	18
-1	208	10	-8	1	329	6	-2	-9	197	9	7	14	43	47	11*	4	343	6	-1
0	265	6	7	2	254	7	-4	-8	275	6	-9	15	183	8	4	5	32	43	-15*
1	215	9	-0	3	313	5	0	-7	230	5	8	16	65	57	39*	6	314	5	-4
2	238	8	-8	4	252	10	3	-6	292	6	1		H,L=	7,	0	7	34	43	-8*
3	203	12	5	5	290	6	5	-5	246	5	-4	-16	91	19	-1*	8	285	6	4
4	236	8	6	6	240	6	4	-4	348	6	-3	-15	126	12	-10	9	86	12	39
5	192	9	4	7	252	6	-8	-3	291	5	-9	-14	84	20	-31*	10	247	6	1
6	219	8	5	8	199	6	-1	-2	349	5	-6	-13	164	8	-9	11	0	47	-43*
7	160	10	-7	9	230	6	5	-1	292	5	-2	-12	133	19	-13	12	202	8	-5
8	188	9	-3	10	154	8	-9	0	334	5	-0	-11	198	6	-5	13	0	49	-44*
9	132	34	-10*	11	206	6	13	1	302	5	5	-10	156	11	-4	14	162	9	-9
10	176	19	16	12	149	9	6	2	357	5	-3	-9	222	6	-5	15	0	52	-31*
	H,L=	7,	-5	13	174	8	9	3	299	5	-1	-8	193	6	3		H,L=	7,	2
-13	184	22	-7	14	132	11	13	4	355	5	6	-7	267	5	0	-13	113	17	13
-12	28	60	1*	15	142	10	12	5	246	5	0	-6	218	6	-2	-12	155	10	9
-11	224	8	7		H,L=	7,	-3	6	291	5	1	-5	303	5	-1	-11	117	12	2
-10	14	57	-15*	-16	159	10	3	7	221	5	-3	-4	236	5	-7	-10	189	8	9
-9	254	17	0	-15	0	52	-34*	8	293	5	8	-3	310	5	4	-9	126	11	-18
-8	38	51	2*	-14	205	20	10	9	192	6	1	-2	264	5	-2	-8	215	7	5
-7	284	6	-9	-13	62	24	36*	10	238	5	1	-1	347	6	-4	-7	163	8	6
-6	50	75	13*	-12	244	7	2	11	143	14	-22	0	273	5	-1	-6	221	7	-5
-5	312	8	-10	-11	0	48	-43*	12	199	10	6	1	352	5	5	-5	176	14	-4
-4	75	20	32*	-10	275	6	-6	13	143	8	8	2	268	5	-1	-4	232	6	-5
-3	333	6	-9	-9	39	54	-16*	14	156	17	-0	3	308	7	5	-3	176	8	-13
-2	71	22	20*	-8	326	8	-4	15	105	13	-7	4	243	6	-1	-2	248	9	1
-1	364	7	-5	-7	57	20	10*	16	126	11	-9	5	308	5	2	-1	195	7	-6
0	57	36	9*	-6	366	6	-5		H,L=	7,	-1	6	211	5	-9	0	249	5	4
1	374	6	4	-5	63	26	15*	-16	0	52	-26*	7	272	5	9	1	201	7	-0
2	33	64	-18*	-4	394	6	-9	-15	174	8	-4	8	180	6	-11	2	246	6	1
3	343	6	-0	-3	74	15	-1*	-14	0	50	-33*	9	223	6	-4	3	194	9	3
4	34	49	-7*	-2	418	6	-9	-13	218	7	-2	10	167	6	8	4	244	6	5
5	317	6	-6	-1	50	37	5*	-12	44	59	-1*	11	195	8	-9	5	172	9	-8
6	0	62	-35*	0	423	6	-4	-11	246	6	-8	12	156	8	12	6	224	11	-4
7	296	6	1	1	44	27	-4*	-10	12	44	-38*	13	172	7	-0	7	162	8	4
8	30	49	-5*	2	428	6	-4	-9	302	8	-4	14	119	14	6	8	201	7	-8
9	253	6	-2	3	85	10	10	-8	0	50	-48*	15	140	10	4	9	152	17	8
10	44	50	16*	4	401	6	-4	-7	332	5	-4	16	90	22	-3*	10	173	8	-6
11	222	7	4	5	50	23	5*	-6	57	18	-22*		H,L=	7,	1	11	120	11	7

STRUCTURE FACTORS CONTINUED FOR
U(BH4)4.O(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
12	153	9	5	2	196	10	6	12	135	10	-1	10	169	14	-3	7	186	6	-1
13	102	15	3	3	167	11	-12	13	114	28	-7*	11	161	8	2	8	191	6	-2
	H,L=	7,	3	4	176	10	-3		H,L=	8,	-3	12	147	9	9	9	174	7	9
-11	169	16	8	5	180	11	-10	-14	0	54	-20*	13	119	20	-19	13	148	8	-13
-10	50	60	9*	6	182	11	-3	-13	168	9	-7	14	113	12	1	11	137	9	-0
-9	187	9	-3	7	157	11	-1	-12	6	51	-9*		H,L=	8,	-1	12	143	9	8
-8	0	55	-38*	8	148	14	1	-11	224	7	2	-14	176	8	15	13	117	15	1
-7	210	8	-18		H,L=	8,	-5	-10	22	48	2*	-13	0	51	-28*	14	115	12	-1
-6	33	56	-18*	-11	61	34	48*	-9	250	9	-8	-12	196	7	-5		H,L=	8,	1
-5	236	12	-2	-10	195	9	-5	-8	58	35	31*	-11	56	27	28*	-13	161	10	9
-4	30	62	-11*	-9	30	54	10*	-7	274	6	-6	-10	223	6	-6	-12	0	58	-23*
-3	229	14	-18	-8	240	7	3	-6	0	72	-19*	-9	65	18	46*	-11	177	8	5
-2	96	17	57	-7	39	57	32*	-5	309	6	-5	-8	268	6	1	-10	62	26	39*
-1	262	8	-3	-6	264	8	1	-4	37	45	17*	-7	50	27	33*	-9	209	8	-7
0	0	49	-25*	-5	73	21	68*	-3	338	6	-3	-6	301	5	-4	-8	36	50	16*
1	266	8	3	-4	266	7	-10	-2	0	70	-8*	-5	40	55	19*	-7	250	6	6
2	74	59	35*	-3	0	52	-9*	-1	319	6	-13	-4	311	6	-4	-6	40	60	9*
3	255	7	9	-2	286	7	-2	0	48	18	35*	-3	52	22	34*	-5	247	7	-9
4	0	52	-41*	-1	41	57	32*	1	332	6	-3	-2	311	5	-8	-4	41	47	17*
5	241	7	2	0	290	6	-5	2	0	43	-9*	-1	0	45	-33*	-3	255	6	-10
6	38	52	-9*	1	0	51	-9*	3	340	7	-2	0	353	5	0	-2	0	51	-20*
7	222	8	3	2	290	6	1	4	71	67	52*	1	56	18	25*	-1	266	6	-6
8	69	24	33*	3	0	56	-8*	5	314	5	3	2	325	5	8	0	35	46	21*
9	190	9	1	4	279	6	3	6	41	59	24*	3	17	42	2*	1	282	6	10
10	34	55	-6*	5	0	50	-11*	7	282	7	1	4	308	5	-6	2	0	45	-19*
11	160	11	-2	6	269	6	4	8	46	51	20*	5	0	43	-20*	3	260	6	-4
	H,L=	7,	4	7	49	50	41*	9	267	6	7	6	302	5	-0	4	18	45	-6*
-7	117	33	-24*	8	239	7	2	10	0	46	-18*	7	0	43	-15*	5	259	6	3
-6	139	17	26	9	0	63	-19*	11	230	6	10	8	269	10	1	6	0	46	-31*
-5	130	23	-29	10	203	9	-1	12	0	49	-15*	9	61	19	43*	7	249	8	4
-4	129	16	12	11	23	53	12*	13	184	9	7	10	216	6	-14	8	42	47	25*
-3	181	11	9		H,L=	8,	-4	14	38	51	18*	11	20	46	-9*	9	202	7	-13
-2	139	15	9	-13	130	28	8*		H,L=	8,	-2	12	203	7	1	10	20	54	-3*
-1	173	14	3	-12	138	11	1	-14	131	12	20	13	51	54	24*	11	176	8	4
0	147	11	4	-11	156	9	11	-13	144	10	7	14	166	13	4	12	14	51	-9*
1	165	13	-5	-10	174	8	2	-12	143	16	3		H,L=	8,	0	13	174	8	20
2	133	15	5	-9	159	9	-6	-11	150	9	-9	-14	110	14	-6		H,L=	8,	2
3	179	19	8	-8	191	7	2	-10	169	7	-3	-13	125	18	9	-11	134	18	18
4	143	13	26	-7	200	8	3	-9	184	7	-4	-12	112	13	-22	-10	132	12	26
5	162	12	4	-6	217	6	7	-8	194	6	7	-11	142	21	4	-9	136	12	4
6	107	19	-7	-5	205	7	-8	-7	218	6	5	-10	154	9	-7	-8	139	13	4
7	151	12	11	-4	226	7	-0	-6	204	6	-1	-9	165	8	1	-7	156	10	-1
	H,L=	8,	-7	-3	223	7	-4	-5	244	5	5	-8	183	7	-9	-6	144	10	-2
-1	222	12	-1	-2	230	11	2	-4	236	5	-7	-7	179	8	-9	-5	162	9	-5
0	76	27	73*	-1	239	6	2	-3	231	6	-3	-6	199	6	-8	-4	155	10	1
1	222	11	-0	0	229	5	7	-2	243	5	-6	-5	196	10	-15	-3	165	9	-5
	H,L=	8,	-6	1	253	6	16	-1	260	8	-1	-4	213	6	-3	-2	158	10	-4
-8	143	14	-6	2	247	6	17	0	235	5	-6	-3	186	6	-11	-1	191	8	11
-7	155	20	-5	3	228	6	2	1	263	5	4	-2	228	6	5	0	183	6	5
-6	166	17	1	4	222	8	-2	2	255	7	4	-1	206	6	-9	1	170	13	-9
-5	158	14	-13	5	228	10	14	3	242	5	8	0	231	4	4	2	168	9	7
-4	168	32	-11*	6	210	7	3	4	241	5	2	1	208	6	-6	3	171	15	2
-3	166	12	-15	7	194	7	-2	5	246	6	10	2	236	7	13	4	158	9	7
-2	184	18	-7	8	186	9	-5	6	207	6	4	3	200	6	1	5	166	8	-3
-1	182	13	-5	9	158	8	-6	7	216	6	4	4	223	6	7	6	146	9	1
0	203	10	10	10	164	7	12	8	191	6	3	5	217	6	7	7	162	9	7
1	198	12	10	11	161	9	16	9	191	6	3	6	205	6	-3	8	125	12	-10

STRUCTURE FACTORS CONTINUED FOR
C(BH4)4.0(C2H5)2.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
9	128	12	-3	-6	176	8	5	0	198	5	2	6	171	7	15	-7	140	15	8
10	86	26	-19*	-5	151	10	-4	1	199	6	1	7	140	9	-1	-6	85	23	-17*
11	124	12	5	-4	201	12	4	2	178	11	0	8	142	9	-3	-5	132	13	-17
	H,L=	8,	3	-3	176	8	6	3	208	6	11	9	103	13	-12	-4	102	16	-5
-7	34	58	21*	-2	192	8	-7	4	170	7	6	10	119	20	2	-3	172	18	2
-6	184	13	6	-1	161	9	-7	5	202	6	10	11	101	14	5	-2	133	11	16
-5	0	60	-15*	0	201	6	6	6	165	7	5		H,L=	9,	1	-1	150	11	-14
-4	161	12	-26	1	176	6	6	7	188	12	14	-10	133	13	-2	0	139	8	17
-3	37	64	9*	2	204	7	6	8	137	9	-3	-9	32	53	13*	1	169	15	4
-2	182	11	-17	3	172	8	1	9	150	9	-5	-8	140	11	-24	2	118	12	1
-1	0	63	-16*	4	199	7	4	10	105	21	-8*	-7	60	31	47*	3	166	9	-4
0	204	10	-2	5	170	8	16	11	135	10	2	-6	194	8	4	4	124	14	17
1	55	57	39*	6	184	8	16	12	118	23	10*	-5	39	51	22*	5	152	17	3
2	215	9	19	7	126	11	-11		H,L=	9,	-1	-4	187	16	-6	6	122	17	20
3	0	56	-27*	8	173	10	19	-12	0	53	-20*	-3	54	59	40*	7	149	10	17
4	207	11	21	9	121	11	-6	-11	147	10	-13	-2	207	8	-4		H,L=	10,	-3
5	72	26	58*	10	146	10	2	-10	0	82	-19*	-1	0	51	-5*	-9	167	9	22
6	175	10	-2	11	121	12	17	-9	183	8	-8	0	236	5	6	-8	56	36	30*
7	0	56	-14*		H,L=	9,	-3	-8	0	49	-19*	1	0	64	-5*	-7	166	10	-3
	H,L=	9,	-5	-12	166	9	11	-7	224	7	2	2	215	7	5	-6	0	52	-24*
-5	154	13	0	-11	0	52	-25*	-6	31	47	9*	3	63	23	51*	-5	174	9	-12
-4	162	15	30	-10	189	13	3	-5	233	6	-4	4	195	17	1	-4	41	57	9*
-3	165	12	5	-9	0	76	-26*	-4	43	46	25*	5	47	49	31*	-3	186	8	-11
-2	147	19	13	-8	204	10	-5	-3	239	7	-7	6	187	8	-3	-2	61	27	31*
-1	177	12	11	-7	16	49	2*	-2	36	60	28*	7	0	50	-14*	-1	197	8	-9
0	149	12	11	-6	228	7	-4	-1	265	6	8	8	170	14	6	0	58	30	36*
1	186	10	22	-5	53	29	31*	0	36	37	33*	9	0	57	-18*	1	210	8	3
2	146	13	11	-4	255	6	-2	1	260	5	2	10	128	15	-7	2	0	60	-32*
3	156	24	-4	-3	62	35	44*	2	54	30	49*		H,L=	9,	2	3	203	9	6
4	143	12	10	-2	261	6	-7	3	251	5	4	-7	114	15	-4	4	75	47	42*
5	151	14	-3	-1	0	58	-3*	4	11	44	-7*	-6	109	16	7	5	180	19	-7
	H,L=	9,	-5	0	267	6	-4	5	239	6	1	-5	132	13	8	6	40	49	16*
-9	178	10	-2	1	35	56	31*	6	43	55	22*	-4	115	15	-4	7	179	8	8
-8	42	56	19*	2	269	9	0	7	231	6	8	-3	131	13	10	8	0	51	-27*
-7	199	9	7	3	63	19	45*	8	43	47	24*	-2	145	16	18	9	157	9	12
-6	0	61	-18*	4	256	6	0	9	187	9	-4	-1	151	12	10		H,L=	10,	-2
-5	216	24	-5	5	50	29	29*	10	59	60	39*	0	125	10	-2	-9	100	15	11
-4	0	55	-11*	6	227	6	-3	11	156	19	-4	1	152	10	12	-8	131	11	5
-3	239	8	7	7	58	25	45*	12	27	51	7*	2	128	13	1	-7	115	12	12
-2	0	68	-19*	8	223	6	12		H,L=	9,	0	3	116	14	-6	-6	153	9	9
-1	245	10	12	9	41	49	14*	-11	93	17	-3	4	112	20	-6	-5	100	15	-9
0	62	45	47*	10	184	16	-2	-10	111	13	-8	5	124	13	-1	-4	183	9	24
1	231	7	-2	11	58	60	32*	-9	118	17	3	6	88	19	-14*	-3	105	13	-5
2	0	53	-16*	12	141	13	-15	-8	145	10	-0	7	128	12	10	-2	175	8	7
3	239	7	7		H,L=	9,	-2	-7	150	9	10		H,L=	10,	-5	-1	136	10	17
4	14	66	4*	-12	90	17	-18*	-6	149	9	-8	-5	32	57	6*	0	166	6	-4
5	218	9	-3	-11	131	11	-3	-5	158	8	11	-4	172	11	-8	1	128	9	9
6	67	32	48*	-10	109	23	-3*	-4	179	7	8	-3	57	51	29*	2	171	13	2
7	210	12	13	-9	151	19	-4	-3	157	8	6	-2	196	9	8	3	135	9	23
8	0	53	-22*	-8	147	9	7	-2	171	8	-9	-1	44	58	16*	4	168	8	9
9	185	9	4	-7	167	8	-7	-1	154	8	-10	0	192	18	8	5	96	14	-14
	H,L=	9,	-4	-6	155	8	-3	0	190	7	6	1	18	56	-10*	6	138	10	-7
-11	106	15	2	-5	199	11	7	1	176	10	12	2	194	12	5	7	91	16	-12
-10	121	34	-23*	-4	164	8	1	2	183	14	3	3	64	73	36*	8	115	12	-11
-9	138	11	10	-3	196	6	-2	3	143	8	-9	4	196	8	16	9	103	13	14
-8	181	8	26	-2	173	7	-5	4	165	10	-4	5	30	54	3*		H,L=	10,	-1
-7	132	11	-4	-1	190	7	-9	5	154	8	5		H,L=	10,	-4	-9	46	53	25*

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