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July 1984

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Dipotassium Bis-[8]Annulene-Ytterbium(II) and -Calcium(II)†

Steven A. Kinsley, Andrew Streitwieser, Jr.* and Allan Zalkin*

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

Abstract:

The title compounds were prepared by stoichiometric reaction of cyclooctatetraene, potassium and either ytterbium or calcium, in liquid ammonia solution. The dimethoxyethane adducts of $K_2[Yb(C_8H_8)_2]$ and $K_2[Ca(C_8H_8)_2]$ are crystalline and have similar x-ray powder patterns; $K_2[Yb(C_8H_8)_2]$ and $K_2[Ca(C_8H_8)_2]$ have identical infrared spectra. X-ray structure analysis of $[K(C_4H_{10}O_2)]_2[Yb(C_8H_8)_2]$ shows planar parallel eclipsed [8]annulene rings sandwiching a centrosymmetric ytterbium. A potassium coordinated with dimethoxyethane is at the opposite side of each ring. Crystals of $[K(C_4H_{10}O_4)]_2[Yb(C_8H_8)_2]$ crystallize in the triclinic system, $P\bar{1}$, with $\underline{a}$ = 9.346(4) Å, $\underline{b}$ = 9.775(4) Å, $\underline{c}$ = 7.740(4) Å, α = 91.72(4)°, β = 109.16(4)°, γ = 86.22(4)° at T = 23 °C.

† Dedicated to the memory of the late Professor Earl L. Muetterties who shared the same birthdate as one of us.

Introduction:

The organolanthanide complexes involving lanthanide(III) ions and the [8]annulene dianion[1] include complexes of the type $K[Ln(C_8H_8)_2]$,[2] $Ce_2(C_8H_8)_3$,[3] $[Ln(C_8H_8)(OC_4H_8)][Ln(C_8H_8)_2]$,[4] $[Ln(C_8H_8)Cl\cdot(OC_4H_8)]_2$,[5] $(C_8H_8)LnR(C_4H_8O)_x$,[6] $(C_8H_8)Ce(O\text{-}i\text{-}C_3H_7)_2Al(C_2H_5)_2$,[7] and $Ln(C_8H_8)(C_5H_5)$.[8] The determination of the structures of $[Ce(C_8H_8)Cl\cdot(OC_4H_8)]_2$,[9] $[K(C_6H_{14}O_3)][Ce(C_8H_8)_2]$[10] and $[Nd(C_8H_8)(OC_4H_8)][Nd(C_8H_8)_2]$[4] have shown that the [8]annulene rings of the complexes are planar with equivalent carbon-carbon bond lengths and that the lanthanide ions in the complexes containing $[Ln(C_8H_8)_2]^-$ are sandwiched by two [8]annulene rings. In contrast to the number of classes of complexes reported involving lanthanide(III) ions, there are reports of only two classes of [8]annulene complexes involving lanthanide(II) ions. The structures of these classes have not been elucidated.

The first lanthanide [8]annulene complexes reported, $Ln(C_8H_8)$ (Ln = Eu, Yb),[11] are the only [8]annulene complexes which have been shown to contain a divalent lanthanide. The characterization of the lanthanide(II) [8]annulene complexes is limited. The infrared spectrum of $Yb(C_8H_8)$[12] suggests a highly symmetric complex (the only bands present between 1000 and 600 cm^{-1} occur at 888 and 678 cm^{-1}), and the low solubility of the complexes in hydrocarbons, ethers and liquid ammonia suggests that the class $Ln(C_8H_8)$ is polymeric. No reactions of the divalent lanthanide complexes have been reported, except for their violent reaction with oxygen.

The report of synthesis of $K_2[Ce(C_8H_8)_2]$ from the reduction of $Ce(C_8H_8)_2$ by two equivalents of potassium in 1,2-dimethoxyethane[13] is the only example of a bis-[8]annulene compound with a central metal atom in a formal 2+ oxidation state. The cerium complex as its di(1,2-dimethoxyethane) adduct was characterized by elemental analysis and infrared spectrum. The structure of $[K(C_4H_{10}O_2)]_2[Ce(C_8H_8)_2]$ is not

known, but the infrared spectrum of the cerium complex does contain bands (887 and 682 cm^{-1}) which are consistent with the presence of an [8]annulene dianion.[14] Although there are reports of Ce(II) from the reduction of Ce(III) in other systems,[15] the presence of the cerium(II) ion in $[K(C_4H_{10}O_2)]_2[Ce(C_8H_8)_2]$ has not been shown by chemical or spectroscopic methods.

In order to study a bis-[8]annulene compound with a divalent central metal atom we have now synthesized and characterized the divalent ytterbium complex $K_2[Yb(C_8H_8)_2]$, **1**, and its calcium analogue, $K_2[Ca(C_8H_8)_2]$, **2**. The determination of the structure of the di(1,2-dimethoxyethane) adduct of **1** by single crystal x-ray diffraction is the first structure solved for a complex of [8]annulene dianion with a divalent lanthanide. In prior work on the bis-cyclopentadienyllanthanide(II) complexes,[16] a comparison of the infrared spectra of $Yb(C_5H_5)_2$ and $Ca(C_5H_5)_2$ had suggested that the ytterbium complex is isostructural with the calcium complex and, therefore, that the ring-metal bonding in the ytterbium complex is highly ionic. In this work the infrared spectra and x-ray powder patterns of **1** and **2** are used to show that **1** and **2** are isostructural.

Experimental Section

General : Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. Ytterbium metal turnings were purchased from Alfa/Ventron. Tetrahydrofuran (THF) was distilled from sodium/benzophenone. 1,2-Dimethoxyethane (DME) was distilled from Na/K alloy. Cyclooctatetraene (COT) (BASF) was vacuum distilled and stored over Molecular Sieves 3Å. Liquid ammonia was vacuum transferred into the reaction vessels from a solution of sodium in liquid ammonia. All air-sensitive compounds were handled in a helium or argon atmosphere glovebox or by standard Schlenk techniques. Infrared spectra were

determined with a Perkin-Elmer Model 283 infrared recording spectrophotometer. Samples for infrared determination were prepared in a glovebox as Nujol mulls. Visible spectra of THF solutions of the organometallic compounds were determined with a Cary Model 118 spectrophotometer; results are expressed as λ_{max} in nm (log ε). ^{1}H-NMR of the organometallic compounds were determined in sealed tubes of THF-$\underline{d}_8$ solutions on a JOEL FX-90Q. The chemical shifts of the proton resonances are referenced to the low field residual proton resonance of THF-$\underline{d}_8$ (set as 3.58 ppm). Samples for x-ray powder pattern determination were prepared by grinding the crystalline sample to a fine powder and sealing the powder into a quartz capillary under argon. X-ray powder pattern data were taken with a Debye-Scherrer camera using nickel filtered copper Kα x-rays. Elemental analyses were performed by the Microanalytical Laboratory of the College of Chemistry, University of California, Berkeley.

Reactions in liquid ammonia: The reaction vessel used for the syntheses in liquid ammonia was a two-necked 100 mL round bottom flask with sidearm. During the reactions, the flask was connected through one neck to a Schlenk line and cooled in a Dry Ice/isopropanol bath. While transferring the liquid ammonia into the reaction vessel and during the course of the reaction, the vacuum manifold was isolated from the vacuum pump. The vacuum manifold was protected from developing high ammonia pressure by a mercury bubbler. After the metals were added to the ammonia, a septum was placed on the free neck of the flask (under argon purge) and cyclooctatetraene was added to the blue solution via syringe. Since cyclooctatetraene freezes on contact with liquid ammonia at that low temperature, the Dry Ice bath was removed to facilitate reaction. When the reaction was complete, the ammonia was allowed to evaporate through the mercury bubbler, leaving the pyrophoric material behind.

X-ray Analysis: With the exception of the ORTEP program, all computer programs

used were written by one of the authors (AZ) for a CDC 7600 computer.

An irregular, orange-red single crystal fragment of 1·2DME with maximum dimensions of 0.2 mm was sealed inside a quartz capillary in an argon atmosphere and examined with a modified Picker FACS-I Automated diffractometer equipped with a graphite monochromator and a Mo x-ray tube. Least squares refinement of the setting angles of 24 centered reflections (27° > 2θ > 20°) using Mo Kα (λ = 0.71073 Å) radiation gave a = 9.346(4) Å, b = 9.775(4), c = 7.740(4) Å, α = 91.72(4)°, β = 109.16(4)°, γ = 86.22(4)°, and V = 666.5 Å^3 at 23 °C. The space group of the crystal is triclinic, P$\bar{1}$, with one formula unit in the unit cell. The calculated density of the crystal (molecular weight of $[K(C_4H_{10}O_2)]_2[Yb(C_8H_8)_2]$ = 639.80) is 1.59 g cm^{-3}.

Intensities were collected to a maximum 2θ value of 50° using a θ − 2θ scan technique. Three standard reflections were measured at every 250th measurement; the three standards showed an isotropic decay of about 5% and the data were adjusted accordingly. A total of 4729 intensities were measured and averaged to give 2361 unique data of which 2312 were used in the least squares with $F^2 > 1\sigma(F^2)$. The data were not corrected for absorption because of the difficulty of seeing the faces and measuring the crystal's irregular dimensions. The absorption coefficient calculates to 38 cm^{-1} and an error of approximately 5% in the intensities is estimated.

Trial positions for the ytterbium and potassium atoms were obtained from a three-dimensional Patterson function and were refined by least squares. An electron density map revealed all of the non-hydrogen atoms. All of the non-hydrogen atoms were refined with anisotropic temperature factors and the hydrogen atoms were included at their estimated positions, but not refined. The F magnitude was used in the full-matrix refinement.

The final weighted R factor[17] was 0.034 for 2312 data with $F^2 > \sigma(F^2)$, and the goodness of fit was 1.33. The assigned weights $w = (\sigma(F))^{-1}$, were derived from $\sigma(F^2) = [\underline{c} + (\underline{p}F^2)^2]^{1/2}$, where $\underline{c}$ is the variance due to counting statistics and $\underline{p} = 0.05$. An empirical extinction correction of the form $F_{corr} = F_{obs}(1 + \underline{k}I)$, where $\underline{k} = 2.13 \times 10^{-7}$, was applied to the data. Scattering factors were taken from literature sources[18] and anomalous scattering terms were applied.[19]

Preparation of 1 and 2. The procedure for the synthesis of the divalent ytterbium complex follows with differences for the procedure for the calcium complex noted. Cyclooctatetraene (1.79 g, 17 mmol) was added to a Dry-Ice/isopropanol-cooled liquid ammonia solution of 0.67 g (17 mmol) of potassium metal and 1.49 g (8.6 mmol) of ytterbium metal. The Dry-Ice/isopropanol bath was removed from the reaction vessel at this time to allow the ammonia solution to warm. As the reaction began, the solution turned green as a bright orange precipitate appeared (the solution and precipitate were bright yellow for the calcium reaction). The ammonia was allowed to evaporate and a bright orange solid was left in the reaction vessel (bright yellow for calcium). When the reaction vessel was warmed with a heat gun, the solid turned bright pink (pale green for calcium). The yield of the solid was 3.57 g (90%). Yields from the liquid ammonia reactions were typically about 90%. Crystals of the THF adducts of 1 and 2 were obtained by the slow cooling of a saturated solution of 1 or 2 in the ether. The THF adducts of 1 and 2 rapidly lost THF of solvation (ca. one hour in an argon atmosphere or ca. 5 minutes, <u>in vacuo</u>) and decomposed to unsolvated powders. Analysis of 2 as a THF complex was not satisfactory, but the analysis does suggest that there are two THF molecules per potassium atom. Anal. of 2·4THF: Calcd. for $C_{32}H_{48}O_4K_2Ca$: C, 62.49; H, 7.87; K, 12.71. Found: C, 61.73; H, 7.40; K, 11.8.

The unsolvated powders were heated at 200°C, <u>in vacuo</u>, for one hour to insure the complete removal of solvated THF. The yield of powder was 57% for 1 (67% for 2) from

the first crop of crystals. The infrared spectra of 1 and 2 are shown in Figure 2. ^{1}H-NMR of 1 δ = 5.47 $\pm$ .03, singlet (2 δ = 5.47 $\pm$ .03, singlet). Visible spectrum of 1 504 nm (850). Satisfactory analyses of the powders were difficult to obtain, especially in the case of the ytterbium complex. Anal: 1: Calcd. for $C_{16}H_{16}K_2Yb$: C, 41.82; H, 3.51; K, 17.01. Found: C, 39.66; H, 3.64; K, 19.2. 2: Calcd. for $C_{16}H_{16}K_2Ca$: C, 58.85; H, 4.94; K, 23.94. Found: C, 58.47; H, 5.22; K, 23.4.

The slow cooling of a saturated solution of 1 or 2 in DME gave crystals of the complexes as DME adducts. The DME adducts of 1 and 2 were stable and gave satisfactory analyses for one DME molecule per potassium. 1·2DME: Calcd. for $C_{24}H_{36}O_4K_2Yb$: C, 45.06; H, 5.67; K, 12.22. Found: C, 44.79; H, 5.59; K, 12.4. 2·2DME: Calcd. for $C_{24}H_{36}O_4K_2Ca$: C, 56.88; H, 7.16; K, 15.43. Found: C, 57.11; H, 7.07; K, 16.07.

Preparation of $K[Yb(C_8H_8)_2]$, 3. In a procedure which is analogous to the procedure used to synthesis 1 and 2, the potassium salt of bis-[8]annuleneytterbium(III) was prepared by the addition of 0.88 g (8.4 mmoles) of cyclooctatetraene to a Dry-Ice/isopropanaol cooled liquid ammonia solution of 0.73 g (4.2 mmoles) of ytterbium metal and 0.16 g (4.2 mmoles) potassium metal. When the reaction was complete and the solvent had evaporated, a bright orange powder was left in the reaction vessel. This powder turned bright blue when the reaction vessel was warmed with a heat gun and exposed to a vacuum. The crude yield of this powder was 1.50 g (86 %). Satisfactory analysis could not be obtained for 3, but the infrared spectrum of 3 (the major absorbances in the 600 to 1000 cm^{-1} region are given in Table III) is similar to the infrared spectra of the other bis[8]annulene lanthanide salts.[2b] λ_{max} of 3 in THF is 574 nm (1400). A portion of this powder was crystallized from DME to give 3·DME. Anal. Calcd. for $C_{20}H_{26}O_2YbK$: C, 47.05; H, 5.13; K, 7.66. Found: C, 46.51; H, 4.91; K, 8.27; N, 0.28.

Results and Discussion

Structure of $[K(C_4H_{10}O_2)]_2[Yb(C_8H_8)_2]$: The atomic parameters and distances are listed in Tables I and II. Figure 1 shows an ORTEP view of a formula unit with the numbering scheme used for the atoms in Table II. Additional atomic distances are available as supplementary material.

The [8]annulene rings of 1·2DME are planar with all the carbon-carbon bond lengths equivalent. The maximum deviation from the least squares plane of the ring for any carbon atom is 0.01 Å. The carbon-carbon distances within the ring range from 1.40 to 1.42 Å with an average of 1.41 ± .01 Å. The bond angles within the ring are all within their standard deviations of 135°.

The ytterbium atom is on the center of symmetry and is sandwiched by two planar [8]annulene ligands; the potassium atoms are each coordinated to one dimethoxyethane ligand and a $[Yb(C_8H_8)_2]$ dianion. The average ytterbium-to-carbon distance is 2.74 ± 0.03 Å; the distance of the ytterbium atom to the least squares plane of the [8]annulene is 2.03 Å. The two sandwiching [8]annulene rings are parallel-planar and exactly eclipsed (being related to each other through the center of symmetry), making the symmetry of the $[Yb(C_8H_8)_2]$ dianion D_{8h}. 1 is the only bis-[8]annulene complex of a lanthanide that exhibits eclipsed rings. In $K(C_6H_{14}O_3)][Ce(C_8H_8)_2]$[10] the [8]annulene rings are in a staggered conformation (i.e., the symmetry of the $[Ce(C_8H_8)_2]$ anion is D_{8d}) and in $[Nd(THF)_2(C_8H_8)][Nd(C_8H_8)_2]$[4] the [8]annulene rings are nearly eclipsed, but not parallel-planar. The eclipsed vs. staggered arrangement of bis-[8]annulene rings is not considered to be indicative of the type of ring-metal bond for these complexes. Wideline NMR studies on crystals of $U(C_8H_8)_2$ indicate that the barrier to ring rotation is essentially 0 kcal mole^{-1}.[20] Any conformational preference for the rings in the bis-[8]annulene complexes is more than likely due to

crystal packing forces, and not due to orbital interactions between the metal and ligands.

The average potassium-to-carbon distance is 3.02 ± 0.02 Å; the distance of the potassium atom to the least squares plane of the [8]annulene ring is 2.39 Å. The potassium atom is also coordinated to two oxygen atoms of a DME ligand at 2.796(4) Å and 2.731(4) Å and to an oxygen atom of an adjacent DME ligand at a distance of 2.928(4) Å.

The average Yb-C distance (2.74 ± .03 Å) in 1·2DME is the same as the average Ce-C distance (2.74 ± .02 Å) in $[K(C_6H_{14}O_3)][Ce(C_8H_8)_2]$.[10] These equal distances are consistent with Raymond's arguments on the ionic nature of the metal-carbon bond in [8]annulenelanthanide complexes,[21] since the ionic radii of Ce(III) and Yb(II) are the same.[22] Note that the addition of the calculated ionic radius of carbon in [8]annulene dianion, 1.49 Å,[23] to the extrapolated ionic radius for a 10-coordinate divalent ytterbium cation, 1.25 Å,[24] gives a Yb-C distance of 2.74 Å.

Physical Properties: The physical properties for 1 and 2 are similar to the properties reported for the trivalent lanthanide complexes, $K[Ln(C_8H_8)_2]$.[2] The most noticable similarity is the air-sensitivity of the compounds $K_2[M(C_8H_8)_2]$; 1 and 2 enflame in contact with air.

Compounds 1 and 2 are thermally stable, showing no sign of decomposition when heated to 360 °C sealed under one atm of argon or to 200 °C <u>in vacuo</u>. In THF solution, 1 is oxidized to $K[Yb(C_8H_8)_2]$, 3, by O_2, CCl_4, COT, and $U(C_8H_8)_2$; the presence of the bright blue ytterbium(III) complex was indicated by its visible spectrum. Compound 3 is thermally unstable and is converted to 1 (by the loss of COT) when heated at 310 °C sealed under one atm of argon, or to 200 °C <u>in vacuo</u>. A mass

spectrum of 1 shows no m/z that can be attributed to the ionization of the sandwich compound.

Compounds 1 and 2 have the same solubility properties; they are insoluble in hydrocarbon solvents such as hexane, toluene and benzene, but soluble in ethers such diethyl ether, THF, and DME. The slow cooling of a saturated solution of 1 or 2 in an ether gives crystals of the ether adduct. The THF adducts of 1 and 2 rapidly lose THF *in vacuo* or in an argon atmosphere (ca. one hour), but the DME adducts are stable at ambident temperatures. As with all of the lanthanide [8]annulene complexes, 1 and 2 exist as powders in the absence of coordinated ether molecules.

^{1}H-NMR: The ^{1}H-NMR of 1 and 2 were determined in THF-d_8 solutions. The eight equivalent protons of 2 occur as a singlet at δ = 5.47 ppm. This resonance is observed upfield from the resonances reported for $K[Y(C_8H_8)_2]$ and $K[La(C_8H_8)_2]$ which occur at 5.75 and 5.90 ppm, respectively, relative to external TMS.[2b] The ring proton resonance of 1 is observed at δ = 5.47 ppm. In its ground state, the ytterbium(II) ion has no unpaired electrons[25] and is diamagnetic; the lack of a shift in the observed ring proton resonance of 1 relative to 2 shows that 1 contains the diamagnetic lanthanide(II) ion.

Visible Spectra: The bright orange 1 in THF solution has an intense, broad absorbance in the visible region at 504 nm. In THF solution, II has no absorbance in the visible region. The pale green color of 2 is due to trace impurities; repeated recrystallization of 2 from THF gives a pure white powder.

The visible spectrum of 1 in THF can be readily interpreted. Earlier studies on the class $K[Ln(C_8H_8)_2]$ led to the conclusion that the broad absorption bands in the visible region of these complexes are due to ligand-to-metal charge transfer.[2] The

visible absorbance of 1 can also be assigned to a ligand-to-metal charge transfer band. Preliminary studies on the di-t-butyl derivative of 1, $K_2[Yb(C_8H_7(C_4H_9))_2]$, show the visible absorbance red-shifted to 520 nm.[26] Alkyl substituents on the [8]annulene dianion make the ligand more reducing and would shift a ligand-to-metal charge transfer band to lower energy. Since the Yb(II) ion in 1 has completely filled 4f orbitals, π-f charge transfer can be ruled out and the visible absorbance of 1 can be assigned as a ligand π-to-metal d charge transfer.

Infrared Spectra: The infrared spectra of 1 and 2 as Nujol mulls are shown in Figure 2. The infrared spectra of 1·2DME and 2·2DME are available as supplementary material.

The infrared spectra of 1 and 2 are identical; the infrared spectra of 1·2DME and 2·2DME are also identical. This similarity of infrared spectra was anticipated, since ytterbium(II) and calcium(II) have almost identical ionic radii[22] and previous work had shown that the infrared spectra of $CaCp_2$ and $YbCp_2$ are similar,[16] even though the sample of $YbCp_2$ may have been contaminated with $YbCp_3$.[27]

Infrared spectra for the 600-1000 cm^{-1} region of some bis-[8]annulene complexes are compared in Table III. It has been noted previously that the infrared spectra of all of the bis-[8]annulene sandwich complexes of the f-transition metals are similar as a result of their similar structures.[2] The assignment of the infrared absorbances of these complexes is still in question; a recent assignment[28] (shown in Table II) is additionally consistent with the fact that 1 and 2 have the same infrared spectra. An earlier assignment attributed the strong band at 698 cm^{-1} to a ring-metal-ring tilt.[29] Such an assignment could not give identical spectra for 1 and 2, since the difference in mass of ytterbium and calcium would cause a difference in energy for any absorbances which involve the central metal. Since the infrared spectra of 1 and

2 are identical in the 400-4000 cm^{-1} region, then any absorbance involving the central metal must occur outside of this range.

Powder Pattern: The measured powder patterns of 1·2DME, 2·2DME and the powder pattern calculated from the single crystal x-ray data of 1·2DME are available as supplementary material. The powder pattern of 1·2DME was calculated using the cell dimensions and the structure factor of the single crystal structure determinations. Only two weak lines out of 21 lines calculated for 1·DME are not observed in the pattern of 2·2DME.[30] Since the ytterbium(II) complex contains 50 more electrons than the calcium complex, one expects and finds intensity differences in the measured powder patterns of 1·2DME and 2·2DME. Nevertheless, the x-ray powder patterns are sufficiently similiar that 1·2DME and 2·2DME are clearly isostructural.

Conclusion

Except for the differences that can be attributed to either the difference in the number of electrons between ytterbium and calcium, or to the availability of a trivalent state for the ytterbium complex, 1 and 2 behave as identical complexes. Since it is highly unlikely that the 4f and 5d orbitals are involved in the ring-metal interaction of 2, these orbitals also play no major role in the ring-metal interaction of 1. The agreement of the ring-metal distance in 1·2DME with the sum of the ionic radius of carbon in [8]annulene dianion and the ionic radius of 10-coordinate ytterbium(II) also suggests the lack of significant covalent interaction between the ring and metal in 1. The results reported in this paper further emphasize the unimportance of the 4f and 5d orbitals in ytterbium(II) chemistry; e.g., the ring-metal interaction in 1 is essentially ionic.

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Supplementary Material Available:

Infrared spectra (1'2DME, 2'2DME), calculated (1'2DME) and measured (1'2DME and 2'2DME) powder patterns, least squares plane ([8]-annulene), listing of anisotropic thermal parameters, calculated hydrogen positions, C-C distances, selected angles and observed structure factors for 1'2DME (18 pages). Ordering information is given on any current masthead.

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17. $R = \Sigma \left| |F_o| - |F_c| \right| / \Sigma |F_o|$

18. For Yb, K, O, and C atoms: International Tables for X-ray Crystallography (1974), Vol. IV, Kynoch Press, Birmingham. For H atoms: Stewart, R.F.; Davidson, E.R.; Simpson, W.T. J. Chem. Phys. 1965, 42, 3175.

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23. In this type of [8]annulene complex, Raymond employs a radius of 1.49 Å for a ring carbon atom; see reference 21.

24. See reference 22. Each [8]annulene dianion is considered to be a ten- electron donor so that each ring formally donates five electron pairs.

25. Ytterbium(II) has a ground state configuration of $[Xe]4f^{14}$.

26. The report of $K_2[Yb(t\text{-}Bu\text{-}C_8H_7)_2]$ and the crystal structure of its diglyme adduct is in preparation.

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29. Hocks, L,; Goffart, J.; Duyckaerts, G.; Teyssie, P. Spectrochim. Acta 1974, 30A, 907. These authors comment that the band at 698 cm^{-1} in $U(C_8H_8)_2$ is unusually high for ring-metal-ring tilt.

30. The powder patterns are compared for lines with a d-spacing between 9.75 and 3.10 Å.

Table I. Positional parameters for $[K(C_4H_{10}O_2)][Yb(C_8H_8)_2]$[a]

Atom	x	y	z
Yb	0	0	0
K	0.35199(13)	−0.34073(12)	0.09645(17)
O(1)	0.5266(4)	−0.5865(4)	0.2003(5)
O(2)	0.6346(4)	−0.3377(4)	0.3517(6)
C(1)	0.2982(6)	−0.0479(6)	0.1970(8)
C(2)	0.2208(7)	−0.1188(6)	0.2916(7)
C(3)	0.1084(7)	−0.2140(6)	0.2420(8)
C(4)	0.0252(7)	−0.2787(6)	0.0758(10)
C(5)	0.0200(6)	−0.2717(6)	−0.1077(9)
C(6)	0.0944(7)	−0.1982(6)	−0.2010(7)
C(7)	0.2084(6)	−0.1027(6)	−0.1517(8)
C(8)	0.2936(6)	−0.0416(6)	0.0138(9)
C(9)	0.4371(9)	−0.7001(7)	0.1946(12)
C(10)	0.6448(7)	−0.5787(6)	0.3691(8)
C(11)	0.7322(7)	−0.4573(7)	0.3771(9)
C(12)	0.7098(8)	−0.2143(7)	0.3748(10)

(a) In this Table and in Table II, the number in parentheses is the estimated standard deviation in the least significant digits.

Table II. Selected interatomic distances (Å)

Atom 1-Atom 2	Distance	Atom 1-Atom 2	Distance
Yb-C(1)	2.719(5)	K-C(1)	2.998(6)
-C(2)	2.736(5)	-C(2)	3.026(6)
-C(3)	2.760(5)	-C(3)	3.036(6)
-C(4)	2.783(5)	-C(4)	3.027(6)
-C(5)	2.773(5)	-C(5)	3.025(6)
-C(6)	2.729(5)	-C(6)	3.025(6)
-C(7)	2.711(5)	-C(7)	3.012(6)
-C(8)	2.715(5)	-C(8)	2.989(6)
O(1)-C(9)	1.425(8)	K-O(1)	2.796(4)
-C(10)	1.411(7)	-O(2)	2.731(4)
O(2)-C(11)	1.415(7)	K-O(1)[a]	2.928(4)
-C(12)	1.414(8)		
C(11)-C(10)	1.481(10)		

(a) Atom at position 1-x, -1-y, -z.

Table III. Comparison of infrared spectra[a,b]

$U(C_8H_8)_2$[c]	$K[La(C_8H_8)^2]$[d]	$K[Yb(C_8H_8)_2]$[e] 3	$K_2[Yb(C_8H_8)_2]$[e,f] 1	Assignment[f]
698 vs	680 vs	690 vs	683 vs	ρ(CH), A_{2u}
746 s	740 m	741 s	740 m	v(CC), A_{2u}
777 m	771 w	770 w		ρ(CH), E_{1u}
792 m				
			879 s	
900 s	892 s	899 s	888 s	β(CH), E_{1u}

(a) vs, very strong; s, strong; m, medium; w, weak. (b) nujol mulls. (c) Ref. 29. (d) Ref. 28. (e) This work. (f) Infrared of 1 and 2 are identical.

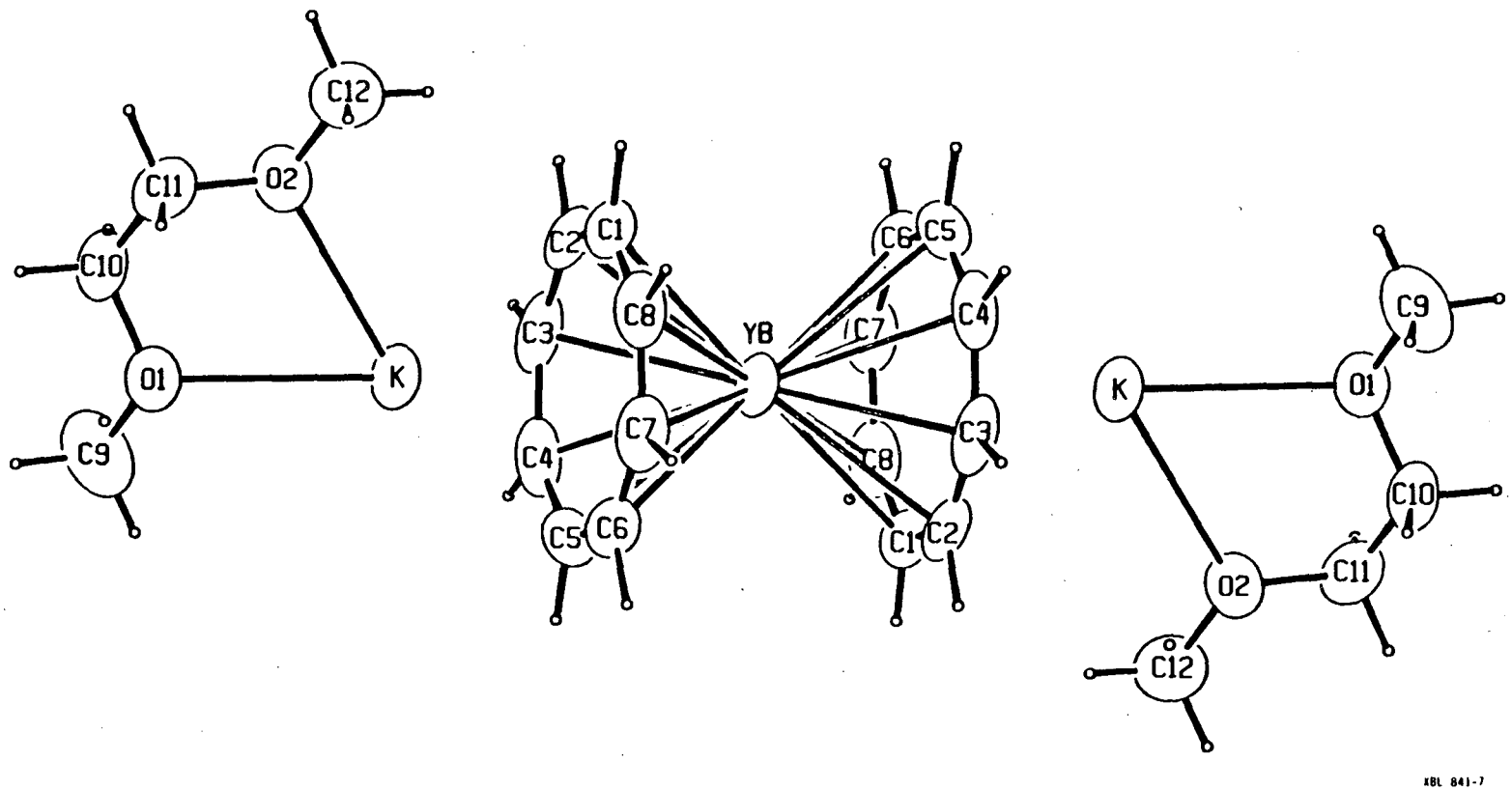

Figure 1: ORTEP drawing of $[K(C_4H_{10}O_2)]_2[Yb(C_8H_8)_2]$ showing atomic numbering scheme.

Figure 2: Infrared spectra[a] of $K_2[Ca(C_8H_8)_2]$ - top,

$K_2[Yb(C_8H_8)_2]$ - bottom.

(a) nujol mulls.

Dipotassium Bis-[8]Annulene-Ytterbium(II) and -Calcium(II)

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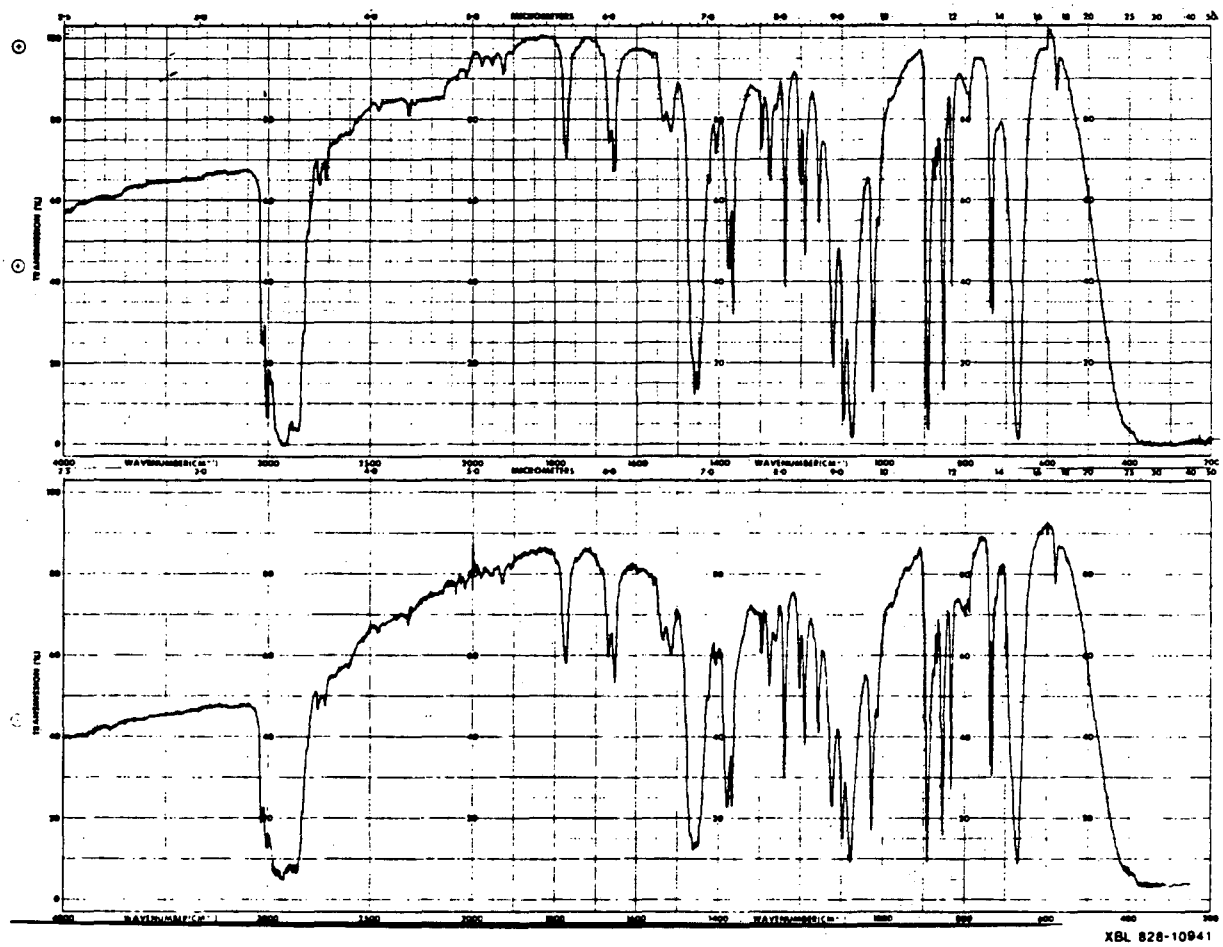
Supplementary Material

1. Infrared Spectra of $[K(C_4H_{10}O_2)]_2[M(C_8H_8)_2]$ M = Ca, Yb
2. Anisotropic Thermal Parameters
3. Calculated Positions for Hydrogen Atoms
4. C-C Distances and Selected Angles
5. Least Squares Plane
6. Powder Patterns
7. Observed Structure Factors

1. Infrared spectra of $[K(C_4H_{10}O_2)]_2[M(C_8H_8)_2]$ M= Ca, Yb



$[K(C_4H_{10}O_2)]_2[Yb(C_8H_8)_2]$ - Top

$[K(C_4H_{10}O_2)]_2[Ca(C_8H_8)_2]$ - Bottom

Nujol mulls

2. Table of Anisotropic Thermal Parameters in $K_2Yb(C_8H_8)_2 \cdot (CH_3COCH_2CH_2OCH_3)_2$[a]

ATOM	B11	B22	B33	B12	B13	B23
YB	3.040(16)	3.324(16)	3.317(16)	1.267(18)	1.163(11)	.594(18)
K	3.47(5)	3.57(5)	4.28(5)	1.16(4)	.81(4)	.28(4)
O(1)	4.26(18)	3.39(16)	4.55(18)	.87(14)	1.85(14)	.42(13)
O(2)	3.57(17)	3.62(17)	6.15(22)	.84(14)	.88(15)	-.26(15)
C(1)	2.41(28)	3.78(24)	5.04(28)	.92(18)	-.28(19)	-.32(21)
C(2)	4.36(26)	4.66(27)	2.75(20)	2.16(23)	.13(18)	.61(19)
C(3)	4.65(27)	4.57(27)	3.88(24)	1.98(23)	2.02(22)	2.38(21)
C(4)	3.69(24)	2.75(21)	6.9(4)	.61(18)	1.87(24)	1.57(22)
C(5)	3.41(23)	3.07(22)	5.5(3)	.46(18)	.56(21)	-1.81(28)
C(6)	4.21(25)	4.51(26)	2.90(20)	1.76(22)	.98(18)	-.59(18)
C(7)	3.96(24)	4.50(26)	4.30(25)	1.77(21)	2.74(21)	.89(28)
C(8)	2.43(28)	3.72(24)	6.5(3)	.82(18)	2.14(21)	.82(22)
C(9)	6.4(4)	4.4(3)	9.2(5)	-.58(28)	3.9(4)	-.3(3)
C(10)	5.28(29)	3.93(25)	4.04(25)	1.42(22)	1.26(22)	.81(28)
C(11)	3.27(24)	5.7(3)	4.83(28)	.98(22)	.37(21)	-.43(24)
C(12)	4.7(3)	5.4(3)	6.3(4)	-1.18(27)	.47(27)	-.33(28)

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[a] The anisotropic temperature factor has the form

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

3. Estimated Positional Parameters for the Hydrogen Atoms in $K_2Yb(C_8H_8)_2 \cdot (CH_3OCH_2CH_2OCH_3)$[a]

H(1)	.374	.811	.2789
H(2)	.2536	-.0968	.423
H(3)	.0733	-.2419	.3465
H(4)	-.0435	-.3442	.0944
H(5)	-.0522	-.3333	-.189
H(6)	.0585	-.2175	-.3334
H(7)	.2338	-.0719	-.2576
H(8)	.3674	.0203	-.0018
H(9)	.390	-.6917	.2908
H(10)	.4993	-.7861	.2097
H(11)	.3549	-.7833	.8743
H(12)	.7113	-.6623	.3875
H(13)	.6003	-.5698	.4788
H(14)	.817	-.4519	.4868
H(15)	.7735	-.4637	.2691
H(16)	.7615	-.2087	.2838
H(17)	.7854	-.2103	.4982
H(18)	.6360	-.1353	.3602

[a] These parameters were included at these calculated positions but not refined in the least-squares procedures. H(1-8) and H(9-18) were assigned isotropic thermal parameters of 8.0 and 10.0 respectively; the isotropic thermal parameters were also not refined. All C-H distances are between 0.98 and 1.00 Å.

4. Selected angles in $K_2Yb(C_8H_8)_2 \cdot (CH_3OCH_2CH_2OCH_3)$

C(1)-C(2)-C(3)	134.8(5)
C(2)-C(3)-C(4)	135.0(5)
C(3)-C(4)-C(5)	134.9(5)
C(4)-C(5)-C(6)	134.9(5)
C(5)-C(6)-C(7)	135.5(5)
C(6)-C(7)-C(8)	134.6(5)
C(7)-C(8)-C(1)	135.0(5)
C(8)-C(1)-C(2)	135.2(5)
O(1)- K -O(2)	92.8(2)
K -O(1)-C(9)	112.9(4)
K -O(1)-C(10)	114.0(3)
K -O(2)-C(12)	117.4(4)
K -O(2)-C(11)	118.1(4)
C(9)-O(1)-C(10)	111.4(5)
C(12)-O(2)-C(11)	113.9(5)
O(1)-C(10)-C(11)	109.6(5)
O(2)-C(11)-C(10)	109.0(5)

C-C Distances in cyclooctatetraene ligand

C(1)-C(2)	1.409(9)
C(2)-C(3)	1.400(10)
C(3)-C(4)	1.421(10)
C(4)-C(5)	1.409(9)
C(5)-C(6)	1.395(9)
C(6)-C(7)	1.413(9)
C(7)-C(8)	1.407(9)
C(8)-C(1)	1.408(9)

5. Cyclooctatetraene Least Squares Plane

Atom	Distances to Plane (Å)
C(1)	0.006
C(2)	-0.010
C(3)	-0.008
C(4)	0.011
C(5)	0.009
C(6)	-0.012
C(7)	-0.008
C(8)	0.012
Yb	-2.032
K	2.391

Plane equation with respect to crystallographic axes:

$$6.005X - 6.898Y - 0.425C = 2.032$$

6. CALCULATED POWDER PATTERN FOR K2YB(C8H8)2.(CH3OCH2CH2OCH3)2
X-RAY WAVE LENGTH = 1.54180 ANGSTROMS.

A = 9.346 B = 9.775 C = 7.740
ALPHA = 91.72 BETA = 109.16 GAMMA = 86.22

H	K	L	D	I	2 THETA	SINSQ
0	1	0	9.753	282.	9.07	.00625
1	0	0	8.813	140.	10.04	.00765
0	0	1	7.311	747.	12.11	.01112
1	0	-1	6.831	282.	12.96	.01274
1	1	0	6.741	1000.	13.13	.01306
1	-1	0	6.354	229.	13.94	.01472
0	-1	1	5.875	161.	15.08	.01722
0	1	1	5.825	365.	15.21	.01751
1	1	-1	5.744	599.	15.43	.01801
1	-1	-1	5.457	77.	16.24	.01995
1	0	1	4.895	150.	18.12	.02480
0	2	0	4.877	24.	18.19	.02499
2	0	-1	4.476	155.	19.83	.02966
1	1	1	4.423	144.	20.08	.03038
2	0	0	4.406	36.	20.15	.03061
1	2	0	4.379	58.	20.28	.03100
1	-1	1	4.328	4.	20.52	.03172
2	1	-1	4.174	38.	21.29	.03412
1	-2	0	4.163	11.	21.34	.03428
2	1	0	4.108	50.	21.63	.03521
1	2	-1	4.075	36.	21.81	.03579
0	-2	1	4.074	37.	21.82	.03581
0	2	1	4.040	46.	22.00	.03640
2	-1	-1	3.971	7.	22.39	.03770
2	-1	0	3.929	7.	22.63	.03850
1	-2	-1	3.871	41.	22.98	.03966
1	0	-2	3.852	232.	23.09	.04006
0	0	2	3.655	14.	24.35	.04447
1	1	-2	3.626	3.	24.55	.04519
1	-1	-2	3.540	2.	25.16	.04742
1	2	1	3.502	17.	25.43	.04845
0	-1	2	3.433	63.	25.95	.05043
2	0	-2	3.415	3.	26.09	.05095
0	1	2	3.413	22.	26.11	.05102
2	2	-1	3.411	34.	26.12	.05107
1	-2	1	3.409	69.	26.14	.05114
2	2	0	3.371	44.	26.44	.05231
2	0	1	3.324	85.	26.82	.05379
2	1	-2	3.280	46.	27.19	.05525
0	3	0	3.251	113.	27.43	.05623
2	-2	-1	3.195	16.	27.93	.05823
2	1	1	3.186	4.	28.01	.05855
2	-2	0	3.177	1.	28.09	.05888
2	-1	-2	3.170	154.	28.15	.05913
1	3	0	3.111	29.	28.70	.06141
2	-1	1	3.108	107.	28.73	.06154
3	0	-1	3.099	80.	28.81	.06189
1	2	-2	3.076	11.	29.03	.06281

X-RAY POWDER PATTERN COMPARISON

$[K(C_4H_{10}O_2)][Yb(C_8H_8)_2]$		$[K(C_4H_{10}O_2)][Yb(C_8H_8)_2]$		$[K(C_4H_{10}O_2)][Ca(C_8H_8)_2]$	
Calculated		Found		Found	
D(Å)	I	D(Å)[b]	I[c]	D(A)[b]	I[c]
9.75	282	9.83(5)	w+		
8.81	140	8.80(4)	w	8.76(4)	w
7.31	747	7.31(3)	s-	7.33(3)	s-
6.76	1282	6.73(2)	s	6.74(2)	s
6.35	229	6.36(2)	w+	6.37(2)	w-
5.79	1125	5.76(2)	s-	5.76(2)	s-
5.46	77	5.45(2)	w-		
4.89	174	4.87(1)	w+	4.90(1)	w-
4.45	392	4.42(1)	m	4.47(1)	m
4.33	4			4.34(1)	w
4.14	99	4.15(1)	w-	4.15(1)	w-
4.06	119	4.07(1)	w-	4.07(1)	w-
3.95	13			3.93(1)	w-
3.85	273	3.85(1)	m	3.85(1)	m
3.65	17			3.61(1)	w-
3.51	19			3.53(1)	w-
3.41	235	3.43(1)	w+	3.43(1)	w
3.31	131	3.31(1)	w-	3.31(1)	w-
3.24	129	3.25(1)	w-	3.25(1)	w-
3.17	155	3.17(1)	w	3.17(1)	m
3.10	227	3.10(1)	w	3.10(1)	w

[a]Adjacent lines combined where 2θ values are less than 0.50° apart. The position of the lines is calculated as $D = \frac{\Sigma(D_i * I_i)}{\Sigma I_i}$. See previous page

[b]The number in brackets is estimated error in the least significant digit.

[c]Estimated relative intensity

% OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 8.0)
K2YB(C8H8)2,(CH3OCH2CH2OCH3)2 F(0,0,0) = 2557

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

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
H,L=		0,	0	4	495	13	-9	H,L=		0,	5	6	63	14	6	4	159	5	-3
1	386	18	6	5	170	5	4	-9	95	6	-7	H,L=		0,	0	5	199	6	1
2	227	6	1	6	371	10	-3	-8	97	6	-4	-4	150	5	0	6	177	5	4
3	755	19	5	7	260	7	21	-7	213	6	1	-3	118	6	1	7	188	5	2
4	330	9	-2	8	181	5	8	-6	126	5	4	-2	82	6	2	8	149	5	4
5	318	8	-1	9	163	5	4	-5	286	8	13	-1	126	5	3	H,L=		1,	-5
6	327	9	-18	10	92	6	-1	-4	290	8	22	0	126	5	5	-9	164	6	-2
7	190	5	-2	11	59	9	-5	-3	151	5	13	1	68	7	-5	-8	39	34	-6
8	131	5	15	H,L=		0,	3	-2	311	8	3	2	135	5	3	-7	82	6	10
9	234	6	-2	-10	91	5	-7	-1	257	7	-8	3	92	6	1	-6	189	6	-7
10	98	6	-8	-9	139	5	-11	0	258	7	-2	4	52	19	-3	-5	101	5	6
11	89	6	-1	-8	241	7	1	1	315	8	-4	H,L=		1,	-0	-4	283	6	11
H,L=		0,	1	-7	144	5	10	2	345	9	2	-5	72	7	1	-3	287	6	-1
-11	131	5	-5	-6	257	7	6	3	141	5	10	-4	117	5	4	-2	153	5	-7
-10	78	6	-7	-5	401	10	-6	4	249	7	17	-3	72	7	0	-1	376	10	-10
-9	84	6	-3	-4	263	7	4	5	258	7	1	-2	112	5	-8	0	368	10	-10
-8	389	8	18	-3	339	3	-8	6	79	6	-3	-1	149	5	-5	1	163	5	-2
-7	130	5	2	-2	679	17	4	7	116	5	2	0	97	6	-6	2	292	8	1
-6	291	8	-2	-1	221	6	5	8	83	6	3	1	106	6	-7	3	300	8	-2
-5	358	9	-6	0	371	10	-11	9	43	34	-7	2	134	5	-4	4	137	5	19
-4	253	7	5	1	559	14	-16	H,L=		0,	6	3	90	6	-3	5	294	8	23
-3	816	21	28	2	188	5	-11	-8	111	5	-3	4	106	6	-3	6	288	7	-1
-2	345	9	7	3	317	8	-15	-7	159	5	5	5	145	5	1	7	79	6	-1
-1	480	12	-2	4	385	10	-7	-6	107	5	-5	H,L=		1,	-7	8	196	6	-8
0	827	22	-2	5	154	5	-3	-5	135	5	1	-7	114	6	0	9	166	5	2
1	717	18	-14	6	268	7	4	-4	178	5	3	-6	78	7	-2	H,L=		1,	-4
2	384	10	5	7	262	7	19	-3	182	5	-2	-5	89	6	-2	-10	54	19	-12
3	737	19	15	8	100	5	1	-2	223	6	8	-4	139	5	-5	-9	182	6	1
4	516	13	4	9	148	5	3	-1	278	7	17	-3	119	5	-7	-8	128	5	0
5	145	4	-7	10	102	6	2	0	156	5	16	-2	114	5	-12	-7	78	6	-2
6	393	10	-2	H,L=		0,	4	1	284	6	19	-1	166	5	-6	-6	262	7	14
7	299	8	6	-10	109	6	-10	2	269	7	7	0	158	5	-9	-5	198	6	6
8	83	6	15	-9	188	6	-8	3	95	5	-4	1	129	5	-11	-4	170	5	-1
9	213	6	-3	-8	199	6	1	4	171	5	-9	2	288	8	-4	-3	292	8	-16
10	115	5	-6	-7	196	6	8	5	187	6	-2	3	159	5	-8	-2	276	7	-17
11	74	7	-7	-6	202	6	24	6	83	6	1	4	117	5	-3	-1	212	6	-18
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-11	157	6	-8	-4	311	8	-3	8	78	14	-7	6	82	6	-5	1	329	9	-13
-10	68	7	-10	-3	158	5	-3	H,L=		0,	7	7	115	6	-6	2	225	6	-6
-9	116	5	-2	-2	507	13	8	-7	129	5	-2	H,L=		1,	-6	3	357	9	-18
-8	222	6	6	-1	277	7	-6	-6	138	5	-0	-8	61	16	-15	4	146	5	5
-7	178	5	14	0	162	5	-9	-5	73	7	2	-7	95	6	0	5	289	8	6
-6	274	7	-7	1	651	17	-24	-4	139	5	5	-6	125	5	3	6	339	9	29
-5	351	9	2	2	257	7	-18	-3	116	5	-8	-5	88	6	-6	7	143	5	0
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0	232	6	-4	7	190	6	-1	2	193	6	-2	0	131	5	28	-10	36	46	-32*
1	296	8	-15	8	98	6	-1	3	96	5	-10	1	177	5	24	-9	131	5	-1
2	298	8	-2	9	54	10	4	4	111	5	0	2	362	10	20	-8	141	5	0
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K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
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-5	282	7	-4	3	538	14	14	11	189	6	-6	-2	111	4	-4	-1	94	5	5
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-3	495	13	-17	5	113	4	-8	-11	118	5	-2	0	298	8	-8	1	188	5	-3
-2	438	11	-8	6	377	10	1	-10	214	6	2	1	281	5	-11	2	90	6	-11
-1	240	6	-12	7	403	11	7	-9	85	6	-4	2	461	12	-5	3	166	5	-3
0	359	9	-14	8	84	5	18	-8	286	6	1	3	286	6	-16	4	74	6	-4
1	325	8	-9	9	190	6	-6	-7	345	9	22	4	168	5	5	5	73	6	3
2	295	8	3	10	125	5	-9	-6	149	5	-5	5	292	8	9	6	63	12	-7
3	538	14	-12	11	55	18	-14	-5	276	7	-2	6	282	6	1	H,L=		1,	8
4	276	7	-3	H,L=		1,	8	-4	331	9	-6	7	186	5	-5	-3	135	5	-8
5	238	6	-2	-11	166	5	-3	-3	318	8	3	8	99	6	-1	-2	119	5	2
6	322	9	1	-10	127	5	-7	-2	718	18	28	9	183	6	-1	-1	66	8	-11
7	195	6	16	-9	110	5	1	-1	664	17	18	10	42	14	-2	0	115	5	4
8	175	5	-4	-8	269	7	8	0	126	4	3	H,L=		1,	5	1	182	6	4
9	152	5	-4	-7	265	7	3	1	503	13	1	-9	142	5	-5	2	50	19	-14
10	121	5	-4	-6	160	5	-0	2	319	8	-23	-8	95	6	-7	3	99	6	-1
11	75	7	-7	-5	371	10	-8	3	213	6	-6	-7	118	5	-2	H,L=		2,	-9
H,L=		1,	-2	-4	445	12	-7	4	377	10	-9	-6	228	6	1	-1	188	6	-5
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-8	169	5	2	0	305	8	8	8	217	6	4	-2	150	5	17	H,L=		2,	-8
-7	172	5	16	11	039	26	-4	9	33	44	-19*	-1	281	7	8	-5	69	7	1
-6	293	8	-6	2	391	18	8	10	153	5	8	0	121	5	3	-4	85	6	1
-5	368	10	-3	3	390	10	-8	11	85	7	-2	1	228	6	16	-3	148	5	-1
-4	214	6	-8	4	760	19	7	H,L=		1,	3	2	262	7	28	-2	69	12	-8
-3	685	18	-4	5	269	7	-6	-10	135	6	-4	3	195	6	20	-1	147	5	-2
-2	594	15	1	6	268	7	1	-9	141	5	-2	4	139	5	15	0	133	5	-3
-1	92	4	5	7	251	7	-5	-8	92	5	3	5	214	6	-7	1	107	6	-10
0	868	22	-27	8	223	6	15	-7	317	8	4	6	210	6	-4	2	124	5	-6
1	111	4	-2	9	110	5	-3	-6	199	6	19	7	50	28	-12	3	129	5	-3
2	248	7	-2	10	178	6	-1	-5	229	6	-2	8	134	5	18	4	96	6	6
3	709	18	9	11	112	5	-3	-4	415	11	-0	9	79	6	7	5	104	5	4
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6	351	9	-5	-10	158	5	-2	-1	625	16	-17	-7	143	5	-2	-6	142	5	-3
7	304	8	8	-9	142	5	-3	0	371	10	-2	-6	211	6	-3	-5	99	6	-4
8	103	5	10	-8	212	6	10	1	151	4	-10	-5	184	5	-1	-4	185	5	-4
9	204	6	1	-7	304	8	12	2	525	14	-27	-4	129	5	3	-3	157	5	-5
10	98	5	2	-6	158	5	-4	3	135	5	-15	-3	168	5	-8	-2	152	5	-10
11	34	43	-15*	-5	322	8	-7	4	243	6	-7	-2	157	5	-7	-1	188	5	-12
H,L=		1,	-1	-4	487	13	-6	5	386	8	-10	-1	157	5	1	0	150	5	-8
-11	150	5	-1	-3	145	4	3	6	82	6	14	0	243	7	3	1	112	5	-3
-10	111	5	-1	-2	571	15	15	7	174	5	4	1	185	5	1	2	151	5	-5
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-8	354	9	5	0	560	14	-0	9	72	7	-4	3	179	5	-2	4	132	5	1
-7	124	5	2	1	595	15	-16	10	85	7	-6	4	69	6	-5	5	118	5	-5
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-4	224	6	2	4	468	12	-8	-9	147	5	-1	7	22	43	-7*	H,L=		2,	-6
-3	532	14	5	5	400	10	4	-8	104	5	-2	H,L=		1,	7	-8	131	5	-2
-2	372	10	-6	6	175	5	-1	-7	151	5	-5	-6	166	6	-7	-7	29	45	-38*
-1	366	9	7	7	299	8	6	-6	232	6	10	-5	132	5	-7	-6	132	5	-6
0	543	14	-3	8	172	5	4	-5	186	6	18	-4	49	28	-8	-5	193	6	-5
1	948	24	-3	9	98	6	-9	-4	352	9	2	-3	166	5	5	-4	92	5	-8

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
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-2	259	7	18	-9	34	41	-12*	-1	142	4	-4	7	121	5	9	-4	216	6	17
-1	64	8	17	-8	236	6	-3	0	629	16	4	8	284	6	0	-3	310	8	5
0	250	7	13	-7	178	5	13	1	328	9	-7	9	75	7	-8	-2	369	10	-3
1	185	6	17	-6	154	5	4	2	377	10	-16	10	58	9	-6	-1	86	5	-14
2	136	5	25	-5	343	9	-3	3	245	6	-6	11	125	6	-4	0	323	8	-10
3	293	8	15	-4	312	3	-5	4	258	7	-9	H,L=	2,	2		1	204	6	-6
4	173	5	2	-3	288	3	-5	5	538	14	-7	-10	129	5	-3	2	161	5	-2
5	148	5	-4	-2	591	15	-1	6	93	5	-3	-9	236	7	3	3	262	7	5
6	190	6	-3	-1	503	13	-9	7	246	7	4	-8	167	5	-2	4	124	5	14
7	146	5	-5	0	118	4	-8	8	273	7	12	-7	233	6	14	5	179	6	0
8	60	16	-19	1	571	15	-16	9	88	6	-3	-6	444	12	14	6	194	6	-9
9	121	5	-8	2	347	9	-6	10	138	5	2	-5	130	5	-6	7	100	5	-5
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-9	117	5	-2	4	437	12	-6	H,L=	2,	0		-3	478	12	-8	9	102	6	1
-8	194	6	-4	5	188	5	3	-11	67	8	-6	-2	174	5	-8	H,L=	2,	5	
-7	105	5	-5	6	235	6	1	-10	212	6	-2	-1	570	15	12	-8	188	6	-2
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5	124	5	23	-6	138	5	-9	2	438	11	-15	11	82	7	-8	4	92	5	1
6	200	6	1	-5	236	6	-5	3	216	6	-9	H,L=	2,	3		5	95	5	-4
7	185	5	2	-4	446	12	-14	4	361	9	-5	-10	84	6	-6	6	156	5	-2
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9	144	5	0	-2	712	15	2	6	152	5	-5	-8	182	6	-3	8	14	43	-11*
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-9	108	6	-11	1	462	12	-14	9	63	7	5	-5	243	7	7	-6	167	6	-9
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-7	163	5	3	3	202	5	-6	11	133	6	-18	-3	374	18	-18	-4	95	5	-2
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-5	349	9	2	5	308	3	1	-11	99	6	-6	-1	317	8	-2	-2	220	6	1
-4	239	6	-9	6	162	5	0	-10	199	6	5	0	389	8	-7	-1	154	5	-6
-3	203	6	1	7	269	7	14	-9	280	6	1	1	384	10	0	0	119	4	2
-2	335	9	-14	8	322	8	12	-8	140	5	5	2	283	5	-18	1	217	6	-1
-1	273	7	-28	9	74	5	4	-7	374	10	20	3	425	11	-23	2	185	5	-4
0	381	10	-26	10	137	5	4	-6	385	10	-2	4	283	6	-7	3	181	5	5
1	381	10	-19	11	91	6	-2	-5	170	5	-1	5	188	5	-2	4	174	5	-1
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3	211	6	-11	-11	55	28	-26	-3	568	14	5	7	91	5	9	6	64	8	-14
4	279	7	-15	-10	183	6	-6	-2	96	4	1	8	135	5	-4	7	78	6	7
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7	199	6	6	-7	398	10	14	1	44	5	5	H,L=	2,	4		-4	143	5	-4
8	47	18	-12	-6	232	6	2	2	465	12	-13	-9	214	6	-3	-3	65	8	-8
9	160	5	1	-5	225	6	-8	3	299	8	-14	-8	141	5	-4	-2	166	5	-1
10	155	5	-4	-4	656	17	0	4	291	8	-4	-7	114	5	1	-1	120	5	-6
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K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
1	138	5	8	5	158	5	1	-2	324	8	-7	8	173	5	-1	-5	464	12	15
2	98	6	2	6	112	5	-8	-1	584	13	-1	9	144	5	3	-4	234	13	13
3	77	6	-2	7	140	5	6	0	643	16	-4	10	48	26	-9	-3	135	4	-4
4	137	5	8	8	99	6	-8	1	135	4	-6	11	105	5	6	-2	488	12	-1
5	86	6	1	9	62	16	-19	2	468	12	-20	H,L=	3,	8		-1	216	6	-5
H,L=	2,	8		H,L=	3,	-5		3	338	9	-17	-10	50	28	-15	0	476	12	-9
0	60	8	7	-9	94	6	-5	4	132	4	-7	-9	228	6	2	1	428	11	-7
H,L=	3,	-9		-8	158	5	-1	5	430	11	-3	-8	208	6	-3	2	211	6	-5
-2	106	6	7	-7	183	6	3	6	141	5	1	-7	168	5	22	3	337	9	-13
-1	56	19	-19	-6	144	5	-1	7	140	5	15	-6	387	10	19	4	439	11	-12
0	136	5	1	-5	239	7	4	8	204	6	-6	-5	227	6	-5	5	283	6	-4
1	146	6	2	-4	365	10	25	9	112	5	5	-4	596	15	0	6	95	6	6
2	68	14	1	-3	164	5	6	10	91	6	7	-3	853	22	-5	7	175	5	3
H,L=	3,	-8		-2	236	6	-18	11	100	6	8	-2	446	12	0	8	100	5	-8
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-1	58	16	-19	3	196	5	0	-7	261	7	18	3	558	14	-11	-8	236	7	1
0	151	5	-1	4	182	5	11	-6	392	18	5	4	94	4	-22	-7	184	5	4
1	155	5	-4	5	228	5	13	-5	289	6	2	5	248	7	-7	-6	184	5	1
2	102	6	0	6	149	5	-7	-4	157	5	-7	6	367	10	-9	-5	374	18	30
3	120	5	-8	7	121	5	-6	-3	659	17	-7	7	115	5	11	-4	284	6	1
4	116	6	-2	8	92	6	7	-2	223	6	2	8	180	5	-2	-3	291	8	-8
5	91	6	-2	9	76	5	2	-1	542	14	5	9	125	5	-6	-2	367	10	-5
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H,L=	3,	-7		-10	126	5	4	1	242	6	-5	11	57	18	-16	0	316	8	3
-7	94	6	-6	-9	119	6	-7	2	366	10	-14	H,L=	3,	1		1	333	9	-6
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-5	179	6	-1	-7	236	7	-4	4	242	6	-6	-9	149	5	6	3	287	6	-11
-4	116	5	-2	-6	168	5	5	5	182	5	-14	-8	257	7	-11	4	292	8	12
-3	158	5	-4	-5	246	7	17	6	176	5	-17	-7	173	5	13	5	154	5	17
-2	223	6	-12	-4	419	11	-6	7	183	6	15	-6	381	8	16	6	123	5	9
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1	151	5	-6	-1	494	13	-13	10	78	7	2	-3	518	13	-2	9	87	6	-7
2	134	5	-13	0	149	4	-4	11	91	6	-2	-2	581	15	-9	10	90	6	2
3	116	5	-5	1	381	10	-19	H,L=	3,	-1		-1	254	7	-8	H,L=	3,	4	
4	209	6	-5	2	533	14	-22	-10	117	5	3	0	537	14	11	-9	88	6	-11
5	94	6	1	3	256	7	-7	-9	198	6	4	1	666	17	9	-8	229	6	-1
6	103	5	-1	4	209	6	-11	-8	179	5	-9	2	161	4	-4	-7	178	6	-3
7	152	5	-3	5	320	8	5	-7	249	7	22	3	493	13	-21	-6	123	5	-8
H,L=	3,	-6		6	168	5	20	-6	431	11	5	4	358	9	-17	-5	245	7	-1
-8	123	6	-1	7	114	5	-2	-5	247	7	4	5	93	5	-9	-4	288	6	9
-7	154	5	-0	8	168	5	8	-4	496	13	-9	6	269	7	-1	-3	235	6	28
-6	118	5	-2	9	44	24	8	-3	746	19	-17	7	196	6	18	-2	367	18	21
-5	189	6	2	10	101	5	-2	-2	224	6	4	8	99	5	-3	-1	347	9	18
-4	251	7	-5	H,L=	3,	-3		-1	585	15	16	9	96	5	5	0	58	8	-6
-3	127	5	18	-10	162	5	8	0	664	17	0	10	63	8	-8	1	352	9	18
-2	252	7	16	-9	212	5	3	1	252	7	5	11	42	13	1	2	229	6	7
-1	314	8	18	-8	61	8	1	2	294	8	-13	H,L=	3,	2		3	92	5	25
0	142	5	22	-7	271	7	9	3	429	11	-9	-10	183	6	-11	4	215	6	4
1	188	6	16	-6	296	8	23	4	365	9	-5	-9	128	5	-7	5	45	17	-1
2	228	6	29	-5	148	5	-5	5	131	4	-12	-8	285	6	-8	6	99	5	-10
3	148	5	16	-4	358	9	-4	6	264	7	-10	-7	211	6	-10	7	136	5	-7
4	213	6	4	-3	319	9	-2	7	182	5	11	-6	271	7	29	8	58	9	-8

STRUCTURE FACTORS CONTINUED FOR
K2YB(C8H8)2,(CH3OCH2CH2OCH3)2

K	FOB	SG	DEL
9	45	26	-5
H,L=	3,		5
-7	198	6	-2
-6	119	5	-10
-5	158	5	-8
-4	277	7	2
-3	96	5	-3
-2	269	7	2
-1	278	7	4
0	124	5	8
1	240	7	1
2	253	7	3
3	64	12	-15
4	95	5	-4
5	134	5	-5
6	39	39	-28*
7	75	6	7
8	75	7	3
H,L=	3,		6
-6	125	5	2
-5	145	5	-5
-4	188	6	-5
-3	126	5	-3
-2	145	5	-2
-1	195	6	-8
0	186	5	-8
1	140	5	-4
2	179	5	1
3	99	5	-3
4	82	6	3
5	148	5	3
6	53	15	-9
H,L=	3,		7
-3	110	5	3
-2	95	6	-2
-1	154	5	8
0	103	5	-0
1	73	6	9
2	187	5	2
3	53	19	-9
4	93	5	10
H,L=	4,		-9
-2	45	27	-14
-1	95	6	-3
0	69	7	-4
1	136	5	-2
2	137	6	-3
H,L=	4,		-8
-5	51	22	-23
-4	161	6	2
-3	83	6	1
-2	183	6	-3
-1	189	6	-8
0	102	5	-3
1	126	5	1
2	158	5	-5

K	FOB	SG	DEL
3	108	5	2
4	105	6	8
5	114	5	8
6	82	6	-1
H,L=	4,		-7
-7	114	6	5
-6	110	5	-3
-5	85	5	-3
-4	167	5	-3
-3	136	5	1
-2	174	5	-6
-1	259	7	-13
0	195	5	-12
1	112	5	-7
2	172	5	-7
3	169	5	-1
4	85	6	-4
5	168	5	4
6	102	6	4
7	87	6	5
H,L=	4,		-6
-8	80	6	3
-7	127	5	-1
-6	146	5	2
-5	150	5	8
-4	178	5	-1
-3	213	6	-1
-2	183	5	9
-1	312	8	27
0	239	7	16
1	159	5	27
2	272	7	28
3	214	6	7
4	131	5	-1
5	191	6	-5
6	144	5	-3
7	89	6	1
8	128	5	-2
H,L=	4,		-5
-9	137	5	-10
-8	88	6	4
-7	96	5	-5
-6	204	6	-4
-5	163	5	8
-4	258	7	21
-3	332	9	16
-2	188	5	9
-1	200	6	-8
0	355	9	-17
1	129	5	-12
2	339	9	2
3	330	9	12
4	131	5	12
5	262	7	8
6	229	6	-7
7	118	5	-1

K	FOB	SG	DEL
8	112	5	11
9	103	6	-1
H,L=	4,		-4
-9	155	5	-4
-8	178	5	8
-7	76	6	-1
-6	258	7	3
-5	230	6	22
-4	152	5	7
-3	476	12	-10
-2	289	6	-0
-1	198	5	-8
0	375	18	-15
1	237	6	-15
2	276	7	-10
3	392	10	-15
4	288	6	-8
5	165	5	14
6	335	9	17
7	180	5	-9
8	57	15	-4
9	132	5	-4
10	64	7	2
H,L=	4,		-3
-10	78	7	-14
-9	151	5	-7
-8	214	6	1
-7	158	5	-5
-6	327	9	24
-5	314	8	8
-4	171	5	-1
-3	274	7	-4
-2	332	9	-3
-1	375	10	-12
0	373	10	-12
1	396	18	-11
2	281	5	-16
3	389	10	-22
4	365	18	-10
5	80	5	-5
6	282	8	11
7	138	5	4
8	114	5	-3
9	148	5	1
10	83	6	-2
H,L=	4,		-2
-10	79	7	-6
-9	157	5	8
-8	214	6	0
-7	189	6	-1
-6	314	8	26
-5	344	9	-4
-4	312	8	-7
-3	216	6	-5
-2	457	12	-14
-1	257	7	-6

K	FOB	SG	DEL
8	623	16	5
1	553	14	-1
2	165	5	-13
3	586	13	-15
4	289	8	-12
5	237	6	-8
6	287	6	9
7	189	5	9
8	181	5	-6
9	133	5	-10
10	185	6	-2
11	36	40	-18*
H,L=	4,		-1
-10	114	5	-4
-9	80	6	1
-8	262	7	-3
-7	203	6	9
-6	184	5	17
-5	413	11	5
-4	177	5	-7
-3	474	12	-1
-2	690	18	2
-1	288	6	-4
0	437	11	8
1	689	18	1
2	273	7	-8
3	337	9	-18
4	433	11	-18
5	173	5	-4
6	173	5	5
7	259	7	12
8	98	6	-14
9	87	6	-1
10	181	6	-4
11	31	48	-7*
H,L=	4,		8
-10	170	6	-1
-9	68	15	-12
-8	223	6	-5
-7	249	7	-7
-6	29	44	-6*
-5	257	7	3
-4	328	9	8
-3	285	8	-6
-2	575	15	-12
-1	360	9	-14
0	353	9	4
1	584	15	-18
2	375	18	-12
3	86	4	-17
4	482	13	-16
5	232	6	-3
6	79	6	2
7	383	8	5
8	162	5	-7
9	55	16	-1

K	FOB	SG	DEL
10	183	6	3
11	56	18	-4
H,L=	4,		1
-10	198	6	-4
-9	75	7	-12
-8	170	5	-4
-7	277	7	-6
-6	183	6	25
-5	228	6	18
-4	396	18	2
-3	271	7	2
-2	226	6	-5
-1	367	18	1
0	306	8	-2
1	379	10	-10
2	345	9	-7
3	187	5	-5
4	317	8	-9
5	261	7	-4
6	126	5	17
7	243	7	5
8	136	5	3
9	71	7	8
10	87	7	-2
H,L=	4,		2
-9	96	6	-1
-8	134	5	2
-7	244	7	-8
-6	218	6	-4
-5	381	8	31
-4	383	18	9
-3	232	6	-4
-2	184	5	-5
-1	457	12	1
0	111	4	-5
1	282	7	4
2	253	7	-6
3	172	5	-5
4	344	9	6
5	175	5	16
6	137	5	3
7	142	5	1
8	127	5	8
9	28	44	-21*
10	83	6	8
H,L=	4,		3
-9	163	5	-3
-8	79	7	-18
-7	239	7	1
-6	280	6	2
-5	144	5	-8
-4	419	11	19
-3	139	5	20
-2	239	6	5
-1	393	18	-8
0	216	6	-1

STRUCTURE FACTORS CONTINUED FOR
K2YB(C8H8)2,(CH3OCH2CH2OCH3)2

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
1	169	5	-2	1	89	5	1	-2	352	9	21	-9	89	6	9	4	158	5	-5
2	279	7	3	H,L=		5,	-9	-1	211	6	4	-8	138	5	4	5	127	5	2
3	165	5	19	-1	47	32	-6	0	101	5	2	-7	258	7	-12	6	160	5	16
4	131	5	18	0	107	5	8	1	266	7	8	-6	197	6	13	7	118	5	-4
5	258	7	2	1	81	5	3	2	155	5	5	-5	309	8	29	8	189	6	-2
6	91	5	-1	2	105	5	-2	3	282	6	18	-4	385	10	1	9	81	6	1
7	49	17	-8	H,L=		5,	-8	4	220	6	20	-3	172	5	-4	10	35	47	-19*
8	122	6	-5	-4	56	9	-13	5	72	6	0	-2	248	7	0	H,L=		5,	1
9	32	45	-7*	-3	153	5	7	6	214	6	-8	-1	430	11	8	-9	218	6	6
H,L=		4,	4	-2	108	5	7	7	178	5	2	0	205	6	0	-8	189	5	2
-8	87	6	-15	-1	112	5	-1	8	89	6	6	1	335	9	-13	-7	231	6	-13
-7	199	6	-5	0	159	5	-2	9	97	6	6	2	372	10	-10	-6	296	8	-5
-6	191	6	-2	1	103	5	-1	H,L=		5,	-4	3	89	4	-6	-5	168	5	19
-5	99	5	2	2	131	5	-1	-9	113	6	-7	4	482	13	-8	-4	412	11	28
-4	172	5	-5	3	136	5	-5	-8	192	6	2	5	300	8	12	-3	289	8	3
-3	244	7	-0	4	104	5	5	-7	181	6	1	6	60	15	5	-2	286	6	1
-2	173	5	9	5	70	13	-17	-6	111	5	-9	7	179	5	0	-1	295	8	-5
-1	247	7	19	H,L=		5,	-7	-5	275	7	14	8	133	5	-6	0	374	10	3
0	248	7	19	-6	154	5	8	-4	314	8	18	9	62	8	2	1	148	5	3
1	137	5	10	-5	126	5	2	-3	122	5	4	10	93	6	3	2	227	6	-8
2	384	8	10	-4	69	13	-8	-2	440	11	-4	H,L=		5,	-1	3	238	6	1
3	223	6	1	-3	121	5	-2	-1	250	7	-7	-10	280	6	1	4	111	5	5
4	42	9	16	-2	141	5	5	0	183	5	-2	-9	154	5	-3	5	230	6	16
5	172	5	-7	-1	167	5	-1	1	283	8	-16	-8	132	5	-7	6	180	5	6
6	94	6	-8	0	248	7	-6	2	221	6	-2	-7	320	8	-14	7	68	14	-8
7	43	26	-12	1	154	5	-4	3	286	6	-8	-6	231	6	13	8	159	5	-1
8	95	6	10	2	122	5	-6	4	169	5	15	-5	35	38	-10*	9	63	15	-5
H,L=		4,	5	3	180	5	-9	5	284	6	20	-4	421	11	5	10	38	42	-8*
-6	182	6	-4	4	143	5	-5	6	158	5	6	-3	328	8	6	H,L=		5,	2
-5	125	5	-2	5	101	5	4	7	187	6	-8	-2	120	4	-4	-9	286	6	-4
-4	86	6	-2	6	114	5	8	8	110	5	-5	-1	433	11	1	-8	112	5	4
-3	206	6	-3	7	61	16	-12	9	74	7	-2	0	278	7	-4	-7	121	5	0
-2	129	5	4	H,L=		5,	-6	10	110	6	3	1	288	8	-6	-6	251	7	-2
-1	164	5	-8	-7	78	5	7	H,L=		5,	-3	2	360	9	-9	-5	211	6	-4
0	170	5	-8	-6	132	5	-8	-9	75	12	-10	3	221	6	-9	-4	243	7	8
1	117	5	6	-5	183	6	4	-8	181	6	4	4	287	6	-6	-3	425	11	22
2	221	6	-0	-4	98	5	2	-7	234	6	1	5	313	8	4	-2	179	5	8
3	172	5	-1	-3	192	6	-3	-6	161	5	2	6	142	5	19	-1	284	6	8
4	93	5	-8	-2	191	5	2	-5	419	11	31	7	144	5	3	0	442	12	2
5	100	5	6	-1	145	5	6	-4	268	7	16	8	177	5	-3	1	123	5	-1
6	104	5	2	0	234	6	9	-3	215	6	-2	9	64	13	-8	2	154	5	-6
7	46	28	-2	1	217	6	5	-2	355	9	-4	10	74	7	4	3	227	6	7
H,L=		4,	6	2	126	5	12	-1	281	7	-5	H,L=		5,	0	4	35	48	6*
-5	101	6	8	3	230	6	4	0	240	6	6	-9	189	6	3	5	215	6	11
-4	112	5	-1	4	170	5	-5	1	386	10	1	-8	161	5	-6	6	156	5	8
-3	156	5	5	5	94	5	1	2	327	9	-10	-7	337	9	-15	7	74	6	8
-2	99	6	-4	6	184	6	4	3	173	5	-8	-6	273	7	7	8	78	7	-0
-1	103	5	1	7	120	5	2	4	313	8	-4	-5	73	7	31	9	68	15	-5
0	159	5	0	8	43	25	-7	5	231	6	13	-4	257	7	8	H,L=		5,	3
1	91	5	6	H,L=		5,	-5	6	112	5	22	-3	372	10	-10	-8	165	6	-6
2	97	5	2	-8	192	5	-0	7	282	6	-8	-2	158	5	6	-7	86	6	1
3	181	5	2	-7	112	5	-8	8	93	5	-2	-1	352	9	-2	-6	233	6	1
4	19	37	-38*	-6	94	5	1	9	63	14	-10	0	283	7	-5	-5	231	6	2
5	101	6	1	-5	243	7	4	10	184	6	-1	1	239	6	2	-4	58	8	-7
H,L=		4,	7	-4	179	5	6	H,L=		5,	-2	2	335	9	-9	-3	326	9	5
0	115	6	-2	-3	194	5	20	-10	178	7	-12	3	300	8	-11	-2	203	6	15

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-1	170	5	17	4	113	5	-1	-6	285	6	0	9	94	6	5	4	294	8	19
0	299	8	21	5	62	8	-11	-5	161	5	0	10	22	44	-21*	5	30	40	12*
1	179	5	27	H,L=		6,	-7	-4	276	7	13	H,L=		6,	-1	6	122	5	-2
2	127	5	6	-6	82	6	-5	-3	262	7	26	-9	186	6	3	7	118	5	-1
3	196	6	6	-5	193	6	-0	-2	221	6	14	-8	198	6	-6	8	36	44	-3*
4	175	5	-7	-4	149	5	-1	-1	428	11	12	-7	221	6	-19	9	64	8	-8
5	52	15	-4	-3	26	40	-27*	0	214	6	-5	-6	333	9	-17	H,L=		6,	2
6	155	5	-6	-2	139	5	-2	1	186	5	2	-5	244	7	9	-8	213	6	2
7	87	6	-8	-1	158	5	-1	2	324	9	4	-4	210	6	26	-7	185	6	-5
8	34	39	-12*	0	112	5	-3	3	159	5	17	-3	357	9	14	-6	128	5	8
H,L=		5,	4	1	172	5	-3	4	188	6	23	-2	302	8	-6	-5	218	6	1
-7	97	6	-6	2	139	5	-1	5	115	5	11	-1	168	5	-3	-4	250	7	1
-6	209	6	-6	3	108	5	-6	6	93	5	-12	0	389	10	-11	-3	136	5	-0
-5	178	6	3	4	169	5	2	7	112	5	-5	1	212	6	-2	-2	301	8	7
-4	106	5	-7	5	99	6	-4	8	124	5	5	2	180	5	3	-1	282	6	17
-3	144	5	-2	6	72	7	-2	9	67	7	4	3	258	7	-3	0	234	6	27
-2	203	6	1	7	82	5	7	H,L=		6,	-3	4	169	5	5	1	372	10	24
-1	102	5	-4	H,L=		5,	-6	-9	180	6	-2	5	158	5	21	2	91	6	16
0	146	5	-4	-7	167	6	0	-8	78	6	10	6	118	5	7	3	187	5	-1
1	173	5	-3	-6	181	6	-5	-7	166	5	0	7	72	6	-13	4	204	6	-2
2	109	5	-7	-5	172	5	-0	-6	278	7	-4	8	184	5	3	5	82	6	-5
3	184	5	-3	-4	247	7	4	-5	130	5	7	9	99	6	7	6	91	6	-7
4	136	5	-5	-3	70	6	-5	-4	433	11	33	10	40	45	-8*	7	110	6	-3
5	67	7	-9	-2	204	6	2	-3	313	8	11	H,L=		6,	0	8	43	32	-3
6	109	5	-4	-1	229	6	-6	-2	125	5	-2	-9	152	5	2	H,L=		6,	3
7	60	15	-8	0	131	5	-1	-1	355	9	-5	-8	213	6	-3	-7	172	6	-9
H,L=		5,	5	1	165	5	-4	0	328	9	-3	-7	208	6	-16	-6	96	6	-10
-5	182	6	-1	2	200	6	-8	1	178	5	-6	-6	332	9	-18	-5	216	6	0
-4	66	14	-18	3	111	5	-5	2	232	6	-4	-5	260	7	-6	-4	188	6	-0
-3	138	5	-2	4	112	5	-10	3	267	7	1	-4	169	5	22	-3	119	5	1
-2	187	6	3	5	164	5	-7	4	100	5	13	-3	439	12	23	-2	226	6	-5
-1	81	6	4	6	54	16	-15	5	252	7	23	-2	293	8	7	-1	175	5	3
0	76	6	4	7	84	6	-3	6	183	5	3	-1	134	5	-6	0	123	5	-8
1	134	5	2	8	64	8	-5	7	57	8	-5	0	359	9	-5	1	223	6	0
2	77	6	1	H,L=		5,	-5	8	127	5	5	1	256	7	-6	2	135	5	-4
3	130	5	-7	-8	134	6	-9	9	73	7	4	2	190	5	-3	3	118	5	-8
4	84	6	8	-7	208	6	2	10	50	16	6	3	285	8	6	4	102	5	2
5	12	44	-33*	-6	126	5	1	H,L=		6,	-2	4	158	5	17	5	96	6	-1
6	86	6	-9	-5	162	5	1	-9	206	6	-1	5	117	5	13	6	82	6	-8
H,L=		5,	6	-4	211	6	4	-8	114	5	1	6	90	6	-4	7	79	12	-11
-3	70	7	-8	-3	237	6	9	-7	182	6	-5	7	74	7	-13	H,L=		6,	4
-2	165	6	3	-2	242	7	14	-6	288	8	-6	8	47	22	-17	-5	217	6	-1
-1	82	6	-4	-1	335	9	34	-5	217	6	10	9	63	15	-13	-4	156	5	-7
0	51	22	-30	0	183	5	22	-4	260	7	26	H,L=		6,	1	-3	93	6	-6
1	136	5	6	1	163	5	16	-3	441	12	3	-8	225	6	5	-2	210	6	-8
2	68	6	10	2	297	8	17	-2	194	5	-2	-7	116	5	0	-1	170	5	-4
3	10	43	-29*	3	134	5	17	-1	211	6	-18	-6	217	6	-8	0	61	13	-2
H,L=		6,	-8	4	95	5	5	0	488	11	-7	-5	314	8	-5	1	97	5	5
-4	109	5	-2	5	130	5	-5	1	148	5	-2	-4	120	5	7	2	138	5	2
-3	88	6	0	6	76	6	-9	2	149	5	-10	-3	383	10	22	3	72	7	6
-2	140	5	8	7	131	5	-0	3	292	8	-16	-2	328	9	20	4	132	5	5
-1	105	6	4	8	81	5	-3	4	110	5	10	-1	169	5	8	5	76	6	6
0	107	5	4	9	42	30	-11	5	180	6	12	0	316	8	4	6	46	10	10
1	147	5	-8	H,L=		5,	-4	6	228	6	4	1	332	9	15	H,L=		6,	5
2	83	6	-1	-8	128	5	-3	7	78	7	-8	2	110	5	11	-3	87	6	-1
3	115	5	1	-7	202	6	4	8	180	6	-6	3	195	6	11	-2	152	5	-1

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
-1	178	6	-2	5	108	5	-3	5	127	5	-4	5	195	6	1	4	77	7	-3
0	53	9	-6	6	136	5	-6	6	118	5	-6	6	63	8	2	5	85	6	-4
1	85	6	-1	7	56	9	-4	7	122	5	-8	7	180	6	2	H,L=		8,	-6
2	132	5	7	8	78	6	9	8	54	17	-4	8	96	6	8	-5	182	6	3
3	42	12	7	H,L=		7,	-4	9	67	8	5	H,L=		7,	2	-4	96	6	-3
4	57	15	3	-8	146	5	-1	H,L=		7,	-1	-6	114	5	-3	-3	148	5	1
H,L=		7,	-8	-7	120	5	0	-8	164	5	6	-5	143	5	-1	-2	177	6	1
-3	98	6	-2	-6	185	6	4	-7	199	6	-7	-4	188	6	-2	-1	110	5	-3
-2	99	6	6	-5	214	6	-1	-6	280	6	-5	-3	164	5	3	0	164	5	1
-1	144	5	-2	-4	103	5	2	-5	294	8	-5	-2	112	5	-1	1	136	5	-5
0	103	6	-8	-3	265	7	2	-4	177	5	-6	-1	191	6	-6	2	126	5	4
1	78	7	-7	-2	234	6	8	-3	270	7	4	0	180	5	-8	3	155	5	-2
2	137	5	8	-1	172	5	24	-2	354	9	23	1	134	5	-3	4	113	5	3
3	78	7	-1	0	316	8	15	-1	217	6	17	2	229	6	-8	5	98	5	9
4	37	49	-42*	1	183	5	25	0	218	6	11	3	85	6	-3	6	129	5	9
H,L=		7,	-7	2	196	6	14	1	348	9	16	4	118	5	-3	H,L=		8,	-5
-5	130	5	-1	3	318	8	3	2	154	5	11	5	112	5	3	-6	118	5	-5
-4	180	6	-3	4	114	5	-5	3	165	5	14	6	37	41	-17*	-5	233	7	1
-3	177	6	1	5	84	5	-10	4	293	8	6	7	85	6	7	-4	97	6	-8
-2	18	46	-61*	6	151	5	-9	5	40	43	-22*	H,L=		7,	3	-3	85	6	-2
-1	167	5	5	7	83	6	-9	6	89	6	-11	-5	180	6	-5	-2	208	6	-1
0	152	5	-6	8	46	26	-12	7	123	5	-5	-4	219	6	-4	-1	155	5	3
1	93	6	-5	9	85	6	2	8	49	31	-14	-3	148	5	-9	0	186	5	-7
2	152	5	3	H,L=		7,	-3	9	34	44	-18*	-2	96	6	-4	1	168	5	1
3	116	5	-1	-8	204	5	3	H,L=		7,	8	-1	210	6	3	2	152	5	-4
4	86	6	-6	-7	62	15	-8	-8	121	5	1	0	121	5	-4	3	147	5	-8
5	138	5	0	-6	152	5	3	-7	289	6	-1	1	112	5	-1	4	216	6	1
6	85	6	-11	-5	290	8	-2	-6	145	5	-13	2	163	5	-2	5	84	6	2
H,L=		7,	-6	-4	158	5	-4	-5	211	6	-1	3	72	7	-4	6	89	6	1
-6	174	6	-1	-3	257	7	12	-4	387	8	-6	4	68	7	3	7	117	5	-1
-5	130	5	-3	-2	326	9	22	-3	125	5	2	5	124	5	18	H,L=		8,	-4
-4	168	5	3	-1	162	5	15	-2	335	9	11	6	44	21	-2	-7	147	5	-4
-3	213	6	2	0	306	8	17	-1	262	7	23	H,L=		7,	4	-6	119	5	-7
-2	130	5	-1	1	271	7	15	0	132	5	15	-4	120	6	-5	-5	186	6	-1
-1	212	6	-1	2	147	5	14	1	315	8	21	-3	177	6	-2	-4	215	6	7
0	204	6	-8	3	163	5	13	2	164	5	19	-2	181	6	-4	-3	99	5	2
1	128	5	-3	4	210	6	4	3	146	5	2	-1	196	6	-8	-2	288	6	-1
2	175	5	-7	5	105	5	-6	4	279	7	-7	0	138	5	-1	-1	219	6	1
3	170	5	-8	6	133	5	-7	5	155	5	-6	1	32	38	-19*	0	74	6	-7
4	131	5	3	7	129	5	-1	6	36	39	-13*	2	114	5	-2	1	220	6	-6
5	100	5	-8	8	48	11	-2	7	186	6	-9	3	112	6	3	2	155	5	-5
6	134	5	-1	9	94	6	5	8	83	6	-0	4	31	43	-3*	3	124	5	-7
7	67	7	7	H,L=		7,	-2	9	46	30	24	H,L=		8,	-8	4	190	6	-4
H,L=		7,	-5	-8	216	6	12	H,L=		7,	1	-1	98	6	1	5	122	5	-2
-7	123	5	-10	-7	130	5	8	-7	245	7	7	0	133	5	-2	6	70	8	-10
-6	214	6	-4	-6	175	5	-1	-6	98	6	6	1	77	14	-18	7	111	5	6
-5	106	5	2	-5	255	7	-9	-5	135	5	4	2	69	8	-4	8	57	9	-9
-4	172	5	8	-4	219	5	-4	-4	276	7	3	H,L=		8,	-7	H,L=		8,	-3
-3	188	6	-4	-3	300	8	24	-3	148	4	-6	-4	134	5	-1	-7	282	6	2
-2	183	5	1	-2	318	8	17	-2	186	5	-0	-3	135	5	-4	-6	96	5	3
-1	233	6	3	-1	211	5	18	-1	251	7	11	-2	147	5	6	-5	158	5	2
0	271	7	6	0	266	7	11	0	161	5	9	-1	183	6	-2	-4	218	6	3
1	173	5	3	1	367	10	4	1	224	6	14	0	154	5	-3	-3	166	5	-0
2	191	6	1	2	141	5	9	2	236	6	5	1	138	5	-8	-2	210	6	1
3	293	8	-12	3	113	5	17	3	144	5	2	2	75	7	5	-1	222	6	1
4	53	18	-38	4	191	6	16	4	124	5	-4	3	123	5	1	0	164	5	4

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
1	242	7	8	6	85	5	-5	4	84	6	9	5	61	16	-6	-3	154	5	-7
2	198	6	8	7	57	17	-7	5	73	7	-5	6	102	6	2	-2	127	5	-2
3	122	5	-5	8	89	7	-5	H,L=		9,	-5	7	0	46	-43*	-1	173	6	1
4	148	5	-4	H,L=		8,	1	-5	136	5	-3	H,L=		9,	-1	0	158	6	-11
5	101	5	1	-6	221	6	-4	-4	199	6	-0	-5	145	5	-1	1	93	6	-10
6	66	15	-27	-5	84	5	-3	-3	134	5	-5	-4	109	5	2	2	69	7	-10
7	104	6	-8	-4	174	5	5	-2	115	5	-8	-3	197	6	1	3	111	5	4
8	71	7	-6	-3	288	6	-3	-1	195	6	2	-2	170	5	8	4	66	7	0
H,L=		8,	-2	-2	94	5	3	0	118	5	-7	-1	94	6	-3	H,L=		10,	-4
-7	200	6	-1	-1	132	5	-2	1	48	10	2	0	180	6	-2	-4	88	6	-8
-6	121	5	1	0	173	5	4	2	116	5	2	1	168	5	-5	-3	169	5	-4
-5	113	5	-2	1	138	5	4	3	122	5	2	2	27	43	-3*	-2	164	5	-3
-4	272	7	1	2	100	5	3	4	66	14	-10	3	112	5	4	-1	113	5	-10
-3	126	5	-5	3	113	5	1	5	88	6	-6	4	189	6	-5	0	177	6	1
-2	195	6	-2	4	99	6	-8	6	73	7	5	5	22	47	-38*	1	122	5	2
-1	241	7	4	5	106	5	6	H,L=		9,	-4	6	86	6	9	2	72	12	-8
0	192	6	9	6	66	15	-10	-5	127	5	-8	7	35	46	-12*	3	125	5	3
1	247	7	7	7	47	22	8	-4	280	6	-6	H,L=		9,	8	4	89	6	-4
2	223	6	8	H,L=		8,	2	-3	165	5	-8	-5	158	5	-10	5	0	46	-45*
3	103	5	-12	-5	112	5	-8	-2	125	5	-3	-4	185	6	-4	H,L=		10,	-3
4	134	5	-8	-4	128	5	-9	-1	200	6	4	-3	176	6	-10	-4	110	6	-10
5	152	5	-3	-3	229	6	-2	0	175	5	-1	-2	190	6	3	-3	150	5	-3
6	38	40	-26*	-2	93	6	-5	1	60	14	-8	-1	96	6	-8	-2	190	6	-10
7	96	6	1	-1	76	7	-4	2	141	5	5	0	174	5	-1	-1	34	45	-38*
8	69	15	-16	0	153	5	1	3	130	5	3	1	155	5	-10	0	113	5	-1
H,L=		8,	-1	1	116	5	2	4	85	6	1	2	17	44	-12*	1	172	6	0
-7	191	6	-5	2	93	6	-9	5	189	6	-0	3	97	6	-1	2	72	7	9
-6	153	5	-2	3	158	5	0	6	57	16	-11	4	65	15	-7	3	113	6	-7
-5	85	6	-4	4	36	39	-18*	7	37	41	-18*	5	59	8	18	4	123	5	2
-4	242	7	2	5	57	9	3	H,L=		9,	-3	6	64	8	5	5	53	9	7
-3	197	6	-7	6	93	5	5	-6	175	6	-6	H,L=		9,	1	H,L=		10,	-2
-2	130	5	0	H,L=		8,	3	-5	189	5	7	-4	102	6	-5	-4	137	5	-11
-1	256	7	-1	-3	145	5	-8	-4	177	6	-1	-3	165	5	-3	-3	139	5	-8
0	179	5	3	-2	151	5	-8	-3	213	6	-2	-2	281	6	-7	-2	196	6	-2
1	129	5	6	-1	72	7	5	-2	87	6	2	-1	44	28	-28	-1	87	6	-11
2	224	6	-10	0	172	6	-0	-1	163	5	-5	0	161	5	-2	0	78	7	-6
3	131	5	-10	1	93	5	-1	0	175	5	3	1	131	5	2	1	163	6	-3
4	93	5	-1	2	38	45	-23*	1	116	5	-0	2	59	8	1	2	86	6	-3
5	210	6	-5	3	129	5	-1	2	195	6	8	3	90	6	-2	3	102	5	9
6	80	6	5	4	78	7	-1	3	150	5	4	4	105	6	-8	4	186	5	9
7	53	20	-19	H,L=		9,	-7	4	48	43	-8*	5	0	47	-28*	5	63	8	2
8	107	6	2	-2	121	5	3	5	119	5	1	H,L=		9,	2	H,L=		10,	-1
H,L=		8,	8	-1	120	6	-4	6	95	6	10	-2	169	6	-6	-3	113	5	-6
-7	148	5	-2	0	80	7	-7	7	29	44	-14*	-1	91	6	-5	-2	174	6	-10
-6	198	6	4	1	125	5	2	H,L=		9,	-2	0	49	18	-9	-1	111	6	-16
-5	118	5	4	2	117	5	3	-6	211	6	1	1	150	5	2	0	145	5	-3
-4	131	5	0	3	45	11	5	-5	124	5	-7	2	72	13	-3	1	138	5	-3
-3	253	7	-2	H,L=		9,	-6	-4	93	6	-2	3	47	36	-11	2	110	5	-1
-2	116	5	3	-4	176	6	-4	-3	255	7	3	4	109	7	9	3	50	20	-9
-1	193	6	-5	-3	84	6	-2	-2	118	5	8	H,L=		10,	-6	4	107	6	4
0	218	6	-7	-2	108	5	-5	-1	83	6	-10	-1	125	5	-0	5	59	9	2
1	19	39	-27*	-1	178	5	1	0	198	6	-4	0	164	6	-0	H,L=		10,	0
2	164	5	-2	0	67	7	-3	1	101	5	-6	1	54	18	-14	-2	126	5	-9
3	114	5	-9	1	123	5	3	2	152	5	-3	2	95	6	-6	-1	157	6	-5
4	130	5	-6	2	121	5	11	3	150	5	-5	3	122	5	12	0	90	6	-13
5	131	5	-4	3	75	7	6	4	91	6	-1	H,L=		10,	-5	1	182	6	-1

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
2	110	6	-3																
3	42	22	7																
4	105	6	0																
H, L=		10,	1																
0	56	19	-18																
1	110	5	4																
H, L=		11,	-4																
0	61	17	-21																
1	115	5	-4																
2	92	9	-5																
H, L=		11,	-3																
-1	135	5	-4																
0	78	7	-6																
1	63	8	2																
2	128	5	7																
H, L=		11,	-2																
0	75	7	0																
1	102	6	4																
2	104	8	-3																

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