## Title

DIGLYME ADDUCT OF DIPOTASSIUM Bis(t-butyl[8]annulene)ytterbate(II) (CH3OCH2CH2OCH2CH2OCH3)2-K2[CH3)3CC8H7]2Yb



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$(CH_3OCH_2CH_2OCH_2CH_2OCH_3)_2K_2[CH_3)_3CC_8H_7]_2Yb$

S.A. Kinsley, A. Streitwieser, Jr.,
and A. Zalkin

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## DISCLAIMER

# Diglyme Adduct of Dipotassium Bis(t-butyl[8]annulene)ytterbate(II)

$(CH_3OCH_2CH_2OCH_2CH_2OCH_3)_2K_2[CH_3)_3CC_8H_7]_2Yb$

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**Abstract.** $M_r$ = 840.12, monoclinic, $P2_1/c$, a = 10.292(4), b = 20.588(6), c = 20.036(6) A, β = 103.28(4)°, V = 4131.9 $A^3$, Z = 4, $D_x$ = 1.350 g $cm^{-3}$, λ(MoKα)=0.71073 A, μ = 16.5 $cm^{-1}$, F(000) = 1728, T = 300 K, R = 0.032 for 3212 unique reflections with $F^2>3\sigma(F^2)$. The ytterbium atom is sandwiched between two parallel [8]annulene rings with a mean Yb-C distance of 2.77(4) A. The potassium atoms cap the other sides of the rings at a mean K-C distance of 3.08(5) A; each potassium atom is also coordinated to four oxygen atoms from the diglyme ligands at distances that range from 2.86 to 3.06 A.

**Experimental.** Red, air sensitive crystals were sealed inside quartz capillaries under argon. Crystal 0.13 x 0.16 x 0.36 mm with 6 faces; modified Picker automatic diffractometer, graphite monochromator; cell dimensions from 32 reflections, $24° < 2\theta < 42°$; analytical absorption correction, range 1.19 to 1.39; max. $(\sin\theta)/\lambda = 0.54$ $Å^{-1}$, h -11 to 11, k 0 to 22, ℓ -21 to 21; three standard reflections, 6% variation in intensities from average, intensities adjusted accordingly; 10798 data, 5413 unique (including 2201, $F^2 < 3\sigma$), $R_{int} = 0.03$; structure solved by Patterson and Fourier methods; refined on F, 462 parameters; 14 cyclooctatetraene hydrogens refined with isotropic thermal parameters, remaining 46 hydrogen atoms in calculated positions and fixed isotropic thermal parameters; anisotropic thermal parameters for non-hydrogen atoms; R = 0.076 for 5413 data, R = 0.032 for 3212 reflections for which $F^2 > 3\sigma$, wR = 0.038, S = 1.34; $w = [\sigma(F)]^{-2}$, p = 0.04 in calc. of $\sigma(F^2)$; max (shift/$\sigma$) = 0.03; empirical extinction correction, $F_{corr} = (1 + 1.65 \times 10^{-7} I)$; max. and min. of $\Delta F$ synthesis 0.7 and -0.8 e $Å^{-3}$; atomic f for neutral Yb, K, O and C, and spherical bonded H from International Tables (1974); local unpublished programs and ORTEP (Johnson, 1965).

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

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*Lists of structure factors, anisotropic thermal parameters, calculated hydrogen positions, deviations from least-squares planes, distances and angles have been deposited with the British Library Lending Division as Supplementary Publication No. (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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**Related literature.** This compound is similar to the dimethoxyethane adduct of $K_2[Yb(C_8H_8)_2]$, (Kinsley, Streitwieser & Zalkin, 1985).

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## References

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

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Kinsley, S. A., Streitwieser Jr., A., & Zalkin, A. (1985). Organometallics 4, 52-57.

Table 1. Atomic Parameters

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

| Atom | x | y | z | $B_{eq}/B$ ($A^2$) |
|---|---|---|---|---|
| Yb | 0.04544(3) | 0.18694(2) | 0.24563(2) | 3.45(1) |
| K(1) | 0.34906(19) | 0.19628(10) | 0.44746(8) | 4.27(5) |
| K(2) | -0.26406(16) | 0.18968(10) | 0.04465(8) | 4.05(5) |
| O(1) | 0.4529(5) | 0.3275(3) | 0.50844(29) | 5.2(2) |
| O(2) | 0.3451(6) | 0.2295(3) | 0.57997(28) | 5.3(2) |
| O(3) | 0.3212(7) | 0.0963(4) | 0.5509(3) | 6.6(3) |
| O(4) | -0.3663(5) | 0.3170(3) | -0.01679(28) | 4.9(2) |
| O(5) | -0.2526(6) | 0.2208(3) | -0.08799(27) | 4.6(2) |
| O(6) | -0.2512(7) | 0.0862(3) | -0.0605(3) | 6.0(2) |
| C(1) | 0.1471(9) | 0.1051(5) | 0.3523(4) | 3.9(2) |
| C(2) | 0.0682(9) | 0.1533(6) | 0.3786(4) | 4.2(3) |
| C(3) | 0.0602(10) | 0.2214(6) | 0.3804(5) | 4.5(3) |
| C(4) | 0.1246(11) | 0.2731(6) | 0.3546(5) | 4.4(3) |
| C(5) | 0.2251(10) | 0.2748(5) | 0.3177(4) | 3.9(3) |
| C(6) | 0.3045(8) | 0.2284(5) | 0.2949(4) | 3.5(3) |
| C(7) | 0.3165(8) | 0.1602(5) | 0.2945(4) | 3.6(3) |
| C(8) | 0.2532(8) | 0.1067(4) | 0.3175(4) | 3.2(3) |
| C(9) | 0.3093(9) | 0.0382(4) | 0.3015(4) | 4.6(3) |
| C(10) | 0.4548(10) | 0.0321(5) | 0.3429(6) | 8.2(4) |
| C(11) | 0.3052(11) | 0.0317(5) | 0.2245(5) | 6.9(4) |
| C(12) | 0.2329(12) | -0.0209(5) | 0.3196(6) | 7.4(4) |
| C(13) | -0.2241(8) | 0.1565(5) | 0.1990(4) | 3.8(3) |
| C(14) | -0.2159(8) | 0.2258(5) | 0.1979(4) | 3.9(3) |
| C(15) | -0.1388(10) | 0.2717(5) | 0.1732(5) | 4.3(3) |

| | | | | |
|---|---|---|---|---|
| C(16) | -0.0375(10) | 0.2681(5) | 0.1353(5) | 4.2(3) |
| C(17) | 0.0264(9) | 0.2162(6) | 0.1090(4) | 4.0(3) |
| C(18) | 0.0173(9) | 0.1479(5) | 0.1125(4) | 3.7(3) |
| C(19) | -0.0568(9) | 0.1014(5) | 0.1401(4) | 3.7(3) |
| C(20) | -0.1589(9) | 0.1022(5) | 0.1767(4) | 3.6(3) |
| C(21) | -0.2120(9) | 0.0356(4) | 0.1947(4) | 4.5(3) |
| C(22) | -0.3623(10) | 0.0285(5) | 0.1541(5) | 6.7(4) |
| C(23) | -0.2045(10) | 0.0297(5) | 0.2712(5) | 6.7(4) |
| C(24) | -0.1424(11) | -0.0239(5) | 0.1726(6) | 6.7(4) |
| C(25) | 0.4333(10) | 0.3749(5) | 0.4539(5) | 6.5(4) |
| C(26) | 0.3666(9) | 0.3408(5) | 0.5541(5) | 5.3(3) |
| C(27) | 0.3941(9) | 0.2908(5) | 0.6097(5) | 5.4(3) |
| C(28) | 0.3351(11) | 0.1813(6) | 0.6293(5) | 6.8(4) |
| C(29) | 0.2546(14) | 0.1262(6) | 0.5956(6) | 7.7(5) |
| C(30) | 0.2563(16) | 0.0378(7) | 0.5240(6) | 9.9(6) |
| C(31) | -0.3517(10) | 0.3642(5) | 0.0379(5) | 6.4(4) |
| C(32) | -0.2846(9) | 0.3319(4) | -0.0633(5) | 5.2(3) |
| C(33) | -0.3034(9) | 0.2815(5) | -0.1177(5) | 5.2(3) |
| C(34) | -0.2393(10) | 0.1725(5) | -0.1372(4) | 5.5(3) |
| C(35) | -0.1686(10) | 0.1152(5) | -0.1000(5) | 5.9(3) |
| C(36) | -0.2009(4) | 0.0265(6) | -0.0324(5) | 8.5(5) |
| H(1) | 0.126(6) | 0.060(3) | 0.368(3) | 2.1(14)* |
| H(2) | 0.014(8) | 0.130(4) | 0.406(4) | 5.5(23)* |
| H(3) | -0.003(9) | 0.242(4) | 0.403(4) | 5.8(26)* |
| H(4) | 0.090(12) | 0.313(6) | 0.357(6) | 10.3(43)* |
| H(5) | 0.244(8) | 0.320(4) | 0.305(4) | 5.2(23)* |
| H(6) | 0.374(8) | 0.248(4) | 0.278(4) | 4.0(20)* |

| | | | | |
|---|---|---|---|---|
| H(7) | 0.395(8) | 0.149(4) | 0.265(4) | 6.4(22)* |
| H(8) | -0.301(7) | 0.144(3) | 0.214(3) | 3.3(17)* |
| H(9) | -0.292(8) | 0.252(4) | 0.228(4) | 6.3(22)* |
| H(10) | -0.159(8) | 0.310(4) | 0.180(4) | 4.1(21)* |
| H(11) | -0.018(7) | 0.315(4) | 0.120(4) | 4.9(19)* |
| H(12) | 0.093(9) | 0.231(4) | 0.079(5) | 6.9(25)* |
| H(13) | 0.095(9) | 0.127(4) | 0.088(4) | 6.5(24)* |
| H(14) | -0.027(8) | 0.052(5) | 0.136(4) | 6.6(25)* |

*Isotropically refined thermal parameters.

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

| | | | |
|---|---|---|---|
| Yb - C(1) | 2.733(8) | Yb - C(19) | 2.767(8) |
| Yb - C(2) | 2.710(8) | Yb - C(20) | 2.836(8) |
| Yb - C(3) | 2.762(10) | Yb - Ring1 | 2.054 |
| Yb - C(4) | 2.786(10) | Yb - Ring2 | 2.056 |
| Yb - C(5) | 2.747(9) | K(1) - Ring1 | 2.456 |
| Yb - C(6) | 2.758(8) | K(2) - Ring2 | 2.468 |
| Yb - C(7) | 2.791(8) | K(1) - O(1) | 3.056(6) |
| Yb - C(8) | 2.821(7) | K(1) - O(2) | 2.751(6) |
| Yb - C(13) | 2.788(8) | K(1) - O(3) | 2.981(6) |
| Yb - C(14) | 2.758(8) | K(1) - O(4)$^{\underline{b}}$ | 2.865(6) |
| Yb - C(15) | 2.735(8) | K(2) - O(1)$^{\underline{b}}$ | 2.857(6) |
| Yb - C(16) | 2.746(8))) | K(2) - O(4) | 22984(7) |
| Yb - C(17) | 2.766(8) | K(2) - O(5) | 2.762(6) |
| Yb - C(18) | 2.737(8) | K(2) - O(6) | 3.020(7) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O(1) | - K(1) | - O(2) | 58.4(2) | Ring1 | - K(1) | - O(1) | 120.5 |
| O(1) | - K(1) | - O(3) | 114.4(2) | Ring1 | - K(1) | - O(2) | 136.9 |
| O(1) | - K(1) | - O(4)[b] | 75.0(2) | Ring 1 | - K(1) | - O(3) | 116.3 |
| O(2) | - K(1) | - O(3) | 58.4(2) | Ring1 | - K(1) | - O(4)[b] | 144.5 |
| O(2) | - K(1) | - O(4)[b] | 91.3(2) | Ring2 | - K(2) | - O(4) | 118.4 |
| O(3) | - K(1) | - O(4)[b] | 90.9(2) | Ring2 | - K(2) | - O(5) | 132.6 |
| O(4) | - K(2) | - O(1)[b] | 76.2(2) | Ring2 | - K(2) | - O(6) | 119.1 |
| O(4) | - K(2) | - O(5) | 59.2(2) | Ring2 | - K(2) | - O(1)[b] | 134.2 |
| O(4) | - K(2) | - O(6) | 113.6(2) | K(1) | - Ring1 | - Yb | 177.3 |
| O(5) | - K(2) | - O(1)[b] | 92.9(2) | K(2) | - Ring2 | - Yb | 176.9 |
| O(5) | - K(2) | - O(6) | 58.3(2) | Ring1 | - Yb | - COT(2) | 176.7 |
| O(6) | - K(2) | - O(1)[b] | 86.6(2) | | | | |

[a] Ring1 and Ring2 are [8]annulene rings C(1)-C(8) and C(13)-C(20) respectively.

[b] Atom at x, 1/2-y, 1/2+z

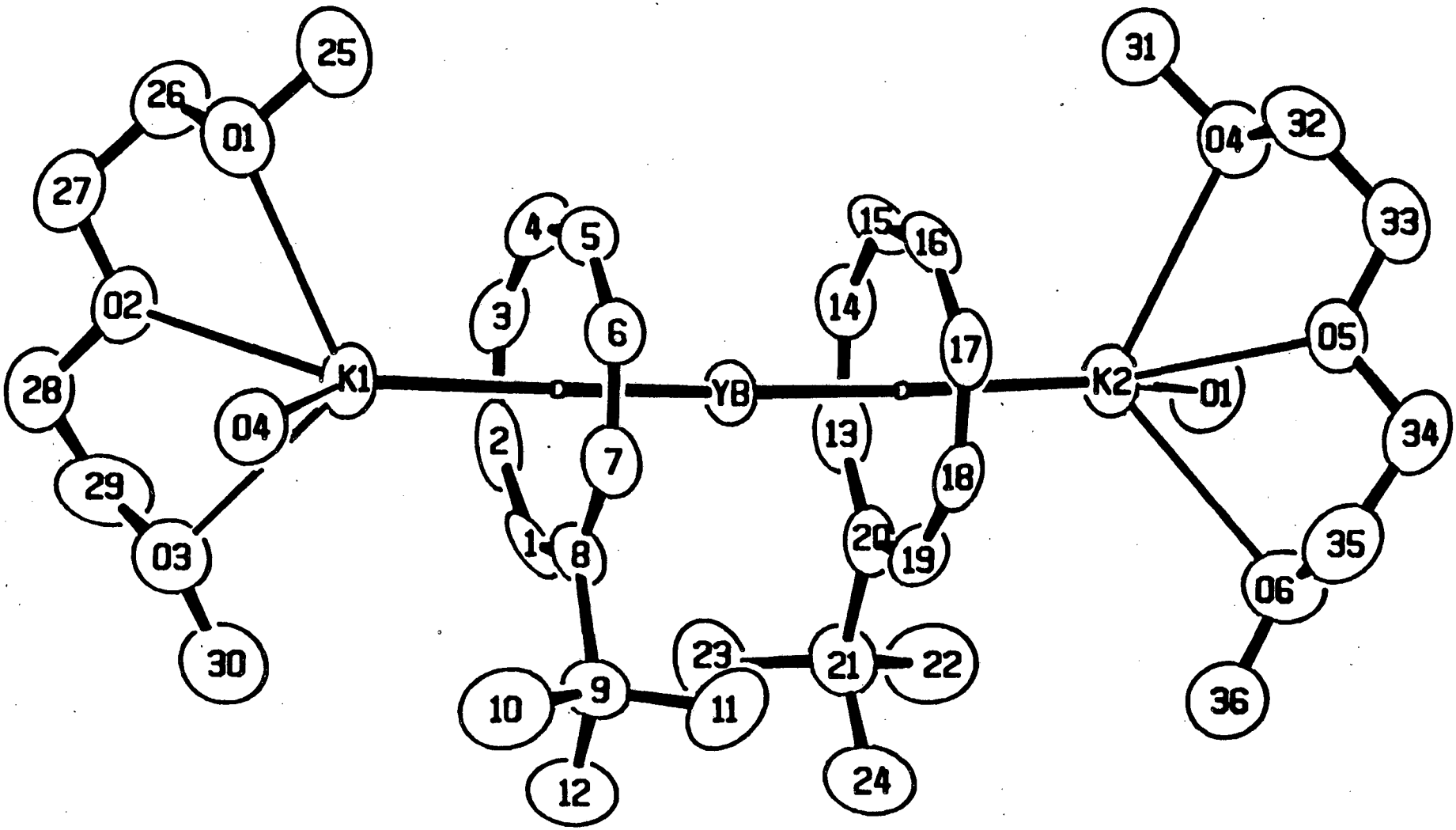


Fig.1. ORTEP (Johnson, 1965) of the molecule showing the atomic numbering scheme.

Supplemental Material for

# Diglyme Adduct of Dipotassium Bis(t-butyl[8]annulene)ytterbate(II)

$(CH_3OCH_2CH_2OCH_2CH_2OCH_3)_2K_2[(CH_3)_3CC_8H_7]_2Yb$

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

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**Abstract.** $M_r$ = 840.12, monoclinic, $P2_1/c$, a = 10.292(4), b = 20.588(6), c = 20.036(6) A, β = 103.28(4)°, V = 4131.9 $A^3$, Z = 4, $D_x$ = 1.350 g $cm^{-3}$, λ(MoKα)=0.71073 A, μ = 16.5 $cm^{-1}$, F(000) = 1728, T = 300 K, R = 0.032 for 3212 unique reflections with $F^2>3\sigma(F^2)$. The ytterbium atom is sandwiched between two parallel [8]annulene rings with a mean Yb-C distance of 2.77(4) A. The potassium atoms cap the other sides of the rings at a mean K-C distance of 3.08(5) A; each potassium atom is also coordinated to four oxygen atoms from the diglyme ligands at distances that range from 2.86 to 3.06 A.

Table S1. Anisotropic Thermal Parameters ($A^2$)[a]

| Atom | $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{13}$ | $B_{23}$ |
|---|---|---|---|---|---|---|
| YB | 3.297(16) | 3.817(17) | 2.788(15) | .143(21) | -.239(10) | .090(19) |
| K(1) | 4.17(8) | 5.30(11) | 3.05(7) | .50(8) | .22(6) | -.27(8) |
| K(2) | 3.89(8) | 4.79(9) | 3.20(7) | -.14(9) | .24(6) | .06(8) |
| O(1) | 4.64(28) | 5.8(4) | 4.90(29) | .63(27) | .93(24) | .73(27) |
| O(2) | 7.4(4) | 5.3(3) | 3.48(28) | -.1(3) | 1.75(26) | -.38(27) |
| O(3) | 8.9(5) | 5.4(4) | 5.5(4) | 1.9(3) | 1.6(3) | .1(3) |
| O(4) | 4.43(26) | 5.2(3) | 4.77(27) | -.25(29) | .76(22) | .4(3) |
| O(5) | 5.7(3) | 4.9(3) | 3.31(26) | -.18(27) | .90(23) | .40(25) |
| O(6) | 7.3(4) | 4.9(4) | 6.2(4) | .6(3) | 2.5(3) | .4(3) |
| C(1) | 4.2(5) | 3.8(5) | 2.9(4) | -.1(4) | -.7(4) | 2.3(4) |
| C(2) | 3.2(4) | 7.7(7) | 1.8(4) | .3(5) | .6(3) | .9(4) |
| C(3) | 4.5(5) | 5.3(7) | 3.2(5) | .9(5) | -.0(4) | -1.3(5) |
| C(4) | 4.6(5) | 4.2(6) | 3.9(5) | .4(5) | -.2(4) | -1.6(4) |
| C(5) | 4.4(5) | 3.0(5) | 3.6(5) | -.2(4) | -.6(4) | -.0(4) |
| C(6) | 2.5(4) | 3.9(5) | 3.7(4) | -.8(4) | -.5(3) | .1(4) |
| C(7) | 2.2(4) | 4.8(5) | 3.4(4) | .2(3) | .1(3) | .3(3) |
| C(8) | 2.4(4) | 3.6(5) | 3.1(4) | .8(3) | -.5(3) | .7(3) |
| C(9) | 4.9(4) | 3.5(4) | 4.7(5) | 1.6(4) | -.1(4) | .1(4) |
| C(10) | 5.7(5) | 7.0(6) | 9.7(7) | 3.7(5) | -2.7(5) | -1.7(6) |
| C(11) | 8.2(6) | 6.7(6) | 5.9(6) | 1.5(5) | 1.6(5) | -2.3(5) |
| C(12) | 9.7(8) | 4.1(6) | 8.0(7) | .8(5) | .9(6) | .2(5) |
| C(13) | 1.9(4) | 6.0(6) | 3.2(4) | -1.1(4) | .0(3) | .3(4) |
| C(14) | 2.6(4) | 5.3(6) | 3.4(4) | .7(4) | -.2(3) | -.0(4) |
| C(15) | 4.0(5) | 3.5(6) | 4.4(5) | 2.5(5) | -1.4(4) | .9(4) |
| C(16) | 5.0(5) | 3.4(5) | 3.5(4) | .1(4) | -.5(4) | 1.5(4) |
| C(17) | 3.9(4) | 5.8(6) | 2.2(4) | -.5(4) | .7(3) | .4(4) |
| C(18) | 4.5(5) | 4.4(5) | 2.1(4) | -.6(4) | .7(3) | -.7(4) |
| C(19) | 4.0(5) | 3.4(5) | 3.4(4) | -.9(4) | .1(4) | -.6(4) |
| C(20) | 3.4(4) | 4.3(5) | 2.5(4) | -1.1(4) | -.1(3) | .3(3) |
| C(21) | 4.3(4) | 4.3(5) | 4.5(5) | -1.6(4) | .4(4) | .6(4) |
| C(22) | 6.1(6) | 5.5(6) | 8.4(7) | -1.8(5) | 1.4(5) | -.1(5) |
| C(23) | 7.6(6) | 6.9(6) | 5.4(5) | -2.3(5) | .8(4) | 1.7(5) |
| C(24) | 7.3(6) | 4.2(6) | 8.1(7) | -.3(5) | 1.0(5) | .7(5) |
| C(25) | 6.0(5) | 7.3(6) | 5.5(5) | -.8(5) | .0(4) | 1.0(5) |
| C(26) | 5.2(5) | 5.6(6) | 5.4(5) | .0(4) | 1.9(4) | -1.0(4) |
| C(27) | 5.7(5) | 6.2(6) | 4.4(5) | -.2(4) | 1.2(4) | -1.2(4) |
| C(28) | 9.9(7) | 6.7(6) | 3.9(4) | .9(6) | 1.8(4) | -.2(5) |
| C(29) | 12.0(9) | 4.9(6) | 7.9(7) | 2.0(6) | 5.7(7) | 1.1(5) |
| C(30) | 16.1(12) | 6.0(7) | 7.0(7) | .7(7) | 1.5(7) | .7(6) |
| C(31) | 7.1(6) | 5.7(6) | 5.6(5) | 1.0(5) | -.1(5) | -1.0(5) |
| C(32) | 4.8(4) | 4.6(6) | 6.2(5) | -.1(4) | 1.3(4) | 1.7(4) |
| C(33) | 5.1(5) | 6.5(6) | 4.1(5) | .1(4) | 1.0(4) | .8(4) |
| C(34) | 6.4(5) | 6.3(7) | 4.0(4) | -1.1(5) | 1.5(4) | -.9(4) |
| C(35) | 6.3(6) | 5.9(6) | 5.7(5) | -.0(5) | 2.0(5) | -1.3(5) |
| C(36) | 14.2(10) | 5.7(7) | 5.6(6) | 1.6(6) | 2.4(6) | -.2(5) |

[a] The anisotropic temperature factor has the form:

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

Table S2. Estimated Hydrogen Positional and Isotropic Thermal Parameters ($A^2$)[a]

| Atom | x | y | z | B |
|---|---|---|---|---|
| H(15) | .2734 | .3383 | .5291 | 10.000 |
| H(16) | .3857 | .3841 | .5742 | 10.000 |
| H(17) | .4902 | .2878 | .6293 | 10.000 |
| H(18) | .348 | .3025 | .6457 | 10.000 |
| H(19) | .2918 | .200 | .6637 | 10.000 |
| H(20) | .4244 | .166 | .6517 | 10.000 |
| H(21) | .2423 | .0949 | .6305 | 10.000 |
| H(22) | .1679 | .1419 | .5701 | 10.000 |
| H(23) | -.1907 | .3329 | -.0384 | 10.000 |
| H(24) | -.3099 | .3744 | -.0841 | 10.000 |
| H(25) | -.3985 | .277 | -.139 | 10.000 |
| H(26) | -.2550 | .2941 | -.1524 | 10.000 |
| H(27) | -.1873 | .1902 | -.1683 | 10.000 |
| H(28) | -.3277 | .1595 | -.1635 | 10.000 |
| H(29) | -.1497 | .0836 | -.1331 | 10.000 |
| H(30) | -.0843 | .1291 | -.0696 | 10.000 |
| H(31) | .4573 | .0353 | .3917 | 12.000 |
| H(32) | .5085 | .0669 | .3294 | 12.000 |
| H(33) | .4907 | -.0101 | .333 | 12.000 |
| H(34) | .3599 | .0660 | .2108 | 12.000 |
| H(35) | .2129 | .0359 | .1982 | 12.000 |
| H(36) | .3404 | -.0109 | .2158 | 12.000 |
| H(37) | .140 | -.0187 | .2936 | 12.000 |
| H(38) | .236 | -.0204 | .3687 | 12.000 |
| H(39) | .2745 | -.0607 | .3077 | 12.000 |
| H(40) | -.3670 | .0313 | .1047 | 12.000 |
| H(41) | -.4153 | .0636 | .1675 | 12.000 |
| H(42) | -.3972 | -.0135 | .1647 | 12.000 |
| H(43) | -.2590 | .0638 | .2853 | 12.000 |
| H(44) | -.1116 | .0344 | .2966 | 12.000 |
| H(45) | -.2384 | -.0130 | .2809 | 12.000 |
| H(46) | -.0468 | -.0226 | .1950 | 12.000 |
| H(47) | -.1528 | -.0232 | .1227 | 12.000 |
| H(48) | -.1818 | -.0637 | .1859 | 12.000 |
| H(49) | .4535 | .4183 | .4738 | 12.000 |
| H(50) | .3402 | .3735 | .428 | 12.000 |
| H(51) | .4926 | .3651 | .4235 | 12.000 |
| H(52) | .1655 | .0474 | .4992 | 12.000 |
| H(53) | .2554 | .0078 | .5619 | 12.000 |
| H(54) | .3062 | .0181 | .4929 | 12.000 |
| H(55) | -.3772 | .4071 | .018 | 12.000 |
| H(56) | -.2584 | .365 | .0635 | 12.000 |
| H(57) | -.4093 | .3521 | .0684 | 12.000 |
| H(58) | -.1121 | .033 | -.0025 | 12.000 |
| H(59) | -.1943 | -.0035 | -.0695 | 12.000 |
| H(60) | -.2609 | .0084 | -.0058 | 12.000 |

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

Table S3. Least-Squares Planes and Deviations (Å) Therefrom

| Plane 1, C(1) - C(8) | | Plane2, C(13) - C(20) | |
|---|---|---|---|
| 5.06 x + 0.63 y + 14.7 z = 6.02 | | 5.24 x - 0.25 y + 14.44 z = 1.68 | |
| atom | dist | atom | dist |
| C(1) | -0.022 | C(13) | -0.022 |
| C(2) | -0.004 | C(14) | -0.011 |
| C(3) | 0.025 | C(15) | 0.024 |
| C(4) | 0.003 | C(16) | 0.009 |
| C(5) | -0.030 | C(17) | -0.024 |
| C(6) | 0.007 | C(18) | -0.005 |
| C(7) | 0.018 | C(19) | 0.018 |
| C(8) | 0.003 | C(20) | 0.011 |
| C(9) | 0.008 | C(21) | 0.010 |
| Yb | -2.054 | Yb | 2.056 |
| K | 2.456 | K | -2.468 |
| H(1) | 0.065 | H(8) | -0.199 |
| H(2) | 0.119 | H(9) | 0.012 |
| H(3) | 0.058 | H(10) | 0.006 |
| H(4) | -0.117 | H(11) | -0.120 |
| H(5) | -0.099 | H(12) | -0.108 |
| H(6) | 0.124 | H(13) | 0.050 |
| H(7) | -0.028 | H(14) | 0.118 |

Table S4. Additional Distances

| Atoms | Dist (A) | Atoms | Dist (A) |
|---|---|---|---|
| C(1) - C(2) | 1.455(13) | C(13) - C(14) | 1.429(12) |
| C(2) - C(3) | 1.404(12) | C(14) - C(15) | 1.396(13) |
| C(3) - C(4) | 1.413(15) | C(15) - C(16) | 1.426(14) |
| C(4) - C(5) | 1.403(14) | C(16) - C(17) | 1.418(13) |
| C(5) - C(6) | 1.400(12) | C(17) - C(18) | 1.412(11)) |
| C(6) - C(7) | 1.410(112 | C(18) - C(19) | 1.415(11) |
| C(7) - C(8) | 1.409(11) | C(19) - C(20) | 1.412(12) |
| C(8) - C(1) | 1.425(12) | C(20) - C(13) | 1.427(12) |
| C(8) - C(9) | 1.584(11) | C(20) - C(21) | 1.549(11) |
| C(9) - C(10) | 1.542(12) | C(21) - C(22) | 1.581(12) |
| C(9) - C(11) | 1.538(12) | C(21) - C(23) | 1.522(12) |
| C(9) - C(12) | 1.538(13) | C(21) - C(24) | 1.536(13) |
| C(26) - C(27) | 1.495(13) | C(32) - C(33) | 1.485(13) |
| C(28) - C(29) | 1.474(15) | C(34) - C(35) | 1.493(13) |
| O(1) - C(25) | 1.444(10) | O(4) - C(31) | 1.445(10) |
| O(1) - C(26) | 1.441(10) | O(4) - C(32) | 1.424(11) |
| O(2) - C(27) | 1.437(10) | O(5) - C(33) | 1.431(11) |
| O(2) - C(28) | 1.420(12) | O(5) - C(34) | 1.429(10) |
| O(3) - C(29) | 1.388(11) | O(6) - C(35) | 1.419(11) |
| O(3) - C(30) | 1.422(14) | O(6) - C(36) | 1.400(12) |
| K(1) - C(1) | 3.107(9) | K(2) - C(13) | 3.101(9) |
| K(1) - C(2) | 3.034(9) | K(2) - C(14) | 3.087(9) |
| K(1) - C(3) | 3.012(10) | K(2) - C(15) | 3.102(10) |
| K(1) - C(4) | 3.054(11) | K(2) - C(16) | 3.066(9) |
| K(1) - C(5) | 3.077(9) | K(2) - C(17) | 3.021(9) |
| K(1) - C(6) | 3.057(9) | K(2) - C(18) | 3.027(9) |
| K(1) - C(7) | 3.096(9) | K(2) - C(19) | 3.105(9) |
| K(1) - C(8) | 3.158(8) | K(2) - C(20) | 3.178(8) |

Table S5. Additional Angles

| Atoms | Angle(°) | Atoms | Angle(°) |
|---|---|---|---|
| C(8) - C(1) - C(2) | 135.7(9) | C(20) - C(13) - C(14) | 138.0(10) |
| C(1) - C(2) - C(3) | 136.9(11) | C(13) - C(14) - C(15) | 136.2(10) |
| C(2) - C(3) - C(4) | 135.0(12) | C(14) - C(15) - C(16) | 134.3(10) |
| C(3) - C(4) - C(5) | 132.5(11) | C(15) - C(16) - C(17) | 134.1(10) |
| C(4) - C(5) - C(6) | 135.4(10) | C(16) - C(17) - C(18) | 133.6(10) |
| C(5) - C(6) - C(7) | 137.7(10) | C(17) - C(18) - C(19) | 137.9(10) |
| C(6) - C(7) - C(8) | 136.8(10) | C(18) - C(19) - C(20) | 136.7(9) |
| C(7) - C(8) - C(1) | 129.9(9) | C(19) - C(20) - C(13) | 129.1(9) |
| C(1) - C(8) - C(9) | 115.8(8) | C(19) - C(20) - C(21) | 117.1(9) |
| C(7) - C(8) - C(9) | 114.3(8) | C(13) - C(20) - C(21) | 113.8(8) |
| C(8) - C(9) - C(10) | 108.5(8) | C(20) - C(21) - C(22) | 108.5(8) |
| C(8) - C(9) - C(11) | 110.7(7) | C(20) - C(21) - C(23) | 111.6(8) |
| C(8) - C(9) - C(12) | 115.3(8) | C(20) - C(21) - C(24) | 115.2(8) |
| C(25) - O(1) - C(26) | 110.7(7) | C(31) - O(4) - C(32) | 112.2(8) |
| O(1) - C(26) - C(27) | 107.7(8) | O(4) - C(32) - C(33) | 109.5(8) |
| C(26) - C(27) - O(2) | 108.0(8) | C(32) - C(33) - O(5) | 109.4(8) |
| C(27) - O(2) - C(28) | 113.6(8) | C(33) - O(5) - C(34) | 113.9(7) |
| O(2) - C(28) - C(29) | 110.0(8) | O(5) - C(34) - C(35) | 108.5(8) |
| C(28) - C(29) - O(3) | 109.1(11) | C(34) - C(35) - O(6) | 109.0(9) |
| C(29) - O(3) - C(30) | 111.2(10) | C(35) - O(6) - C(36) | 112.3(9) |

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