Title

STRUCTURE OF TRIS (METHYLCYCLOPENTADIENYL) CERIUM (III) TRIMETHYLPHOSPHINE, (CH3C5H4)3 Ce.P(CH3)3

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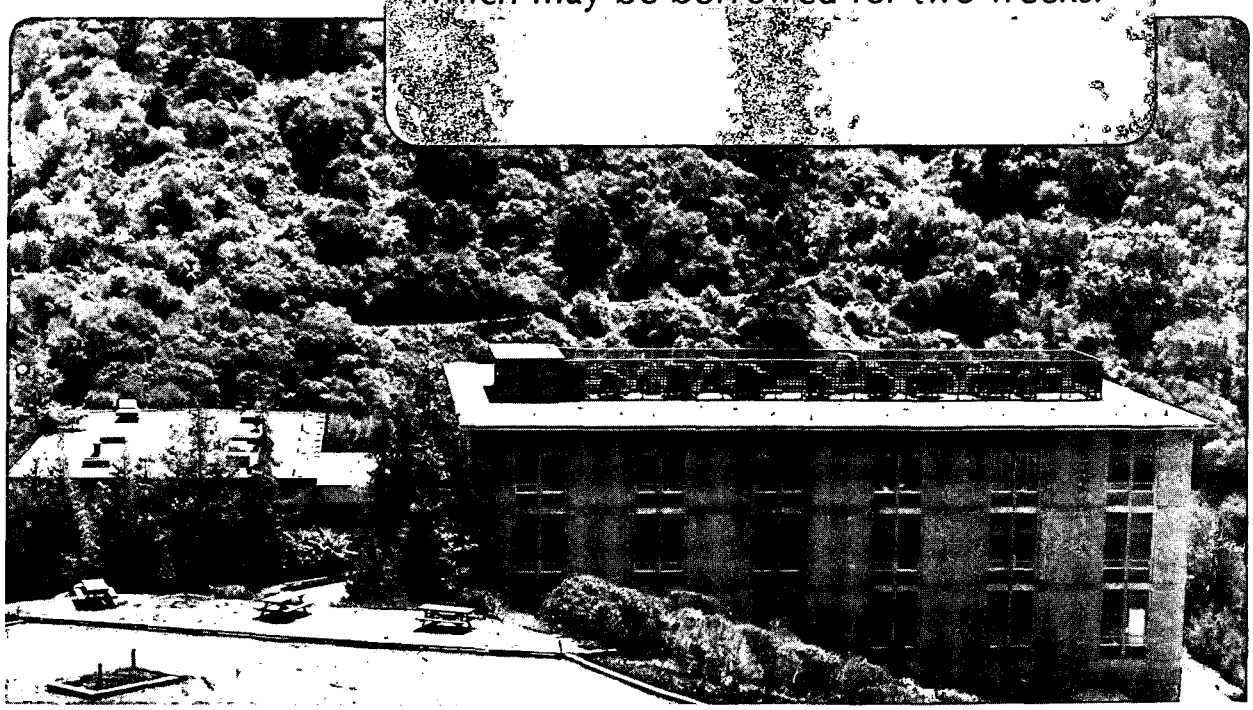
S. Stults and A. Zalkin

March 1986



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DISCLAIMER

STRUCTURE OF TRIS(METHYLCYCLOPENTADIENYL)CERIUM(III)TRIMETHYLPHOSPHINE, $(CH_3C_5H_4)_3Ce\cdot P(CH_3)_3$

By Stephen Stults & Allan Zalkin

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Abstract. M_r = 453.57 monoclinic, Cc, a = 14.017(4), b = 9.351(3), c = 16.348(6) Å, β = 103.92(3)°, V = 2080(3) $Å^3$, Z = 4, D_x = 1.448(3) g cm^{-3}, Mo Kα, λ(α_1) = 0.70930 Å, μ = 23.0 cm^{-1}, F(000) = 916, T = 296 K, R = 0.024 for 1232 reflections ($F^2 > \sigma$). The structure consists of cerium centered monomolecular units in which the cerium atom is coordinated in a pentahapto fashion to three cyclopentadiene rings and to the phosphorus atom of the trimethyl phosphine molecule. The average Ce-C distance is 2.82 ± 0.04 Å and the Ce-P distance is 3.072(4) Å.

Introduction. Recently we reported the structure of $(CH_3C_5H_4)_3U.P(CH_3)$ (Brennan & Zalkin,1985) as part of a study of the relative affinity of Lewis bases toward $(CH_3C_5H_4)_3U$. A parallel experiment using $(CH_3C_5H_4)_3Ce{\cdot}P(CH_3)_3$ is being done to study what effect a different metal atom has on the molecular structure and chemistry. Interligand contacts influence the ability of a ligand to coordinate to a metal ion and must be considered when comparing ligand basicities. As part of this study we report here the X-ray structure of $(CH_3C_5H_4)_3Ce.P(CH_3)_3$, which is isomorphous with the uranium complex.

Experimental. Yellow, air sensitive needles of the phosphine complex were prepared by reacting $(CH_3C_5H_4)_3Ce{\cdot}OC_4H_8$, isolated from the reaction of $CeCl_3$ with 3 equivalents of $NaCH_3C_5H_4$ in tetrahydrofuran, with $P(CH_3)_3$ in diethylether (Andersen, 1979) and crystallizing from diethyl ether at 253K. Crystals were sealed inside quartz capillaries because of their reactivity in the atmosphere, and no measured density is reported for the same reason. Crystal 0.18 x 0.18 x 0.17 mm with 6 faces; modified Picker automatic diffractometer, graphite monochromator; cell dimensions from 20 reflections, $21° < 2\theta < 36°$; analytical absorption correction, range 1.37 to 1.54; max. $(\sin\theta)/\lambda$ = 0.54 A^{-1}, h -15 to 15, k 0 to 10, ℓ -17 to 17; three standard reflections, <2% variation in intensities from average, intensities adjusted accordingly; 2878 data, 1366 unique (including 134, $F^2 < \sigma$), R_{int} = 0.021; refinements started with parameters of the uranium isomorph (Brennan & Zalkin, 1985); refined on F, 206 parameters, non-methyl hydrogen atoms in calculated positions with isotropic thermal parameters, methyl hydrogen atoms not included, anisotropic thermal parameters for non-hydrogen atoms; R = 0.032 for 1366 reflections (0.024

for 1232 for which $F^2 > \sigma$), wR = 0.026, S = 1.0; $w = [\sigma(F)]^{-2}$, p = 0.04 in calc. of $\sigma(F^2)$; max. (shift/σ) = 0.03, max. correction for extinction 1% of F, $F_{corr}=F_{obs}(1+3.1\times10^{-8}I)$; max. and min. of ΔF synthesis 0.18 and -0.24 e A^{-3}; atomic f for neutral Ce, 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. On the assumption that the crystal was twinned with both enantiomers present in equal amounts, the data were averaged. The f" term of the anomalous dispersion was set to zero, and the f' term was applied as usual.

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. (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. The complex $(CH_3C_5H_4)_3Ce.P(CH_3)_3$ is monomolecular in the crystalline state and consists of a cerium atom coordinated to the three methylcyclopentadienyl groups in a pentahapto bonding mode and to the phosphorus atom of the trimethyl phosphine molecule in a distorted

trigonal pyramidal arrangement with the phosphorus atom at the apex and cyclopentadienyl ring centers on the base; the plane through the cyclopentadienyl centers is 0.34 Å below the Ce atom. The angles about the Ce atom are given in Table 2. The cerium atom is 3.072(4) Å from the phosphorus atom and 2.54 to 2.58 Å from the least-squares planes of the cyclopentadienyl rings; the average Ce-C distance is 2.82 ± 0.04 Å. There are no observed close contacts between the phosphine ligand and the Cp rings.

Although 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), this represents the first structurally characterized organometallic tertiary phosphine complex of cerium.

Although $(CH_3C_5H_4)_3Ce{\cdot}P(CH_3)_3$ and $(CH_3C_5H_4)_3U{\cdot}P(CH_3)_3$ are crystallographically isomorphous there is a significant structural difference in the two molecules. The angles made by the four ligands about the metal atom are close to being tetrahedral in the uranium complex (average Cp-U-Cp angles, 112±7°; average P-U-Cp angle, 106.4±9°) and trigonal pyramidal in the cerium complex (average Cp-Ce-Cp angle, 118±1°; average P-Ce-Cp angle 98.1±1°). These Ce angles are within a degree of the comparable angles in $(CH_3C_5H_4)_3U{\cdot}OC_4H_8$ (Wasserman et al., 1983).

The published U(III) and Ce(III) ionic radii (Shannon & Prewitt, 1969) show the U(III) radius to be 0.03 Å larger than the Ce(III) radius. Assuming a purely ionic model, this structure indicates the reverse to be true. The average Ce-Cp distance (2.56 ± 0.03 Å) is

larger than the average U-Cp distance (2.52 ± 0.02 Å) by an amount that is barely significant. However, the Ce-P distance (3.07(4) Å) is a full 0.1 Å larger than the U-P distance (2.972(6) Å). Further structural studies are currently underway to ascertain the nature of this discrepancy.

Helpful discussions with Dr. John Brennan and Professor R. A. Andersen are 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.

References

Andersen, R. A. (1979). Inorg. Chem. **18**, 1507-1509.

Brennan, J. & Zalkin, A. (1985). Acta Cryst. C**41**, 1038-1040.

Burns, J. H. & Baldwin, W. H. (1976). J. Organomet. Chem. **120**, 361-367.

International Tables for X-ray Crystallography (1974). Vol.IV; Table 2.2, pp 71-102. Birmingham: Kynoch Press.

Johnson, C. K. (1965). ORTEP. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

Rogers, R.D., Atwood, J.L., Emad, A., Sikora, D.J., & Rauch, M.D. (1981). J. Organomet. Chem. **216**, 383-392.

Rogers, R.D., Bynum, R.V., & Atwood, J.L. (1980). J. Organomet. Chem. **192**, 65-73.

Shannon, R. D. & Prewitt, C. T. (1969). Acta Cryst. B**25**, 925-945.

Wasserman, H.J., Zozulin, A.J., Moody, D.C., Ryan, R.R., & Salazar, K. V. (1983). J. Organomet. Chem., **254**, 305-311.

Table 1. Atomic parameters for

Tris(methylcyclopentadienyl)cerium(III)trimethylphosphine

$$B_{eq} = \sum_i \sum_j B_{ij} a_i^* a_j^* a_i \cdot a_j / 3, \quad A^2.$$

Atom	x	y	z	B_{eq}
Ce	1/4	0.33939(4)	1/4	3.20
P	0.2804(3)	0.1697(4)	0.41521(26)	4.79
C(1)	0.3852(13)	0.6059(20)	0.4224(12)	9.01
C(2)	0.3989(9)	0.5285(16)	0.3429(10)	5.19
C(3)	0.4454(11)	0.3971(19)	0.3426(12)	5.83
C(4)	0.4500(16)	0.3631(19)	0.2595(16)	6.10
C(5)	0.4063(12)	0.4749(24)	0.2089(10)	6.56
C(6)	0.3754(15)	0.5754(23)	0.2638(16)	6.32
C(7)	0.1115(11)	0.6595(16)	0.1293(11)	7.20
C(8)	0.1026(13)	0.5608(23)	0.2020(13)	5.07
C(9)	0.1434(10)	0.5774(16)	0.2873(9)	4.82
C(10)	0.1158(11)	0.4677(16)	0.3350(8)	5.32
C(11)	0.0595(17)	0.3735(23)	0.2753(15)	6.48
C(12)	0.0516(11)	0.4258(21)	0.1973(12)	5.72
C(13)	0.1557(14)	0.2923(18)	0.0147(10)	7.46
C(14)	0.1926(16)	0.2143(20)	0.0931(14)	7.14
C(15)	0.1428(8)	0.1277(11)	0.1423(8)	5.45
C(16)	0.2074(12)	0.0492(12)	0.2044(8)	7.27
C(17)	0.3026(10)	0.0699(14)	0.1941(10)	7.09
C(18)	0.2958(10)	0.1630(16)	0.1259(9)	6.88
C(19)	0.3296(14)	0.2547(22)	0.5212(10)	7.78
C(20)	0.3671(10)	0.0201(16)	0.4248(9)	8.51
C(21)	0.1661(10)	0.0946(18)	0.4348(10)	9.74

Table 2. Selected distances and angles

Distances

Atoms	d(A)	Atoms	d(A)
Ce - P	3.072(4)	Ce - C(14)	2.757(18)
Ce - C(2)	2.875(13)	Ce - C(15)	2.829(10)
Ce - C(3)	2.844(16)	Ce - C(16)	2.840(11)
Ce - C(4)	2.779(20)	Ce - C(17)	2.837(10)
Ce - C(5)	2.751(15)	Ce - C(18)	2.807(10)
Ce - C(6)	2.797(20)	Ce - Cp_1[a]	2.55
Ce - C(8)	2.896(19)	Ce - Cp_2	2.59
Ce - C(9)	2.828(13)	Ce - Cp_3	2.54
Ce - C(10)	2.858(13)	P - C(19)	1.880(18)
Ce - C(11)	2.817(23)	P - C(20)	1.836(13)
Ce - C(12)	2.824(16)	P - C(21)	1.847(13)

Angles

P	- Ce - Cp_1	97.3	Cp_2	- Ce - Cp_3	117.8
P	- Ce - Cp_2	98.8	C(19)	- P - C(20)	98.9(8)
P	- Ce - Cp_3	96.7	C(19)	- P - C(21)	98.2(8)
Cp_1	- Ce - Cp_2	118.8	C(20)	- P - C(21)	106.2(8)
Cp_1	- Ce - CP_3	118.2			

[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.

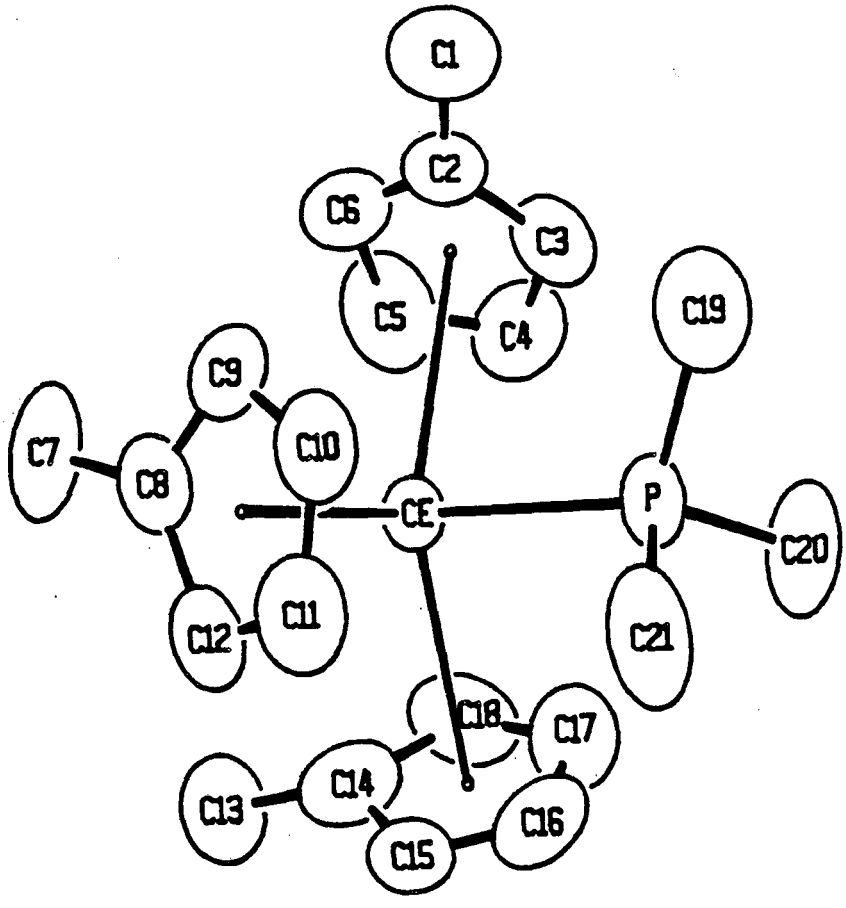

Fig. 1. ORTEP drawing of tris(methylcyclopentadienyl)cerium(III)-trimethylphosphine; thermal ellipsoids at 50% probability level.

Supplementary Material

for

STRUCTURE OF TRIS(METHYLCYCLOPENTADIENYL)CERIUM(III)TRIMETHYLPHOSPHINE, $(CH_3C_5H_4)_3Ce.P(CH_3)_3$

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Abstract. M_r = 453.57 monoclinic, Cc, a = 14.017(4), b = 9.351(3), c = 16.348(6) Å, β = 103.92(3)°, V = 2080(3) $Å^3$, Z = 4, D_x = 1.448(3) g cm^{-3}, Mo Kα, λ(α_1) = 0.70930 Å, μ = 23.0 cm^{-1}, F(000) = 916, T = 296 K, R = 0.024 for 1232 reflections ($F^2 > \sigma$). The structure consists of cerium centered monomolecular units in which the cerium atom is coordinated in a pentahapto fashion to three cyclopentadiene rings and to the phosphorus atom of the trimethyl phosphine molecule. The average Ce-C distance is 2.82 ± 0.04 Å and the Ce-P distance is 3.072(4) Å.

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

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ce	2.584(16)	3.196(19)	3.830(18)	0.20(7)	0.776(12)	-0.46(6)
P	4.86(18)	4.52(19)	4.59(14)	-0.41(16)	0.33(13)	1.42(15)
C(1)	8.7(10)	7.8(9)	9.8(11)	-1.3(8)	0.7(9)	-3.8(9)
C(2)	2.7(5)	4.6(8)	7.9(9)	-1.7(5)	0.6(6)	-0.8(7)
C(3)	2.5(5)	6.5(9)	7.9(10)	-0.4(5)	-0.0(6)	-1.0(7)
C(4)	3.2(6)	5.5(9)	10.2(16)	-0.5(7)	2.9(9)	-1.2(9)
C(5)	5.3(8)	9.1(11)	6.0(9)	-1.2(8)	2.7(7)	1.0(9)
C(6)	4.3(10)	4.6(8)	9.6(16)	-1.3(7)	0.7(11)	-1.4(12)
C(7)	7.1(7)	6.3(8)	8.6(9)	2.3(7)	2.9(7)	2.7(8)
C(8)	3.1(7)	5.5(9)	6.4(11)	1.2(6)	0.8(8)	-0.7(8)
C(9)	3.4(6)	3.8(6)	7.7(9)	1.0(5)	2.3(6)	-1.0(7)
C(10)	4.9(6)	6.5(7)	5.3(7)	1.6(5)	2.6(6)	-0.7(7)
C(11)	3.7(7)	7.7(11)	8.8(13)	0.9(7)	2.9(8)	-0.1(9)
C(12)	2.3(5)	6.3(10)	8.1(13)	1.0(6)	0.3(7)	0.2(8)
C(13)	10.1(11)	6.8(9)	4.5(8)	-0.5(7)	-0.1(7)	0.5(6)
C(14)	8.4(12)	4.9(8)	8.0(10)	-0.8(8)	1.9(8)	-3.4(7)
C(15)	4.6(5)	4.6(6)	6.7(6)	-1.0(4)	0.6(5)	-1.9(5)
C(16)	10.1(9)	3.9(5)	7.6(7)	-0.4(6)	1.9(6)	-2.2(5)
C(17)	7.4(8)	6.1(7)	7.3(8)	2.5(6)	0.9(6)	-3.3(6)
C(18)	6.0(7)	8.6(9)	6.3(6)	-0.2(6)	1.9(6)	-5.0(7)
C(19)	9.6(9)	8.6(10)	5.4(9)	0.0(8)	2.3(8)	-0.1(8)
C(20)	9.6(8)	6.6(7)	8.8(8)	3.1(7)	1.1(7)	1.1(7)
C(21)	6.6(7)	0.9(10)	10.9(10)	-2.4(7)	0.5(7)	6.7(9)

[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)	C(3)	0.4710	0.3372	0.3923	10.000
H(2)	C(4)	0.4784	0.2764	0.2410	10.000
H(3)	C(5)	0.3980	0.4840	0.1479	10.000
H(4)	C(6)	0.3417	0.6663	0.2454	10.000
H(5)	C(9)	0.1864	0.6570	0.3115	10.000
H(6)	C(10)	0.1323	0.4584	0.3965	10.000
H(7)	C(11)	0.0302	0.2843	0.2884	10.000
H(8)	C(12)	0.0164	0.3795	0.1450	10.000
H(9)	C(15)	0.0711	0.1240	0.1332	10.000
H(10)	C(16)	0.1892	-0.0102	0.2476	10.000
H(11)	C(17)	0.3629	0.0271	0.2284	10.000
H(12)	C(18)	0.3514	0.1909	0.1026	10.000

[a] 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)

$$12.246\,a + 4.330\,b - 1.061\,c = 6.809$$

C(2)	-0.0003
C(3)	0.0009
C(4)	-0.0018
C(5)	-0.0010
C(6)	0.0004
Ce	-2.543(10)
C(1)	0.08(4)

Plane 2, C(8) - C(12)

$$12.100\,a - 4.685\,b - 4.377\,c = -2.244$$

C(8)	-0.026
C(9)	0.164
C(10)	-0.012
C(11)	0.009
C(12)	0.010
Ce	2.585(9)
C(7)	-0.06(4)

Plane 3, C(14) - C(18)

$$-.563\,a + 7.187\,b + 10.289\,c = 2.3223$$

C(14)	0.068
C(15)	-0.021
C(16)	0.018
C(17)	0.007
C(18)	-0.022
Ce	2.548(7)
C(13)	-0.16(3)

Table D. C-C distances and C-C-C angles

Distances

Atoms	d(A)	Atoms	d(A)
C(2) - C(3)	1.391(23)	C(12) - C(8)	1.443(28)
C(3) - C(4)	1.411(29)	C(14) - C(15)	1.434(25)
C(4) - C(5)	1.382(26)	C(15) - C(16)	1.396(17)
C(5) - C(6)	1.436(29)	C(16) - C(17)	1.399(18)
C(6) - C(2)	1.331(24)	C(17) - C(18)	1.400(19)
C(8) - C(9)	1.382(23)	C(18) - C(14)	1.495(22)
C(9) - C(10)	1.398(21)	C(1) - C(2)	1.539(23)
C(10) - C(11)	1.407(27)	C(7) - C(8)	1.533(27)
C(11) - C(12)	1.345(26)	C(13) - C(14)	1.458(26)

Angles(°)

C(1) -C(2) -C(3)	124.9(16)	C(9) -C(10)-C(11)	104.8(14)
C(1) -C(2) -C(6)	127.8(20)	C(10)-C(11)-C(12)	109.5(19)
C(3) -C(2) -C(6)	107.1(19)	C(8) -C(12)-C(11)	109.9(19)
C(2) -C(3) -C(4)	109.4(16)	C(13)-C(14)-C(15)	131.1(18)
C(3) -C(4) -C(5)	106.8(15)	C(13)-C(14)-C(18)	125.7(20)
C(2) -C(6) -C(5)	110.5(20)	C(15)-C(14)-C(18)	100.3(17)
C(4) -C(5) -C(6)	106.1(16)	C(14)-C(15)-C(16)	112.8(13)
C(7) -C(8) -C(9)	128.5(19)	C(15)-C(16)-C(17)	108.0(13)
C(7) -C(8) -C(12)	128.1(17)	C(16)-C(17)-C(18)	107.4(12)
C(9) -C(8) -C(12)	103.4(19)	C(14)-C(18)-C(17)	111.0(14)
C(8) -C(9) -C(10)	112.2(17)		

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 8.0)
(CH3C5H4)CE.P(CH3)3 F(0,0,0) = 3369

SG = Estimated standard deviation of Fob. DEL = /Fob/- /Fca/, where
Fob and Fca are the observed and calculated structure factors.
* 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		7	105	9	-6	11	349	8	0	-4	183	5	-4	-1	69	24	-23
21185	24	-109		8	342	8	-2	12	165	7	8	-3	461	10	-8	0	198	6	5
4	779	16	23	9	32	54	-12*	13	251	7	6	-2	157	5	-5	1	100	9	-2
6	780	16	8	10	246	6	-7	14	140	8	-4	-1	541	12	6	2	240	6	5
8	491	10	9	11	46	59	-9*	15	135	8	-2	0	88	7	-8	3	122	8	1
10	381	8	-1	12	236	7	9	16	53	67	-40*	1	516	11	-16	4	214	6	5
12	390	8	-1	13	50	62	16*	H,K=	1,	3		2	229	5	-1	5	100	10	12
14	207	6	-6	H,K=	0,	8		-16	200	7	8	3	351	8	7	6	161	7	5
16	159	6	4	0	119	11	2	-15	0	63	-27*	4	167	5	-3	7	36	56	-31*
H,K=	0,	2		1	265	7	-6	-14	239	6	2	5	433	9	1	H,K=	2,	0	
0	123	5	25	2	56	42	-24	-13	47	63	22*	6	42	56	-2*	-16	158	6	1
1	402	9	-16	3	330	8	1	-12	252	7	1	7	426	9	1	-14	271	6	1
2	238	5	34	4	84	11	11	-11	44	61	2*	8	163	7	4	-12	409	9	2
31	126	25	60	5	279	7	-2	-10	409	9	-7	9	327	8	-3	-10	331	7	7
4	336	7	26	6	60	35	-13	-9	15	56	-42*	10	75	26	-15	-8	515	11	-14
5	574	12	4	7	216	6	6	-8	488	10	9	11	252	7	-4	-6	685	14	1
6	379	8	12	8	34	60	13*	-7	14	51	-46*	12	63	28	4	-4	558	11	10
7	448	9	-2	9	208	7	11	-6	481	10	-9	13	199	7	3	-2	812	16	16
8	380	8	1	10	41	54	36*	-5	165	5	8	14	71	27	6	01	116	23	42
9	510	11	0	H,K=	0,	10		-4	828	17	12	H,K=	1,	7		2	210	4	-11
10	147	7	-8	0	179	9	9	-3	202	5	4	-12	131	8	-2	4	720	15	15
11	328	7	1	1	47	64	-40*	-2	794	16	-6	-11	119	9	1	6	841	17	11
12	178	7	0	2	169	7	7	-1	53	18	-1	-10	146	7	-18	8	450	9	11
13	254	7	-5	H,K=	1,	1		0	567	12	41	-9	129	8	0	10	344	7	-9
14	116	9	-1	-17	132	9	-8	1	232	5	9	-8	167	6	-6	12	339	7	0
15	207	7	-3	-16	77	25	-22	2	633	13	-36	-7	279	7	0	14	192	5	4
16	60	20	-16	-15	160	7	3	3	91	5	1	-6	187	7	0	16	182	6	0
H,K=	0,	4		-14	134	8	1	4	850	17	30	-5	265	7	-2	H,K=	2,	2	
0	538	12	12	-13	289	7	-3	5	135	5	2	-4	217	6	-2	-17	150	8	0
1	518	11	0	-12	156	7	2	6	464	10	-9	-3	136	8	-7	-16	61	19	-3
2	468	10	5	-11	325	7	1	7	43	49	-17*	-2	257	6	1	-15	224	7	2
3	689	14	2	-10	259	6	-1	8	494	10	2	-1	293	7	-3	-14	121	8	6
4	276	6	-3	-9	314	7	4	9	58	30	-17	0	222	6	0	-13	227	7	9
5	507	11	14	-8	300	6	-8	10	372	8	-5	1	306	7	-5	-12	176	7	-5
6	407	9	11	-7	543	12	9	11	32	64	-42*	2	278	7	3	-11	328	7	-3
7	261	6	-2	-6	215	5	1	12	238	7	-3	3	237	6	0	-10	138	7	-4
8	308	7	1	-5	681	14	45	13	44	60	15*	4	248	7	6	-9	480	10	0
9	318	7	-6	-4	676	14	24	14	226	7	-3	5	308	7	4	-8	257	6	2
10	239	6	6	-3	377	8	7	15	64	47	39	6	220	6	-14	-7	416	9	-10
11	228	7	4	-2	804	16	37	16	172	7	-2	7	201	6	1	-6	246	6	-17
12	163	7	-10	-1	1036	21	-19	H,K=	1,	5		8	181	6	0	-5	724	15	46
13	148	7	-5	0	459	9	-14	-15	143	8	1	9	76	25	-35	-4	255	6	23
14	95	19	-35	1	876	19	3	-14	46	63	-25*	10	145	7	1	-3	568	12	-10
15	152	8	1	2	582	15	7	-13	230	7	-4	11	144	8	7	-2	218	5	2
H,K=	0,	6		3	490	10	43	-12	34	61	-35*	12	109	14	-7	1	216	5	8
0	455	10	4	4	594	12	49	-11	268	7	-2	H,K=	1,	9		0	521	11	0
1	168	6	-8	5	560	12	-14	-10	189	7	-3	-7	56	42	-29	1	389	8	-4
2	342	7	-8	6	220	5	-2	-9	321	7	4	-6	176	7	6	2	176	5	4
3	141	6	2	7	604	13	5	-8	116	8	3	-5	77	13	9	3	808	20	18
4	285	7	6	8	343	7	2	-7	443	10	5	-4	241	7	9	4	203	5	-8
5	134	7	-5	9	297	7	0	-6	22	56	-17*	-3	96	9	8	5	407	9	1
6	426	9	-3	10	266	6	-6	-5	473	10	10	-2	235	6	-3	6	296	6	9

STRUCTURE FACTORS continued for
(CH3C5H4)CE.P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	449	10	2	-1	125	7	-1	2	156	5	-9	-7	440	10	2	2	204	7	2
8	164	6	-4	0	494	10	5	3	525	11	18	-6	118	7	3	3	57	61	-10*
9	449	10	-7	1	84	9	-1	4	427	9	21	-5	380	8	1	4	198	7	-2
10	163	7	7	2	342	7	0	5	536	11	-1	-4	289	6	-3	5	0	62	-44*
11	274	7	1	3	98	9	14	6	314	7	4	-3	359	8	-8	6	173	7	2
12	176	7	9	4	369	8	0	7	481	10	-11	-2	191	5	0	H,K=	4,	0	
13	251	7	0	5	81	21	-17	8	322	7	7	-1	448	10	9	-16	195	5	7
14	34	61	-45*	6	409	9	1	9	242	6	2	0	173	5	-3	-14	332	7	1
15	198	7	2	7	86	12	5	10	217	6	-2	1	416	9	-20	-12	380	8	-2
16	36	58	-30*	8	260	7	-1	11	321	7	0	2	249	6	-9	-10	357	8	2
H,K=	2,	4		9	0	60	-47*	12	149	8	-1	3	263	6	-1	-8	645	13	0
-16	106	10	10	10	226	6	2	13	187	7	-7	4	125	7	-3	-6	736	15	-3
-15	177	7	8	11	17	60	-18*	14	150	7	-4	5	392	8	-6	-4	536	11	30
-14	153	7	7	12	219	7	8	15	126	9	-4	6	125	7	-5	-2	546	11	-9
-13	156	7	-6	13	24	57	-1*	H,K=	3,	3		7	348	8	0	0	294	6	-37
-12	177	7	-14	H,K=	2,	8		-16	203	7	11	8	159	7	6	2	728	15	42
-11	234	7	8	-10	21	64	-8*	-15	0	61	-30*	9	251	7	-2	4	736	15	0
-10	215	6	-1	-9	220	7	6	-14	212	6	-2	10	40	60	-28*	6	632	13	2
-9	313	7	-11	-8	0	60	-48*	-13	60	34	25	11	248	7	-6	8	314	7	2
-8	227	6	-1	-7	202	6	-1	-12	248	7	-1	12	45	62	-15*	10	327	7	-8
-7	238	6	4	-6	113	9	-5	-11	35	60	-33*	13	186	7	3	12	297	7	3
-6	267	6	-2	-5	224	6	-1	-10	432	9	-13	H,K=	3,	7		14	171	6	-1
-5	457	10	10	-4	65	28	10	-9	37	48	-21*	-12	134	8	7	H,K=	4,	2	
-4	307	7	-3	-3	261	7	-1	-8	394	8	1	-11	136	8	10	-17	169	7	2
-3	597	13	-11	-2	81	12	4	-7	59	19	0	-10	161	7	1	-16	71	27	18
-2	398	8	-2	-1	228	6	1	-6	389	8	-5	-9	136	7	-8	-15	190	7	-6
-1	493	11	-6	0	123	8	3	-5	115	5	-6	-8	157	7	0	-14	134	7	8
0	339	7	4	1	308	7	-6	-4	734	15	14	-7	262	7	-4	-13	187	7	-1
1	448	9	-5	2	66	27	-4	-3	167	5	12	-6	197	7	3	-12	170	7	-9
2	247	6	-10	3	316	7	-8	-2	797	16	14	-5	209	7	10	-11	389	8	2
3	587	12	-7	4	53	54	2*	-1	124	5	17	-4	277	7	-3	-10	95	16	-15
4	256	6	13	5	237	6	-5	0	538	11	-5	-3	202	7	-4	-9	486	10	-1
5	270	6	6	6	65	28	1	1	234	5	2	-2	257	7	-2	-8	185	5	3
6	335	7	0	7	197	6	9	2	763	16	-2	-1	324	7	-3	-7	486	10	-5
7	260	6	-8	8	60	32	19	3	60	16	-19	0	263	7	-2	-6	347	8	7
8	226	6	-7	9	195	7	1	4	601	13	-6	1	276	7	-7	-5	669	14	14
9	314	7	5	H,K=	3,	1		5	125	5	3	2	276	7	1	-4	199	5	-1
10	185	7	2	-17	129	8	-2	6	316	7	4	3	226	6	5	-3	688	14	-5
11	192	7	0	-16	136	8	3	7	60	13	-8	4	235	7	4	-2	565	12	1
12	163	7	-6	-15	175	7	-6	8	436	9	-9	5	231	6	3	-1	820	17	20
13	146	7	-1	-14	159	7	0	9	22	60	-1*	6	182	6	0	0	601	12	33
14	115	9	5	-13	311	7	2	10	324	7	5	7	151	7	-11	1	777	16	-10
H,K=	2,	6		-12	175	7	-4	11	63	37	-11	8	144	7	3	2	316	7	-5
-14	179	7	1	-11	287	7	2	12	201	6	-6	9	140	7	-2	3	658	14	16
-13	0	62	-49*	-10	309	7	-1	13	0	60	-31*	10	122	8	-5	4	219	5	-7
-12	242	6	8	-9	362	8	-4	14	221	7	6	11	152	8	5	5	413	9	-4
-11	8	60	-64*	-8	312	7	-6	15	58	39	35	H,K=	3,	9	6	273	6	-4	
-10	232	6	-5	-7	622	13	24	H,K=	3,	5		-7	68	44	-21	7	413	9	1
-9	105	10	-7	-6	356	8	2	-15	155	8	-3	-6	168	7	4	8	99	9	15
-8	323	8	-3	-5	650	13	22	-14	61	35	-9	-5	42	55	-12*	9	359	8	-5
-7	106	9	2	-4	291	6	-7	-13	243	7	-7	-4	235	7	2	10	177	7	-8
-6	405	9	2	-3	277	6	-5	-12	58	37	-25	-3	57	62	-17*	11	225	7	2
-5	122	8	-1	-2	124	5	-1	-11	257	7	0	-2	201	7	-6	12	138	8	-4
-4	293	7	8	-1	865	18	18	-10	188	7	0	-1	56	37	-6	13	195	6	2
-3	120	7	-3	0	340	7	21	-9	276	7	4	0	168	7	0	14	40	63	-20*
-2	417	9	-7	1	571	12	5	-8	93	10	16	1	73	13	12	15	176	7	4

STRUCTURE FACTORS continued for
(CH3C5H4)CE.P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	4,	4		10	217	6	-2	-16	204	7	6	10	34	61	-35*	-16	75	26	-2
-16	91	12	3	11	30	62	-24*	-15	39	60	9*	11	239	7	-6	-15	189	6	8
-15	169	7	-3	H,K=	4,	8		-14	201	6	-2	12	49	64	-2*	-14	124	8	-5
-14	149	7	-14	-10	19	62	-8*	-13	56	60	12*	H,K=	5,	7		-13	203	7	-2
-13	152	7	4	-9	220	7	2	-12	290	7	3	-12	133	8	2	-12	162	7	3
-12	183	7	-3	-8	48	55	-3*	-11	42	63	16*	-11	126	9	-8	-11	360	8	-6
-11	271	7	2	-7	192	7	5	-10	479	10	-7	-10	183	7	-1	-10	133	7	5
-10	200	6	-1	-6	50	59	-9*	-9	44	58	-15*	-9	124	8	-3	-9	361	8	-2
-9	359	8	-4	-5	241	6	2	-8	387	8	-6	-8	194	6	-2	-8	255	6	6
-8	251	6	4	-4	52	18	42	-7	108	7	4	-7	221	6	2	-7	301	7	-5
-7	223	6	3	-3	286	7	1	-6	453	10	-8	-6	228	6	0	-6	310	7	-1
-6	289	6	2	-2	41	58	5*	-5	148	5	5	-5	209	6	0	-5	564	12	4
-5	369	8	-5	-1	232	6	3	-4	699	15	3	-4	279	7	-1	-4	72	8	-7
-4	284	6	-8	0	25	60	-55*	-3	303	7	-1	-3	232	7	2	-3	766	16	6
-3	468	10	4	1	248	6	-3	-2	608	13	-4	-2	245	7	-2	-2	272	6	0
-2	288	6	-3	2	45	58	25*	-1	214	5	7	-1	262	7	-2	-1	645	13	-17
-1	254	6	-19	3	220	6	-6	0	550	12	-21	0	271	7	3	0	181	5	1
0	410	9	10	4	63	15	0	1	218	5	3	1	176	7	-4	1	544	12	-11
1	418	9	-2	5	193	6	-3	2	739	15	-8	2	238	6	-2	2	175	5	-9
2	364	8	-6	6	73	14	-2	3	105	6	0	3	148	7	-3	3	416	9	7
3	437	9	-13	7	223	7	9	4	440	9	-3	4	215	6	-3	4	285	6	4
4	311	7	-5	8	52	55	15*	5	8	53	-26*	5	189	6	2	5	344	7	-4
5	205	6	5	H,K=	5,	1		6	372	8	8	6	156	7	-1	6	274	6	1
6	265	6	7	-17	128	9	10	7	40	58	-4*	7	161	7	2	7	399	9	0
7	358	8	-5	-16	122	9	-1	8	435	9	-9	8	167	7	-3	8	108	9	3
8	191	6	0	-15	172	7	-9	9	33	55	6*	9	134	8	13	9	322	7	-6
9	292	7	4	-14	115	9	-4	10	270	7	-1[illegible]	H,K=	5,	9		10	164	7	1
10	163	7	-4	-13	304	7	1	11	0	61	-32*	-6	169	7	10	11	186	6	0
11	145	7	-1	-12	176	7	-1	12	184	7	3	-5	87	21	2	12	100	10	9
12	156	7	-12	-11	263	7	-3	13	0	63	-37*	-4	222	7	7	13	170	7	2
13	170	7	8	-10	277	6	6	H,K=	5,	5		-3	66	35	-27	H,K=	6,	4	
H,K=	4,	6		-9	383	8	-7	-15	160	7	0	-2	184	7	4	-15	150	8	-3
-14	179	7	2	-8	218	5	0	-14	25	62	-31*	-1	34	63	-26*	-14	156	7	-4
-13	60	61	12*	-7	603	13	6	-13	233	7	-5	0	152	7	-6	-13	137	8	-6
-12	214	7	-2	-6	317	7	0	-12	0	55	-45*	1	34	62	-13*	-12	160	7	-10
-11	45	58	-24*	-5	547	12	1	-11	249	7	0	2	205	7	-2	-11	310	7	5
-10	197	6	1	-4	410	9	3	-10	130	8	9	3	62	32	9	-10	159	7	-2
-9	54	54	-29*	-3	673	14	4	-9	307	7	0	H,K=	6,	0		-9	341	8	-3
-8	345	8	8	-2	351	8	-18	-8	111	9	-5	-16	182	6	8	-8	283	7	-4
-7	110	10	6	-1	984	20	28	-7	444	10	-14	-14	302	7	-1	-7	254	6	5
-6	461	10	-7	0	460	10	9	-6	174	6	-3	-12	313	7	-3	-6	320	7	0
-5	33	62	-58*	1	609	13	9	-5	335	7	2	-10	298	7	-3	-5	352	14	1
-4	377	8	-2	2	410	9	-12	-4	201	6	2	-8	536	11	7	-4	281	6	-2
-3	78	11	10	3	549	12	6	-3	330	7	-7	-6	606	13	-15	-3	371	8	-6
-2	455	10	-13	4	260	6	3	-2	125	6	6	-4	549	11	0	-2	250	6	1
-1	108	8	-5	5	540	11	-8	-1	452	10	-1	-2	862	18	12	-1	224	6	0
0	453	10	-11	6	223	6	-7	0	54	38	-12	0	692	14	-7	0	338	7	3
1	116	8	-9	7	348	8	3	1	420	9	-1	2	642	13	-27	1	439	9	4
2	307	7	2	8	240	6	1	2	186	6	-4	4	508	10	-7	2	243	6	2
3	39	61	-36*	9	235	6	-9	3	373	8	-1	6	444	9	7	3	401	9	1
4	380	8	-10	10	172	7	-4	4	129	8	0	8	267	6	-2	4	302	7	3
5	91	11	-5	11	287	7	-4	5	446	10	-2	10	341	7	-5	5	260	6	-6
6	340	8	3	12	110	9	-8	6	127	8	-2	12	259	6	6	6	239	6	-2
7	45	53	8*	13	159	7	-7	7	306	7	3	14	131	6	-4	7	328	8	2
8	204	6	-3	14	103	10	-6	8	115	8	9	H,K=	6,	2		8	188	6	5
9	44	53	-24*	H,K=	5,	3		9	215	6	0	-17	157	8	0	9	201	6	-4

STRUCTURE FACTORS continued for
(CH3C5H4)CE.P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
10	148	7	0	-7	456	10	0	-10	117	8	10	12	195	6	3	10	131	8	6
11	101	10	-16	-6	211	5	3	-9	245	6	5	H,K=	8,	2		H,K=	8,	6	
12	133	8	-7	-5	347	8	-2	-8	88	22	-26	-16	55	58	-18*	-12	189	7	-1
H,K=	6,	6		-4	352	8	-4	-7	369	8	-3	-15	188	7	-4	-11	44	61	-26*
-13	27	63	-20*	-3	472	10	-19	-6	66	50	-30	-14	114	9	4	-10	179	7	1
-12	208	7	5	-2	392	8	-5	-5	337	8	4	-13	214	6	1	-9	42	54	0*
-11	56	40	-18	-1	414	9	6	-4	114	9	-11	-12	98	10	-7	-8	232	6	-5
-10	194	6	7	0	423	9	-6	-3	361	8	-2	-11	316	7	2	-7	65	38	14
-9	96	9	12	1	293	6	-7	-2	125	8	0	-10	112	9	-6	-6	227	6	1
-8	321	7	7	2	276	6	-9	-1	422	9	-8	-9	304	7	0	-5	94	10	-6
-7	42	59	-9*	3	393	8	-11	0	138	7	1	-8	197	6	2	-4	242	7	3
-6	363	8	2	4	142	6	2	1	333	8	-2	-7	249	6	2	-3	108	9	12
-5	75	26	-13	5	443	10	-10	2	202	6	2	-6	201	6	-2	-2	317	7	-6
-4	292	7	-1	6	212	6	1	3	364	8	0	-5	384	8	-1	-1	61	35	-10
-3	82	13	-4	7	230	6	2	4	85	22	-20	-4	167	6	2	0	314	7	-4
-2	366	8	0	8	210	7	-1	5	333	8	7	-3	345	7	-8	1	38	55	18*
-1	138	8	16	9	250	7	-8	6	101	9	25	-2	241	6	-4	2	232	6	-1
0	400	9	-7	10	120	8	-13	7	203	6	6	-1	209	5	10	3	43	59	2*
1	53	63	-38*	11	239	7	0	8	108	8	12	0	149	6	-4	4	256	7	0
2	304	7	0	12	89	11	-5	9	174	7	2	1	427	9	1	5	3	61	-38*
3	85	23	-6	13	144	8	13	10	59	62	-3*	2	186	6	-6	6	214	7	-4
4	342	8	2	H,K=	7,	3		H,K=	7,	7		3	364	8	-9	7	16	61	-19*
5	81	12	-9	-16	207	7	3	-11	144	8	1	4	220	6	-1	8	163	7	4
6	264	7	-3	-15	53	54	6*	-10	163	7	-2	5	300	7	-6	H,K=	8,	8	
7	62	26	11	-14	192	7	0	-9	149	7	1	6	140	8	7	-7	178	7	2
8	182	6	1	-13	42	60	-25*	-8	144	7	3	7	348	8	1	-6	68	29	4
9	56	60	-13*	-12	269	7	0	-7	192	7	-2	8	86	11	-4	-5	221	7	0
10	208	7	6	-11	47	58	-27*	-6	126	8	-9	9	224	6	-2	-4	55	55	-18*
H,K=	6,	8		-10	405	9	-1	-5	179	6	-3	10	120	8	4	-3	213	7	-1
-9	197	7	-2	-9	44	61	-11*	-4	172	6	-3	11	134	8	-5	-2	90	11	-9
-8	57	59	-16*	-8	347	8	-5	-3	195	6	3	H,K=	8,	4		-1	196	7	-4
-7	186	7	6	-7	33	57	-33*	-2	184	6	5	-15	135	8	11	0	40	62	-23*
-6	65	43	13	-6	440	9	-9	-1	239	6	-1	-14	128	8	0	1	213	7	-15
-5	242	7	1	-5	104	7	8	0	180	6	5	-13	144	7	5	2	24	63	-8*
-4	37	59	10*	-4	529	11	0	1	179	6	1	-12	129	8	-5	H,K=	9,	1	
-3	273	7	5	-3	49	33	1	2	169	6	2	-11	224	6	-6	-16	94	11	-3
-2	79	12	6	-2	332	7	-4	3	146	7	-13	-10	137	8	-7	-15	181	7	8
-1	214	6	4	-1	64	19	-11	4	156	7	-5	-9	251	7	4	-14	89	20	-17
0	41	59	-29*	0	401	9	-11	5	200	7	6	-8	277	7	-3	-13	234	7	-6
1	214	6	0	1	53	46	-13	6	141	8	-3	-7	283	7	-8	-12	160	7	-7
2	46	59	17*	2	474	10	0	7	122	9	1	-6	276	7	0	-11	234	7	-1
3	233	7	6	3	0	56	-42*	H,K=	8,	0		-5	418	9	-4	-10	211	7	-7
4	63	17	-1	4	297	7	0	-16	164	6	8	-4	190	6	-1	-9	332	8	3
5	200	7	6	5	0	60	-28*	-14	256	6	-5	-3	407	9	-5	-8	207	6	2
6	43	54	-9*	6	380	8	-4	-12	317	7	7	-2	221	6	0	-7	403	9	-3
H,K=	7,	1		7	79	24	6	-10	332	7	-6	-1	340	8	3	-6	235	6	1
-17	119	10	-1	8	355	8	-2	-8	514	11	7	0	221	6	4	-5	297	7	5
-16	114	9	12	9	28	51	-17*	-6	496	10	-3	1	374	8	-4	-4	293	7	-2
-15	183	7	2	10	182	6	-4	-4	365	8	3	2	208	6	7	-3	365	8	-7
-14	72	26	-30	11	40	59	7*	-2	599	13	13	3	243	6	1	-2	241	6	4
-13	289	7	5	12	166	7	7	0	488	10	-20	4	260	7	6	-1	369	8	1
-12	164	7	5	H,K=	7,	5		2	374	8	7	5	186	6	-3	0	267	6	0
-11	231	6	-3	-14	48	56	-7*	4	473	10	-9	6	176	6	-8	1	345	8	2
-10	208	6	0	-13	210	7	10	6	365	8	1	7	226	6	6	2	284	7	-2
-9	315	7	4	-12	68	26	-1	8	236	6	-2	8	127	7	10	3	375	8	-7
-8	151	6	2	-11	182	7	-9	10	300	7	3	9	169	7	-3	4	208	6	-3

STRUCTURE FACTORS continued for
(CH3C5H4)CE.P(CH3)3 page 5

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	350	8	3	8	106	10	2	H,K=	10,	4		1	255	7	-1	2	231	6	-1
6	198	7	7	H,K=	9,	7		-13	144	8	-3	2	213	6	0	4	294	7	-3
7	167	7	-7	-9	152	8	-4	-12	134	8	1	3	253	7	-10	6	211	6	1
8	150	7	-2	-8	141	8	5	-11	197	7	-2	4	145	7	2	H,K=	12,	2	
9	221	7	-2	-7	178	7	3	-10	162	7	1	5	240	7	1	-13	149	8	-8
10	81	12	7	-6	155	7	0	-9	212	6	3	6	148	7	10	-12	90	12	-10
11	184	7	3	-5	136	8	-2	-8	199	6	-6	7	165	7	4	-11	203	7	-4
H,K=	9,	3		-4	157	7	-13	-7	266	7	-6	8	137	8	16	-10	114	9	-5
-15	48	64	3*	-3	175	7	1	-6	203	6	5	H,K=	11,	3		-9	213	6	-3
-14	161	7	-8	-2	155	7	2	-5	317	7	1	-13	24	55	7*	-8	126	8	0
-13	44	53	14*	-1	192	7	-2	-4	242	7	3	-12	248	7	7	-7	281	7	3
-12	254	7	-2	0	135	8	3	-3	240	7	3	11	52	53	13*	-6	114	8	5
-11	28	60	-27*	1	140	7	3	-2	325	8	1	-10	261	7	1	-5	325	7	2
-10	327	8	-1	2	153	7	8	-1	225	7	0	-9	33	60	-28*	-4	150	7	-4
-9	78	14	5	3	176	7	7	0	269	7	-4	-8	244	7	-6	-3	271	7	-7
-8	314	7	-4	4	136	8	0	1	256	7	1	-7	41	60	-23*	-2	160	7	-3
-7	34	62	-32*	H,K=	10,	0		2	206	6	-4	-6	330	8	0	-1	272	7	-12
-6	399	9	-1	-14	234	6	4	3	187	6	-6	-5	110	9	14	0	133	7	-3
-5	0	60	-27*	-12	281	6	8	4	191	6	5	-4	351	8	1	1	274	7	1
-4	465	10	2	-10	350	8	-1	5	190	6	6	-3	81	21	-17	2	121	8	2
-3	106	9	-5	-8	471	10	0	6	141	7	7	-2	312	7	-7	3	188	6	3
-2	376	8	3	-6	443	9	4	7	210	7	-4	-1	117	8	2	4	142	7	9
-1	0	59	-10*	-4	432	9	-1	8	114	9	3	0	362	8	-9	5	191	7	7
0	454	10	-8	-2	533	11	-1	H,K=	10,	6		1	19	59	-20*	6	60	43	-14
1	42	53	0*	0	400	8	-5	-10	189	7	-5	2	320	7	-4	H,K=	12,	4	
2	411	9	6	2	333	7	8	-9	65	28	15	3	0	58	-16*	-11	174	7	-3
3	67	31	-13	4	441	9	-3	-8	243	7	1	4	226	6	4	-10	112	9	-7
4	282	7	7	6	280	6	-6	-7	59	19	-13	5	34	60	24*	-9	173	7	4
5	52	54	10*	8	208	6	2	-6	233	7	6	6	241	7	5	-8	118	8	0
6	305	7	-2	10	225	6	2	-5	82	11	14	7	26	62	5*	-7	172	7	2
7	30	59	-10*	H,K=	10,	2		-4	238	7	1	H,K=	11,	5		-6	124	8	2
8	250	7	-7	-15	167	7	6	-3	54	61	-20*	-11	171	7	-2	-5	178	6	5
9	66	42	24	-14	99	11	-5	-2	276	7	5	-10	100	10	10	-4	165	7	-2
10	154	7	1	-13	202	6	4	-1	62	31	-1	-9	219	7	-3	-3	114	9	-9
H,K=	9,	5		-12	84	11	-11	0	214	6	3	-8	77	23	-10	-2	180	6	7
-13	173	7	-7	-11	267	7	-6	1	45	59	-12*	-7	211	6	4	-1	187	6	7
-12	62	32	-14	-10	110	9	-4	2	199	6	0	-6	104	10	-16	0	109	9	-10
-11	164	7	-5	-9	296	7	-6	3	42	55	-17*	-5	199	6	2	1	231	6	-6
-10	78	21	-13	-8	130	8	7	4	251	7	1	-4	92	10	-8	2	119	8	5
-9	230	6	-4	-7	317	7	-3	5	49	62	3*	-3	252	6	4	3	176	7	0
-8	65	27	-4	-6	132	8	10	H,K=	11,	1		-2	40	51	7*	4	131	8	-1
-7	312	7	0	-5	401	9	-5	-14	90	12	-1	-1	271	7	7	H,K=	12,	6	
-6	126	8	14	-4	193	6	-2	-13	197	7	11	0	110	9	0	-5	38	62	4*
-5	330	8	-4	-3	360	8	-1	-12	100	10	-10	1	211	6	-3	-4	218	7	12
-4	80	26	-28	-2	234	6	-4	-11	205	6	-5	2	52	61	-27*	-3	61	52	52
-3	376	8	2	-1	377	8	3	-10	133	8	-7	3	237	7	-3	-2	243	7	0
-2	87	11	23	0	202	6	7	-9	272	7	-7	4	41	63	-22*	H,K=	13,	1	
-1	384	8	-4	1	485	10	-7	-8	167	7	3	5	234	7	5	-12	99	11	2
0	108	9	15	2	152	7	-1	-7	312	7	5	H,K=	12,	0		-11	167	7	-4
1	264	7	-7	3	326	8	-2	-6	222	7	0	-12	193	6	0	-10	101	10	0
2	58	39	-29	4	169	7	4	-5	284	7	-7	-10	216	6	-2	-9	215	7	-1
3	277	7	5	5	232	6	-3	-4	248	7	10	-8	273	6	0	-8	97	10	1
4	43	51	0*	6	97	18	-1	-3	390	8	-4	-6	271	6	1	-7	220	6	6
5	232	6	1	7	258	7	6	-2	169	7	6	-4	330	7	0	-6	119	8	-1
6	81	21	-12	8	108	9	5	-1	366	8	-6	-2	317	7	-3	-5	224	6	-1
7	165	7	-7	9	165	7	4	0	203	7	8	0	218	6	-1	-4	83	21	-17

STRUCTURE FACTORS continued for
(CH3C5H4)CE.P(CH3)3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	273	7	-2																
-2	81	20	-16																
-1	219	6	2																
0	155	7	3																
1	157	7	1																
2	144	7	-1																
3	220	7	6																
4	120	9	7																
H,K= 13, 3																			
-10	205	7	0																
-9	17	61	-9*																
-8	229	7	3																
-7	39	60	4*																
-6	287	7	5																
-5	56	40	-5																
-4	228	6	0																
-3	47	60	2*																
-2	187	6	1																
-1	44	60	31*																
0	252	7	7																
1	59	61	39*																
2	233	6	10																
3	0	65	-24*																
H,K= 13, 5																			
-5	163	7	5																
-4	113	9	0																
-3	203	7	-1																
-2	120	8	16																
H,K= 14, 0																			
-10	214	6	-2																
-8	231	6	2																
-6	202	6	5																
-4	253	6	2																
-2	275	6	8																
0	238	6	8																
2	240	6	-3																
H,K= 14, 2																			
-9	186	7	0																
-8	140	8	9																
-7	230	7	4																
-6	117	9	1																
-5	231	7	10																
-4	126	8	7																
-3	183	7	0																
-2	112	9	4																
-1	214	7	-4																
0	69	16	-6																
1	238	7	9																
H,K= 15, 1																			
-5	187	7	1																
-4	116	9	-4																
-3	213	7	-5																

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