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BIS [TRIS (CYCLOPENTADIENYL)URANIUM (IV) [1,2-BIS (DIMETHYLDIPHOSPHINO)ETHANE] [(C5H5)3U]2. (CH3)2PCH2CH2P(CH3)2

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BIS[TRIS(CYCLOPENTADIENYL)URANIUM(IV)]
[1,2-BIS(DIMETHYLDIPHOSPHINO)ETHANE]
$[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

A. Zalkin, J.G. Brennan and R.A. Andersen

November 1986

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Bis[tris(cyclopentadienyl)uranium(IV)][1,2-bis(dimethyldiphosphino)ethane]

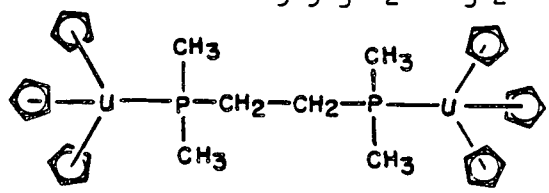
$[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

By Allan Zalkin, John G. Brennan & Richard A. Andersen

Materials and Molecular Research Division, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley CA 94720

Abstract. $[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$, M_r = 1016.78, triclinic, $P\bar{1}$, a = 14.467(8), b = 14.819(6), c = 8.378(3) A, α = 102.72(3)°, β = 90.03(3)°, γ = 96.69(3)°, V = 1739.5 A^3, Z = 2, D_x = 1.941 g cm^{-3}, λ(MoKα) = 0.71073 A, μ = 89.3 cm^{-1}, F(000) = 952, T = 296 K, R = 0.035 for 1987 unique reflections with $F^2 > 2\sigma(F^2)$ of 3241 total unique data. The phosphorus atom at each end of the bis(dimethylphosphino)ethane ligand is coordinated to a trivalent uranium atom of a triscyclopentadienyluranium fragment; a center of inversion is located at the midpoint of the CH_2CH_2 bridge of the $(CH_3)_2PCH_2CH_2P(CH_3)_2$ ligand. Distances (A) are: ave U-C(Cp) 2.77 ± 0.03; ave U-P 3.022 ± 0.002; ave U-Cp(ring) 2.518 ± 0.011 A.

Introduction. The title complex, $[(C_5H_5)_3U]_2\cdot(CH_3)_2PCH_2CH_2P(CH_3)_2$,



was prepared during the course of studies on the coordination chemistry of tetra- and tri-valent uranium complexes with bidentate amine, phosphine, and arsine ligands. The crystal structures of the tetravalent complexes with bidentate ligands, $UCl_4[(CH_3)_2NCH_2CH_2N(CH_3)_2]_2$ (Zalkin, Edwards, Zhang & Andersen, 1986), $U(OC_6H_5)_4[(CH_3)_2PCH_2CH_2P(CH_3)_2]_2$ (Edwards, Andersen & Zalkin, 1981), $UCl_4[1,2\text{-}(CH_3)_2AsC_6H_4]_2$ (Edwards, Andersen & Gellert, 1986), and $U(CH_3)(CH_2C_6H_5)_3\cdot(CH_3)_2PCH_2CH_2P(CH_3)_2$ (Edwards, Andersen & Zalkin, 1984) have been described. In all of the above cases the ligands are bidentate, chelating ligands towards the uranium atom. In the title compound the $(CH_3)_2PCH_2CH_2P(CH_3)_2$ ligand is not acting as a bidentate, chelating ligand but it is acting as a bridging monodentate ligand towards each trivalent uranium atom.

Experimental. The compound was prepared from $(C_5H_5)_3U\cdot OC_4H_8$ and $(CH_3)_2PCH_2CH_2P(CH_3)_2$. Crystals suitable for X-ray diffraction studies were grown from a mixture of toluene and hexane (Brennan, 1985). Dark red, air sensitive crystals were sealed inside quartz capillaries under argon. Crystal 0.06 x 0.15 x 0.21 mm with 10 faces; modified Picker automatic diffractometer, graphite monochromator; cell dimensions from 49 reflections, $20° < 2\theta < 36°$; analytical absorption correction, range 1.75 to 4.04; max. $(\sin\theta)/\lambda = 0.48$ Å; h -13 to 13, k -13 to 13, l -8 to 8; three standard reflections, average decay 3%, intensities adjusted accordingly; 6454 data, 3242 unique, $R_{int} = 0.05$; structure solved by Patterson and Fourier methods; refined on F, f' & f" terms included, 355 parameters;

calculated positional coordinates of the cyclopentadienyl hydrogen atoms with isotropic thermal parameters were included but not refined; anisotropic thermal parameters for non-hydrogen and non-disordered atoms; large thermal anisotropies and unsatisfactory distances in the dimethylphosphinoethane ligand suggested disorder; difference electron density maps were used to locate alternate atomic positions for the dimethylphosphinoethane carbon atoms; each of the carbon atoms in the ligand were placed in two positions and refined as half atoms with isotropic thermal parameters; distance restraints (Waser, 1963) imposed on disordered atoms, C-P 1.85 ± 0.02, C-C 1.54 ± 0.02, C-C(next neighbor) 3.03 ± 0.04 Å; $R = 0.035$ for 1987 reflections for which $F^2 > 2\sigma(F^2)$; $R = 0.086$ all data; $wR = 0.040$; $S = 1.0$; $w = 4F_o/[\sigma^2(F_o^2)^2+(0.06F_o^2)^2]$; max (shift/σ) < 0.04; no extinction correction; max. and min. of ΔF synthesis 2.4 and -1.2 e Å; atomic f, f' & f" for neutral U, Cℓ, P, and C, and spherical bonded H from International Tables (1974); local unpublished programs and ORTEP (Johnson, 1965).

Atomic parameters are listed in Table 1,* and distances and angles are listed in Table 2. Fig.1 shows the molecule and numbering scheme.

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*Lists of structure factors, anisotropic thermal parameters, calculated hydrogen positions, distances and angles, and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. The structure consists of a $(C_5H_5)_3U$ fragment coordinated to the phosphorus atoms at each end of the $(CH_3)_2PCH_2CH_2P(CH_3)_2$ ligand. The

phosphine ligand bridges the two $(C_5H_5)_3U$ fragments so that $(CH_3)_2PCH_2CH_2P(CH_3)_2$ acts as a monodentate ligand towards each uranium center. There are two crystallographically independent, though chemically equivalent, molecules in the unit cell across the inversion centers at (0,0,0) and (1/2,1/2,0).

The geometry of the complex is unusual since $(CH_3)_2PCH_2CH_2P(CH_3)_2$ usually acts as a bidentate ligand towards a given metal center, rather than as a bridging ligand as found in the title compound. The reason for this structural change presumably is steric, since in a hypothetical molecule, $(C_5H_5)_3U\cdot(CH_3)_2PCH_2CH_2P(CH_3)_2$ in which the phosphine acts as a bidentate ligand, the coordination number of the uranium is one greater than found in the title compound. Inspection of the ORTEP diagram in Figure 1 clearly shows that the molecule is economically packed and that increasing the coordination number by one will require a substantial reorganization of the coordination sphere about uranium so that the intramolecular ligand-ligand repulsions are minimized. The coordination geometry about each uranium atom is similar to that found in $(CH_3C_5H_4)_3U\cdot P(CH_3)_3$ (Brennan & Zalkin, 1985), in which the U-P distance is 2.972(6) A. In the title compound the averaged U-P distance is 3.022 ± 0.002 A. The other bond parameters in these two molecules also are similar. The averaged U-C($CH_3C_5H_4$) distance in $(CH_3C_5H_4)_3U\cdot P(CH_3)_3$ is 2.79 ± 0.04 A and the U-ring centroid distance is 2.52 ± 0.01 A, the (ring centroid)-U-(ring centroid) angle is 112 ± 7° and the (ring centroid)-U-P angle is 106 ± 9°. In the title complex, the averaged U-C(C_5H_5) distance is 2.77 ± 0.03 A, the U-(ring centroid) distance is 2.52 ± 0.01 A, the (ring centroid)-U-(ring centroid) angle is 118 ± 1° and the (ring centroid)-U-P angle is 98 ± 1°. Given the large uncertainty in the bond parameters and the range in individual paramters, the

coordination geometrys about the trivalent uranium atoms in $[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$ and in $(CH_3C_5H_4)_3U \cdot P(CH_3)_3$ are identical or nearly so.

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References

Brennan, J. G. (1985). Ph. D. Thesis, University of California at Berkeley.

Brennan, J. G., Zalkin, A. (1985). Acta Cryst. C41, 1038-1040.

Edwards, P. G., Andersen, R. A., Gellert, R. W. (1986) Submitted for publication.

Edwards, P. G., Andersen, R. A., Zalkin, A. (1981). J. Am. Chem. Soc. 103, 7792-7793.

Edwards, P. G., Andersen, R. A., Zalkin, A. (1984). Organometallics 3, 293-298.

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.

Waser, J. (1963) Acta Cryst. 16, 1091-1094.

Zalkin, A., Edwards, P. G., Zhang, D., Andersen, R. A. (1986). Acta Cryst. in press.

Table 1. Atomic Parameters

$B_{eq} = \Sigma_i \Sigma_j B_{ij} a_i^* a_j^* a_i \cdot a_j / 3$, A^2.

molecule 1

Atom	x	y	z	B/Beq
U(1)	-0.03723(5)	0.28914(6)	0.54961(9)	3.19
P(1)	-0.1054(4)	0.0982(4)	0.6049(7)	4.67
C(1)	0.1520(18)	0.350(3)	0.603(4)	7.85
C(2)	0.1105(21)	0.3966(17)	0.736(4)	5.76
C(3)	0.0786(16)	0.3304(28)	0.8264(27)	6.05
C(4)	0.1012(23)	0.2433(20)	0.741(4)	6.29
C(5)	0.1462(21)	0.2575(23)	0.605(4)	6.24
C(6)	0.0309(25)	0.288(4)	0.244(3)	8.27
C(7)	0.0261(27)	0.2003(28)	0.248(3)	5.95
C(8)	-0.064(3)	0.1709(20)	0.2382(27)	5.55
C(9)	-0.1162(19)	0.243(4)	0.2391(28)	7.40
C(10)	-0.054(4)	0.3199(23)	0.240(3)	6.76
C(11)	-0.153(3)	0.354(3)	0.801(4)	7.23
C(12)	-0.2067(27)	0.302(3)	0.698(7)	11.69
C(13)	-0.2138(29)	0.345(5)	0.568(5)	14.60
C(14)	-0.145(4)	0.426(3)	0.615(5)	10.00
C(15)	-0.1178(20)	0.4281(24)	0.757(6)	7.50
C(31)	-0.0226(23)	0.0081(24)	0.5841(23)	4.7(10)
C(32)	-0.2149(20)	0.041(3)	0.488(5)	5.0(12)
C(33)	-0.140(3)	0.108(3)	0.8241(26)	5.9(14)
C(31')	-0.0531(7)	-0.0060(17)	0.486(4)	3.7(9)
C(32')	-0.2332(14)	0.067(3)	0.545(5)	6.0(15)
C(33')	-0.1021(29)	0.0856(29)	0.8223(24)	3.8(10)

Table 1. Atomic Parameters(continued)

molecule 2

Atom	x	y	z	B/Beq
U(2)	0.45618(5)	0.21069(6)	0.02519(9)	3.34
P(2)	0.3991(4)	0.4051(4)	0.1139(7)	4.87
C(16)	0.5210(28)	0.1505(28)	-0.286(3)	7.48
C(17)	0.5171(22)	0.2443(24)	-0.2770(27)	5.75
C(18)	0.4277(25)	0.2602(20)	-0.2729(27)	4.97
C(19)	0.3734(19)	0.1765(23)	-0.287(3)	5.48
C(20)	0.4306(29)	0.1103(22)	-0.294(3)	6.87
C(21)	0.5700(23)	0.260(4)	0.300(4)	9.10
C(22)	0.5969(21)	0.176(4)	0.220(6)	9.20
C(23)	0.6414(23)	0.1925(27)	0.085(5)	8.48
C(24)	0.6404(16)	0.2826(26)	0.086(3)	5.60
C(25)	0.6014(23)	0.3267(23)	0.217(5)	7.04
C(26)	0.295(3)	0.2077(23)	0.205(8)	10.59
C(27)	0.2724(22)	0.150(4)	0.068(6)	9.00
C(28)	0.3096(27)	0.0762(27)	0.024(4)	7.30
C(29)	0.3649(23)	0.0727(27)	0.154(6)	8.25
C(30)	0.3524(28)	0.151(3)	0.2671(29)	8.25
C(34)	0.4905(24)	0.5015(23)	0.0905(14)	5.6(11)
C(35)	0.2916(20)	0.425(3)	0.008(5)	4.8(11)
C(36)	0.373(3)	0.433(4)	0.3377(25)	7.4(17)
C(34')	0.4473(7)	0.4971(24)	0.004(5)	5.7(12)
C(35')	0.2710(13)	0.4003(29)	0.061(5)	4.6(11)
C(36')	0.407(3)	0.465(3)	0.3361(24)	5.7(13)

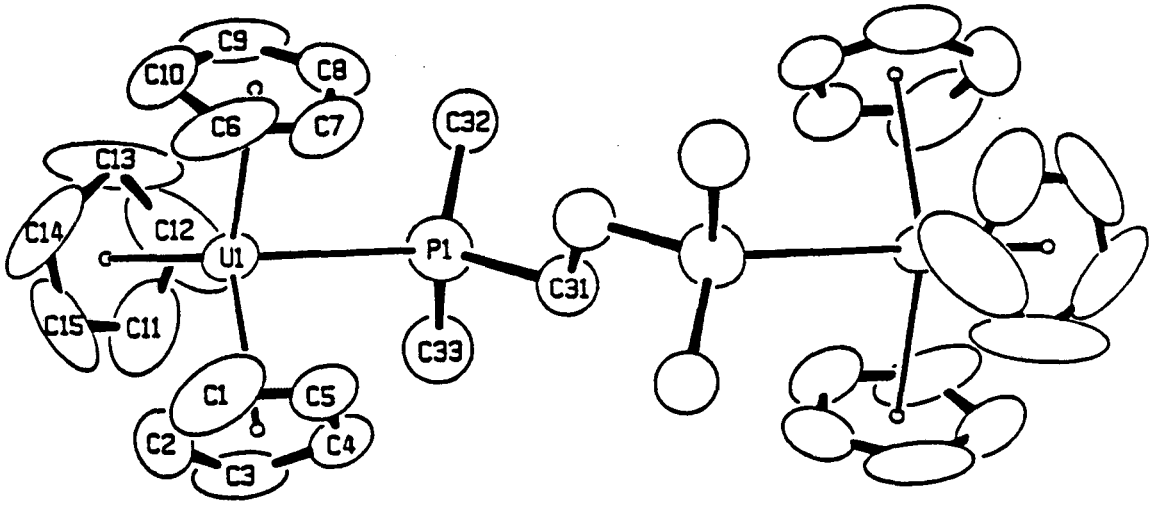
Primed atoms indicate the alternate disorder sites.

Table 2. Selected distances(Å) and angles(°)

U(1) - P(1)	3.020(06)	U(2) - P(2)	3.024(06)
U(1) - C(1)	2.784(28)	U(2) - C(16)	2.766(25)
U(1) - C(2)	2.765(25)	U(2) - C(17)	2.809(20)
U(1) - C(3)	2.774(22)	U(2) - C(18)	2.797(23)
U(1) - C(4)	2.801(25)	U(2) - C(19)	2.795(26)
U(1) - C(5)	2.803(27)	U(2) - C(20)	2.759(27)
U(1) - C(6)	2.738(25)	U(2) - C(21)	2.742(30)
U(1) - C(7)	2.787(26)	U(2) - C(22)	2.771(27)
U(1) - C(8)	2.803(24)	U(2) - C(23)	2.780(27)
U(1) - C(9)	2.752(24)	U(2) - C(24)	2.755(24)
U(1) - C(10)	2.744(23)	U(2) - C(25)	2.810(30)
U(1) - C(11)	2.768(21)	U(2) - C(26)	2.779(28)
U(1) - C(12)	2.758(33)	U(2) - C(27)	2.754(28)
U(1) - C(13)	2.772(30)	U(2) - C(28)	2.734(26)
U(1) - C(14)	2.666(27)	U(2) - C(29)	2.727(25)
U(1) - C(15)	2.758(23)	U(2) - C(30)	2.763(22)
U(1) - Cp(1)	2.527	U(2) - Cp(4)	2.533
U(1) - Cp(2)	2.516	U(2) - Cp(5)	2.523
U(1) - Cp(3)	2.505	U(2) - Cp(6)	2.506
Cp(1) - U(1) - Cp(2)	117.31	Cp(4) - U(2) - Cp(5)	119.42
Cp(1) - U(1) - Cp(3)	117.61	Cp(4) - U(2) - Cp(6)	116.12
Cp(2) - U(1) - Cp(3)	119.77	Cp(5) - U(2) - Cp(6)	119.49

[a] Cp(1), Cp(2), Cp(3), Cp(4), Cp(5) and Cp(6) represent the centroids of cyclopentadienyl atoms C(1)-C(5), C(6)-C(10), C(11)-C(15), C(16)-C(20), C(21)-C(25) and C(26)-C30) respectively.

Fig.1. ORTEP (Johnson, 1965) drawing of molecule 1; 50% probability ellipsoids.



Supplemental Material

for

Bis[tris(cyclopentadienyl)uranium(IV)][1,2-bis(dimethyldiphosphino)ethane]

$[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

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Supplemental Table 1. Anisotropic Thermal Parameters (A^2)[a]

$[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
U(1)	2.33(5)	4.36(6)	3.05(4)	0.70(4)	0.31(4)	1.04(4)
U(2)	2.55(5)	4.84(6)	2.80(4)	0.54(4)	0.45(4)	1.14(4)
P(1)	3.8(3)	5.4(4)	4.7(3)	0.60(27)	1.20(25)	0.85(27)
P(2)	3.2(3)	5.7(4)	5.4(3)	0.51(27)	0.34(25)	0.62(27)
C(1)	3.2(14)	13.3(30)	9.0(23)	1.1(17)	0.9(13)	6.6(22)
C(2)	5.6(17)	3.5(14)	7.9(18)	-1.1(12)	-1.3(14)	1.5(14)
C(3)	2.5(12)	11.3(24)	3.9(13)	0.3(15)	-0.8(10)	1.1(16)
C(4)	7.6(20)	4.8(17)	6.8(18)	-1.5(14)	-4.1(15)	2.9(15)
C(5)	6.9(19)	6.2(19)	5.8(17)	1.8(15)	-2.4(14)	1.1(15)
C(6)	6.8(22)	15.7(35)	4.2(15)	1.7(24)	0.2(13)	6.1(20)
C(7)	6.6(22)	8.3(22)	3.7(13)	3.5(19)	0.0(13)	1.7(14)
C(8)	8.6(23)	5.5(18)	2.0(11)	0.4(18)	-0.1(13)	-0.1(10)
C(9)	4.2(17)	15.5(33)	2.0(11)	2.5(22)	-0.3(11)	0.1(17)
C(10)	11.3(28)	7.4(20)	2.9(12)	3.3(21)	-0.3(15)	2.6(13)
C(11)	8.1(24)	9.0(25)	6.4(18)	6.6(21)	5.2(18)	2.5(19)
C(12)	4.8(21)	10.9(28)	14.9(36)	-5.2(20)	2.0(22)	-3.8(29)
C(13)	4.8(21)	28.5(64)	7.0(22)	11.0(31)	-3.9(19)	-8.1(31)
C(14)	14.3(36)	14.0(34)	6.1(20)	11.9(30)	4.7(21)	6.3(22)
C(15)	5.4(17)	3.7(16)	11.1(27)	0.8(14)	2.4(18)	-3.4(17)
C(16)	9.5(25)	9.7(24)	6.3(16)	6.8(22)	3.7(16)	5.4(17)
C(17)	4.8(17)	10.2(24)	2.6(11)	-1.0(16)	0.5(10)	3.1(13)
C(18)	6.9(19)	4.9(16)	2.9(11)	1.0(15)	-0.4(11)	0.4(11)
C(19)	6.4(17)	5.8(17)	5.2(14)	2.2(17)	1.1(12)	2.6(13)
C(20)	8.4(23)	7.1(21)	4.5(14)	0.1(19)	1.7(15)	0.3(13)
C(21)	5.5(21)	17.7(40)	4.5(17)	4.1(25)	-1.3(14)	2.0(21)
C(22)	1.8(15)	16.2(37)	13.1(30)	-0.4(18)	-1.6(16)	11.5(30)
C(23)	5.7(19)	6.5(21)	12.4(29)	5.3(17)	-2.8(18)	-2.1(19)
C(24)	2.6(12)	10.5(24)	3.2(13)	2.0(14)	0.2(10)	-0.1(14)
C(25)	5.5(19)	9.3(24)	6.4(20)	1.3(17)	-2.2(15)	1.5(18)
C(26)	7.0(25)	3.4(18)	20.4(44)	1.7(18)	10.0(28)	-0.1(24)
C(27)	4.1(17)	6.9(26)	16.0(37)	-1.5(19)	2.7(21)	3.7(24)
C(28)	7.7(22)	6.1(20)	6.3(17)	-4.1(17)	0.6(16)	0.2(16)
C(29)	7.2(20)	8.2(23)	12.2(27)	2.2(17)	2.6(21)	7.8(22)
C(30)	9.5(25)	10.4(26)	2.6(12)	-5.1(21)	2.9(14)	-0.1(15)

[a] The anisotropic temperature factor has the form:

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

Supplemental Table 2. Estimated Hydrogen Positional and Isotropic Thermal Parameters (A^2)[a] $[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

Atom	x	y	z	B
H(1)	0.1791	0.3842	0.5249	10.0
H(2)	0.1021	0.4635	0.7733	10.0
H(3)	0.0459	0.3353	0.9297	10.0
H(4)	0.0894	0.181	0.7649	10.0
H(5)	0.1725	0.214	0.5165	10.0
H(6)	0.0927	0.325	0.2441	10.0
H(7)	0.0742	0.1619	0.2475	10.0
H(8)	-0.0924	0.106	0.2386	10.0
H(9)	-0.1828	0.2414	0.2310	10.0
H(10)	-0.0664	0.3840	0.2433	10.0
H(11)	-0.1426	0.3284	0.9036	10.0
H(12)	-0.2512	0.2438	0.6746	10.0
H(13)	-0.2444	0.345	0.4656	10.0
H(14)	-0.1170	0.4825	0.5674	10.0
H(15)	-0.073	0.4742	0.8458	10.0
H(16)	0.5799	0.1243	-0.2853	10.0
H(17)	0.5693	0.2944	-0.2706	10.0
H(18)	0.4037	0.3206	-0.2612	10.0
H(19)	0.3059	0.1643	-0.2926	10.0
H(20)	0.4158	0.0425	-0.3063	10.0
H(21)	0.5397	0.2634	0.4027	10.0
H(22)	0.5888	0.1138	0.2413	10.0
H(23)	0.6676	0.1514	-0.0072	10.0
H(24)	0.6669	0.3167	0.0014	10.0
H(25)	0.592	0.3945	0.2586	10.0
H(26)	0.2812	0.2624	0.2703	10.0
H(27)	0.2254	0.1767	-0.0065	10.0
H(28)	0.296	0.0302	-0.0824	10.0
H(29)	0.4003	0.0166	0.1516	10.0
H(30)	0.3855	0.1654	0.3782	10.0

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

Supplemental Table 3. Additional Distances(A)

$[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

P(1)	- C(33')	1.873(17)	P(2)	- C(36')	1.874(18)
P(1)	- C(31)	1.874(17)	P(2)	- C(35)	1.874(18)
P(1)	- C(32)	1.876(18)	P(2)	- C(34)	1.874(18)
P(1)	- C(31')	1.881(17)	P(2)	- C(36)	1.876(18)
P(1)	- C(33)	1.883(18)	P(2)	- C(34')	1.877(18)
P(1)	- C(32')	1.893(18)	P(2)	- C(35')	1.894(18)
C(1)	- C(2)	1.356(36)	C(12)	- C(13)	1.387(65)
C(1)	- C(5)	1.360(39)	C(13)	- C(14)	1.444(61)
C(2)	- C(1)	1.356(36)	C(14)	- C(15)	1.249(42)
C(2)	- C(3)	1.405(33)	C(16)	- C(20)	1.367(40)
C(3)	- C(4)	1.406(34)	C(16)	- C(17)	1.383(38)
C(4)	- C(5)	1.362(35)	C(17)	- C(18)	1.342(32)
C(6)	- C(7)	1.298(43)	C(23)	- C(24)	1.336(38)
C(6)	- C(10)	1.374(40)	C(24)	- C(25)	1.314(34)
C(7)	- C(8)	1.328(39)	C(26)	- C(27)	1.287(52)
C(8)	- C(9)	1.375(38)	C(26)	- C(30)	1.420(49)
C(10)	- C(10)	1.363(39)	C(27)	- C(28)	1.261(43)
C(11)	- C(12)	1.231(45)	C(28)	- C(29)	1.364(41)
C(11)	- C(15)	1.280(39)	C(29)	- C(30)	1.355(42)
C(31)	- C(31')	0.900(33)	C(34)	- C(34')	0.943(34)
C(31)	- C(31)	1.537(19)	C(34)	- C(34)	1.534(20)
C(31')	- C(31')	1.536(19)	C(34')	- C(34')	1.521(20)
C(32)	- C(32')	0.627(57)	C(35)	- C(35')	0.682(50)
C(33)	- C(33')	0.668(52)	C(36)	- C(36')	0.641(65)
H(1)	- C(1)	0.972(00)	H(16)	- C(16)	0.977(00)
H(2)	- C(2)	0.994(00)	H(17)	- C(17)	0.988(00)
H(3)	- C(3)	0.980(00)	H(18)	- C(18)	0.982(00)
H(4)	- C(4)	0.981(00)	H(19)	- C(19)	0.972(00)
H(5)	- C(5)	0.977(00)	H(20)	- C(20)	0.985(00)
H(6)	- C(6)	0.996(00)	H(21)	- C(21)	0.961(00)
H(7)	- C(7)	0.947(00)	H(22)	- C(22)	0.971(00)
H(8)	- C(8)	0.999(00)	H(23)	- C(23)	0.978(00)
H(9)	- C(9)	0.963(00)	H(24)	- C(24)	1.006(00)
H(10)	- C(10)	0.980(00)	H(25)	- C(25)	1.013(00)
H(11)	- C(11)	1.030(00)	H(26)	- C(26)	0.915(00)
H(12)	- C(12)	1.000(00)	H(27)	- C(27)	1.085(00)
H(13)	- C(13)	0.965(00)	H(28)	- C(28)	1.001(00)
H(14)	- C(14)	1.045(00)	H(29)	- C(29)	1.023(00)
H(15)	- C(15)	1.053(00)	H(30)	- C(30)	1.015(00)

Primed labels indicate alternate disorder atoms.

Supplemental Table 4. Additional Angles (°)

$[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

C(31)	-P(1)	-C(32)	107.1(16)	C(34)	-P(2)	-C(35)	105.7(15)
C(31)	-P(1)	-C(33)	100.8(14)	C(34)	-P(2)	-C(36)	104.0(16)
C(31')	-P(1)	-C(32')	102.2(14)	C(34')	-P(2)	-C(35')	99.1(13)
C(31')	-P(1)	-C(33')	104.5(14)	C(34')	-P(2)	-C(36')	104.8(16)
C(32)	-P(1)	-C(33)	102.8(16)	C(35)	-P(2)	-C(36)	105.1(16)
C(32')	-P(1)	-C(33')	102.9(15)	C(35')	-P(2)	-C(36')	102.8(15)
C(2)	-C(1)	-C(5)	110.3(25)	C(17)	-C(16)	-C(20)	106.0(26)
C(1)	-C(2)	-C(3)	106.2(25)	C(16)	-C(17)	-C(18)	108.9(27)
C(2)	-C(3)	-C(4)	107.8(22)	C(17)	-C(18)	-C(19)	108.0(25)
C(3)	-C(4)	-C(5)	106.8(24)	C(18)	-C(19)	-C(20)	107.8(27)
C(1)	-C(5)	-C(4)	108.9(27)	C(16)	-C(20)	-C(19)	109.3(28)
C(7)	-C(6)	-C(10)	114.2(34)	C(22)	-C(21)	-C(25)	108.9(31)
C(6)	-C(7)	-C(8)	104.5(30)	C(21)	-C(22)	-C(23)	106.0(33)
C(7)	-C(8)	-C(9)	111.2(31)	C(22)	-C(23)	-C(24)	107.5(30)
C(8)	-C(9)	-C(10)	106.5(28)	C(23)	-C(24)	-C(25)	111.8(29)
C(6)	-C(10)	-C(9)	103.6(28)	C(21)	-C(25)	-C(24)	105.6(32)
C(12)	-C(11)	-C(15)	113.5(41)	C(27)	-C(26)	-C(30)	96.8(28)
C(11)	-C(12)	-C(13)	107.5(44)	C(26)	-C(27)	-C(28)	121.4(45)
C(12)	-C(13)	-C(14)	101.8(27)	C(27)	-C(28)	-C(29)	105.2(33)
C(13)	-C(14)	-C(15)	106.8(36)	C(28)	-C(29)	-C(30)	104.1(29)
C(11)	-C(15)	-C(14)	109.9(37)	C(26)	-C(30)	-C(29)	112.0(32)
P(1)	-C(31)	-C(31)	111.6(17)	P(2)	-C(34)	-C(34)	111.1(18)
P(1)	-C(31')	-C(31')	111.1(17)	P(2)	-C(34')	-C(34')	111.2(18)

Supplemental Table 5. Least-squares Planes
$[(C_5H_5)_3U]_2 \cdot (CH_3)_2PCH_2CH_2P(CH_3)_2$

Equation of plane No. 1
12.445 a - 0.625 b + 4.026 c = 4.093
Distance to the plane from atoms in the plane

atom	d(A)	σ(d)
C(1)	0.0075	(596)
C(2)	-0.0045	(457)
C(3)	0.0054	(522)
C(4)	-0.0019	(475)
C(5)	-0.0012	(452)
not in the plane		
U(1)	-2.525	(17)

Equation of plane No. 2
-0.539 a + 0.052 b + 8.165 c = 2.009
Distance to the plane from atoms in the plane

atom	d(A)	σ(d)
C(6)	-0.0160	(673)
C(7)	0.0150	(538)
C(8)	-0.0202	(608)
C(9)	0.0187	(719)
C(10)	-0.0005	(679)
not in the plane		
U(1)	2.514	(23)

Equation of plane No. 3:
-11.810 a + 7.481 b + 2.540 c =6.495
Distance to the plane from atoms in the plane

atom	d(A)	σ(d)
C(11)	-0.0049	(641)
C(12)	-0.0197	(785)
C(13)	0.0563	(954)
C(14)	-0.0314	(684)
C(15)	0.0215	(625)
not in the plane		
U(1)	-2.497	(27)

Equation of plane No. 4
-0.119 a - 1.071 b + 8.284 c = -2.604
Distance to the plane from atoms in the plane

atom	d(A)	σ(d)
C(16)	-0.0103	(525)
C(17)	-0.0135	(461)
C(18)	0.0134	(450)
C(19)	-0.0081	(442)
C(20)	0.0010	(523)
not in the plane		
U(2)	2.533	(17)

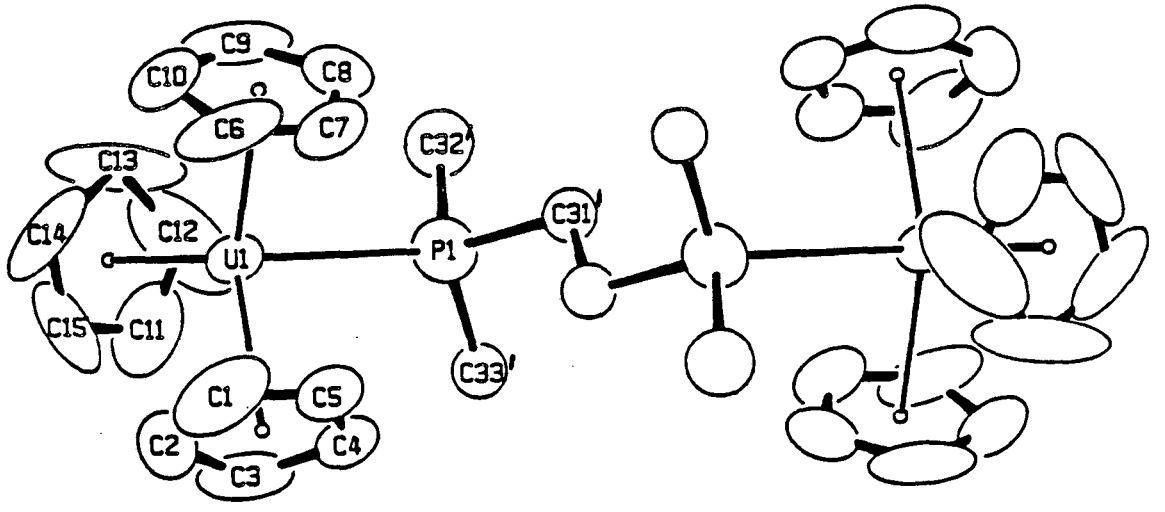
Equation of plane No. 5
12.380 a - 0.196 b + 4.001 c = 8.233
Distance to the plane from atoms in the plane

atom	d(A)	σ(d)
C(21)	-0.0265	(733)
C(22)	0.0215	(673)
C(23)	0.0104	(518)
C(24)	-0.0174	(499)
C(25)	0.0183	(520)
not in the plane		
U(2)	2.514	(23)

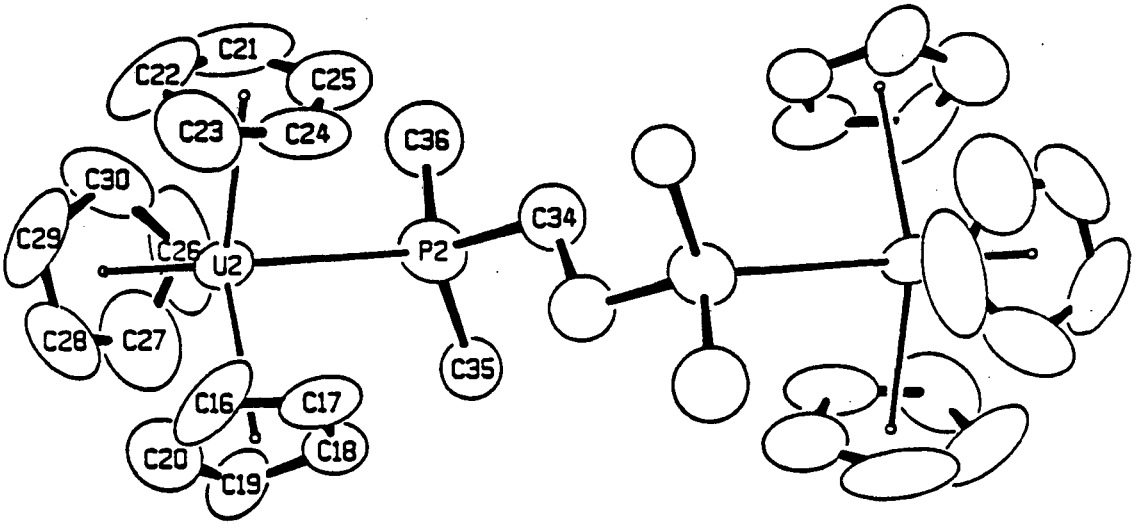
Equation of plane No. 6
10.439 a + 7.258 b - 4.193 c = 3.679
Distance to the plane from atoms in the plane

atom	d(A)	σ(d)
C(26)	0.0484	(804)
C(27)	-0.0289	(661)
C(28)	0.0058	(529)
C(29)	0.0123	(662)
C(30)	-0.0246	(662)
not in the plane		
U(2)	2.507	(23)

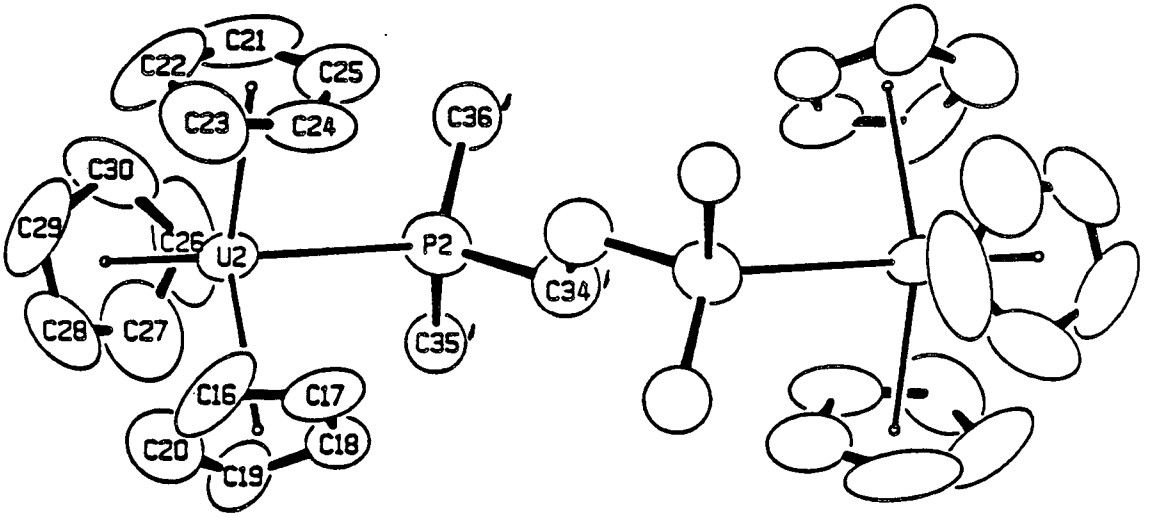
Supplemental Fig. 1. ORTEP drawing of molecule 1 using alternate disorder configuration (primed atoms); 50% probablility ellipsoids.



Supplemental Fig. 2. ORTEP drawing of molecule 2; 50% probability ellipsoids.



Supplemental Fig. 3. ORTEP drawing of molecule 2 using alternate disorder configuration (primed atoms); 50% probablility ellipsoids.



OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
(C5H5)3 U (CH2)PCH2CH2P(CH3)2 U (C5H5)3 F(0,0,0) = 2636

SG = Estimated standard deviation of Fob. DEL = /Fob/- /Fca/, where
Fob and Fca are the observed and calculated structure factors.
* indicates zero weighted data.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
H,L=	0,	0		-14	61	94	23*	6	286	12	2	2	49	65	-3*	1	867	27	24	-13	69	89	44*	2	124	8	4	-6	60	63	-6*
3	26	71	-3*	-13	30	89	-6*	7	150	13	2	3	0	75	-19*	2	422	13	6	-12	107	21	58	3	508	16	-28	-5	275	10	17
4	346	12	9	-12	97	41	-4*	8	166	14	-3	4	189	10	-11	3	469	15	-7	-11	138	30	-23	4	133	9	-5	-4	259	10	4
5	0	73	-1*	-11	156	13	-7	H,L=	0,	6		5	59	75	35*	4	390	12	0	-10	74	75	-2*	5	654	21	-19	-3	319	11	-8
6	134	11	-3	-10	194	10	12	-11	160	12	3	6	328	12	-2	5	240	9	-6	-9	280	11	5	6	183	10	-2	-2	286	10	5
7	50	74	22*	-9	310	11	-17	-10	0	71	-5*	7	48	78	11*	6	53	60	16*	-8	74	45	-3*	7	439	15	-17	-1	396	13	12
8	201	11	-8	-8	215	9	-7	-9	76	44	40*	8	401	13	-10	7	61	64	32*	-7	473	15	-29	8	54	82	17*	0	143	9	5
9	72	73	56*	-7	427	14	-12	-8	26	80	25*	9	57	80	14*	8	31	61	4*	-6	215	9	-2	9	199	13	-4	1	291	11	3
10	350	13	2	-6	360	12	-8	-7	76	44	-29*	10	267	11	7	9	152	10	6	-5	612	19	-56	10	15	92	-16*	2	148	11	-6
11	0	93	-9*	-5	411	13	-14	-6	37	73	19*	11	50	76	46*	10	79	82	3*	-4	310	11	-4	11	127	28	24	3	86	33	-17*
12	233	13	20	-4	348	11	-20	-5	292	11	0	H,L=	1,	-5		11	253	11	23	-3	723	23	-14	12	82	57	47*	4	22	80	-44*
13	63	80	54*	-3	347	11	11	-4	71	63	21*	-8	0	89	-40*	12	146	26	-6	-2	107	6	-17	H,L=	1,	3		5	63	81	18*
H,L=	0,	1		-2	0	56	-41*	-3	484	15	11	-7	175	13	3	13	193	13	7	2	102	15	-30	-14	184	14	10	6	109	32	7*
-14	35	81	11*	-1	29	46	4*	-2	26	72	2*	-6	42	74	9*	H,L=	1,	-2		3	673	29	4	-13	67	82	-14*	7	136	14	28
-13	69	89	57*	0	145	7	-1	-1	457	15	12	-5	44	80	35*	-12	67	77	36*	4	274	10	-5	-12	218	12	12	8	123	29	-1
-12	75	94	45*	1	283	9	-9	0	24	65	-8*	-4	69	54	27*	-11	46	95	14*	5	645	20	-40	-11	148	13	9	H,L=	1,	6	
-11	207	13	18	2	257	9	1	1	328	12	6	-3	248	10	-4	-10	119	20	7	6	191	10	-18	-10	213	10	-5	-11	94	18	15
-10	68	78	-4*	3	514	16	9	2	66	77	56*	-2	60	70	32*	-9	224	12	-3	7	513	16	-28	-9	101	25	-32	-10	267	11	4
-9	277	12	-9	4	431	14	-8	3	184	11	10	-1	347	12	2	-8	165	11	6	8	66	29	4*	-8	28	66	-13*	-9	185	11	5
-8	88	20	-21	5	324	11	-4	4	80	82	70*	0	75	27	38*	-7	376	13	8	9	276	11	-2	-7	47	63	-2*	-8	338	12	-8
-7	490	16	-4	6	338	12	-6	5	59	72	27*	1	431	14	-1	-6	374	12	16	10	68	86	31*	-6	225	8	-5	-7	177	10	11
-6	209	9	-7	7	243	11	-6	6	31	73	5*	2	55	67	-14*	-5	437	14	-5	11	175	14	13	-5	165	7	-4	-6	281	11	-10
-5	643	20	-30	8	146	13	1	H,L=	0,	7		3	540	17	8	-4	415	13	-18	12	97	44	62*	-4	446	14	-5	-5	70	73	-14*
-4	297	10	11	9	165	14	8	-9	40	80	27*	4	116	11	-2	-3	435	14	-15	13	70	76	53*	-3	354	11	3	-4	199	10	8
-3	670	21	0	10	77	95	-15*	-8	320	11	12	5	355	12	-6	-2	244	9	3	H,L=	1,	1		-2	637	20	11	-3	44	65	-28*
-2	90	6	-19	11	40	83	27*	-7	46	76	37*	6	65	70	44*	-1	79	17	-2	-14	228	13	15	-1	499	16	5	-2	44	71	9*
-1	56	6	-23	H,L=	0,	4		-6	251	10	1	7	46	77	-44*	0	96	8	15	-13	0	92	-4*	0	876	28	36	-1	45	73	38*
0	28	36	-8*	-13	194	12	15	-5	74	21	55	8	51	87	26*	1	33	54	13*	-12	274	13	21	1	393	12	5	0	216	10	-4
1	174	6	-13	-12	148	13	17	-4	160	11	5	9	53	55	-21*	2	118	7	19	-11	58	82	54*	2	458	14	8	1	143	11	14
2	121	10	-12	-11	203	11	9	-3	25	76	18*	10	20	81	-2*	3	274	9	-11	-10	369	13	7	3	145	9	-9	2	318	12	2
3	561	18	14	-10	84	37	-1*	-2	63	67	59*	11	201	11	3	4	338	11	-18	-9	62	83	49*	4	138	10	3	3	155	13	2
4	207	10	0	-9	103	29	-39	-1	64	80	59*	12	51	80	11*	5	313	45	-57	-8	201	10	3	5	53	65	5*	4	287	11	3
5	674	21	-29	-8	0	69	-51*	0	208	10	9	H,L=	1,	-4		6	447	14	-2	-7	55	69	43*	6	67	76	2*	5	58	85	-47*
6	174	13	-4	-7	76	18	-5	1	47	67	37*	-10	74	91	2*	7	425	14	-14	-6	195	8	-13	7	0	82	-41*	6	233	11	5
7	571	18	-11	-6	81	13	14	2	287	11	1	-9	100	20	14	8	334	11	1	-5	23	53	19*	8	191	12	4	H,L=	1,	7	
8	0	79	-36*	-5	321	11	-3	3	39	81	32*	-8	240	12	-7	9	285	11	-1	-4	400	13	3	9	150	16	22	-9	37	79	9*
9	265	11	-13	-4	374	12	1	4	257	11	14	-7	152	13	-3	10	227	11	8	-3	33	53	11*	10	231	13	7	-8	60	78	55*
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11	151	15	7	-2	556	17	9	-5	225	11	-5	-5	68	63	-13*	12	100	48	17*	-1	33	39	7*	H,L=	1,	4		-6	55	66	15*
12	41	93	-7*	-1	600	19	16	-4	89	36	3*	-4	455	15	1	13	83	92	48*	0	1218	37	36	-13	74	85	39*	-5	286	11	13
13	66	87	46*	0	449	14	-4	-3	295	11	10	-3	156	9	-17	14	74	96	29*	1	37	49	24*	-12	71	75	-35*	-4	71	73	-20*
H,L=	0,	2		1	414	13	-4	-2	51	82	-26*	-2	412	13	10	H,L=	1,	-1		2	361	12	-7	-11	171	11	3	-3	416	14	11
-14	207	14	11	2	301	10	3	H,L=	1,	-8		-1	240	9	9	-13	0	93	-80*	3	67	32	46*	-10	162	11	-9	-2	112	15	8
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-11	125	32	-16	5	0	73	-2*	4	63	75	-29*	2	148	8	7	-10	274	12	14	6	46	75	-11*	-7	340	11	-11	1	210	11	1
-10	249	11	-2	6	86	40	-9*	H,L=	1,	-7		3	148	8	-18	-9	147	15	-3	7	14	78	-16*	-8	368	12	-11	2	57	44	2*
-9	171	10	7	7	108	17	4	-4	0	88	-18*	4	422	13	-5	-8	151	12	-1	8	215	11	3	-5	324	11	-4	3	77	60	-21*
-8	78	30	9*	8	99	59	-26*	-3	94	37	-11*	5	126	9	3	-7	38	74	19*	9	61	77	54*	-4	289	10	8	H,L=	1,	8	
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-6	143	8	4	10	109	35	4*	-1	256	11	5	7	228	9	-12	-5	131	9	-1	11	79	80	76*	-2	45	51	13*	-3	15	69	11*
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-4	443	14	-4	-12	117	15	9	1	383	13	8	9	152	11	-7	-3	60	16	10	13	73	89	65*	0	69	30	-22*	H,L=	2,	-7	
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2	347	11	14	-6	379	12	-7	7	0	81	-50*	-11	182	13	12	3	113	8	13	-10	80	47	17*	6	257	11	0	1	27	79	-13*
3	195	9	9	-5	50	63	0*	8	0	83	-10*	-10	156	14	21	4	510	16	0	-9	347	12	0	7	240	12	-17	2	0	81	-4*
4	258	9	2	-4	299	10	7	9	49	68	10*	-9	203	13	-11	5	233	9	9	-8	68	37	-12*	8	105	21	-13	3	45	69	1*
5	50	66	-32*	-3	62	47	-18*	H,L=	1,	-6		-8	113	31	-24	6	24	65	-27*	-7	577	18	-24	9	133	16	15	4	158	11	14
6	0	72	-22*	-2	78	28	-20*	-6	226	11	-4	-7	120	13	23	7	45	72	-2*	-6	166	8	0	10	79	33	7*	5	80	81	-9*
7	54	37	32*	-1	78	22	39	-5	75	37	52*	-6	108	14	2	8	131	13	14	-5	623	20	-25	H,L=	1,	5		6	231	10	3
8	199	11	-14	0	181	9	-4	-4	300	11	-6	-5	90	25	4	9	225	11	15	-4	156	7	-12	-12	157	12	6	7	160	11	1
9	148	15	3	1	106	12	12	-3	41	70	18*	-4	189	8	-2	10	287	12	0	-3	369	12	-13	-11	171	11	9	8	226	11	7
10	255	13	-7	2	353	12	-7	-2	361	12	1	-3	256	9	-5	11	157	15	9	-2	102	8	29	-10	40	72	-45*	9	171	11	5
11	100	52	-23*	3	126	12	1	-1	0	78	-66*	-2	419	13	3	12	240	13	8	-1	45	49	19*	-9	72	56	-11*	H,L=	2,	-6	
12	225	12	21	4	330	12	-5	0	194	10	-12	-1	725	22	13	13	75	96	-19*	0	80	10	9	-8	47	75	35*	-6	15	73	-22*
H,L=	0,	3		5	105	32	-20*	1	55	73	18*	0	422	13	22	H,L=	1,	0		1	174	7	9	-7	134	10	1	-5	61	79	43*

STRUCTURE FACTORS continued for
(C5H5)3 U (CH2)PCH2CH2P(CH3)2 U (C5H5)3

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-4	35	81	-23*	-1	220	8	9	-10	269	12	-6	7	43	72	33*	3	298	11	-12	-5	69	79	65*	-7	205	9	-2	11	0	97	-78*
-3	184	11	0	0	144	7	-1	-9	187	12	1	8	223	12	3	4	242	11	-6	-4	82	36	3*	-6	427	14	3	12	80	89	41*
-2	137	12	19	1	107	8	11	-8	117	14	5	9	91	44	83*	5	268	12	-20	-3	268	10	-1	-5	142	8	-8	13	84	54	69*
-1	322	11	-1	2	190	7	-11	-7	62	75	3*	10	318	13	10	6	183	13	8	-2	135	11	4	-4	524	16	0	H,L=	3,	1	
0	141	11	0	3	216	8	10	-8	58	65	38*	11	36	89	26*	7	212	12	-1	-1	326	11	-1	-3	273	9	3	-14	215	13	18
1	386	14	-14	4	446	14	-6	-5	227	9	7	12	232	12	10	8	38	81	-45*	0	63	46	-6*	-2	359	11	-8	-13	94	54	-11*
2	208	9	4	5	141	8	-7	-6	523	16	21	H,L=	2,	3		H,L=	2,	6		1	392	13	9	-1	143	7	-5	-12	263	13	12
3	435	14	4	6	457	14	-12	-3	102	8	13	-14	0	94	-18*	-11	126	14	-6	2	165	9	3	0	77	13	18	-11	136	32	-5
4	170	10	-10	7	222	9	-2	-2	869	27	17	-13	13	89	-19*	-10	64	70	7*	3	508	16	8	1	104	7	2	-10	263	12	8
5	295	11	0	8	414	14	-2	-1	581	18	37	-12	38	86	-8*	-9	58	81	24*	4	177	9	-9	2	230	8	10	-9	172	13	-3
6	23	80	-35*	9	164	11	-18	0	1013	31	66	-11	240	11	-6	-8	46	68	2*	5	285	10	-7	3	281	9	13	-8	73	40	-14*
7	78	46	3*	10	264	11	-11	1	532	17	22	-10	0	79	-30*	-7	96	32	-12*	6	26	75	-20*	4	529	17	-6	-7	94	12	-1
8	45	81	44*	11	94	56	27*	2	592	19	7	-9	391	13	-17	-6	123	13	-3	7	41	75	2*	5	121	9	-6	-6	107	9	8
9	5	54	-33*	12	101	41	3*	3	59	75	22*	-8	0	67	-70*	-5	222	10	8	8	28	78	26*	6	643	20	-15	-5	181	7	4
10	36	80	-3*	13	48	80	24*	4	364	12	-7	-7	611	19	-28	-4	262	10	0	9	92	19	9	7	186	9	6	-4	440	14	9
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-8	212	12	-1	-11	235	12	23	7	33	78	5*	-4	87	33	-16*	-1	360	12	9	12	115	16	21	10	256	12	0	-1	674	21	4
-7	49	75	22*	-10	126	17	1	8	138	14	-5	-3	282	9	-12	0	181	10	6	H,L=	3,	-4		11	47	96	9*	0	385	12	11
-6	314	12	2	-9	237	11	21	9	193	11	8	-2	32	47	17*	1	239	11	-10	-10	53	89	-25*	12	102	64	32*	1	569	18	-21
-5	76	42	40*	-8	113	15	1	10	274	12	6	-1	64	28	-20*	2	163	12	2	-9	69	75	23*	13	0	97	-3*	2	309	11	-11
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-1	56	60	-16*	-4	251	9	3	H,L=	2,	1		3	473	15	-11	6	91	46	2*	-5	50	73	-3*	-11	265	13	19	6	46	51	43*
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1	58	63	47*	-2	330	11	-6	-13	51	93	27*	5	483	16	-5	-8	183	12	6	-3	58	60	8*	-9	209	11	5	8	165	13	-14
2	147	9	8	-1	391	18	10	-12	70	98	8*	6	146	12	7	-8	287	11	4	-2	426	14	-10	-8	98	26	18	9	156	14	2
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4	250	9	-6	1	540	17	13	-10	121	32	7	8	52	81	12*	-6	233	10	5	0	145	8	-2	-6	119	9	9	11	154	15	10
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6	418	14	-11	3	488	15	32	-8	138	12	9	10	72	94	27*	-4	78	84	-43*	2	232	9	-2	-4	317	10	13	H,L=	3,	2	
7	24	74	-23*	4	375	12	-10	-7	513	16	-14	11	0	92	-42*	-3	58	78	14*	3	65	15	19	-3	526	17	31	-14	0	94	-6*
8	476	15	-12	5	262	9	-10	-6	228	8	0	H,L=	2,	4		-2	76	78	57*	4	320	11	6	-2	581	18	21	-13	40	84	5*
9	73	74	-10*	6	68	16	7	-5	620	19	-34	-13	75	51	1*	-1	64	78	17*	5	75	27	8*	-1	374	12	15	-12	89	52	31*
10	278	11	0	7	14	68	-28*	-4	228	9	-5	-12	213	11	0	0	172	11	7	6	394	13	-10	0	431	14	29	-11	218	11	-7
11	0	74	-49*	8	51	71	10*	-3	478	15	13	-11	98	19	-33	1	117	29	-19	7	40	72	-6*	1	388	12	26	-10	79	38	-2*
12	98	55	-17*	9	173	11	-5	-2	103	8	5	-10	183	11	-7	2	230	11	0	8	436	14	-9	2	610	19	30	-9	364	12	-6
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-8	0	88	-36*	13	183	14	4	2	144	13	-8	-6	187	9	-8	-2	154	11	14	12	66	84	-8*	6	89	29	-5*	-5	617	19	-25
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6	46	64	20*	-1	158	6	25	-12	255	12	18	8	172	14	9	-4	264	11	-2	1	723	22	7	-8	341	12	-16	9	145	16	-8
7	22	70	-4*	0	0	40	-19*	-11	41	58	35*	9	127	17	14	-3	195	10	-1	2	55	30	14*	-7	407	13	-14	10	66	91	29*
8	0	76	-18*	1	139	6	24	-10	325	12	-9	10	191	14	17	-2	275	11	-6	3	657	21	-1	-6	545	17	-7	11	22	92	-53*
9	119	14	-11	2	76	19	3	-9	23	74	4*	H,L=	2,	5		-1	176	10	-6	4	72	12	18	-5	361	12	5	H,L=	3,	3	
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12	78	40	67*	5	361	12	-1	-6	255	9	-21	-10	185	11	-1	2	58	73	14*	7	63	45	9*	-2	72	27	7*	-12	250	11	7
13	267	12	23	6	505	16	-12	-5	45	53	20*	-9	281	11	-7	3	95	28	13*	8	67	72	56*	-1	66	16	25	-11	24	56	12*
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-11	57	90	42*	8	307	12	13	-3	35	48	4*	-7	272	10	-15	5	149	10	16	10	52	84	47*	1	80	29	28*	-9	73	36	68*
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-7	172	11	-5	12	55	98	-13*	1	63	37	45*	-3	176	9	8	9	177	12	-17	H,L=	3,	-2		5	411	14	-8	-5	67	35	39*
-6	426	14	9	13	0	90	-27*	2	527	16	36	-2	35	69	8*	10	209	11	-1	-12	86	45	79*	6	386	13	-9	-4	507	16	-13
-5	132	10	7	H,L=	2,	0		3	29	63	19*	-1	20	68	2*	H,L=	3,	-5		-11	51	94	29*	7	403	14	-2	-3	41	59	1*
-4	527	17	-11	-13	0	96	-93*	4	222	9	-18	0	116	11	4	-8	99	30	33*	-10	178	13	-1	8	163	13	-9	-2	742	23	12
-3	253	9	-3	-12	242	12	9	5	44	68	38*	1	263	10	-10	-7	144	24	-7	-9	119	15	17	9	258	11	-2	-1	29	54	-11*
-2	445	14	0	-11	129	32	1	6	47	74	2*	2	185	10	3	-6	88	38	35*	-8	345	12	6	10	147	15	24	0	809	25	-10

STRUCTURE FACTORS continued for
(C5H5)3 U (CH2)PCH2CH2P(CH3)2 U (C5H5)3

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
1	0	63	-25*	6	136	28	5	-3	341	11	-3	-8	448	15	9	10	118	18	13	5	30	74	10*	1	62	64	30*	10	94	41	21*
2	467	15	2	H,L=	3,	7		-2	171	9	-1	-7	181	9	6	11	38	79	-11*	6	84	53	39*	2	36	66	30*	11	170	15	-19
3	20	69	-8*	-9	87	79	54*	-1	391	13	0	-6	623	20	-8	12	63	77	48*	7	72	81	49*	3	138	13	-17	12	106	21	26
4	141	11	-9	-8	50	78	-1*	0	142	9	6	-5	115	8	-3	H,L=	4,	2		8	200	14	0	4	143	12	-10	H,L=	5,	-2	
5	60	77	58*	-7	125	13	14	1	471	15	2	-4	591	19	-14	-14	189	14	15	9	69	93	55*	5	252	11	-10	-12	58	80	29*
6	74	81	42*	-6	122	14	-3	2	245	9	3	-3	311	10	5	-13	90	58	-6*	H,L=	4,	5		6	191	11	2	-11	0	91	-35*
7	46	88	28*	-5	224	10	2	3	478	15	0	-2	296	10	7	-12	226	12	11	-12	44	82	13*	7	306	11	1	-10	182	12	5
8	222	13	22	-4	240	11	4	4	210	9	5	-1	152	7	1	-11	158	12	15	-11	244	11	9	8	110	29	-29	-9	57	82	4*
9	44	85	29*	-3	283	11	6	5	210	9	5	0	45	57	42*	-10	221	10	-7	-10	77	22	22	9	227	11	-6	-8	385	13	-3
10	242	13	2	-2	258	11	1	6	46	61	30*	1	143	8	-10	-8	131	11	3	-9	294	11	-5	H,L=	5,	-5		-7	42	65	-3*
H,L=	3,	4		-1	244	11	0	7	0	77	-18*	2	310	10	18	-8	69	17	19	-8	66	69	17*	-8	130	15	6	-6	421	14	-8
-13	79	58	-9*	0	156	12	-12	8	74	48	35*	3	296	10	11	-7	81	24	1*	-7	379	13	-8	-7	54	83	-10*	-5	140	9	0
-12	31	73	-5*	1	182	11	22	9	101	33	-21*	4	554	17	-12	-6	203	8	-5	-8	79	50	-12*	-6	70	77	-23*	-4	519	16	-12
-11	278	11	-7	2	124	15	-1	10	64	86	-9*	5	93	14	-32	-5	181	10	-10	-5	363	12	-13	-5	81	63	65*	-3	144	8	9
-10	36	73	10*	3	54	86	6*	11	201	12	1	6	530	17	3	-4	423	13	10	-4	41	65	-19*	-4	135	12	14	-2	492	15	7
-9	340	12	-7	H,L=	4,	-7		12	83	27	-2*	7	197	11	0	-3	435	14	29	-3	101	13	4	-3	88	38	-7*	-1	0	55	-7*
-8	56	72	-20*	-3	241	11	-6	H,L=	4,	-3		8	369	13	6	-2	609	19	27	-2	69	40	6*	-2	264	10	-4	0	53	17	10*
-7	424	14	-18	-2	101	30	-1*	-11	73	88	60*	9	143	15	19	-1	574	18	13	-1	69	70	-61*	-1	266	10	-9	1	56	28	43*
-6	140	9	-4	-1	196	11	-8	-10	123	31	-21	10	213	12	11	0	837	26	25	0	52	64	43*	0	310	11	11	2	450	14	17
-5	426	14	-2	0	84	38	18*	-9	31	88	-50*	11	56	96	47*	1	440	15	-4	1	262	10	-3	1	354	12	-2	3	111	10	-3
-4	59	43	4*	1	51	77	3*	-8	374	13	-3	12	0	81	-31*	2	417	13	-9	2	55	79	44*	2	408	13	9	4	582	18	6
-3	155	9	-9	2	24	77	14*	-7	51	76	-18*	13	85	91	84*	3	188	9	-1	3	379	13	-8	3	229	9	-3	5	184	9	-3
-2	36	64	-22*	3	86	18	-2	-6	398	13	-15	H,L=	4,	0		4	101	28	-7	4	71	33	-18*	4	344	12	7	6	500	16	-13
-1	125	9	6	4	95	34	6*	-5	62	50	-10*	-13	194	13	9	5	48	70	0*	5	341	13	-4	5	126	12	-17	7	63	75	-7*
0	25	64	13*	5	197	11	-4	-4	396	13	-7	-12	194	13	8	6	15	86	-22*	6	90	45	51*	6	87	18	2	8	435	14	-5
1	237	9	-8	6	148	12	12	-3	101	10	7	-11	282	12	12	7	60	77	2*	7	166	15	-11	7	0	79	-27*	9	79	86	40*
2	60	61	47*	7	260	11	-2	-2	462	15	-6	-10	115	36	-20*	8	165	14	5	H,L=	4,	6		8	46	81	25*	10	187	14	-14
3	417	14	-11	H,L=	4,	-6		-1	44	55	10*	-9	186	11	-5	9	158	15	4	-11	62	72	13*	9	60	75	-17*	11	24	94	-14*
4	113	14	-9	-6	59	85	-35*	0	111	8	-3	-8	59	75	-18*	10	215	13	8	-10	101	17	8	10	101	30	-5*	12	0	96	-44*
5	449	15	-16	-5	70	78	55*	1	20	56	-3*	-7	66	32	51*	11	139	16	10	-9	43	80	22*	11	143	14	18	H,L=	5,	-1	
6	60	79	-6*	-4	71	80	16*	2	331	11	4	-6	114	9	7	H,L=	4,	3		-8	53	80	-5*	H,L=	5,	-4		-13	264	13	36
7	278	12	-1	-3	68	70	-7*	3	83	20	2	-5	257	9	-3	-13	52	83	1*	-7	56	80	-22*	-9	135	14	16	-12	0	92	-26*
8	49	91	24*	-2	191	11	-1	4	444	14	-2	-4	354	11	-6	-12	69	75	19*	-6	242	10	3	-8	228	11	5	-11	292	12	22
9	136	17	7	-1	233	10	1	5	153	9	-3	-3	507	16	23	-11	256	11	-1	-5	18	82	-106*	-7	249	11	1	-10	59	74	54*
H,L=	3,	5		0	255	10	2	6	469	15	-12	-2	410	13	14	-10	43	79	-32*	-4	376	13	3	-6	326	12	-7	-9	228	10	13
-12	183	12	-7	1	298	11	-4	7	86	26	19*	-1	572	18	30	-9	367	12	-6	-3	131	12	14	-5	205	10	-2	-8	83	72	23*
-11	104	28	1	2	344	12	9	8	477	15	-5	0	154	9	29	-8	139	10	6	-2	405	14	-5	-4	311	11	-18	-7	132	10	7
-10	139	13	1	3	248	10	14	9	10	72	-4*	1	626	20	19	-7	509	16	-17	-1	198	11	5	-3	239	9	-4	-6	14	65	1*
-9	47	76	-8*	4	314	11	5	10	240	11	-3	2	334	11	1	-6	226	9	2	0	311	12	-7	-2	274	10	2	-5	201	8	-3
-8	76	35	65*	5	194	10	6	11	92	72	74*	3	374	12	11	-5	494	16	-2	1	138	13	8	-1	200	9	2	-4	43	58	8*
-7	84	17	-3	6	80	43	-19*	12	23	81	-16*	4	270	10	8	-4	99	11	-9	2	191	11	9	0	88	21	11	-3	730	23	8
-6	214	9	14	7	66	79	-7*	H,L=	4,	-2		5	129	12	-6	-3	229	9	-8	3	0	76	-12*	1	34	58	-27*	-2	49	57	38*
-5	147	10	-1	8	48	79	37*	-12	0	93	-6*	6	58	79	-4*	-2	0	60	-7*	4	0	85	-10*	2	165	8	6	-1	798	25	43
-4	384	13	5	9	66	81	11*	-11	269	12	5	7	31	80	-23*	-1	65	68	-34*	5	0	86	-10*	3	192	9	-1	0	108	9	16
-3	39	72	-30*	10	61	73	-21*	-10	31	77	17*	8	92	41	-7*	0	56	63	28*	H,L=	4,	7		4	221	9	-4	1	794	25	50
-2	449	14	3	H,L=	4,	-5		-9	217	11	14	9	232	12	3	1	266	10	-11	-8	150	12	5	5	176	9	-2	2	63	52	41*
-1	203	9	7	-8	158	12	16	-8	50	77	25*	10	113	38	9*	2	51	72	-9*	-7	225	11	8	6	287	11	-13	3	612	19	12
0	365	12	6	-7	166	12	-13	-7	166	10	15	11	233	12	14	3	411	14	-23	-6	165	11	1	7	266	10	-5	4	47	59	18*
1	153	11	5	-6	270	11	1	-6	0	76	-21*	12	121	32	-5	4	160	11	-16	-5	134	13	5	8	317	12	-4	5	104	14	5
2	252	10	-1	-5	181	11	3	-5	53	56	-26*	H,L=	4,	1		5	446	15	-19	-4	80	22	12	9	205	12	-9	6	18	68	-18*
3	0	83	-19*	-4	333	12	-10	-4	45	60	15*	-14	65	83	52*	6	149	14	8	-3	52	82	17*	10	167	12	-3	7	157	12	15
4	55	72	14*	-3	212	10	-6	-3	572	18	2	-13	49	86	29*	7	266	12	-10	-2	38	79	-16*	11	62	88	-2*	8	78	84	65*
5	72	86	66*	-2	278	10	-4	-2	46	49	27*	-12	134	19	1	8	63	64	4*	-1	88	41	5*	H,L=	5,	-3		9	190	13	-7
6	104	39	-7*	-1	178	9	-4	-1	750	23	23	-11	147	16	12	9	133	31	-6	0	113	15	4	-11	213	12	9	10	77	93	48*
7	60	87	36*	0	90	26	-11	0	126	7	15	-10	217	13	-12	10	0	82	-37*	1	187	11	12	-10	112	16	32	11	259	13	9
8	174	14	18	1	36	69	10*	1	795	25	44	-9	272	11	-8	H,L=	4,	4		2	133	27	-7	-9	181	12	-6	12	0	82	-7*
H,L=	3,	6		2	79	16	-13	2	11	55	-4*	-8	274	10	-4	-13	60	82	42*	H,L=	5,	-7		-8	0	81	-56*	H,L=	5,	0	
-11	141	14	-9	3	114	12	-10	3	755	23	14	-7	416	13	-10	-12	233	11	-2	-2	176	11	14	-7	149	11	6	-13	88	91	84*
-10	180	11	-1	4	234	9	-11	4	53	59	25*	-6	414	13	3	-11	55	81	53*	-1	40	69	-21*	-6	41	66	-10*	-12	86	67	24*
-9	278	11	-5	5	141	11	-9	5	226	9	-6	-5	407	13	-4	-10	206	11	12	0	295	11	6	-5	74	30	1*	-11	57	95	14*
-8	163	12	-23	6	323	11	-9	6	36	68	13*	-4	350	12	-13	-9	50	75	39*	1	72	80	-6*	-4	113	11	-6	-10	274	12	8
-7	319	11	3	7	271	10	-6	7	110	13	9	-3	283	10	6	-8	66	70	61*	2	331	12	6	-3	347	11	-3	-9	161	11	0
-6	212	10	-5	8	298	11	-10	8	25	80	-12*	-2	106	12	13	-7	46	68	29*	3	0	79	-19*	-2	261	9	-7	-8	492	16	13
-5	201	10	-4	9	209	11	-7	9	210	11	10	-1	67	71	47*	-6	251	9	0	4	270	11	7	-1	493	15	10	-7	184	8	11
-4	113	14	-14	10	200	11	-6	10	77	30	74*	0	136	14	18	-5	37	58	10*	5	0	84	-42*	0	301	10	18	-6	579	18	-11
-3	58	75	-47*	11	99	18	10	11	273	12	18	1	100	14	-3	-4	429	14	0	8	159	11	13	1	581	18	13	-5	110	10	3
-2	62	67	21*	H,L=	4,	-4		12	39	95	17*	2	308	11	8	-3	40	68	-13*	H,L=	5,	-6		2	288	10	-4	-4	514	16	-15
-1	81	38	17*	-10	69	87	8*	13	234	13	15	3	445	14	-20	-2	530	17	-11	-6	97	35	-18*	3	487	15	1	-3	250	9	19
0	105	30	-23	-9	162	13	-14	H,L=	4,	-1		4	440	26	-40	-1	48	61	22*	-5	219	11	-16	4	188	9	1	-2	229	9	3
1	255	11	-3	-8	88	21	29	-13	30	64	-1*	5	362	12	-23	0	564	18	-5	-4	147	12	-4	5	257	10	-6	-1	77	29	-19*
2	169	12	-5	-7	151	13	-12	-12	73	36	43*	6	395	13	-8	1	0	72	-28*	-3	296	11	1	6	45	71	32*	0	80	29	13*
3	253	11	2	-6	72	77	21*	-11	46	94	39*	7	271	11	-2	2	293	11	1	-2	24	80	-75*	7	68	74	39*	1	152	9	3
4	194	12	-6	-5	41	72	2*	-10	210	12	-2	8	174	12	2	3	0	79	-40*	-1	216	10	-10	8	64	71	14*	2	385	13	-6
5	197	12	8	-4	86	16	-22	-9	160	12	8	9	183	13	0	4	63	84	-15*	0	0	78	-51*	9	153	13	0	3	230	10	4

STRUCTURE FACTORS continued for
(C5H5)3 U (CH2)PCH2CH2P(CH3)2 U (C5H5)3

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
4	554	18	-7	-1	290	10	-6	-7	48	81	-27*	-10	123	15	13	-13	243	13	17	9	216	12	8	-4	296	11	0	-6	58	68	30*
5	115	15	-3	0	596	19	5	-6	176	11	0	-9	174	11	23	-12	63	91	37*	10	64	84	-25*	-3	41	82	-9*	-5	62	64	-8*
6	412	14	-13	1	240	10	2	-5	80	83	-26*	-8	222	11	-11	-11	266	12	5	H,L=	6,	3		-2	372	13	7	-4	243	10	-3
7	181	12	-11	2	260	10	-23	-4	256	11	3	-7	252	10	-5	-10	37	73	31*	-13	53	75	26*	-1	0	87	-36*	-3	201	9	-5
8	333	12	1	3	16	73	-50*	-3	76	62	-33*	-6	292	11	-7	-9	178	10	2	-12	134	13	8	0	337	12	18	-2	318	11	0
9	100	61	-4*	4	62	83	-9*	-2	288	11	8	-5	199	9	-2	-8	53	62	20*	-11	141	14	-5	1	24	84	6*	-1	339	11	7
10	150	30	-17	5	55	75	36*	-1	133	27	0	-4	289	10	-7	-7	73	19	-10	-10	210	11	-7	2	107	31	-10	0	352	12	10
11	44	82	37*	6	72	90	31*	0	212	11	7	-3	280	10	-7	-6	24	67	-8*	-9	246	11	-14	3	79	80	68*	1	380	12	22
12	0	85	-14*	7	28112		-49*	1	104	32	20*	-2	288	10	-3	-5	219	9	-2	-8	271	11	-7	4	87	86	29*	2	327	11	0
H,L=	5,	1		8	171	15	13	H,L=	6,	-7		-1	180	8	2	-4	55	25	30*	-7	242	10	-6	H,L=	6,	7		3	318	11	7
-13	198	14	7	9	148	18	-1	-1	163	12	4	0	37	55	-14*	-3	648	20	8	-8	394	13	-2	-6	54	70	11*	4	275	10	-4
-12	153	17	-4	10	183	14	24	0	38	70	16*	1	93	11	-7	-2	67	48	61*	-5	229	10	-15	-5	176	12	5	5	165	11	-11
-11	245	13	16	H,L=	5,	4		1	51	70	-10*	2	215	9	0	-1	749	23	36	-4	280	10	8	-4	0	72	-8*	6	62	75	12*
-10	112	20	-1	-13	133	13	27	2	35	76	15*	3	277	10	18	0	120	11	17	-3	207	10	5	-3	0	86	-15*	7	37	79	25*
-9	139	12	-10	-12	11	75	-70*	3	106	15	9	4	277	10	-8	1	703	22	31	-2	33	62	19*	-2	22	85	-2*	8	77	66	-3*
-8	78	17	-3	-11	245	11	-6	4	0	82	-10*	5	190	9	-9	2	89	16	12	-1	46	64	30*	-1	104	29	-1	9	138	15	17
-7	59	74	26*	-10	90	35	-16*	5	238	11	7	6	382	13	-8	3	477	15	0	0	103	26	1	0	0	84	-30*	10	129	17	-6
-6	70	74	60*	-9	280	11	-9	H,L=	6,	-6		7	258	11	-9	4	79	24	-24*	1	222	10	-17	H,L=	7,	-6		11	112	41	-14*
-5	241	10	-4	-8	106	14	-19	-5	87	35	70*	8	341	12	-16	5	77	48	-20*	2	191	11	-8	-4	54	80	51*	H,L=	7,	-2	
-4	373	13	6	-7	383	12	-4	-4	92	33	41*	9	217	12	0	6	80	82	25*	3	256	11	-8	-3	272	11	-2	-11	63	86	6*
-3	475	15	-6	-6	176	10	0	-3	82	32	74*	10	153	14	11	7	156	13	16	4	322	12	-21	-2	63	79	9*	-10	102	33	7*
-2	357	12	-4	-5	390	13	-3	-2	212	10	2	11	61	80	-1*	8	67	89	61*	5	267	12	-3	-1	165	11	0	-9	203	11	0
-1	874	37	5	-4	62	64	-28*	-1	71	26	5*	H,L=	6,	-2		9	203	14	-15	6	248	13	-1	0	30	73	14*	-8	290	11	-2
0	388	13	22	-3	114	12	-11	0	411	14	15	-11	212	11	18	10	53	82	29*	7	237	13	11	1	58	70	11*	-7	264	10	5
1	755	40	-8	-2	48	69	3*	1	91	33	-9*	-10	0	87	-66*	11	246	12	11	8	99	45	-10*	2	45	71	16*	-6	373	12	-8
2	359	12	-11	-1	133	10	5	2	403	13	8	-8	175	11	-6	H,L=	6,	1		9	106	37	22*	3	172	10	18	-5	184	10	-17
3	280	10	4	0	47	72	19*	3	60	71	6*	-8	50	69	7*	-13	0	93	-18*	H,L=	6,	4		4	82	49	67*	-6	323	11	2
4	166	11	-9	1	232	10	10	4	303	11	4	-7	118	12	4	-12	70	88	-26*	-12	168	12	2	5	287	11	-1	-3	282	10	-5
5	91	34	-9*	2	68	58	-6*	5	44	71	-29*	-6	34	61	-5*	-11	21	87	9*	-11	116	15	20	6	55	70	51*	-2	267	10	6
6	73	26	7*	3	403	14	-8	6	103	35	-35*	-5	195	9	1	-10	257	11	-14	-10	153	12	22	7	297	11	6	-1	150	8	14
7	79	53	6*	4	154	13	-13	7	5	81	-30*	-4	135	9	4	-9	121	19	-19	-9	79	39	24*	H,L=	7,	-5		0	0	65	-4*
8	119	31	18	5	422	14	-11	8	67	70	50*	-3	459	15	7	-8	373	13	-7	-8	43	80	37*	-7	47	82	37*	1	146	9	9
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10	79	82	-32*	7	224	13	2	-7	217	11	-7	-1	645	20	32	-6	430	14	-18	-6	191	10	3	-5	41	80	14*	3	275	10	3
11	158	28	-32	8	62	95	11*	-6	174	11	7	0	283	10	28	-5	81	52	-17*	-5	191	10	-7	-4	141	12	11	4	269	10	1
H,L=	5,	2		H,L=	5,	5		-5	282	11	-14	1	659	21	36	-4	480	16	-14	-4	332	11	9	-3	56	80	40*	5	192	10	-5
-13	65	87	50*	-12	177	12	-10	-4	194	11	-7	2	283	10	4	-3	168	11	-5	-3	172	10	10	-2	299	11	-6	6	324	12	1
-12	144	14	21	-11	0	83	-7*	-3	335	13	-9	3	482	15	4	-2	182	11	-4	-2	406	14	2	-1	123	13	2	7	273	12	4
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-10	179	11	-11	-9	56	81	50*	-1	221	10	-6	5	210	10	6	0	140	12	2	0	373	13	6	1	155	11	20	9	193	14	9
-9	298	11	-13	-8	75	44	60*	0	63	63	19*	6	74	44	45*	1	213	10	2	1	207	11	-5	2	461	15	10	10	117	21	-17
-8	235	9	3	-7	77	56	68*	1	25	71	16*	7	105	29	19	2	416	30	-9	2	217	11	-4	3	70	74	52*	11	99	57	56*
-7	381	12	6	-6	315	11	-9	2	75	50	56*	8	86	50	32*	3	159	12	-20	3	33	87	12*	4	323	12	4	H,L=	7,	-1	
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-5	383	12	-1	-4	410	13	7	4	157	11	-18	10	110	22	17	5	75	80	22*	5	62	91	58*	6	125	13	15	-11	202	11	15
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-3	319	11	10	-2	475	15	8	6	160	12	0	12	71	97	-60*	7	127	18	-5	7	56	94	-2*	8	48	84	-3*	-9	174	11	5
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-1	71	29	41*	0	484	16	12	8	79	51	-8*	-12	56	87	43*	9	68	94	-14*	H,L=	6,	5		H,L=	7,	-4		-7	59	73	1*
0	123	11	-15	1	34	81	14*	9	250	11	0	-11	58	86	29*	10	117	36	7*	-11	201	11	3	-9	129	16	-21	-6	57	70	50*
1	284	10	-7	2	207	11	2	10	79	59	-13*	-10	205	11	-1	11	59	89	46*	-10	72	73	-37*	-8	102	16	20	-5	251	10	13
2	251	10	-4	3	38	75	17*	H,L=	6,	-4		-9	62	68	24*	H,L=	6,	2		-9	289	11	0	-7	280	11	-14	-4	191	9	2
3	364	13	-19	4	77	27	69*	-9	122	30	-32	-8	470	15	-3	-13	197	12	6	-8	114	15	8	-6	129	27	-15	-3	459	15	5
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5	235	11	-15	6	58	82	-4*	-7	0	84	-70*	-6	498	16	-17	-11	200	11	-2	-6	131	13	-10	-4	142	23	-42	-1	569	18	21
6	322	12	-16	7	59	92	42*	-6	86	35	22*	-5	194	8	0	-10	87	38	-12*	-5	337	12	-9	-3	333	11	-20	0	340	11	25
7	211	12	4	H,L=	5,	6		-5	30	77	-9*	-4	555	17	1	-9	137	12	-9	-4	79	21	4	-2	59	72	-14*	1	506	16	27
8	145	16	0	-10	65	77	19*	-4	210	10	-3	-3	120	9	3	-8	68	69	10*	-3	78	45	12*	-1	220	9	3	2	300	11	0
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H,L=	5,	3		-6	80	45	16*	0	403	13	16	1	43	61	33*	-4	321	11	12	1	238	11	10	3	241	10	-4	6	67	85	23*
-13	110	17	6	-5	276	11	-8	1	358	12	8	2	478	15	8	-3	473	15	9	2	68	79	-38*	4	184	10	1	7	101	63	-4*
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-11	132	15	-11	-3	86	34	34*	3	222	9	1	4	435	14	6	-1	682	21	28	4	106	40	-15*	6	208	11	-9	9	158	16	9
-10	156	12	-20	-2	65	70	27*	4	320	11	5	5	116	26	-17	0	416	14	8	5	256	13	-16	7	396	13	1	10	118	19	17
-9	92	17	-1	-1	136	13	10	5	133	11	-2	6	389	13	-12	1	461	15	-19	6	16	97	-59*	8	91	44	-10*	11	165	28	-29
-8	82	30	68*	0	62	83	36*	6	63	67	-3*	7	0	89	-55*	2	249	11	-11	H,L=	6,	6		9	281	12	-10	H,L=	7,	0	
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-6	172	9	-3	2	80	24	54*	8	68	85	15*	9	51	93	-18*	4	90	52	0*	-9	60	80	57*	H,L=	7,	-3		-11	71	73	26*
-5	223	9	-5	3	257	11	-2	9	91	22	-4	10	169	15	1	5	52	83	37*	-8	0	73	-52*	-10	137	14	4	-10	235	10	0
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-3	257	10	1	H,L=	5,	7		11	102	44	-26*	12	79	81	59*	7	76	85	-31*	-6	270	11	11	-8	140	13	9	-8	441	14	-10
-2	586	18	11	-8	64	83	10*	H,L=	6,	-3		H,L=	6,	0		8	46	84	-40*	-5	73	53	37*	-7	70	24	2*	-7	68	75	-17*

STRUCTURE FACTORS continued for
(C5H5)3 U (CH2)PCH2CH2P(CH3)2 U (C5H5)3 page 5

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-6	401	13	-7	-6	85	72	32*	3	44	82	-27*	3	236	10	5	6	379	14	-4	-4	113	33	-17*	7	0	78	-15*	-6	51	97	-11*
-5	154	10	3	-5	279	11	11	4	232	10	5	4	272	11	4	7	76	85	-9*	-3	76	58	23*	8	85	65	-29*	-5	268	12	10
-4	373	12	-3	-4	204	10	8	5	58	71	-6*	5	78	85	-18*	8	275	12	3	-2	65	77	6*	9	66	94	28*	-4	234	13	4
-3	39	75	-43*	-3	352	12	4	6	120	27	-10	6	17	76	13*	9	46	90	19*	-1	63	89	-11*	H,L=	9,	-2		-3	498	16	15
-2	338	11	7	-2	215	10	7	H,L=	8,	-5		7	0	94	-34*	H,L=	8,	2		0	129	31	-12	-10	74	46	22*	-2	214	13	7
-1	53	61	33*	-1	447	15	6	-6	47	82	37*	8	77	95	-33*	-12	0104		-18*	1	120	38	-52*	-9	244	11	-13	-1	377	14	9
0	113	12	5	0	73	26	-4*	-5	324	12	-12	9	128	30	16	-11	219	12	-4	2	189	13	5	-8	84	44	1*	0	149	16	16
1	34	65	24*	1	332	12	-7	-4	51	73	45*	10	156	15	10	-10	65	86	60*	3	157	15	-1	-7	401	14	-16	1	326	13	5
2	443	14	1	2	122	16	-17	-3	303	11	-13	H,L=	8,	-1		-9	109	37	6*	4	217	13	-5	-6	216	11	-25	2	181	14	1
3	40	84	-72*	3	115	30	11	-2	0	79	-60*	-11	55	81	-27*	-8	50	95	16*	H,L=	8,	6		-5	313	11	-9	3	295	13	1
4	393	14	-7	4	0	96	-59*	-1	163	11	9	-10	120	16	-3	-7	50	93	-20*	-8	48	86	10*	-4	218	10	-6	4	89	92	-5*
5	94	41	-28*	5	0	98	-33*	0	58	67	39*	-9	249	11	-1	-6	68	79	3*	-7	80	67	-20*	-3	266	11	-21	5	0	94	-17*
6	435	15	-17	6	106	43	28*	1	80	62	48*	-8	326	12	1	-5	356	13	-1	-6	158	13	9	-2	35	72	4*	6	0	96	-41*
7	75	80	-12*	7	140	16	21	2	57	69	25*	-7	272	11	-12	-4	79	86	9*	-5	163	12	11	-1	150	10	15	7	158	15	13
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-13	241	13	7	-9	241	11	3	8	67	84	4*	-1	119	12	-1	2	63	89	60*	1	143	14	15	5	318	12	-7	-8	439	15	-24
-12	61	62	55*	-8	254	11	1	H,L=	8,	-4		0	0	74	-39*	3	262	12	-11	H,L=	9,	-6		6	137	16	5	-7	91	67	-15*
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-7	87	87	36*	-3	56	81	-54*	-4	190	10	1	5	219	11	3	8	60	82	53*	3	101	31	-5*	-11	135	14	1	-2	89	78	-14*
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6	50	90	-1*	-10	101	36	-12*	9	0	88	-45*	-6	23	70	0*	-2	68	31	-8*	6	97	35	-5*	2	404	14	12	-10	70	78	54*
7	161	14	2	-9	37	82	7*	H,L=	8,	-3		-5	180	11	8	-1	74	63	25*	7	0	87	-17*	3	159	12	20	-9	86	60	14*
8	0	83	-1*	-8	42	83	2*	-9	200	11	13	-4	224	10	0	0	185	12	-9	H,L=	9,	-4		4	244	11	11	-8	0	99	-33*
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10	34	82	14*	-6	224	11	0	-7	348	12	-13	-2	284	11	7	2	323	13	-16	-6	76	54	25*	6	44	84	-11*	-6	64	80	40*
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-6	450	15	-15	3	94	42	74*	2	11	73	-26*	7	115	21	-29	-9	67	76	20*	3	249	11	-5	-7	287	12	-8	3	190	15	5
-5	0	84	-39*	4	55	89	50*	3	254	10	-11	8	0	98	-84*	-8	57	87	34*	4	25	81	13*	-6	282	11	0	4	95	52	75*
-4	398	13	8	5	0	91	-11*	4	220	10	0	9	32102		-121*	-7	120	29	-10	5	373	13	-18	-5	180	12	-4	5	48	98	15*
-3	103	16	-8	H,L=	7,	6		5	293	11	-8	10	83	90	-7*	-6	66	76	-16*	6	61	83	47*	-4	228	11	-9	6	59	95	46*
-2	93	32	-16*	-9	251	11	3	6	227	11	-4	H,L=	8,	1		-5	248	11	8	7	314	12	-12	-3	204	11	9	H,L=	9,	4	
-1	78	37	27*	-8	59	75	-28*	7	395	14	-3	-12	75	86	-14*	-4	203	11	-3	8	63	76	14*	-2	171	11	-1	-10	258	12	4
0	153	12	0	-7	246	11	-9	8	105	33	29*	-11	21	96	-52*	-3	363	13	1	H,L=	9,	-3		-1	55	82	-6*	-9	148	13	22
1	118	16	-3	-6	87	44	-15*	9	256	12	8	-10	246	13	-11	-2	195	12	1	-9	39	84	10*	0	81	45	18*	-8	318	12	-8
2	332	12	-15	-5	230	10	12	10	59	81	-4*	-9	86	86	-30*	-1	415	14	3	-8	136	13	-1	1	212	11	2	-7	76	92	-39*
3	81	86	1*	-4	79	82	30*	H,L=	8,	-2		-8	465	16	0	0	102	41	-4*	-7	54	79	28*	2	262	11	0	-6	303	12	8
4	383	14	-17	-3	32	73	2*	-10	137	13	8	-7	20117		-79*	1	292	12	1	-6	30	80	24*	3	242	12	-6	-5	63	92	14*
5	0	89	-54*	-2	83	22	56	-9	95	39	-44*	-6	414	14	-7	2	148	16	10	-5	57	79	50*	4	302	12	-5	-4	186	13	2
6	334	13	-22	-1	58	88	-47*	-8	100	33	-4*	-5	96	49	-23*	3	105	23	16	-4	222	10	-9	5	224	13	-10	-3	57	88	17*
7	120	38	-12*	0	66	86	-3*	-7	56	70	12*	-4	307	12	-1	4	63	98	27*	-3	24	53	15*	6	282	13	-18	-2	26	94	16*
8	233	12	27	1	183	12	3	-6	0	78	-33*	-3	62	90	12*	5	71	93	40*	-2	377	13	6	7	232	13	-12	-1	50	91	46*
9	61	82	-18*	2	87	84	-10*	-5	154	10	2	-2	223	12	12	6	74	79	8*	-1	109	26	-4	8	186	14	0	0	197	13	-10
H,L=	7,	3		H,L=	8,	-6		-4	289	10	1	-1	26	88	4*	H,L=	8,	5		0	455	15	10	9	66	84	-56*	1	110	42	7*
-12	107	19	-19	-3	82	41	56*	-3	291	11	7	0	140	15	9	-10	206	12	-7	1	104	24	2	H,L=	9,	1		2	282	13	-4
-11	200	11	13	-2	209	11	-1	-2	322	11	6	1	22	87	1*	-9	224	11	-4	2	401	13	8	-11	185	14	1	3	108	44	38*
-10	0	87	-65*	-1	84	51	18*	-1	366	12	14	2	378	13	-1	-8	217	15	3	3	0	81	-19*	-10	46100		-27*	4	272	13	-16
-9	122	15	18	0	361	12	9	0	371	12	20	3	117	30	13	-7	222	12	-13	4	260	11	-4	-9	83	98	-2*	5	0	94	-19*
-8	0	84	-18*	1	66	80	-18*	1	359	12	26	4	363	13	-24	-6	234	11	-1	5	23	84	19*	-8	46	98	31*	H,L=	9,	5	
-7	144	12	8	2	303	11	-1	2	349	12	0	5	128	17	3	-5	151	13	-4	8	0	89	-27*	-7	75	97	65*	-9	49	75	43*

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-8	0	88	-8*	3	21	88	0*	-3	419	15	4	3	130	27	3	6	74	83	-20*	-5	325	13	-15	0	70	75	49*				
-7	153	13	7	4	234	12	2	-2	260	13	0	4	141	15	0	H,L=	11,	2		-4	57	80	37*	1	40	82	0*				
-6	59	87	-10*	5	75	78	72*	-1	365	14	-8	5	23	75	-20*	-9	209	15	-9	-3	206	12	2	2	93	78	7*				
-5	263	11	13	6	78	90	75*	0	239	13	21	6	0	90	-35*	-8	222	15	-9	-2	38	91	-18*	H,L=	13,	-1					
-4	156	14	-18	7	98	56	66*	1	312	14	0	H,L=	11,	-2		-7	232	14	-5	-1	30	92	21*	-5	98	42	15*				
-3	317	12	7	8	121	20	-12	2	134	35	-37	-8	47	75	-9*	-6	230	15	-3	0	23	89	1*	-4	201	13	-4				
-2	191	13	-7	H,L=	10,	-1		3	188	27	-13	-7	305	12	-11	-5	151	37	-18	1	141	16	6	-3	68	95	-39*				
-1	304	12	2	-10	66	85	6*	4	73	97	14*	-6	0	86	-58*	-4	173	19	0	2	62	84	0*	-2	298	12	-8				
0	125	24	6	-9	256	11	-8	5	56	94	48*	-5	374	13	-14	-3	65	98	-47*	3	286	12	-2	-1	71	85	-41*				
1	214	12	16	-8	67	82	1*	6	0	85	-37*	-4	65	74	37*	-2	68110		11*	4	71	89	60*	0	362	13	10				
2	37	95	-46*	-7	384	13	5	7	105	50	-13*	-3	254	11	-5	-1	102	70	72*	5	296	13	-12	1	81	96	-24*				
3	77	35	17*	-6	164	12	4	H,L=	10,	3		-2	65	36	-11*	0	150	32	22	H,L=	12,	0		2	218	13	4				
H,L=	9,	6		-5	301	12	-3	-10	229	13	8	-1	22	77	-17*	1	179	17	0	-8	0	82	-62*	3	88	56	22*				
-5	80	86	-18*	-4	165	12	-2	-9	76	96	11*	0	42	77	30*	2	243	14	-5	-7	0	91	-23*	H,L=	13,	0					
-4	77	88	5*	-3	274	11	-1	-8	325	13	-13	1	17	91	-75*	3	201	14	-9	-6	137	16	16	-6	70	78	60*				
-3	35	77	20*	-2	85	56	72*	-7	53	86	-14*	2	89	41	27*	4	205	14	-4	-5	86	27	43*	-5	281	12	-6				
-2	74	86	12*	-1	92	40	5*	-6	285	13	-5	3	285	12	-14	5	129	37	-33	-4	305	12	7	-4	84	90	78*				
-1	17	89	-50*	0	5	83	-5*	-5	22100		-33*	4	0	93	-32*	H,L=	11,	3		-3	32	95	27*	-3	137	31	-6				
H,L=	10,	-5		1	212	11	1	-4	196	14	-3	5	351	13	1	-9	56	86	-12*	-2	398	14	-5	-2	82	29	30*				
-3	193	11	-7	2	55	79	-13*	-3	63	96	43*	6	22	79	-26*	-8	35	84	18*	-1	81	83	27*	-1	29	84	7*				
-2	87	20	-6	3	334	13	-9	-2	70	84	22*	7	258	13	-1	-7	55	67	37*	0	400	14	3	0	48	94	8*				
-1	79	81	5*	4	180	13	-8	-1	63	66	13*	H,L=	11,	-1		-6	66	90	-21*	1	57	94	23*	1	120	21	-24				
0	51	71	17*	5	335	13	0	0	198	14	4	-9	61	74	19*	-5	227	14	1	2	244	13	-9	2	114	21	22				
1	48	79	19*	6	151	17	-3	1	92	97	21*	-8	83	43	-15*	-4	179	16	-8	3	0	87	-16*	3	248	13	9				
2	28	72	-4*	7	285	13	-5	2	322	14	-5	-7	0	89	-3*	-3	382	15	6	4	101	57	3*	H,L=	13,	1					
3	140	13	-1	8	87	95	-5*	3	31102		-35*	-6	0	90	-81*	-2	190	16	-7	5	0	98	-26*	-6	102	60	-34*				
4	157	12	7	H,L=	10,	0		4	288	13	3	-5	0	89	-8*	-1	354	14	6	H,L=	12,	1		-5	35105		25*				
5	251	11	6	-10	107	18	-17	5	107	55	16*	-4	305	12	8	0	150	18	12	-8	29103		-73*	-4	241	14	-11				
H,L=	10,	-4		-8	71	78	-35*	H,L=	10,	4		-3	77	86	58*	1	260	14	13	-7	307	14	-3	-3	59	99	31*				
-6	45	72	30*	-8	64	92	5*	-8	44	91	18*	-2	460	15	12	2	0102		-87*	-6	82	91	-53*	-2	330	14	1				
-5	50	70	17*	-7	98	38	96*	-8	85	44	64*	-1	129	15	27	3	92	94	-29*	-5	263	14	7	-1	0105		-35*				
-4	97	36	-12*	-6	0	91	-59*	-7	105	36	4*	0	518	17	9	4	53	86	35*	-4	24105		-67*	0	307	14	3				
-3	122	14	14	-5	108	33	-6*	-6	75	79	65*	1	88	53	2*	H,L=	11,	4		-3	193	15	13	1	73	85	46*				
-2	278	11	3	-4	351	13	12	-5	271	12	-4	2	362	13	12	-7	86	94	18*	-2	64103		59*	2	204	14	0				
-1	151	12	1	-3	184	13	3	-4	54	96	36*	3	64	82	59*	-6	224	13	-8	-1	68102		58*	H,L=	13,	2					
0	436	14	7	-2	437	15	8	-3	410	15	-4	4	171	15	1	-5	80	84	28*	0	43	90	19*	-6	154	17	72				
1	175	12	-1	-1	324	12	16	-2	0	95	-25*	5	0	83	-31*	-4	164	15	20	1	228	14	13	-5	164	33	-19				
2	322	12	5	0	334	13	9	-1	356	14	3	6	78	93	61*	-3	74	91	67*	2	98	53	44*	-4	98106		45*				
3	156	13	15	1	252	12	0	0	87	54	74*	7	24	95	0*	-2	44	95	16*	3	250	14	-25	-3	0113		-108*				
4	174	12	-7	2	312	13	2	1	234	13	-1	H,L=	11,	0		-1	66	95	28*	4	96	26	15	-2	0	98	-5*				
5	0	88	-33*	3	110	22	-7	2	72	85	38*	-9	226	13	-7	0	120	38	-29*	5	235	13	8	-1	44109		17*				
6	86	72	21*	4	104	86	-46*	3	84101		-20*	-8	76	78	-12*	1	76	95	45*	H,L=	12,	2		0	78	86	40*				
7	48	90	21*	5	0101		-26*	4	84	94	68*	-7	339	13	0	2	240	14	5	-8	68	91	63*	1	213	14	7				
H,L=	10,	-3		6	68	87	-22*	H,L=	10,	5		-6	178	13	22	H,L=	12,	-4		-7	102	71	88*								
-8	57	77	2*	7	89	26	28	-7	31	90	-17*	-5	304	13	0	-1	256	12	-11	-6	131	20	22								
-7	285	11	-14	8	138	30	19	-6	224	12	-2	-4	146	16	-10	0	277	12	11	-5	108	51	16*								
-6	12	81	-21*	H,L=	10,	1		-5	0	90	-23*	-3	228	13	-7	1	268	12	-4	-4	282	15	-1								
-5	382	13	-20	-11	101	45	12*	-4	76	80	-45*	-2	67	81	54*	H,L=	12,	-3		-3	202	17	14								
-4	62	33	49*	-10	191	14	3	-3	27	80	3*	-1	68	93	46*	-5	243	11	-14	-2	332	15	15								
-3	299	11	1	-9	218	14	-11	-2	0	93	-41*	0	72	92	61*	-4	175	12	2	-1	261	15	18								
-2	89	37	16*	-8	302	13	0	-1	9	80	-7*	1	226	13	-7	-3	193	11	8	0	245	14	-4								
-1	57	81	-13*	-7	301	13	-1	0	130	35	-27	2	92	56	25*	-2	78	85	-3*	1	168	17	-12								
0	60	77	50*	-6	299	14	-14	1	82	33	-4*	3	315	13	-8	-1	24	77	-5*	2	168	16	-15								
1	41	81	-27*	-5	201	14	4	H,L=	11,	-4		4	98	70	-49*	0	28	72	18*	3	33102		-44*								
2	97	18	22	-4	230	14	-2	-4	163	13	-5	5	281	13	-1	1	18	77	-11*	H,L=	12,	3									
3	285	11	-6	-3	144	18	-4	-3	190	12	-9	6	66	87	-54*	2	101	36	17*	-7	184	16	0								
4	83	70	70*	-2	103	81	-3*	-2	65	74	-26*	7	217	14	-14	3	184	12	8	-6	158	18	-17								
5	376	13	-8	-1	0100		-10*	-1	75	79	28*	H,L=	11,	1		4	183	13	0	-5	122	23	-2								
6	53	91	-8*	0	63	99	-29*	0	0	81	-9*	-10	71	99	-20*	H,L=	12,	-2		-4	128	37	8								
7	283	12	-7	1	166	29	-25	1	52	81	35*	-9	78	84	8*	-6	80	83	13*	-3	77102		17*								
8	95	44	14*	2	245	13	-3	2	52	74	-17*	-8	57	97	26*	-5	103	31	25*	-2	40102		2*								
H,L=	10,	-2		3	222	14	-15	3	189	11	0	-7	54	88	14*	-4	184	12	9	-1	38	69	-11*								
-9	0103		-26*	4	251	13	0	4	153	13	-10	-6	81	94	-9*	-3	115	34	-34*	0	118	24	13								
-8	110	17	-7	5	191	14	-5	5	259	12	3	-5	141	20	5	-2	303	12	-2	1	160	18	-2								
-7	24	74	-3*	6	189	14	7	H,L=	11,	-3		-4	331	14	5	-1	124	16	-7	2	205	15	17								
-6	0	85	-44*	7	178	14	9	-6	52	80	17*	-3	198	15	11	0	413	14	12	H,L=	12,	4									
-5	60	81	57*	H,L=	10,	2		-5	41	79	8*	-2	369	14	-2	1	96	39	-18*	-4	157	16	12								
-4	276	11	-2	-10	48	99	2*	-4	140	14	-4	-1	270	13	14	2	269	12	0	-3	274	13	14								
-3	0	82	-10*	-9	73	96	0*	-3	154	12	10	0	309	13	20	3	93	42	9*	-2	139	18	8								
-2	418	14	5	-8	57103		41*	-2	298	11	-5	1	197	15	-3	4	60	95	-72*	H,L=	13,	-2									
-1	92	36	-9*	-7	56105		38*	-1	169	12	-2	2	234	14	-8	5	57	92	33*	-4	139	30	-24								
0	512	16	10	-6	115	69	24*	0	429	14	5	3	127	37	38	H,L=	12,	-1		-3	98	63	-46*								
1	96	19	2	-5	252	14	-3	1	169	12	4	4	95	52	6*	-7	295	12	4	-2	46	74	-3*								
2	414	14	11	-4	215	15	-12	2	315	12	27	5	32	83	26*	-6	43	79	-15*	-1	63	86	47*								

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