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THE SYNTHESIS AND STRUCTURE OF Di-n- PROPYIAMMONIUM ETHOXYBIS (DI-n-PROPYILMONOTHIOCARBAMATO)DIOXOURANATE(VI), A MIXED CHELATE ALKOXIDE OF URANIUM

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Dale L. Perry, David H. Templeton and Allan Zalkin

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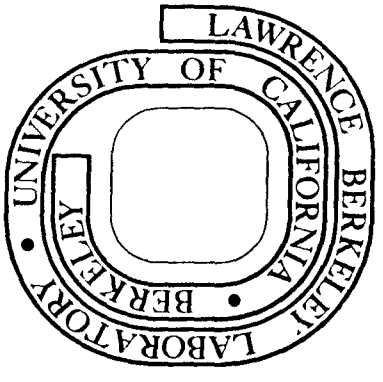

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THE SYNTHESIS AND STRUCTURE OF DI-n-PROPYLAMMONIUM ETHOXYBIS(DI-n-PROPYLMONOTHIOCARBAMATO)DIOXOURANATE(VI), A MIXED CHELATE ALKOXIDE OF URANIUM

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Although many reports involving the uranyl ion, UO_2^{+2}, have appeared in the chemical literature, most concern the chemistry of the simple salts (and adducts of these compounds)[1] and complexes which exhibit uranyl-oxygen and uranyl-nitrogen linkages.[2,3] The chemistry of the common organic chelating species such as tropolonates,[4] β-diketonates,[5] and Schiff bases[6] has been described, and much attention has also been focused on the structural aspects[2,3] of such compounds. Photochemical studies[7] and the use of the uranyl ion (in the form of complex species of the type $UO_2F_5^{-3}$, for example) in studies of the binding of heavy metals to proteins[8] have also been reported.

Uranyl complexes involving heavier donor atoms in Group VA (such as phosphorous and arsenic) and Group VIA (such as sulfur and selenium), however, are not so well known. The UO_2^{+2} ion is considered to be a "hard" acid[9] and thus does not easily form simple acceptor-donor adducts with the heavy congeners of nitrogen and oxygen and, as a

result, virtually all uranyl-sulfur compounds found in the research literature involve sulfur as the sulfide[1] or some other anionic form such as the thiocarbamate involved in this investigation.

The present report details the synthesis and structural study of one of the members of a new set of compounds[10] of the type $[R_2NH_2]^+[UO_2(R_2NCOS)_2OR']^-$ (the uranyl thiocarbamate alkoxides), where R = n - C_3H_7 and R' = C_2H_5 in this case. These compounds represent (1) the first air and moisture stable class of actinide alkoxides, (2) the first actinide alkloxide existing in conjunction with a chelating anion, and (3) the first UO_5S_2 metal center. Consequently, since these compounds also possess the uranium-oxygen bond in three separate environments in the same molecule, they are of considerable structural interest.

EXPERIMENTAL

The title compound was prepared by bubbling carbonyl sulfide (Matheson, 97.5% purity) through a solution of di-n-proylamine (Eastman, reagent grade) in absolute ethanol at 0°C for 5-10 minutes followed by the addition of a saturated, ethanolic solution of $UO_2Cl_2 \cdot 3H_2O$ (Alfa Products) with stirring. The bright yellow complex that precipitated from solution was filtered on a Buchner funnel, washed with several portions of cold diethyl ether, and allowed to dry in the open air.

Anal. Calcd. for $[(\underline{n}\text{-}C_3H_7)_2NH_2]^+[UO_2((\underline{n}\text{-}C_3H_7)_2NCOS)_2OC_2H_5]^-$: C, 35.83; H, 6.65; N, 5.70; S, 8.70. Found: C, 35.72; H, 6.52; N, 5.71; S, 8.34.

A small yellow crystal, of approximately 0.14 × 0.11 × 0.08 mm in size, was glued to a glass fiber and examined with a Picker FACS-I automatic diffractometer equipped with a graphite monochromator and a Cu X-ray tube ($\lambda(K\alpha_1)$ 1.54056 Å). Omega scans of several low angle reflections showed peaks with half-widths of 0.1°. The space group is C2/c. The setting angles of 12 manually centered reflections ($91° < 2\theta < 95°$) were used to determine the least-squares the following cell parameters: $\underline{a}$ = 23.217(7) Å, $\underline{b}$ = 15.238(3) Å, $\underline{c}$ = 19.567(6) Å, β = 109.50(4)° and V = 6525 $Å^3$. For Z=8 and a molecular weight of 713.8 the calculated density is 1.45 gm cm^{-3}.

Intensity data were collected using the θ-2θ scan technique with a scan speed of 2°/min on 2θ. Each peak was scanned 0.7° before the $K\alpha_1$ peak to 0.7° after the $K\alpha_2$ peak, and backgrounds were counted for 10 seconds at each end of the scan range. The temperature during the data collection was 22 ± 1°C. Three standard reflections were measured every 200th scan. A total of 8674 scans were performed, but the last 3245 were deleted because of the severity of the crystal decomposition and lack of consistency among the standard reflections. The 5071 scans, excluding the standard reflections, resulted in 4046 unique data of which 2815 had $I > 3\sigma$. An absorption correction (μ = 165 cm^{-1}) was applied[11] which ranged from 2.4 to 4.4. The crystal decay factor based on the variations of the three standard reflections ranged from 1.0 to

2.1. This large variation was alleviated to some extent by the averaging of equivalent reflections, but remains one of the limiting factors in the accuracy of the data.

A three-dimensional Patterson calculation showed the uranium atom position, and subsequent least-squares refinements and Fourier calculations revealed all of the atoms in the structure. Least-squares refinements in which the function $\Sigma w(|F_o|-|F_c|)^2/\Sigma wF_o^2$ was minimized converged rapidly to the final structure. The expressions that were used in proccessing the data and estimating weights are given in the supplementary material; the "ignorance factor", p was set to 0.05. Scattering factors from Doyle and Turner[12] were used, and anomalous dispersion corrections[13] were applied. Anisotropic thermal parameters were applied only to the uranium atom. Hydrogen atoms were included at calculated positions of 0.95 ± 0.01 Å from the carbon or nitrogen atoms to which they are bonded, but they were not refined.

The discrepancy indices for 2739 data where $F^2 > 3\sigma$ and $25° < 2\theta < 110°$ are

$$R = \Sigma||F_o|-|F_c||/\Sigma|F_o| = 0.044$$

$$R_w = [\Sigma w(|F_o|-|F_c|)^2/\Sigma|F_o|^2]^{1/2} = 0.054$$

R for all 4046 data is 0.069. The error in an observation of unit weight is 1.29. In the last cycle no parameter changed more than 0.17 σ. The largest peak in the final difference Fourier was 1.4 e/Å^3 and is a ripple near the uranium atom.

RESULTS AND DISCUSSION

Atomic parameters, distances and angles are listed in Tables I-III. Figure 1 shows an ORTEP view of the non-hydrogen atoms and the numbering scheme used for the atoms in the tables.

The uranium atom is heptacoordinate and is at the center of a pentagonal bipyramid consisting of two sulfur atoms and five oxygen atoms (See Fig. 1). The overall molecular structure of the title compound is remarkably similar to that of diethylammonium ethoxy-bis(diethylmonocarbamato)dioxouranate(VI),[10] which has ethyl groups in place of n-propyl groups. In each compound two formula units form a hydrogen bonded dimer about a crystallographic center of symmetry. These dimers pack in the two crystal lattices with different symmetry, yet corresponding bond distances and angles (excepting the alkyl groups) are in close agreement for the two structures. This consistency indicates that we are observing a structure which is characteristic of the complex, and not one which is dominated by molecular packing effects or subject to excessive error. On the other hand, the alkyl groups are poorly defined with some large thermal parameters and some bond lengths which clearly are in error.

ACKNOWLEDGEMENT

This work was supported by the Division of Nuclear Sciences, Office of Basic Energy Sciences, U.S. Department of Energy. D.L.P. was a National Science Foundation Postdoctoral Fellow, 1976-1977 and a Miller Fellow, 1977-79.

Supplementary material available: Data processing formulas and the listing of structure factor amplitudes (17 pages). Ordering information is given on any current masthead page.

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Table I. Positional and Thermal Parameters with Estimated Deviations[a] for the Non-hydrogen Atoms.

	x	y	z	B
U	.14583(2)	.04975(3)	.11598(3)	[b]
S(1)	.1140(2)	.1771(3)	.2058(2)	6.84(9)
S(2)	.1487(2)	-.0406(3)	.2455(2)	7.49(9)
O(1)	.1272(4)	.2011(6)	.0813(5)	6.2(2)
O(2)	.1693(4)	-.1029(6)	.1325(5)	6.3(2)
O(3)	.1575(4)	.0261(5)	.0112(5)	5.8(2)
O(4)	.0662(4)	.0272(5)	.0706(5)	5.6(2)
O(5)	.2244(4)	.0738(6)	.1556(5)	6.0(2)
N(1)	.1128(6)	.327(1)	.1335(8)	8.6(3)
N(2)	.1924(6)	-.199(1)	.2265(8)	8.5(3)
N(3)	-.0501(5)	.0136(8)	.0911(6)	6.2(3)
C(1)	.1168(6)	.238(1)	.1340(8)	6.6(3)
C(2)	.1711(6)	-.120(1)	.1962(8)	6.1(3)
C(3)	.2105(9)	.020(1)	-.012(1)	9.9(5)
C(4)	.234(2)	-.079(2)	-.007(2)	19.1(11)
C(5)	.1232(9)	.378(1)	.073(1)	9.7(5)
C(6)	.062(1)	.389(2)	.016(1)	11.9(6)
C(7)	.074(1)	.450(2)	-.046(2)	14.4(8)
C(8)	.0935(9)	.378(1)	.190(1)	9.9(5)
C(9)	.150(1)	.411(2)	.237(1)	11.6(6)
C(10)	.126(1)	.469(2)	.294(1)	13.1(7)
C(11)	.2161(8)	-.257(1)	.186(1)	9.3(5)
C(12)	.181(2)	-.337(3)	.159(2)	19.6(12)
C(13)	.130(2)	-.334(3)	.114(2)	22.4(15)
C(14)	.213(1)	-.214(1)	.308(1)	11.1(6)
C(15)	.162(1)	-.252(2)	.313(1)	13.3(7)
C(16)	.186(1)	-.267(2)	.407(1)	14.3(7)
C(17)	-.0326(7)	-.063(1)	.1415(8)	6.8(3)
C(18)	-.0239(7)	-.147(1)	.1014(9)	8.4(4)
C(19)	-.002(1)	-.223(2)	.152(1)	12.5(6)
C(20)	-.0556(7)	.096(1)	.128(1)	8.3(4)
C(21)	-.0639(8)	.169(1)	.073(1)	9.4(5)
C(22)	-.074(1)	.261(2)	.107(1)	14.4(7)

[a] Here and in the following tables the number in parenthesis is the estimated standard deviations for the least significant figures.

[b] The anisotropic temperature factor for U has the form $\exp(-0.25(B_{11}h^2a^{*2}+2B_{12}hka^*b^*+...))$, with B_{11} = 4.43(2), B_{22} = 4.71(3), B_{33} = 5.00(3), B_{12} = -0.31(2), B_{13} = 1.43(2) and B_{23} = -0.08(2).

Table II. Estimated Hydrogen Positional Parameters[a]

	x	y	z
H(1)	.2425	.0568	.0182
H(2)	.1995	.0398	-.0616
H(3)	.2032	-.1162	-.0376
H(4)	.2461	-.0992	.0422
H(5)	.2699	-.0817	-.0228
H(6)	.1505	.3458	.0546
H(7)	.1408	.434	.0906
H(8)	.0344	.4166	.0355
H(9)	.0464	.3327	-.004
H(10)	.1023	.4217	-.065
H(11)	.0903	.5057	-.0254
H(12)	.0359	.4593	-.0846
H(13)	.075	.3402	.216
H(14)	.0659	.425	.1683
H(15)	.1697	.4484	.2115
H(16)	.1774	.3656	.2612
H(17)	.1055	.4304	.3174
H(18)	.0977	.5133	.2677
H(19)	.1600	.4961	.3297
H(20)	.2563	-.2742	.216
H(21)	.2188	-.2255	.1445
H(22)	.1774	-.3664	.2008
H(23)	.2055	-.3721	.1383
H(24)	.1321	-.3060	.0711
H(25)	.104	-.3002	.1336
H(26)	.1143	-.3920	.1033
H(27)	.2223	-.160	.3351
H(28)	.2478	-.2524	.3244
H(29)	.1536	-.3069	.2873
H(30)	.1273	-.2143	.2960
H(31)	.1953	-.211	.4303
H(32)	.2215	-.3036	.4216
H(33)	.1537	-.2945	.4194
H(34)	-.0637	-.0735	.1627
H(35)	.0053	-.0494	.1792
H(36)	.0059	-.135	.0782
H(37)	-.0621	-.1617	.0655
H(38)	-.0317	-.2356	.1756
H(39)	.0363	-.2088	.1884
H(40)	.0026	-.2737	.1255
H(41)	-.0187	.1056	.1684
H(42)	-.0897	.094	.1448
H(43)	-.0987	.1570	.0315
H(44)	-.028	.1733	.0592
H(45)	-.0389	.2737	.1492
H(46)	-.1097	.2574	.1215
H(47)	-.0791	.3066	.072
H(48)	-.0891	0	.0543
H(49)	-.0119	.0180	.084

[a]Isotropic temperature parameters assigned were B = 10.0 $Å^2$ for atoms H(1)-H(47) and B = 8.0 $Å^2$ for H(47) and H(48).

Table III. Distances (Å)

U	-O(1)	2.40(1)	C(17)-N(3)	1.49(2)
	-O(2)	2.39(1)	C(20)-N(3)	1.47(2)
	-O(3)	2.19(1)	C(3) -C(4)	1.61(4)
	-O(4)	1.80(1)	C(5) -C(6)	1.49(3)
	-O(5)	1.77(1)	C(6) -C(7)	1.62(3)
	-S(1)	2.877(4)	C(8) -C(9)	1.42(3)
	-S(2)	2.865(4)	C(9) -C(10)	1.67(3)
S(1)	-C(1)	1.70(2)	C(11)-C(12)	1.46(4)
S(2)	-C(2)	1.73(2)	C(12)-C(13)	1.22(5)
O(1)	-C(1)	1.26(2)	C(14)-C(15)	1.35(3)
O(2)	-C(2)	1.26(2)	C(15)-C(16)	1.74(3)
O(3)	-C(3)	1.45(2)	C(17)-C(18)	1.55(2)
N(1)	-C(1)	1.37(2)	C(18)-C(19)	1.50(3)
N(2)	-C(2)	1.35(2)	C(20)-C(21)	1.51(3)
C(5)	-N(1)	1.50(2)	C(21)-C(22)	1.60(3)
C(8)	-N(1)	1.54(2)	N(3) -O(3)[a]	2.70(2)
C(11)	-N(2)	1.43(2)	N(3) -O(4)	2.87(2)
C(14)	-N(2)	1.53(3)		

[a]At position -x, -y, -z.

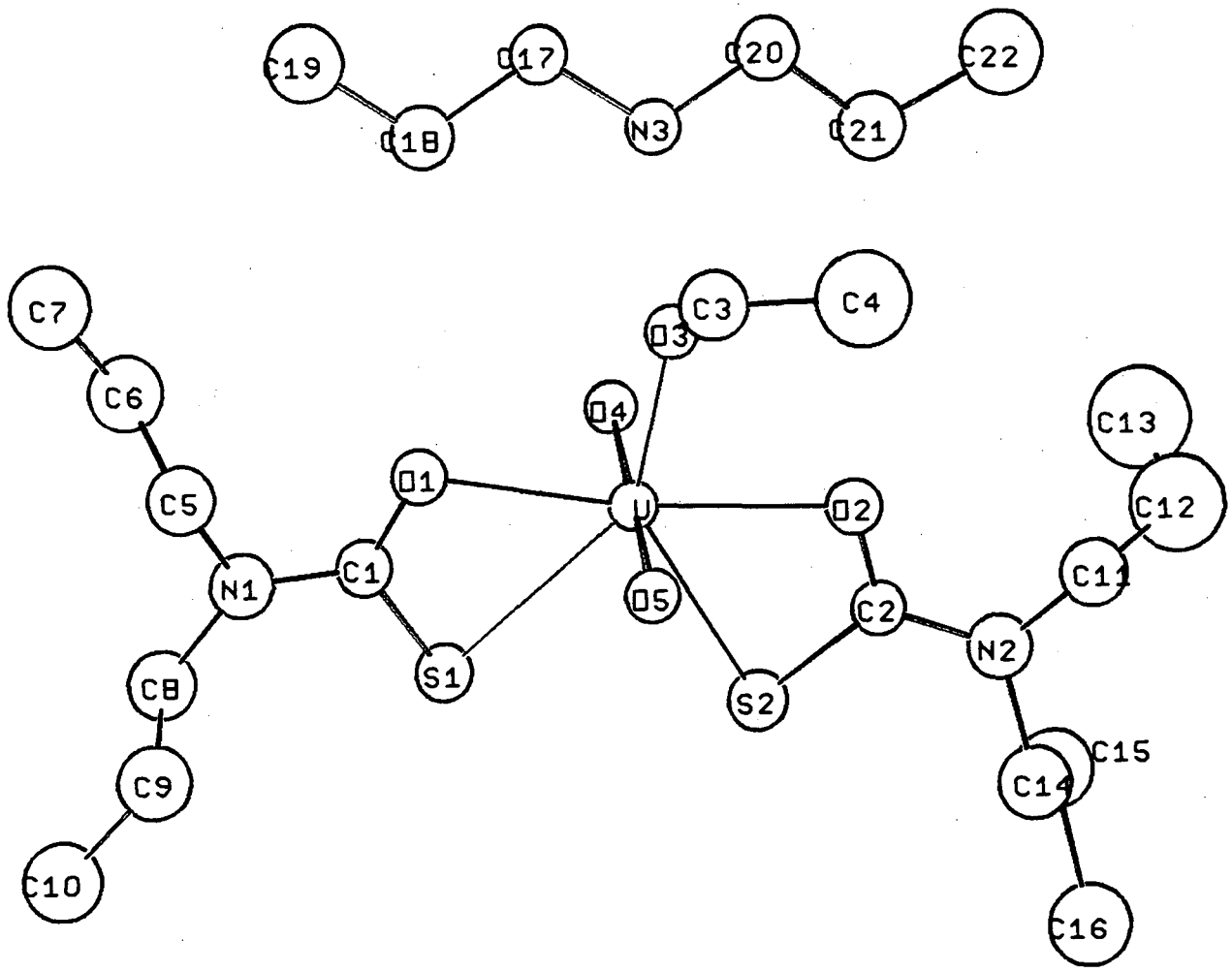
Table IV. Selected angles (deg).

O(4) -U	-O(5)	176.6(4)
O(4) -U	-O(1)	89.2(4)
	-O(2)	91.8(4)
	-O(3)	86.2(4)
	-S(1)	90.0(3)
	-S(2)	93.6(3)
O(5) -U	-O(1)	89.3(4)
	-O(2)	89.3(4)
	-O(3)	90.7(4)
	-S(1)	91.7(3)
	-S(2)	89.7(3)
O(1) -U	-O(3)	87.7(3)
O(3) -U	-O(2)	82.7(3)
O(2) -U	-S(2)	58.3(2)
S(2) -U	-S(1)	73.6(2)
S(1) -U	-O(1)	57.7(3)
O(1) -C(1)	-S(1)	120(1)
O(2) -C(2)	-S(2)	119(1)
C(1) -N(1)	-C(5)	119(2)
C(1) -N(1)	-C(8)	122(2)
C(5) -N(1)	-C(8)	118(2)
C(2) -N(2)	-C(11)	118(2)
C(2) -N(2)	-C(14)	122(2)
C(11) -N(2)	-C(14)	117(2)
O(3)[a] -N(3)	-O(4)	126(1)

[a]Atom at -x, -y, -z.

FIGURE CAPTION

Fig. 1. ORTEP view of the structure.



$UO_2(SOCN(C_3H_7)_2)_2(O(C_2H_5))-(C_3H_7)_2NH_2^+$

XBL 788-10657

Fig. 1

Supplementary materials for the paper:

The Synthesis and Structure of Di-n-propylammoniumethoxybis (di-n-propylmonothiocarbamato) dioxouranate(VI), A Mixed Chelate Alkoxide of Uranium

by Dale L. Perry, David H. Templeton and Allan Zalkin

DATA PROCESSING FORMULAE

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

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

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

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

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

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

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

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

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 1.0)
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ F(0,0,0) = 2702

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		H,K=	0,	6		12	106	5	-3	-3	289	0	-2*	9	214	6	0
2	66	0	-31*	0	143	5	7	13	26	24	24*	-2	545	0	-29*	10	100	6	0
4	702	0	24*	1	322	9	7	14	102	5	4	-1	59	0	-19*	11	131	5	5
6	224	6	14	2	34	5	9	15	8	24	7*	0	669	0	35*	12	106	4	4
8	430	11	-8	3	560	14	14	H,K=	0,	12		1	351	0	2*	13	137	5	9
10	225	6	-12	4	238	6	30	0	199	7	10	2	507	0	-4*	14	19	24	14*
12	197	6	-7	5	194	5	9	1	86	5	11	3	16	0	-16*	15	99	7	-6
14	119	5	2	6	51	4	7	2	0	22	-19*	4	432	0	13*	16	115	6	0
16	132	5	4	7	271	8	-5	3	93	5	7	5	104	3	1	17	67	13	-5*
18	83	6	5	8	139	5	1	4	132	6	-2	6	154	4	3	18	14	27	5*
H,K=	0,	2		9	20	21	4*	5	71	6	1	7	80	3	-8	H,K=	1,	5	
0	536	0	27*	10	18	28	1*	6	81	7	4	8	416	14	4	-18	0	28	0*
1	148	0	11*	11	268	8	-1	7	101	6	7	9	68	3	3	-17	116	6	-6
2	229	0	-5*	12	38	11	-15*	8	115	5	-13	10	140	4	7	-16	17	26	15*
3	459	0	29*	13	30	25	5*	9	42	8	-3*	11	92	4	3	-15	91	5	-4
4	228	0	-1*	14	54	7	-2	10	53	7	0	12	223	6	5	-14	38	9	14*
5	165	5	16	15	123	8	-4	11	64	6	-4	13	79	5	-4	-13	165	6	-1
6	164	5	-1	16	9	29	-21*	12	48	7	-11	14	35	16	-1*	-12	42	8	15
7	216	6	19	17	35	18	22*	13	20	29	18*	15	9	30	-2*	-11	205	7	-7
8	445	12	15	18	21	26	-6*	H,K=	0,	14		16	154	6	-3	-10	49	5	2
9	14	21	2*	H,K=	0,	8		0	85	15	-4	17	19	24	-5*	-9	196	6	-7
10	86	4	0	0	353	10	8	1	72	6	-8	18	9	28	6*	-8	142	5	11
11	206	6	14	1	158	5	-3	2	18	22	6*	19	7	26	-24*	-7	422	11	-16
12	118	4	2	2	32	8	2*	3	117	6	-3	H,K=	1,	3	-6	23	8	11*	
13	33	8	11*	3	210	6	-2	4	27	12	-2*	-19	38	10	7*	-5	161	5	-16
14	152	5	11	4	247	7	1	5	66	6	-3	-18	75	7	-6	-4	137	4	3
15	86	5	0	5	97	4	5	6	30	17	11*	-17	108	7	-5	-3	562	14	-8
16	102	5	4	6	112	4	3	7	100	8	-12	-16	5	32	-17*	-2	34	4	7
17	30	14	2*	7	115	5	-7	8	31	13	-9*	-15	64	6	-1	-1	250	7	-6
18	86	6	2	8	206	7	-3	9	25	14	-4*	-14	132	5	0	0	168	5	6
19	65	6	2	9	17	23	7*	H,K=	0,	16	-13	157	6	16	1	541	16	14	
H,K=	0,	4		10	69	6	-8	0	42	7	12	-12	52	6	4	2	29	8	10*
0	291	0	7*	11	149	5	-1	1	61	5	-5	-11	181	5	-2	3	130	4	8
1	219	0	5*	12	125	5	3	2	20	14	16*	-10	150	5	-5	4	56	4	1
2	34	4	-1	13	6	28	-20*	3	65	5	-11	-9	194	6	1	5	498	15	7
3	560	14	11	14	86	5	11	H,K=	1,	1	-8	199	5	7	6	144	5	5	
4	96	3	-9	15	46	19	-19*	-19	9	31	2*	-7	274	7	0	7	78	4	3
5	337	9	25	16	54	6	6	-18	107	5	1	-6	315	8	-9	8	10	19	-3*
6	102	4	4	17	4	28	-3*	-17	24	24	6*	-5	130	4	-17	9	259	8	-5
7	340	9	13	H,K=	0,	10	-16	48	12	23*	-4	117	3	-3	10	37	7	15	
8	126	4	9	0	314	9	16	-15	30	11	-2*	-3	358	0	-15*	11	143	5	-2
9	122	4	3	1	79	4	19	-14	200	6	0	-2	466	0	15*	12	15	29	-16*
10	47	6	-11	2	22	16	10*	-13	37	13	7*	-1	49	0	-12*	13	148	6	-8
11	275	8	4	3	62	5	-2	-12	10	20	-7*	0	253	0	-6*	14	16	31	11*
12	12	24	-5*	4	265	8	10	-11	78	4	5	1	487	0	5*	15	95	8	-4
13	0	24	-3*	5	22	17	15*	-10	390	10	19	2	243	0	25*	16	8	26	0*
14	61	7	9	6	84	5	-4	-9	107	4	0	3	71	0	9*	17	60	9	-18
15	161	6	-5	7	32	9	10*	-8	130	4	6	4	301	13	21	18	19	26	12*
16	0	27	-35*	8	207	6	-3	-7	79	3	-4	5	374	16	-4	H,K=	1,	7	
17	44	11	4*	9	30	11	13*	-6	527	14	8	6	186	5	11	-17	63	21	-8*
18	27	29	-1*	10	72	6	-10	-5	123	0	-3*	7	17	15	-6*	-16	21	24	4*
19	94	6	-9	11	21	23	14*	-4	426	0	38*	8	213	6	-8	-15	68	8	-7

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
-14	70	6	-6	7	33	6	14*	4	54	6	-8	-9	244	11	-18	8	23	14	8*
-13	96	5	-14	8	207	7	-1	5	156	6	1	-8	302	15	-9	9	252	7	8
-12	5	25	-13*	9	70	5	-8	6	33	9	3*	-7	41	4	-5	10	121	4	1
-11	156	7	-1	10	48	7	-9	7	18	24	-8*	-6	426	11	-1	11	105	5	-2
-10	110	5	-12	11	20	24	-1*	8	86	5	-1	-5	365	10	-20	12	0	24	-13*
-9	228	7	0	12	142	6	-14	9	78	10	-12	-4	219	0	-16*	13	174	7	-2
-8	51	5	-2	13	54	5	10	10	28	24	-3*	-3	105	0	14*	14	45	9	-4*
-7	220	7	-2	14	31	10	20*	11	21	30	-16*	-2	341	0	4*	15	19	27	6*
-6	185	5	-8	15	0	24	-13*	H,K=	1,	15		-1	273	0	16*	16	0	30	-25*
-5	98	4	4	16	86	5	-11	-7	66	10	-19	0	94	0	-1*	17	120	8	-13
-4	94	3	1	H,K=	1,	11		-6	18	20	15*	1	151	0	-9*	18	28	20	-9*
-3	383	10	17	-14	98	7	-8	-5	40	11	-5*	2	502	0	43*	H,K=	2,	6	
-2	230	6	-1	-13	34	10	9*	-4	18	21	14*	3	365	0	28*	-18	0	25	-15*
-1	104	3	-4	-12	14	25	0*	-3	120	6	-2	4	105	3	5	-17	80	6	-19
0	180	5	7	-11	66	5	10	-2	3	23	3*	5	116	4	0	-16	46	10	-3*
1	451	12	7	-10	135	10	-5	-1	19	22	-2*	6	356	9	19	-15	15	27	1*
2	298	8	11	-9	26	13	5*	0	10	22	-2*	7	107	4	11	-14	8	26	-8*
3	49	4	4	-8	79	5	14	1	125	7	-3	8	50	4	2	-13	197	7	-17
4	213	6	-6	-7	61	6	2	2	0	21	-9*	9	175	5	1	-12	39	11	0*
5	281	7	6	-6	228	7	10	3	17	24	16*	10	231	6	5	-11	72	6	13
6	177	5	8	-5	13	22	-2*	4	20	24	14*	11	31	18	-6*	-10	36	12	-1*
7	34	6	12	-4	74	5	5	5	113	11	-9	12	92	5	-4	-9	311	9	-22
8	167	6	-7	-3	78	6	-1	6	7	20	6*	13	147	5	0	-8	26	11	13*
9	156	5	-8	-2	198	6	-2	7	33	6	5*	14	128	6	0	-7	48	6	-5
10	65	5	-3	-1	0	21	-3*	H,K=	2,	0		15	35	9	21*	-6	105	4	-7
11	122	6	6	0	139	6	-3	-20	93	10	-1	16	90	5	1	-5	452	12	-4
12	101	7	-4	1	84	4	18	-18	51	7	2	17	73	8	-1	-4	131	4	0
13	155	6	-1	2	172	5	4	-16	142	6	4	18	77	6	-7	-3	194	5	16
14	9	25	6*	3	74	5	-3	-14	115	4	3	H,K=	2,		4	-2	90	3	1
15	37	9	2*	4	187	6	-2	-12	192	5	-5	-19	57	8	4	-1	521	13	-6
16	71	10	-3	5	74	5	-1	-10	326	9	7	-18	29	14	8*	0	129	4	11
17	45	8	-8	6	121	6	1	-8	383	10	1	-17	117	6	-12	1	406	10	8
H,K=	1,		9	7	33	14	19*	-6	507	13	-5	-16	57	7	-3	2	85	4	1
-16	0	24	-28*	8	179	8	0	-4	117	0	24*	-15	39	11	-9*	3	365	10	-11
-15	17	24	-6*	9	63	7	1	-21	007	0	-33*	-14	25	21	18*	4	17	21	9*
-14	122	5	-5	10	75	5	-1	0	252	0	22*	-13	221	7	0	5	165	5	-1
-13	12	24	-20*	11	17	22	6*	2	746	0	44*	-12	54	6	10	6	181	5	3
-12	21	24	10*	12	97	6	-10	4	17	0	-23*	-11	50	6	15	7	170	5	-6
-11	48	8	3	13	32	21	-4*	6	343	9	20	-10	46	6	2	8	38	8	8*
-10	208	7	3	14	14	21	12*	8	94	3	3	-9	330	9	0	9	212	7	-11
-9	54	8	-3	H,K=	1,	13		10	364	10	-1	-8	68	4	3	10	84	5	9
-8	4	22	-24*	-11	48	6	-11	12	100	5	5	-7	202	6	9	11	65	5	-13
-7	92	4	-2	-10	75	8	-2	14	195	6	-5	-6	189	6	0	12	42	9	8*
-6	233	7	1	-9	58	5	7	16	65	6	4	-5	514	13	-6	13	170	7	5
-5	33	10	-3*	-8	14	23	8*	18	87	7	-7	-4	80	4	0	14	13	25	-19*
-4	103	4	-2	-7	102	7	-7	H,K=	2,	2		-3	160	4	13	15	48	9	-7
-3	87	4	1	-6	88	5	-3	-19	44	18	-6*	-2	43	4	3	16	37	12	-3*
-2	242	7	7	-5	79	5	8	-18	51	10	6*	-1	438	0	6*	17	88	6	-8
-1	58	5	-7	-4	37	7	7*	-17	50	8	-3	0	101	0	12*	H,K=	2,	8	
0	222	6	4	-3	139	5	0	-16	164	6	13	1	243	6	-1	-17	44	9	-12*
1	96	4	-6	-2	90	6	-2	-15	16	29	-7*	2	45	4	1	-16	80	6	-2
2	248	7	2	-1	54	6	0	-14	57	8	-15	3	261	7	9	-15	23	24	8*
3	90	4	-4	0	88	5	6	-13	134	5	2	4	144	4	1	-14	40	11	-10*
4	154	5	-10	1	119	5	-1	-12	191	6	-1	5	306	8	-2	-13	119	6	0
5	113	5	6	2	106	5	7	-11	57	4	8	6	150	4	5	-12	106	5	-8
6	85	5	-9	3	17	22	13*	-10	215	6	6	7	277	8	17	-11	38	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
-10	154	6	6	13	14	23	6*	2	25	31	-8*	-5	332	9	3	12	28	13	22*
-9	184	6	-9	14	79	16	-21*	H,K=	3,	1		-4	411	14	-14	13	26	31	-19*
-8	225	6	15	H,K=	2,	12	-20	58	12	-11*		-3	381	0	10*	14	21	25	17*
-7	28	8	12*	-13	57	7	-9	-19	42	9	9*	-2	79	0	12*	15	115	6	-9
-6	174	6	-5	-12	71	7	-10	-18	59	7	-4	-1	562	0	42*	16	15	27	-3*
-5	177	6	-4	-11	15	22	7*	-17	16	26	7*	0	408	0	13*	17	62	9	-8
-4	112	4	-1	-10	52	8	-13	-16	164	6	-5	1	73	0	-11*	H,K=	3,	7	
-3	93	4	-1	-9	83	7	-5	-15	0	24	-15*	2	289	7	2	-18	23	25	-10*
-2	318	9	9	-8	111	5	7	-14	82	5	-4	3	319	8	12	-17	21	27	5*
-1	225	6	-6	-7	47	6	17	-13	62	5	6	4	138	4	8	-16	60	6	-4
0	86	3	-6	-6	105	5	-7	-12	255	7	-13	5	33	5	-1	-15	74	8	-18
1	157	5	-19	-5	143	6	0	-11	91	4	12	6	181	5	5	-14	15	27	-24*
2	323	9	4	-4	92	5	-5	-10	52	5	0	7	259	7	-1	-13	106	5	6
3	157	5	5	-3	58	5	13	-9	111	4	-2	8	269	7	1	-12	135	6	4
4	21	13	-9*	-2	176	6	-2	-8	548	17	-20	9	74	4	6	-11	217	7	-6
5	69	5	-1	-1	140	5	0	-7	164	5	-9	10	116	4	4	-10	46	8	7*
6	235	7	-13	0	55	6	-1	-6	55	3	-3	11	214	7	1	-9	115	5	-11
7	110	7	-7	1	47	6	10	-5	26	0	4*	12	54	6	4	-8	208	6	-6
8	76	4	4	2	164	8	-8	-4	365	0	1*	13	77	5	4	-7	154	5	-13
9	129	6	-6	3	106	7	-20	-3	105	0	2*	14	125	5	3	-6	45	5	-11
10	170	6	0	4	30	10	4*	-2	106	0	17*	15	106	6	-7	-5	334	9	-2
11	61	6	-11	5	93	7	-1	-1	213	0	9*	16	30	14	2*	-4	296	8	-4
12	61	8	-12	6	146	10	-12	0	663	0	2*	17	74	6	3	-3	186	5	-1
13	78	5	-10	7	78	7	-5	1	113	0	9*	18	74	7	-6	-2	112	4	12
14	84	5	-9	8	32	10	8*	2	173	0	9*	H,K=	3,	5	-1	356	9	12	
15	21	28	-14*	9	68	7	-4	3	294	0	4*	-19	95	9	-5	0	290	8	11
16	55	7	-3	10	83	12	-17	4	220	6	2	-18	0	31	-1*	1	107	4	-7
H,K=	2,	10	11	31	10	-1*	5	125	4	1	-17	25	26	-10*	2	140	4	8	
-15	14	22	12*	12	25	16	-8*	6	157	4	8	-16	24	26	5*	3	373	10	-14
-14	52	8	-4	H,K=	2,	14	7	95	3	0	-15	144	6	-3	4	165	5	1	
-13	20	24	11*	-10	28	11	-3*	8	297	8	-4	-14	18	26	5*	5	101	4	5
-12	107	5	-14	-9	87	6	-18	9	40	6	-5	-13	112	6	-2	6	165	6	-3
-11	30	12	17*	-8	40	7	-1	10	245	7	1	-12	27	17	16*	7	162	6	-14
-10	128	5	-7	-7	25	11	12*	11	89	5	-6	-11	245	18	-12	8	74	4	3
-9	2	22	-6*	-6	27	12	2*	12	106	4	3	-10	19	21	-5*	9	66	9	6
-8	134	5	-2	-5	141	8	-7	13	33	11	16*	-9	190	5	-15	10	98	6	-2
-7	41	7	4	-4	31	11	20*	14	187	7	-5	-8	24	10	2*	11	215	10	-16
-6	227	7	7	-3	21	22	-19*	15	62	10	13	-7	194	11	-26	12	43	8	17*
-5	17	21	-9*	-2	59	6	-7	16	54	7	-3	-6	122	4	8	13	16	25	-8*
-4	110	4	-7	-1	114	9	-14	17	25	30	10*	-5	509	16	-6	14	70	6	-14
-3	37	7	5*	0	0	24	-16*	18	103	5	1	-4	190	5	0	15	81	6	-14
-2	254	7	-2	1	80	5	1	H,K=	3,	3	-3	393	13	-12	16	0	32	-12*	
-1	13	19	11*	2	58	6	-7	-19	81	11	-17	-2	157	4	1	H,K=	3,	9	
0	60	5	-9	3	109	5	-11	-18	13	26	-14*	-1	394	10	0	-16	81	5	-7
1	28	8	-7*	4	17	22	3*	-17	0	29	-14*	0	51	3	-3	-15	17	26	-15*
2	256	8	-4	5	100	9	-9	-16	116	6	-2	1	116	4	4	-14	62	7	3
3	36	7	-12	6	37	10	1*	-15	133	6	-6	2	73	3	-7	-13	38	12	10*
4	18	23	11*	7	66	12	-7*	-14	89	5	1	3	431	11	-5	-12	152	6	-9
5	28	11	-6*	8	31	7	27*	-13	85	7	-4	4	56	4	-3	-11	84	5	7
6	233	9	-14	9	78	10	-8	-12	80	5	-14	5	104	4	11	-10	28	12	3*
7	26	14	-11*	H,K=	2,	16	-11	250	7	-7	6	24	17	8*	-9	0	24	-29*	
8	33	9	-1*	-3	25	12	-13*	-10	32	8	5*	7	331	10	5	-8	255	8	-10
9	17	30	16*	-2	18	27	-14*	-9	129	4	-14	8	16	20	4*	-7	35	8	2*
10	163	11	-9	-1	80	6	-3	-8	319	9	-11	9	16	21	-3*	-6	59	6	1
11	19	24	2*	0	22	13	15*	-7	230	13	-7	10	8	23	-2*	-5	110	4	-6
12	57	9	-7	1	41	13	-14*	-6	22	8	-5*	11	257	8	-2	-4	239	7	-2

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	82	4	7	-6	19	23	6*	-18	100	6	-8	-1	167	5	1	H,K=		4,	8
-2	108	4	-7	-5	133	6	-3	-17	81	6	8	0	137	4	4	-17	39	11	-7*
-1	60	5	1	-4	87	5	-6	-16	36	13	-12*	1	270	7	-6	-16	15	28	7*
0	289	9	-5	-3	117	7	4	-15	70	7	-6	2	51	4	9	-15	57	7	-4
1	26	11	9*	-2	62	5	5	-14	216	6	-11	3	292	8	-7	-14	101	6	-15
2	106	4	-8	-1	123	5	-9	-13	39	13	-13*	4	111	4	-8	-13	41	10	2*
3	120	4	-9	0	137	8	-3	-12	34	18	-3*	5	364	10	-4	-12	89	7	5
4	199	7	-5	1	45	6	1	-11	204	6	-11	6	29	11	7*	-11	146	6	-12
5	23	14	0*	2	36	12	-10*	-10	240	14	-22	7	190	6	3	-10	190	7	-10
6	155	6	-7	3	139	9	-11	-9	80	4	-8	8	160	5	2	-9	75	5	-3
7	88	4	-1	4	70	6	4	-8	250	7	0	9	266	8	0	-8	143	5	2
8	120	5	3	5	16	24	13*	-7	321	9	-5	10	28	17	3*	-7	169	5	-6
9	11	24	-22*	6	52	7	-16	-6	365	17	-7	11	207	7	7	-6	225	6	-10
10	150	9	-1	7	127	6	3	-5	35	5	20	12	60	7	-10	-5	17	20	3*
11	69	7	-6	8	60	6	-1	-4	243	0	16*	13	97	6	-8	-4	161	5	-7
12	46	9	-4*	9	14	21	2*	-3	355	0	10*	14	39	10	5*	-3	204	6	-13
13	17	30	13*	10	35	12	-15*	-2	256	0	-8*	15	136	8	-4	-2	139	4	-4
14	100	10	-17	H,K=		3,	15	-1	41	0	3*	16	30	18	-16*	-1	13	22	5*
15	21	23	-11*	-7	59	6	-18	0	401	0	9*	17	19	34	-10*	0	295	8	5
H,K=		3,	11	-6	18	23	13*	1	382	0	21*	H,K=		4,	6	1	204	6	-14
-15	36	8	6*	-5	84	6	-4	2	345	0	6*	-19	57	7	-7	2	134	4	-7
-14	51	10	-8*	-4	37	6	26	3	228	6	2	-18	37	12	0*	3	96	4	-10
-13	38	9	1*	-3	51	6	-11	4	231	6	2	-17	57	8	-11	4	222	9	-6
-12	100	5	-8	-2	33	8	21*	5	234	6	11	-16	29	16	10*	5	164	7	-12
-11	31	11	-3*	-1	104	8	-15	6	77	3	8	-15	108	8	-8	6	25	29	15*
-10	32	12	20*	0	28	9	14*	7	95	4	4	-14	105	8	6	7	44	8	-1
-9	70	6	9	1	32	8	1*	8	334	9	8	-13	79	6	-7	8	170	8	-4
-8	192	7	-6	2	28	8	26*	9	70	4	9	-12	30	13	-3*	9	90	5	-14
-7	41	9	-5*	3	134	7	-2	10	54	7	11	-11	244	7	-4	10	31	13	2*
-6	17	26	2*	4	4	21	-1*	11	189	6	6	-10	83	5	-3	11	105	8	-3
-5	48	7	-5	5	24	18	1*	12	173	6	-4	-9	113	4	-9	12	102	9	-16
-4	218	6	-3	6	15	20	8*	13	65	9	-9	-8	114	4	0	13	64	6	7
-3	16	24	-1*	H,K=		4,	0	14	70	9	-1	-7	331	9	-6	14	47	10	9*
-2	93	5	3	-20	0	32	-3*	15	74	6	-3	-6	177	5	1	15	43	9	-9*
-1	92	5	0	-18	110	6	-10	16	115	5	0	-5	48	5	11	H,K=		4,	10
0	219	8	-7	-16	41	8	-9*	17	28	16	8*	-4	177	5	8	-16	20	25	3*
1	70	5	2	-14	201	6	3	18	41	11	-5*	-3	493	13	3	-15	18	26	14*
2	117	4	1	-12	166	5	-5	H,K=		4,	4	-2	165	5	2	-14	128	7	-4
3	70	5	-2	-10	448	13	10	-19	66	10	-7	-1	101	3	0	-13	20	24	5*
4	142	6	1	-8	304	8	27	-18	45	9	8*	0	34	6	12	-12	44	8	-5*
5	20	22	-1*	-6	689	20	-7	-17	97	6	8	1	446	12	-1	-11	27	18	7*
6	159	9	-8	-4	353	0	2*	-16	30	15	28*	2	49	4	4	-10	150	6	-1
7	78	6	1	-2	373	0	-37*	-15	139	6	-12	3	247	7	-3	-9	36	17	27*
8	144	12	0	0	888	0	-25*	-14	61	7	7	4	78	4	-3	-8	164	5	8
9	20	22	7*	2	620	0	16*	-13	110	5	-2	5	320	9	-2	-7	23	23	13*
10	100	10	-3	4	407	11	1	-12	20	30	1*	6	20	13	10*	-6	185	6	2
11	44	8	3*	6	41	4	3	-11	264	7	-18	7	112	5	-4	-5	63	5	0
12	43	17	-7*	8	391	11	-4	-10	88	5	-3	8	92	5	2	-4	167	5	-5
13	21	23	5*	10	22	19	17*	-9	63	4	-22	9	143	5	-11	-3	34	8	4*
H,K=		3,	13	12	252	9	3	-8	136	4	9	10	21	24	4*	-2	134	5	-4
-12	46	8	-6	14	56	7	5	-7	367	10	-21	11	185	6	-14	-1	38	7	4
-11	66	5	-8	16	145	8	-10	-6	99	4	-8	12	25	26	-8*	0	255	7	9
-10	27	13	8*	18	35	12	0*	-5	108	4	16	13	113	8	-8	1	28	11	-2*
-9	60	6	-6	H,K=		4,	2	-4	71	3	4	14	0	26	-17*	2	125	5	9
-8	106	5	3	-20	0	33	-4*	-3	543	14	-12	15	92	6	-3	3	45	8	-6*
-7	87	5	0	-19	28	20	-16*	-2	53	4	-2	16	24	25	-7*	4	226	7	6

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
5	20	24	13*	-19	23	24	11*	0	13	17	-10*	-17	81	8	-10	5	83	5	-2
6	31	33	4*	-17	31	13	3*	1	176	6	5	-16	39	12	-9*	6	185	7	-9
7	0	26	-15*	-16	119	7	6	2	244	7	-16	-15	43	7	38	7	65	7	-8
8	206	7	-1	-15	0	24	-4*	3	81	3	2	-14	89	14	-11	8	105	7	0
9	51	9	4	-14	180	6	3	4	161	6	10	-13	135	6	-18	9	62	6	1
10	20	23	19*	-13	55	5	9	5	320	9	5	-12	52	8	-1	10	101	6	-6
11	0	26	-4*	-12	180	6	-13	6	229	8	-3	-11	39	11	-6*	11	0	25	-12*
12	129	6	-1	-11	53	5	-3	7	77	4	4	-10	167	7	-8	12	96	6	-6
13	21	23	19*	-10	440	12	29	8	97	8	-8	-9	276	12	7	13	12	37	-24*
H,K=	4,	12	-9	204	6	-4	9	259	8	-6	-8	56	6	-1	14	66	6	3	
-13	29	15	0*	-8	214	6	-4	10	181	8	0	-7	157	8	3	H,K=	5,	11	
-12	0	25	-14*	-7	15	16	-5*	11	0	26	-12*	-6	230	11	-14	-15	0	25	-13*
-11	78	9	3	-6	591	15	7	12	95	6	3	-5	252	9	-8	-14	82	13	-2
-10	113	7	6	-5	121	4	2	13	165	6	-2	-4	0	19	-23*	-13	42	10	-2*
-9	0	25	-5*	-4	9	0	-4*	14	10	28	-24*	-3	158	9	-11	-12	82	6	4
-8	76	6	-3	-3	184	0	5*	15	16	29	-19*	-2	266	8	-8	-11	27	28	-7*
-7	100	6	-3	-2	667	0	12*	16	69	8	-10	-1	204	7	-4	-10	121	12	-11
-6	123	9	-4	-1	215	0	1*	17	75	8	-16	0	25	10	-2*	-9	57	6	15
-5	37	8	18*	0	149	0	13*	H,K=	5,	5	1	303	9	0	-8	22	24	-9*	
-4	131	6	7	1	570	0	-8*	-18	17	26	-1*	2	184	7	0	-7	41	8	20*
-3	156	6	9	2	649	18	6	-17	134	12	-5	3	155	6	-2	-6	198	13	-6
-2	113	5	15	3	18	12	-30*	-16	0	29	-2*	4	73	5	-8	-5	30	10	0*
-1	23	24	-11*	4	126	4	8	-15	11	28	-5*	5	193	6	-4	-4	20	22	13*
0	168	6	2	5	193	6	4	-14	34	19	-20*	6	136	5	-8	-3	67	5	11
1	101	5	-2	6	314	9	6	-13	244	14	-25	7	76	5	-2	-2	236	11	1
2	66	5	10	7	31	6	15*	-12	0	26	-2*	8	87	5	-1	-1	48	7	4
3	47	6	-2	8	186	8	6	-11	29	12	-1*	9	183	8	-1	0	17	22	6*
4	127	6	-2	9	70	5	7	-10	9	25	5*	10	73	7	-1	1	46	7	1
5	93	5	0	10	247	8	-8	-9	331	10	-24	11	0	29	-13*	2	195	7	5
6	14	24	6*	11	54	6	13	-8	126	5	5	12	48	10	-14*	3	47	8	6
7	96	5	13	12	183	9	-3	-7	278	9	11	13	124	17	-15	4	70	6	-2
8	126	6	-3	13	76	7	-8	-6	62	4	9	14	47	8	0	5	58	6	3
9	53	7	-3	14	89	6	-10	-5	323	9	-15	15	0	24	-4*	6	161	13	-4
10	9	23	-7*	15	13	26	6*	-4	15	17	-10*	H,K=	5,	9	7	0	32	-10*	
11	48	9	6*	16	104	9	2	-3	338	11	-6	-17	7	27	-24*	8	100	7	5
H,K=	4,	14	17	22	36	-17*	-2	19	11	9*	-16	69	8	-10	9	38	20	-9*	
-10	44	7	8	H,K=	5,	3	-1	340	10	-21	-15	16	25	11*	10	116	10	-2	
-9	25	15	1*	-19	0	29	-19*	0	78	4	-9	-14	80	12	-23	11	0	23	-5*
-8	35	9	5*	-18	66	7	7	1	377	11	-2	-13	58	10	-4	12	64	6	-4
-7	130	5	8	-17	130	10	3	2	20	10	-1*	-12	62	8	-7	H,K=	5,	13	
-6	39	9	3*	-16	74	8	-5	3	164	6	-2	-11	23	25	20*	-12	26	31	-12*
-5	0	21	-5*	-15	21	26	11*	4	52	4	12	-10	212	11	-1	-11	24	14	3*
-4	13	33	-17*	-14	92	6	-9	5	374	12	0	-9	74	8	6	-10	69	12	-5
-3	154	6	7	-13	208	7	0	6	49	5	-6	-8	117	6	1	-9	78	10	-9
-2	17	22	8*	-12	111	7	-4	7	105	5	-1	-7	80	7	-1	-8	43	7	11
-1	30	10	-3*	-11	73	5	-2	8	0	22	-8*	-6	230	8	-6	-7	56	11	-7*
0	91	6	11	-10	180	6	-13	9	304	9	-8	-5	61	4	7	-6	87	8	-3
1	130	7	4	-9	306	9	-12	10	0	25	-25*	-4	57	5	-1	-5	107	14	-14
2	28	15	-11*	-8	24	9	8*	11	25	19	18*	-3	93	8	1	-4	26	17	19*
3	63	6	-4	-7	191	6	-8	12	11	31	2*	-2	229	9	-13	-2	111	7	0
4	34	12	-2*	-6	370	10	-6	13	176	9	-9	-1	72	5	-2	-1	95	5	0
5	115	6	1	-5	351	10	-2	14	0	26	-5*	0	83	5	8	0	0	22	-11*
6	26	13	11*	-4	72	4	7	15	32	14	-1*	1	78	5	-1	1	87	11	-5
7	64	7	-7	-3	147	4	-5	16	12	25	9*	2	274	9	-6	2	103	5	0
8	49	5	11	-2	270	8	-5	H,K=	5,	7	3	30	17	3*	3	46	8	0	
H,K=	5,	1	-1	284	8	5	-18	51	8	9	4	50	7	-15	4	15	23	-6*	

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
5	119	7	-1	1	203	6	10	-18	0	28	-13*	3	209	6	-4	1	0	31	-16*
6	59	7	-11	2	181	5	11	-17	58	7	-3	4	130	6	-1	2	93	9	-4
7	21	22	3*	3	265	8	-3	-16	68	12	4	5	47	7	-1	3	84	5	0
8	38	9	5*	4	131	5	3	-15	111	7	-6	6	186	7	-5	5	54	6	10
9	69	7	-14	5	23	10	7*	-14	31	13	12*	7	110	8	0	6	128	8	6
H,K=		5,	15	6	306	9	1	-13	162	10	1	8	58	6	5	7	92	10	5
-7	38	39	-7*	7	116	5	-1	-12	64	7	-4	9	41	21	6*	8	56	7	2
-6	0	22	-1*	8	162	6	-7	-11	215	8	-2	10	139	10	2	9	47	7	8
-4	16	21	13*	9	128	5	-9	-10	43	7	11	11	89	6	-1	10	77	13	-3
-2	0	22	-4*	10	239	9	3	-9	272	11	-4	12	11	27	9*	H,K=		6,	14
-1	70	6	3	11	113	11	-3	-8	42	11	-3*	13	49	8	0	-10	27	21	5*
0	24	26	18*	12	7	25	-3*	-7	201	6	6	14	104	6	-2	-9	60	26	-26*
1	105	12	-7	13	103	6	4	-6	54	5	-2	H,K=		6,	10	-8	35	37	-18*
2	28	10	14*	14	128	8	3	-5	441	13	-11	-16	90	30	-19*	-7	49	7	-2
3	61	10	-2	15	60	8	-3	-4	133	4	-11	-15	0	24	-1*	-6	0	22	-11*
4	8	22	-4*	16	31	13	16*	-3	118	4	3	-14	35	9	24*	-4	3	30	-18*
H,K=		6,	0	17	57	8	8	-2	58	5	-4	-13	27	20	20*	-3	26	16	-9*
-18	39	9	10*	H,K=		6,	4	-1	379	10	2	-12	119	9	-21	-2	48	6	11
-16	163	6	-11	-19	100	8	1	0	109	4	-2	-11	0	29	-15*	-1	135	11	0
-14	41	7	18	-18	25	28	12*	1	99	4	-2	-9	23	24	16*	0	15	29	-28*
-12	284	8	-10	-17	76	10	-11	2	27	7	7*	-8	209	9	2	1	7	22	-2*
-10	151	5	2	-16	49	15	-4*	3	405	12	-5	-7	77	5	12	2	34	9	2*
-8	678	17	10	-15	118	6	-16	4	42	5	-1	-6	96	6	-7	3	124	8	-5
-6	240	6	-3	-14	44	8	10*	5	62	5	6	-5	43	6	5	4	22	32	-12*
-4	540	14	6	-13	205	9	-19	6	142	5	-6	-4	187	8	-9	5	30	9	1*
-2	856	0	21*	-12	52	8	-18	7	218	8	12	-3	26	10	22*	6	23	23	-1*
0	431	0	-27*	-11	235	7	-8	8	26	10	5*	-2	179	6	10	H,K=		7,	1
2	535	15	18	-10	35	8	-2*	9	129	8	-6	-1	32	7	31*	-19	42	8	10*
4	128	4	-3	-9	229	7	-11	10	71	8	-3	0	194	7	-2	-18	143	6	7
6	416	12	5	-8	118	4	7	11	171	9	0	1	0	22	-4*	-17	21	27	-10*
8	122	4	-6	-7	35	12	7*	12	18	25	-5*	2	183	8	1	-16	104	8	-5
10	280	11	2	-6	149	5	2	13	92	6	-1	3	33	9	26*	-15	37	12	15*
12	0	25	-4*	-5	441	12	-16	14	29	15	-7*	4	109	6	-3	-14	239	7	3
14	201	10	12	-4	75	3	-1	15	62	9	-10	5	0	24	-10*	-13	5	22	0*
16	37	11	23*	-3	103	4	-12	H,K=		6,	8	6	192	9	-12	-12	204	6	6
H,K=		6,	2	-2	87	4	-3	-18	16	27	-3*	7	40	7	12	-11	77	4	-1
-19	83	7	8	-1	337	9	-1	-17	25	27	-4*	8	68	6	-3	-10	231	6	1
-18	15	27	6*	0	132	4	-7	-16	90	7	-3	9	15	24	7*	-9	0	17	-14*
-17	35	13	0*	1	59	3	5	-15	45	10	-11*	10	152	12	-3	-8	457	12	9
-16	208	7	10	2	93	3	-2	-14	12	27	6*	11	35	9	16*	-7	166	5	8
-15	67	10	-7	3	350	11	-4	-13	105	6	2	12	0	38	-10*	-6	205	6	-8
-14	37	12	-5*	4	7	20	-19*	-12	142	8	-6	H,K=		6,	12	-5	42	4	-10
-13	108	5	-9	5	137	4	11	-11	108	6	-6	-13	33	34	-25*	-4	341	9	0
-12	249	7	-15	6	104	4	4	-10	72	6	10	-12	84	16	-12*	-3	82	3	2
-11	149	5	7	7	322	9	2	-9	157	7	-7	-11	43	7	4	-2	22	11	-2*
-10	101	4	8	8	74	5	2	-8	251	8	1	-10	34	6	19*	-1	138	5	-21
-9	250	7	4	9	165	7	2	-7	72	5	6	-9	55	7	-6	0	485	13	-13
-8	404	11	7	10	80	5	-3	-6	45	6	0	-8	129	14	-2	1	57	3	-1
-7	120	4	-1	11	193	11	-4	-5	205	6	-6	-7	43	7	7	2	23	8	0*
-6	168	5	10	12	27	28	16*	-4	182	7	-2	-6	54	7	-7	3	186	6	-5
-5	279	7	7	13	133	6	6	-3	26	10	-5*	-5	105	8	-7	4	348	10	0
-4	303	8	9	14	31	17	-10*	-2	190	6	-7	-4	134	12	0	5	79	4	-4
-3	101	3	0	15	42	14	-25*	-1	181	6	3	-3	46	10	9*	6	83	4	3
-2	246	7	4	16	0	26	-2*	0	164	6	-9	-2	120	7	6	7	48	5	-1
-1	205	6	9	H,K=		6,	6	1	15	23	8*	-1	117	6	4	8	324	10	-2
0	326	9	-7	-19	85	12	-6	2	218	7	-2	0	156	8	6	9	0	23	-12*

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
10	95	6	0	-7	277	8	-8	H,K=	7,	9		8	173	12	8	-19	18	27	6*
11	94	5	-4	-6	56	4	9	-17	26	31	14*	9	18	22	9*	-18	115	7	-12
12	158	6	-7	-5	253	7	0	-16	9	30	-40*	10	48	9	6*	-17	87	10	-12
13	16	25	3*	-4	26	9	9*	-15	0	28	-40*	11	18	24	-14*	-16	65	8	12
14	107	11	3	-3	487	13	-3	-14	102	7	-5	H,K=	7,	13	-15	20	28	-12*	
15	53	8	-2	-2	84	3	7	-13	34	10	30*	-12	51	6	15	-14	236	8	8
16	87	6	-2	-1	143	4	3	-12	114	6	-3	-11	97	5	5	-13	113	5	-7
H,K=	7,	3	0	20	17	-1*	-11	92	7	8	-10	44	7	-2	-12	62	9	-8	
-19	94	6	-1	1	317	9	-4	-10	134	5	10	-9	0	22	-4*	-11	160	5	4
-18	70	6	2	2	20	11	-4*	-9	11	25	-1*	-8	89	10	5	-10	326	9	-5
-17	55	8	4	3	289	9	7	-8	224	7	6	-7	124	11	5	-9	180	6	3
-16	73	9	-13	4	24	8	7*	-7	26	13	-5*	-6	62	6	7	-8	59	5	6
-15	160	6	0	5	176	5	6	-6	189	7	11	-5	47	7	4	-7	195	5	0
-14	144	6	4	6	28	10	-3*	-5	99	6	2	-4	89	7	8	-6	283	7	-9
-13	0	26	-8*	7	256	11	10	-4	181	6	-1	-3	160	8	4	-5	174	5	-3
-12	100	6	6	8	13	21	1*	-3	129	5	14	-2	25	17	-5*	-4	63	4	-2
-11	292	8	-9	9	84	5	-4	-2	4	20	-10*	-1	78	5	10	-3	112	4	-10
-10	67	4	-5	10	32	13	7*	-1	32	6	15*	0	112	9	-6	-2	312	8	0
-9	0	20	-9*	11	227	11	3	0	282	9	-1	1	105	6	5	-1	55	3	-3
-8	264	7	10	12	13	25	0*	1	72	4	3	2	33	10	2*	0	110	3	-1
-7	332	9	3	13	34	10	-1*	2	25	9	21*	3	98	6	10	1	311	8	6
-6	80	4	-8	14	26	14	16*	3	68	5	7	4	66	12	-8*	2	361	10	-12
-5	161	5	8	15	100	8	-1	4	235	10	-8	5	56	6	-2	3	7	16	-12*
-4	201	6	5	H,K=	7,	7	5	78	6	-3	6	6	22	-3*	4	146	5	7	
-3	302	8	-8	-18	36	14	-11*	6	42	7	-4	7	88	5	-1	5	266	7	3
-2	19	12	1*	-17	59	8	10	7	27	16	-8*	8	72	9	3	6	153	5	5
-1	112	4	-2	-16	47	10	10*	8	168	10	-1	H,K=	7,	15	7	6	19	-3*	
0	284	8	7	-14	72	8	-1	9	39	9	-11*	-6	24	19	15*	8	217	6	-5
1	190	5	3	-13	31	17	29*	10	64	7	-2	-5	45	6	9	9	147	5	13
2	26	7	-13*	-12	55	8	-14	11	63	8	9	-4	0	22	-15*	10	126	5	-5
3	318	9	-9	-11	270	8	3	12	90	10	-6	-3	109	7	3	11	83	8	0
4	186	6	1	-10	104	5	5	13	0	23	-11*	-2	0	20	-1*	12	155	6	14
5	164	5	1	-9	42	8	-2*	H,K=	7,	11	-1	81	5	9	13	93	7	-2	
6	94	4	-4	-8	110	5	1	-15	43	7	6	0	9	23	0*	14	6	35	-8*
7	219	7	-2	-7	268	7	1	-14	112	8	13	1	76	5	-6	15	35	13	-3*
8	239	10	1	-6	133	5	5	-13	17	22	13*	2	0	21	-19*	16	83	10	-1
9	89	5	-1	-5	129	5	-2	-12	71	6	0	H,K=	8,	0	H,K=	8,	4		
10	26	28	-5*	-4	202	6	-1	-11	39	12	-1*	-18	139	6	-6	-19	0	27	-23*
11	184	9	-2	-3	274	7	-2	-10	67	7	-13	-16	90	5	0	-18	38	13	7*
12	108	6	10	-2	55	5	-5	-9	11	32	2*	-14	218	6	6	-17	118	16	-15
13	0	30	-19*	-1	144	5	-1	-8	157	10	3	-12	30	7	-10*	-16	35	12	23*
14	67	6	3	0	220	6	-4	-7	56	6	5	-10	421	11	0	-15	117	6	1
15	95	10	-5	1	220	7	0	-6	79	5	7	-8	64	4	6	-14	39	20	-13*
16	58	7	10	2	53	5	-2	-5	21	22	14*	-6	403	10	-6	-13	232	8	-5
H,K=	7,	5	3	225	8	-3	-4	203	8	2	-4	30	4	-11	-12	18	25	10*	
-18	0	28	-9*	4	192	6	-9	-3	54	6	-8	-2	279	7	21	-11	144	6	-2
-17	54	7	16	5	204	9	-5	-2	30	31	-15*	0	273	7	12	-10	105	6	12
-16	37	10	11*	6	84	5	6	-1	48	8	7	2	384	10	-7	-9	174	6	-9
-15	187	7	-18	7	110	6	7	0	254	8	10	4	351	9	11	-8	53	5	-6
-14	23	27	6*	8	139	6	1	1	62	5	7	6	232	7	12	-7	252	7	-4
-13	0	26	-20*	9	67	6	8	2	24	16	-4*	8	258	7	10	-6	40	5	-8
-12	12	24	11*	10	54	6	6	3	35	16	2*	10	141	5	7	-5	47	4	-7
-11	339	10	-4	11	165	11	2	4	165	7	-2	12	205	9	13	-4	23	8	7*
-10	30	14	25*	12	66	7	-6	5	35	13	2*	14	0	26	-35*	-3	402	11	-5
-9	0	22	-10*	13	9	25	-22*	6	74	5	8	16	112	6	4	-2	78	4	8
-8	83	4	-6	14	51	7	5	7	65	6	8	H,K=	8,	2	-1	226	6	-1	

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
0	51	4	-3	-13	95	6	4	H,K=	8,	12	-3	61	3	0	-17	117	12	-6	
1	326	10	16	-12	38	11	8*	-13	54	7	-4	-2	362	9	2	-16	0	34	-17*
2	134	4	-4	-11	115	5	9	-12	33	11	0*	-1	91	3	6	-15	44	10	-17*
3	14	28	-13*	-10	207	7	9	-11	44	7	1	0	245	7	-20	-14	32	15	15*
4	91	4	0	-9	102	6	-8	-10	117	6	6	1	200	6	-13	-13	246	10	6
5	359	11	0	-8	0	32	-9*	-9	64	5	6	2	399	10	14	-12	48	7	-2
6	93	4	-2	-7	139	7	-13	-8	12	22	3*	3	160	5	-4	-11	95	5	-13
7	33	10	-4*	-6	222	7	-6	-6	149	8	-1	4	110	4	-8	-10	40	5	13
8	90	7	-3	-5	79	5	1	-5	48	14	-8*	5	99	4	-5	-9	247	7	-12
9	272	10	8	-4	53	5	-3	-4	57	7	-4	6	351	10	3	-8	34	7	3*
10	59	8	-1	-3	161	6	11	-3	123	8	-4	7	61	5	7	-7	103	4	8
11	90	6	21	-2	193	7	-8	-2	183	7	11	8	0	21	-12*	-6	34	6	5
12	49	9	-14*	-1	134	5	2	-1	33	36	-6*	9	58	6	-5	-5	367	10	-9
13	126	6	-7	0	194	6	3	0	73	5	6	10	219	10	3	-4	40	4	14
14	0	24	-4*	1	180	6	10	1	96	5	-4	11	0	25	-20*	-3	97	4	1
15	32	21	-24*	2	187	7	-1	2	124	5	1	12	63	7	-1	-2	51	4	9
H,K=	8,	6		3	73	6	6	3	18	23	16*	13	47	9	-9*	-1	376	10	-4
-19	13	30	-11*	4	159	7	-9	4	79	6	0	14	116	8	3	0	24	12	-2*
-18	11	28	-18*	5	159	8	-11	5	93	5	0	15	37	9	18*	1	135	4	7
-17	117	12	-9	6	112	5	-3	6	63	10	1	H,K=	9,		3	2	62	4	-4
-16	0	31	-17*	7	19	24	-12*	7	6	26	-20*	-19	72	10	-3	3	321	9	8
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-7	316	10	2	-15	0	28	-8*	-4	6	22	-1*	-10	121	4	9	12	31	13	8*
-6	115	4	1	-14	123	6	1	-3	132	10	0	-9	271	7	6	14	20	23	13*
-5	165	6	-5	-13	0	23	-4*	-2	36	9	3*	-8	150	5	-8	H,K=	9,		7
-4	26	6	10*	-12	0	25	-15*	-1	44	7	8	-7	34	5	24	-18	0	31	-6*
-3	308	9	-6	-11	12	22	9*	0	23	21	3*	-6	150	5	-3	-17	82	8	-2
-2	142	5	-10	-10	181	6	2	1	130	8	1	-5	335	9	12	-16	80	6	-3
-1	120	5	-5	-9	25	18	8*	2	51	7	-5	-4	73	3	6	-15	50	8	2
0	42	5	6	-8	43	7	7	3	10	30	4*	-3	68	3	17	-14	32	13	5*
1	345	10	-6	-7	0	23	-4*	4	28	10	12*	-2	250	7	-7	-13	142	10	-1
2	46	5	-1	-6	218	7	6	5	102	12	-1	-1	267	7	0	-12	129	5	-3
3	11	18	1*	-5	39	7	-2*	H,K=	9,	1	0	223	6	8	-11	46	7	5	
4	82	4	1	-4	52	5	-11	-19	55	8	20	1	185	5	-4	-10	74	5	7
5	294	10	-7	-3	0	21	-6*	-18	53	10	10	2	190	5	3	-9	214	9	-9
6	26	12	-7*	-2	190	7	-3	-17	22	27	-6*	3	294	8	-9	-8	159	6	-1
7	23	12	16*	-1	42	7	2	-16	219	7	13	4	19	13	13*	-7	25	29	9*
8	105	6	7	0	143	5	4	-15	33	12	-8*	5	232	7	8	-6	151	5	2
9	186	10	-5	1	16	27	-6*	-14	76	7	-2	6	226	7	8	-5	269	7	0
10	49	7	4	2	189	7	3	-13	24	13	4*	7	203	6	3	-4	100	4	-4
11	62	10	2	3	26	9	23*	-12	255	7	2	8	28	10	9*	-3	27	11	-3*
12	0	31	-27*	4	150	8	-1	-11	9	19	-2*	9	171	6	9	-2	196	6	3
13	114	8	-6	5	12	22	11*	-10	224	6	14	10	174	6	3	-1	234	7	10
H,K=	8,	8		6	110	8	-6	-9	153	5	4	11	82	7	-12	0	24	8	10*
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-17	84	8	9	8	154	10	0	-7	34	5	5	13	115	8	7	2	189	6	13
-16	58	15	5*	9	20	23	0*	-6	192	5	1	14	65	6	6	3	266	7	1
-15	47	12	2*	10	64	6	0	-5	140	4	-4	H,K=	9,		5	4	27	10	9*
-14	111	6	-4	11	15	22	13*	-4	256	7	1	-18	0	29	-9*	5	116	5	5

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	147	5	2	2	157	6	9	-14	111	5	6	8	54	7	-3	-3	189	6	-1
7	136	6	4	3	46	6	6	-13	53	7	-7	9	7	27	-8*	-2	62	6	-6
8	17	23	5*	4	11	21	2*	-12	181	6	0	10	41	11	-11*	-1	81	4	0
9	122	5	3	5	46	7	4	-11	161	5	4	11	205	7	7	0	212	6	7
10	75	7	-7	6	148	8	1	-10	74	4	5	12	25	16	14*	1	91	5	6
11	47	8	-8	7	43	10	12*	-9	125	4	9	13	21	26	3*	2	108	5	-2
12	25	13	5*	8	20	22	6*	-8	318	8	5	14	34	10	-2*	3	172	7	0
13	93	10	5	9	24	15	-9*	-7	182	5	-6	H,K=	10,			6	4	174	6	1
H,K=	9,	9		H,K=	9,	13	-6	54	4	-7	-19	116	8	9	5	63	5	3	
-17	0	26	-27*	-11	34	9	4*	-5	171	5	-4	-18	31	12	13*	6	84	5	-2
-16	110	9	-1	-10	51	6	0	-4	297	8	-7	-17	0	26	-5*	7	85	7	-3
-15	26	15	21*	-9	99	6	1	-3	114	4	-13	-16	60	7	8	8	105	5	3
-14	48	6	9	-8	83	5	8	-2	26	6	11*	-15	129	6	-6	9	0	22	-5*
-13	72	6	9	-7	4	20	2*	-1	250	7	-16	-14	27	23	-11*	10	71	6	0
-12	118	6	-1	-6	68	5	2	0	506	13	-19	-13	62	6	9	11	75	6	-2
-11	35	10	3*	-5	140	6	2	1	21	12	3*	-12	102	5	1	12	34	14	-7*
-10	143	8	3	-4	70	6	10	2	23	7	-9*	-11	238	7	7	H,K=	10,	10	
-9	55	7	4	-3	51	6	4	3	350	9	4	-10	42	7	2	-16	85	7	0
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-6	154	5	-6	0	65	6	7	6	183	6	3	-7	238	7	4	-13	8	23	-7*
-5	93	5	7	1	52	6	-1	7	164	6	16	-6	37	6	1	-12	115	6	-13
-4	142	5	6	2	82	5	4	8	195	6	-10	-5	226	7	1	-11	33	10	11*
-3	36	6	4	3	72	5	-4	9	26	14	6*	-4	95	4	-7	-10	33	8	3*
-2	202	6	-2	4	16	22	-3*	10	129	6	10	-3	253	7	-3	-9	36	7	15*
-1	94	5	2	5	67	5	3	11	119	8	10	-2	80	4	3	-8	186	7	-2
0	66	8	-2	6	68	7	2	12	75	6	7	-1	272	7	14	-7	28	17	-1*
1	26	9	21*	H,K=	9,	15	13	33	12	9*	0	119	4	2	-6	32	8	4*	
2	250	7	8	-4	0	19	-4*	14	87	6	8	1	126	5	11	-5	15	20	13*
3	107	5	20	-3	36	5	13	H,K=	10,	4	2	29	7	17*	-4	181	7	3	
4	36	8	8*	-2	17	19	11*	-18	27	18	2*	3	334	10	4	-3	30	8	9*
5	41	7	8	-1	94	6	6	-17	8	25	-4*	4	45	7	-3	-2	67	8	8
6	190	6	1	H,K=	10,	0	-16	46	10	-3*	5	84	5	9	-1	0	22	-9*	
7	60	6	8	-18	97	6	-5	-15	174	7	6	6	59	5	10	0	235	7	12
9	41	8	-4*	-16	185	6	19	-14	44	9	13*	7	188	7	5	1	39	7	6
10	118	6	6	-14	159	6	17	-13	94	5	3	8	64	5	2	2	59	6	1
11	22	24	-2*	-12	183	6	9	-12	65	5	-2	9	22	26	18*	3	34	6	32
12	30	12	-9*	-10	84	4	-5	-11	258	7	-2	10	27	28	-7*	4	166	6	13
H,K=	9,	11	-8	523	13	21	-10	41	6	11	11	148	7	-2	5	0	23	-5*	
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-14	23	25	-16*	-4	402	10	-18	-8	94	4	3	13	0	22	-16*	7	22	17	21*
-13	25	29	-12*	-2	72	4	-7	-7	103	4	-2	H,K=	10,	8	8	112	10	-2	
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-11	0	25	-2*	2	230	6	-14	-5	303	8	1	-16	75	7	-2	10	95	6	12
-10	76	9	-7	4	314	8	26	-4	75	4	8	-15	79	10	3	H,K=	10,	12	
-9	31	12	-7*	6	237	7	9	-3	265	7	-3	-14	76	5	5	-13	17	27	-2*
-8	111	7	-2	8	230	8	4	-2	54	4	-7	-13	43	13	-1*	-12	81	8	0
-7	24	12	23*	10	142	6	20	-1	256	7	2	-12	120	5	-7	-11	76	5	9
-6	136	5	4	12	83	6	11	0	155	5	6	-11	132	6	3	-10	33	9	-1*
-5	38	9	-15*	14	112	6	-3	1	152	5	15	-10	18	23	-8*	-9	33	10	1*
-4	73	5	3	H,K=	10,	2	2	52	5	-3	-9	81	5	11	-8	137	5	8	
-3	40	8	-4*	-19	94	6	8	3	367	10	3	-8	230	7	7	-7	57	6	4
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-1	63	5	11	-17	0	26	-14*	5	71	5	-3	-6	49	7	5	-5	80	5	-2
0	102	5	8	-16	173	6	8	6	88	4	-2	-5	105	6	0	-4	157	6	13
1	44	7	0	-15	103	5	8	7	279	9	6	-4	213	7	-1	-3	57	6	12

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ PAGE10

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	0	26	-13*	13	30	18	5*	1	360	10	6	-6	216	6	9	H,K=	12,	0	
-1	81	7	-9	14	22	32	2*	2	29	8	-7*	-5	0	22	-3*	-18	86	6	9
0	154	7	4	H,K=	11,	3		3	117	4	7	-4	110	6	-9	-16	188	7	15
1	33	25	3*	-18	73	7	-6	4	20	21	-3*	-3	97	7	4	-14	75	5	-6
2	34	9	17*	-17	82	6	-6	5	246	7	5	-2	130	6	-1	-12	142	5	-2
3	65	6	-2	-16	43	9	16*	6	12	21	3*	-1	54	6	-1	-10	281	8	9
4	77	5	0	-15	128	8	9	7	128	5	-4	0	200	6	3	-8	135	4	-12
5	18	21	12*	-14	136	5	13	8	33	8	8*	1	79	5	5	-6	412	11	-1
6	72	5	7	-13	95	5	6	9	150	6	7	2	115	5	3	-4	93	3	-13
7	71	5	1	-12	21	24	-12*	10	15	23	11*	3	16	21	-2*	-2	364	9	-1
H,K=	10,		14	-11	210	6	4	11	114	9	1	4	183	6	-1	0	50	4	-5
-8	49	7	-3	-10	175	5	11	12	15	21	12*	5	47	6	-4	2	355	9	7
-7	82	5	-4	-9	103	4	-1	13	75	6	-3	6	75	5	4	4	136	5	2
-6	27	12	6*	-8	105	4	0	H,K=	11,		7	8	131	6	0	6	249	7	3
-5	79	7	-4	-7	235	6	6	-18	48	7	-4	9	26	13	-2*	8	73	5	12
-4	34	8	8*	-6	118	4	1	-17	102	6	11	10	42	5	24	10	133	5	6
-3	79	5	9	-5	0	16	-7*	-16	20	22	19*	H,K=	11,		11	12	91	5	8
-2	15	25	13*	-4	112	4	2	-15	83	5	-3	-14	111	7	6	H,K=	12,	2	
-1	103	6	5	-3	306	8	0	-14	104	5	7	-13	33	8	7*	-19	20	26	-6*
0	48	6	3	-2	187	5	9	-13	90	6	9	-12	38	6	15	-18	82	10	10
1	40	7	-1*	-1	30	6	6*	-12	25	32	-2*	-11	0	23	-28*	-17	86	7	2
2	17	21	10*	0	218	6	-6	-11	172	6	6	-10	123	5	0	-16	122	5	10
3	91	5	0	1	324	9	5	-10	121	5	8	-9	20	24	15*	-15	21	26	13*
H,K=	11,		1	2	145	5	1	-9	106	5	-2	-8	53	6	-8	-14	130	5	2
-19	0	25	-24*	3	137	5	0	-8	74	5	-6	-7	38	12	-3*	-13	114	5	-1
-18	154	6	9	4	164	5	10	-7	223	7	-3	-6	125	7	-1	-12	109	6	3
-17	67	6	9	5	248	7	3	-6	125	5	-1	-5	11	20	10*	-11	44	5	0
-16	0	24	-6*	6	15	27	-1*	-5	89	4	9	-4	123	6	16	-10	217	6	-3
-15	21	22	6*	7	101	5	5	-4	142	5	-4	-3	47	7	1	-9	169	5	6
-14	223	7	7	8	167	6	2	-3	245	7	13	-2	137	5	8	-8	114	4	-8
-13	26	11	3*	9	130	6	1	-2	103	4	5	-1	0	25	-20*	-7	109	4	-5
-12	10	21	-17*	10	0	25	-24*	-1	22	13	-2*	0	150	5	10	-6	243	7	6
-11	53	9	0	11	113	5	10	0	161	5	3	1	20	24	-12*	-5	184	5	-1
-10	284	8	11	12	74	9	-1	1	226	8	6	2	116	5	9	-4	0	17	-14*
-9	0	18	-7*	13	67	7	1	2	64	5	3	3	0	23	-10*	-3	135	4	10
-8	234	6	12	14	0	23	-11*	3	87	5	-4	4	121	5	7	-2	372	10	0
-7	148	4	-8	H,K=	11,		5	4	139	5	8	5	53	7	13	-1	94	4	-2
-6	335	9	-16	-18	18	35	14*	5	196	6	3	6	9	22	-10*	0	56	3	-2
-5	0	16	-25*	-17	108	6	1	6	30	10	-6*	7	16	22	-8*	1	191	6	-10
-4	210	6	5	-16	9	27	0*	7	50	9	6*	8	126	5	4	2	308	9	1
-3	99	3	5	-15	144	7	7	8	102	5	6	H,K=	11,		13	3	116	4	-5
-2	325	9	4	-14	23	24	7*	9	89	5	9	-10	66	5	4	4	63	4	10
-1	119	4	-13	-13	134	6	9	10	0	22	-9*	-9	52	9	10	5	154	5	-7
0	394	10	3	-12	39	8	14*	11	65	6	-5	-8	47	5	12	6	189	7	6
1	99	4	7	-11	209	6	0	12	54	13	-8*	-7	97	6	5	7	62	6	-3
2	226	7	-5	-10	11	20	-14*	H,K=	11,		9	-6	90	5	9	8	85	5	5
3	131	4	-5	-9	122	5	-1	-16	0	22	-4*	-5	3	19	-7*	9	89	5	4
4	340	9	13	-8	35	7	-6*	-15	45	7	1	-4	40	7	6	10	135	7	3
5	79	4	2	-7	237	7	-7	-14	110	5	-4	-3	136	5	16	11	26	11	22*
6	92	4	10	-6	70	7	-2	-13	32	9	9*	-2	65	5	0	12	50	11	-3*
7	38	7	4*	-5	26	6	11*	-12	50	13	5*	-1	8	19	-2*	13	58	8	-12
8	234	8	14	-4	26	7	-7*	-11	59	7	6	0	59	6	1	H,K=	12,	4	
9	37	8	1*	-3	404	11	-4	-10	156	7	2	1	103	5	8	-18	33	14	13*
10	21	24	-10*	-2	14	18	11*	-9	33	13	-8*	2	48	9	-2	-17	120	6	0
11	31	15	-8*	-1	15	17	-11*	-8	132	5	12	3	24	11	3*	-16	0	25	-27*
12	132	6	9	0	18	20	-12*	-7	48	6	-3	4	59	5	5	-15	13	25	-18*

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ PAGE11

L	FCB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-14	45	8	-9*	9	149	6	16	8	66	5	5	10	128	5	11	1	9	20	-6*
-13	233	7	15	10	46	7	2	H,K=	12,	12	11	36	8	7*	2	34	7	-1*	
-12	35	8	4*	11	21	21	-3*	-12	63	5	2	12	25	15	5*	3	270	8	-1
-11	5	21	-3*	12	33	13	16*	-11	6	21	-4*	H,K=	13,	3	4	27	8	15*	
-10	81	4	4	H,K=	12,	8	-10	84	8	0	-18	0	26	-18*	5	40	7	10	
-9	208	6	-9	-17	81	7	6	-9	62	6	-1	-17	59	6	5	6	27	12	26*
-8	64	4	2	-16	88	5	9	-8	74	5	11	-16	104	5	12	7	155	6	-5
-7	120	4	-7	-15	0	22	-11*	-7	0	22	-27*	-15	92	5	4	8	0	25	-18*
-6	63	4	-3	-14	68	7	4	-6	117	6	2	-14	0	23	-14*	9	68	5	4
-5	242	7	-1	-13	99	5	2	-5	68	5	1	-13	128	5	-1	10	0	25	-9*
-4	20	10	11*	-12	71	7	5	-4	39	6	6	-12	121	5	4	11	114	5	-2
-3	208	6	13	-11	0	27	-14*	-3	69	5	5	-11	145	5	1	H,K=	13,	7	
-2	116	4	9	-10	145	7	0	-2	146	6	6	-10	16	20	0*	-18	12	23	-11*
-1	269	7	-6	-9	145	5	6	-1	67	5	4	-9	176	6	-1	-17	39	8	-7*
0	0	22	-14*	-8	72	5	4	0	0	33	-19*	-8	187	6	8	-16	59	7	1
1	245	7	3	-7	76	5	4	1	54	7	2	-7	83	4	9	-15	90	7	0
2	125	4	-5	-6	201	6	-1	2	116	6	7	-6	24	7	10*	-14	45	6	14
3	183	6	3	-5	160	6	3	3	45	6	1	-5	275	7	-20	-13	91	7	2
4	34	10	7*	-4	42	6	5	4	25	28	2*	-4	93	4	4	-12	89	6	-6
5	215	8	-2	-3	36	6	9	5	67	5	13	-3	87	4	-10	-11	125	5	7
6	57	6	-4	-2	179	6	-4	H,K=	12,	14	-2	151	5	-9	-10	0	31	-14*	
7	51	6	-4	-1	135	5	2	-5	92	5	-2	-1	304	8	3	-9	140	5	7
8	7	23	-16*	0	30	12	-10*	-4	31	7	2*	0	219	6	-15	-8	129	5	-2
9	174	7	2	1	105	5	8	-3	69	5	4	1	17	19	4*	-7	91	5	-2
10	26	16	-12*	2	206	6	5	-2	0	22	-22*	2	102	4	14	-6	61	8	-2
11	12	23	-8*	3	89	5	3	-1	88	5	14	3	264	7	3	-5	224	7	2
12	17	24	-7*	5	94	5	3	H,K=	13,	1	4	65	5	1	-4	148	6	-1	
13	100	5	1	6	155	5	1	-19	33	35	-7*	5	15	20	5*	-3	123	5	-2
H,K=	12,	6	7	48	7	-4	-18	57	9	13	6	118	5	6	-2	105	4	1	
-18	0	26	-10*	8	47	6	7	-17	0	30	-5*	7	153	5	7	-1	170	5	7
-17	122	11	-4	9	64	5	0	-16	202	6	17	8	53	7	0	0	108	4	8
-16	0	24	-19*	10	80	5	11	-15	50	6	8	9	39	10	-10*	1	15	20	4*
-15	0	23	-15*	H,K=	12,	10	-14	41	7	3	10	87	6	-5	2	95	5	-3	
-14	45	8	5	-15	26	12	6*	-13	22	11	13*	11	92	6	-6	3	205	6	-2
-13	182	6	2	-14	74	8	-3	-12	164	5	-7	12	22	23	-3*	4	67	6	0
-12	43	8	1	-13	0	23	-9*	-11	31	7	-2*	H,K=	13,	5	5	19	21	11*	
-11	25	12	16*	-12	74	5	1	-10	25	10	-12*	-19	103	6	2	6	75	8	-11
-10	42	6	5	-11	0	24	-22*	-9	89	4	3	-18	14	24	8*	7	125	6	10
-9	250	7	-8	-10	123	10	-11	-8	347	9	-2	-17	43	9	-11*	8	37	6	4
-8	38	6	8	-9	0	24	-2*	-7	61	4	-4	-16	0	25	-8*	9	40	8	14*
-7	137	5	0	-8	76	5	-4	-6	99	5	5	-15	109	5	4	10	65	5	2
-6	47	6	-2	-7	0	23	-21*	-5	83	4	-6	-14	16	22	11*	H,K=	13,	9	
-5	291	8	6	-6	159	8	-5	-4	270	7	-14	-13	158	6	11	-16	107	5	11
-4	25	13	-4*	-5	32	8	8*	-3	51	5	-4	-12	43	7	9	-15	17	21	1*
-3	162	6	3	-4	35	7	8*	-2	154	5	-12	-11	186	6	2	-14	34	11	9*
-2	135	5	-3	-3	15	26	14*	-1	74	4	4	-10	0	23	-28*	-13	43	8	7*
-1	245	7	0	-2	211	6	4	0	311	8	0	-9	183	6	4	-12	112	6	-12
0	0	19	-24*	-1	0	22	-23*	1	45	4	-5	-8	42	7	1	-11	59	6	5
1	225	7	8	0	14	19	9*	2	216	6	11	-7	124	5	5	-10	46	14	0*
2	78	5	-10	1	0	21	-6*	3	102	4	5	-6	0	19	-15*	-9	0	21	-15*
3	132	6	12	2	193	6	0	4	154	5	2	-5	319	9	-4	-8	197	7	3
4	0	28	-5*	3	13	20	10*	5	30	7	10*	-4	0	18	-9*	-7	24	14	-1*
5	190	7	5	4	45	5	5	6	192	6	1	-3	125	4	-2	-6	57	6	-1
6	55	6	1	5	16	19	11*	7	71	5	3	-2	15	18	6*	-5	70	5	15
7	69	5	6	6	150	6	8	8	92	5	-11	-1	305	8	1	-4	181	6	6
8	49	8	10	7	0	22	-13*	9	0	23	-10*	0	0	26	-17*	-3	66	6	4

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ PAGE12

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	121	5	-3	6	0	37	-26*	1	259	7	7	-1	12	24	-8*	-11	38	6	5
0	146	5	-6	8	170	7	3	2	39	5	17	0	165	6	3	-10	243	7	7
1	0	23	-10*	10	37	9	16*	3	154	6	-4	1	104	5	5	-9	65	4	-3
2	148	5	5	12	87	6	3	4	78	5	1	2	0	21	-6*	-8	41	6	16
3	70	6	6	H,K=	14,		2	5	156	5	0	3	89	6	-4	-7	108	5	7
4	115	5	11	-18	93	7	1	6	18	24	9*	4	140	5	-6	-6	357	9	-6
5	32	5	31	-17	42	7	6	7	122	6	6	5	84	6	2	-5	67	4	1
6	125	7	-4	-16	84	5	12	8	47	8	-8	6	13	20	1*	-4	27	7	10*
7	45	10	12*	-15	78	6	-2	9	64	5	4	7	53	7	3	-3	106	4	0
8	53	6	-7	-14	118	6	1	10	0	23	-10*	8	94	7	5	-2	290	8	-7
H,K=	13,		11	-13	14	22	7*	11	107	5	-8	H,K=	14,		10	-1	21	12	-1*
-13	9	20	-10*	-12	90	4	-7	H,K=	14,		6	-14	90	5	-1	0	88	4	2
-12	111	7	5	-11	140	5	4	-18	29	11	4*	-13	13	26	9*	1	79	4	7
-11	0	25	-7*	-10	174	6	6	-17	69	6	13	-12	75	6	1	2	224	8	-1
-10	14	19	6*	-9	10	19	-10*	-15	107	6	-7	-11	22	24	14*	3	25	8	0*
-9	49	5	8	-8	187	6	0	-14	50	7	-1	-10	93	5	-2	4	136	5	-2
-8	144	6	2	-7	207	6	-7	-13	26	13	-7*	-9	45	7	-4	5	57	10	-14
-7	24	10	8*	-6	164	5	-4	-12	68	5	7	-8	118	5	0	6	131	5	2
-6	27	9	-6*	-5	55	4	-7	-11	187	6	0	-7	27	9	11*	7	0	22	-5*
-5	52	6	3	-4	204	6	-4	-10	69	6	1	-6	98	5	6	8	103	7	4
-4	120	5	-1	-3	221	6	0	-9	0	25	-14*	-5	11	19	0*	9	47	6	12
-3	0	21	-13*	-2	139	5	3	-8	35	9	-5*	-4	142	5	1	10	70	8	-4
-2	106	5	-2	-1	82	4	3	-7	251	7	2	-3	23	16	10*	11	20	22	11*
-1	39	8	0*	0	291	8	-11	-6	24	14	-3*	-2	52	8	8	H,K=	15,		3
0	149	5	6	1	142	5	-6	-5	80	4	-5	-1	12	20	4*	-18	32	20	-13*
1	0	23	-8*	2	90	4	-7	-4	84	4	-7	0	170	6	-2	-17	94	5	9
2	85	5	0	3	147	6	-13	-3	275	8	-6	1	19	21	8*	-16	26	14	-3*
3	37	9	-4*	4	166	5	3	-2	17	19	7*	2	28	8	1*	-15	54	6	0
4	64	5	2	5	128	5	-4	-1	88	4	8	3	26	8	23*	-14	88	11	-6
5	0	31	-8*	6	27	12	-4*	0	89	5	-4	4	126	5	-4	-13	130	5	8
6	99	5	-2	7	74	6	1	1	163	5	3	5	0	20	-4*	-12	39	8	-3*
H,K=	13,		13	8	158	6	0	2	37	7	-9*	6	32	7	9*	-11	111	6	7
-9	74	4	6	9	43	8	-4	3	144	5	-12	H,K=	14,		12	-10	147	5	-7
-8	86	5	3	10	36	8	15*	4	46	7	5	-11	63	5	-3	-9	160	5	1
-7	54	6	7	11	62	9	-1	5	118	8	-3	-10	66	6	-8	-8	75	6	10
-6	0	20	-5*	12	75	6	-6	6	13	20	4*	-9	0	19	-9*	-7	191	6	2
-5	96	6	-2	H,K=	14,		4	7	109	5	11	-8	77	5	-2	-6	145	5	7
-4	64	6	-6	-18	35	9	12*	8	48	7	10	-7	49	7	-12	-5	140	6	2
-3	16	19	0*	-17	48	8	7	9	60	6	-4	-6	72	5	5	-4	56	4	6
-2	27	10	-4*	-16	22	24	-8*	10	0	25	-21*	-5	26	9	0*	-3	232	7	-10
-1	108	5	0	-15	145	5	8	H,K=	14,		8	-4	106	8	8	-2	191	7	-4
0	72	5	6	-14	44	6	13	-16	19	23	-11*	-3	64	5	-6	-1	115	4	0
1	7	20	-4*	-13	0	23	-8*	-15	64	6	-1	-2	33	7	-1*	0	57	4	-2
H,K=	14,		0	-12	0	25	-18*	-14	102	5	4	-1	44	7	1	1	231	7	-15
-18	144	6	12	-11	230	7	2	-13	16	22	0*	0	120	5	8	2	160	5	-3
-16	77	5	5	-10	68	5	-2	-12	66	5	-5	1	65	4	6	3	62	5	9
-14	184	6	-6	-9	0	20	-19*	-11	91	5	3	2	17	21	-6*	4	62	5	5
-12	49	5	-6	-8	48	6	5	-10	78	5	-7	3	36	6	4	5	168	6	-3
-10	178	5	8	-7	223	6	-4	-9	32	8	8*	H,K=	15,		1	7	26	20	24*
-8	279	8	0	-6	39	6	-8	-8	153	5	-1	-18	108	5	7	8	78	5	-1
-6	251	7	6	-5	108	4	-11	-7	130	5	2	-17	54	6	12	9	117	5	3
-4	257	7	-6	-4	50	5	5	-6	122	5	2	-16	84	5	12	10	47	6	1
-2	143	5	0	-3	293	8	-5	-5	0	21	-15*	-15	16	21	11*	H,K=	15,		5
0	332	9	5	-2	20	14	9*	-4	153	5	-4	-14	157	5	11	-18	0	24	-1*
2	0	24	-20*	-1	127	5	1	-3	144	5	-3	-13	63	5	11	-17	101	7	0
4	229	7	12	0	136	5	-4	-2	47	8	-1	-12	76	5	10	-16	19	21	8*

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ PAGE13

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-15	62	6	2	-13	43	12	5*	-16	125	6	18	H,K=	16,	6	-8	120	6	3	
-14	41	7	17	-12	30	17	4*	-15	43	7	7	-17	56	17	-10*	-7	0	20	-19*
-13	134	6	-10	-11	19	20	14*	-14	40	14	-8*	-16	23	14	-2*	-6	83	5	1
-12	30	8	9*	-10	144	6	0	-13	98	5	-3	-15	77	5	4	-5	14	21	4*
-11	108	5	3	-9	56	6	-10	-12	137	5	-1	-14	36	8	1*	-4	82	5	-9
-10	12	21	-2*	-8	13	20	1*	-11	52	6	6	-13	120	8	-9	-3	0	20	-6*
-9	207	6	10	-7	31	15	11*	-10	108	5	1	-12	50	10	-2*	-2	118	6	-6
-8	23	11	22*	-6	191	7	7	-9	157	5	2	-11	103	5	3	-1	0	24	-9*
-7	169	6	-11	-5	34	9	-6*	-8	250	7	-3	-10	44	6	0	0	80	4	-4
-6	37	6	1	-4	26	12	-5*	-7	9	20	-20*	-9	181	6	2	2	109	6	-3
-5	139	5	2	-3	37	6	5	-6	151	5	12	-8	39	6	3	3	28	8	16*
-4	26	9	18*	-2	169	6	0	-5	193	6	-16	-7	0	20	-12*	4	30	8	-5*
-3	217	7	-6	-1	22	20	-13*	-4	128	5	-3	-6	28	28	6*	H,K=	16,	12	
-2	0	20	-7*	0	61	7	-3	-3	0	19	-18*	-5	248	7	-9	-7	10	24	1*
-1	125	5	4	1	58	6	-2	-2	197	6	-15	-4	36	10	6*	-6	55	5	2
0	26	11	-8*	2	131	6	4	-1	138	5	2	-3	0	21	-6*	-5	58	6	4
1	235	7	-2	3	19	16	4*	0	141	5	-13	-2	67	7	-9	-4	61	5	5
2	17	21	6*	4	71	5	-8	1	74	5	-12	-1	180	7	-3	-3	0	19	-11*
3	33	11	-13*	5	31	9	-4*	2	185	6	4	0	41	7	-5	-2	87	5	5
4	34	18	11*	H,K=	15,	11	3	114	5	-2	1	65	5	-3	H,K=	17,	1		
5	169	6	-2	-12	26	9	-1*	4	26	15	-15*	2	36	7	-3*	-18	86	6	7
6	0	21	-9*	-11	22	12	-8*	5	75	5	4	3	136	5	-3	-17	0	22	-8*
7	0	21	-3*	-10	118	6	3	6	136	5	1	4	0	23	-24*	-16	103	5	0
8	2	21	-7*	-9	0	19	-8*	7	70	5	-4	5	67	7	-2	-15	50	7	-5
9	112	5	-12	-8	25	8	5*	8	28	10	12*	6	3	22	-31*	-14	117	5	3
10	25	10	17*	-7	26	29	-7*	9	53	6	5	7	86	5	-5	-13	18	21	14*
H,K=	15,	7	-6	113	5	0	10	88	5	-3	8	32	7	14*	-12	132	6	-1	
-17	92	6	3	-5	25	12	-3*	H,K=	16,	4	H,K=	16,	8	-10	86	5	7		
-16	37	8	3*	-4	35	6	7	-18	31	8	27*	-15	36	9	-6*	-9	21	21	-12*
-15	18	22	-3*	-3	29	10	-1*	-17	71	6	0	-14	28	18	4*	-8	268	8	-14
-14	91	6	9	-2	128	5	5	-16	42	11	-2*	-13	64	6	0	-7	58	5	-1
-13	108	9	-1	-1	0	22	-9*	-15	0	26	-42*	-12	102	5	7	-6	58	4	-3
-12	0	32	-22*	0	47	5	-2	-14	15	22	10*	-11	63	8	4	-5	73	8	-11
-11	25	30	-10*	1	25	10	-3*	-13	169	6	8	-10	94	5	6	-4	238	7	6
-10	122	5	-3	2	104	5	-2	-12	49	7	-4	-9	88	5	-3	-3	74	5	7
-9	137	6	-2	3	0	20	-3*	-11	96	7	11	-8	126	5	3	-2	25	8	18*
-8	0	21	-8*	H,K=	16,	0	-10	0	21	-17*	-7	16	20	5*	-1	38	7	11*	
-7	144	7	0	-18	17	21	2*	-9	196	6	3	-6	101	5	-9	0	213	6	-9
-6	132	5	-8	-16	194	6	16	-8	107	5	9	-5	135	5	-4	1	19	20	12*
-5	136	5	-7	-14	0	23	-22*	-7	32	7	7*	-4	117	5	3	2	59	5	15
-4	22	18	-9*	-12	172	6	2	-6	64	5	7	-3	30	7	16*	3	38	7	-10*
-3	131	6	-7	-10	108	5	-1	-5	233	7	-5	-2	115	5	0	4	133	6	-2
-2	106	5	-9	-8	283	8	3	-4	26	9	6*	-1	99	5	4	5	11	21	2*
-1	102	5	2	-6	240	7	-1	-3	19	14	2*	0	65	5	2	6	65	7	-6
0	52	7	-4	-4	196	6	-7	-2	90	5	5	1	42	6	5	7	45	7	5
1	152	5	4	-2	216	6	-1	-1	234	7	5	2	120	5	3	8	114	7	1
2	91	5	1	0	139	5	10	0	43	6	-4	3	84	5	0	9	0	24	-10*
3	14	18	5*	2	179	6	7	1	80	4	2	4	14	22	-15*	H,K=	17,	3	
4	57	6	7	4	17	22	0*	2	62	6	-18	5	38	7	5	-18	44	9	-2*
5	133	5	-1	6	157	6	-2	3	187	6	-9	6	99	5	-2	-17	0	22	-2*
6	58	6	5	8	31	7	3*	4	22	16	15*	H,K=	16,	10	-16	58	6	2	
7	22	14	7*	10	105	7	3	5	69	8	-2	-13	14	20	9*	-15	114	5	6
8	43	7	-7	H,K=	16,	2	6	41	13	3*	-12	106	5	10	-14	56	5	13	
H,K=	15,	9	-19	40	9	1*	7	89	5	2	-11	32	7	5*	-13	44	7	-8	
-15	0	28	-13*	-18	24	16	19*	8	0	26	-6*	-10	64	5	1	-12	100	5	-1
-14	55	5	-3	-17	53	8	1	9	102	6	5	-9	25	6	25*	-11	167	6	-1

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ PAGE14

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-10	75	5	4	-7	141	5	10	6	45	7	-1	H,K=	18,	6		H,K=	19,	1	
-9	57	5	-6	-6	45	5	16	8	113	5	0	-16	25	9	22*	-17	36	9	0*
-8	146	5	-1	-5	127	5	-1	H,K=	18,	2	-15	76	7	4	-16	120	5	3	
-7	158	5	-3	-4	105	5	-3	-18	80	5	5	-14	34	8	5*	-15	0	31	-8*
-6	44	5	7	-3	136	5	-6	-17	60	5	11	-13	95	5	-6	-14	69	5	-3
-5	130	5	-13	-2	0	22	-17*	-16	0	21	-4*	-12	17	20	4*	-13	64	6	-2
-4	112	5	0	-1	62	10	-1	-15	62	6	-6	-11	107	7	-9	-12	111	7	-2
-3	140	5	0	0	96	5	-1	-14	136	5	14	-10	55	6	-4	-11	15	20	-5*
-2	17	21	-30*	1	63	5	10	-13	62	9	-5	-9	96	5	5	-10	127	6	-8
-1	135	5	-6	2	21	25	-2*	-12	29	11	-2*	-8	31	9	25*	-9	50	6	-5
0	157	5	-12	3	116	5	2	-11	91	5	0	-7	187	6	8	-8	120	6	2
1	89	5	-3	4	60	6	-7	-10	166	5	-4	-6	58	5	11	-7	28	9	0*
2	0	25	-7*	5	47	5	5	-9	55	5	7	-5	40	6	8	-6	176	6	-5
3	134	5	-7	6	37	12	1*	-8	42	12	-8*	-4	0	23	-20*	-5	70	5	-2
4	77	9	-1	H,K=	17,	9	-7	127	5	-11	-3	168	7	-8	-4	74	4	10	
5	46	6	-5	-13	0	23	-7*	-6	154	5	3	-2	44	5	5	-3	39	5	13
6	26	15	-8*	-12	89	5	0	-5	36	5	11	-1	25	11	-2*	-2	162	5	0
7	93	5	-2	-10	34	6	3*	-4	108	5	6	0	39	7	-8	-1	37	7	-9*
8	56	8	-3	-9	0	23	-6*	-3	123	5	-12	1	130	6	0	0	44	7	-2
H,K=	17,	5	-8	130	5	-11	-2	116	5	2	2	17	21	-10*	1	40	6	15	
-17	27	10	11*	-7	25	13	-16*	-1	29	9	1*	3	0	22	-32*	2	146	5	-1
-16	16	22	9*	-6	35	8	9*	0	125	5	-1	4	30	9	0*	3	29	10	7*
-15	127	5	11	-5	29	10	-5*	1	98	5	0	5	110	5	-1	4	27	9	-2*
-14	17	23	-7*	-4	154	5	-4	2	114	6	-2	6	10	20	8*	5	47	6	9
-13	32	10	-9*	-3	31	7	1*	3	0	22	-34*	H,K=	18,	8	6	122	6	2	
-12	6	22	-4*	-2	12	18	6*	4	100	5	-1	-14	88	5	0	7	25	11	3*
-11	198	6	2	-1	0	22	-28*	5	87	7	-2	-13	51	10	5*	H,K=	19,	3	
-10	20	17	17*	0	132	5	-12	6	46	7	-1	-12	0	24	-10*	-17	61	8	-15
-9	47	6	-4	1	29	8	0*	7	37	7	14	-11	57	5	4	-16	57	6	2
-8	36	8	-1*	2	31	7	4*	8	89	6	1	-10	95	5	-7	-15	0	21	-4*
-7	194	6	0	3	30	9	-9*	H,K=	18,	4	-9	42	6	1	-14	54	7	3	
-6	21	22	5*	4	108	5	2	-17	84	7	6	-8	47	6	-7	-13	130	5	0
-5	134	6	-10	H,K=	17,	11	-16	0	21	-5*	-7	93	6	2	-12	58	6	-1	
-4	8	20	1*	-9	17	19	-5*	-15	89	5	2	-6	120	5	3	-11	0	20	-10*
-3	161	6	-7	-8	109	5	4	-14	35	16	-6*	-5	30	11	10*	-10	81	5	-6
-2	32	15	8*	-7	25	9	-2*	-13	91	5	7	-4	66	5	-2	-9	156	5	-1
-1	135	5	-6	-6	47	6	9	-12	33	6	24	-3	91	4	7	-8	95	5	1
0	5	21	5*	-5	15	18	7*	-11	154	6	-5	-2	100	5	5	-7	52	6	-1
1	100	5	3	-4	110	4	9	-10	75	5	12	-1	38	6	13	-6	82	9	4
2	24	10	17*	-3	29	8	-1*	-9	134	6	12	0	92	5	4	-5	156	5	0
3	149	6	-12	-2	25	6	11*	-8	25	13	-3*	1	77	5	3	-4	24	11	9*
4	18	19	14*	-1	20	15	-1*	-7	180	6	-3	2	51	6	-4	-3	69	5	-10
5	43	10	-12*	0	125	5	3	-6	56	6	-3	3	0	20	-12*	-2	87	5	-9
6	0	19	-8*	H,K=	18,	0	-5	55	9	-6	4	78	7	-8	-1	140	5	11	
7	107	5	2	-18	124	5	12	-4	46	5	7	H,K=	18,	10	0	16	32	-16*	
8	16	21	5*	-16	51	6	13	-3	171	6	-7	-10	113	6	8	1	87	5	-7
H,K=	17,	7	-14	190	7	14	-2	41	11	5*	-9	30	7	10*	2	99	10	-9	
-16	39	8	-6*	-12	18	20	2*	-1	36	6	21	-8	44	5	5	3	90	5	-10
-15	104	7	4	-10	189	6	-6	0	35	9	-10*	-7	13	19	7*	4	0	21	-8*
-14	42	7	1	-8	96	4	1	1	175	6	-11	-6	110	5	-2	5	76	5	-6
-13	13	21	6*	-6	239	7	-8	2	41	6	-5	-5	0	18	-9*	6	72	5	5
-12	81	5	1	-4	109	6	-2	3	29	9	10*	-4	58	8	-9	H,K=	19,	5	
-11	130	5	2	-2	159	5	1	4	33	8	4*	-3	0	18	-10*	-16	0	22	-7*
-10	31	8	-1*	0	94	9	-9	5	125	5	4	-2	99	5	-1	-15	0	22	-13*
-9	41	7	-4	2	92	5	-2	6	28	8	8*	-1	0	20	-2*	-14	0	22	-5*
-8	99	5	-3	4	124	5	-2	7	42	6	4	0	93	5	4	-13	143	6	-1

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ PAGE15

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-12	24	9	21*	-4	158	8	-2	-7	71	5	-2	-5	0	29	-30*	-8	0	22	-28*
-11	19	22	15*	-2	60	5	-1	-6	13	20	4*	-4	62	6	2	-7	66	5	2
-10	0	21	-5*	0	140	5	-1	-5	142	5	-4	-3	121	5	0	-6	110	9	-5
-9	185	6	4	2	71	5	3	-4	30	9	2*	-2	36	7	1*	-5	59	5	6
-8	0	21	-7*	4	83	5	11	-3	65	6	-3	-1	38	6	-10	-4	27	7	18*
-7	40	7	-7	H,K=	20,		2	-2	29	8	2*	0	89	5	-5	-3	53	6	-22
-6	22	15	2*	-16	76	6	-11	-1	102	5	2	1	98	8	-6	-2	103	5	-2
-5	165	7	-1	-15	69	5	5	0	25	26	0*	2	40	14	-1*	-1	41	10	-3*
-4	15	21	-3*	-14	29	13	0*	1	0	19	-20*	3	62	8	-6	0	30	7	0*
-3	61	9	-10	-13	46	8	-6	2	20	25	-9*	H,K=	21,		5	1	59	6	-2
-2	26	11	23*	-12	115	5	5	3	107	7	-5	-14	27	8	14*	2	103	7	1
-1	124	5	0	-11	88	5	7	H,K=	20,		8	-13	35	10	5*	H,K=	22,		4
0	20	21	3*	-10	0	21	-4*	-11	55	5	-1	-12	7	19	2*	-13	86	5	-6
1	101	6	-8	-9	62	5	-2	-10	0	26	-1*	-11	118	5	-8	-12	0	25	-12*
2	0	21	-1*	-8	167	6	3	-9	28	9	-7*	-10	6	20	1*	-11	43	6	-5
3	94	5	-10	-7	56	5	13	-8	99	5	-1	-9	20	21	-5*	-10	42	7	-5
4	22	11	17*	-6	22	11	16*	-7	47	5	4	-8	0	19	-10*	-9	106	5	-4
5	96	5	6	-5	124	5	-5	-6	27	7	3*	-7	131	5	-4	-8	14	21	0*
H,K=	19,		7	-4	118	5	2	-5	70	5	-3	-6	0	19	-1*	-7	56	6	-13
-14	38	7	0	-3	52	6	-5	-4	101	5	2	-5	29	6	11*	-6	53	5	5
-13	98	5	2	-2	45	6	-15	-3	40	6	-5	-4	22	10	8*	-5	85	6	-8
-12	59	5	-1	-1	92	5	-1	-2	39	6	-10	-3	114	5	-13	-4	26	7	21*
-11	26	11	10*	0	130	5	-7	-1	59	5	5	-2	0	19	-5*	-3	75	5	-12
-10	67	6	-1	1	10	25	0*	0	72	8	-5	-1	31	8	-10*	-2	32	9	-11*
-9	106	5	6	2	66	5	-2	H,K=	21,		1	0	0	20	-2*	-1	51	6	-6
-8	43	7	-10	3	91	5	2	-16	0	22	-27*	1	108	7	-2	0	0	20	-2*
-7	49	6	-7	4	70	6	-11	-15	43	7	-5	2	24	14	10*	1	105	7	-6
-6	71	5	-3	5	6	20	-2*	-14	127	5	7	H,K=	21,		7	H,K=	22,		6
-5	139	7	2	H,K=	20,		4	-13	29	10	-3*	-11	76	5	-7	-11	32	8	-3*
-4	23	14	-2*	-16	40	5	12	-12	46	6	-7	-10	66	5	9	-10	27	10	-8*
-3	37	6	1	-15	80	6	1	-11	55	5	6	-9	6	19	-9*	-9	84	5	-8
-2	83	6	-2	-14	25	9	11*	-10	104	5	-9	-8	52	5	2	-8	0	28	-11*
-1	95	5	-1	-12	30	8	-6*	-9	0	20	-12*	-7	99	5	-3	-7	72	5	-5
0	12	19	8*	-11	114	5	-1	-8	106	5	-5	-6	37	16	-7*	-6	34	6	4
1	63	7	7	-9	99	5	-9	-7	43	8	-2	-5	8	20	-14*	-5	84	5	1
2	64	5	-2	-8	55	8	-11	-6	112	5	-2	-4	45	11	-13*	-4	0	26	-2*
3	66	7	5	-7	104	5	3	-5	27	9	-5*	-3	102	5	-8	-3	65	5	-12
H,K=	19,		9	-6	0	20	-2*	-4	120	5	-2	-2	26	9	4*	-2	24	10	-3*
-11	17	19	6*	-5	128	5	-6	-3	43	6	-15	-1	0	19	-7*	H,K=	23,		1
-10	81	7	-3	-4	44	5	5	-2	64	6	-3	H,K=	22,		0	-13	41	6	3
-9	37	6	1	-3	63	7	3	-1	0	21	-8*	-14	103	5	1	-12	84	5	-7
-8	54	5	-2	-2	25	8	7*	0	124	5	-2	-12	79	4	20	-11	21	16	-10*
-7	0	20	-1*	-1	137	5	-4	1	34	7	4*	-10	123	5	-9	-10	38	6	-4
-6	115	5	1	0	48	6	-12	2	39	8	2*	-8	35	8	7*	-9	32	7	3*
-5	37	6	7	1	14	21	-10*	3	0	25	-21*	-6	143	8	-1	-8	102	5	-7
-4	45	5	10	2	37	5	20	4	114	9	6	-4	17	20	-3*	-7	0	27	-7*
-3	0	19	-6*	3	138	6	-9	H,K=	21,		3	-2	139	5	6	-6	53	8	-11
-2	121	6	-2	4	35	8	1*	-15	76	5	0	0	9	19	-6*	-5	40	7	-10
-1	26	9	-5*	H,K=	20,		6	-14	65	5	3	2	107	5	5	-4	84	5	1
H,K=	20,		0	-14	0	20	-1*	-13	18	20	-3*	H,K=	22,		2	-3	0	20	-2*
-16	139	5	9	-13	61	5	-2	-12	46	6	2	-14	72	5	-1	-2	82	5	-6
-14	80	5	12	-12	48	7	4	-11	109	5	-5	-13	77	5	-3	-1	38	7	-1
-12	143	5	3	-11	104	5	-7	-10	86	5	3	-12	19	20	-7*	0	69	6	-8
-10	13	21	2*	-10	0	21	-2*	-9	21	11	6*	-11	23	11	1*	H,K=	23,		3
-8	205	6	-5	-9	83	5	-1	-7	117	8	-8	-10	110	7	0	-12	47	5	-4
-6	13	20	-15*	-8	42	11	-5*	-6	74	5	-9	-9	55	6	0	-11	47	5	2

STRUCTURE FACTORS CONTINUED FOR
(C2H5O)UO2(SOCN(C3H7)2)2- (C3H7)2NH2+ PAGE16

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-10	35	10	0*																
-9	80	5	-7																
-8	70	5	-8																
-7	8	26	-15*																
-6	30	7	0*																
-5	87	5	-13																
-4	52	5	4																
-3	18	19	16*																
-2	41	6	-8																
-1	94	4	2																
H,K=	23,	5																	
-10	25	7	24*																
-9	96	5	-3																
-8	0	19	-1*																
-7	37	6	5																
-6	19	22	16*																
-5	114	5	-4																
-4	17	20	13*																
-3	21	11	9*																
H,K=	24,	0																	
-10	59	6	1																
-8	82	7	-20																
-6	33	8	-8*																
-4	101	8	-8																
H,K=	24,	2																	
-10	32	8	-2*																
-9	22	11	10*																
-8	66	7	-16																
-7	48	6	-3																
-6	33	8	-8*																
-5	39	7	-11*																
-4	80	5	1																
-3	56	5	-7																

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