Title

CRYSTAL AND MOLECULAR STRUCTURE OF BIS-n-(CYCLOBUTENOCYCLOOCTATETRANE)URANIUM(IV), U[C8H6(CH2)2]2.

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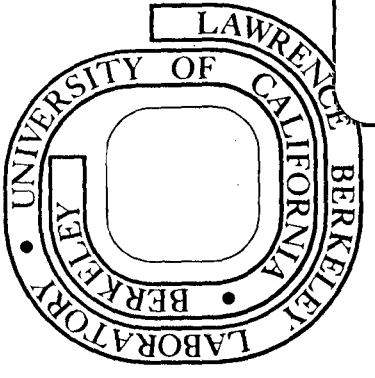

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CRYSTAL AND MOLECULAR STRUCTURE OF BIS-π-(CYCLOBUTENOCYCLOOCTATETRAENE)URANIUM(IV), $U[C_8H_6(CH_2)_2]_2$ [1]

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ABSTRACT

Crystals of bis-π-(bicyclo[6.2.0]deca-1,3,5,7-tetraene)uranium(IV), $U[C_8H_6(CH_2)_2]_2$, are monoclinic, space group $P2_1/n$, $\underline{a}$ = 9.906(8) Å, $\underline{b}$ = 11.039(9) Å, $\underline{c}$ = 7.221(6) Å, β = 98.89(5)°, V = 780.15 Å^3, Z = 2, Dx = 2.122 g cm^{-3}, at 22°C. X-ray diffraction data were measured with counter methods and MoKα radiation. With anisotropic temperature factors for the uranium and carbon atoms, and isotropic temperature factors for the hydrogen atoms, R = 0.020 for 1315 independent reflections ($I > 3\sigma$). The molecule is a sandwich compound with the C_8 rings in an eclipsed configuration about the uranium atom which is on a center of symmetry. The average U-C distance is 2.64 ± 0.02 Å, and the average C-C distance in the C_8 ring is 1.39 ± 0.01 Å (uncorrected for thermal motion). The cylcobuteno ring is planar and at an angle

of 6.8° to the plane of the C_8 ring. The C-C bond length is 1.47(2) Å in the $-CH_2-CH_2-$ moiety, and it is 1.55(2) Å where this group is fused to the C_8 ring.

INTRODUCTION

Following the initial characterization of bis(cyclooctatetraene) uranium(IV), "uranocene", by Streitwieser and Müller-Westerhoff,[2] its crystal and molecular structure was determined.[3] Subsequently the preparation[4] and structure[5] of bis(cyclooctatetraene)thorium (IV), "thoracene," was reported as well as the preparations and structures of octamethyl uranocene,[6,7] $U(C_8H_4(CH_3)_4)_2$, and octaphenyl uranocene,[8,9] $U(C_8H_4(C_6H_5)_4)_2$.

As part of a program to extend knowledge of the chemical and structural properties of compounds of actinide elements, we undertook a study of the structure of butenouranocene synthesized by Berryhill and Streitwieser.[10] The immediate objective was a description of the molecular geometry for use in the interpretation of the n.m.r. spectra.[10]

EXPERIMENTAL SECTION

Crystals grown from a hexane solution were dark green. As the material is extremely air sensitive they were manipulated and kept in an argon filled dry box until they could be inserted into 0.2 mm quartz capillaries and sealed. Weissenberg photographs were taken of the crystals from which the space group and rough cell dimensions were obtained. Some of the crystals exhibited twinning and were rejected for data collection. A wedge shaped crystal fragment was placed on a Picker FACS-I automated diffractometer equipped with graphite monochromated MoKα radiation, (λ = 0.70930 Å), for study.

Cell dimensions were obtained from carefully centered settings on the $K\alpha_1$ peaks of 12 reflections where $35° < 2\theta < 38°$. The cell dimensions, crystal description and other details of the experiment are given in Table I. The width of omega scans at half-height were typically 0.1°. Intensity data were collected using the θ-2θ scan method. Three standards were measured after each 200th scan, and the maximum variation of these measurements from their mean value was about 2%. The data were corrected for absorption.[11] Several azimuthal scans in diverse regions of reciprocal space were performed to test the validity of the absorption correction and to make minor adjustments on the crystal dimensions. The data were processed, averaged, and given estimated standard deviations using formulas presented in the Supplementary Material. The factor p = 0.04 was used in the calculations of $\sigma(F^2)$.

The position of the uranium atom at the origin was evident from the strong pseudo-body-centering exhibited by the data. A Patterson function and subsequent Fourier maps after least-squares refinement of part of the structure revealed the positions of all the carbon atoms. The structure was refined by full-matrix least squares where the function $\Sigma w||F_o|-|F_c||^2/\Sigma wF_o^2$ was minimized. The two reflections below $\sin\theta/\lambda$ of 0.08 were zero weighted because of excessively large discrepancies. Because the observed values of the larger intensities were consistently below the calculated values, an empirical extinction correction was applied; the largest correction to F due to extinction was 1.2. The uranium and carbon atom parameters were refined using

anisotropic temperature factors. The hydrogen atom positions were estimated from the carbon atom geometry and were refined with isotropic temperature factors. All of the hydrogen atoms with the exception of H(1) refined to acceptable positions; H(1) shifted to a position about 0.5 Å from C(1), and it was then restrained to a distance of 0.95 ± 0.05 Å from the carbon atom in the least-squares refinement in the manner suggested by Waser[12] and described in one of our previous papers.[13] Scattering factors for U, C and H were taken from references 14, 15 and 16 respectively; dispersion corrections used were from reference 17.

The R indices are given in Table I and the parameters in Table II. In the last cycle the largest shift was 0.26σ. The largest peak in the final difference map was 1.1 eÅ^3. A list of distances and angles is given in Tables III and IV, with atoms numbered as in Fig. 1.

DISCUSSION

The title compound exists as discrete molecules in the solid state. With the uranium at the origin of the unit cell, the molecule has a center of symmetry imposed on it by the space group and the C_8 rings are exactly eclipsed. The molecular symmetry is close to $\underline{C_{2h}}$. The uranium atom is sandwiched by the two cyclobutenocyclooctatetraene moieties, and it is accurately centered on the cyclooctatetraene (C_8) rings; i.e., the U atom is very nearly equidistant from all of the

atoms in the C_8 ring; see Fig. 1 and Table III. The cyclobuteno (C_4) ring is planar and the plane of the ring is bent about 6.8° from the plane of the C_8 ring toward the center of the molecule, i.e., the two most distant carbon atoms are both 0.18 Å below the least-squares plane through the C_8 ring; none of the atoms in the C_8 ring is more than 0.016 Å from its least-squares plane.

Bond angles and distances are comparable to those found in other uranocenes. The mean U-C value in this compound is 2.64 ± 0.02 Å: this compares with a value of 2.65 Å in uranocene,[5] 2.66 Å in $U(C_8H_4(CH_3)_4)_2$[7] and 2.65 ± 0.03 Å in octaphenyluranocene.[9] Variations in the U-C bond length in the title compound are statistically significant. They result from a slight distortion of the C_8 ring caused by the cyclobuteno adduct; i.e., where C(9) and C(10) are attached to the COT ring the angles inside the ring are 2 or 3 degrees more than the ideal value of 135°, while the other angles around the ring compensate to maintain planarity. The mean C-C bond length, uncorrected for thermal motion is 1.39 ± 0.02 Å. It is evident from the ORTEP drawing in Fig. 1 that there is considerable torsional motion in the plane of the ring. We estimate an increase to 1.41 Å for the average C-C bond length due to this motion.[9] This compares to 1.42 Å in octaphenyluranocene,[9] 1.41 Å in $U[C_8H_4(CH_3)_4]_2$,[7] 1.41 Å in a potassium salt of $C_8H_4(CH_3)_4$ dianion,[18] and 1.42 Å (after correction for torsional motion) in thoracene and uranocene.[5] The bond lengths of C(8)-C(9), C(7)-C(10) and C(9)-C(10) are aliphatic in nature with the first two being close to the accepted C-C bond length. The C(9)-C(10) bond length is

1.47(2) Å, which would increase to 1.49 Å with a correction for torsional motion, and is still somewhat short of the expected value of 1.54 Å.

Although the four membered cyclobuteno ring is very nearly planar, the hydrogen atoms of the CH_2 groups, H(7) through H(10) in Fig. 1, are not symmetrically disposed across that plane. The H(7)-C(9)-H(8) and H(9)-C(10)-H(10) groups are twisted in such a way as to move H(7) away from the uranium atom and H(10) towards it. This distortion results in a staggered configuration of the hydrogen atoms of the two methylene groups.

If the molecules are regarded as spheres, their packing corresponds approximately to the tetragonal protactinium metal structure[19] with 10 nearest neighbors at distances, measured between uranium atoms: 2 at 7.22 Å, 4 at 7.91 Å, and 4 at 8.58 Å. Other nearby molecules are 2 at 9.91 Å, 2 at 11.04 Å, and 2 at 11.32 Å. Inspection of intermolecular hydrogen-hydrogen distances shows that each molecule is in van der Waals contact with its ten nearest neighbors and also, through the hydrogen atoms on the C_4 rings, with the neighbors at 9.91 Å and 11.32 Å.

We thank Professor A. Streitwieser for suggesting this study and for his cooperation in it.

Supplementary Materials Available: Data processing formulas, calculated powder pattern, and a listing of observed structure factors (12 pages). Ordering information is given on an current masthead page.

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Table I. Summary of Crystal Data and Intensity Collection

Compound	$U(C_{10}H_{10})_2$
Formula Weight	498.41
a	9.906(8) Å
b	11.309(9) Å
c	7.221(6) Å
β	98.89(5)°
V	780.15 $Å^3$
Density (calc)	2.12 g/cm^3
Space Group[a]	$P2_1/n$ (alternate setting of $P2_1/c$)
Crystal Shape and Size	Wedge shaped fragment approximately described by the 5 faces; 110, $\bar{1}10$, $1\bar{1}0$, 528, $\bar{1}\bar{1}5$. Dimensions - 0.2 mm long x 0.2 mm width x 0.1 mm deep.
Crystal Volume	.0047 mm^3
Temperature	21 ± 1°C
Radiation	MoKα(λ 0.70930 and 0.71357 Å), monochromated from (002) face of mosaic graphite
μ	99 cm^{-1}
Transmission Factor	0.16 - 0.45
Data Collection Method	θ-2θ scan (2°/min along 2θ)
Scan Range	0.6° below $K\alpha_1$ to 0.6° above $K\alpha_2$
Background Counts	8 sec. Background offset from scan limits by 0.5°
2θ limits	3 - 60°

Table I (Continued)

No. of Scans	4872 (including standards)
No. of unique data	2296
Unique data used $F_o^2 > 3\sigma(F_o^2)$; $.706 > \sin\theta/\lambda > 0.08$	1315
Final No. of Variables	135
Extinction Factor, k $F_{corr} = F_o(1 + kI)$	1.8×10^{-6}
R_w[b]	0.027
R[c] (1315 data used in R_w)	0.020
R (all 2296 data)	0.061
Goodness of Fit	1.06

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[a] The general positions are $\pm(x,y,z;\ 1/2 + x,\ 1/2 - y,\ 1/2 + z)$.

[b] $R_w = [\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2]^{1/2}$.

[c] $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$.

Table II. Positional and Thermal Parameters[a]

Atom	x	y	z
U	0	0	0
C(1)	.0848(9)	.1002(8)	.335(1)
C(2)	-.0244(9)	.1694(8)	.254(1)
C(3)	-.0605(9)	.2235(7)	.077(2)
C(4)	-.005(1)	.2313(7)	-.089(2)
C(5)	.112(1)	.1843(7)	-.152(1)
C(6)	.2240(8)	.1138(7)	-.074(1)
C(7)	.2569(6)	.0648(6)	.103(1)
C(8)	.1993(8)	.0598(6)	.268(1)
C(9)	.308(1)	-.0316(9)	.356(2)
C(10)	.370(1)	-.0269(9)	.183(2)
H(1)	.051(9)	.07(1)	.43(1)
H(2)	-.096(8)	.186(8)	.33(1)
H(3)	-.146(9)	.260(9)	.04(2)
H(4)	-.064(6)	.274(5)	-.177(9)
H(5)	.114(8)	.199(7)	-.27(1)
H(6)	.287(7)	.104(7)	-.13(1)
H(7)	.302(8)	-.134(9)	.39(1)
H(8)	.38(1)	.006(8)	.47(2)
H(9)	.46(1)	-.006(7)	.20(2)
H(10)	.370(6)	-.113(6)	.09(1)

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
U	1.920(9)	1.692(9)	2.26(1)	0	-.062(6)	0
C(1)	6.0(4)	4.0(3)	2.1(2)	-1.9(3)	1.0(2)	-.9(2)
C(2)	4.2(3)	4.0(3)	5.0(4)	-.8(3)	1.9(3)	-2.4(3)
C(3)	2.3(3)	2.1(3)	9.0(7)	.1(2)	.0(4)	-1.3(4)
C(4)	4.3(4)	2.1(2)	5.9(4)	.6(3)	-2.2(3)	.5(3)
C(5)	6.6(5)	2.9(3)	2.6(3)	-1.1(3)	.3(3)	.0(2)
C(6)	4.3(3)	3.4(3)	4.7(4)	-1.2(3)	2.4(3)	-.9(3)
C(7)	2.0(2)	2.3(2)	5.6(4)	-.3(2)	-.3(2)	-.2(2)
C(8)	4.0(3)	2.5(3)	3.5(3)	-.9(2)	-1.7(2)	.3(2)
C(9)	6.4(6)	3.8(4)	9.0(8)	-.8(3)	-5.0(6)	1.6(4)
C(10)	3.2(3)	4.9(6)	10.3(9)	1.0(3)	-1.9(4)	-1.5(5)
H(1)	6.6(26)					
H(2)	4.1(18)					
H(3)	6.7(28)					
H(4)	1.3(11)					
H(5)	3.4(18)					
H(6)	3.2(17)					
H(7)	5.7(22)					
H(8)	7.2(32)					
H(9)	5.6(23)					
H(10)	2.3(14)					

[a] The anisotropic temperature factor has the form $\exp(-0.25(B_{11}h^2a^{*2}+2B_{12}hka^*b^*+\ldots))$.

Table III. Interatomic Distances (Å)

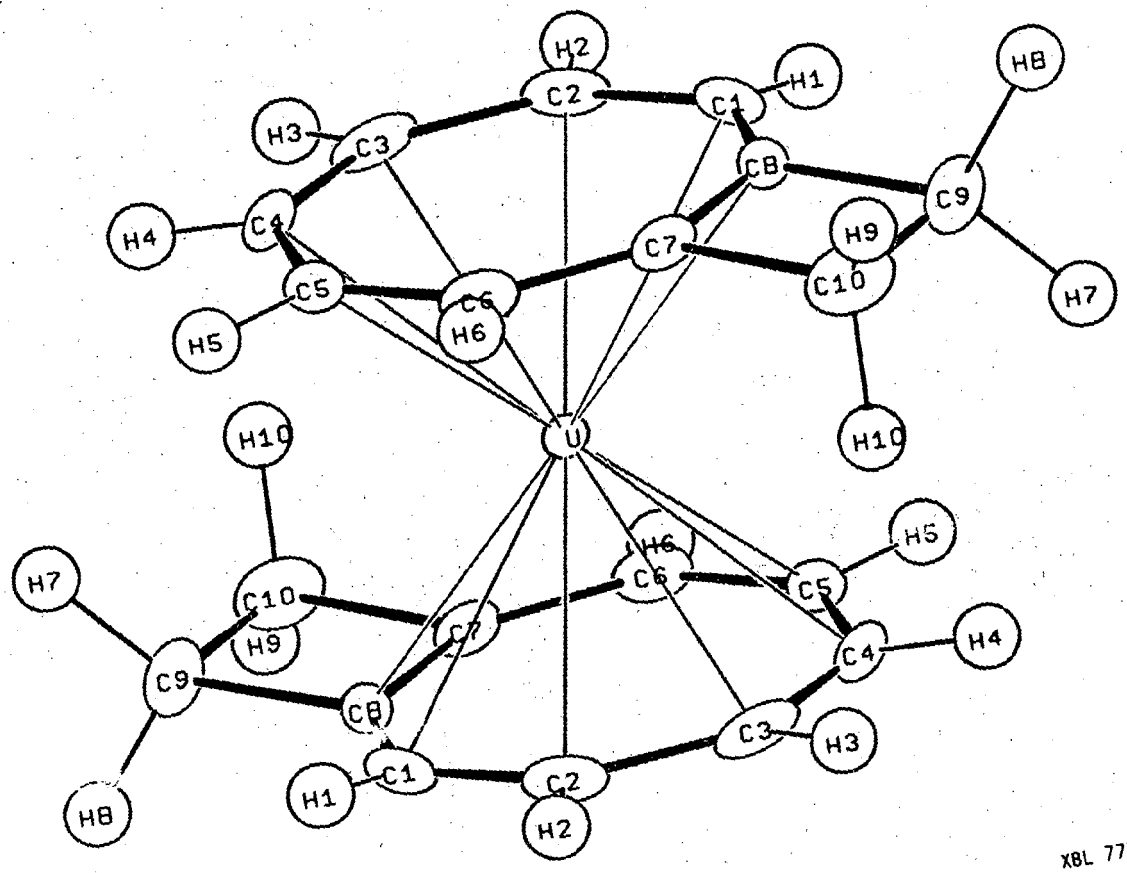
U	-2C(1)	2.675(7)	C(1)-H(1)	0.87(5)
	-2C(2)	2.654(7)	C(2)-H(2)	0.96(8)
	-2C(3)	2.618(7)	C(3)-H(3)	0.94(9)
	-2C(4)	2.631(8)	C(4)-H(4)	0.93(6)
	-2C(5)	2.637(8)	C(5)-H(5)	0.87(9)
	-2C(6)	2.674(7)	C(6)-H(6)	0.79(8)
	-2C(7)	2.637(6)	C(9)-H(7)	1.16(9)
	-2C(8)	2.626(6)	-H(8)	1.06(14)
			C(10)-H(9)	0.92(11)
C(1)-C(2)		1.38(2)	-H(10)	1.15(8)
C(2)-C(3)		1.41(2)		
C(3)-C(4)		1.39(2)		
C(4)-C(5)		1.41(2)		
C(5)-C(6)		1.40(2)		
C(6)-C(7)		1.38(2)		
C(7)-C(8)		1.40(2)		
C(8)-C(1)		1.38(2)		
C(8)-C(9)		1.54(2)		
C(9)-C(10)		1.47(2)		
C(10)-C(7)		1.55(2)		

Table IV. Selected Angles

C(8)-C(1) -C(2)	131.7(8)
C(1)-C(2) -C(3)	134.0(8)
C(2)-C(3) -C(4)	136.7(8)
C(3)-C(4) -C(5)	135.0(9)
C(4)-C(5) -C(6)	135.7(8)
C(5)-C(6) -C(7)	130.6(7)
C(6)-C(7) -C(8)	137.2(7)
C(7)-C(8) -C(1)	139.0(7)
C(6)-C(7) -C(10)	131.0(9)
C(1)-C(8) -C(9)	129.2(11)
C(8)-C(7) -C(10)	91.3(9)
C(7)-C(8) -C(9)	91.4(10)
C(8)-C(9) -C(10)	89.0(9)
C(7)-C(10)-C(9)	88.4(8)
C(8)-C(9) -H(7)	132(4)
C(8)-C(9) -H(8)	112(6)
H(7)-C(9) -H(8)	106(6)
C(7)-C(10)-H(9)	121(5)
C(7)-C(10)-H(10)	113(4)
H(9)-C(10)-H(10)	102(6)

FIGURE CAPTION

Fig. 1. An ORTEP drawing of the molecule.



XBL 7711-10665

$C_{10}H_{10}U\ C_{10}H_{10}$

Fig. 1

DATA PROCESSING FORMULAE

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

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

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

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

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

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

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

When $S(F_a^2) > 4\sigma(F_a^2)$, $\sigma(F_a^2)$ is replaced by $S(F_a^2)$.

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

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

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

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

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

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

C = counts recorded during a scan

I = individual raw intensity, background removed.

t_c = scan count time

t_b = background count time

B_1 = individual background count

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

F = structure factor

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

A = absorption correction

Lp = Lorentz and polarization corrections

θ_m = monochromater angle

θ = crystal diffraction angle

S = scatter

a = average

q = additional uncertainty that affects the weak intensities

p = estimate of non-statistical errors

wtg = weighting factors in least squares

CALCULATED POWDER PATTERN FOR U C(20) H(20)
X-RAY WAVE LENGTH = 1.54180 ANGSTROMS.

A = 9.906 B = 11.039 C = 7.221
ALPHA = 90.00 BETA = 98.89 GAMMA = 90.00

H	K	L	D	I	2 THETA	SINSQ
1	1	0	7.323	1000.	12.09	.01109
1	0	-1	6.243	605.	14.19	.01525
0	1	1	5.992	645.	14.78	.01655
0	2	0	5.519	240.	16.06	.01951
1	1	-1	5.434	0.	16.31	.02013
1	0	1	5.383	174.	16.47	.02051
2	0	0	4.893	155.	18.13	.02482
1	1	1	4.838	12.	18.34	.02539
1	2	0	4.808	30.	18.45	.02571
2	1	0	4.474	4.	19.85	.02969
0	2	1	4.366	3.	20.34	.03118
1	2	-1	4.135	257.	21.49	.03476
2	1	-1	4.057	108.	21.91	.03611
1	2	1	3.854	20.	23.08	.04002
2	2	0	3.662	38.	24.31	.04432
2	1	1	3.570	154.	24.94	.04663
0	0	2	3.567	44.	24.96	.04670
1	3	0	3.444	40.	25.37	.05010
2	2	-1	3.422	2.	26.04	.05074
0	1	2	3.394	7.	26.25	.05158
1	1	-2	3.364	80.	26.50	.05252
0	3	1	3.270	79.	27.27	.05557
1	3	-1	3.170	0.	28.15	.05914
3	0	-1	3.157	43.	28.27	.05962
3	1	0	3.129	132.	28.53	.06072
2	0	-2	3.121	20.	28.60	.06100
2	2	1	3.115	1.	28.66	.06126
1	1	2	3.070	108.	29.08	.06305
1	3	1	3.038	15.	29.40	.06440
3	1	-1	3.035	6.	29.43	.06450
2	1	-2	3.004	0.	29.74	.06588
0	2	2	2.996	67.	29.82	.06621
1	2	-2	2.975	2.	30.04	.06715
2	3	0	2.941	10.	30.39	.06871
2	3	-1	2.813	82.	31.82	.07512
3	2	0	2.808	1.	31.86	.07535
3	0	1	2.807	50.	31.88	.07541
1	2	2	2.766	2.	32.37	.07768
0	4	0	2.760	44.	32.44	.07803
3	2	-1	2.740	68.	32.68	.07913
3	1	1	2.721	2.	32.92	.08028
2	2	-2	2.717	73.	32.97	.08051
2	0	2	2.691	50.	33.29	.08204
1	4	0	2.656	1.	33.74	.08423
2	3	1	2.634	58.	34.03	.08565
2	1	2	2.615	2.	34.29	.08692
0	4	1	2.574	0.	34.86	.08971
0	3	2	2.561	0.	35.03	.09060
1	3	-2	2.548	89.	35.22	.09154
3	1	-2	2.547	49.	35.24	.09164

THE TEN STRONGEST DIFFRACTION LINES ARE

H	K	L	D	I	2 THETA	SINSQ
1	1	0	7.323	1000.	12.09	.01108
0	1	1	5.992	645.	14.78	.01655
1	0	-1	6.243	605.	14.19	.01525
1	2	-1	4.135	257.	21.49	.03476
0	2	0	5.519	240.	16.06	.01951
1	0	1	5.383	174.	16.47	.02051
2	0	0	4.893	155.	18.13	.02482
2	1	1	3.570	154.	24.94	.04663
3	1	0	3.129	132.	28.53	.06072
2	1	-1	4.057	108.	21.91	.03611

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 6.0)
U(C20H20). F(0,0,0) = 2659

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

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	0,	0		4	0	30	-21*	7	57	21	32*	-1	18	27	-0*	-9	166	9	-2
2	654	13	1	5	450	13	-5	H,K=	0,	11		0	944	0	-102*	-8	28	42	28*
4	507	18	5	6	28	33	9*	1	318	7	-8	1	177	6	0	-7	276	7	-5
6	387	17	7	7	303	15	3	2	40	15	19*	2	827	19	-25	-6	13	41	-18*
8	255	7	1	8	2	40	-5*	3	295	6	-2	3	112	5	12	-5	451	16	1
10	133	9	7	9	152	9	-4	4	46	17	34*	4	595	12	19	-4	46	11	16*
H,K=	0,	1		H,K=	0,	6		5	267	7	2	5	8	36	8*	-3	630	13	11
11	007	34	-24	0	559	12	-7	6	13	41	6*	6	412	16	3	-2	13	22	11*
2	202	6	7	1	29	10	13*	7	162	7	-8	7	37	30	28*	-1	967	23	-3
3	760	15	19	2	497	10	-15	H,K=	0,	12		8	244	6	-10	0	109	3	5
4	53	8	-3	3	31	14	1*	0	306	7	-0	9	6	42	4*	1	770	21	-39
5	443	10	10	4	491	11	2	1	12	32	-33*	H,K=	1,	2		2	22	25	8*
6	37	23	33*	5	56	13	-13*	2	296	7	2	-10	36	42	21*	3	546	16	-14
7	311	7	-1	6	342	7	-2	3	26	34	11*	-9	204	6	2	4	22	31	0*
8	18	38	3*	7	68	11	37	4	254	6	-1	-8	24	37	10*	5	426	9	3
9	188	8	-6	8	225	8	5	5	41	28	36*	-7	303	8	-4	6	45	19	-12*
10	30	44	21*	9	43	44	41*	6	182	7	1	-6	0	47	-15*	7	297	7	5
H,K=	0,	2		H,K=	0,	7		H,K=	0,	13		-5	491	10	6	8	19	38	10*
0	968	20	0	1	487	10	-4	1	290	6	-1	-4	86	6	1	9	165	8	-4
1	110	3	5	2	36	18	-21*	2	33	34	1*	-3	780	38	-7	H,K=	1,	5	
2	686	22	-1	3	476	10	-5	3	250	6	4	-2	136	5	4	-9	46	52	42*
3	140	4	8	4	44	12	13*	4	5	38	1*	-1	990	20	34	-8	226	7	-3
4	615	13	24	5	397	9	-4	5	181	9	8	0	291	10	10	-7	32	37	30*
5	16	32	-7*	6	36	38	34*	H,K=	0,	14		1	295	9	5	-6	342	17	5
6	412	15	6	7	249	6	-1	0	228	7	-2	2	154	5	29	-5	36	28	33*
7	37	25	29*	8	46	40	43*	1	38	46	30*	3	728	21	-6	-4	508	15	13
8	244	6	-5	H,K=	0,	8		2	234	6	-1	4	40	15	17*	-3	16	24	5*
9	42	33	38*	0	476	10	-1	3	35	40	33*	5	539	11	31	-2	658	13	-6
H,K=	0,	3		1	44	8	2	4	185	7	-1	6	51	14	43*	-1	10	20	-10*
1	687	16	6	2	543	11	-18	H,K=	0,	15		7	331	7	8	0	737	26	-18
2	43	6	7	3	17	29	-2*	1	202	6	6	8	42	26	25*	1	30	8	29*
3	662	25	-3	4	371	8	-1	2	0	45	-15*	9	180	6	-2	2	633	13	-24
4	28	19	0*	5	31	37	-19*	H,K=	1,	0		H,K=	1,	3		3	12	31	-5*
5	512	11	3	6	269	6	-9	-9	197	6	0	-9	22	40	22*	4	488	13	-6
6	60	11	15	7	16	39	-7*	-7	321	21	9	-8	244	6	0	5	59	22	11*
7	298	7	-0	8	161	9	5	-5	431	14	16	-7	30	35	5*	6	300	7	10
8	0	38	-4*	H,K=	0,	9		-3	731	18	20	-6	371	8	2	7	13	54	-9*
9	168	6	-17	1	486	10	-11	-11	121	0	-233*	-5	0	35	-25*	8	232	6	1
H,K=	0,	4		2	21	29	11*	1	833	21	-11	-4	589	23	10	9	56	18	52*
0	869	18	3	3	408	9	-8	3	819	17	8	-3	52	6	12	H,K=	1,	6	
1	56	3	-0	4	48	15	27*	5	438	10	-4	-2	944	22	-7	-9	143	7	1
2	721	17	-8	5	288	7	-0	7	332	8	2	-1	2	18	-21*	-8	12	41	-6*
3	7	25	-32*	6	26	36	13*	9	187	8	-4	0	457	19	0	-7	294	7	3
4	504	17	-21	7	189	6	12	H,K=	1,	1		1	325	7	-0	-6	0	35	-26*
5	46	12	9*	8	16	45	-9*	-10	139	8	4	2	710	14	-41	-5	432	9	11
6	357	8	-1	H,K=	0,	10		-9	10	41	6*	3	10	24	-22*	-4	54	9	17
7	11	36	9*	0	402	9	1	-8	237	8	-6	4	591	13	23	-3	518	11	1
8	239	8	1	1	66	7	2	-7	0	36	-9*	5	108	6	10	-2	35	9	-4*
9	66	14	56*	2	381	8	-17	-6	396	9	2	6	393	9	12	-1	535	11	-3
H,K=	0,	5		3	18	35	11*	-5	77	8	7	7	3	36	2*	0	40	6	-2
1	715	15	-20	4	288	6	2	-4	642	26	20	8	216	6	-8	1	632	18	-26
2	74	3	-4	5	32	47	8*	-3	54	7	10	9	43	28	39*	2	39	8	20*
3	479	10	-6	6	256	7	2	-2	665	29	1	H,K=	1,	4		3	459	10	-9

STRUCTURE FACTORS CONTINUED FOR
U(C20H20).

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	15	30	6*	5	45	47	33*	2	249	6	1	-6	414	9	1	-9	159	7	12
5	392	12	0	6	238	6	-7	3	0	41	-10*	-5	32	21	1*	-8	0	39	-7*
6	53	15	44*	7	15	40	10*	4	210	7	1	-4	629	16	-7	-7	246	6	-1
7	281	6	4	8	165	9	18	5	59	16	55*	-3	0	25	-2*	-6	10	35	-24*
8	25	41	11*	H,K=	1,	10		H,K=	1,	14		-2	845	40	41	-5	437	9	11
9	151	7	-4	-7	191	6	3	-4	42	28	40*	-1	113	6	5	-4	90	5	12
H,K=	1,	7		-6	11	53	7*	-3	217	6	1	0	412	9	-6	-3	532	11	2
-9	0	46	-7*	-5	266	6	6	-2	32	36	25*	1	94	5	4	-2	17	22	16*
-8	203	6	6	-4	38	40	9*	-1	245	6	-3	2	709	22	-19	-1	649	20	-4
-7	56	16	2*	-3	334	7	-8	0	30	39	-3*	3	0	26	-29*	0	41	5	9
-6	319	7	-0	-2	0	31	-3*	1	222	6	-5	4	558	12	12	1	910	32	-67
-5	26	35	-18*	-1	352	7	2	2	35	37	35*	5	35	20	22*	2	175	4	9
-4	423	9	4	0	69	10	-0	3	202	6	2	6	451	9	10	3	493	10	-15
-3	25	29	11*	1	419	9	-14	4	31	40	31*	7	43	20	24*	4	45	11	29*
-2	506	11	10	2	26	30	-3*	H,K=	1,	15		8	215	6	-3	5	329	7	4
-1	24	25	13*	3	340	7	-8	-2	201	6	3	9	25	42	25*	6	0	39	-25*
0	472	10	-2	4	9	34	0*	-1	14	39	-6*	H,K=	2,		3	7	281	7	2
1	30	12	-17*	5	280	7	-5	0	186	6	3	-9	184	6	-4	8	0	41	-7*
2	512	14	-10	6	0	39	-5*	1	47	39	41*	-8	0	37	-2*	9	153	8	-13
3	85	8	19	7	176	6	8	2	163	6	-5	-7	280	7	-2	H,K=	2,		6
4	479	10	-5	H,K=	1,	11		H,K=	2,	0		-6	32	39	17*	-9	0	42	-18*
5	27	39	-15*	-7	35	42	20*	-10	133	8	-10	-5	484	10	-2	-8	206	7	-5
6	278	6	-8	-6	236	7	8	-8	227	7	2	-4	29	30	-6*	-7	49	18	35*
7	53	19	52*	-5	17	41	-2*	-6	436	9	13	-3	639	18	19	-6	306	7	5
8	183	7	-2	-4	287	7	0	-4	711	27	46	-2	17	36	4*	-5	56	10	20
H,K=	1,	8		-3	0	35	-15*	-2	498	10	-6	-1	859	21	40	-4	512	11	9
-8	0	50	-4*	-2	288	6	-2	0	913	20	32	0	272	9	-5	-3	38	10	31*
-7	231	7	1	-1	25	37	23*	2	941	19	-3	1	701	19	-40	-2	525	11	1
-6	0	37	-1*	0	349	7	-4	4	576	12	25	2	82	4	14	-1	41	6	-1
-5	278	7	-0	1	17	31	12*	6	412	16	4	3	603	23	16	0	645	23	-17
-4	25	32	1*	2	299	6	-6	8	250	6	1	4	0	30	-16*	1	92	5	13
-3	457	9	-1	3	9	35	-18*	H,K=	2,	1		5	465	10	7	2	485	10	-7
-2	0	27	-3*	4	276	7	3	-10	0	44	-14*	6	0	46	-21*	3	80	6	23
-1	492	10	8	5	48	35	38*	-9	191	6	-7	7	302	7	4	4	459	10	-11
0	68	8	1	6	219	7	3	-8	39	26	33*	8	0	48	-20*	5	29	32	25*
1	541	16	-14	H,K=	1,	12		-7	328	7	4	9	154	8	-13	6	288	7	7
2	21	34	-6*	-6	32	43	26*	-6	21	34	1*	H,K=	2,		4	7	0	37	-30*
3	474	10	-8	-5	221	6	4	-5	533	11	9	-9	39	43	22*	8	212	6	-2
4	12	31	2*	-4	57	12	47*	-4	75	9	-2	-8	213	6	-14	H,K=	2,		7
5	331	8	-14	-3	297	7	0	-3	643	38	11	-7	33	36	-24*	-9	133	9	-4
6	0	37	-17*	-2	37	21	9*	-2	14	33	-1*	-6	323	7	3	-8	29	42	24*
7	188	6	-2	-1	299	7	4	-1	655	29	21	-5	38	39	6*	-7	265	6	4
8	66	15	53*	0	23	33	6*	0	106	4	-4	-4	491	10	18	-6	43	18	39*
H,K=	1,	9		1	307	8	-3	1	849	24	-16	-3	25	18	-2*	-5	346	8	5
-8	164	11	14	2	18	41	6*	2	170	8	19	-2	815	17	5	-4	31	38	13*
-7	15	40	6*	3	255	6	-7	3	716	24	15	-1	43	6	-7	-3	497	11	4
-6	263	6	4	4	0	37	-0*	4	34	15	13*	0	812	38	-31	-2	13	29	5*
-5	0	35	-13*	5	215	6	3	5	492	10	9	1	139	3	3	-1	496	10	-9
-4	275	7	-4	6	0	43	-21*	6	60	15	10*	2	696	14	-42	0	53	7	-7
-3	0	29	-3*	H,K=	1,	13		7	302	7	-4	3	116	5	-20	1	545	17	-3
-2	429	9	-9	-5	41	32	35*	8	28	39	24*	4	513	11	21	2	57	8	11
-1	0	29	-15*	-4	211	7	-7	9	186	8	-5	5	78	7	15	3	444	9	-5
0	485	10	-3	-3	39	23	27*	H,K=	2,	2		6	328	7	2	4	43	14	11*
1	10	28	7*	-2	288	6	-4	-10	140	7	0	7	0	38	-7*	5	335	8	-5
2	499	11	-9	-1	20	34	13*	-9	0	40	-6*	8	205	6	1	6	19	36	3*
3	33	19	22*	0	293	7	-6	-8	233	6	-9	9	0	49	-4*	7	250	6	2
4	341	7	-6	1	0	34	-5*	-7	29	44	20*	H,K=	2,		5	8	39	42	33*

STRUCTURE FACTORS CONTINUED FOR
U(C20H20).

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	2,	8		-2	23	31	-3*	3	644	13	7	1	211	5	24	-1	494	14	3
-8	176	7	-3	-1	312	7	-4	5	475	10	10	2	604	18	-10	0	61	6	6
-7	52	17	32*	0	34	18	11*	7	230	6	-1	3	146	4	-2	1	531	19	-9
-6	265	7	3	1	313	7	3	9	203	6	2	4	503	11	0	2	16	27	-25*
-5	31	36	25*	2	25	31	3*	H,K=	3,	1		5	39	29	13*	3	482	10	-17
-4	351	7	-2	3	282	6	-6	-10	143	7	-3	6	388	9	-1	4	67	8	23
-3	0	31	-12*	4	32	47	15*	-9	48	20	47*	7	38	39	18*	5	345	8	2
-2	474	10	0	5	244	6	-0	-8	215	6	-3	8	206	6	6	6	44	51	30*
-1	0	26	-14*	6	15	49	6*	-7	18	36	-5*	9	63	16	59*	7	261	7	-2
0	540	18	-10	H,K=	2,	12		-6	414	9	3	H,K=	3,	4		8	40	42	37*
1	39	10	-13*	-6	171	7	1	-5	52	11	36*	-9	174	8	0	H,K=	3,	7	
2	440	14	-3	-5	44	23	31*	-4	567	37	15	-8	30	38	22*	-9	39	49	13*
3	54	9	22	-4	255	6	-3	-3	50	8	9	-7	246	6	-5	-8	189	9	-0
4	384	8	1	-3	37	40	16*	-2	693	19	-11	-6	20	33	18*	-7	15	39	1*
5	0	34	-7*	-2	276	6	1	-1	202	5	5	-5	416	9	9	-6	282	6	7
6	260	6	-5	-1	0	32	-20*	0	914	19	-9	-4	13	29	-2*	-5	18	45	17*
7	54	16	43*	0	333	7	4	1	150	4	11	-3	506	10	21	-4	444	9	1
8	167	7	-2	1	44	23	-19*	2	714	20	-12	-2	28	9	17*	-3	49	8	27
H,K=	2,	9		2	279	6	0	3	35	10	-7*	-1	713	22	12	-2	525	11	1
-8	44	35	35*	3	2	42	-10*	4	514	11	20	0	83	3	5	-1	55	6	-1
-7	218	6	5	4	240	7	1	5	25	40	1*	1	752	16	-38	0	524	19	-12
-6	31	37	28*	5	22	41	16*	6	372	8	13	2	20	28	-17*	1	32	13	-14*
-5	246	6	4	6	148	15	-14	7	41	22	21*	3	593	13	-12	2	352	7	2
-4	43	23	41*	H,K=	2,	13		8	241	6	-2	4	20	31	9*	3	58	34	47*
-3	369	8	-5	-5	178	6	14	9	15	44	5*	5	394	9	1	4	399	9	-6
-2	39	13	32*	-4	0	40	-29*	H,K=	3,	2		6	48	15	30*	5	44	31	30*
-1	469	12	-7	-3	246	6	5	-10	18	41	8*	7	257	6	-3	6	295	7	-3
0	26	35	25*	-2	36	40	29*	-9	180	7	-5	8	38	41	16*	7	38	39	34*
1	462	16	-4	-1	298	7	-1	-8	13	37	6*	9	161	8	-1	8	180	8	-2
2	40	12	28*	0	20	44	-1*	-7	320	8	-2	H,K=	3,	5		H,K=	3,	8	
3	393	8	-10	1	271	7	3	-6	86	8	4	-9	37	41	30*	-8	31	43	24*
4	26	34	16*	2	32	35	29*	-5	467	10	-6	-8	214	7	-4	-7	225	6	3
5	282	6	-3	3	247	8	3	-4	38	15	7*	-7	26	36	3*	-6	49	16	42*
6	0	42	-21*	4	21	39	3*	-3	646	21	18	-6	304	7	9	-5	299	7	2
7	186	6	1	5	176	7	-3	-2	111	4	4	-5	61	20	30*	-4	0	34	-21*
H,K=	2,	10		H,K=	2,	14		-1	745	31	-24	-4	442	9	8	-3	423	9	-5
-7	0	41	-13*	-4	163	7	-5	0	110	3	3	-3	24	27	21*	-2	35	14	-8*
-6	246	8	9	-3	29	38	16*	1	615	19	16	-2	585	12	10	-1	561	17	-3
-5	21	43	9*	-2	233	6	-1	2	11	23	0*	-1	68	4	-1	0	14	28	1*
-4	313	7	2	-1	0	40	-27*	3	584	21	-3	0	741	33	-4	1	386	8	-5
-3	17	32	-10*	0	231	7	2	4	58	8	23	1	264	10	24	2	43	12	-32*
-2	310	7	-5	1	40	35	38*	5	496	11	3	2	563	12	-12	3	395	8	2
-1	44	10	3*	2	223	6	-1	6	45	17	-20*	3	33	34	-26*	4	31	33	27*
0	414	9	-6	3	61	15	48*	7	264	6	-6	4	483	11	-6	5	291	7	-5
1	13	29	6*	H,K=	2,	15		8	0	44	-5*	5	28	33	19*	6	52	19	16*
2	361	8	-6	-2	7	39	4*	9	164	9	-8	6	301	7	1	7	216	6	-10
3	10	38	-23*	-1	183	6	-1	H,K=	3,	3		7	11	40	10*	8	46	53	46*
4	280	7	0	0	37	39	19*	-9	0	40	-28*	8	211	6	12	H,K=	3,	9	
5	0	48	-1*	1	180	6	13	-8	229	6	-8	H,K=	3,	6		-8	157	9	8
6	220	6	1	2	0	49	-1*	-7	27	35	11*	-9	146	12	5	-7	38	54	33*
7	62	30	56*	H,K=	3,	0		-6	379	8	-11	-8	20	49	18*	-6	244	6	12
H,K=	2,	11		-9	175	10	-2	-5	23	31	6*	-7	233	7	-0	-5	0	35	-11*
-7	165	9	-4	-7	331	7	4	-4	417	9	11	-6	29	35	26*	-4	334	8	-3
-6	36	41	28*	-5	483	20	33	-3	22	25	20*	-5	408	9	9	-3	32	32	13*
-5	243	6	-2	-3	623	16	-36	-2	800	21	24	-4	43	12	22*	-2	414	12	-12
-4	46	15	8*	-1	737	19	4	-1	40	5	3	-3	538	11	4	-1	11	31	-13*
-3	315	7	1	1	918	25	13	0	727	23	-32	-2	31	11	18*	0	462	15	2

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	63	8	25	0	281	6	6	-4	531	11	17	-6	39	21	30*	-4	333	7	-4
2	389	11	-4	1	44	20	23*	-3	48	11	2*	-5	406	9	18	-3	32	17	14*
3	15	42	9*	2	270	6	-2	-2	673	20	-7	-4	8	31	3*	-2	442	11	8
4	299	7	15	3	57	18	36*	-1	140	3	12	-3	522	11	5	-1	43	12	32*
5	0	36	-6*	4	221	8	8	0	691	14	13	-2	27	27	25*	0	455	14	-1
6	236	8	-5	H,K=	3,	14		1	9	23	-35*	-1	460	15	-5	1	90	9	-27
7	55	26	51*	-4	6	44	3*	2	631	20	-19	0	80	4	7	2	420	9	-12
H,K=	3,	10		-3	170	7	-1	3	66	6	18	1	567	13	-12	3	39	24	19*
-7	177	8	-1	-2	33	37	26*	4	462	10	6	2	47	12	-2*	4	309	7	-1
-6	4	41	-1*	-1	224	6	3	5	26	42	14*	3	552	13	-1	5	34	37	30*
-5	279	6	10	0	0	37	-4*	6	331	8	5	4	44	14	30*	6	258	8	-4
-4	23	33	23*	1	238	6	-5	7	36	41	18*	5	354	8	0	7	2	52	1*
-3	327	8	-5	2	31	38	8*	8	226	10	-8	6	31	53	30*	H,K=	4,	9	
-2	39	15	35*	3	198	6	0	9	0	49	-21*	7	247	6	7	-8	36	45	33*
-1	392	8	-4	H,K=	3,	15		H,K=	4,	3		8	35	43	31*	-7	186	6	8
0	27	29	9*	-1	22	41	18*	-9	170	6	-3	H,K=	4,	6		-6	0	39	-15*
1	333	7	0	0	174	8	12	-8	52	16	41*	-9	0	47	-10*	-5	288	7	5
2	47	12	10*	1	0	39	-13*	-7	280	6	-7	-8	199	8	-3	-4	25	34	9*
3	310	7	-2	H,K=	4,	0		-6	59	17	15*	-7	28	43	25*	-3	313	7	2
4	0	37	-23*	-10	135	10	-14	-5	406	8	-8	-6	301	7	11	-2	14	29	-14*
5	243	7	-7	-8	203	6	-2	-4	24	32	-11*	-5	0	34	-10*	-1	442	11	-6
6	40	43	30*	-6	301	7	7	-3	575	15	18	-4	461	9	5	0	43	11	10*
7	180	12	3	-4	564	12	-8	-2	48	15	14*	-3	40	11	-6*	1	381	12	-10
H,K=	3,	11		-2	658	16	0	-1	675	30	-30	-2	480	10	8	2	62	11	23
-7	25	43	17*	0	850	21	22	0	24	24	15*	-1	52	8	-1	3	368	8	2
-6	196	6	8	2	786	16	-28	1	603	21	9	0	454	16	-14	4	8	36	-13*
-5	13	39	-3*	4	496	11	5	2	134	5	1	1	60	7	-25	5	247	6	-4
-4	314	7	0	6	243	6	4	3	522	12	-5	2	445	19	-19	6	38	40	31*
-3	42	17	36*	8	246	6	-8	4	0	31	-17*	3	85	10	33	7	170	11	-11
-2	291	6	-2	H,K=	4,	1		5	416	10	3	4	431	9	-1	H,K=	4,	10	
-1	0	31	-10*	-10	14	42	13*	6	33	35	32*	5	19	38	10*	-7	49	40	47*
0	305	7	5	-9	159	7	-1	7	288	7	7	6	298	7	6	-6	221	9	22
1	38	16	24*	-8	43	20	18*	8	0	53	-16*	7	40	49	31*	-5	52	24	37*
2	301	7	-6	-7	295	7	-6	9	149	11	-4	8	180	7	7	-4	311	7	1
3	11	34	-3*	-6	66	12	-0	H,K=	4,	4		H,K=	4,	7		-3	15	36	-11*
4	258	6	-2	-5	374	9	5	-9	23	63	-5*	-8	0	44	-6*	-2	330	7	-2
5	0	44	-2*	-4	34	16	1*	-8	230	7	4	-7	219	6	-1	-1	24	29	18*
6	189	9	10	-3	701	20	-14	-7	0	44	-5*	-6	19	37	13*	0	317	11	-4
H,K=	3,	12		-2	35	9	10*	-6	332	7	-7	-5	350	8	3	1	58	9	-3
-6	38	42	29*	-1	793	20	-8	-5	12	33	-4*	-4	45	17	18*	2	365	8	-0
-5	190	8	-1	0	141	4	3	-4	414	9	12	-3	464	13	1	3	50	17	13*
-4	25	36	3*	1	748	15	0	-3	47	12	13*	-2	28	24	20*	4	267	7	-0
-3	258	7	-1	2	0	23	-11*	-2	571	12	-1	-1	480	19	1	5	13	39	7*
-2	26	33	8*	3	533	11	13	-1	24	25	-16*	0	41	9	0*	6	197	6	-7
-1	298	8	1	4	85	6	12	0	599	12	-13	1	381	8	-7	H,K=	4,	11	
0	41	16	-11*	5	447	9	12	1	0	26	-31*	2	105	5	-23	-6	38	45	38*
1	293	6	-3	6	0	42	-21*	2	623	13	-5	3	422	12	-15	-5	237	7	1
2	12	48	-1*	7	250	7	-4	3	0	29	-24*	4	28	33	19*	-4	38	24	-3*
3	252	6	-3	8	49	21	32*	4	460	10	4	5	316	7	-3	-3	294	7	4
4	0	43	-10*	9	160	7	-10	5	0	45	-15*	6	36	51	19*	-2	0	32	-19*
5	201	7	-1	H,K=	4,	2		6	311	7	1	7	226	7	1	-1	295	6	-2
H,K=	3,	13		-10	130	8	-0	7	33	39	-2*	8	20	43	14*	0	12	35	10*
-5	19	46	-5*	-9	8	39	5*	8	197	7	3	H,K=	4,	8		1	287	6	-4
-4	181	6	7	-8	201	7	-15	H,K=	4,	5		-8	169	9	15	2	46	23	12*
-3	39	26	17*	-7	52	14	32*	-9	171	9	3	-7	19	55	15*	3	267	6	-7
-2	249	6	3	-6	367	8	-2	-8	40	34	28*	-6	260	9	5	4	45	26	38*
-1	25	47	23*	-5	42	16	31*	-7	234	6	5	-5	0	34	-10*	5	223	7	-0

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	0	45	-10*	5	36	20	25*	5	326	7	5	6	254	7	-3	1	0	33	-31*
H,K=	4,	12		6	299	7	9	6	38	42	21*	7	30	46	26*	2	278	6	0
-6	152	9	-4	7	30	47	24*	7	245	9	0	H,K=	5,	8		3	0	37	-36*
-5	0	42	-4*	8	206	7	-6	8	10	46	5*	-8	60	18	54*	4	234	8	-2
-4	229	6	3	H,K=	5,	2		H,K=	5,	5		-7	201	6	8	5	26	42	17*
-3	48	14	32*	-9	145	7	-4	-9	41	53	36*	-6	0	39	-1*	H,K=	5,	12	
-2	262	6	-2	-8	43	28	-5*	-8	200	7	2	-5	265	7	-1	-5	174	6	-0
-1	14	35	6*	-7	261	6	-9	-7	60	15	51*	-4	51	11	12*	-4	56	21	42*
0	284	6	3	-6	22	38	3*	-6	301	7	-1	-3	289	6	-1	-3	250	7	3
1	0	36	-14*	-5	429	9	4	-5	25	36	16*	-2	36	16	20*	-2	24	34	6*
2	252	7	-1	-4	26	32	16*	-4	426	9	10	-1	446	14	1	-1	259	7	-1
3	0	41	-10*	-3	527	11	1	-3	0	32	-5*	0	18	27	2*	0	33	38	19*
4	233	6	1	-2	53	6	-3	-2	483	10	-4	1	443	15	-16	1	253	6	2
5	45	31	22*	-1	663	16	6	-1	22	25	7*	2	45	15	36*	2	7	36	-28*
H,K=	4,	13		0	59	4	-4	0	525	11	-6	3	355	8	-12	3	220	7	5
-5	166	8	13	1	633	13	0	1	0	31	-2*	4	0	36	-36*	4	27	47	25*
-4	0	40	-14*	2	22	24	19*	2	489	11	-1	5	254	8	-4	H,K=	5,	13	
-3	202	6	6	3	441	9	8	3	80	12	18	6	34	39	33*	-4	171	6	-2
-2	38	24	29*	4	66	8	8	4	399	9	2	7	172	7	1	-3	22	38	17*
-1	242	6	-0	5	374	8	6	5	21	34	19*	H,K=	5,	9		-2	219	6	3
0	0	35	-20*	6	48	17	36*	6	281	6	-1	-7	11	54	7*	-1	19	39	14*
1	274	7	-2	7	292	7	-6	7	20	51	17*	-6	216	8	2	0	240	6	-8
2	27	37	23*	8	0	46	-19*	8	158	8	-7	-5	40	28	26*	1	55	22	49*
3	217	6	9	H,K=	5,	3		H,K=	5,	6		-4	247	6	2	2	203	7	6
4	31	42	16*	-9	67	13	62*	-9	140	8	-5	-3	0	32	-9*	3	37	40	17*
H,K=	4,	14		-8	186	7	-10	-8	17	41	7*	-2	332	7	-2	H,K=	5,	14	
-3	42	26	28*	-7	9	36	7*	-7	219	6	-3	-1	14	29	8*	-3	185	6	4
-2	195	7	-5	-6	350	8	-8	-6	64	11	56	0	368	13	-7	-2	0	41	-2*
-1	19	43	16*	-5	56	12	-6*	-5	333	8	4	1	42	16	24*	-1	199	7	8
0	222	6	-4	-4	473	10	8	-4	38	19	27*	2	425	9	-16	0	19	43	-3*
1	22	38	-2*	-3	34	15	23*	-3	460	10	-2	3	31	36	20*	1	187	6	4
2	190	6	0	-2	566	15	-12	-2	0	30	-2*	4	250	6	-3	H,K=	6,	0	
H,K=	5,	0		-1	86	3	-5	-1	441	12	-3	5	27	43	20*	-8	238	6	5
-9	154	6	2	0	615	13	-4	0	28	19	7*	6	207	7	0	-6	273	6	5
-7	294	7	17	1	110	5	-8	1	481	10	-9	H,K=	5,	10		-4	447	9	4
-5	337	8	2	2	507	11	3	2	100	6	31	-7	155	8	1	-2	503	10	-14
-3	553	11	7	3	38	40	27*	3	416	9	1	-6	10	41	8*	0	534	11	2
-1	690	14	4	4	423	9	4	4	47	15	34*	-5	245	6	13	2	464	10	4
1	752	21	-4	5	15	33	8*	5	318	7	-2	-4	31	35	9*	4	491	10	0
3	476	10	2	6	319	7	-5	6	30	38	26*	-3	266	6	2	6	307	7	7
5	402	9	17	7	48	24	8*	7	204	6	6	-2	11	38	-0*	8	167	7	-4
7	267	6	1	8	186	7	-10	8	44	58	32*	-1	320	7	-12	H,K=	6,	1	
H,K=	5,	1		H,K=	5,	4		H,K=	5,	7		0	19	30	18*	-9	138	10	-8
-9	52	19	43*	-9	156	7	-5	-8	165	7	-0	1	329	8	-2	-8	18	39	-11*
-8	210	6	-0	-8	39	32	36*	-7	29	48	23*	2	103	8	13	-7	276	19	5
-7	36	40	33*	-7	233	6	-4	-6	278	7	6	3	296	7	-0	-6	16	34	11*
-6	279	7	3	-6	61	11	43	-5	18	42	13*	4	49	17	46*	-5	377	8	-8
-5	38	38	29*	-5	396	17	-3	-4	329	7	-2	5	231	6	-7	-4	43	22	5*
-4	544	17	1	-4	41	16	4*	-3	11	35	-13*	6	28	49	1*	-3	441	9	-7
-3	111	4	-1	-3	479	10	-1	-2	428	9	1	H,K=	5,	11		-2	39	8	-2*
-2	576	14	-1	-2	28	22	9*	-1	89	5	14	-6	167	7	4	-1	552	12	-1
-1	32	9	-14*	-1	526	17	-23	0	459	17	-6	-5	28	44	12*	0	80	4	8
0	671	14	1	0	154	4	-11	1	61	11	-22	-4	254	6	4	1	493	11	6
1	24	18	21*	1	604	13	14	2	425	9	-15	-3	31	34	29*	2	22	31	6*
2	558	12	-1	2	66	7	21	3	25	33	15*	-2	291	7	-4	3	521	12	-11
3	74	5	4	3	460	11	1	4	321	7	-4	-1	31	39	20*	4	29	30	-2*
4	513	11	-2	4	0	32	-8*	5	0	36	-2*	0	267	6	1	5	356	9	2

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	52	18	49*	6	270	6	-3	-7	24	45	19*	-5	38	50	21*	-2	25	28	-9*
7	235	6	-8	7	49	22	41*	-6	235	7	11	-4	200	6	3	-1	480	10	-7
8	43	44	23*	8	177	9	12	-5	29	36	28*	-3	26	41	9*	0	84	4	4
H,K=	6,	2		H,K=	6,	5		-4	253	6	-6	-2	241	6	2	1	470	10	-8
-9	50	21	47*	-9	129	8	-13	-3	19	31	12*	-1	34	35	31*	2	21	28	-7*
-8	199	6	10	-8	34	40	26*	-2	351	7	-11	0	251	6	4	3	447	10	-5
-7	20	37	17*	-7	208	7	3	-1	35	14	12*	1	0	36	-21*	4	0	32	-20*
-6	315	7	-2	-6	27	37	19*	0	383	14	-10	2	216	6	1	5	301	7	-5
-5	54	11	6*	-5	289	6	-2	1	0	55	-19*	3	54	29	3*	6	47	19	45*
-4	434	9	-3	-4	64	9	8	2	369	8	-9	4	204	7	12	7	215	6	6
-3	85	6	13	-3	469	10	1	3	35	35	-9*	H,K=	6,	13		H,K=	7,	3	
-2	538	11	5	-2	12	35	9*	4	263	6	2	-4	16	51	4*	-9	25	47	22*
-1	19	23	17*	-1	485	14	-5	5	50	18	46*	-3	191	6	3	-8	152	7	-5
0	547	12	-2	0	26	31	25*	6	196	9	3	-2	45	19	44*	-7	21	38	-3*
1	50	10	-3*	1	482	10	6	H,K=	6,	9		-1	207	6	3	-6	272	7	2
2	453	10	1	2	109	8	13	-7	166	8	4	0	62	12	50*	-5	30	42	22*
3	0	30	-1*	3	407	9	-3	-6	66	14	62*	1	211	6	-6	-4	355	8	-1
4	432	9	8	4	27	33	18*	-5	233	7	2	2	48	20	4*	-3	81	6	1
5	28	36	8*	5	299	7	-5	-4	0	45	-22*	H,K=	6,	14		-2	453	9	-5
6	313	7	-3	6	29	44	25*	-3	256	6	-3	-1	27	39	25*	-1	39	9	26*
7	0	54	-7*	7	179	7	-2	-2	4	30	-4*	0	167	8	-11	0	466	10	-4
8	174	8	-4	H,K=	6,	6		-1	337	7	3	H,K=	7,	0		1	13	27	1*
H,K=	6,	3		-8	161	8	-1	0	5	33	-13*	-9	133	8	0	2	512	11	-10
-9	150	10	7	-7	10	39	7*	1	352	12	-16	-7	256	6	-5	3	12	36	-34*
-8	44	34	27*	-6	250	7	1	2	50	16	44*	-5	339	7	-4	4	323	7	13
-7	214	6	-4	-5	18	36	-8*	3	269	6	0	-3	412	9	-11	5	40	25	17*
-6	40	40	13*	-4	350	8	7	4	33	45	13*	-1	458	10	-7	6	245	6	-3
-5	400	8	4	-3	63	22	-5*	5	230	6	-2	1	484	10	-2	7	0	42	-9*
-4	33	38	27*	-2	462	12	1	6	10	46	8*	3	431	9	-3	H,K=	7,	4	
-3	455	10	-2	-1	42	10	8*	H,K=	6,	10		5	324	7	1	-9	138	8	-0
-2	19	27	-10*	0	485	11	-7	-7	23	48	20*	7	198	7	-5	-8	34	40	23*
-1	570	12	-3	1	111	5	19	-6	167	7	1	H,K=	7,	1		-7	183	6	-5
0	72	6	-5	2	381	8	7	-5	20	41	14*	-9	28	42	23*	-6	18	43	9*
1	488	10	1	3	43	15	30*	-4	247	6	6	-8	195	6	-6	-5	276	6	-3
2	25	27	-4*	4	328	8	-3	-3	33	40	25*	-7	45	31	35*	-4	21	32	-11*
3	484	11	-11	5	20	36	17*	-2	300	6	-3	-6	278	7	-8	-3	394	12	-11
4	16	35	-10*	6	246	8	1	-1	18	31	4*	-5	0	33	-4*	-2	102	5	2
5	305	7	4	7	17	43	-2*	0	268	6	-3	-4	389	8	6	-1	459	10	-2
6	3	37	-16*	H,K=	6,	7		1	58	10	21	-3	41	16	8*	0	32	14	17*
7	231	11	-2	-8	36	45	33*	2	290	7	-3	-2	463	10	-2	1	442	10	2
8	43	52	29*	-7	197	6	-2	3	26	46	21*	-1	41	8	18*	2	0	42	-28*
H,K=	6,	4		-6	0	40	-10*	4	239	8	0	0	447	9	-6	3	416	9	3
-9	53	19	52*	-5	253	6	1	5	24	41	22*	1	76	7	7	4	11	39	-21*
-8	171	6	2	-4	44	14	43*	H,K=	6,	11		2	516	11	-18	5	278	6	-1
-7	29	37	22*	-3	376	8	-8	-6	52	21	44*	3	36	42	10*	6	46	47	38*
-6	284	6	-6	-2	18	40	-4*	-5	181	6	1	4	335	7	-0	7	178	7	-7
-5	45	48	15*	-1	426	13	4	-4	16	41	11*	5	30	35	20*	H,K=	7,	5	
-4	385	8	8	0	43	12	12*	-3	262	7	2	6	267	8	5	-8	153	7	2
-3	25	33	23*	1	424	10	-11	-2	50	12	32*	7	32	45	23*	-7	33	39	33*
-2	517	11	-1	2	19	38	2*	-1	270	6	-0	H,K=	7,	2		-6	238	6	9
-1	43	8	-11	3	329	7	5	0	0	33	-3*	-9	139	8	2	-5	39	24	1*
0	566	12	5	4	16	36	2*	1	266	6	-3	-8	39	42	37*	-4	324	8	-6
1	48	11	12*	5	274	7	-6	2	26	36	-20*	-7	207	8	-7	-3	0	34	-4*
2	454	10	1	6	64	14	54*	3	207	6	2	-6	32	35	31*	-2	391	8	-6
3	30	38	16*	7	168	7	-1	4	55	18	44*	-5	353	8	-8	-1	0	30	-4*
4	352	8	-4	H,K=	6,	8		5	197	11	-9	-4	0	47	-12*	0	457	9	-2
5	38	31	26*	-8	127	10	-9	H,K=	6,	12		-3	410	9	-2	1	46	14	1*

STRUCTURE FACTORS CONTINUED FOR
U(C2OH2O).

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	407	10	9	-5	0	39	-5*	4	300	7	-0	-7	51	19	41*	3	295	7	1
3	37	22	9*	-4	266	6	2	6	235	6	12	-6	242	6	12	4	40	27	18*
4	302	7	-3	-3	30	33	19*	H,K=	8,	1		-5	29	35	9*	5	225	6	5
5	19	49	2*	-2	284	6	-6	-9	102	14	-12	-4	293	6	-11	6	36	54	22*
6	232	7	2	-1	9	37	-2*	-8	14	44	13*	-3	67	10	-9	H,K=	8,		8
7	25	45	-10*	0	277	7	-6	-7	197	6	-2	-2	341	7	-1	-7	38	44	28*
H,K=	7,	6		1	2	34	-26*	-6	0	38	-13*	-1	0	35	-10*	-6	181	7	2
-8	18	42	14*	2	257	7	-1	-5	301	7	4	0	401	9	2	-5	45	59	31*
-7	199	8	4	3	45	29	9*	-4	0	36	-13*	1	19	29	-15*	-4	262	6	-0
-6	16	55	16*	4	241	8	-4	-3	389	8	-8	2	378	8	0	-3	32	34	15*
-5	243	6	9	5	46	37	40*	-2	49	13	-1*	3	41	16	4*	-2	273	6	-5
-4	38	40	-10*	H,K=	7,	10		-1	458	10	-8	4	295	7	-0	-1	40	25	33*
-3	400	9	-7	-6	42	43	39*	0	58	7	3	5	30	38	5*	0	285	8	-6
-2	19	38	-2*	-5	199	6	-8	1	502	10	-2	6	208	6	-6	1	38	42	9*
-1	394	8	5	-4	19	36	15*	2	40	16	12*	H,K=	8,		5	2	276	10	2
0	35	21	1*	-3	252	6	-0	3	284	6	8	-8	50	41	46*	3	31	37	4*
1	389	9	9	-2	32	33	23*	4	15	38	-9*	-7	196	6	-5	4	247	7	2
2	36	22	7*	-1	262	6	-4	5	289	7	3	-6	25	64	16*	5	25	42	23*
3	327	7	6	0	0	36	-13*	6	16	40	6*	-5	231	6	-3	H,K=	8,		9
4	26	39	26*	1	262	6	2	7	196	8	4	-4	0	34	-8*	-6	71	15	59*
5	282	7	-9	2	63	12	50	H,K=	8,	2		-3	315	12	-5	-5	223	6	4
6	25	43	24*	3	213	7	-6	-9	46	53	45*	-2	32	32	30*	-4	37	31	36*
7	182	7	3	4	66	16	40*	-8	161	7	9	-1	365	8	3	-3	234	6	-4
H,K=	7,	7		5	193	7	-0	-7	0	39	-24*	0	0	29	-18*	-2	44	15	39*
-8	142	7	12	H,K=	7,	11		-6	234	6	-10	1	365	9	10	-1	278	6	4
-7	20	41	3*	-5	41	49	29*	-5	19	34	5*	2	34	28	14*	0	27	34	18*
-6	222	7	3	-4	205	6	1	-4	326	7	-0	3	305	8	5	1	240	6	1
-5	32	42	26*	-3	32	36	23*	-3	18	41	-3*	4	0	36	-11*	2	71	12	37
-4	313	7	1	-2	247	6	-3	-2	439	9	2	5	262	8	-0	3	258	6	8
-3	28	32	4*	-1	36	24	30*	-1	45	8	33*	6	0	52	-7*	4	25	41	23*
-2	351	7	-2	0	254	9	-3	0	451	9	0	H,K=	8,		6	H,K=	8,		10
-1	26	34	14*	1	13	41	0*	1	9	30	-16*	-8	141	7	7	-6	147	11	5
0	381	8	-3	2	201	7	-2	2	415	9	0	-7	21	41	7*	-5	40	37	25*
1	0	34	-21*	3	36	50	23*	3	38	26	36*	-6	222	6	9	-4	213	7	7
2	322	7	6	4	207	7	-6	4	318	7	-2	-5	47	25	39*	-3	0	47	-21*
3	14	35	1*	H,K=	7,	12		5	0	39	-0*	-4	288	7	-5	-2	242	6	-0
4	282	7	-9	-4	0	40	-14*	6	226	8	-3	-3	26	43	20*	-1	19	34	14*
5	0	40	-3*	-3	195	6	4	7	5	43	4*	-2	294	7	-3	0	245	7	2
6	188	7	-6	-2	18	40	9*	H,K=	8,	3		-1	19	34	-12*	1	46	49	19*
H,K=	7,	8		-1	223	6	4	-8	3	51	-8*	0	370	8	5	2	215	6	-3
-7	163	8	2	0	49	20	49*	-7	176	7	-3	1	0	33	-13*	3	61	26	29*
-6	39	41	32*	1	241	7	1	-6	0	39	-8*	2	319	7	6	4	211	6	9
-5	249	6	-3	2	0	40	-43*	-5	280	6	-9	3	38	23	28*	H,K=	8,		11
-4	27	38	1*	3	195	9	9	-4	23	38	8*	4	286	7	-6	-5	154	7	1
-3	302	7	-8	H,K=	7,	13		-3	339	7	-0	5	42	29	18*	-4	33	38	13*
-2	38	16	37*	-3	0	45	-0*	-2	31	21	-10*	6	188	7	-17	-3	192	6	-3
-1	320	11	2	-2	176	6	7	-1	430	9	-3	H,K=	8,		7	-2	0	36	-6*
0	0	32	-17*	-1	28	38	23*	0	38	50	29*	-7	159	8	-4	-1	226	6	1
1	322	7	-3	0	207	6	-2	1	429	9	-1	-6	0	40	-1*	0	0	37	-11*
2	26	36	-20*	1	0	43	-17*	2	25	29	-29*	-5	222	7	-7	1	222	6	-0
3	271	6	-2	H,K=	8,	0		3	331	7	-4	-4	60	14	10*	2	36	43	5*
4	49	18	44*	-8	162	7	-6	4	37	23	15*	-3	302	7	6	3	201	7	-4
5	222	6	5	-6	240	7	-3	5	270	7	-1	-2	0	34	-27*	H,K=	8,		12
6	8	47	1*	-4	337	7	1	6	23	39	23*	-1	323	8	2	-3	32	49	27*
H,K=	7,	9		-2	460	10	-8	7	183	7	0	0	47	15	41*	-2	185	9	3
-7	61	20	56*	0	474	10	-1	H,K=	8,	4		1	314	7	4	-1	0	38	-3*
-6	196	7	13	2	386	8	-1	-8	149	10	-2	2	52	13	41*	0	212	6	-3

STRUCTURE FACTORS CONTINUED FOR
U(C20H20).

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	47	22	45*	H,K=	9,	4		5	57	21	45*	-1	269	6	0	-1	291	6	-0
H,K=	9,	0		-8	0	46	-3*	H,K=	9,	8		0	0	33	-6*	0	0	34	-6*
-7	166	6	-6	-7	181	7	1	-6	47	27	33*	1	318	7	-5	1	289	7	9
-5	250	6	9	-6	38	39	23*	-5	183	6	-3	2	20	32	-2*	2	52	21	17*
-3	382	8	-8	-5	242	6	-5	-4	0	54	-27*	3	301	7	-1	3	220	6	2
-1	357	7	-7	-4	47	14	44*	-3	223	6	9	4	0	45	-20*	4	24	39	20*
1	383	8	-0	-3	300	6	-2	-2	50	17	30*	5	215	7	-1	5	193	6	10
3	287	6	-1	-2	0	31	-1*	-1	284	9	4	H,K=	10,	2		H,K=	10,	6	
5	238	7	2	-1	345	7	1	0	49	16	41*	-8	117	9	-9	-6	159	10	3
H,K=	9,	1		0	0	30	-11*	1	269	6	4	-7	30	40	16*	-5	26	41	26*
-8	150	11	12	1	302	7	-1	2	53	15	23*	-6	191	7	5	-4	212	8	-3
-7	34	39	34*	2	22	32	-16*	3	252	7	-1	-5	0	36	-4*	-3	17	36	-6*
-6	210	7	0	3	292	7	-12	4	37	41	33*	-4	251	6	-4	-2	268	6	6
-5	22	35	14*	4	33	37	5*	H,K=	9,	9		-3	0	40	-15*	-1	0	38	-2*
-4	293	7	2	5	214	6	0	-6	146	8	12	-2	275	6	-4	0	280	6	1
-3	47	10	10*	6	48	55	44*	-5	52	20	43*	-1	27	30	4*	1	18	40	5*
-2	406	8	-3	H,K=	9,	5		-4	183	6	-2	0	314	7	-6	2	275	6	5
-1	35	26	-5*	-7	49	22	44*	-3	0	37	-14*	1	18	46	5*	3	42	26	2*
0	389	8	4	-6	210	7	3	-2	236	6	-3	2	310	7	-4	4	188	6	3
1	0	32	-19*	-5	0	38	-6*	-1	41	27	19*	3	40	19	-3*	H,K=	10,	7	
2	287	7	-0	-4	269	6	-4	0	229	7	-7	4	261	6	4	-6	33	56	11*
3	51	16	3*	-3	0	33	-17*	1	31	41	20*	5	23	44	5*	-5	157	7	-5
4	313	7	1	-2	293	7	-0	2	249	7	10	H,K=	10,	3		-4	33	42	22*
5	29	47	26*	-1	16	30	1*	3	7	42	0*	-7	136	8	-8	-3	208	6	-3
6	211	6	4	0	319	7	1	4	168	10	-7	-6	19	40	2*	-2	31	40	15*
H,K=	9,	2		1	36	18	33*	H,K=	9,	10		-5	218	6	-12	-1	264	6	6
-8	0	56	-7*	2	298	7	3	-5	157	7	-0	-4	15	34	12*	0	8	35	3*
-7	167	6	5	3	29	41	11*	-4	39	48	3*	-3	265	6	-8	1	279	7	7
-6	47	18	46*	4	246	6	4	-3	179	6	-3	-2	25	31	20*	2	38	51	35*
-5	255	7	-3	5	36	46	23*	-2	25	43	23*	-1	306	7	-3	3	213	6	-1
-4	32	33	28*	H,K=	9,	6		-1	222	6	-1	0	25	31	15*	4	28	44	23*
-3	345	8	2	-7	171	7	-0	0	0	38	-5*	1	284	6	-5	H,K=	10,	8	
-2	60	8	-14	-6	38	58	34*	1	222	7	4	2	27	33	21*	-5	39	56	37*
-1	374	8	-4	-5	203	6	-0	2	19	43	-2*	3	289	7	-2	-4	163	7	-2
0	0	28	-18*	-4	29	46	7*	3	212	7	15	4	0	40	-20*	-3	34	42	21*
1	352	8	-2	-3	268	6	4	H,K=	9,	11		5	210	6	3	-2	237	6	4
2	16	30	8*	-2	29	31	-4*	-3	28	38	15*	H,K=	10,	4		-1	18	36	1*
3	327	7	-10	-1	309	7	3	-2	185	6	2	-7	21	57	12*	0	237	6	-1
4	54	13	16*	0	35	37	33*	-1	0	38	-8*	-6	180	7	4	1	34	38	28*
5	251	6	4	1	317	7	7	0	201	6	0	-5	27	37	22*	2	223	6	0
6	2	42	-4*	2	23	40	20*	1	26	41	8*	-4	265	7	-3	3	26	41	25*
H,K=	9,	3		3	282	7	1	H,K=	10,	0		-3	26	33	16*	H,K=	10,	9	
-8	141	8	3	4	64	13	28*	-8	122	13	-10	-2	288	6	-2	-5	153	7	4
-7	0	43	-2*	5	201	6	-4	-6	200	6	0	-1	36	28	13*	-4	34	42	22*
-6	211	6	-0	H,K=	9,	7		-4	250	6	-7	0	301	7	5	-3	177	8	1
-5	33	35	28*	-7	2	44	1*	-2	268	6	-4	1	26	34	11*	-2	0	38	-15*
-4	285	6	-5	-6	163	11	-1	0	321	7	-6	2	278	7	-3	-1	223	7	2
-3	28	30	15*	-5	26	47	-2*	2	298	7	-1	3	22	36	-5*	0	38	46	27*
-2	356	7	-2	-4	224	6	2	4	243	6	4	4	200	6	7	1	218	7	12
-1	16	38	10*	-3	0	40	-2*	H,K=	10,	1		5	17	51	-7*	2	34	41	27*
0	347	8	6	-2	270	7	3	-8	0	45	-10*	H,K=	10,	5		H,K=	10,	10	
1	52	9	19	-1	17	41	-2*	-7	150	10	-10	-7	146	12	-2	-3	37	42	34*
2	305	7	-11	0	293	7	-1	-6	44	24	40*	-6	0	60	-3*	-2	187	6	0
3	0	38	-5*	1	17	38	16*	-5	222	6	1	-5	201	6	-0	-1	0	39	-21*
4	295	7	-3	2	302	7	2	-4	0	35	-7*	-4	25	36	-1*	0	191	7	0
5	0	44	-4*	3	0	38	-28*	-3	284	6	-10	-3	262	6	-8	1	42	54	39*
6	197	6	-2	4	234	7	7	-2	35	18	-21*	-2	29	32	24*	H,K=	11,	0	

STRUCTURE FACTORS CONTINUED FOR
U(C20H20).

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	146	7	-4	H,K=	11,	5		-3	232	6	6	-3	165	6	6				
-5	186	8	-11	-6	136	8	1	-2	27	38	20*	-2	23	39	20*				
-3	239	6	-5	-5	30	39	24*	-1	237	6	-7	-1	157	6	7				
-1	268	6	1	-4	206	6	3	0	38	23	28*	0	0	41	-1*				
1	274	6	-5	-3	0	37	-17*	1	218	6	-4	1	179	9	-3				
3	223	6	-1	-2	255	6	4	2	48	16	44*	H,K=	12,	8					
H,K=	11,	1		-1	40	18	35*	3	200	6	-0	-1	0	47	-6*				
-7	36	50	33*	0	250	6	8	H,K=	12,	2		H,K=	13,	0					
-6	179	6	0	1	39	22	25*	-6	127	8	-6	-5	129	8	-5				
-5	36	37	35*	2	224	7	8	-5	0	43	-8*	-3	211	7	2				
-4	209	7	-2	3	0	39	-5*	-4	179	6	5	-1	202	7	4				
-3	46	18	42*	4	186	8	11	-3	9	40	-9*	1	198	7	4				
-2	244	6	5	H,K=	11,	6		-2	231	6	7	H,K=	13,	1					
-1	29	41	16*	-6	31	45	21*	-1	25	34	15*	-5	28	41	21*				
0	288	7	-6	-5	151	7	-1	0	219	6	-4	-4	156	7	-7				
1	29	32	24*	-4	19	39	8*	1	0	42	-10*	-3	32	37	31*				
2	258	6	-2	-3	216	6	5	2	217	6	-4	-2	192	6	-6				
3	35	37	23*	-2	23	43	15*	3	34	45	19*	-1	37	42	20*				
4	209	6	-6	-1	233	6	9	H,K=	12,	3		0	200	6	9				
H,K=	11,	2		0	25	37	21*	-6	43	35	36*	1	35	37	30*				
-7	128	13	-4	1	241	6	11	-5	153	9	-0	2	181	7	4				
-6	25	40	23*	2	46	22	21*	-4	18	38	10*	H,K=	13,	2					
-5	194	6	4	3	185	7	5	-3	184	5	3	-4	31	48	29*				
-4	55	12	33*	H,K=	11,	7		-2	38	23	10*	-3	168	6	3				
-3	207	6	-3	-5	28	43	25*	-1	234	6	-0	-2	29	47	14*				
-2	20	32	17*	-4	168	9	2	0	31	43	25*	-1	183	6	5				
-1	283	6	-4	-3	0	38	-1*	1	218	7	2	0	27	36	20*				
0	30	32	20*	-2	215	6	7	2	41	24	26*	1	181	6	-4				
1	264	6	-3	-1	0	36	-1*	3	200	6	-5	2	47	23	47*				
2	17	34	9*	0	210	6	7	H,K=	12,	4		H,K=	13,	3					
3	240	6	-8	1	19	39	8*	-5	0	58	0*	-4	155	6	3				
4	10	52	-13*	2	197	6	0	-4	168	6	-3	-3	26	40	21*				
H,K=	11,	3		3	22	51	9*	-3	0	36	-7*	-2	172	6	7				
-7	42	50	42*	H,K=	11,	8		-2	209	6	-5	-1	0	38	-7*				
-6	141	7	-6	-4	0	61	-1*	-1	34	38	17*	0	190	7	6				
-5	39	29	37*	-3	183	7	2	0	208	6	-1	1	28	38	21*				
-4	203	6	-4	-2	35	37	31*	1	39	40	35*	H,K=	13,	4					
-3	28	33	7*	-1	208	7	14	2	207	6	6	-4	32	40	29*				
-2	245	6	-2	0	58	14	49*	3	0	40	-27*	-3	151	9	-5				
-1	47	16	5*	1	182	7	-0	H,K=	12,	5		-2	31	39	26*				
0	279	6	-2	2	37	47	31*	-5	142	7	3	-1	178	6	-0				
1	38	42	37*	H,K=	11,	9		-4	21	43	16*	0	0	38	-13*				
2	244	7	-8	-3	0	43	-2*	-3	192	7	6	1	185	7	2				
3	8	38	-19*	-2	194	8	8	-2	50	22	45*	H,K=	13,	5					
4	207	6	-4	-1	27	40	11*	-1	188	5	-6	-3	11	56	10*				
H,K=	11,	4		0	178	7	7	0	0	36	-25*	-2	159	6	-4				
-6	0	50	-4*	1	68	23	66*	1	207	6	3	-1	33	38	7*				
-5	181	6	0	H,K=	12,	0		2	0	38	-5*	0	173	6	-1				
-4	0	40	-11*	-6	149	7	-0	H,K=	12,	6									
-3	227	6	1	-4	194	6	-3	-4	152	7	1								
-2	41	17	11*	-2	264	6	4	-3	38	38	35*								
-1	287	7	1	0	236	6	4	-2	180	6	5								
0	44	15	30*	2	204	7	-5	-1	0	37	-16*								
1	253	6	11	H,K=	12,	1		0	174	6	1								
2	35	48	18*	-6	0	53	-11*	1	0	38	-9*								
3	194	6	1	-5	163	6	1	2	190	6	4								
4	37	41	-11*	-4	13	42	-0*	H,K=	12,	7									

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