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DIVALENT LANTHANIDE CHEMISTRY; BIS(PENTAMETHYLCYCLOPENTADIENYL) EUROPIUM(II) AND YTTERBIUM(II) DERIVATIVES: CRYSTAL STRUCTURE OF BIS(PENTAMETHYLCYCLOPENTADIENYL)YTTERBIUM(II)TETRAHYDROFURAN HEMI(TOLUENE) AT 176K

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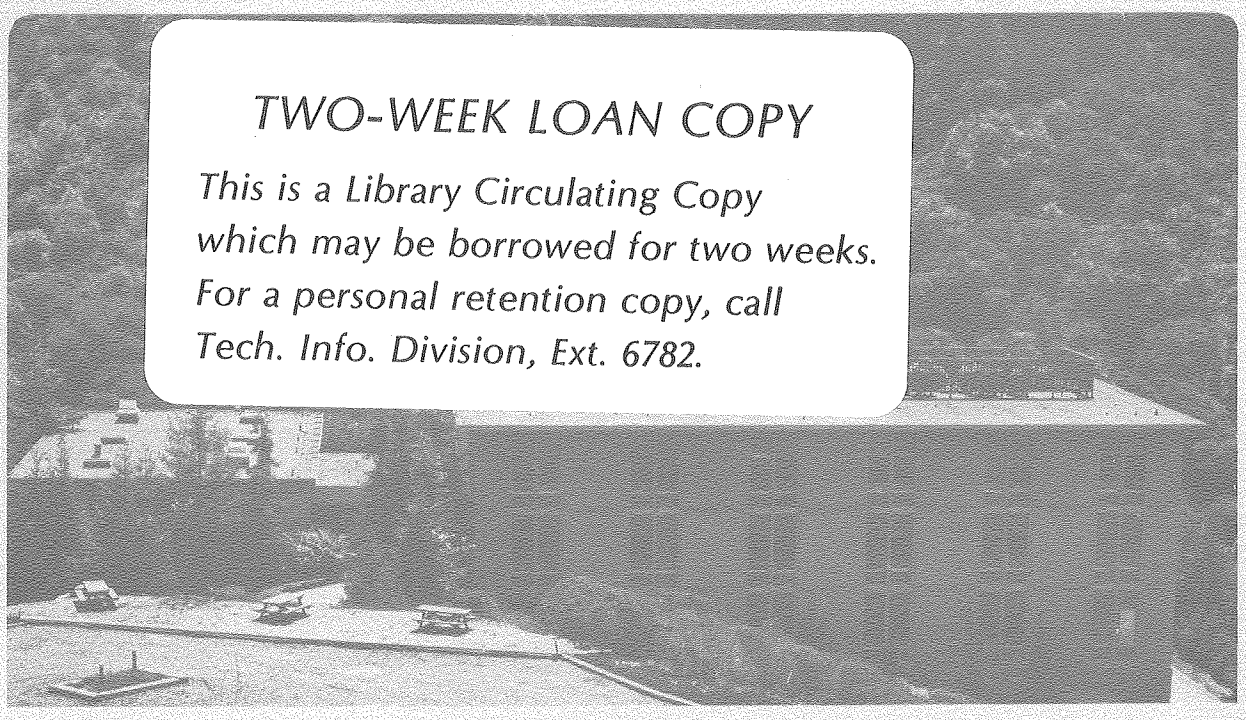

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DIVALENT LANTHANIDE CHEMISTRY; BIS(PENTAMETHYL CYCLOPENTADIENYL)EUROPIUM(II) AND YTTERBIUM(II) DERIVATIVES: CRYSTAL STRUCTURE OF BIS(PENTAMETHYLCYCLO-PENTADIENYL)YTTERBIUM(II)TETRAHYDROFURAN HEMI (TOLUENE) AT 176K

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Abstract

Red, paramagnetic (μ_B = 7.99 B.M., 5-50K) bis(pentamethyl-cyclopentadienyl)europium(II)(tetrahydrofuran)(diethylether), $(Me_5C_5)_2Eu(THF)(Et_2O)$ is isolated from reaction of three molar equivalents of sodium pentamethylcyclopentadienide and europium trichloride in refluxing tetrahydrofuran, after crystallization from diethyl ether. The monotetrahydrofuran complex, $(Me_5C_5)_2Eu(THF)$, may be isolated by use of toluene rather than diethyl ether as the crystallization solvent. Red, diamagnetic bis(pentamethylcyclo-pentadienyl)ytterbium(II)(tetrahydrofuran) is isolated from the reaction of ytterbium dichloride and sodium pentamethylcyclopen-tadienide in refluxing tetrahydrofuran. The diethyl ether complex, $(Me_5C_5)_2Yb(OEt_2)$, may be isolated by crystallization of the tetrahydro-furan complex from diethylether. The hemi-toluene complex, $(Me_5C_5)_2$ Yb(THF)·1/2 toluene, can be isolated by recrystallization of the tetrahydrofuran complex from toluene. As these divalent metallocenes are the first hydrocarbon-soluble lanthanide derivatives to be isolated we have examined the latter complex by X-ray crystallography.

Crystals of $(Me_5C_5)_2Yb(OC_4H_8)\cdot 1/2(C_6H_5CH_3)$ crystalline in the monoclinic system, $P2_1/n$, with $\underline{a}$ = 11.358(8) Å, $\underline{b}$ = 21.756(19) Å, $\underline{c}$ = 10.691(7) Å, and β = 101.84(5)° at 176K. For Z = 4 the calculated density is 1.37 g cm^{-3}. The ytterbium atom is coordinated to the oxygen atom of a tetrahydrofuran molecule and to two pentamethyl cyclopentadienyl rings. The molecule has approximate C_2 symmetry about the Yb - O bond. The Yb - O distance is 2.41 Å, the Yb - C distances average 2.66 Å, and the Yb-Cp (centroid) distances average 2.37 Å. The Me_5C_5 rings are in a staggered configuration with respect to each other. The methyl groups of the Me_5C_5 groups are displaced by .03 to .21 Å from the planes of the five-membered rings away from the ytterbium atom. The toluene molecule is not coordinated to the complex and is on a center of symmetry in a disordered configuration. The 3466 data with $F^2 > 3\sigma$ refined by full matrix least-squares to a conventional R factor of 0.036.

Introduction

In contrast to the reasonably extensive literature associated with trivalent lanthanide organometallic compounds, the divalent oxidation state of these metals has been largely ignored.[1] Yellow, paramagnetic (μ_B = 7.63 B.M.) and red, diamagnetic biscyclopentadienyl-europium and -ytterbium, respectively, were first prepared from the metal and cyclopentadiene in liquid ammonia.[2] The compounds are insoluble in solvents with which they do not react, though some coordination complexes with, for example ammonia, have been isolated. The preparation of Cp_2Yb from the metal and diene in liquid ammonia is not straightforward since two other cyclopentadienyl-containing products, Cp_3Yb and a species formulated as $Cp_4Yb_2N_2H_4$, have been isolated.[3] Alternative synthetic schemes have been devised which give Cp_2Yb in good yield.[4] The latter paper also reports that Cp_2Yb is green when pure, rather than red as was initially reported.[2] An insoluble, purple, paramagnetic (μ_B = 3.6 B.M.) derivative of samarium(II), $Cp_2Sm(THF)$, has also been described.[5] The insoluble cyclooctatetraene (COT) derivatives, (COT)Eu and (COT)Yb, have been briefly mentioned.[6] An ether-soluble pentafluorophenylytterbium species, $(C_6F_5)_2Yb(THF)_4$[7] and some insoluble alkynyl derivatives, $(RC \equiv C)_2M$, of ytterbium[8,9] and europium[9] have also been described.

The general pattern which dominates the rather meager knowledge of divalent lanthanide organometallic chemistry is their lack of volatility and solubility. This is doubtless due to some type of polymer

formation, possibly similar to that found for Cp_2Ca.[10] Use of sterically demanding ligands to stabilize low coordination numbers is a strategy that can be used to prevent polymerization. Replacement of the five hydrogen atoms of a cyclopentadienyl group with five methyl groups, giving the pentamethylcyclopentadienyl group, greatly increases the steric bulk of the ligand. This is shown, by way of example, by the observation that dicyclopentadienylmanganese[11] has a polymeric constitution in the solid state[12] whereas bis(pentamethylcyclopentadienyl)manganese is monomeric.[13] In this paper we describe some coordination complexes of bis(pentamethylcyclopentadienyl)-europium(II) and -ytterbium(II) and the crystal structure of one of them, $(Me_5C_5)_2Yb(THF)\cdot 1/2$ toluene.

Experimental Section

Microanalyses were performed by the microanalytical laboratory of this department. The ^{1}H(90 MHz) and $^{13}C\{^{1}H\}$ (22.5 MHz) nuclear magnetic resonance spectra were recorded on a Joel FX-90 in toluene-d_8 solution and referenced to Me_4Si ($\delta = 0$). Infrared spectra were recorded on a Perkin-Elmer 597 machine as Nujol mulls between cesium iodide windows. The magnetic susceptibility measurements were performed as previously described.[14] All operations were performed under nitrogen.

Bis(pentamethylcyclopentadienyl)europium(II)(tetrahydrofuran) (diethyl ether). Sodium pentamethylcyclopentadienide[15] (9.72g, 0.0614 mol) in tetrahydrofuran (75 mL) was added to a suspension of europium trichloride (5.30g, 0.0205 mol) in tetrahydrofuran (75 mL). A blue colored solution developed immediately which slowly turned brown-red at room temperature. The suspension was refluxed for 12 h. Tetrahydrofuran was removed in vacuum, the residue was extracted with diethyl ether (2 x 150 mL), and the combined extracts were concentrated to ca. 100 mL. Cooling (-10°C) afforded red prisms in 65 percent yield (7.5g), mp 181-182°C. The complex is soluble in aliphatic and aromatic hydrocarbons and in ethereal solvents. The complex decomposed upon attempted sublimation in vacuum at ca. 140°C. Anal. Calcd for $C_{28}H_{48}EuO_2$: C, 59.1; H, 8.51. Found: C, 59.1; H, 8.43. A sample of the complex was dissolved in benzene and hydrolyzed with water. The ^{1}H NMR spectrum of the benzene solution showed tetrahydrofuran and diethylether present in ca. equal amounts. The compound

follows Curie behavior from 5-50K with μ_{eff} = 7.99 B.M. and C = 7.91. IR, 2713w, 1627w, 1313w, 12896w, 1248w, 1208w, 1185w, 1147m, 1119w, 1089w, 1054m, 1032s, 1003w, sh, 927w, 896s, 837w, 828w, 818w, 795m, 777m, 766w, 721m, 649w, br, 624w, 585m, 506m, br, 353w, br, and 248s, br cm^{-1}.

Bis(pentamethylcyclopentadienyl)europium(II)(tetrahydrofuran). Bis(pentamethylcyclopentadienyl)europium(tetrahydrofuran)(diethyl ether) (1.5g, 0.0027mol) was dissolved in toluene (25mL) and the solution was concentrated to ca. 10mL. Cooling (-70°C) yielded red prisms in quantitative yield, mp 178-181°C, Anal. Calcd for $C_{24}H_{38}EuO$: C, 58.3, H, 7.74. Found: C, 58.6; H, 7.56 IR: 2714w, 1637w, br, 1292w, sh, 1281w, 1243m, 1209m, 1027s, br, 952w, 928w, 898s, br, 834w, sh, 794w, 723m, 691w, 637m, br, 587w, 462w, 357m, br, 258s, br cm^{-1}. Crystallization of the monotetrahydrofuran complex from diethyl ether yields $(Me_5C_5)_2Eu(THF)(OEt_2)$.

Bis(pentamethylcyclopentadienyl)ytterbium(II)tetrahydrofuran. Sodium pentamethylcyclopentadienide (3.97g, 0.0251 mol) in tetrahydrofuran (75mL) was added to a suspension of ytterbium dichloride[16] (3.06g, 0.0125mol) in tetrahydrofuran (75mL). After refluxing for 12h, the deep purple suspension was evaporated to dryness, and the residue was extracted with diethyl ether (2 x 100mL). The combined, green extracts were concentrated to ca. 100mL and cooled (-10°C). The red prisms were collected and dried in vacuum, yield 5.5g (85%). When heated in a sealed capillary the complex shrank at ca. 120°C and melted at 206-209°C. Anal. Calcd for $C_{24}H_{38}OYb$: C, 55.9; H, 7.43.

Found: C, 56.2; H, 7.32. The complex is soluble in aliphatic and aromatic hydrocarbons and ethereal solvents. The complex decomposed upon attempted sublimation in vacuum at ca. 125°C. The ^{1}H nuclear magnetic resonance spectrum (-25°C) consists of multiplets at δ 3.42 and δ 1.41 due to the α- and β- protons of tetrahydrofuran, respectively, and a singlet at δ 2.12 due to the methyl protons of the Me_5C_5 rings in area ratio 4:4:30, respectively. The $^{13}C\{^{1}H\}$ nuclear resonance spectrum (-25°C) consists of singlets at δ 111, 69.5, 25.7, and 11.5 due to $(Me_5C_5)_2Yb$,

$Yb(O\overline{CH_2CH_2CH_2CH_2})$, $Yb(O\overline{CH_2CH_2CH_2CH_2})$,

and $(Me_5C_5)_2Yb$, respectively. IR: 2719w, 1646w, br, 1322w, 1297w, 1249m, br, 1221w, 1151w, 1093w, 1067w, sh, 1034s, br, 916w, 882s, br, 801w, 783w, 723m, 669m, br, 627w, 592m, 483w, 472w, 361m, br, 308m and 258s, br cm^{-1}.

Bis(pentamethylcyclopentadienyl)ytterbium(II)(diethylether). This complex was crystallized from the mother liquor which yielded the monotetrahydrofuran complex (above). Green needles in ca. 5% yield were isolated after most of the tetrahydrofuran complex had crystallized. The complex decomposed without melting at ca. 145°C. Anal. Calcd for $C_{24}H_{40}OYb$: C, 55.7; H, 7.79. Found: C, 55.7; H, 7.58. The ^{1}H nuclear magnetic resonance spectrum (PhH-d_6, +35°C) consisted of a quartet centered at δ 3.15, a singlet at δ 2.16, and a triplet at δ 1.04 due to CH_3CH_2OYb, $(Me_5C_5)_2Yb$, and CH_3CH_2OYb in area ratio 4:30:6, respectively. IR: 2720w, 1633w, 1284w, 1262w, 1180w, sh,

1163w, sh, 1149s, 1123w, 1097w, sh, 1977s, br, 1041m, 1019w, 980w, sh, 948w, 929m, 839s, 829w, sh, 797w, 722m, 592m, 552w, 482w, 443w, 355m, br, 303m, and 268s, br cm^{-1}.

Bis(pentamethylcyclopentadienyl)ytterbium(II)(tetrahydrofuran)(hemi-toluene). Sodium pentamethylcyclopentadienide (3.52g, 0.0227mol) in tetrahydrofuran (75mL) and ytterbium dichloride (2.71g, 0.0111mol) in tetrahydrofuran (75mL) were refluxed for 12h. Tetrahydrofuran was removed in vacuum and the residue was extracted with toluene (150mL), the solution was concentrated to ca. 80mL, and was cooled to -70°C. The brown-red prisms were collected and dried in vacuum, yield was 4.6g (74%). When heated in a sealed capillary the complex darkened at ca. 195°C and melted at 204-206°C. Anal. calcd for $C_{27.5}H_{42}OYb$: C, 58.8; H, 7.54; Found: 58.5; H, 7.27. IR: 2719m, 1604m, 1337w, 1259m, 1242w, sh, 1174m, br, 1079w, 1022s, 918m, 868s, br, 843w, sh, 795w, 730s, 694s, 671m, 589w, 481w, sh, 466m, 360m, br, 304s, br, 282w, sh, and 268s cm^{-1}.

X-Ray

Crystals were sealed in quartz capillaries and mounted on a Picker FACS-I automated diffractometer equipped with a graphite monochromater, a Mo x-ray tube, and a Syntex LT-1 temperature controller. ω-scans of several low-angle reflections had a width at half-height of 0.15°. Least-squares refinement of the setting angles of 9 manually centered reflections ($40<2\theta<50°$) using $MoK\alpha_1$ (λ = 0.70930 Å) radiation gave a = 11.358(8) Å, b = 21.756(19) Å, c = 10.691(7) Å, β = 101.84(5)°, and V = 2585.6 $Å^3$ at 176(5)K. The observed

extinctions are unique to space group $P2_1/n$. With $Z = 4$ and a molecular weight of 533.62 g mol^{-1}, the calculated density is 1.37 g cm^{-3}.

Intensity data were collected for two forms to 50° in 2θ using θ-2θ scans with a scan speed of 2°/min on 2θ, a scan range from 1.5° below the $K\alpha_1$ peak to 1.5° above the $K\alpha_2$ peak, and with backgrounds counted for 10 seconds at each end of the scan range. Three standard reflections, measured after every 200 reflections, decreased in intensity by 6 percent during data collection and the measured intensities were corrected accordingly. Data were collected at low temperature (176K) to minimize severe crystal movement, which was evident at room temperature. Due to occasional problems with the temperature controller, data for portions of the second form were unreliable and not used. Absorption corrections to the data were not applied, because attempts to fit an analytical absorption correction to the intensity variation of azimuthal scans were unsuccessful as the crystal shape permitted a re-entrant beam in some orientations (μ = 36.2 cm^{-1} for Mo Kα radiation and approximate crystal dimensions were 0.12 x 0.16 x 0.22 mm). Intensities of the 8544 reflections measured were corrected for Lorentz and polarization factors, extinctions were removed, and equivalent reflections were averaged to yield a set of 4592 unique reflections.

Trial coordinates for the ytterbium atom were obtained from a three-dimensional Patterson function and were refined by least-squares. A Fourier calculation then revealed all non-hydrogen atoms

of the pentamethylcyclopentadienyl (Cp) rings and the tetrahydrofuran (THF). A series of isotropic and anisotropic least-squares refinements, followed by a difference synthesis, gave a difference Fourier map with peaks of electron density (3 to 5 $e/Å^3$) near a center of symmetry. These peaks could be interpreted in terms of two partially overlapping sets of toluene carbon atoms as shown in Figure 1. In the final cycles of refinement, all non-hydrogen atoms except those for toluene were refined anisotropically; the carbon atoms for toluene were refined isotropically and were not restrained except to assign full occupancy to atoms C(25) and C(26), and half occupancy to atoms C(27), C(28), and C(29). The refinement converged to the positions given in Table I with the changes in parameters in the last cycle all 0.07σ or less. The data were inspected for evidence of extinction, but an extinction correction was not indicated. Thermal parameters and structure factor amplitudes are included in the supplementary material.

The full-matrix least squares program minimizes the function $\Sigma w|\Delta F|^2/\Sigma wF_o^2$ where the assigned weights, $w = [\sigma(F)]^{-2}$, are derived from $\sigma(F^2) = [S^2 + (pF^2)^2]^{1/2}$ where S^2 is the variance due to counting statistics and $p = 0.04$. Scattering factors for neutral atoms were those of Doyle and Turner[17] corrected for anomolous dispersion.[18] Discrepancy indicies for 255 parameters varied with 3466 data having $F^2 > 3\sigma(F^2)$ are

$$R = \Sigma||F_o| - |F_c| / \Sigma|F_o|| = 0.037$$

$$R_w = \Sigma[w(|F_o| - |F_c|)^2 / \Sigma w F_o^2]^{1/2} = 0.049$$

R for all 4592 data is 0.053 and the estimated standard deviation in an observation of unit weight is 1.58. A difference Fourier calculation after the final cycle of least-squares refinement had a maximum electron density of 2.0 e/Å^3 located near the ytterbium atom.

Results and Discussion

Addition of three molar equivalents of sodium pentamethylcyclopentadienide to europium trichloride in refluxing tetrahydrofuran yields the divalent species, $(Me_5C_5)_2Eu(THF)(OEt_2)$ upon crystallization from diethyl ether. In contrast the mono-tetrahydrofuran complex, $(Me_5C_5)_2Eu(THF)$, is obtained when toluene is used as a solvent for crystallization. These two compounds can be interconverted, e.g., crystallization of the mono-tetrahydrofuran complex from diethyl ether yields $(Me_5C_5)_2Eu(THF)(Et_2O)$, whereas crystallization of the latter complex from toluene yields $(Me_5C_5)_2Yb(THF)$. Thus the diethyl ether ligand is rather labile, suggesting that it might be present in the solid state as solvent of crystallization. The sensitivity of these compounds to reaction or isolation conditions is further illustrated by our inability to isolate compounds from reaction of europium trichloride with $NaMe_5C_5$ in refluxing toluene or with $LiMe_5C_5$ in refluxing tetrahydrofuran. We have also been unable to isolate compounds from europium dichloride and $NaMe_5C_5$ in refluxing tetrahydrofuran.

The magnetic moment of $(Me_5C_5)_2Eu(THF)(OEt_2)$, μb = 7.99 B.M., follows Curie behavior from 5-50K. This is consistent with the $^8S_{7/2}$ ground state expected for a europous (f^7) ion. The ability of sodium pentamethylcyclopentadienide to reduce europium(III) to europium(II) is not surprising as this reduction potential in aqueous acid solution is -0.6v.[19a] Even lower values (-0.35v) have been estimated.[19b]

The divalent ytterbium derivative, $(Me_5C_5)_2Yb(THF)$, is most readily prepared from sodium pentamethylcyclopentadienide and ytterbium dichloride in refluxing tetrahydrofuran. Again, reaction and crystallization conditions are critical. If diethyl ether is used as crystallization solvent green $(Me_5C_5)_2Yb(OEt_2)$ and red $(Me_5C_5)_2Yb(THF)$ are isolated by fractional crystallization. If toluene is used for crystallization $(Me_5C_5)_2Yb(THF)\cdot 1/2$ PhMe is isolated. Further, ytterbium dichloride and $NaMe_5C_5$ (1:2 molar ratio) in refluxing diethyl ether or $LiMe_5C_5$ (1:2 molar ratio) in refluxing tetrahydrofuran do not yield any isolable compounds.

The divalent ytterbium(II) species (f^{14}) is rigorously diamagnetic (5-50K) as expected for a $^1S_0$ ground state ytterbous ion and normal, diamagnetic ^1H and $^{13}C\{^1H\}$ nuclear magnetic resonance parameters are observed (see experimental section). However, the proton chemical shift of the methyl resonance of the Me_5C_5 group is temperature dependent, ranging from δ 1.98 at 80°C to δ 2.18 at -50°C. The tetrahydrofuran resonances are also temperature dependent; between 80° and -50°C the α-protons range from δ 4.02 to δ 3.30 and the β-protons range from δ 1.81 to δ 1.32.

Tables of atomic positions, distances and angles, and least-squares planes are given in Tables I-IV. The three-fold coordination of the Yb(II) ion is planar (see Plane 4 in Table IV) with the ytterbium Cp(centroid) average distance of 2.37 Å and an angle between the centroids of the two Cp-rings of 144°. In addition, the average

Cp-Yb-O angle is 108°, giving approximate C_2 symmetry about the Yb-O axis as can be seen in Figure 2. The approximate C_2 symmetry is carried further in the THF molecule and in the staggered conformation of the C_5Me_5 groups (see Figure 3). The Cp-rings are planar and normal to the Yb-Cp axis in both cases as indicated by the lack of significant systematic variation in Yb-C (ring) distances. The methyl groups, however, are bent out of the plane of each Cp-ring away from the Yb(II) ion with the largest deviation in each ring (0.18 Å for C(9) and 0.21 Å for C(17)) occurring for those methyl groups with the closest intramolecular contacts. Otherwise, the C_5Me_5-groups have normal geometry. The THF molecule is probably disordered since the rms amplitudes of displacement for C(22) and C(23) are much larger than for other carbon atoms and are highly anisotropic. Such disorder is normal for THF molecules.[20] Although the apparent bond angles in the disordered toluene molecules are reasonably close to the expected 120°, the apparent bond distances are less satisfactory because they are derived from averaged positions of several atoms that are not necessarily coincident. A better test of the model uses the positions of carbon atoms that are not overlapped by others, C(27), C(28)', and C(29)' in Figure 1, to calculate a C-C bond distance for the toluene ring. With distances of 2.47, 2.43, and 2.32 Å between these atoms, which would form an equilateral triangle if the toluene ring were exactly a hexagon, the calculated C-C bond distance in the ring is 1.39 Å, the expected value.

The average ytterbium-carbon bond lengths in the complex, 2.66 Å, less the seven coordinate ionic radius of the ytterbous ion (1.08 Å),[21] yields 1.58 Å for the effective ionic radius of a pentamethylcyclopentadienide group. This value is similar to those observed for other lanthanide and actinide cyclopentadienyl compounds (1.64 ± 0.04 Å) in which the metal-ring bonding is considered to be primarily ionic.[22-24] Further, the ytterbium-oxygen bond length, 2.41 Å, less the ytterbous ionic radius, yields 1.33 Å as the ionic radius of a three coordinate oxygen atom. A value of 1.36 Å has been suggested.[21]

We have been informed recently that a 1:2 complex, $(Me_5C_5)_2Yb(THF)_2$, has been isolated.[25]

Acknowledgement

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Supplementary Material Available: Listing of atomic thermal parameters, listing of structure factor amplitudes (19 pages). Ordering information is given on any current masthead page.

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Table I. Positional Parameters[a]

ATOM	x	y	z
YB	.68910(3)	.64148(1)	.30066(3)
O	.9038(43)	.6472(2)	.3172(5)
C(1)	.6798(7)	.7042(3)	.0842(7)
C(2)	.6761(7)	.7487(3)	.1800(7)
C(3)	.5646(6)	.7425(3)	.2186(7)
C(4)	.4987(7)	.6941(3)	.1460(8)
C(5)	.5690(7)	.6696(3)	.0648(7)
C(6)	.7800(9)	.6958(4)	.0100(9)
C(7)	.7678(9)	.7977(4)	.230(1)
C(8)	.5228(9)	.7833(4)	.3187(9)
C(9)	.3702(8)	.6773(4)	.145(1)
C(10)	.5317(9)	.6187(4)	-.0330(9)
C(11)	.5689(7)	.5485(3)	.3764(7)
C(12)	.5574(6)	.5975(3)	.4573(8)
C(13)	.6705(8)	.6105(4)	.5355(7)
C(14)	.7541(7)	.5678(4)	.5021(7)
C(15)	.6907(7)	.5303(3)	.4034(8)
C(16)	.4690(9)	.5162(4)	.287(1)
C(17)	.4413(8)	.6267(4)	.478(1)
C(18)	.696(1)	.6568(5)	.642(1)
C(19)	.8853(8)	.5611(5)	.5679(9)
C(20)	.748(1)	.4770(4)	.343(1)
C(21)	.9948(8)	.6869(5)	.392(1)
C(22)	1.112(1)	.6661(8)	.369(2)
C(23)	1.092(1)	.6210(6)	.262(2)
C(24)	.9642(7)	.6009(4)	.254(1)
C(25)	.0195(9)	.4595(5)	.077(1)
C(26)	.191(1)	.5126(5)	.020(1)
C(27)	.059(2)	.5002(9)	.005(2)
C(28)	.113(2)	.5520(9)	-.059(2)
C(29)	.151(2)	.473(1)	.090(2)

[a] The estimated standard deviation of the least significant digit is given in parenthesis here and in the following tables.

Table II. Selected Interatomic Distances (Å)

Pentamethylcyclopentadienyl Ring 1		Pentamethylcyclopentadienyl Ring 2		Tetrahydrofuran	
Yb-C(1)	2.670(7)	Yb-C(11)	2.658(7)	Yb-O	2.412(5)
-C(2)	2.654(7)	-C(12)	2.643(7)	O-C(21)	1.45(1)
-C(3)	2.663(7)	-C(13)	2.649(8)	O-C(24)	1.46(1)
-C(4)	2.694(8)	-C(14)	2.664(7)	C(21)-C(22)	1.47(2)
-C(5)	2.680(8)	-C(15)	2.654(7)	C(22)-C(23)	1.49(2)
Average	2.672	Average	2.654	C(23)-C(24)	1.51(2)
C(ring) - C(ring)				**Toluene**	
C(1)-C(2)	1.42(1)	C(11)-C(12)	1.40(1)	C(25)-C(27)	1.32(2)
C(2)-C(3)	1.42(1)	C(12)-C(13)	1.41(1)	C(25)-C(27)'	1.42(2)
C(3)-C(4)	1.43(1)	C(13)-C(14)	1.42(1)	C(25)-C(28)	1.50(2)
C(4)-C(5)	1.40(1)	C(14)-C(15)	1.41(1)	C(25)-C(29)	1.51(2)
C(5)-C(1)	1.45(1)	C(15)-C(1)	1.41(1)	C(26)-C(27)	1.51(2)
Average	1.42	Average	1.41	C(26)-C(28)	1.39(2)
				C(26)-C(29)	1.29(2)
C(ring) - CH_3					
C(1)-C(6)	1.53(1)	C(11)-C(16)	1.50(1)		
C(2)-C(7)	1.51(1)	C(12)-C(17)	1.52(1)		
C(3)-C(8)	1.54(1)	C(13)-C(18)	1.50(1)		
C(4)-C(9)	1.50(1)	C(14)-C(19)	1.52(1)		
C(5)-C(10)	1.52(1)	C(15)-C(20)	1.54(1)		
Average	1.52	Average	1.52		

Table III. Selected Angles (deg)

Yb-Coordination		Tetrahydrofuran	
Cp(1)[a]-Yb-Cp(2)	143.5(3)	C(21)-O-C(24)	108.4(6)
Cp(1)-Yb-O	107.7(3)	O-C(21)-C(22)	106.9(8)
Cp(3)-Yb-O	108.8(3)	C(21)-C(22)-C(23)	109.5(10)
		C(22)-C(23)-C(24)	102.8(9)
		C(23)-C(24)-O	108.4(7)
	Pentamethylcyclopentadienyl		
Ring 1		Ring 2	
	Internal Angles		
C(5)-C(1)-C(2)	107.8(6)	C(15)-C(11)-C(12)	107.4(7)
C(1)-C(2)-C(3)	107.9(7)	C(11)-C(12)-C(13)	109.3(6)
C(2)-C(3)-C(4)	108.1(7)	C(12)-C(13)-C(14)	107.2(7)
C(3)-C(4)-C(5)	108.5(7)	C(13)-C(14)-C(15)	107.5(7)
C(4)-C(5)-C(1)	107.7(7)	C(14)-C(15)-C(11)	108.6(7)
Average	108.0	Average	108.0
	External Angles		
C(2)-C(1)-C(6)	126.4(7)	C(12)-C(11)-C(16)	126.7(8)
C(5)-C(1)-C(6)	125.8(8)	C(15)-C(11)-C(16)	125.6(8)
C(1)-C(2)-C(7)	128.1(7)	C(11)-C(12)-C(17)	127.1(8)
C(3)-C(2)-C(7)	123.9(7)	C(13)-C(12)-C(17)	122.9(8)
C(2)-C(3)-C(8)	124.7(7)	C(12)-C(13)-C(18)	126.3(8)
C(4)-C(3)-C(8)	127.2(7)	C(14)-C(13)-C(18)	126.3(8)
C(3)-C(4)-C(9)	125.8(8)	C(13)-C(14)-C(19)	126.1(8)
C(5)-C(4)-C(9)	125.3(8)	C(15)-C(14)-C(19)	126.3(8)
C(4)-C(5)-C(10)	126.0(7)	C(14)-C(15)-C(20)	123.9(8)
C(1)-C(5)-C(10)	126.1(7)	C(11)-C(15)-C(20)	127.4(8)
Average	125.9	Average	125.9
Toluene			
C(25)-C(29)-C(26)	123(2)		
C(29)-C(26)-C(28)'[b]	121(2)		
C(28)'-C(25)'-C(27)	119(2)		
C(25)'-C(27)-C(25)	122(2)		
C(27)-C(25)-C(29)	115(2)		
Average	120		

a Cp_1 and Cp_2 represent the centroids of the cyclopentadienyl moieties C(1)-C(5) and C(11)-C(15), respectively.

b Primed carlon atoms are at positions x, y, z.

Table IV. Perpendicular Distances (Å) from Least-Squares Planes

Plane 1. Ring 1: C(1)-C(5)

Deviation of Atoms in Plane		Distance to Plane	
C(1)	-.006	C(6)	-.079
C(2)	+.002	C(7)	-.072
C(3)	+.004	C(8)	-.028
C(4)	-.007	C(9)	-.179
C(5)	+.008	C(10)	-.049
		Yb	2.383

Plane 2. Ring 2: C(11)-C(15)

Deviations of Atoms in Plane		Distance to Plane	
C(11)	+.002	C(16)	+.137
C(12)	+.001	C(17)	+.208
C(13)	-.003	C(18)	+.088
C(14)	+.005	C(19)	+.108
C(15)	-.004	C(20)	+.043
		Yb	-2.367

Plane 3. Toluene: C(25), C(25)', C(26), C(26)', C(27), C(28), C(29)'

Deviations of Atoms in Plane	
C(25)	+.022
C(25)'[b]	+.001
C(26)	-.011
C(26)'	+.034
C(27)	-.062
C(28)	+.054
C(20)'	-.038

Plane 4. Cp_1-Cp_2-Yb-O

Cp(1)[a]	.008
Cp(2)	.008
Yb	-.020
O	.005

[a] See comment a in Table III.

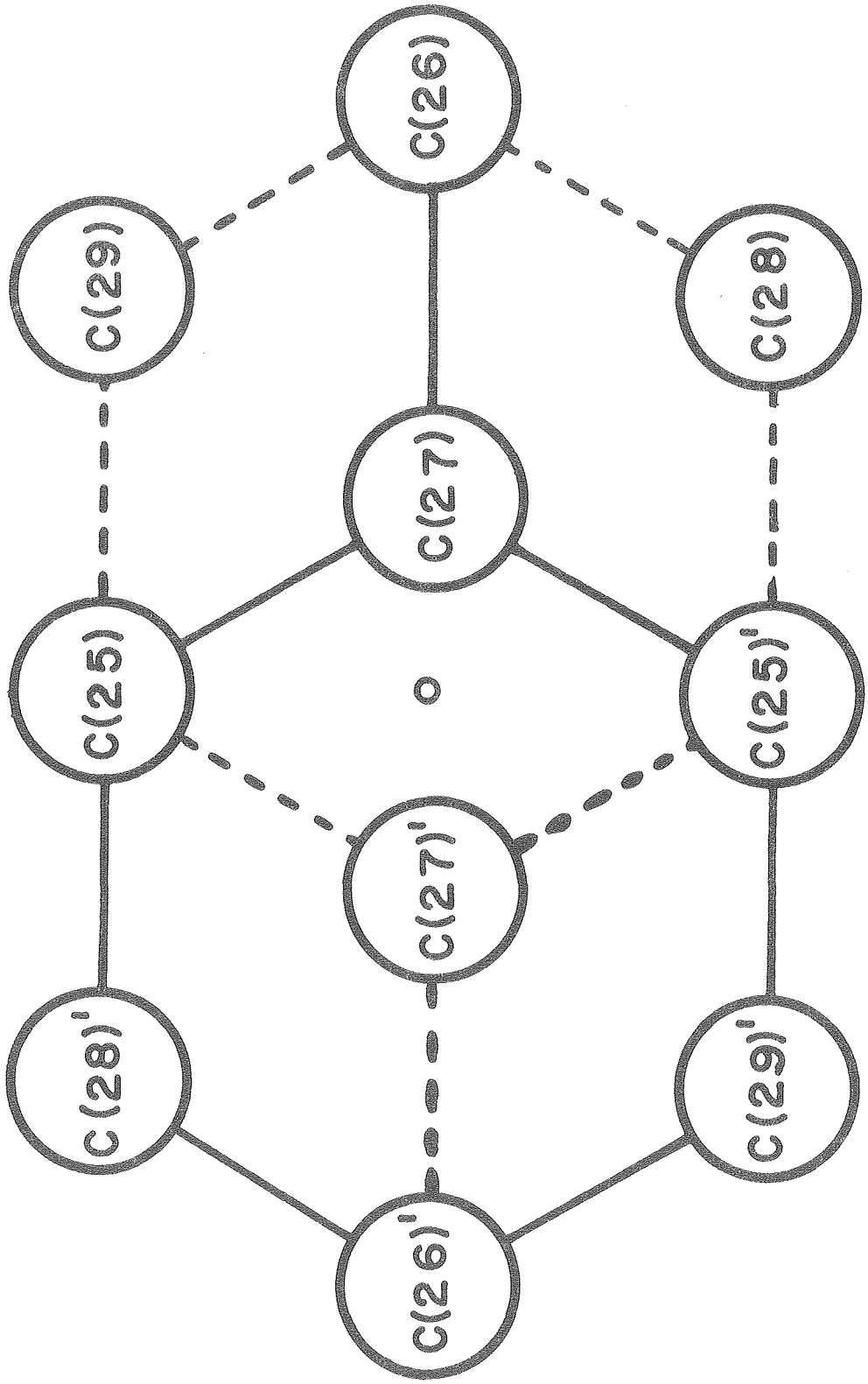
[b] See comment b in Table III.

Figure Captions

Fig. 1. Disordered model for the toluene molecule. Carbons C(25) and C(26) were given full occupancy and C(27), C(28), and C(29) were given half occupancy, corresponding to two toluene molecules per unit cell containing four ytterbium ions.

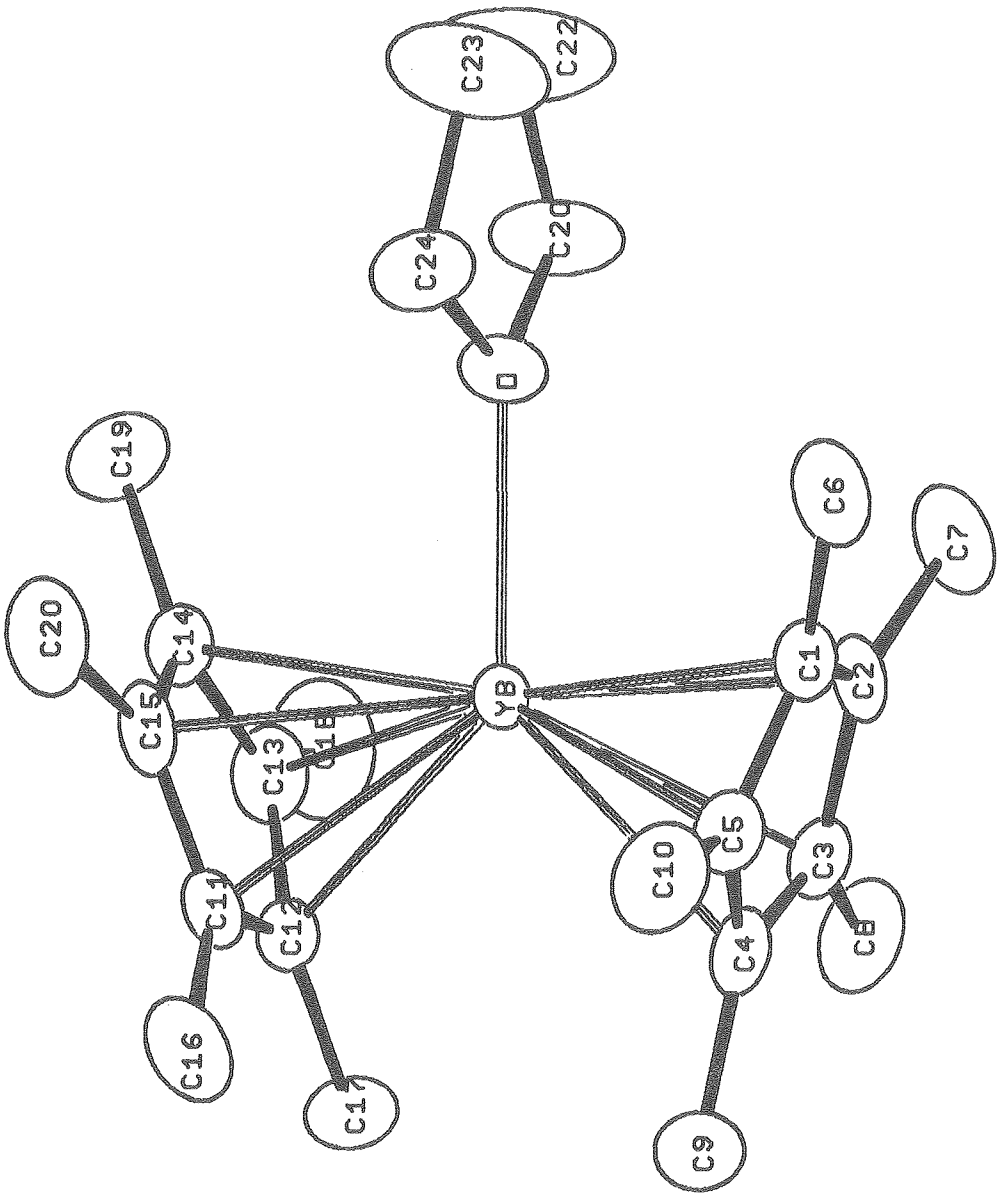
Fig. 2. ORTEP diagram showing atom numbering.

Fig. 3. ORTEP diagram showing the staggered configurations of the Cp rings.



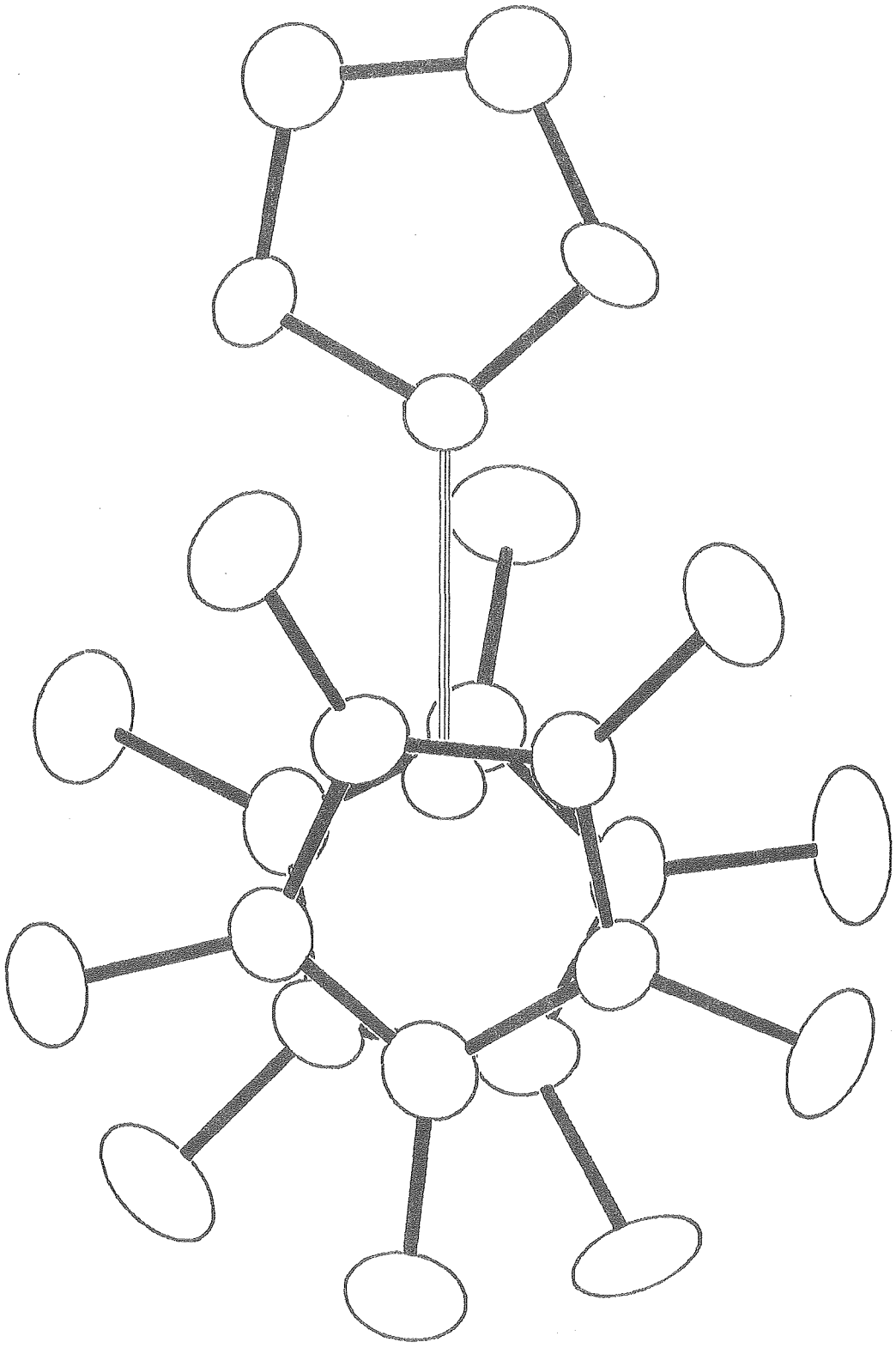
XBL 803-8701

Fig. 1



XBL 799-11775

Fig. 2



XBL 799-11777

Fig. 3

SUPPLEMENTARY MATERIALS FOR THE PAPER

DIVALENT LANTHANIDE CHEMISTRY; BIS(PENTAMETHYL CYCLOPENTADIENYL)EUROPIUM(II) AND YTTERBIUM(II) DERIVATIVES: CRYSTAL STRUCTURE OF BIS(PENTAMETHYLCYCLOPENTADIENYL)YTTERBIUM(II)TETRAHYDROFURAN HEMI (TOLUENE) AT 176K

by

T. Don Tilley, Richard A. Andersen, Brock Spencer, Helena Ruben, Allan Zalkin and D. H. Templeton

Thermal Parameters[a]

ATOM	B11	B22	B33	B12	B13	B23
YB	1.72(1)	1.65(1)	2.20(1)	.02(1)	.354(9)	.46(1)
O	2.0(2)	2.9(2)	3.0(2)	-.2(2)	.8(2)	-.6(2)
C(1)	2.7(3)	2.4(3)	2.5(3)	.4(3)	.7(3)	.9(3)
C(2)	3.2(3)	1.6(3)	2.3(3)	-.2(3)	.7(3)	.6(2)
C(3)	2.7(3)	2.1(3)	2.2(3)	.7(2)	.5(2)	.5(2)
C(4)	3.1(3)	2.0(3)	2.7(3)	.4(3)	-.0(3)	.8(3)
C(5)	2.8(3)	2.3(3)	2.3(3)	.2(3)	.1(3)	.2(3)
C(6)	5.2(5)	3.7(4)	3.1(4)	.4(4)	2.4(4)	1.3(3)
C(7)	5.1(5)	2.3(3)	4.7(5)	-1.2(3)	.8(4)	-.1(3)
C(8)	5.6(5)	2.7(4)	4.0(4)	1.7(3)	1.8(5)	-.2(3)
C(9)	2.5(3)	4.1(4)	4.5(5)	-.1(3)	.2(3)	.8(4)
C(10)	4.8(4)	3.4(4)	2.8(4)	.3(3)	-.2(3)	-1.0(3)
C(11)	2.6(3)	2.1(3)	2.3(3)	-.6(2)	.2(2)	.6(2)
C(12)	2.3(3)	2.5(3)	3.0(3)	.3(2)	.8(3)	1.1(3)
C(13)	4.1(4)	2.5(3)	1.9(3)	.3(3)	.8(3)	-.2(3)
C(14)	2.7(3)	2.8(3)	2.1(3)	.2(3)	.4(2)	.9(3)
C(15)	3.9(4)	1.5(3)	2.9(3)	.0(3)	1.1(3)	.5(3)
C(16)	4.4(4)	3.4(4)	4.5(5)	-1.9(4)	-.3(4)	.3(4)
C(17)	2.5(3)	4.8(5)	4.9(5)	1.1(3)	2.1(3)	1.3(4)
C(18)	8.3(7)	4.3(5)	2.7(4)	-.1(4)	.7(4)	-1.4(4)
C(19)	3.0(4)	6.1(5)	3.3(4)	.6(4)	-.3(3)	1.2(4)
C(20)	6.1(5)	1.8(3)	6.1(6)	.4(4)	2.1(5)	-.2(4)
C(21)	2.4(4)	4.8(5)	7.9(7)	-1.2(3)	.6(4)	-3.1(5)
C(22)	4.2(6)	10.5(10)	12.9(13)	-1.4(6)	2.7(7)	-7.7(10)
C(23)	4.6(5)	6.5(7)	11.2(11)	-2.0(5)	3.6(6)	-5.0(7)
C(24)	2.8(3)	3.2(4)	4.9(5)	.4(3)	1.2(3)	-1.4(3)

ATOM	B
C(25)	4.6(2)
C(26)	5.2(2)
C(27)	4.1(4)
C(28)	4.3(4)
C(29)	4.7(4)

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

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
Y8.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3)) F(0.0.0) = 2907

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

L	FOB	SG	DEL
H,K=	0,	0	
2	474	10	8
4	241	5	-3
6	213	5	-10
8	333	7	-3
10	293	6	-3
12	160	5	3
H,K=	0,	1	
1	310	19	3
2	278	15	0
3	540	20	8
4	446	16	-31
5	409	12	-1
6	378	13	-10
7	224	5	-1
8	180	7	10
9	88	8	4
10	16	27	-3*
11	48	11	4*
12	143	5	0
H,K=	0,	2	
0	188	5	20
1	1010	40	-10
2	404	28	-2
3	422	26	19
4	37	20	16*
5	20	22	-14*
6	94	7	-0
7	250	12	1
8	102	4	5
9	320	8	-15
10	51	7	1
11	229	6	2
12	34	19	9*
H,K=	0,	3	
1	204	6	-4
2	422	23	-5
3	414	32	-26
4	256	15	-21
5	552	32	-10
6	283	14	-1
7	315	12	1
8	132	4	-8
9	91	19	10*
10	13	29	-9*
11	83	8	1
12	60	7	2
H,K=	0,	4	
0	739	15	57
1	420	9	24
2	416	18	-15
3	157	5	48
4	258	19	7
5	21	15	9*
6	157	5	-7
7	170	4	6
8	276	17	-13
9	156	5	-4
10	211	12	-2
11	61	8	2
12	177	5	6
H,K=	0,	5	
1	417	10	28
2	354	14	-6
3	57	7	26
4	672	47	-11
5	214	11	-3
6	532	34	-14
7	89	4	14
8	187	9	-3
9	26	32	12*
10	13	27	-14*
11	24	27	1*
12	147	6	-4
H,K=	0,	6	
0	679	14	68
1	697	14	73
2	340	12	35
3	474	22	8
4	58	4	0
5	55	10	-7
6	144	8	0
7	228	15	-1
8	169	13	-1
9	282	15	-11
10	166	4	4
11	154	5	-1
12	82	6	5
H,K=	0,	7	
1	274	6	30
2	0	22	-17*
3	735	34	17
4	0	21	-3*
5	556	36	-6
6	48	8	-3
7	337	24	4
8	56	7	7
9	48	39	-12*
10	22	36	-4*
11	102	7	1
H,K=	0,	8	
0	436	9	-2
1	529	11	11
2	490	12	35
3	257	12	-13
4	295	15	7
5	37	37	-4*
6	135	5	-3
7	215	14	-8
8	218	12	-7
9	246	21	-1
10	186	16	-0
11	191	6	8
H,K=	0,	9	
1	112	3	8
2	494	12	29
3	137	4	6
4	430	21	-12
5	82	4	1
6	423	25	5
7	19	37	-2*
8	223	5	1
9	18	27	-3*
10	30	18	18*
11	58	8	-7
H,K=	0,	10	
0	516	11	23
1	282	6	10
2	489	14	31
3	279	6	18
4	28	10	14*
5	32	22	-21*
6	129	12	-9
7	78	5	11
8	292	25	-0
9	149	16	-4
10	247	17	6
11	136	5	3
H,K=	0,	11	
1	226	5	2
2	76	5	-2
3	433	16	24
4	192	5	12
5	457	26	19
6	97	4	-1
7	229	15	13
8	28	30	9*
9	95	5	5
10	0	28	-28*
11	62	8	-13
H,K=	0,	12	
0	280	6	32
1	472	10	22
2	112	4	6
3	341	7	13
4	68	5	3
5	36	14	-5*
6	21	27	3*
7	232	6	-4
8	69	10	10
9	263	20	-6
10	79	6	-1
11	206	6	4
H,K=	0,	13	
1	123	3	-2
2	327	7	19
3	230	5	-2
4	444	19	14
5	227	10	-1
6	314	14	-5
7	115	4	7
8	100	5	-13
9	41	15	37*
10	26	35	21*
H,K=	0,	14	
0	425	9	15
1	59	6	14
2	419	9	18
3	23	24	0*
4	155	4	-2
5	65	6	-9
6	171	7	1
7	31	14	6*
8	241	15	-5
9	0	30	-6*
10	252	20	2
H,K=	0,	15	
1	63	17	-6*
2	221	5	2
3	261	6	11
4	352	12	-6
5	307	14	8
6	259	14	-9
7	220	5	-3
8	103	5	-0
9	76	6	-3
10	27	38	-28*
H,K=	0,	16	
0	21	29	8*
1	410	9	12
2	58	12	-2*
3	213	5	4
4	64	8	-9
5	22	34	9*
6	0	26	-7*
7	215	13	-2
8	50	9	-15
9	233	15	-4
5	36	14	-5*
6	21	27	3*
7	232	6	-4
8	69	10	10
9	263	20	-6
10	79	6	-1
11	206	6	4
H,K=	0,	17	
1	127	11	-4
2	67	6	-2
3	333	7	8
4	173	5	11
5	318	14	2
6	171	5	3
7	186	6	-1
8	104	7	-9
9	38	22	15*
H,K=	0,	18	
0	425	9	7
1	89	7	2
2	360	8	0
3	0	40	-15*
4	75	9	-6
5	26	29	0*
6	107	4	7
7	90	8	9
8	190	6	-3
H,K=	0,	19	
1	22	29	-19*
2	219	6	-1
3	90	5	5
4	247	6	0
5	103	5	-3
6	228	5	-2
7	104	6	-1
8	105	8	-4
H,K=	0,	20	
0	221	5	0
1	344	7	7
2	158	4	1
3	163	4	-1
4	32	33	-6*
5	7	27	-4*
6	61	8	-15
7	140	5	3
H,K=	0,	21	
1	87	13	-10
2	77	6	6
3	250	6	-6
4	41	11	13*
5	254	6	-0
6	66	7	-2
7	186	6	-12
H,K=	0,	22	
0	172	6	2
1	235	5	3
2	180	5	-1
3	119	6	-3
4	44	10	-12*

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	18	36	-20*	12	0	26	-15*	-10	104	5	2	-6	345	23	3	0	457	9	21
6	37	20	4*	H,K=	1,	2		-9	319	13	-15	-5	174	4	8	1	601	13	35
H,K=	0,	23		-12	85	5	1	-8	196	5	-8	-4	70	8	19	2	528	15	29
1	0	28	-37*	-11	37	17	10*	-7	331	17	-11	-3	130	4	22	3	361	13	10
2	198	6	-3	-10	306	7	-11	-6	196	5	-2	-2	335	10	-3	4	281	14	3
3	22	27	-6*	-9	88	12	13	-5	185	5	7	-1	349	7	12	5	37	8	14*
4	263	6	-2	-8	360	8	-23	-4	22	29	14*	0	577	12	54	6	16	32	-0*
5	0	34	-17*	-7	101	4	-1	-3	252	12	-8	1	272	6	3	7	88	5	-3
H,K=	0,	24		-6	385	15	-13	-2	474	19	14	2	863	29	107	8	144	8	1
0	206	7	-12	-5	20	36	-17*	-1	452	14	2	3	262	14	6	9	173	16	-10
1	153	5	-7	-4	88	4	15	0	219	5	9	4	296	17	18	10	166	4	-7
2	166	5	-0	-3	187	6	8	1	397	9	-5	5	218	22	7	11	129	5	-8
3	93	5	-1	-2	374	17	-15	2	93	10	41	6	20	25	16*	H,K=	1,	9	
4	51	10	7*	-1	490	17	-23	3	494	34	1	7	65	8	1	-11	181	5	2
H,K=	0,	25		0	948	24	-2	4	108	3	2	8	188	16	-15	-1(	37	12	7*
1	107	5	-2	1	84	3	3	5	204	11	2	9	125	4	-4	-9	36	11	14*
2	49	11	-4*	2	311	26	-26	6	20	22	13*	10	172	13	2	-8	29	43	-3*
3	178	5	-2	3	68	6	2	7	110	4	-7	11	138	4	-0	-7	255	21	-10
H,K=	1,	0		4	294	18	-9	8	110	6	6	H,K=	1,	7	-6	0	24	-30*	
-11	170	5	-11	5	165	12	3	9	251	15	-1	-12	198	5	-3	-5	472	27	-5
-9	426	9	-18	6	33	34	-3*	10	105	6	-4	-11	35	16	26*	-4	63	6	-3
-7	372	8	1	7	101	5	13	11	192	5	-3	-10	133	4	-1	-3	584	22	14
-5	253	5	-13	8	240	14	3	12	79	8	-4	-9	25	34	19*	-2	186	4	8
-3	413	9	-14	9	98	10	-5	H,K=	1,	5	-8	39	49	-20*	-1	479	10	23	
-1	658	14	-80	10	231	5	-8	-12	63	10	7	-7	0	39	-11*	0	36	9	25*
1	989	20	16	11	71	6	5	-11	145	7	-1	-6	401	26	-8	1	39	10	2*
3	514	11	44	12	203	5	2	-10	51	13	0*	-5	12	29	7*	2	72	4	11
5	213	5	-3	H,K=	1,	3	-9	34	38	-6*	-4	571	29	-18	3	268	10	14	
7	131	4	3	-12	156	5	-3	-8	30	33	-9*	-3	28	12	-2*	4	136	3	8
9	296	7	-1	-11	83	5	-7	-7	213	6	-2	-2	621	19	32	5	396	25	1
11	241	6	0	-10	80	7	-4	-6	36	16	5*	-1	102	3	16	6	72	5	-4
H,K=	1,	1		-9	36	42	34*	-5	528	31	-15	0	341	9	68	7	340	23	2
-12	169	5	-0	-8	86	15	5	-4	196	11	1	1	100	3	7	8	0	40	-7*
-11	107	5	4	-7	148	4	-6	-3	934	46	58	2	282	11	14	9	213	19	0
-10	64	8	2	-6	381	12	-2	-2	202	5	40	3	146	4	10	10	23	27	16*
-9	71	13	1	-5	328	15	0	-1	85	7	-5	4	401	25	13	11	36	19	12*
-8	94	6	7	-4	685	36	-22	0	109	3	17	5	79	4	6	H,K=	1,	10	
-7	123	10	14	-3	30	30	-22*	1	203	6	22	6	461	36	-15	-1:	155	4	-3
-6	185	14	5	-2	58	3	-22	2	282	12	47	7	67	7	1	-1(	148	5	-9
-5	376	11	-16	-1	344	12	3	3	511	30	14	8	308	26	-4	-9	277	21	-8
-4	437	12	-7	0	352	8	14	4	53	5	-11	9	21	28	-11*	-8	167	4	4
-3	468	15	-5	1	413	8	25	5	543	45	-8	10	57	13	-4*	-7	302	18	-2
-2	403	13	-15	2	314	20	20	6	168	5	-10	11	49	10	4*	-6	80	4	-9
-1	405	13	-44	3	330	24	12	7	384	28	-3	H,K=	1,	8	-5	81	6	-11	
0	187	4	-1	4	517	37	9	8	105	5	-9	-12	65	7	8	-4	42	9	1*
1	164	7	15	5	274	17	6	9	135	11	-0	-11	116	5	-3	-3	89	4	-6
2	269	12	8	6	466	27	-8	10	36	23	7*	-10	207	5	-1	-2	131	3	-1
3	409	17	19	7	181	4	-3	11	6	27	5*	-9	224	10	-8	-1	433	9	14
4	367	14	-8	8	297	11	-4	12	29	34	17*	-8	298	20	-3	0	273	6	20
5	394	16	-4	9	111	7	-7	H,K=	1,	6	-7	210	16	-9	1	549	11	29	
6	323	7	-3	10	39	43	4*	-12	122	5	3	-6	186	9	-12	2	381	11	17
7	305	6	-5	11	10	28	7*	-11	78	6	-9	-5	200	11	5	3	437	13	2
8	203	6	7	12	53	9	1	-10	164	4	-2	-4	197	15	10	4	82	4	-4
9	169	8	11	H,K=	1,	4	-9	254	6	-11	-3	182	8	14	5	20	39	1*	
10	38	12	-11*	-12	27	31	7*	-8	292	15	-10	-2	370	12	7	6	66	5	8
11	41	10	36*	-11	196	6	7	-7	246	14	-6	-1	282	6	17	7	175	5	-11

STRUCTURE FACTORS CONTINUED FOR
Y8.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
8	104	7	-2	-6	239	12	-5	6	255	6	-2	2	93	9	-3	6	263	13	-2
9	192	6	-7	-5	353	15	-2	7	196	12	-4	3	244	5	1	7	64	7	-6
10	84	7	-2	-4	248	11	3	8	153	4	-3	4	33	19	26*	H,K=		1,	22
11	192	5	-1	-3	446	13	11	9	87	11	1	5	91	4	-3	-6	149	5	-2
H,K=		1,	11	-2	251	5	7	H,K=		1,	16	6	35	15	-21*	-5	64	7	8
-11	77	6	0	-1	267	6	1	-9	37	12	34*	7	63	8	11	-4	28	29	22*
-10	125	4	8	0	22	59	-24*	-8	295	17	4	8	71	9	-2	-3	48	11	-10*
-9	37	28	31*	1	0	34	-9*	-7	45	10	-4*	H,K=		1,	19	-2	104	7	-3
-8	149	4	-3	2	6	23	-2*	-6	260	12	1	-8	35	14	-5*	-1	133	5	3
-7	49	8	20	3	291	6	1	-5	27	39	17*	-7	128	6	6	0	204	5	0
-6	294	16	-3	4	174	5	-1	-4	30	37	-8*	-6	73	6	-5	1	224	5	-2
-5	219	5	-8	5	373	19	1	-3	72	7	-2	-5	241	5	-2	2	189	5	-1
-4	498	19	-3	6	187	6	1	-2	212	5	-4	-4	127	4	-2	3	175	5	-1
-3	227	5	4	7	252	17	-6	-1	17	24	5*	-3	320	7	-3	4	95	7	6
-2	503	10	50	8	107	5	1	0	405	8	11	-2	181	5	-7	5	87	6	-10
-1	193	4	6	9	118	4	-6	1	107	4	7	-1	198	6	3	6	29	33	-8*
0	145	11	-13	10	0	49	-17*	2	403	9	-1	0	68	7	-13	H,K=		1,	23
1	42	53	-19*	H,K=		1,	14	3	46	8	9	1	0	61	-47*	-5	236	7	-6
2	160	4	8	-10	58	8	-3	4	213	5	7	2	32	16	-5*	-4	34	14	11*
3	116	3	0	-9	274	18	12	5	0	41	-11*	3	229	5	-1	-3	272	6	-2
4	345	14	11	-8	21	29	3*	6	50	7	10	4	38	10	-4*	-2	21	27	-5*
5	109	5	5	-7	291	14	4	7	23	34	-4*	5	239	5	5	-1	194	5	-2
6	366	24	-5	-6	42	17	-6*	8	124	5	0	6	99	6	-0	0	24	28	8*
7	101	11	10	-5	197	11	1	9	47	12	-5*	7	219	6	-11	1	0	38	-13*
8	207	16	-4	-4	14	29	-11*	H,K=		1,	17	8	89	6	-7	2	26	28	24*
9	28	22	-11*	-3	82	4	-4	-9	30	25	-3*	H,K=		1,	20	3	161	5	-6
10	101	6	-3	-2	34	9	3*	-8	39	18	-5*	-8	183	5	-3	4	0	28	-21*
11	34	16	7*	-1	392	8	18	-7	116	4	3	-7	124	4	2	5	227	7	-9
H,K=		1,	12	0	70	4	0	-6	225	5	-7	-6	146	4	4	H,K=		1,	24
-11	60	13	-9*	1	503	11	8	-5	168	5	-2	-5	43	15	9*	-4	17	29	15*
-10	206	16	-0	2	12	25	2*	-4	309	10	-0	-4	15	29	13*	-3	29	39	-25*
-9	96	4	8	3	430	14	13	-3	242	5	7	-3	71	13	-8	-2	97	5	-9
-8	292	18	-9	4	50	7	4	-2	323	7	3	-2	201	5	1	-1	147	7	-5
-7	89	6	13	5	172	4	-7	-1	139	9	0	-1	140	7	-5	0	113	7	-3
-6	266	13	11	6	22	36	6*	0	83	18	-11*	0	299	6	4	1	201	5	-1
-5	35	12	-13*	7	103	5	-2	1	64	9	-9	1	216	5	-6	2	185	5	-13
-4	21	23	3*	8	20	26	6*	2	133	4	-3	2	304	7	2	3	150	5	-2
-3	29	10	-13*	9	178	13	-2	3	30	15	8*	3	93	8	-3	4	108	5	-6
-2	338	7	16	10	7	28	-10*	4	261	6	2	4	157	5	-8	H,K=		1,	25
-1	117	3	6	H,K=		1,	15	5	166	4	3	5	25	27	7*	-3	74	8	5
0	578	12	23	-10	29	29	-1*	6	261	11	-2	6	13	27	-12*	-2	198	6	-13
1	285	6	12	-9	30	33	-16*	7	148	5	-5	7	57	13	-19*	-1	26	34	-11*
2	598	12	26	-8	54	9	-19	8	164	5	-1	H,K=		1,	21	0	54	16	-11*
3	155	3	4	-7	87	5	-2	9	94	5	-6	-7	49	10	-19*	1	45	11	-8*
4	240	5	15	-6	228	10	1	H,K=		1,	18	-6	179	5	-6	2	84	6	-10
5	50	3	3	-5	308	7	-9	-9	205	5	-5	-5	57	7	4	H,K=		2,	0
6	104	9	-2	-4	334	14	1	-8	74	12	-6	-4	263	6	-2	-12	15	29	8*
7	36	37	-24*	-3	334	7	1	-7	259	14	0	-3	79	6	6	-11	253	6	-10
8	156	6	-10	-2	284	6	5	-6	69	5	9	-2	292	6	-5	-8	350	7	-11
9	14	33	-17*	-1	188	4	-10	-5	96	4	-4	-1	11	33	-21*	-6	432	9	-14
10	193	6	-16	0	104	8	5	-4	67	10	11	0	109	7	-4	-4	209	4	-17
H,K=		1,	13	1	0	62	-15*	-3	120	4	-5	1	0	27	-18*	-2	32	8	11*
-10	79	6	-5	2	26	17	6*	-2	33	35	-22*	2	48	12	-11*	0	304	6	-33
-9	17	31	-2*	3	170	4	2	-1	365	8	-1	3	35	21	-19*	2	675	15	60
-8	5	26	-5*	4	268	10	4	0	144	5	-6	4	231	5	-5	4	482	10	2
-7	190	5	4	5	267	6	1	1	417	9	-8	5	44	10	14*	6	89	4	13

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
8	68	9	20	-9	185	7	-9	-3	87	3	-19	3	89	4	23	10	173	18	-2
10	21€	6	-4	-8	55	8	-2	-2	646	23	29	4	17	21	14*	11	20	28	8*
H,K=		2,	1	-7	105	7	-10	-1	211	5	33	5	255	20	-11	H,K=		2,	10
-12	154	6	4	-6	58	4	-9	0	443	11	42	6	33	11	16*	-11	45	10	-15*
-11	150	4	-4	-5	461	16	-3	1	10	35	-22*	7	353	32	-17	-1€	137	4	-3
-10	177	4	4	-4	339	10	8	2	14	33	-21*	8	93	12	-3	-9	150	4	-5
-9	133	5	-7	-3	783	34	27	3	192	11	17	9	229	16	-2	-8	291	15	-10
-8	56	6	9	-2	154	5	-1	4	263	20	-13	10	34	18	7*	-7	229	12	-10
-7	87	6	3	-1	427	13	-9	5	148	12	-8	11	101	10	2	-€	353	14	11
-6	18€	6	10	0	200	5	-9	6	342	25	-7	H,K=		2,	8	-5	99	6	1
-5	273	10	-12	1	280	7	20	7	82	5	-12	-12	37	14	-11*	-4	104	3	-12
-4	411	10	-26	2	0	39	-6*	8	333	25	-7	-11	64	6	4	-3	96	4	7
-3	30ę	7	10	3	124	4	7	9	97	4	-6	-10	94	5	-7	-2	138	4	7
-2	303	9	-54	4	161	13	-10	10	120	7	-3	-9	221	13	-3	-1	166	4	4
-1	499	11	-62	5	334	21	-0	11	44	13	29*	-8	309	15	-6	0	399	8	16
0	531	16	-68	6	166	4	1	H,K=		2,	6	-7	260	18	8	1	290	6	22
1	162	5	5	7	352	18	0	-12	29	21	21*	-6	223	13	-9	2	520	14	12
2	289	8	60	8	164	5	0	-11	106	8	-7	-5	78	4	-8	3	134	3	-1
3	214	6	24	9	258	6	4	-10	102	5	-3	-4	286	11	-18	4	242	5	6
4	243	5	-3	10	32	18	1*	-9	202	6	-1	-3	139	3	-1	5	130	4	-2
5	200	4	-1	11	100	7	-7	-8	202	5	-1	-2	237	5	15	6	57	7	-0
6	25ę	5	-10	H,K=		2,	4	-7	361	16	-13	-1	170	4	-6	7	83	14	-2
7	19ę	5	-3	-12	45	10	-3*	-€	194	5	-6	0	258	5	-2	8	50	23	2*
8	31ę	12	-11	-11	71	8	4	-5	409	26	20	1	418	9	18	ę	64	9	-2
9	191	5	4	-10	205	5	-2	-4	226	6	2	2	314	8	7	10	132	5	-5
10	13€	4	7	-9	107	8	-2	-3	26	72	-15*	3	500	19	3	H,K=		2,	11
11	60	7	15	-8	380	15	-10	-2	129	13	7	4	116	4	4	-11	194	5	-2
H,K=		2,	2	-7	157	4	-6	-1	306	6	37	5	219	13	-6	-1€	29	23	-24*
-12	13	27	12*	-6	434	21	-2	0	367	8	45	6	112	4	-3	-9	114	5	4
-11	143	4	-5	-5	191	4	10	1	564	11	43	7	39	25	21*	-8	47	9	13*
-10	52	12	-9*	-4	302	7	-12	2	388	11	7	8	20	27	-17*	-7	165	4	5
-9	367	8	-8	-3	46	6	15	3	489	22	-7	9	82	7	6	-6	134	4	3
-8	66	5	18	-2	210	5	16	4	353	24	-5	10	103	5	1	-5	306	7	-7
-7	371	12	-22	-1	64	12	-34*	5	232	17	2	11	155	16	-1	-4	101	4	-4
-6	36	15	8*	0	331	7	6	6	82	4	-4	H,K=		2,	9	-3	513	16	16
-5	361	8	0	1	210	6	28	7	105	6	-7	-11	49	14	3*	-2	288	6	3
-4	15	33	-7*	2	764	29	59	8	55	20	16*	-10	175	5	2	-1	569	12	25
-3	181	5	17	3	312	25	8	9	100	5	-9	-9	45	10	11*	0	132	3	13
-2	157	4	0	4	443	35	3	10	92	5	2	-8	33	46	-10*	1	221	5	11
-1	102	9	-9	5	163	15	3	11	153	7	-3	-7	0	25	-12*	2	30	12	8*
0	94	9	10	6	189	13	-6	H,K=		2,	7	-6	223	13	-3	3	71	4	-0
1	434	9	-15	7	55	7	-3	-12	15	28	8*	-5	29	10	-28*	4	76	6	1
2	61	16	7*	8	42	26	6*	-11	210	7	2	-4	436	20	5	5	321	21	0
3	€52	36	-1	9	75	7	-0	-10	18	27	5*	-3	53	5	6	6	214	14	-6
4	198	12	8	10	189	6	5	-9	151	6	-5	-2	604	18	21	7	312	23	1
5	337	13	14	11	97	5	5	-8	47	8	8	-1	105	3	2	8	86	7	-2
6	66	5	0	H,K=		2,	5	-7	69	14	-10*	0	499	10	21	9	210	14	-7
7	8	43	-9*	-12	201	5	-0	-6	51	9	1*	1	0	27	-16*	10	48	10	-6*
8	73	5	21	-11	77	7	7	-5	303	8	12	2	156	4	12	H,K=		2,	12
9	17€	4	4	-10	207	5	4	-4	188	5	16	3	58	5	19	-11	55	9	-13
10	45	14	17*	-9	23	34	18*	-3	618	25	2	4	186	11	-5	-1€	95	7	7
11	191	6	2	-8	69	10	5	-2	150	4	24	5	15	25	0*	-ę	236	12	-0
H,K=		2,	3	-7	21	31	4*	-1	531	15	6	6	388	28	-0	-8	112	4	-12
-12	14ę	4	5	-6	281	11	-5	0	125	3	13	7	76	7	12	-7	332	16	-2
-11	13€	4	-1	-5	61	8	-5	1	199	4	1	8	326	30	-12	-6	79	5	10
-10	114	4	-2	-4	557	27	1	2	48	4	11	9	16	28	-6*	-5	282	13	11

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	55	6	5	7	26	28	18*	1	146	5	6	3	265	6	-2	-2	58	8	-8
-3	40	7	4	8	29	38	5*	2	70	5	1	4	95	6	-6	-1	168	10	-12
-2	21	22	-3*	9	6	30	-6*	3	158	6	-9	5	174	5	4	0	41	16	29*
-1	395	8	7	H,K=	2,	15		4	53	9	-7	6	24	37	-10*	1	87	13	-5
0	128	4	15	-10	121	5	3	5	175	5	3	7	49	9	-5*	2	11	29	-24*
1	474	10	10	-9	56	7	-2	6	125	4	4	H,K=	2,	21		H,K=	3,	0	
2	224	5	17	-8	27	25	-14*	7	207	13	3	-7	23	37	-9*	-11	57	9	-0
3	449	15	-1	-7	31	14	-24*	8	137	5	-4	-6	74	7	-6	-9	249	7	1
4	208	5	7	-6	75	13	-9	H,K=	2,	18		-5	176	5	-4	-7	356	7	-15
5	236	14	-6	-5	249	6	-0	-9	79	7	4	-4	70	12	7	-5	481	10	-7
6	158	4	-2	-4	171	4	5	-8	233	5	-7	-3	304	7	-1	-3	195	4	-44
7	22	36	14*	-3	337	7	2	-7	74	6	-3	-2	99	6	8	-1	65	7	25
8	15	26	8*	-2	259	6	9	-6	240	5	-7	-1	230	5	0	1	617	13	56
9	99	7	-4	-1	260	6	9	-5	81	5	-3	0	0	26	-14*	3	539	12	28
10	33	16	-9*	0	173	4	5	-4	104	5	7	1	175	6	-3	5	468	10	8
H,K=	2,	13		1	169	6	-4	-3	7	31	-12*	2	0	27	-11*	7	161	5	-7
-11	139	4	9	2	0	36	-4*	-2	85	5	-5	3	49	9	-16	9	52	8	32
-10	126	4	-10	3	0	26	-19*	-1	30	40	3*	4	23	27	21*	11	122	8	2
-9	37	12	-7*	4	110	7	-4	0	321	7	-3	5	185	5	-3	H,K=	3,	1	
-8	25	26	-0*	5	208	5	-2	1	141	4	0	6	41	13	16*	-12	110	6	-0
-7	56	14	3*	6	202	12	2	2	323	7	4	H,K=	2,	22	-11	180	6	8	
-6	185	5	-4	7	173	5	-4	3	50	10	-6*	-6	158	5	4	-10	194	5	0
-5	208	5	9	8	151	6	-5	4	263	12	5	-5	127	4	-1	-9	232	7	-2
-4	348	8	1	9	145	19	-5	5	36	11	-3*	-4	66	8	-4	-8	101	4	-2
-3	226	9	10	H,K=	2,	16		6	116	4	-5	-3	10	39	-11*	-7	24	31	-7*
-2	446	9	-0	-10	0	32	-17*	7	0	40	-14*	-2	26	34	-5*	-6	114	4	9
-1	219	5	6	-9	201	5	-6	8	56	8	4	-1	21	27	-15*	-5	186	19	25
0	246	7	3	-8	19	28	14*	H,K=	2,	19		0	85	5	-10	-4	167	4	-9
1	54	16	-14*	-7	305	7	-3	-8	54	15	-13*	1	125	6	-3	-3	310	6	-31
2	102	4	-0	-6	22	26	-8*	-7	32	28	-14*	2	260	6	-4	-2	507	10	1
3	63	7	11	-5	220	6	5	-6	111	4	-4	3	146	6	2	-1	482	10	-47
4	218	12	-1	-4	85	5	-5	-5	91	6	1	4	194	5	-2	0	369	8	-16
5	152	14	3	-3	58	6	0	-4	267	6	4	5	97	6	-3	1	378	8	-0
6	254	18	-5	-2	13	25	10*	-3	159	4	-6	H,K=	2,	23		2	239	6	-4
7	167	12	-4	-1	224	5	-4	-2	332	7	-2	-5	8	28	-7*	3	124	4	-2
8	183	12	-7	0	27	30	-16*	-1	142	4	3	-4	242	7	-5	4	81	4	0
9	109	6	3	1	342	7	12	0	246	7	7	-3	25	27	5*	5	145	4	2
10	136	17	-2	2	24	26	-7*	1	65	6	-8	-2	252	6	-1	6	189	5	-3
H,K=	2,	14		3	338	11	10	2	12	48	-33*	-1	18	26	1*	7	252	7	-7
-10	135	4	-7	4	28	37	-6*	3	34	36	27*	0	165	4	5	8	225	7	-6
-9	59	11	-12	5	255	13	-2	4	184	5	-3	1	14	27	-6*	9	261	7	-16
-8	280	14	8	6	31	15	19*	5	37	13	-4*	2	18	39	-3*	10	129	4	-3
-7	59	6	-0	7	62	7	1	6	234	12	11	3	20	33	-9*	11	121	8	-8
-6	319	14	-5	8	20	33	7*	7	87	32	-10*	4	114	5	-5	H,K=	3,	2	
-5	23	31	3*	9	113	5	-6	H,K=	2,	20		5	20	29	-9*	-12	58	8	-5
-4	145	4	4	H,K=	2,	17		-8	126	4	4	H,K=	2,	24	-11	51	8	0	
-3	33	11	15*	-9	108	6	5	-7	213	5	-2	-4	78	8	-3	-10	100	4	-8
-2	79	4	3	-8	23	29	12*	-6	120	5	-6	-3	0	28	-3*	-9	20	37	-0*
-1	83	4	5	-7	18	27	-3*	-5	142	4	0	-2	0	44	-9*	-8	314	7	-4
0	415	9	16	-6	92	5	1	-4	38	10	10*	-1	90	6	-10	-7	74	5	4
1	45	11	8*	-5	181	5	-1	-3	39	10	17*	0	162	6	5	-6	497	13	-21
2	415	9	10	-4	217	5	-1	-2	0	30	-35*	1	141	5	-9	-5	106	6	0
3	71	7	5	-3	332	7	4	-1	118	4	-4	2	185	5	6	-4	432	12	-28
4	370	14	1	-2	289	6	5	0	104	6	-4	3	184	5	-5	-3	27	36	-33*
5	135	8	8	-1	269	6	3	1	289	6	7	H,K=	2,	25	-2	120	4	-14	
6	200	5	-6	0	133	15	3	2	133	5	-1	-3	210	5	-10	-1	33	42	14*

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
0	252	6	3	6	127	4	-1	H,K=	3,	7		-5	162	4	-6	5	106	4	10
1	0	40	-13*	7	207	15	1	-12	217	6	3	-4	90	4	4	6	261	7	-9
2	491	11	9	8	10	44	3*	-11	20	36	9*	-3	410	16	-8	7	152	5	2
3	120	3	14	9	53	8	13	-10	222	6	3	-2	37	5	5	8	272	23	-3
4	612	13	26	10	38	22	21*	-9	24	28	-15*	-1	681	14	39	9	90	7	-1
5	78	5	-6	11	146	9	-5	-8	187	5	3	0	69	3	-3	10	193	7	-9
6	257	7	7	H,K=	3,	5	-7	21	24	-7*		1	387	8	35	H,K=	3,	12	
7	51	7	5	-12	76	6	-0	-6	31	9	22*	2	36	11	2*	-11	31	18	-3*
8	151	6	-0	-11	220	6	0	-5	53	5	2	3	150	4	-3	-10	52	8	-5
9	61	6	24	-10	54	7	3	-4	270	11	5	4	78	4	7	-9	68	6	2
10	159	6	3	-9	284	7	3	-3	185	4	18	5	204	14	-7	-8	226	6	-2
11	27	28	15*	-8	38	15	26*	-2	563	18	-15	6	91	5	-6	-7	107	9	-1
H,K=	3,	3	-7	97	6	-6	-1	129	3	16		7	363	29	-5	-6	433	22	-7
-12	186	6	5	-6	49	13	-10*	0	497	10	-6	8	28	24	3*	-5	64	9	13
-11	151	4	7	-5	130	12	-3	1	40	5	-8	9	268	24	-16	-4	312	12	8
-10	241	6	7	-4	169	7	-7	2	287	6	5	10	22	31	18*	-3	70	4	-3
-9	83	9	-2	-3	544	23	-17	3	44	5	-8	H,K=	3,	10	-2	144	4	8	
-8	146	5	-8	-2	140	3	-9	4	26	28	-8*	-11	25	33	12*	-1	54	5	-8
-7	41	11	-11*	-1	735	22	36	5	75	5	9	-10	50	8	-6	0	214	5	9
-6	77	20	37*	0	104	4	-14	6	273	23	-11	-9	163	6	2	1	173	11	4
-5	158	4	-16	1	366	8	-1	7	0	45	-8*	-8	197	5	-7	2	356	8	8
-4	266	6	-14	2	192	5	11	8	281	8	-19	-7	341	17	-12	3	176	4	13
-3	217	5	-28	3	172	11	1	9	24	38	-6*	-6	116	4	3	4	427	11	-7
-2	595	17	-1	4	73	4	-5	10	205	24	-13	-5	327	18	6	5	236	6	-4
-1	386	11	20	5	107	4	0	11	13	29	-14*	-4	200	5	1	6	293	10	-1
0	722	15	42	6	49	8	-3	H,K=	3,	8		-3	290	6	5	7	24	35	-16*
1	232	5	19	7	313	26	-5	-12	53	14	5*	-2	65	5	7	8	45	33	-13*
2	431	20	32	8	64	16	-8*	-11	46	10	-0*	-1	22	12	1*	9	8	30	1*
3	202	6	12	9	236	7	-5	-10	47	10	4*	0	99	3	4	10	78	7	-6
4	10	21	-16*	10	15	33	-29*	-9	129	4	-6	1	190	4	4	H,K=	3,	13	
5	127	4	1	11	172	8	-5	-8	207	6	2	2	249	6	11	-11	179	8	-2
6	260	17	3	H,K=	3,	6	-7	294	17	-2	3	398	9	1	-10	103	5	3	
7	93	5	-4	-12	31	22	25*	-6	321	17	3	4	289	7	2	-9	167	4	-4
8	328	10	-3	-11	0	36	-5*	-5	261	10	-10	5	340	16	7	-8	83	5	-7
9	146	5	-5	-10	68	6	7	-4	136	3	-2	6	182	14	-5	-7	122	6	12
10	203	7	-4	-9	63	18	-4*	-3	165	4	1	7	152	5	-6	-6	86	10	0
11	43	13	-1*	-8	295	11	-4	-2	60	6	-3	8	0	28	-18*	-5	216	6	3
H,K=	3,	4	-7	197	10	3	-1	0	30	-6*		9	56	8	18	-4	86	6	-9
-12	41	23	13*	-6	293	14	-4	0	176	4	10	10	28	26	-12*	-3	284	7	9
-11	47	10	5*	-5	240	14	-17	1	290	6	13	H,K=	3,	11	-2	268	6	9	
-10	35	17	0*	-4	415	23	-10	2	400	9	14	-11	72	6	-4	-1	362	8	6
-9	159	5	4	-3	156	17	-18	3	256	6	-3	-10	213	5	2	0	210	5	3
-8	59	6	-7	-2	60	19	-7*	4	287	16	0	-9	61	8	-2	1	302	8	6
-7	378	14	-13	-1	48	20	20*	5	264	16	-3	-8	187	5	9	2	122	4	-2
-6	243	12	-3	0	278	6	34	6	269	24	-6	-7	162	6	4	3	108	4	6
-5	453	20	-22	1	426	10	21	7	149	8	4	-6	60	6	10	4	0	27	-10*
-4	316	8	-10	2	372	9	-1	8	54	17	-10*	-5	47	9	-15*	5	100	7	3
-3	328	9	8	3	399	17	16	9	0	27	-10*	-4	266	6	-1	6	189	6	4
-2	84	6	-2	4	442	30	-2	10	92	11	5	-3	188	4	3	7	180	15	-2
-1	37	9	10*	5	218	19	-11	H,K=	3,	9		-2	494	15	25	8	131	8	-2
0	245	6	40	6	268	25	-7	-11	219	6	6	-1	240	5	7	9	180	7	-12
1	421	10	21	7	93	7	-9	-10	61	14	-7*	0	503	11	24	H,K=	3,	14	
2	157	4	-18	8	108	5	-10	-9	195	5	-3	1	128	3	2	-10	32	15	-8*
3	567	44	-27	9	36	27	12*	-8	43	21	-1*	2	288	6	27	-9	127	8	-6
4	169	13	0	10	84	5	1	-7	77	5	1	3	58	6	-3	-8	55	7	3
5	466	35	-3	11	121	8	-2	-6	31	12	24*	4	38	13	12*	-7	271	14	1

STRUCTURE FACTORS CONTINUED FOR
Y8.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	46	23	14*	H,K=	3,	17		-7	83	5	7	-2	21	44	6*	-6	105	3	-1
-5	320	11	3	-9	79	6	-1	-6	229	5	3	-1	0	28	-4*	-5	535	15	-25
-4	18	25	14*	-8	137	6	4	-5	142	7	-1	0	49	19	-7*	-4	83	3	1
-3	255	5	5	-7	15	27	-21*	-4	185	5	6	1	168	5	5	-3	473	10	-40
-2	36	9	-16*	-6	24	26	19*	-3	96	4	-0	2	147	5	-6	-2	70	3	0
-1	81	4	3	-5	115	4	9	-2	103	4	-7	3	187	5	-2	-1	434	9	37
0	79	6	4	-4	202	5	3	-1	8	27	-11*	H,K=	3,	25	0	16	27	13*	
1	255	7	4	-3	140	5	4	0	72	63	-33*	-2	248	6	1	1	251	6	-6
2	32	12	-5*	-2	303	6	-3	1	40	19	-4*	-1	69	9	10	2	46	5	5
3	442	11	4	-1	258	6	2	2	256	6	-0	0	211	7	-7	3	446	9	10
4	126	4	-6	0	337	7	1	3	163	4	2	1	16	31	-12*	4	59	5	-8
5	392	10	-10	1	178	5	6	4	232	6	-9	H,K=	4,	0	5	560	14	9	
6	30	15	23*	2	166	9	5	5	139	7	-1	-12	139	5	2	6	125	4	-2
7	140	6	-4	3	34	12	-2*	6	162	7	-8	-10	32	12	23*	7	306	8	3
8	32	23	24*	4	58	8	-4	H,K=	3,	21	-8	236	5	-8	8	15	32	-4*	
9	69	7	23	5	85	5	-1	-7	30	19	-7*	-6	542	11	-15	9	78	6	23
H,K=	3,	15	6	108	5	-6	-6	29	30	3*	-4	494	10	-47	10	48	11	11*	
-10	142	4	2	7	131	5	0	-5	43	10	0*	-2	299	6	-22	11	66	11	-4
-9	124	5	-1	8	194	7	1	-4	189	5	-5	0	138	4	-6	H,K=	4,	3	
-8	114	5	0	H,K=	3,	18		-3	32	17	-10*	2	324	7	2	-12	68	6	-2
-7	77	6	8	-9	171	5	4	-2	242	5	-5	4	685	15	47	-11	203	5	6
-6	53	8	-7	-8	64	6	8	-1	90	5	5	6	404	10	6	-10	123	6	1
-5	61	7	3	-7	230	7	-4	0	262	6	-2	8	270	7	-14	-9	294	7	-7
-4	199	5	-1	-6	86	5	-0	1	23	27	-13*	10	56	11	19*	-8	133	4	5
-3	207	10	1	-5	264	13	6	2	171	6	-14	H,K=	4,	1	-7	202	5	-6	
-2	307	6	0	-4	130	6	-7	3	17	28	-9*	-12	128	6	5	-6	16	22	-13*
-1	259	6	1	-3	224	5	-2	4	20	30	-0*	-11	166	6	3	-5	130	17	8
0	249	5	6	-2	30	38	-7*	5	17	28	8*	-10	247	5	-5	-4	108	15	9
1	186	4	7	-1	41	9	-14*	6	147	6	-7	-9	210	6	0	-3	318	7	-8
2	181	5	-0	0	8	43	2*	H,K=	3,	22	-8	250	5	-13	-2	258	5	-13	
3	44	22	2*	1	268	6	3	-6	141	4	-1	-7	180	4	-4	-1	467	11	-31
4	9	39	4*	2	74	8	-7	-5	171	5	-3	-6	125	13	-13	0	382	8	19
5	70	13	-4*	3	328	8	-7	-4	156	4	2	-5	70	39	29*	1	531	24	-42
6	137	6	6	4	80	7	-1	-3	101	5	-2	-4	92	66	66*	2	281	13	10
7	128	4	-1	5	245	7	-1	-2	81	8	12	-3	316	6	-6	3	356	7	9
8	178	7	-2	6	62	10	1	-1	17	44	-1*	-2	416	8	-29	4	198	5	9
9	155	7	1	7	118	6	3	0	31	37	-9*	-1	393	8	-37	5	26	28	7*
H,K=	3,	16	H,K=	3,	19		1	87	9	-14	0	492	10	-42	6	77	5	-3	
-9	11	30	7*	-8	44	21	22*	2	127	5	-6	1	455	9	19	7	239	8	1
-8	166	4	-1	-7	75	6	6	3	220	5	-6	2	353	7	-11	8	116	5	2
-7	23	35	8*	-6	31	15	-5*	4	159	6	-2	3	267	6	27	9	255	6	-4
-6	303	7	-1	-5	72	5	2	5	157	7	-8	4	105	3	-0	10	124	8	0
-5	46	16	-9*	-4	80	5	-1	H,K=	3,	23	5	25	20	5*	11	178	6	2	
-4	266	6	2	-3	301	6	3	-5	88	10	-14	6	157	4	1	H,K=	4,	4	
-3	57	6	7	-2	143	4	-6	-4	21	28	18*	7	131	6	-2	-12	141	5	10
-2	128	6	-12	-1	294	7	3	-3	245	6	-8	8	229	6	-2	-11	0	27	-17*
-1	7	25	-11*	0	98	4	-3	-2	50	8	46	9	219	6	-0	-10	47	11	-1*
0	189	17	-7	1	302	7	-7	-1	217	6	-11	10	181	6	-8	-9	0	36	-6*
1	19	26	14*	2	24	27	-16*	0	0	30	-8*	11	126	5	3	-8	181	4	1
2	314	7	-4	3	20	33	-24*	1	214	6	-11	H,K=	4,	2	-7	81	4	-1	
3	49	10	2*	4	34	12	12*	2	15	28	-20*	-12	17	28	9*	-6	366	15	-12
4	377	10	-4	5	82	8	-2	3	55	8	-6	-11	79	9	-2	-5	296	14	-1
5	0	27	-10*	6	26	28	-15*	4	45	10	10*	-10	48	8	12	-4	501	20	-17
6	221	6	-5	7	198	7	-4	H,K=	3,	24	-9	85	8	5	-3	231	6	-13	
7	22	27	1*	H,K=	3,	20		-4	89	9	0	-8	19	29	-3*	-2	395	10	-23
8	0	28	-7*	-8	185	6	-7	-3	131	4	1	-7	323	7	1	-1	275	6	37

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
0	129	4	26	8	70	8	7	-7	106	6	-4	3	239	5	3	-5	136	5	-4
1	84	3	6	9	59	10	7	-6	162	5	-12	4	15	30	11*	-4	408	14	10
2	274	6	-0	10	18	46	-22*	-5	13	27	-11*	5	31	27	25*	-3	31	12	23*
3	183	11	3	H,K=		4,	7	-4	170	5	-4	6	105	8	-5	-2	251	6	7
4	516	25	5	-12	0	34	-19*	-3	51	7	-1	7	199	6	2	-1	158	158	156*
5	182	5	1	-11	244	6	-9	-2	383	9	8	8	101	7	-0	0	21	29	-8*
6	353	16	-5	-10	26	46	12*	-1	56	5	6	9	236	6	4	1	4	25	-27*
7	97	6	7	-9	308	7	-8	0	674	14	12	H,K=		4,	12	2	269	6	3
8	171	5	7	-8	45	55	5*	1	25	29	4*	-11	81	8	3	3	82	7	-5
9	30	20	3*	-7	268	6	-13	2	431	9	13	-10	8	33	-8*	4	423	9	17
10	52	10	3*	-6	0	28	-17*	3	108	4	-1	-9	46	17	-3*	5	35	17	6*
H,K=		4,	5	-5	35	12	33*	4	128	5	-1	-8	61	18	-1*	6	278	9	3
-12	197	18	14	-4	42	10	-18*	5	61	14	19*	-7	264	6	-12	7	0	32	-6*
-11	85	8	3	-3	367	8	-5	6	216	6	7	-6	126	5	-14	8	94	10	-5
-10	253	18	5	-2	55	5	9	7	46	17	5*	-5	419	9	-8	9	11	34	-12*
-9	53	11	-4*	-1	554	12	-26	8	262	8	3	-4	163	7	-4	H,K=		4,	15
-8	287	13	2	0	59	5	28	9	71	8	23	-3	392	9	-1	-10	161	4	2
-7	91	4	-6	1	575	12	12	10	254	7	14	-2	45	13	-7*	-9	140	4	3
-6	206	5	-10	2	0	24	-7*	H,K=		4,	10	-1	170	6	3	-8	138	15	14
-5	10	34	-9*	3	250	5	-0	-11	27	33	19*	0	59	7	-6	-7	139	4	4
-4	122	27	-10*	4	34	20	19*	-10	46	13	28*	1	131	5	6	-6	85	6	0
-3	125	5	18	5	34	37	28*	-9	68	9	0	2	85	6	-6	-5	61	7	-1
-2	493	17	-6	6	55	12	26*	-8	163	5	-8	3	389	8	26	-4	73	9	-10
-1	78	6	-8	7	267	7	7	-7	152	6	-13	4	114	7	-1	-3	128	6	-3
0	619	13	-17	8	20	31	-6*	-6	377	8	-23	5	415	9	17	-2	222	5	6
1	124	4	-9	9	240	6	1	-5	255	7	-12	6	87	6	5	-1	323	7	5
2	561	11	29	10	0	36	-16*	-4	356	8	-0	7	224	6	5	0	347	8	-2
3	170	5	11	H,K=		4,	8	-3	181	5	-10	8	47	18	2*	1	324	7	10
4	154	4	5	-12	53	13	8*	-2	356	8	11	9	38	52	14*	2	280	6	15
5	45	26	7*	-11	59	21	-11*	-1	142	4	3	H,K=		4,	13	3	142	4	-3
6	159	5	-5	-10	0	32	-3*	0	128	4	1	-10	188	6	-15	4	14	27	-13*
7	24	44	10*	-9	68	8	5	1	94	4	5	-9	134	6	13	5	0	28	-11*
8	227	6	8	-8	215	5	-17	2	257	6	9	-8	220	6	-11	6	91	5	6
9	64	11	10	-7	247	6	-19	3	228	5	12	-7	171	5	-9	7	136	7	-5
10	262	7	16	-6	210	5	-26	4	343	8	12	-6	74	7	-2	8	141	7	-3
H,K=		4,	6	-5	289	7	2	5	230	5	2	-5	41	33	27*	H,K=		4,	16
-12	103	7	8	-4	380	9	-14	6	366	8	13	-4	121	6	1	-9	77	5	-0
-11	62	15	12*	-3	328	7	-5	7	150	5	1	-3	98	5	-3	-8	40	17	10*
-10	55	10	4	-2	220	5	-17	8	134	5	6	-2	280	7	3	-7	212	5	6
-9	88	9	3	-1	244	5	14	9	66	11	1	-1	260	6	2,	-6	22	29	19*
-8	99	8	-8	0	52	5	21	10	33	34	-8*	0	391	8	7	-5	377	13	-4
-7	238	6	-12	1	160	4	6	H,K=		4,	11	1	197	7	3	-4	44	24	-7*
-6	270	6	-12	2	251	5	17	-11	189	6	-2	2	263	6	6	-3	377	8	2
-5	395	9	-36	3	396	8	14	-10	79	20	-2*	3	176	5	-0	-2	24	26	13*
-4	267	6	-27	4	338	7	23	-9	245	6	-10	4	122	7	15	-1	106	4	5
-3	299	7	-14	5	339	7	10	-8	115	5	-1	5	62	31	-5*	0	0	26	-2*
-2	288	6	1	6	258	6	9	-7	264	6	-11	6	77	7	14	1	91	32	-30*
-1	219	5	-5	7	226	6	5	-6	151	5	-2	7	116	6	4	2	78	12	3
0	29	37	16*	8	135	6	7	-5	8	29	-23*	8	213	7	15	3	330	7	3
1	236	5	-4	9	0	49	-9*	-4	28	25	-11*	9	133	6	15	4	37	20	3*
2	301	6	22	10	21	34	-6*	-3	192	5	1	H,K=		4,	14	5	302	8	1
3	424	9	31	H,K=		4,	9	-2	213	6	11	-10	37	12	22*	6	39	11	8*
4	266	6	13	-11	31	50	-9*	-1	436	10	9	-9	15	31	6*	7	174	7	-2
5	397	8	28	-10	253	6	-5	0	139	4	-4	-8	119	4	7	8	56	8	25
6	292	6	12	-9	0	68	-55*	1	500	11	20	-7	35	13	-2*	H,K=		4,	17
7	224	6	2	-8	284	6	-14	2	175	5	13	-6	387	16	-10	-9	224	5	11

STRUCTURE FACTORS CONTINUED FOR
Y8.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-8	112	4	13	-1	52	19	-7*	-3	570	12	-69	-12	107	5	-3	-4	41	7	23
-7	115	5	5	0	0	31	-1*	-1	309	9	-46	-11	86	8	2	-3	247	9	-2
-6	64	7	9	1	83	17	-11*	1	211	6	-0	-10	210	5	1	-2	66	3	-1
-5	0	29	-6*	2	65	7	-9	3	331	7	-1	-9	104	13	-13	-1	381	9	-19
-4	59	6	-4	3	214	5	2	5	508	12	31	-8	291	12	-5	0	171	5	-10
-3	171	5	6	4	158	4	1	7	390	9	13	-7	125	4	0	1	677	14	33
-2	159	5	7	5	209	7	-5	9	169	6	-6	-6	274	6	-11	2	39	7	-7
-1	364	8	-3	6	118	7	8	H,K=	5,	1	-5	51	5	-13	3	437	9	28	
0	251	6	2	H,K=	4,	21	-12	62	13	-4*	-4	61	80	9*	4	131	5	-2	
1	359	7	3	-7	119	5	3	-11	177	4	10	-3	129	6	-3	5	139	4	0
2	161	5	5	-6	32	18	11*	-10	172	5	10	-2	319	8	-4	6	36	26	-13*
3	155	5	4	-5	5	29	-4*	-9	328	11	-6	-1	171	6	-15	7	138	6	-10
4	43	9	-7*	-4	42	10	-15*	-8	278	6	-14	0	573	12	-17	8	26	30	-2*
5	11	28	-6*	-3	171	5	-6	-7	308	7	-8	1	273	6	-5	9	198	5	-7
6	42	11	-8*	-2	60	7	-3	-6	167	4	-6	2	563	12	15	10	59	8	-5
7	137	4	1	-1	249	6	-4	-5	244	7	-13	3	265	6	5	H,K=	5,	6	
H,K=	4,	18	0	25	27	-5*	-4	101	12	28	4	254	6	12	-12	135	5	-4	
-8	127	4	-4	1	278	6	5	-3	234	25	10	5	59	8	6	-11	128	6	-1
-7	51	12	21*	2	9	30	-14*	-2	325	7	-17	6	52	8	-6	-10	108	4	-6
-6	277	14	4	3	156	4	-9	-1	354	10	-38	7	16	42	11*	-9	45	7	19
-5	104	4	-0	4	26	29	-5*	0	442	9	-13	8	177	5	3	-8	133	5	-6
-4	318	7	-2	5	8	28	-10*	1	548	11	-13	9	143	5	2	-7	104	5	-6
-3	106	5	-0	H,K=	4,	22	2	348	7	8	10	189	6	-1	-6	237	5	-1	
-2	238	5	7	-6	155	6	-6	3	361	9	20	H,K=	5,	4	-5	364	14	-6	
-1	16	28	-6*	-5	185	5	4	4	218	6	11	-12	71	12	-5	-4	488	10	3
0	24	84	-27*	-4	193	5	0	5	87	6	15	-11	159	5	-4	-3	386	13	-17
1	0	42	-7*	-3	181	5	0	6	32	34	28*	-10	73	9	8	-2	394	9	2
2	220	5	1	-2	125	5	-3	7	98	15	8	-9	36	14	2*	-1	288	7	-5
3	111	5	5	-1	4	38	-4*	8	113	4	-3	-8	35	14	4*	0	142	5	5
4	276	8	6	0	0	87	-9*	9	196	5	2	-7	193	4	1	1	58	5	1
5	86	10	-2	1	57	16	-10*	10	142	6	0	-6	176	4	-5	2	281	6	11
6	231	5	-5	2	121	6	-3	H,K=	5,	2	-5	400	8	-16	3	174	4	5	
7	0	29	-5*	3	157	5	3	-12	204	5	9	-4	251	5	-4	4	295	26	-22
H,K=	4,	19	4	164	5	-3	-11	47	8	36	-3	595	13	-24	5	206	15	-13	
-8	204	5	8	H,K=	4,	23	-10	132	4	4	-2	193	5	-1	6	315	29	-11	
-7	44	11	-1*	-5	24	32	-4*	-9	0	30	-4*	-1	296	7	-32	7	148	5	-6
-6	102	5	10	-4	117	7	-1	-8	77	6	-2	0	103	37	-9*	8	169	4	-8
-5	0	34	-25*	-3	40	11	23*	-7	24	24	15*	1	12	22	7*	9	65	7	0
-4	46	10	1*	-2	246	6	1	-6	382	8	-14	2	56	12	-6*	10	56	9	3
-3	55	7	0	-1	0	31	-16*	-5	125	5	-1	3	341	7	9	H,K=	5,	7	
-2	245	6	-3	0	259	6	4	-4	559	12	-42	4	117	4	8	-13	124	5	2
-1	150	4	-2	1	0	27	-17*	-3	46	48	-20*	5	389	8	4	-11	29	32	0*
0	342	7	6	2	220	5	3	-2	466	10	-57	6	188	5	7	-10	273	6	1
1	93	5	-2	3	0	30	-28*	-1	35	6	17	7	274	12	-5	-9	35	75	-14*
2	269	7	-1	H,K=	4,	24	0	97	5	-25	8	43	10	-18*	-8	354	14	-11	
3	33	15	15*	-3	101	10	-5	1	37	6	16	9	110	7	3	-7	0	31	-6*
4	24	27	-25*	-2	126	5	-0	2	68	81	-45*	10	0	29	-20*	-6	322	13	-14
5	6	36	-3*	-1	0	62	-10*	3	116	14	-5	H,K=	5,	5	-5	30	15	11*	
6	81	6	2	0	27	37	1*	4	453	10	20	-12	60	9	10	-4	34	17	9*
H,K=	4,	20	1	23	29	-1*	5	160	5	5	-11	172	5	2	-3	54	5	-17	
-7	184	5	-0	2	141	7	-2	6	411	9	3	-10	71	8	4	-2	333	9	-18
-6	109	7	9	H,K=	5,	0	7	34	51	-16*	-9	307	7	-0	-1	58	5	2	
-5	272	14	5	-11	180	5	-1	8	263	6	9	-8	123	4	0	0	593	14	-1
-4	165	4	2	-9	64	11	7	9	41	11	11*	-7	284	12	-10	1	13	21	-2*
-3	228	5	8	-7	252	5	-7	10	59	15	-5*	-6	34	9	-11*	2	611	13	24
-2	42	18	1*	-5	530	11	-32	H,K=	5,	3	-5	186	8	-2	3	16	24	13*	

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	223	6	-7	-7	129	8	-9	5	76	5	-2	0	326	7	12	2	25	31	-1*
5	19	27	15*	-6	136	4	-2	6	280	33	-17	1	280	6	4	3	165	5	-0
6	37	17	4*	-5	328	15	3	7	106	5	1	2	275	6	2	4	76	5	3
7	10	29	5*	-4	230	5	6	8	176	21	-7	3	207	5	-1	5	232	5	-7
8	137	15	-7	-3	484	15	1	9	60	8	0	4	162	6	4	6	71	6	-2
9	0	33	-21*	-2	198	5	4	H,K=	5,	13		5	54	8	-2	H,K=	5,	19	
10	210	13	-6	-1	342	7	3	-10	131	4	2	6	35	14	-5*	-8	73	8	-6
H,K=	5,	8		0	204	5	2	-9	205	12	-2	7	76	6	-14	-7	207	12	1
-11	94	5	12	1	22	34	7*	-8	152	5	5	8	118	8	-11	-6	62	8	7
-10	106	5	-5	2	87	5	-3	-7	232	6	-5	H,K=	5,	16		-5	106	5	-5
-9	38	10	10*	3	252	6	4	-6	170	5	-10	-9	54	8	-4	-4	21	26	-9*
-8	78	19	2*	4	146	4	-3	-5	100	5	2	-8	55	8	4	-3	45	8	6
-7	136	5	-5	5	247	21	-6	-4	38	14	3*	-7	27	19	12*	-2	60	7	-2
-6	254	6	-4	6	173	6	-15	-3	149	4	-4	-6	285	6	3	-1	285	6	0
-5	274	6	-2	7	256	30	-19	-2	109	5	5	-5	0	23	-4*	0	96	5	-5
-4	416	16	-12	8	120	5	-10	-1	343	8	2	-4	343	7	0	1	275	6	-1
-3	364	8	1	9	64	20	-20*	0	233	5	-0	-3	83	10	-11	2	142	4	-2
-2	438	9	4	H,K=	5,	11		1	368	8	5	-2	355	8	3	3	166	5	-1
-1	293	8	14	-11	75	8	3	2	248	6	3	-1	46	13	1*	4	54	9	-1
0	161	4	9	-10	230	13	4	3	248	6	8	0	200	5	-10	5	74	6	0
1	42	6	0	-9	47	14	-6*	4	66	15	-6*	1	65	6	-2	6	18	35	-19*
2	179	4	10	-8	289	15	-4	5	107	5	-0	2	65	8	-2	H,K=	5,	20	
3	237	5	4	-7	196	8	-16	6	26	35	17*	3	65	8	1	-7	30	22	-2*
4	234	6	-4	-6	233	5	-13	7	57	8	0	4	267	7	6	-6	182	5	-1
5	236	23	-16	-5	5	25	-4*	8	86	9	-7	5	12	27	-20*	-5	93	5	-8
6	270	36	-23	-4	28	13	25*	H,K=	5,	14		6	240	13	-12	-4	250	6	-4
7	205	21	-10	-3	53	8	3	-10	26	27	-4*	7	31	18	4*	-3	101	4	-1
8	144	17	-9	-2	266	6	6	-9	7	27	-2*	H,K=	5,	17		-2	198	5	3
9	118	5	2	-1	158	4	1	-8	18	29	13*	-9	127	4	3	-1	61	11	2
H,K=	5,	9		0	491	10	9	-7	163	4	0	-8	196	5	2	0	42	56	-26*
-11	186	5	-2	1	105	4	3	-6	96	4	5	-7	115	4	3	1	7	26	6*
-10	30	35	6*	2	375	8	7	-5	399	9	-10	-6	147	6	-4	2	76	6	-11
-9	327	16	-5	3	167	4	3	-4	90	6	-8	-5	68	7	-2	3	74	10	-8
-8	40	44	2*	4	244	6	-2	-3	417	13	1	-4	52	7	4	4	173	5	0
-7	324	16	-1	5	25	45	-4*	-2	0	29	-21*	-3	51	8	-1	5	174	5	5
-6	108	4	-3	6	39	11	-1*	-1	284	7	1	-2	195	5	0	H,K=	5,	21	
-5	152	4	-12	7	51	8	-7	0	20	26	-11*	-1	179	4	1	-6	176	5	5
-4	32	11	17*	8	130	5	-15	1	39	14	11*	0	331	7	5	-5	35	14	-10*
-3	174	4	9	9	67	7	-4	2	60	9	7	1	230	5	5	-4	0	28	-35*
-2	40	7	-8	H,K=	5,	12		3	260	6	1	2	274	6	2	-3	15	26	-9*
-1	418	9	-2	-11	25	28	-12*	4	0	27	-3*	3	174	4	-2	-2	182	5	-6
0	62	5	-10	-10	77	8	-0	5	302	14	-10	4	100	4	1	-1	34	16	8*
1	629	17	10	-9	22	26	6*	6	21	29	7*	5	74	6	1	0	257	6	1
2	80	6	3	-8	57	6	1	7	220	6	-12	6	31	16	17*	1	60	9	-4
3	352	7	-4	-7	84	13	-20	8	26	29	-15*	7	21	29	-4*	2	240	5	-1
4	22	26	7*	-6	275	6	0	H,K=	5,	15		H,K=	5,	18		3	48	9	2
5	148	5	-7	-5	218	5	13	-10	151	5	7	-8	30	38	13*	4	145	5	-7
6	26	38	5*	-4	421	15	-9	-9	192	5	9	-7	129	5	-6	H,K=	5,	22	
7	71	6	-5	-3	86	5	4	-8	164	4	0	-6	18	27	-16*	-5	185	5	-5
8	63	7	-10	-2	363	8	5	-7	176	5	2	-5	277	6	-1	-4	170	5	-5
9	193	21	-13	-1	70	5	2	-6	117	4	7	-4	98	5	2	-3	202	5	-0
H,K=	5,	10		0	122	4	1	-5	81	12	-1	-3	257	6	0	-2	124	4	-5
-11	133	5	7	1	31	18	-8*	-4	18	33	9*	-2	61	6	-7	-1	108	5	-6
-10	20	26	-2*	2	146	4	1	-3	33	35	24*	-1	207	5	2	0	41	16	2*
-9	21	39	-8*	3	86	5	1	-2	211	5	4	0	23	36	-7*	1	0	42	-15*
-8	93	4	1	4	292	7	-6	-1	286	6	-3	1	25	39	-8*	2	59	13	9*

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	80	7	-9	-6	39	8	3*	4	207	5	6	-7	386	19	-12	5	8	35	-3*
H,K=	5,	23		-5	280	6	-16	5	182	5	-5	-6	0	27	-5*	6	96	5	-7
-4	46	10	-7*	-4	21	28	-3*	6	358	9	17	-5	290	7	-10	7	28	37	24*
-3	66	7	-14	-3	490	11	-52	7	75	6	3	-4	23	20	9*	8	37	26	3*
-2	11	39	0*	-2	55	15	-13*	8	219	6	5	-3	21	27	-11*	9	45	13	0*
-1	206	5	-6	-1	391	12	-36	9	82	6	7	-2	25	48	-16*	H,K=	6,	10	
0	48	9	-0*	0	116	9	-5	H,K=	6,	5		-1	210	5	-2	-11	73	7	-0
1	230	5	-0	1	127	39	-50*	-12	45	9	12*	0	21	22	7*	-10	160	5	1
2	0	30	-6*	2	19	27	-6*	-11	72	7	13	1	480	13	-4	-9	67	6	6
H,K=	5,	24		3	78	50	-20*	-10	163	5	1	2	0	24	-17*	-8	32	14	-5*
-1	121	5	1	4	109	6	2	-9	56	66	-8*	3	437	9	11	-7	42	8	-15*
0	0	33	-32*	5	324	8	13	-8	349	15	-2	4	116	4	9	-6	119	6	2
H,K=	6,	0		6	158	7	5	-7	123	4	-2	5	214	23	-4	-5	97	4	1
-12	251	6	17	7	284	7	7	-6	354	8	-6	6	34	13	6*	-4	376	16	-11
-10	198	5	8	8	53	12	12*	-5	105	5	-3	7	24	30	16*	-3	245	5	-6
-8	83	6	-1	9	202	5	4	-4	160	4	-9	8	20	28	16*	-2	373	9	-4
-6	237	5	-10	H,K=	6,	3	-3	96	15	30	9	126	5	0	-1	167	4	4	
-4	369	8	-28	-12	17	28	-17*	-2	174	4	3	H,K=	6,	8	0	187	4	2	
-2	424	11	-39	-11	96	6	6	-1	45	13	0*	-11	188	5	6	1	96	4	-1
0	310	7	-30	-10	47	49	1*	0	357	12	-17	-10	152	5	6	2	38	10	-7*
2	64	43	-23*	-9	298	18	6	1	78	6	-5	-9	81	6	-2	3	67	6	8
4	306	17	-10	-8	166	8	-8	2	436	19	-21	-8	20	27	0*	4	181	5	2
6	329	9	15	-7	329	12	-9	3	162	13	-17	-7	31	33	3*	5	94	4	-7
8	289	7	22	-6	136	4	-4	4	335	7	9	-6	99	5	-2	6	226	8	1
10	127	7	-7	-5	249	5	-7	5	38	29	4*	-5	224	12	-14	7	115	7	-5
H,K=	6,	1		-4	118	5	9	6	82	11	-10	-4	294	10	3	8	205	22	-14
-12	73	6	21	-3	47	70	-11*	7	0	31	-4*	-3	416	9	-9	H,K=	6,	11	
-11	86	5	2	-2	71	6	40	8	77	6	-3	-2	310	7	-4	-11	118	5	-0
-10	166	4	8	-1	217	19	-16	9	60	9	15	-1	279	7	-14	-10	40	16	-12*
-9	205	5	5	0	177	9	-9	H,K=	6,	6	0	232	5	2	-9	242	5	-3	
-8	371	8	-11	1	471	10	-2	-11	169	5	5	1	103	5	0	-8	94	7	4
-7	276	6	-6	2	158	4	-4	-10	146	4	6	2	43	9	8*	-7	276	13	7
-6	313	7	-15	3	398	8	-7	-9	126	4	-6	3	115	4	5	-6	148	4	-0
-5	189	4	-10	4	148	8	-3	-8	34	38	-8*	4	60	7	1	-5	252	6	-2
-4	200	6	-3	5	196	5	2	-7	95	4	-10	5	196	22	4	-4	10	25	-12*
-3	74	22	3*	6	35	23	-6*	-6	148	13	-16	6	195	19	-11	-3	36	14	31*
-2	184	22	28	7	0	27	-12*	-5	287	15	0	7	227	19	-11	-2	96	6	-15
-1	238	6	-18	8	25	28	1*	-4	269	6	-14	8	154	6	-10	-1	285	6	1
0	376	8	-19	9	139	5	2	-3	507	11	-17	9	124	5	-4	0	165	4	-1
1	215	5	-10	H,K=	6,	4	-2	219	5	-10	H,K=	6,	9	1	360	8	-1		
2	362	8	-3	-12	216	14	8	-1	242	6	-4	-11	7	27	0*	2	183	5	-1
3	239	6	4	-11	110	6	8	0	203	6	-9	-10	190	5	-4	3	394	8	15
4	230	13	1	-10	156	4	6	1	126	4	-5	-9	6	33	2*	4	63	7	-1
5	149	4	11	-9	50	7	28	2	14	31	-6*	-8	302	15	-9	5	198	6	-5
6	115	10	7	-8	31	32	25*	3	106	4	-14	-7	83	7	-6	6	43	11	-3*
7	32	23	-6*	-7	31	13	12*	4	145	5	-7	-6	329	14	-3	7	47	11	-1*
8	57	7	7	-6	259	14	-4	5	264	19	-13	-5	26	28	-5*	8	53	8	8
9	87	5	-2	-5	197	10	-12	6	172	5	-9	-4	139	4	9	H,K=	6,	12	
10	106	7	-4	-4	421	17	-23	7	224	7	-5	-3	7	24	1*	-10	10	32	-9*
H,K=	6,	2		-3	122	4	-10	8	135	4	-4	-2	118	4	5	-9	128	7	11
-12	40	8	12	-2	448	11	-32	9	167	5	-6	-1	76	5	4	-8	21	28	10*
-11	204	5	8	-1	126	5	-5	H,K=	6,	7	0	406	8	11	-7	11	29	-31*	
-10	52	11	14*	0	219	7	-27	-11	103	4	1	1	97	4	-7	-6	99	6	-0
-9	168	5	7	1	168	8	-13	-10	29	30	-21*	2	486	10	11	-5	308	14	-8
-8	40	17	18*	2	14	25	-19*	-9	298	13	2	3	70	6	10	-4	148	4	-3
-7	149	5	1	3	47	13	-13*	-8	32	70	-16*	4	319	7	1	-3	423	9	2

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.0C4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	142	4	7	-4	143	5	6	2	0	31	-6*	-5	165	4	-13	-9	60	35	2*
-1	292	7	-3	-3	14	34	-0*	3	0	41	-15*	-3	402	8	-20	-8	267	6	1
0	114	4	-2	-2	0	44	-13*	4	142	5	-3	-1	609	13	-34	-7	199	5	-12
1	79	5	10	-1	168	5	-3	5	57	17	-9*	1	292	6	-7	-6	310	7	-15
2	66	9	9	0	202	6	5	H,K=	6,	19		3	47	8	-6	-5	160	5	-9
3	125	8	-4	1	207	6	2	-7	86	7	-15	5	159	8	-0	-4	269	6	-22
4	67	6	-10	2	254	6	4	-6	214	6	2	7	165	7	-1	-3	160	4	-16
5	193	5	-2	3	283	7	0	-5	53	10	2*	9	236	12	-13	-2	60	66	14*
6	52	8	-9	4	189	5	4	-4	108	6	2	H,K=	7,	1		-1	41	10	-14*
7	252	27	-15	5	133	5	1	-3	22	31	19*-12		0	34	-15*	0	133123		-57*
8	83	6	-8	6	54	8	12	-2	106	6	-8	-11	53	11	-7*	1	143	7	2
H,K=	6,	13		7	16	30	-18*	-1	70	8	-3	-10	77	7	9	2	285	6	-6
-10	149	4	-2	H,K=	6,	16		0	204	8	1	-9	182	5	4	3	206	6	7
-9	99	5	-1	-9	80	8	-5	1	126	6	9	-8	224	5	3	4	412	9	7
-8	222	5	5	-8	0	32	-11*	2	245	6	-5	-7	256	7	-5	5	128	6	-0
-7	207	5	-2	-7	38	18	-2*	3	122	5	-1	-6	206	5	-5	6	213	7	4
-6	256	6	-1	-6	32	23	-0*	4	181	8	0	-5	230	5	-14	7	47	13	-6*
-5	105	7	3	-5	263	6	0	5	30	34	-24*	-4	171	4	-5	8	39	51	24*
-4	153	4	-1	-4	57	9	2	H,K=	6,	20		-3	209	10	-15	9	0	35	-5*
-3	52	17	22*	-3	320	8	-1	-6	35	22	5*	-2	101	9	-8	H,K=	7,	4	
-2	157	4	-3	-2	37	15	-6*	-5	165	8	-9	-1	184	5	119	-11	179	6	2
-1	105	4	-2	-1	344	7	-1	-4	105	6	-7	0	175	4	-19	-10	110	6	7
0	253	5	10	0	0	31	-23*	-3	223	6	-0	1	202	5	-13	-9	165	5	-6
1	194	5	-7	1	187	5	-5	-2	128	5	-2	2	240	6	-7	-8	84	8	11
2	335	7	0	2	43	9	-5*	-1	238	6	1	3	307	7	2	-7	34	19	21*
3	224	5	-5	3	110	5	2	0	91	7	-4	4	154	7	8	-6	22	29	11*
4	259	6	5	4	0	35	-4*	1	79	8	-3	5	306	8	18	-5	202	5	-10
5	102	5	1	5	182	6	-10	2	47	12	40*	6	198	5	12	-4	142	5	-14
6	116	5	-4	6	35	13	7*	3	37	21	-22*	7	102	8	10	-3	394	9	-36
7	47	11	20*	H,K=	6,	17		4	90	7	4	8	28	34	9*	-2	160	7	-8
8	64	7	3	-8	144	5	-5	H,K=	6,	21		9	35	32	0*	-1	432	9	-29
H,K=	6,	14		-7	182	6	-4	-5	185	5	-2	H,K=	7,	2		0	186	5	-7
-10	145	5	3	-6	103	6	1	-4	13	47	-2*-11		46	13	-2*	1	299	7	-5
-9	26	28	19*	-5	156	5	4	-3	24	42	2*-10		163	6	-3	2	70	7	1
-8	48	11	7*	-4	58	8	6	-2	0	32	-3*	-9	81	12	14	3	86	6	-4
-7	40	10	-3*	-3	31	23	-2*	-1	143	6	-11	-8	171	5	-3	4	80	7	16
-6	188	4	1	-2	74	7	8	0	31	32	-5*	-7	77	16	-8*	5	136	6	-1
-5	41	10	-12*	-1	158	5	-5	1	242	6	-10	-6	88	6	-18	6	70	12	-2
-4	375	8	-2	0	123	5	-1	2	97	6	4	-5	32	30	27*	7	215	6	1
-3	55	8	10	1	236	7	3	3	220	6	0	-4	265	6	-15	8	78	15	4*
-2	420	9	1	2	191	6	-8	H,K=	6,	22		-3	71	6	-8	9	198	8	4
-1	63	12	-6	3	211	5	2	-4	179	5	-9	-2	509	11	-39	H,K=	7,	5	
0	231	6	10	4	143	13	4	-3	150	5	-2	-1	144	4	-18	-11	0	33	-8*
1	41	44	5*	5	147	6	0	-2	200	6	-6	0	497	11	-26	-10	0	31	-21*
2	41	29	4*	6	74	10	-10	-1	172	5	-6	1	132	4	7	-9	201	5	-8
3	19	32	8*	H,K=	6,	18		0	116	12	-5	2	173	5	7	-8	52100		-27*
4	219	5	6	-8	23	33	2*	1	36	43	-13*	3	0	31	-11*	-7	369	8	-15
5	0	28	-19*	-7	0	36	-5*	2	22	53	-6*	4	58	10	8	-6	169	5	-21
6	232	17	-9	-6	132	11	-10	H,K=	6,	23		5	43	45	3*	-5	307	7	-11
7	22	28	-14*	-5	89	7	1	-2	36	46	-14*	6	181	6	4	-4	83	10	-4
H,K=	6,	15		-4	208	5	4	-1	29	32	23*	7	67	9	13	-3	229	5	-16
-9	153	4	4	-3	101	6	-1	0	157	6	-12	8	224	7	2	-2	99	5	-8
-8	162	5	4	-2	288	7	-5	H,K=	7,	0		9	56	12	9*	-1	39	19	31*
-7	155	6	-4	-1	108	7	-3	-11	202	6	6	H,K=	7,	3	0	62	8	-3	
-6	210	5	7	0	211	5	-7	-9	237	6	5	-11	57	13	13*	1	293	7	-16
-5	167	4	3	1	10	38	-11*	-7	103	4	-0	-10	99	6	-9	2	104	5	-1

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	36?	8	15	-5	119	7	-11	-10	92	9	-11	H,K=		7,	14	-3	45	21	-2*
4	139	7	8	-4	122	7	-9	-9	58	10	3	-9	167	5	2	-2	31	27	1*
5	33?	7	2	-3	251	6	-4	-8	228	7	-0	-8	31	32	15*	-1	45	12	2*
6	40	15	-6*	-2	295	7	-15	-7	104	5	7	-7	31	37	-1*	0	114	5	-1
7	121	6	8	-1	274	6	-5	-6	322	7	-10	-6	19	31	-17*	1	71	8	-15
8	49	13	9*	0	267	6	0	-5	36	41	-15*	-5	152	5	-5	2	213	6	8
9	69	9	19	1	223	6	1	-4	230	6	0	-4	61	8	-5	3	164	5	-1
H,K=		7,	6	2	126	5	10	-3	54	9	16	-3	252	6	3	4	200	6	-0
-11	129	7	0	3	168	5	-1	-2	54	9	-11	-2	80	7	-8	5	109	10	2
-10	168	5	7	4	114	13	9	-1	87	8	-1	-1	307	7	-8	H,K=		7,	18
-9	87	7	-2	5	110	5	-3	0	216	6	-7	0	30	25	-17*	-7	38	19	-5*
-8	106	12	2	6	145	5	-2	1	77	17	-5*	1	229	6	-0	-6	0	35	-24*
-7	48	20	-9*	7	142	5	-5	2	310	7	-6	2	0	30	-6*	-5	129	7	-6
-6	71	7	-2	8	201	6	12	3	141	5	10	3	48	13	10*	-4	59	9	7
-5	91	6	-17	H,K=		7,	9	4	275	6	2	4	27	32	10*	-3	224	6	-2
-4	303	7	-18	-11	0	36	-31*	5	63	8	2	5	110	6	-9	-2	51	20	-6*
-3	209	5	-6	-10	0	40	-21*	6	163	6	4	6	0	32	-15*	-1	283	7	-6
-2	28?	7	-17	-9	168	5	-7	7	0	36	-34*	H,K=		7,	15	0	112	5	6
-1	217	5	-8	-8	45	12	10*	H,K=		7,	12	-9	76	12	2	1	173	5	1
0	35?	8	11	-7	285	7	-6	-10	203	6	-1	-8	137	5	4	2	23	31	18*
1	100	5	0	-6	17	43	-15*	-9	45	13	-0*	-7	165	5	-3	3	0	39	-18*
2	203	6	-11	-5	277	7	-16	-8	111	6	-2	-6	201	5	1	4	8	31	1*
3	24	31	-3*	-4	59	11	6*	-7	32	35	-9*	-5	200	5	-9	H,K=		7,	19
4	46	13	19*	-3	154	7	5	-6	23	34	-12*	-4	169	5	-4	-6	78	8	-5
5	127	7	4	-2	73	6	-9	-5	51	13	-17*	-3	123	5	-4	-5	220	6	-1
6	235	7	1	-1	88	6	6	-4	235	6	-2	-2	0	30	-11*	-4	48	12	8*
7	103	6	0	0	65	7	7	-3	126	7	1	-1	23	42	4*	-3	85	14	-3
8	183	6	-9	1	310	7	3	-2	327	7	-3	0	45	12	-5*	-2	0	32	-21*
H,K=		7,	7	2	65	13	12*	-1	143	5	6	1	163	5	2	-1	40	30	6*
-11	45	14	4*	3	364	8	2	0	254	6	10	2	210	6	3	0	53	10	12*
-10	89	7	-7	4	32	38	15*	1	79	17	17*	3	213	5	3	1	179	6	-8
-9	0	34	-18*	5	236	6	7	2	211	8	0	4	209	6	-2	2	90	7	-0
-8	273	7	-8	6	52	11	8*	3	19	30	-8*	5	143	7	-3	3	220	6	4
-7	86	54	-15*	7	100	6	-5	4	88	6	19	6	126	6	-3	4	90	7	-2
-6	375	8	-5	8	0	37	-4*	5	22	34	-28*	H,K=		7,	16	H,K=		7,	20
-5	26	29	12*	H,K=		7,	10	6	189	6	9	-8	116	6	4	-5	17	33	-20*
-4	293	7	-14	-10	110	6	-6	7	59	15	13*	-7	0	37	-5*	-4	148	5	-2
-3	54	10	19*	-9	161	5	-2	H,K=		7,	13	-6	79	7	4	-3	93	7	-7
-2	98	5	-3	-8	61	16	9*	-10	48	12	23*	-5	0	31	-20*	-2	263	6	2
-1	0	28	-28*	-7	81	6	5	-9	132	6	-3	-4	178	5	2	-1	154	6	-1
0	170	5	-2	-6	76	6	-7	-8	110	6	3	-3	42	12	38*	0	216	6	-4
1	44	11	-0*	-5	104	7	12	-7	240	6	1	-2	310	8	-8	1	79	12	8
2	337	7	6	-4	126	5	1	-6	191	5	2	-1	0	30	-12*	2	93	8	5
3	15	31	9*	-3	322	7	-10	-5	311	8	-4	0	243	6	4	3	0	33	-2*
4	34?	8	2	-2	177	6	-13	-4	109	7	-12	1	0	30	-28*	H,K=		7,	21
5	30	26	2*	-1	313	7	11	-3	191	5	1	2	155	10	2	-4	174	7	2
6	201	6	11	0	227	5	1	-2	34	39	26*	3	32	33	14*	-3	25	34	-6*
7	0	32	-17*	1	275	6	1	-1	78	7	-1	4	55	11	-8*	-2	0	34	-50*
8	40	51	-4*	2	54	28	-10*	0	79	16	-1*	5	0	43	-11*	-1	0	32	-9*
H,K=		7,	8	3	24	46	-16*	1	141	7	2	6	156	6	4	0	100	6	-3
-11	150	7	2	4	0	30	-25*	2	165	7	1	H,K=		7,	17	1	32	32	-4*
-10	164	5	-0	5	100	8	-2	3	320	7	5	-8	143	6	-3	2	218	6	1
-9	159	5	-4	6	94	6	-2	4	138	5	-8	-7	119	6	-14	H,K=		7,	22
-8	73	12	2	7	211	8	8	5	200	7	4	-6	200	6	-7	-2	165	5	1
-7	23	29	11*	8	110	7	2	6	68	17	-1*	-5	107	7	-5	-1	187	6	-3
-6	27	40	9*	H,K=		7,	11	7	117	6	8	-4	173	5	8	H,K=		8,	0

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-10	247	16	7	-8	93	4	-1	6	285	6	12	1	278	6	-5	0	18	35	16*
-8	236	6	4	-7	171	4	4	7	83	6	3	2	193	7	-0	1	130	6	-0
-6	69	5	-0	-6	165	5	-3	8	111	6	5	3	135	5	8	2	58	58	35*
-4	174	4	-0	-5	381	8	-26	H,K=	8,	6	4	73	6	7	3	253	6	5	
-2	357	8	-21	-4	148	6	-14	-11	152	6	0	5	34	18	7*	4	90	5	8
0	472	10	-22	-3	284	6	-15	-10	153	5	9	6	96	5	4	5	257	7	9
2	258	6	-8	-2	113	7	-6	-9	166	5	-4	7	121	5	4	6	58	8	-1
4	143	11	3	-1	106	7	5	-8	138	4	7	H,K=	8,	9	H,K=	8,	12		
6	100	8	-2	0	31	49	-19*	-7	151	4	3	-10	9	27	-8*	-9	229	6	13
8	239	8	3	1	151	16	-8	-6	72	8	0	-9	44	20	22*	-8	27	36	12*
H,K=	8,	1	2	197	5	-19	-5	35	11	14*	-8	178	12	8	-7	164	4	4	
-11	36	12	27*	3	269	8	0	-4	89	6	-8	-7	20	25	16*	-6	30	13	28*
-10	21	26	11*	4	152	7	-3	-3	241	6	8	-6	272	7	5	-5	30	30	-5*
-9	41	9	9*	5	361	9	5	-2	128	4	-4	-5	57	8	-8	-4	28	16	20*
-8	93	5	5	6	153	5	-1	-1	289	6	-13	-4	297	13	4	-3	200	5	2
-7	172	5	-6	7	128	7	-2	0	211	5	-1	-3	138	4	5	-2	99	8	3
-6	219	5	0	8	84	8	7	1	289	6	5	-2	237	5	1	-1	345	11	7
-5	192	4	-3	H,K=	8,	4	2	131	5	1	-1	41	13	0*	0	115	5	6	
-4	324	7	-11	-11	100	5	9	3	209	6	-4	0	49	13	-6*	1	334	7	4
-3	204	5	-6	-10	170	5	-2	4	63	7	-7	1	32	43	-1*	2	47	9	-8*
-2	137	8	-8	-9	146	4	5	5	26	32	-0*	2	211	6	4	3	158	4	2
-1	80	38	38*	-8	226	5	-6	6	61	9	-2	3	51	12	-12*	4	60	7	25
0	90	90	79*	-7	110	6	8	7	146	5	-5	4	297	7	2	5	26	35	-7*
1	141	4	-3	-6	99	6	-8	8	131	5	5	5	0	33	-13*	6	27	29	17*
2	197	5	-4	-5	40	12	6*	H,K=	8,	7	6	242	6	4	H,K=	8,	13		
3	243	6	-8	-4	145	4	-3	-11	68	8	6	7	18	29	5*	-9	34	14	12*
4	262	7	-1	-3	134	4	-7	-10	25	31	10*	H,K=	8,	10	-8	142	5	-1	
5	205	7	-1	-2	272	6	-6	-9	81	5	-12	-10	209	6	8	-7	114	4	-0
6	225	6	11	-1	157	4	-2	-8	20	26	11*	-9	116	5	10	-6	275	6	6
7	121	7	1	0	388	8	-16	-7	270	12	2	-8	178	4	-1	-5	146	4	-6
8	93	8	14	1	68	11	3	-6	0	50	-39*	-7	39	10	-17*	-4	271	6	1
H,K=	8,	2	2	295	17	-5	-5	349	16	3	-6	122	6	3	-3	176	4	-6	
-11	213	5	8	3	147	8	-11	-4	79	14	-20	-5	17	32	13*	-2	184	5	-3
-10	55	13	9*	4	95	9	0	-3	324	7	5	-4	48	25	1*	-1	22	30	-5*
-9	243	6	-1	5	31	16	3*	-2	65	6	5	-3	127	5	10	0	24	31	-0*
-8	102	5	-8	6	93	9	1	-1	125	13	-12	-2	346	11	-8	1	22	31	12*
-7	209	5	-9	7	76	12	-2	0	27	31	-9*	-1	259	6	2	2	162	5	2
-6	34	34	17*	8	184	6	-1	1	140	5	0	0	345	8	1	3	141	4	-0
-5	90	4	-9	H,K=	8,	5	2	21	39	-2*	1	213	6	1	4	227	7	-0	
-4	52	6	-1	-11	0	40	-11*	3	295	6	11	2	307	7	3	5	197	69	73*
-3	238	5	-7	-10	0	27	-2*	4	36	21	19*	3	97	6	13	6	181	7	-7
-2	62	5	8	-9	36	10	26*	5	327	8	1	4	45	12	4*	H,K=	8,	14	
-1	413	13	-26	-8	160	5	-0	6	43	13	1*	5	53	9	13	-9	35	14	16*
0	82	5	-5	-7	93	12	-6	7	199	5	7	6	99	7	1	-8	174	5	8
1	389	13	-24	-6	374	8	-8	H,K=	8,	8	7	65	8	1	-7	32	16	19*	
2	93	7	-4	-5	63	6	-11	-10	161	5	2	H,K=	8,	11	-6	86	5	0	
3	197	6	11	-4	409	9	-3	-9	180	12	6	-10	24	37	-5*	-5	37	11	5*
4	28	40	-13*	-3	56	11	7*	-8	124	4	-1	-9	91	5	-2	-4	53	7	-6
5	40	16	11*	-2	182	5	-11	-7	149	4	3	-8	33	18	-7*	-3	15	26	1*
6	34	15	29*	-1	91	6	3	-6	92	4	-3	-7	241	6	7	-2	248	6	-6
7	160	7	-3	0	19	26	5*	-5	30	32	17*	-6	103	4	2	-1	48	10	1*
8	67	8	1	1	68	7	-15	-4	168	4	1	-5	298	13	-7	0	293	7	-4
H,K=	8,	3	2	231	12	-0	-3	135	6	-6	-4	84	5	5	1	41	9	31*	
-11	58	8	6	3	38	42	3*	-2	209	5	9	-3	271	6	11	2	255	7	2
-10	33	13	10*	4	361	8	-2	-1	282	6	9	-2	75	11	-9	3	25	39	-15*
-9	60	11	2	5	125	4	5	0	391	8	5	-1	129	7	-8	4	54	8	3

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	0	67	-21*	-4	207	5	-2	-1	103	4	-0	-2	87	5	4	-2	158	5	1
H,K=	8,	15		-3	63	10	-6	0	386	8	-13	-1	210	6	-7	-1	197	5	-1
-8	86	5	2	-2	153	4	-1	1	45	19	1*	0	61	11	2	0	304	6	-0
-7	149	6	-4	-1	22	40	-4*	2	390	13	-12	1	24	38	20*	1	248	6	3
-6	202	5	-4	0	17	30	11*	3	86	5	7	2	64	10	4	2	272	6	-3
-5	210	5	-2	1	30	26	4*	4	160	5	-1	3	215	6	-9	3	141	4	-3
-4	187	5	-3	2	137	5	-1	5	0	34	-4*	4	51	13	9*	4	118	5	-1
-3	182	5	-5	H,K=	8,	20		6	54	10	30	5	293	7	8	5	61	8	-11
-2	145	6	-1	-4	0	32	-8*	7	63	8	6	6	68	12	-3	6	41	13	14*
-1	39	10	16*	-3	139	4	2	H,K=	9,	3		7	215	6	6	H,K=	9,	9	
0	9	36	6*	-2	101	6	-5	-10	118	6	0	H,K=	9,	6	-10	0	33	-24*	
1	40	16	-7*	-1	215	5	-4	-9	25	27	20*	-10	180	5	9	-9	27	22	25*
2	119	7	5	0	135	7	-6	-8	69	5	12	-9	175	5	6	-8	21	31	19*
3	181	5	-2	1	192	5	-6	-7	92	6	-6	-8	232	6	6	-7	144	4	-3
4	191	5	-1	H,K=	9,	0		-6	229	5	-2	-7	142	4	8	-6	47	8	-0
5	177	6	-1	-11	206	6	18	-5	120	5	-2	-6	219	5	7	-5	273	11	-3
H,K=	8,	16		-9	308	8	11	-4	398	9	-10	-5	72	20	-13*	-4	11	41	-12*
-8	26	29	15*	-7	228	5	3	-3	195	5	-15	-4	36	29	13*	-3	382	8	1
-7	125	4	5	-5	118	8	2	-2	203	5	-20	-3	32	36	23*	-2	58	6	11
-6	32	15	12*	-3	64	6	5	-1	118	4	-9	-2	171	5	-0	-1	300	7	-4
-5	17	32	4*	-1	287	6	-16	0	160	6	-2	-1	203	5	-3	0	36	15	3*
-4	61	9	19	1	467	10	-26	1	46	21	-8*	0	258	6	1	1	7	33	-23*
-3	168	5	-6	3	249	6	12	2	98	29	-14*	1	234	7	-3	2	15	27	-3*
-2	0	26	-12*	5	77	6	3	3	130	4	-2	2	234	5	-5	3	189	5	10
-1	295	7	-6	7	122	5	2	4	246	5	5	3	191	5	-10	4	55	17	4*
0	50	13	3*	H,K=	9,	1		5	147	6	3	4	128	4	-3	5	269	9	4
1	253	7	0	-11	116	5	11	6	242	6	7	5	52	12	-5*	6	30	36	11*
2	22	28	20*	-10	53	8	11	7	118	5	6	6	29	29	21*	H,K=	9,	10	
3	148	5	-3	-9	28	34	4*	H,K=	9,	4		7	70	7	9	-9	241	5	14
4	6	29	-10*	-8	53	10	6*	-10	85	7	0	H,K=	9,	7	-8	122	4	1	
H,K=	8,	17		-7	138	4	11	-9	235	6	9	-10	61	8	-6	-7	213	5	12
-7	150	5	1	-6	189	6	4	-8	114	7	0	-9	14	27	10*	-6	124	4	3
-6	138	4	-5	-5	286	6	-11	-7	302	7	4	-8	100	4	3	-5	82	5	5
-5	239	6	7	-4	249	6	-19	-6	77	7	-1	-7	28	17	10*	-4	0	27	-10*
-4	130	4	-4	-3	274	6	-15	-5	175	4	-4	-6	261	6	1	-3	104	4	8
-3	164	4	7	-2	158	5	-3	-4	17	28	-4*	-5	0	42	-20*	-2	131	6	2
-2	79	6	1	-1	213	5	-12	-3	85	6	-2	-4	378	12	-0	-1	306	7	1
-1	86	7	3	0	161	18	-1	-2	79	6	15	-3	2	53	-2*	0	180	5	7
0	35	12	31*	1	103	41	42*	-1	230	6	-0	-2	341	7	-11	1	310	7	-9
1	92	7	-1	2	118	11	-2	0	204	5	-14	-1	32	37	28*	2	154	5	-4
2	105	5	3	3	158	4	-6	1	358	8	-12	0	95	6	-8	3	206	7	-2
3	189	5	-6	4	184	5	2	2	146	7	-1	1	27	35	17*	4	77	7	-3
4	123	5	-6	5	215	6	9	3	251	6	4	2	89	5	-4	5	32	36	-11*
H,K=	8,	18		6	166	5	10	4	103	6	-5	3	50	8	14	6	20	30	5*
-6	57	7	16	7	178	5	10	5	82	6	-11	4	254	23	-1	H,K=	9,	11	
-5	35	13	7*	H,K=	9,	2		6	41	16	13*	5	13	36	0*	-9	32	17	-5*
-4	106	7	1	-11	26	28	-5*	7	98	5	14	6	277	7	7	-8	92	5	8
-3	0	29	-16*	-10	238	6	10	H,K=	9,	5		H,K=	9,	8		-7	24	26	0*
-2	247	6	-2	-9	49	8	23	-10	27	29	24*	-10	145	5	1	-6	207	5	6
-1	77	12	-4	-8	284	7	-2	-9	11	28	-11*	-9	193	5	10	-5	64	6	4
0	253	6	-7	-7	74	9	16	-8	29	17	-3*	-8	199	5	16	-4	324	7	1
1	79	6	2	-6	217	5	-2	-7	153	4	4	-7	182	5	9	-3	149	4	6
2	187	5	-4	-5	28	34	24*	-6	0	54	-30*	-6	154	4	7	-2	317	7	7
3	22	29	17*	-4	98	5	8	-5	400	12	-9	-5	98	5	1	-1	48	10	-5*
H,K=	8,	19		-3	27	19	11*	-4	113	6	-7	-4	38	43	8*	0	126	4	-1
-5	89	5	3	-2	201	5	-4	-3	327	7	-7	-3	170	4	-10	1	27	28	-10*

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	105	5	3	-1	132	4	6	-6	160	4	4	-4	165	5	-2	1	74	8	-9
3	83	6	9	0	43	10	1*	-5	140	5	1	-3	37	19	8*	2	43	14	-10*
4	223	5	4	1	4	28	-17*	-4	287	6	-6	-2	140	4	-10	3	71	7	-7
5	83	9	-4	2	70	9	-2	-3	265	6	-4	-1	161	5	-9	4	16	39	12*
H,K=		9,	12	3	149	6	5	-2	292	6	-7	0	246	5	-1	5	177	17	-8
-9	76	6	7	4	141	5	-3	-1	209	5	2	1	102	6	-6	H,K=		10,	8
-8	237	5	14	H,K=		9,	16	0	245	5	-9	2	317	7	-11	-9	176	5	4
-7	45	9	7*	-7	0	34	-30*	1	117	20	-1	3	98	6	-6	-8	181	5	4
-6	183	12	13	-6	154	5	0	2	50	8	46	4	218	6	-5	-7	197	5	1
-5	40	10	11*	-5	31	16	3*	3	78	6	2	5	71	7	0	-6	157	5	0
-4	14	26	13*	-4	23	34	18*	4	143	7	1	6	85	9	13	-5	124	5	-10
-3	0	28	-14*	-3	37	22	11*	5	120	6	8	H,K=		10,	5	-4	49	9	-5
-2	209	5	-1	-2	188	5	-4	6	175	5	12	-10	147	6	15	-3	27	33	2*
-1	72	7	2	-1	0	29	-17*	H,K=		10,	2	-9	17	33	4*	-2	77	7	-0
0	299	7	5	0	267	7	-5	-10	36	21	4*	-8	25	33	5*	-1	170	4	0
1	87	5	2	1	27	28	19*	-9	238	6	2	-7	48	8	2	0	151	5	3
2	270	9	4	2	257	6	-0	-8	38	12	16*	-6	157	4	4	1	215	5	-7
3	58	10	-6	3	18	29	16*	-7	286	6	4	-5	61	31	-21*	2	205	5	-10
4	135	7	-2	H,K=		9,	17	-6	87	7	9	-4	321	7	-0	3	191	5	-14
5	57	9	9	-6	145	5	-4	-5	246	11	-6	-3	158	4	0	4	152	5	2
H,K=		9,	13	-5	163	5	8	-4	19	32	-2*	-2	337	7	-10	5	97	5	-2
-8	35	13	25*	-4	210	6	2	-3	30	23	26*	-1	51	13	13*	H,K=		10,	9
-7	164	5	7	-3	155	5	-0	-2	76	6	1	0	174	5	7	-9	58	7	21
-6	135	5	8	-2	193	5	3	-1	210	5	-8	1	32	33	-7*	-8	37	14	9*
-5	228	5	2	-1	93	9	9	0	84	10	-4	2	35	13	27*	-7	18	36	15*
-4	153	5	7	0	31	19	-14*	1	332	7	-7	3	11	28	6*	-6	148	5	-1
-3	285	6	6	1	19	28	0*	2	24	32	5*	4	148	6	-3	-5	11	26	2*
-2	196	5	-2	2	86	9	-1	3	284	6	-2	5	59	8	13	-4	292	6	-1
-1	137	5	4	H,K=		9,	18	4	30	22	13*	6	210	6	-1	-3	47	8	11
0	59	8	20	-5	46	12	-4*	5	150	5	9	H,K=		10,	6	-2	370	8	5
1	13	30	11*	-4	30	30	10*	6	0	33	-12*	-9	200	5	15	-1	48	9	-2*
2	51	16	14*	-3	57	8	-17	H,K=		10,	3	-8	150	4	4	0	190	5	-2
3	136	5	-1	-2	21	31	11*	-10	82	6	18	-7	224	5	-2	1	20	28	1*
4	135	6	6	-1	215	6	-3	-9	117	4	8	-6	180	4	-4	2	0	29	-20*
5	195	5	-3	0	88	6	3	-8	43	14	38*	-5	157	5	-6	3	49	9	10*
H,K=		9,	14	1	232	5	-4	-7	51	8	-3	-4	85	12	-6	4	144	5	-5
-8	37	12	22*	H,K=		9,	19	-6	72	9	-5	-3	35	15	-8*	5	61	7	23
-7	206	5	5	-3	216	7	6	-5	238	6	-9	-2	62	7	7	H,K=		10,	10
-6	18	30	2*	-2	75	7	-2	-4	158	4	-3	-1	144	4	1	-8	224	6	6
-5	110	5	7	-1	163	5	3	-3	330	7	-8	0	197	5	-7	-7	118	4	4
-4	34	14	26*	0	49	14	24*	-2	143	5	-4	1	245	5	-9	-6	191	5	3
-3	111	5	0	H,K=		10,	0	-1	289	6	-4	2	172	5	-3	-5	92	5	8
-2	12	31	-1*	-10	187	5	10	0	112	4	5	3	214	16	-11	-4	70	7	-1
-1	237	6	-2	-8	334	8	17	1	95	6	-8	4	141	7	-6	-3	37	15	3*
0	24	27	16*	-6	221	5	8	2	0	44	-4*	5	135	5	-0	-2	70	6	1
1	273	7	2	-4	203	5	5	3	112	10	-9	H,K=		10,	7	-1	70	6	-9
2	42	11	-1*	-2	168	4	-3	4	85	6	1	-9	100	5	12	0	222	6	3
3	226	7	-0	0	288	6	-0	5	182	5	0	-8	0	27	-10*	1	153	5	-8
4	13	33	-25*	2	309	7	-1	6	72	7	-4	-7	76	6	11	2	250	6	1
H,K=		9,	15	4	202	5	5	H,K=		10,	4	-6	32	13	20*	3	131	6	-1
-7	63	9	-8	6	55	9	4	-10	149	5	7	-5	266	6	1	4	168	5	0
-6	165	5	3	H,K=		10,	1	-9	88	5	11	-4	66	6	-10	H,K=		10,	11
-5	203	5	7	-10	136	4	14	-8	261	6	1	-3	365	8	-4	-8	49	9	-6
-4	213	5	2	-9	65	7	11	-7	123	4	1	-2	22	40	-15*	-7	83	6	5
-3	210	5	5	-8	19	27	9*	-6	254	6	-2	-1	307	7	1	-6	52	12	18*
-2	158	4	0	-7	80	7	-4	-5	101	8	-1	0	13	26	-5*	-5	205	5	6

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	79	6	-7	H,K=	10,	16		-8	105	5	1	4	189	6	-4	-5	50	8	6
-3	306	7	7	-5	171	5	12	-7	18	32	2*	H,K=	11,	7		-4	159	5	0
-2	118	6	1	-4	4	28	-5*	-6	54	7	0	-8	118	6	2	-3	94	6	3
-1	237	6	5	-3	53	8	13	-5	39	39	-3*	-7	40	17	38*	-2	232	5	4
0	49	12	-7*	-2	18	28	-5*	-4	199	5	3	-6	69	6	-7	-1	80	6	-1
1	93	5	1	-1	173	5	3	-3	140	5	7	-5	30	16	22*	0	212	5	2
2	20	28	9*	0	22	31	5*	-2	280	6	-12	-4	187	5	0	1	38	16	-3*
3	59	8	-1	1	241	6	2	-1	104	5	-1	-3	49	8	0	2	95	6	-0
4	62	8	-1	H,K=	10,	17		0	213	5	-4	-2	310	7	-5	H,K=	11,	12	
H,K=	10,	12		-3	183	5	-1	1	102	5	3	-1	35	15	24*	-6	233	5	11
-8	84	5	2	-2	151	5	5	2	68	7	-7	0	222	5	-3	-5	51	9	2*
-7	219	5	-2	-1	156	5	2	3	29	35	2*	1	49	11	4*	-4	159	4	4
-6	39	22	16*	0	100	7	6	4	22	34	-14*	2	103	5	2	-3	24	27	-5*
-5	156	4	2	H,K=	11,	0		H,K=	11,	4		3	25	31	23*	-2	35	24	-6*
-4	23	27	-7*	-9	177	5	18	-9	135	6	5	4	21	31	-14*	-1	55	8	13
-3	2	33	-6*	-7	276	6	13	-8	59	7	8	H,K=	11,	8		0	111	5	-3
-2	26	27	15*	-5	244	6	2	-7	238	6	0	-8	153	4	-2	1	74	6	3
-1	124	4	-5	-3	93	4	-0	-6	159	5	13	-7	165	5	4	2	200	5	-2
0	91	5	6	-1	71	5	14	-5	227	5	4	-6	206	6	10	H,K=	11,	13	
1	238	5	-3	1	169	5	1	-4	69	10	-6	-5	145	4	6	-5	116	5	0
2	112	10	7	3	263	6	-7	-3	98	6	-4	-4	114	4	0	-4	112	7	2
3	245	7	-2	5	187	6	5	-2	25	35	21*	-3	99	5	-1	-3	168	5	4
4	77	11	-3	H,K=	11,	1		-1	80	6	-0	-2	25	31	-19*	-2	123	7	-5
H,K=	10,	13		-9	154	5	16	0	42	10	-16*	-1	20	28	-11*	-1	203	5	0
-7	18	38	10*	-8	64	6	6	1	211	5	-6	0	109	5	3	0	101	6	2
-6	153	4	6	-7	23	29	17*	2	66	8	-12	1	152	5	1	1	157	6	10
-5	120	5	-2	-6	65	6	6	3	265	7	-2	2	185	7	-4	H,K=	11,	14	
-4	210	6	0	-5	127	5	5	4	108	9	-2	3	134	5	-2	-4	9	28	3*
-3	177	5	-1	-4	119	7	-4	H,K=	11,	5		4	146	5	-2	-3	103	5	1
-2	203	5	0	-3	260	6	5	-9	150	6	14	H,K=	11,	9		-2	43	12	38*
-1	135	5	6	-2	183	5	-1	-8	37	12	7*	-7	42	11	-1*	-1	73	7	-0
0	111	6	-4	-1	243	5	-9	-7	54	12	8*	-6	8	27	7*	0	20	29	-14*
1	28	33	-6*	0	155	4	-5	-6	32	17	-1*	-5	131	5	-6	H,K=	11,	15	
2	17	29	-1*	1	141	5	-7	-5	145	4	4	-4	55	7	2	-3	147	6	6
3	59	13	14*	2	91	5	8	-4	92	12	6	-3	229	6	3	-2	161	5	8
H,K=	10,	14		3	55	9	51	-3	255	6	-8	-2	39	11	8*	H,K=	12,	0	
-6	225	6	11	4	36	24	5*	-2	115	4	10	-1	274	6	-3	-8	155	5	12
-5	24	27	12*	5	90	6	2	-1	258	6	-14	0	34	15	7*	-6	252	6	10
-4	111	5	3	H,K=	11,	2		0	65	10	2	1	155	5	-2	-4	227	6	3
-3	38	12	23*	-9	22	27	2*	1	149	4	-5	2	31	18	21*	-2	137	4	5
-2	76	7	-10	-8	238	6	10	2	53	10	-8*	3	25	29	5*	0	44	10	30*
-1	35	35	5*	-7	66	6	3	3	46	10	9*	H,K=	11,	10		2	152	5	-8
0	224	6	4	-6	245	6	1	4	22	31	7*	-7	214	5	4	H,K=	12,	1	
1	48	10	-5*	-5	79	9	12	H,K=	11,	6		-6	120	5	4	-8	128	5	8
2	257	10	-6	-4	212	5	3	-8	179	5	8	-5	187	5	9	-7	51	12	6*
3	56	12	12*	-3	29	16	-4*	-7	146	4	3	-4	78	6	-5	-6	45	9	1*
H,K=	10,	15		-2	38	12	30*	-6	208	6	-2	-3	93	5	3	-5	0	33	-6*
-6	77	7	2	-1	53	7	8	-5	135	6	0	-2	51	9	8	-4	83	8	2
-5	146	6	10	0	145	5	5	-4	148	5	0	-1	0	29	-9*	-3	117	5	5
-4	187	5	0	1	33	14	14*	-3	63	7	-11	0	83	7	-4	-2	188	5	3
-3	174	5	-8	2	240	5	-2	-2	29	24	9*	1	168	5	1	-1	150	5	0
-2	165	5	-2	3	48	10	11*	-1	34	15	-2*	2	97	8	3	0	213	5	-4
-1	129	5	-1	4	258	6	6	0	134	5	-4	3	208	5	1	1	148	5	-2
0	84	7	2	5	53	9	14	1	112	5	-5	H,K=	11,	11		2	127	6	-5
1	78	6	9	H,K=	11,	3		2	200	5	-11	-7	15	28	-4*	3	66	8	3
2	0	29	-10*	-9	89	6	12	3	149	7	-4	-6	75	7	5	H,K=	12,	2	

STRUCTURE FACTORS CONTINUED FOR
YB.(C5(CH3)5)2.OC4H4.1/2(C6H5(CH3))

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-8	7	33	2*	1	106	6	2	0	129	6	-7								
-7	210	5	13	2	88	6	-7	H,K=	13,		2								
-6	76	9	-0	H,K=	12,		7	-5	29	23	-0*								
-5	244	6	-3	-7	127	5	7	-4	233	5	4								
-4	73	7	15	-6	33	14	29*	-3	58	10	15								
-3	191	5	9	-5	31	22	-3*	-2	190	5	2								
-2	37	13	1*	-4	25	33	23*	-1	35	35	-12*								
-1	60	11	7*	-3	166	5	2	0	72	7	-10								
0	20	28	7*	-2	2	38	-21*	H,K=	13,		3								
1	107	5	11	-1	256	6	-2	-5	43	18	6*								
2	26	35	0*	0	36	24	20*	-4	18	28	16*								
3	202	5	-3	1	231	5	7	-3	46	11	3*								
H,K=	12,		3	2	0	29	-7*	-2	133	5	11								
-7	120	4	15	H,K=	12,		8	-1	79	11	-4								
-6	34	13	22*	-6	158	5	14	0	203	6	-0								
-5	0	27	-6*	-5	185	5	9	H,K=	13,		4								
-4	57	7	3	-4	154	5	7	-5	200	5	10								
-3	156	4	0	-3	139	6	3	-4	85	11	9								
-2	106	4	4	-2	106	5	-1	-3	230	6	8								
-1	229	6	-2	-1	61	17	-1*	-2	83	10	-8								
0	104	6	-5	0	32	18	5*	-1	113	5	-7								
1	197	5	-7	1	95	6	3	0	25	30	-9*								
2	86	6	-4	H,K=	12,		9	H,K=	13,		5								
3	108	9	-1	-6	53	8	9	-5	76	8	3								
H,K=	12,		4	-5	23	35	22*	-4	20	28	16*								
-7	88	5	7	-4	94	5	-2	-3	92	6	8								
-6	229	6	9	-3	18	36	-3*	-2	40	14	0*								
-5	110	4	6	-2	195	5	-0	-1	174	5	-2								
-4	232	5	12	-1	44	10	5*	0	47	32	-5*								
-3	71	13	-6*	0	241	6	2	H,K=	13,		6								
-2	121	4	-0	1	44	11	8*	-4	199	5	2								
-1	59	12	17*	H,K=	12,		10	-3	128	5	4								
0	46	10	8*	-5	110	5	0	-2	143	5	-2								
1	48	12	12*	-4	190	5	9	-1	105	5	1								
2	159	5	-0	-3	98	6	4	H,K=	13,		7								
3	84	6	3	-2	122	5	-4	-3	4	29	-3*								
H,K=	12,		5	-1	46	9	22*	-2	133	5	-5								
-7	32	23	3*	0	28	28	11*												
-6	50	8	4	H,K=	12,		11												
-5	34	13	27*	-4	35	16	17*												
-4	70	6	-12	-3	138	5	5												
-3	80	8	3	-2	53	10	-8*												
-2	212	6	-4	-1	218	5	2												
-1	85	5	12	0	58	12	11*												
0	256	6	-5	H,K=	12,		12												
1	83	6	11	-2	40	20	6*												
2	176	5	1	H,K=	13,		0												
H,K=	12,		6	-5	197	5	5												
-7	156	4	15	-3	244	6	8												
-6	156	5	5	-1	149	5	1												
-5	209	5	14	H,K=	13,		1												
-4	121	6	9	-5	68	6	-8												
-3	175	5	1	-4	14	35	10*												
-2	89	5	1	-3	75	6	5												
-1	41	12	-14*	-2	93	5	-4												
0	27	28	10*	-1	145	5	-5												