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STRUCTURE OF
TRIS(METHYLCYCLOPENTADIENYL)URANIUM(III)TRIMETHYLPHOSPHINE,
$(CH_3C_5H_4)_3U.P(CH_3)_3$

J.G. Brennan and A. Zalkin

September 1984

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STRUCTURE OF TRIS(METHYLCYCLOPENTADIENYL)URANIUM(III)TRIMETHYLPHOSPHINE, $(CH_3C_5H_4)_3U.P(CH_3)_3$

By John G. Brennan & Allan Zalkin

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Abstract. M_r = 551.5, monoclinic, Cn, a = 13.949(5), b = 9.280(4), c = 16.194(6) Å, β = 104.09(4)°, V = 2033(3) $Å^3$, Z = 4, D_x = 1.801(3) g cm^{-3}, Mo Kα, $\lambda(\alpha_1)$ = 0.70930 Å, μ = 76.4 cm^{-1}, F(000) = 1052, T = 296 K, R = 0.024 for 1568 reflections. The structure consists of uranium centered monomolecular units in which the uranium atom is coordinated in a penta-hapto fashion to three cyclopentadiene rings and to the phosphorus atom of the trimethyl phosphine molecule. The average U-C distance is 2.79 ± 0.06 Å and the U-P distance is 2.972(6) Å.

Introduction. We are currently studying the relative affinity of Lewis bases toward $(CH_3C_5H_4)_3U$. Trimethylphosphine, $P(CH_3)_3$, is found to be a better base towards U(III) than are ethers or tertiary amines. This is surprising, as ether and amine complexes of the actinide metals have been known since the early 1900's, yet the first unequivocal characterization of an actinide phosphine complex was just recently published (Edwards, Andersen & Zalkin, 1981). To try to determine what extent ligand-ligand repulsions may influence competitive basicity, we are studying the molecular structure of these $(CH_3C_5H_4)_3U$ complexes, and report here the X-ray structure of $(CH_3C_5H_4)_3U.P(CH_3)$.

Experimental. Red, air sensitive needles of the phosphine complex were prepared by reacting UCl_3 (Andersen, 1979) with $Na(CH_3C_5H_4)$ in tetrahydrofuran (THF), adding $P(CH_3)_3$, and crystallizing from pentane at 253K. Crystal 0.15 x 0.23 x 0.38 mm with 9 faces; modified Picker automatic diffractometer, graphite monochromator; cell dimensions from 31 reflections, $20° < 2\theta < 27°$; analytical absorption correction, range 2.78 to 3.41; max. $(\sin\theta)/\lambda = 0.60$, h -16 to 16, k 0 to 11, ℓ -19 to 19; three standard reflections, <2% variation in intensities from average; 3650 data, 1798 unique (including 230, $F^2 < 2\sigma$, $R_{int} = 0.029$; structure solved by Patterson and Fourier methods; refined on F, 207 parameters, non-methyl hydrogen atoms in calculated positions with isotropic thermal parameters, anisotropic thermal parameters for non-hydrogen atoms, ring C-C and $C-CH_3$ bond distances restrained to 1.40(2) & 1.52(2) Å; R = 0.024 for 1568 reflections

(0.033 for 1568 for which $F^2 > 2\sigma$), wR = 0.032, S = 1.07; $w = [\sigma(F)]^{-2}$, p = 0.04 in calc. of $\sigma(F^2)$; max. (shift/σ) = 0.08, max. correction for extinction 3% of F; max. and min. of ΔF synthesis 0.34 and -0.37 e A^{-3}; atomic f for neutral U, P and C, and spherical bonded H from International Tables (1974); local unpublished programs and ORTEP (Johnson, 1965).

In an effort to determine the absolute configuration of the molecule, the full unaveraged data set was used to refine both enantiomorphic structures, but the results showed no significant differences in the R factors for the two structures. The Friedel pairs of selected reflections with large differences were investigated, but again there was no significant correlation with the observed data. On the assumption that the crystal was twinned with both enantiomers present in equal amounts, the data were averaged and $\Delta f''$ for all atoms set to zero.

The cyclopentadienyl rings suffered considerable thermal motion. The carbon atoms in the ring were not well resolved resulting in unrealistic C-C bond lengths and slow convergence of the least-squares refinements, and it was necessary to apply distance restraints (Waser,1963) to the atoms of the methylcyclopentadiene ligands.

Atomic parameters are listed in Table 1.*

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*Lists of structure factors, anisotropic thermal parameters and H-atom parameters, deviations from least squares planes, distances and angles have been deposited with the British Library Lending Division as Supplementary Publication No. (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. The complex $(CH_3C_5H_4)_3.P(CH_3)_3$ is monomolecular in the crystalline state and consists of a uranium atom coordinated to the three methylcyclopentadienyl groups in a penta-hapto bonding mode and to the phosphorus atom of the trimethyl phosphine molecule in a distorted tetrahedral arrangement; the angles about the U atom are given in Table 2. The uranium atom is 2.972(6) Å from the phosphorus atom and 2.51 to 2.54 Å from the least squares planes of the cyclopentadienyl rings; the average U-C distance is 2.79 ± 0.06 Å.

While there are a number of similar trivalent lanthanide structures in the literature ($(C_5H_5)_3Gd.OC_4H_8$ (Rogers et al., 1980), $(C_5H_5)_3Y.OC_4H_8$, $(C_5H_5)_3La.OC_4H_8$ (Rogers et al., 1981), and $(C_5H_5)_3Nd.CNC_6H_{11}$ (Burns & Baldwin, 1965), there is currently only one related trivalent uranium compound, $(C_5H_5)_3U.OC_4H_8$, structurally characterized (Wasserman et al., 1983). The average U to cyclopentadiene ring distance is 2.52 ± 0.02 Å in both $(CH_3C_5H_4)_3U.P(CH_3)_3$ and $(C_5H_5)_3U.OC_4H_8$. In the trimethylphosphine complex, the average Cp-U-P angle is 106 ± 9°, and the average Cp-U-Cp angle, 112 ± 7°. This compares to 99 ± 3° for the Cp-U-O angle and 118 ± 2° for the Cp-U-Cp

angle in the tetrahydrofuran complex, and reflects the sterically more demanding nature of the phosphine ligand relative to tetrahydrofuran.

In comparison to three U(III) alkylphosphine structures described in the literature, the uranium(III) phosphorus distance in $(CH_3C_5H_4)_3U.P(CH_3)_3$, 2.972(6), is significantly shorter than the U-P distances of 3.211(8) and 3.092(8) in $((CH_3C)_5)_2UH.((CH_3)_2PCH_2CH_2P(CH_3)_2)$(Duttera et al., 1981), 3.057(9) and 3.139(9), in $U(BH_4)_2.((CH_3)_2PCH_2CH_2P(CH_3)_2)_2$, (Wasserman et al., 1984), 3.085(3) and 3.174(3), in $U(CH_3BH_3)_2.((CH_3)_2PCH_2CH_2P(CH_3)_2)_2$(Brennan et al., 1984).

Helpful discussions with Professor R. A. Andersen are greatly appreciated. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

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Wasserman, H.J., Moody, D.C., & Ryan, R.R. (1984). J. Chem. Soc. Chem. Comm. pp. 532-533.

Table 1. Atomic parameters for

Tris(methylcyclopentadienyl)uranium(III)trimethylphosphine

$$B_{eq} = \Sigma(B_{ii})/3,\ A^2.$$

Atom	x	y	z	B_{eq}
U	1/4	0.08828(3)	1/4	2.90
P	0.2795(5)	-0.0741(6)	0.4124(4)	4.88
C(1)	0.3866(17)	0.4028(20)	0.3706(14)	6.75
C(2)	0.3884(18)	0.3026(23)	0.2977(13)	6.69
C(3)	0.4381(15)	0.1715(27)	0.3031(14)	8.11
C(4)	0.4393(14)	0.1257(16)	0.2249(12)	4.08
C(5)	0.3819(12)	0.2171(18)	0.1635(12)	5.11
C(6)	0.3564(17)	0.3289(22)	0.2077(11)	7.01
C(7)	0.1118(18)	0.3483(26)	0.0735(15)	8.32
C(8)	0.1035(13)	0.2746(18)	0.1569(12)	5.65
C(9)	0.1227(19)	0.3241(17)	0.2414(17)	6.30
C(10)	0.0919(16)	0.2149(26)	0.2921(14)	10.62
C(11)	0.0536(16)6	0.0944(20)	0.2398(15)	5.87
C(12)	0.0494(13)	0.1473(21)	0.1572(14)	5.85
C(13)	0.1536(25)	0.024(3)	0.0135(15)	9.08
C(14)	0.1978(16)	-0.0603(27)	0.0916(1)	11.26
C(15)	0.1437(12)	-0.1256(16)	0.1435(11)	5.37
C(16)	0.2094(12)	-0.2007(16)	0.2061(12)	6.54
C(17)	0.3030(12)	-0.1787(17)	0.1946(12)	7.00
C(18)	0.2964(13)	-0.0850(17)	0.1271(10)	5.66
C(19)	0.3336(25)	0.025(5)	0.5188(20)	10.53
C(20)	0.3698(19)	-0.2218(21)	0.4288(15)	9.42
C(21)	0.1669(16)	-0.1561(29)	0.4345(18)	9.23

Table 2. Selected distances and angles

Distances

Atoms	d(Å)	Atoms	d(Å)
U - P	2.972(6)	U - C(14)	2.847(23)
U - C(2)	2.748(23)	U - C(15)	2.805(15)
U - C(3)	2.668(22)	U - C(16)	2.797(15)
U - C(4)	2.789(19)	U - C(17)	2.795(16)
U - C(5)	2.834(16)	U - C(18)	2.756(15)
U - C(6)	2.856(20)	U - Cp(1)[a]	2.51
U - C(8)	2.817(17)	U - Cp(2)	2.51
U - C(9)	2.800(21)	U - Cp(3)	2.54
U - C(10)	2.728(21)	P - C(19)	1.933(26)
U - C(11)	2.704(21)	P - C(20)	1.837(18)
U - C(12)	2.889(17)	P - C(21)	1.857(20)

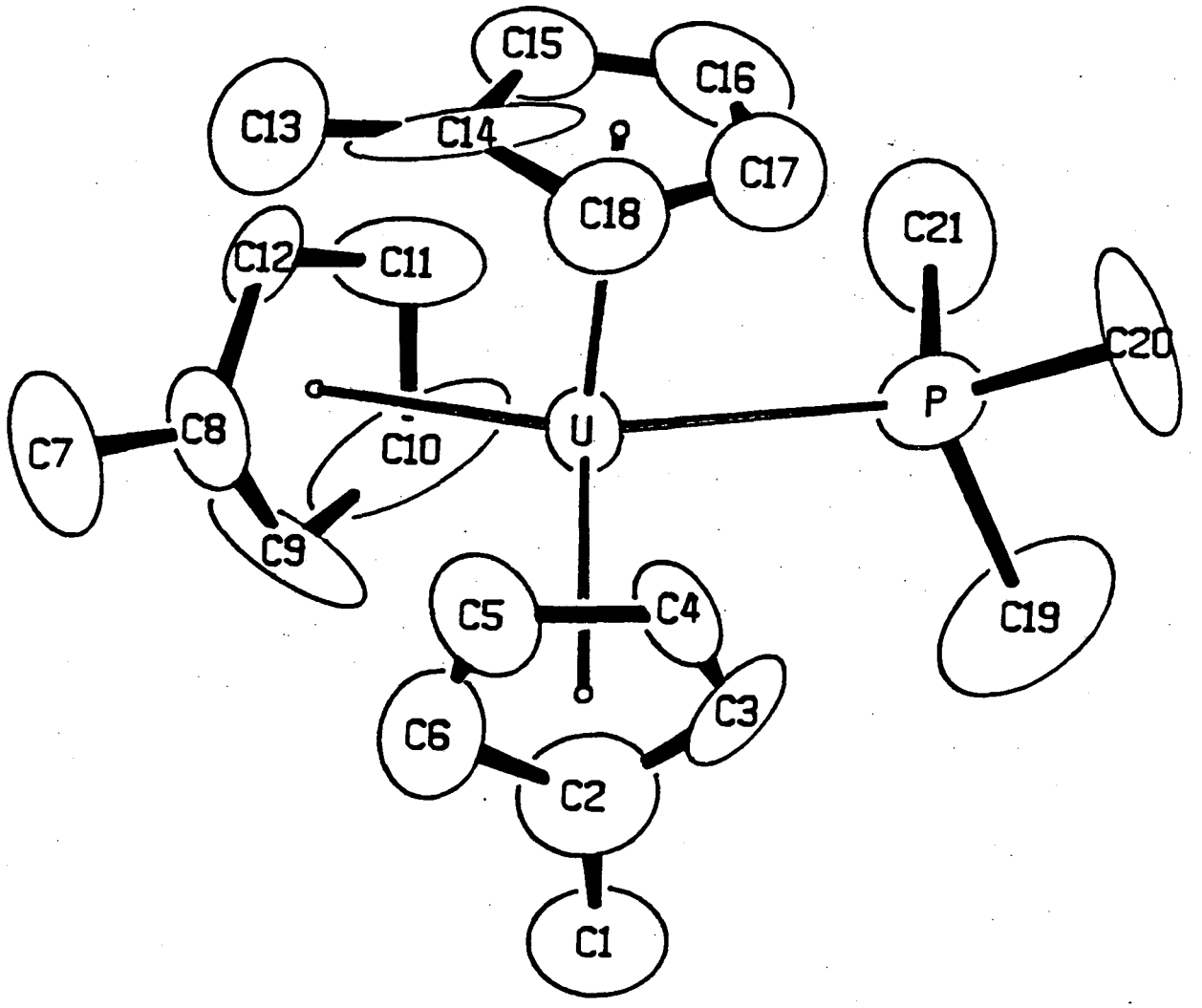
Angles

P - U - Cp_1	112.7	Cp_2 - U - Cp_3	106.0
P - U - Cp_2	109.7	C(19) - P - C(20)	97(2)
P - U - Cp_3	96.7	C(19) - P - C(21)	101(2)
Cp_1 - U Cp_2	119.4	C(20) - P - C(21)	104(2)
Cp_1 - U CP_3	109.8		

[a] Cp_1, Cp_2 and Cp_3 represents the centers of atom groups C(2)-C(6), C(8)-C(12) and C(14)-C(18) respectively.

Figure caption

Fig. 1. ORTEP drawing of tris(methylcyclopentadienyl)uranium(III)-trimethylphosphine; thermal ellipsoids at 50% probability level.



Supplementary Material

for

STRUCTURE OF TRIS(METHYLCYCLOPENTADIENYL)URANIUM(III)TRIMETHYLPHOSPHINE, $(CH_3C_5H_4)_3U.P(CH_3)_3$

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Table A. Anisotropic Thermal Parameters ($Å^2$)[a]

ATOM	B11	B22	B33	B12	B13	B23
U	2.438(13)	2.735(15)	3.496(16)	.30(6)	.673(10)	.46(5)
P	4.81(20)	4.95(22)	4.47(21)	-.41(18)	.33(17)	-.72(17)
C(1)	6.9(10)	6.1(10)	7.3(11)	-.6(8)	1.7(9)	-1.8(9)
C(2)	4.8(10)	8.6(16)	7.5(16)	-2.7(10)	3.1(13)	1.2(12)
C(3)	2.5(7)	8.0(14)	10.7(20)	-.7(8)	-4.6(11)	.9(14)
C(4)	4.4(7)	3.1(7)	5.1(9)	-.4(6)	1.9(8)	2.2(6)
C(5)	4.0(7)	4.9(7)	7.2(11)	.5(5)	2.8(8)	1.2(7)
C(6)	5.2(9)	8.2(14)	7.0(12)	-2.8(9)	.4(9)	4.5(11)
C(7)	9.4(14)	7.2(11)	8.5(14)	1.8(11)	2.4(12)	5.5(11)
C(8)	3.4(6)	4.3(8)	8.8(13)	1.1(6)	.7(9)	2.8(9)
C(9)	6.9(14)	1.4(5)	13.4(25)	-.2(6)	8.0(18)	-.8(9)
C(10)	4.3(10)	17.6(30)	9.5(17)	1.2(13)	.7(18)	-10.8(20)
C(11)	3.9(8)	5.0(9)	9.5(17)	-.7(7)	3.3(11)	-4.0(10)
C(12)	2.2(7)	5.6(9)	7.8(12)	-1.3(6)	-2.6(7)	2.6(9)
C(13)	11.1(19)	10.1(14)	4.6(12)	-4.2(13)	-.9(12)	4.3(12)
C(14)	10.5(23)	13.2(24)	11.2(23)	-9.7(20)	5.0(18)	-9.4(20)
C(15)	5.4(7)	4.3(7)	6.4(8)	-1.3(6)	1.4(7)	-.7(6)
C(16)	7.6(10)	3.9(6)	9.0(11)	-.3(6)	3.5(8)	-1.6(7)
C(17)	7.1(10)	4.9(8)	8.1(11)	1.7(7)	.2(8)	-1.8(8)
C(18)	5.9(9)	5.9(8)	5.3(7)	.6(7)	1.5(7)	-1.5(7)
C(19)	8.1(14)	15.5(22)	7.5(18)	3.0(14)	.9(13)	-7.2(17)
C(20)	12.9(16)	6.0(10)	9.8(13)	6.4(11)	3.7(12)	4.5(10)
C(21)	6.4(10)	9.8(13)	11.5(17)	-1.5(10)	2.3(11)	4.6(13)

[a] The anisotropic temperature factor has the form

$$\exp[-0.25(B_{11}h^2a^{*2} + 2B_{12}hka^*b^* + \ldots].$$

Table B. Hydrogen Positional and Isotropic Thermal Parameters[a]

Atom	x	y	z	B (A^2)
H(1)	.4725	.1265	.3558	10.000
H(2)	.4729	.0384	.2130	10.000
H(3)	.3646	.2033	.1013	10.000
H(4)	.3216	.4157	.1819	10.000
H(5)	.1515	.4173	.2628	10.000
H(6)	.0978	.2188	.3539	10.000
H(7)	.0327	0	.2560	10.000
H(8)	.0165	.0949	.1042	10.000
H(9)	.0720	-.1194	.1368	10.000
H(10)	.1927	-.2596	.2589	10.000
H(11)	.364	-.2217	.2285	10.000
H(12)	.3521	-.0433	.108	10.000

[b] The isotropic temperature factor has the form $\exp[-B\sin^2\theta/\lambda]$.

Table C. Deviations (Å) from Least-Squares Planes

Plane 1, C(2) - C(6)	
C(2)	-0.002
C(3)	-0.021
C(4)	0.036
C(5)	-0.037
C(6)	0.025
U	-2.510
C(1)	0.199

Plane 2, C(8) - C(12)	
C(8)	0.065
C(9)	-0.021
C(10)	-0.027
C(11)	0.067
C(12)	-0.085
U	2.509
C(7)	-0.015

Plane 3, C(14) - C(18)	
C(14)	-0.035
C(15)	0.020
C(16)	0.002
C(17)	-0.023
C(18)	0.036
U	2.541
C(13)	-0.113

Table D. C-C distances and C-C-C angles[a]

Distances

Atoms	d(Å)	Atoms	d(Å)
C(2) - C(3)	1.392(18)	C(12) - C(8)	1.403(17)
C(3) - C(4)	1.341(18)	C(14) - C(15)	1.398(18)
C(4) - C(5)	1.400(17)	C(15) - C(16)	1.379(16)
C(5) - C(6)	1.357(18)	C(16) - C(17)	1.378(16)
C(6) - C(2)	1.438(18)	C(17) - C(18)	1.382(17)
C(8) - C(9)	1.406(19)	C(18) - C(14)	1.374(18)
C(9) - C(10)	1.434(19)	C(1) - C(2)	1.507(18)
C(10) - C(11)	1.427(16)	C(7) - C(8)	1.543(17)
C(11) - C(12)	1.412(19)	C(13) - C(14)	1.489(19)

Angles(°)

C(1) -C(2) -C(3)	126(2)	C(9) -C(10)-C(11)	104(2)
C(1) -C(2) -C(6)	132(2)	C(10)-C(11)-C(12)	107(2)
C(3) -C(2) -C(6)	100(2)	C(8) -C(12)-C(11)	113(2)
C(2) -C(3) -C(4)	112(2)	C(13)-C(14)-C(15)	126(2)
C(3) -C(4) -C(5)	110(2)	C(13)-C(14)-C(18)	126(2)
C(2) -C(6) -C(5)	116(2)	C(15)-C(14)-C(18)	107(2)
C(4) -C(5) -C(6)	102(2)	C(14)-C(15)-C(16)	107(2)
C(7) -C(8) -C(9)	129(2)	C(15)-C(16)-C(17)	108(2)
C(7) -C(8) -C(12)	125(2)	C(16)-C(17)-C(18)	108(2)
C(9) -C(8) -C(12)	103(2)	C(14)-C(18)-C(17)	108(2)
C(9) -C(10)-C(11)	104(2)		

[a] Distances were restrained in the least-squares, therefore the quoted e.s.d's in parentheses are not significant.

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 6.0)
U(CH3C5H4)3.P(CH3)3 F(0,0,0) = 2814

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	2	437	11	-8	-5	692	18	7	9	56	11	-11	-6	218	6	2
21	176	30	-82	3	124	5	2	-4	616	16	39	10	419	11	-4	-5	294	8	5
4	811	26	-3	4	365	10	-5	-3	506	13	2	11	27	53	-8*	-4	247	7	-2
6	799	20	6	5	128	5	-4	-2	725	18	15	12	292	8	8	-3	212	6	-3
8	565	15	-11	6	458	12	-11	-1	1024	26	-26	13	0	56	-44*	-2	281	7	-1
10	428	11	5	7	93	7	7	0	499	13	0	14	263	7	2	-1	340	9	-5
12	409	11	-1	8	384	10	-10	1	903	24	1	15	19	52	-6*	0	265	7	-6
14	247	7	1	9	49	27	20*	2	577	15	21	16	200	7	-1	1	347	9	-2
16	187	6	-6	10	294	8	7	3	602	23	31	17	54	61	24*	2	290	8	-2
18	186	6	12	11	47	47	-5*	4	559	19	39	H,K=	1,		5	3	290	8	2
H,K=	0,		2	12	260	7	2	5	608	25	0	-16	87	21	11	4	265	7	3
0	216	6	11	13	30	58	-24*	6	279	7	-4	-15	183	7	6	5	332	9	-4
1	560	17	9	14	188	7	0	7	633	21	4	-14	74	21	-14	6	248	7	-6
2	149	7	68	15	0	63	-39*	8	351	9	6	-13	260	7	4	7	246	7	7
31	032	27	42	H,K=	0,		8	9	368	10	-12	-12	85	9	2	8	198	6	-4
4	344	9	18	0	136	7	-1	10	282	8	11	-11	303	15	4	9	158	6	-0
5	624	16	-4	1	325	9	-0	11	367	10	-7	-10	201	8	9	10	165	6	-3
6	378	10	15	2	101	7	-4	12	177	6	-4	-9	357	15	0	11	174	6	1
7	487	15	12	3	363	10	2	13	278	8	-2	-8	141	5	-1	12	139	7	2
8	372	10	20	4	75	15	-22	14	149	6	-8	-7	460	12	-8	13	151	7	7
9	530	14	8	5	318	8	0	15	168	6	-6	-6	48	20	-12*	14	80	22	-38
10	185	5	1	6	99	7	-11	16	110	8	0	-5	512	13	10	H,K=	1,		9
11	364	9	4	7	256	7	-9	17	154	7	-8	-4	232	6	-1	-11	19	56	-37*
12	186	6	-6	8	44	47	-0*	18	61	34	-5*	-3	540	14	20	-10	207	7	0
13	284	8	-2	9	232	7	2	H,K=	1,		3	-2	189	5	15	-9	28	59	-39*
14	135	5	4	10	49	48	7*	-18	144	8	5	-1	600	15	15	-8	221	7	3
15	232	6	1	11	200	7	3	-17	35	60	12*	0	148	5	-2	-7	69	21	-3*
16	81	13	-3	12	71	13	13	-16	224	7	8	1	579	15	6	-6	214	7	-7
17	136	6	-8	H,K=	0,		18	-15	33	58	6*	2	255	7	-8	-5	69	11	-11
18	53	28	-26*	0	184	8	0	-14	265	8	6	3	439	12	2	-4	279	8	-0
H,K=	0,		4	1	128	7	2	-13	44	49	27*	4	208	6	0	-3	93	8	8
0	531	14	-5	2	186	6	5	-12	315	8	2	5	474	12	-11	-2	279	8	3
1	573	16	-10	3	143	7	-3	-11	36	51	-13*	6	90	6	2	-1	95	8	11
2	476	12	8	4	163	6	-4	-10	450	12	-11	7	455	12	0	0	254	7	7
3	699	20	4	5	122	7	-1	-9	31	48	-19*	8	175	6	-7	1	85	9	-3
4	316	8	2	6	136	7	-4	-8	539	14	2	9	363	10	3	2	283	8	-1
5	546	18	-19	7	108	8	-5	-7	42	11	-11	10	131	6	5	3	115	7	2
6	397	10	13	8	121	11	-6	-6	564	20	0	11	288	13	-8	4	256	7	2
7	340	9	-11	H,K=	1,		1	-5	122	4	21	12	78	10	3	5	84	9	-3
8	316	8	15	-18	36	54	-40*	-4	832	21	-7	13	225	7	-5	6	205	6	-5
9	356	9	-14	-17	157	7	-2	-3	166	5	18	14	106	8	18	7	63	26	10*
10	246	7	-2	-16	108	8	-8	-2	834	23	-2	15	156	7	-0	8	204	7	3
11	269	7	-1	-15	197	6	2	-1	61	4	-3	16	43	64	-22*	9	58	16	-8
12	171	6	-9	-14	148	6	-4	0	689	18	53	H,K=	1,		7	10	181	7	5
13	188	6	4	-13	321	9	1	1	191	5	6	-14	118	8	4	H,K=	1,		11
14	139	6	2	-12	180	6	-5	2	708	18	-42	-13	187	7	9	-1	177	7	2
15	186	6	3	-11	351	14	-11	3	73	4	-0	-12	140	7	-3	0	31	60	-0*
16	108	7	-0	-10	281	13	-5	4	857	25	8	-11	168	6	-3	1	174	7	-1
17	122	7	-5	-9	388	10	-7	5	111	4	40	-10	176	6	-6	H,K=	2,		0
H,K=	0,		6	-8	315	13	12	6	546	22	-20	-9	183	6	-0	-18	180	7	-5
0	526	14	7	-7	577	15	-10	7	45	19	-14*	-8	195	6	-1	-16	197	6	0
1	160	5	2	-6	270	7	-7	8	537	14	-0	-7	316	8	-4	-14	308	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
-12	419	11	-12	-15	192	7	4	7	69	16	8	-17	151	7	-6	2	786	22	-2
-10	390	10	14	-14	164	5	2	8	319	8	7	-16	141	7	3	3	88	4	10
-8	584	15	-2	-13	204	6	6	9	5	53	-51*	-15	212	7	-6	4	668	17	-1
-6	714	18	-16	-12	196	6	0	10	262	7	1	-14	162	6	6	5	104	5	-3
-4	652	18	26	-11	280	8	-10	11	40	55	-3*	-13	331	9	-1	6	407	17	1
-2	872	22	-5	-10	234	7	-9	12	242	7	-10	-12	206	6	1	7	60	18	-16*
0	1143	29	50	-9	347	9	-9	13	56	58	3*	-11	317	8	-11	8	476	20	12
2	420	11	-26	-8	262	7	5	14	165	7	-3	-10	308	8	2	9	32	51	-19*
4	784	20	7	-7	313	12	17	15	0	75	-35*	-9	424	11	0	10	372	10	-8
6	851	22	33	-6	304	8	-3	H,K=	2,	8	-8	326	9	-4	11	59	13	0	
8	526	14	-4	-5	505	18	12	-13	156	7	-4	-7	630	16	-6	12	257	7	-3
10	392	10	-27	-4	342	9	5	-12	70	13	6	-6	372	10	-12	13	16	57	-41*
12	371	10	2	-3	634	16	6	-11	205	7	-4	-5	673	23	-2	14	242	7	-4
14	234	7	-12	-2	415	11	-0	-10	0	59	-52*	-4	337	9	-22	15	0	61	-33*
16	191	7	-10	-1	545	14	-5	-9	241	7	-5	-3	394	10	-3	16	167	7	-5
18	159	7	0	0	372	10	-2	-8	88	17	1	-2	111	4	12	H,K=	3,	5	
H,K=	2,	2	1	511	13	4	-7	242	7	-14	-1	855	22	8	-17	137	8	-4	
-18	82	11	4	2	315	8	1	-6	127	6	-8	0	132	4	21	-16	71	27	-11*
-17	167	7	-8	3	616	16	-5	-5	273	7	-5	1	660	18	22	-15	191	7	2
-16	63	42	-17*	4	298	8	6	-4	51	51	-18*	2	258	10	-13	-14	82	11	-1
-15	244	7	-2	5	353	9	-5	-3	303	8	-6	3	610	26	33	-13	261	7	-4
-14	144	6	4	6	352	9	-9	-2	95	7	1	4	444	12	26	-12	103	7	-3
-13	255	7	-8	7	327	14	-7	-1	281	8	-9	5	588	26	28	-11	289	13	2
-12	192	6	8	8	262	7	-12	0	147	6	5	6	345	9	18	-10	191	6	14
-11	367	10	-9	9	348	14	-10	1	347	9	-1	7	540	14	15	-9	326	14	-1
-10	175	6	-7	10	202	6	-6	2	102	7	-8	8	327	9	12	-8	103	6	-24
-9	511	13	-5	11	234	7	10	3	357	9	6	9	309	8	10	-7	453	12	-15
-8	283	7	4	12	176	6	0	4	63	63	-53*	10	240	7	11	-6	152	5	8
-7	482	13	-6	13	177	6	-5	5	287	8	7	11	345	9	6	-5	437	11	8
-6	281	7	-10	14	123	8	-9	6	84	9	-14	12	168	6	2	-4	307	8	10
-5	727	19	24	15	172	7	-0	7	240	7	6	13	235	7	-3	-3	434	11	3
-4	284	7	3	16	113	9	10	8	51	56	-9*	14	159	7	6	-2	218	6	-11
-3	630	16	-41	H,K=	2,	6	9	212	7	-10	15	157	7	-5	-1	510	13	9	
-2	284	7	20	-16	138	8	-2	10	0	59	-57*	16	99	10	-3	0	199	6	5
-1	371	10	31	-15	64	43	8*	11	181	7	2	17	153	7	4	1	491	13	-2
0	507	13	17	-14	208	7	4	12	69	27	6*	H,K=	3,	3	2	267	7	5	
1	512	13	2	-13	56	57	-12*	H,K=	2,	10	-18	155	7	7	3	357	9	17	
2	244	6	-6	-12	268	8	3	-8	128	8	-6	-17	30	54	2*	4	170	5	3
3	801	20	-2	-11	38	47	-33*	-7	127	7	5	-16	217	7	-3	5	427	11	-8
4	255	7	2	-10	284	8	-2	-6	134	7	-13	-15	49	57	7*	6	156	5	8
5	494	18	-22	-9	83	8	34	-5	141	7	-5	-14	253	7	6	7	385	10	-4
6	318	14	9	-8	372	10	3	-4	156	7	-5	-13	30	55	17*	8	176	6	-2
7	506	24	22	-7	93	7	-13	-3	186	6	-1	-12	314	8	-2	9	300	8	3
8	213	6	-10	-6	436	11	-3	-2	171	6	3	-11	56	12	-3	10	96	8	4
9	482	19	15	-5	103	8	-1	-1	146	7	-3	-10	465	12	-22	11	278	8	7
10	171	6	7	-4	367	10	-6	0	167	6	-6	-9	45	29	-7*	12	75	11	-0
11	320	9	-17	-3	109	5	7	1	139	7	1	-8	455	18	6	13	212	7	4
12	176	6	-10	-2	489	13	7	2	167	6	-4	-7	45	19	-13*	14	93	10	8
13	278	8	17	-1	111	5	4	3	138	7	-7	-6	479	12	-12	15	145	8	6
14	106	8	6	0	549	14	13	4	138	7	-15	-5	91	5	6	H,K=	3,	7	
15	210	7	-7	1	84	6	-1	5	134	7	6	-4	753	19	5	-14	106	9	-14
16	39	54	-42*	2	411	11	2	6	128	7	0	-3	137	4	21	-13	161	7	6
17	136	8	-1	3	84	6	34	7	116	8	-2	-2	812	21	6	-12	153	6	6
H,K=	2,	4	4	415	11	6	H,K=	3,	1	-1	90	4	15	-11	163	6	2		
-17	145	8	5	5	102	6	13	-19	131	8	-0	0	618	16	5	-10	171	6	-3
-16	96	10	-19	6	435	11	-13	-18	87	11	-5	1	182	5	-3	-9	195	6	2

STRUCTURE FACTORS CONTINUED FOR
U(CH3C5H4)3.P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-8	181	6	-5	4	779	20	24	-5	438	11	9	-10	59	29	19*	1	651	17	-3
-7	301	13	0	6	690	18	8	-4	326	9	-8	-9	241	15	8	2	418	11	-8
-6	227	14	6	8	406	11	4	-3	515	13	-20	-8	74	10	2	3	604	15	20
-5	248	7	0	10	375	10	-0	-2	326	9	1	-7	239	7	8	4	305	8	-0
-4	291	8	3	12	331	9	-4	-1	366	9	-4	-6	86	8	8	5	572	15	-5
-3	260	7	2	14	206	7	-10	0	419	11	10	-5	284	8	4	6	264	7	-2
-2	280	7	2	16	173	7	5	1	471	12	6	-4	38	51	-3*	7	414	11	10
-1	364	10	0	H,K=	4,		2	2	380	10	9	-3	329	9	6	8	258	7	6
0	286	8	5	-18	50	55	-23*	3	492	13	-7	-2	66	18	-8	9	292	8	-3
1	321	8	-2	-17	179	7	-8	4	335	9	2	-1	287	8	-2	10	198	6	0
2	282	8	-1	-16	72	23	-9*	5	290	8	5	0	110	6	3	11	314	8	5
3	273	7	1	-15	221	7	1	6	279	7	-4	1	301	8	4	12	135	7	-5
4	256	7	2	-14	136	7	-1	7	380	10	-9	2	43	52	-15*	13	202	7	5
5	272	7	0	-13	240	7	-3	8	223	6	-8	3	270	7	-9	14	118	8	-3
6	207	6	-5	-12	174	6	-9	9	330	9	9	4	69	19	-7	15	138	8	1
7	202	6	-2	-11	411	11	-5	10	177	6	-10	5	241	7	-9	16	77	24	-2*
8	164	6	-9	-10	154	6	2	11	197	6	7	6	99	8	-2	H,K=	5,		3
9	177	6	-3	-9	502	13	-10	12	177	6	-4	7	239	7	-7	-18	142	8	-7
10	143	7	-7	-8	228	6	-2	13	184	7	6	8	44	55	-15*	-17	0	61	-19*
11	183	7	5	-7	537	14	5	14	112	9	1	9	219	7	1	-16	221	7	2
12	115	8	-16	-6	347	9	-10	15	157	7	4	10	58	37	-3*	-15	0	57	-17*
13	135	8	4	-5	685	18	-3	H,K=	4,		6	H,K=	4,		10	-14	239	7	0
H,K=	3,		9	-4	247	6	-7	-16	136	8	-8	-7	115	8	1	-13	44	53	25*
-11	28	61	-31*	-3	698	18	-7	-15	52	61	20*	-6	153	7	1	-12	331	9	-0
-10	198	7	1	-2	520	13	27	-14	213	7	6	-5	149	7	1	-11	26	52	-29*
-9	32	59	-37*	-1	780	28	-4	-13	46	57	-5*	-4	162	7	-2	-10	492	13	-12
-8	203	7	1	0	547	18	12	-12	256	7	-0	-3	179	6	6	-9	42	42	5*
-7	72	21	6	1	774	20	4	-11	44	54	-3*	-2	164	6	3	-8	445	12	-2
-6	213	7	3	2	333	9	28	-10	257	7	0	-1	136	7	-3	-7	83	6	13
-5	57	25	-10*	3	687	25	14	-9	73	16	1	0	162	7	5	-6	524	14	-10
-4	271	8	2	4	262	13	1	-8	380	10	5	1	154	7	4	-5	119	5	-1
-3	47	54	-30*	5	491	13	17	-7	107	6	-7	2	151	7	-2	-4	722	18	-12
-2	256	7	1	6	297	8	7	-6	480	12	-12	3	166	7	2	-3	236	6	13
-1	64	12	6	7	464	20	20	-5	68	8	20	4	141	7	-2	-2	673	17	-19
0	228	7	-6	8	143	5	-2	-4	424	11	-4	5	121	8	-4	-1	163	5	9
1	59	25	5*	9	399	21	-0	-3	65	14	12	H,K=	5,		1	0	617	19	-27
2	245	7	-5	10	191	6	-3	-2	502	13	8	-19	123	8	-6	1	173	5	-1
3	63	23	-15*	11	277	8	0	-1	108	6	-2	-18	103	9	16	2	756	19	-11
4	235	7	1	12	159	6	3	0	584	13	-7	-17	142	7	-4	3	88	6	-8
5	51	55	-6*	13	227	7	6	1	108	6	2	-16	140	7	10	4	510	13	-0
6	211	7	-2	14	44	61	-38*	2	381	10	8	-15	212	7	-5	5	0	47	-34*
7	45	59	-5*	15	197	7	7	3	74	8	6	-14	135	7	-5	6	435	11	5
8	212	7	9	16	79	23	4	4	428	11	-7	-13	317	8	-6	7	21	47	-12*
9	45	55	-30*	H,K=	4,		4	5	87	8	12	-12	196	6	-4	8	468	17	0
H,K=	4,		0	-17	139	8	-2	6	377	10	-0	-11	306	8	0	9	15	54	-11*
-18	172	7	3	-16	99	9	-12	7	44	52	-5*	-10	285	8	-4	10	329	9	2
-16	224	7	15	-15	190	7	5	8	261	7	4	-9	431	11	8	11	0	56	-8*
-14	359	9	-4	-14	162	7	-8	9	49	31	-19*	-8	246	7	-1	12	224	7	1
-12	398	11	-6	-13	198	6	-0	10	249	7	-7	-7	612	16	-18	13	25	58	8*
-10	425	11	14	-12	197	6	-3	11	51	46	4*	-6	330	9	-5	14	219	7	3
-8	674	17	-5	-11	309	8	5	12	224	7	2	-5	563	14	-24	15	47	62	30*
-6	750	19	-24	-10	226	6	1	13	43	55	0*	-4	391	10	-11	H,K=	5,		5
-4	623	16	6	-9	381	10	-9	H,K=	4,		8	-3	677	22	-16	-17	135	8	-0
-2	649	17	-20	-8	275	7	-2	-13	156	7	4	-2	363	9	-12	-16	49	63	-29*
0	482	12	-26	-7	297	8	1	-12	67	27	8*	-1	918	25	8	-15	190	7	10
2	800	20	37	-6	303	8	7	-11	201	7	4	0	451	12	27	-14	49	52	-19*

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
-13	256	7	3	-10	174	7	2	1	591	15	-18	-8	362	9	-9	-17	147	7	6
-12	85	9	-9	-9	39	59	-15*	2	227	6	-10	-7	49	50	-10*	-16	112	8	-5
-11	284	8	-2	-8	191	6	2	3	492	13	4	-6	354	10	-1	-15	214	7	-4
-10	147	6	6	-7	20	57	-32*	4	300	8	-4	-5	64	16	5	-14	127	7	-2
-9	351	9	3	-6	210	7	5	5	417	11	13	-4	357	9	4	-13	299	8	4
-8	139	6	-8	-5	74	19	-10	6	279	7	14	-3	87	7	-0	-12	182	6	1
-7	459	12	-9	-4	257	7	5	7	423	11	2	-2	421	11	1	-11	273	7	1
-6	196	6	-1	-3	73	19	-17	8	139	6	-3	-1	120	6	1	-10	216	6	-9
-5	381	10	-11	-2	230	7	0	9	355	9	2	0	449	12	5	-9	357	9	-11
-4	220	6	-3	-1	56	15	-2	10	172	6	2	1	66	17	-20	-8	181	6	6
-3	401	10	-4	0	207	6	-4	11	220	7	1	2	363	10	-8	-7	476	12	-15
-2	159	5	-3	1	77	10	16	12	108	8	-9	3	78	9	5	-6	255	7	5
-1	507	13	-5	2	242	7	5	13	189	7	-6	4	384	10	-10	-5	410	11	1
0	119	5	-3	3	55	57	-13*	14	47	73	-28*	5	79	9	-7	-4	361	9	-4
1	469	12	-3	4	230	7	-3	15	161	7	0	6	312	8	3	-3	523	14	-9
2	211	6	-8	5	67	35	13*	H,K=	6,	4		7	71	10	-5	-2	389	10	-7
3	410	11	-10	6	203	7	11	-17	147	8	4	8	226	7	-7	-1	492	13	2
4	160	5	-5	7	52	61	-15*	-16	110	9	-3	9	23	58	-34*	0	419	11	-14
5	456	12	-6	H,K=	6,	0		-15	169	7	4	10	226	7	-6	1	394	10	-10
6	161	6	-3	-18	150	7	-1	-14	159	7	-1	11	52	52	2*	2	314	8	-0
7	331	9	-6	-16	213	7	3	-13	198	6	8	12	188	7	3	3	456	12	17
8	135	6	-9	-14	325	9	-6	-12	177	6	-11	H,K=	6,	8		4	203	6	-0
9	255	7	-5	-12	339	9	-16	-11	335	9	14	-12	65	27	6*	5	476	12	-9
10	67	27	-17*	-10	371	10	-8	-10	191	6	1	-11	195	7	-1	6	230	6	9
11	262	8	4	-8	566	15	-6	-9	366	10	-9	-10	66	13	16	7	300	8	3
12	53	41	-8*	-6	624	16	-35	-8	289	8	8	-9	216	7	-8	8	230	7	9
13	174	7	-1	-4	601	15	-21	-7	309	8	-5	-8	91	8	14	9	294	8	12
14	61	29	-15*	-2	843	21	-18	-6	328	9	-3	-7	222	7	-1	10	158	6	2
H,K=	5,	7		0	731	19	-14	-5	401	10	-23	-6	73	10	2	11	263	8	5
-14	105	9	-5	2	707	18	7	-4	311	8	1	-5	276	8	3	12	106	9	-8
-13	160	7	6	4	581	15	30	-3	416	11	-13	-4	20	53	-42*	13	165	7	-7
-12	147	7	4	6	511	13	-3	-2	295	8	3	-3	259	8	8	14	95	10	-12
-11	158	6	1	8	335	9	-3	-1	316	8	6	-2	104	7	7	H,K=	7,	3	
-10	195	6	15	10	378	10	7	0	349	9	2	-1	268	7	-1	-18	156	7	-1
-9	183	6	-3	12	282	8	-1	1	467	12	-20	0	97	7	7	-17	29	62	6*
-8	211	6	-10	14	172	7	2	2	277	7	-3	1	258	7	-3	-16	212	7	-3
-7	263	7	3	H,K=	5,	2		3	429	11	-0	2	46	48	8*	-15	38	58	9*
-6	242	7	-3	-18	46	56	-27*	4	304	8	-5	3	267	7	3	-14	229	7	-0
-5	260	7	3	-17	179	7	1	5	312	8	-14	4	97	8	18	-13	65	22	19*
-4	282	8	-1	-16	86	10	-3	6	259	7	4	5	234	7	-2	-12	312	8	-8
-3	281	8	0	-15	206	7	3	7	353	9	2	6	60	27	-19*	-11	41	55	3*
-2	272	7	2	-14	142	6	-4	8	209	6	5	7	226	7	7	-10	423	11	-11
-1	307	8	2	-13	252	7	1	9	257	7	0	8	0	53	-29*	-9	37	51	2*
0	286	8	0	-12	173	6	6	10	163	6	-6	9	187	7	7	-8	400	11	-4
1	244	7	-2	-11	381	10	-11	11	166	6	1	H,K=	6,	10	-7	33	49	-5*	
2	263	7	-2	-10	150	6	-7	12	141	7	-3	-6	132	10	-8	-6	500	13	4
3	212	6	8	-9	399	11	0	13	164	7	-1	-5	148	7	5	-5	75	8	24
4	234	7	-2	-8	271	7	6	14	95	19	2	-4	138	7	-4	-4	575	15	-2
5	232	7	-8	-7	378	10	-18	H,K=	6,	6		-3	147	7	13	-3	42	21	20*
6	187	6	-5	-6	304	11	-15	-15	0	63	-26*	-2	151	7	9	-2	418	11	-3
7	201	6	-2	-5	577	24	-3	-14	212	7	8	-1	117	8	3	-1	12	46	-15*
8	170	6	-7	-4	148	5	-6	-13	44	59	5*	0	156	7	5	0	469	12	-5
9	168	6	12	-3	748	23	-16	-12	244	7	8	1	150	7	6	1	52	11	-0
10	145	7	5	-2	303	8	-10	-11	33	56	-18*	2	151	7	6	2	535	14	9
11	155	7	0	-1	675	23	-6	-10	250	7	0	H,K=	7,	1		3	45	36	-33*
H,K=	5,	9		0	239	6	19	-9	67	19	-17	-18	87	11	-2	4	377	10	-12

STRUCTURE FACTORS CONTINUED FOR
U(CH3C5H4)3.P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	0	50	-47*	1	221	6	-2	-7	314	8	-8	-12	217	7	9	-6	250	7	-3
6	420	11	4	2	195	6	0	-6	220	6	7	-11	52	17	8*	-5	346	9	-2
7	48	50	-13*	3	198	6	-6	-5	435	11	-5	-10	232	7	2	-4	299	8	-4
8	388	10	2	4	185	6	0	-4	202	6	6	-9	49	37	-19*	-3	412	11	-3
9	51	32	10*	5	226	7	-4	-3	399	10	-19	-8	284	8	1	-2	267	7	4
10	242	7	4	6	169	6	-4	-2	256	7	-1	-7	56	22	3*	-1	421	11	5
11	40	57	11*	7	153	7	0	-1	314	8	9	-6	279	8	5	0	287	8	-3
12	195	7	7	8	154	7	-10	0	191	5	-10	-5	93	7	7	1	392	10	7
13	33	54	15*	9	131	8	7	1	473	12	7	-4	306	8	1	2	296	8	8
14	195	7	7	10	127	8	5	2	214	6	13	-3	88	7	3	3	398	10	-5
H,K=		7,	5	H,K=		7,	9	3	424	19	7	-2	365	10	-1	4	226	6	5
-16	64	34	0*	-9	61	30	12*	4	233	7	4	-1	56	24	-13*	5	381	10	-0
-15	180	7	2	-8	176	7	-5	5	347	9	-5	0	353	9	-2	6	207	6	-3
-14	38	53	-20*	-7	46	50	-1*	6	165	6	-8	1	33	52	-25*	7	237	7	3
-13	231	7	4	-6	203	7	6	7	368	10	5	2	281	8	-8	8	166	6	-3
-12	95	9	7	-5	66	22	-9*	8	105	8	-8	3	41	45	-23*	9	248	7	10
-11	238	7	-2	-4	231	7	2	9	268	8	1	4	298	8	-1	10	108	8	0
-10	131	6	5	-3	43	50	-24*	10	130	7	7	5	0	56	-70*	11	208	7	-2
-9	290	8	-1	-2	218	7	2	11	176	7	-4	6	256	7	-3	12	64	32	-31*
-8	132	6	9	-1	65	23	7*	12	77	21	-16	7	0	54	-69*	13	132	8	-4
-7	387	10	6	0	230	7	7	13	171	7	-10	8	202	7	4	H,K=		9,	3
-6	123	6	-11	1	65	24	-15*	H,K=		8,	4	9	40	61	3*	-17	0	63	-20*
-5	374	10	-0	2	234	7	-6	-17	134	8	0	10	195	7	-2	-16	190	7	4
-4	148	5	3	3	53	41	-14*	-16	92	19	-20	H,K=		8,	8	-15	68	24	51*
-3	403	11	-2	4	187	7	4	-15	148	7	4	-11	183	7	2	-14	201	7	-9
-2	151	5	4	5	55	19	1*	-14	123	8	-20	-10	66	25	12*	-13	36	57	9*
-1	444	12	-11	H,K=		3,	0	-13	174	7	-2	-9	201	7	-1	-12	294	8	5
0	161	5	-11	-18	155	7	3	-12	158	6	-6	-8	75	20	-9	-11	20	52	-45*
1	373	10	-4	-16	199	7	5	-11	266	7	2	-7	209	6	-5	-10	358	9	-2
2	212	6	-8	-14	287	8	2	-10	171	6	-7	-6	43	56	-42*	-9	54	54	-4*
3	387	10	-11	-12	337	9	2	-9	286	8	15	-5	239	7	-3	-8	357	9	-9
4	136	6	13	-10	375	10	-13	-8	280	8	6	-4	82	9	1	-7	29	51	-18*
5	364	10	-2	-8	516	14	-28	-7	330	9	-1	-3	239	7	-8	-6	432	11	-15
6	103	7	-1	-6	528	14	-20	-6	274	7	-7	-2	101	6	-10	-5	44	47	16*
7	246	7	-6	-4	456	12	-1	-5	420	11	-15	-1	240	7	-2	-4	479	12	-14
8	122	7	-4	-2	630	16	-3	-4	221	6	-14	0	90	9	10	-3	82	6	13
9	218	7	1	0	552	14	0	-3	420	11	3	1	249	7	-1	-2	414	11	0
10	58	40	-27*	2	461	12	27	-2	238	7	-6	2	67	24	10*	-1	21	47	-2*
11	199	7	-17	4	505	13	-7	-1	361	9	-7	3	247	7	7	0	480	13	-1
12	65	30	1*	6	414	11	11	0	240	7	-5	4	88	10	-11	1	16	49	-14*
H,K=		7,	7	8	291	8	-1	1	395	18	-12	5	189	7	4	2	444	12	1
-14	64	65	-48*	10	320	9	12	2	226	7	4	6	33	62	-23*	3	76	9	7
-13	157	7	0	12	234	7	2	3	298	8	-3	7	174	10	-3	4	338	9	5
-12	139	7	-2	14	131	8	-16	4	269	7	4	H,K=		9,	1	5	48	67	11*
-11	169	6	5	H,K=		8,	2	5	244	7	3	-18	75	14	-10	6	344	9	13
-10	175	6	5	-18	65	33	0*	6	202	6	3	-17	150	7	17	7	24	54	-21*
-9	190	6	-0	-17	172	7	1	7	255	7	6	-16	101	9	-5	8	295	8	-0
-8	164	6	-22	-16	88	10	0	8	146	7	1	-15	193	7	-6	9	63	36	7*
-7	229	7	1	-15	212	7	5	9	202	7	-5	-14	137	7	12	10	190	7	-6
-6	165	6	-6	-14	126	7	-8	10	135	7	-9	-13	260	7	3	11	47	54	-8*
-5	221	6	0	-13	247	7	-2	11	134	8	-6	-12	176	6	8	12	178	7	6
-4	197	6	8	-12	126	7	4	12	114	9	-0	-11	269	7	-4	H,K=		9,	5
-3	240	7	3	-11	335	9	-5	H,K=		8,	6	-10	219	6	-5	-15	174	7	7
-2	199	6	-8	-10	138	6	-2	-15	40	64	-2*	-9	357	9	-6	-14	65	28	6*
-1	282	8	5	-9	335	9	-6	-14	196	7	6	-8	225	6	-2	-13	202	7	3
0	208	6	2	-8	213	6	-2	-13	40	54	-12*	-7	412	11	-18	-12	35	61	-52*

STRUCTURE FACTORS CONTINUED FOR
U(CH3C5H4)3,P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-11	208	7	-2	-10	372	10	-5	-3	288	8	-5	-13	212	7	1	-10	109	8	4
-10	108	8	-3	-8	472	12	-17	-2	309	8	-1	-12	125	7	-8	-9	251	7	6
-9	276	8	10	-6	457	12	-11	-1	279	8	-9	-11	237	7	-5	-8	107	8	7
-8	83	9	-4	-4	467	12	-2	0	277	8	8	-10	157	6	0	-7	244	7	1
-7	338	9	9	-2	549	14	4	1	303	8	4	-9	302	8	-6	-6	136	7	-2
-6	133	6	20	0	452	12	3	2	233	7	4	-8	190	6	4	-5	245	7	-4
-5	356	9	-4	2	398	10	17	3	237	7	-1	-7	332	9	-4	-4	119	7	7
-4	137	6	-0	4	462	12	4	4	205	6	6	-6	233	7	5	-3	296	8	3
-3	397	10	5	6	323	9	8	5	218	7	7	-5	325	9	-5	-2	45	57	-22*
-2	102	7	-1	8	246	7	-0	6	158	7	5	-4	248	7	0	-1	306	8	7
-1	395	10	-2	10	241	7	5	7	230	7	-4	-3	400	11	-8	0	116	8	-2
0	123	6	-6	12	170	8	1	8	128	8	-7	-2	193	6	-1	1	259	7	3
1	312	8	-4	H,K=	10,		2	9	180	7	4	-1	385	10	-11	2	103	9	0
2	123	7	7	-17	163	7	12	10	126	8	-5	0	223	6	9	3	259	7	-6
3	314	8	-2	-16	73	26	-4*	H,K=	10,		6	1	309	8	6	4	89	10	2
4	82	10	0	-15	180	7	-2	-13	20	63	-23*	2	233	7	5	5	246	7	4
5	270	8	-1	-14	116	8	2	-12	204	7	10	3	303	8	4	6	87	11	-15
6	104	8	0	-13	224	7	8	-11	49	54	11*	4	170	6	0	7	184	7	-3
7	203	7	-2	-12	102	8	-8	-10	231	7	11	5	285	8	9	8	84	12	11
8	125	8	2	-11	296	8	2	-9	0	57	-55*	6	155	6	3	H,K=	11,		7
9	187	7	-3	-10	133	6	-2	-8	276	8	12	7	199	6	0	-10	138	7	1
10	31	54	-35*	-9	323	9	2	-7	57	38	-9*	8	135	7	9	-9	162	7	1
H,K=	9,		7	-8	154	6	0	-6	263	7	-9	9	196	7	5	-8	151	7	-3
-12	126	8	4	-7	348	9	-5	-5	59	21	-3*	10	90	11	9	-7	175	6	4
-11	146	7	6	-6	148	5	-1	-4	290	8	-3	H,K=	11,		3	-6	174	6	1
-10	153	6	9	-5	413	11	-15	-3	60	13	-13	-16	166	7	8	-5	158	6	-0
-9	184	6	6	-4	208	6	-7	-2	314	8	-0	-15	9	54	-9*	-4	167	6	-1
-8	162	6	4	-3	377	10	-8	-1	70	11	8	-14	197	7	8	-3	196	7	5
-7	201	6	-2	-2	246	7	-4	0	264	7	1	-13	47	59	25*	-2	153	7	-3
-6	169	6	-0	-1	395	10	-2	1	58	43	8*	-12	269	8	10	-1	173	7	4
-5	177	6	-6	0	213	6	-6	2	242	7	-5	-11	24	57	-14*	0	155	7	-2
-4	182	6	-0	1	485	13	-3	3	68	21	19*	-10	293	8	7	1	132	8	-4
-3	215	6	5	2	176	6	1	4	278	8	-5	-9	0	37	-33*	2	161	7	1
-2	183	6	-0	3	360	9	-1	5	56	59	6*	-8	294	8	-8	3	175	7	-2
-1	228	7	0	4	183	6	-4	6	229	7	4	-7	49	15	-2*	4	129	8	-1
0	157	6	-3	5	279	9	4	7	59	62	11*	-6	372	10	1	H,K=	12,		0
1	171	6	3	6	119	7	-10	8	165	7	3	-5	59	17	-14	-16	165	7	0
2	163	6	-3	7	278	8	2	H,K=	10,		8	-4	386	10	-6	-14	218	7	4
3	193	7	-5	8	115	8	4	-9	182	7	4	-3	79	7	14	-12	228	7	4
4	150	7	-6	9	200	7	-8	-8	77	11	10	-2	363	10	-6	-10	270	7	2
5	193	7	-5	10	114	8	7	-7	203	7	1	-1	89	7	7	-8	312	8	-2
6	147	7	-0	11	149	7	-3	-6	39	58	-12*	0	401	11	-13	-6	313	8	-3
7	116	9	-3	H,K=	10,		4	-5	227	7	7	1	37	46	-1*	-4	373	10	-3
H,K=	9,		9	-16	85	12	2	-4	58	48	-4*	2	359	9	3	-2	366	10	-3
-6	178	7	-2	-15	142	8	3	-3	208	7	1	3	0	49	-45*	0	288	8	-5
-5	54	42	-13*	-14	115	9	2	-2	38	60	-34*	4	276	8	9	2	280	8	3
-4	205	7	7	-13	180	7	3	-1	219	7	14	5	0	56	-52*	4	328	9	3
-3	65	24	9*	-12	141	7	-5	0	39	59	6*	6	263	8	-3	6	243	7	-3
-2	180	7	-7	-11	234	7	2	1	225	7	-1	7	44	59	7*	8	210	7	2
-1	70	25	8*	-10	182	6	6	2	25	61	-22*	8	237	7	-8	H,K=	12,		2
0	205	7	-1	-9	247	7	9	3	191	7	-1	9	55	61	28*	-15	158	7	5
1	45	63	-30*	-8	215	7	5	H,K=	11,		1	H,K=	11,		5	-14	97	10	3
H,K=	10,		0	-7	299	8	-0	-17	110	10	-11	-14	47	64	-11*	-13	181	7	-6
-16	171	7	-1	-6	209	6	-2	-16	80	23	-18	-13	196	7	13	-12	117	7	12
-14	257	7	3	-5	341	9	3	-15	168	7	-3	-12	103	9	14	-11	235	7	12
-12	307	8	1	-4	242	7	-1	-14	122	7	9	-11	209	7	4	-10	130	7	-3

STRUCTURE FACTORS CONTINUED FOR
U(CH3C5H4)3,P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	248	7	5	2	231	7	3	-5	183	6	-8	2	129	7	-8				
-8	141	6	-4	3	43	53	-4*	-4	118	7	9	3	141	7	1				
-7	304	8	-1	4	234	7	8	-3	222	7	-6	H,K= 15,			1				
-6	129	6	-1	H,K= 13,			1	-2	104	8	-3	-12	113	8	0				
-5	338	9	-6	-15	156	7	6	-1	217	7	3	-11	165	7	-3				
-4	172	6	5	-14	86	11	-5	0	115	8	-16	-10	126	7	10				
-3	307	8	-6	-13	185	7	13	1	199	7	3	-9	204	7	-0				
-2	181	6	-3	-12	118	7	14	2	64	50	-22*	-8	115	7	-5				
-1	312	8	-11	-11	194	7	-5	3	214	7	2	-7	199	6	1				
0	159	6	1	-10	112	8	7	4	80	12	25	-6	138	6	6				
1	309	8	-0	-9	245	7	3	H,K= 14,			0	-5	206	6	-1				
2	138	6	-7	-8	111	7	-8	-14	182	7	1	-4	126	6	-3				
3	237	7	-1	-7	246	7	3	-12	199	7	2	-3	230	7	-2				
4	153	6	1	-6	152	6	5	-10	233	7	-3	-2	149	6	-1				
5	222	7	11	-5	254	7	-5	-8	244	7	-5	-1	209	6	-0				
6	98	9	-2	-4	137	6	0	-6	232	7	-3	0	163	6	3				
7	220	7	4	-3	300	8	0	-4	278	8	-3	1	195	6	3				
8	62	37	-24*	-2	129	6	-5	-2	291	17	-0	2	117	7	-6				
9	163	7	8	-1	258	7	0	0	258	7	-1	3	196	7	-2				
H,K= 12,			4	0	167	6	2	2	259	17	-1	H,K= 15,			3				
-14	120	9	16	1	199	6	-0	4	244	7	-1	-10	193	7	2				
-13	164	7	9	2	166	6	7	6	189	7	2	-9	45	58	23*				
-12	125	8	2	3	243	7	8	H,K= 14,			2	-8	217	7	0				
-11	207	7	6	4	130	7	3	-13	177	7	7	-7	0	56	-13*				
-10	140	7	1	5	214	7	2	-12	95	9	17	-6	246	7	-3				
-9	193	7	-5	6	132	7	8	-11	196	7	-1	-5	36	54	15*				
-8	138	7	3	7	163	7	3	-10	119	7	14	-4	217	7	-3				
-7	215	7	4	H,K= 13,			3	-9	206	7	-3	-3	22	54	-1*				
-6	153	6	-1	-14	171	7	8	-8	135	6	-1	-2	211	6	-1				
-5	222	6	5	-13	0	61	-31*	-7	243	7	-2	-1	42	55	24*				
-4	183	6	-11	-12	212	7	-2	-6	124	6	-2	0	235	7	-8				
-3	174	6	-1	-11	0	59	-32*	-5	240	7	-4	1	0	58	-36*				
-2	195	6	-4	-10	228	7	-2	-4	131	6	-1	2	202	7	-4				
-1	223	7	3	-9	27	55	5*	-3	214	6	-5	H,K= 16,			0				
0	153	6	0	-8	254	7	-4	-2	122	6	-3	-8	222	7	-2				
1	259	7	5	-7	29	46	-6*	-1	237	7	-2	-6	208	7	-6				
2	152	6	5	-6	308	8	6	0	101	7	3	-4	242	7	-4				
3	205	7	4	-5	29	52	-25*	1	240	7	-1	-2	245	7	-5				
4	137	7	-14	-4	266	7	-2	2	108	7	4	0	207	6	2				
5	179	7	-3	-3	57	20	17*	3	210	7	4	H,K= 16,			2				
6	139	7	2	-2	239	7	-2	4	112	8	4	-8	61	26	-23*				
7	187	7	5	-1	40	45	26*	5	183	7	-1	-7	182	6	-8				
H,K= 12,			6	0	286	8	8	H,K= 14,			4	-6	81	10	2				
-11	0	65	-38*	1	49	53	31*	-11	161	7	12	-5	192	6	1				
-10	208	7	14	2	258	7	-1	-10	124	8	1	-4	87	9	-3				
-9	22	61	-26*	3	0	52	-31*	-9	154	7	-0	-3	186	6	5				
-8	239	7	6	4	204	7	-5	-8	140	7	1	-2	97	8	3				
-7	59	30	20*	5	49	54	25*	-7	182	6	-2	-1	195	6	-5				
-6	225	7	-0	6	207	7	-1	-6	140	6	-2								
-5	28	56	17*	H,K= 13,			5	-5	209	6	-0								
-4	241	7	-0	-11	165	7	2	-4	147	6	7								
-3	18	59	-6*	-10	70	14	-1	-3	178	6	1								
-2	267	8	-1	-9	198	7	1	-2	136	6	10								
-1	69	35	25*	-8	63	44	-14*	-1	194	6	0								
0	222	7	3	-7	185	7	-4	0	119	7	-0								
1	64	35	20*	-6	112	7	2	1	183	7	-6								

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