trispyrazolylborate or with potassium tris(3,5-dimethyl-pyrazolyl)borate arises from weaker acidity of bis(3,5-dimethylpyrazolyl)borane because of the electron-releasing effect of the methyl substituents on the pyrazolyl rings or from the increased steric demands of three 3,5-dimethylpyrazolyl rings relative to three pyrazolyl rings is presently unclear.

The major products from reactions between $C_3H_5Fe(CO)_3I$ and potassium trispyrazolylborates are the iron-(II) complexes $(HBPz_3)_2Fe$ where all of the ligands originally bonded to the iron atom (i.e., allyl, carbonyl, and iodine) have been displaced by trispyrazolylborate ligands. These products are not listed in the scheme in Figure 1, since their origin is ambiguous. The $(HBPz_3)_2Fe$ compounds may arise from displacement of the propenyl and two carbonyl groups in an intermediate of type D with a second trispyrazolylborate anion or by displacement of the allyl group in an intermediate of type A with a second trispyrazolylborate anion followed by attack of the uncomplexed nitrogen atoms of both trispyrazolylborate ligands on the metal atom with loss of all of the carbonyl groups. The latter pathway is made more probable by the observed reaction of $C_3H_5Fe(CO)_3I$ with potassium bispyrazolylborate to give the dicarbonyl cis-$[H_2B(C_3H_3N_2)_2]_2$-$Fe(CO)_2$ (II). In the bispyrazolylborate system there are insufficient nitrogens on the bispyrazolylborate ligands after displacement of both the allyl and iodine in $C_3H_5Fe(CO)_3I$ to replace all of the carbonyl groups then remaining on the iron. In this system two carbonyl groups must remain on the iron atom after all available nitrogen atoms for coordination from the bispyrazolylborate ligands are used.

Structure of the 10π Electron Cyclooctatetraene Dianion in Potassium Diglyme 1,3,5,7-Tetramethylcyclooctatetraene Dianion, $[K((CH_3OCH_2CH_2)_2O)]_2[C_8H_4(CH_3)_4]$

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Abstract: The structure of the potassium salt of a cyclooctatetraene dianion has been determined. As predicted by the Hückel theory this 10π electron system is aromatic with eightfold molecular symmetry and average C–C bond lengths of 1.407 (6) Å. Yellow air-sensitive crystals of potassium diglyme bis(1,3,5,7-tetramethylcyclooctatetraene) dianion, $[K((CH_3OCH_2CH_2)_2O)]_2[C_8H_4(CH_3)_4]$, crystallize in space group $P\bar{1}$ (C_i^1) with $a = 9.757$ (3), $b = 10.026$ (4), $c = 8.793$ (3) Å, $\alpha = 97.15$ (1)°, $\beta = 112.35$ (1)°, and $\gamma = 109.95$ (1)° with $\rho_{calcd} = 1.16$ g cm^{-3} for $Z = 1$. All atoms, including hydrogen atoms, have been located and their positions and thermal parameters refined by full-matrix least-squares procedures to a conventional R factor of 5.5% for 855 reflections with $F^2 > 3\sigma(F^2)$ collected with an automated X-ray diffractometer. The structure consists of an ion trimer which lies on an inversion center. The two potassium ions are related by inversion and lie on either side of the cyclooctatetraene ring such that all the K–C bond lengths are equal and average 3.003 (8) Å. The opposite side of each potassium ion is coordinated by the three ether oxygens at an average distance of 2.835 (14) Å. All atoms in the carbocyclic ring lie in the plane to within experimental error and the ring is not significantly puckered; the two independent methyl groups are bent out of the plane of the ring by only 0.5 and 2.6°.

O ne of the first successes of quantum chemistry in its application to organic compounds was the explanation of the unusual stability of "aromatic" compounds. The Hückel $4n + 2$ rule for single carbocyclic rings is the most generally used result.[2] Probably the two most important predictions of this rule were the instability of uncomplexed cyclobutadiene and the conversion of the alternating double bond tub geometry of the 8π electron cyclooctatetraene molecule to a symmetrical planar 10π electron dianion.[3] Although

many physical studies have been carried out on the dianion, much speculation has been made regarding its planar geometry, and structures have been determined for some of its complexes;[4–11] no definitive structural data have been available for cyclooctatetraene dianion itself. We report here the results of such a

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study. The anion, a tetramethyl substituted derivative of cyclooctatetraene, offers two advantages: the puckering of the ring can be determined by observing the deviation of the methyl groups from the carbocyclic ring and the thermal libration of the ring in the solid state is expected to be diminished relative to the unsubstituted ring due to intermolecular interactions.

Experimental Section

The compound was obtained as a by-product in the synthesis of the cerium complex, $[K((CH_3OCH_2CH_2)_2O)][Ce(C_8H_4(CH_3)_4)_2].$[12] When crystallized from the dimethyl ether of diethylene glycol, diglyme, potassium bis(1,3,5,7-tetramethylcyclooctatetraene) dianion, $[K((CH_3OCH_2CH_2)_2O)]_2[C_8H_4(CH_3)_4]$, is obtained as bright yellow crystals which are extremely sensitive to oxygen and water. The composition and structure of the compound were established by the diffraction analysis.

Several crystals were mounted in thin-walled quartz capillaries under an argon atmosphere. Precession photographs revealed no systematic absences and showed triclinic symmetry, implying the space groups $P1(C_1^1)$ or $P\bar{1}(C_i^1)$.[13] The subsequent structure analysis shows the space group is $P\bar{1}$. The crystal orientation and unit cell constants were determined by a least-squares refinement of the diffractometer setting angles for 12 carefully centered reflections.[14,15] The crystal data are summarized in Table I.

Table I. Crystal Data for $[K((CH_3OCH_2CH_2)_2O)]_2[C_8H_4(CH_3)_4]$

Molecular weight	506.82 g/mol
Linear absorption coefficient, μ(Mo Kα)	3.55 cm^{-1}
Calculated density	1.16 g/cm^3
Space group	$P\bar{1}$
Molecules/unit cell	1
Cell constants[a]	
a	9.757 (3) Å
b	10.026 (4) Å
c	8.793 (3) Å
α	97.15 (1)°
β	112.35 (1)°
γ	109.95 (1)°
Cell volume	727.9 (5) Å^3

[a] Reduced cell. Ambient temperature = 23°. Mo Kα_1 λ 0.70926 Å.

The mosaicity of the data crystal, which was mounted along the a axis, was determined using the narrow source, open counter ω-scan technique.[16] The widths of ω scans at half maximum for typical strong reflections were 0.1–0.16°. Intensity data were collected on an automated Picker four-circle diffractometer using graphite crystal monochromatized Mo Kα radiation. Data were collected and processed as described previously,[15] with a scan rate of 1°/min from 0.50° below the Kα_1 peak to 0.50° above the Kα_2 peak and background counts of 10 sec each at the start and end of each scan. A full sphere of data was collected for $2\theta < 30°$ and the half sphere with $l > 0$ was collected for $30° < 2\theta < 45°$. Crystal and instrumental stability were monitored by measuring the intensities of the 301, 020, and 002 reflections after every 70 reflections. The crystal showed no evidence of decomposition. The range of scatter in the intensities of the standards during data collection was roughly 6%. On the basis of the scatter in the standards the p factor introduced to prevent overweighting the strong reflections was chosen as 0.06.[16,17] A total of 2654 data was collected, which

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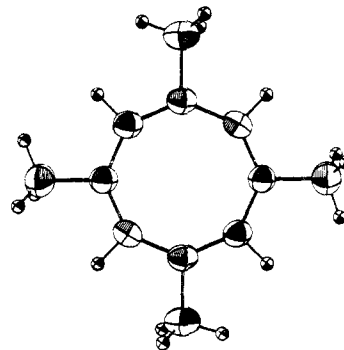(17) P. W. R. Corfield, R. J. Doedens, and J. A. Ibers, Inorg. Chem., 6, 197 (1967).

Figure 1. A perspective drawing of the 1,3,5,7-tetramethylcyclooctatetraene dianion. Thermal ellipsoids enclose 40% of the electron distribution. For clarity the isotropic thermal parameters for the hydrogens were set as 1.0 Å^2. The ring carbon at the far left is C_1 and the atoms are numbered in sequence for counterclockwise motion around the ring.

after averaging gave 1875 independent reflections, of which 855 had $F^2 > 3\sigma(F^2)$. The agreement factor for averaging was 1.9%. No absorption correction was necessary since, for $\mu = 3.56$ cm^{-1} and a maximum crystal dimension of 0.04 cm, the transmission factor range is smaller than from 0.87 to 0.93.

Solution and Refinement of the Structure. The structure was solved from an origin-removed sharpened Patterson map followed by full-matrix least-squares refinements and difference Fourier calculations.[18] Refinement with anisotropic thermal parameters reduced R_1 and R_2 to 7.9 and 9.8%.[22] A difference Fourier showed electron density near the expected hydrogen positions. The hydrogens were positioned on the basis of ideal geometries for the various groups involved. All hydrogens were positioned 1.0 Å from the atoms to which they are bonded.[23] The hydrogens on the ring and in the methylene groups were positioned assuming trigonal and tetrahedral geometries for the central carbon atoms. The three hydrogens in each methyl were treated as a rigid tetrahedral group, and the rotational angle about the threefold axis was refined. The thermal parameters for the hydrogens were fixed. The final refinement converged to $R_1 = 5.45\%$ and $R_2 = 6.81\%$.[24] The final positional and thermal parameters are given in Table II.[25]

Discussion

Potassium diglyme 1,3,5,7-tetramethylcyclooctatetraenide exists as a discrete ion trimer. Each tetramethylcyclooctatetraene dianion ring has its center on the crystallographic inversion center. A drawing of the ring is shown in Figure 1. Associated with each ring are the two centrosymmetrically related potassium diglyme units. All three of the diglyme oxygen are coordinated to the metal. A drawing of an entire $[K((CH_3OCH_2CH_2)_2O)]_2[C_8H_4(CH_3)_4]$ unit is shown in

(18) Scattering factors for K, O, and C were those of Cromer and Mann (ref 19) and for hydrogen were those of Stewart, et al. (ref 20). Real and imaginary contributions from anomalous scattering were included (ref 21). In addition to local programs for the CDC 6400 and 7600 computers, modifications of the following programs were used: Ibers' NUCLS, a group least-squares version of the Busing–Levy ORFLS program; Zalkin's FORDAP Fourier program; ORFFE, a function and error program by Busing, Martin, and Levy; Johnson's ORTEP thermal ellipsoid plot program.

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(20) R. F. Stewart, E. R. Davidson, and W. T. Simpson, J. Chem. Phys., 42, 3175 (1965).

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(24) On the final cycle no parameter shifted by more than 0.2 of its estimated standard deviation. The error in an observation of unit weight (ref 6) was 1.64 and did not show any systematic variation as a function of either F_o or sin θ. A final difference Fourier was featureless. The highest peak had a density of 0.25 e/Å^3 or roughly 5% of a carbon atom.

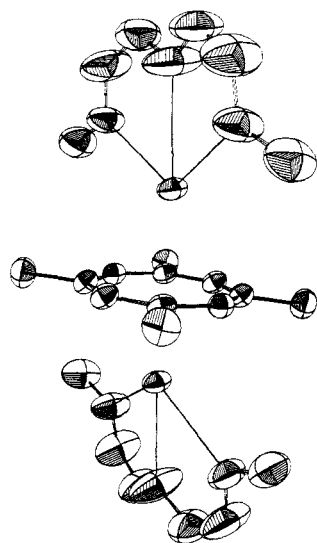(25) See paragraph at end of paper regarding supplementary material.

Figure 2. A perspective drawing of [K((CH₃OCH₂CH₂)₂O)]₂-[C₈H₄(CH₃)₄]. Thermal ellipsoids enclose 30% of the electron density. Hydrogen atoms are not shown. The left-most ring carbon is C_3 and numbering proceeds in sequence for clockwise motion around the ring. In the lower diglyme molecule the left-most atom is C_7 and the left-most oxygen atom is O_1 and the remainder of the numbering is sequential.

Figure 2. A crystal packing diagram is shown in Figure 3.

The crystallographic symmetry requires that the two potassium atoms be equidistant from the ring center. The observed distance is 2.375 (3) Å. There is no crystallographic requirement that the two metal atoms be equidistant from any of the ring carbon atoms. The average K–C distance is 3.003 (8) Å with individual distances deviating from this value by at most three or four times their standard deviations. This is slightly
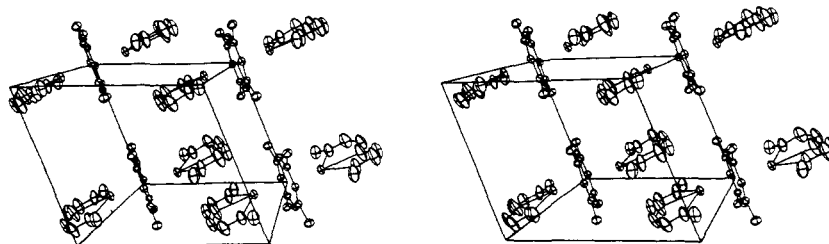
Table II. Position and Thermal Parameters for [K((CH₃OCH₂CH₂)₂O)]₂[C₈H₄(CH₃)₄]

| Atom | Positional parameters | | |
	x	y	z
K	0.27022 (19)ᵃ	0.01643 (17)	0.10410 (24)
C₁	0.0443 (8)	0.1214 (9)	-0.1305 (12)
C₂	-0.0212 (8)	-0.0264 (9)	-0.2185 (8)
C₃	-0.0750 (8)	-0.1613 (8)	-0.1838 (10)
C₄	-0.0821 (8)	-0.1960 (7)	-0.0377 (12)
C₅	0.0828 (10)	0.2238 (8)	-0.2377 (10)
C₆	-0.1438 (9)	-0.2933 (8)	-0.3344 (10)
O₁	0.3500 (10)	-0.2117 (8)	0.1951 (11)
O₂	0.5993 (10)	0.0464 (11)	0.2591 (15)
O₃	0.5475 (8)	0.2876 (7)	0.2280 (11)
C₇	0.2256 (15)	-0.3523 (13)	0.1324 (18)
C₈	0.5069 (21)	-0.1848 (16)	0.2888 (22)
C₉	0.6275 (15)	-0.0562 (19)	0.3171 (19)
C₁₀	0.7201 (16)	0.1786 (22)	0.3108 (22)
C₁₁	0.6928 (16)	0.2913 (17)	0.3047 (24)
C₁₂	0.5277 (13)	0.4086 (12)	0.2173 (17)

| Atom | Thermal parameters ᵇ | | | | | |
	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
K	137 (3)	157 (3)	303 (5)	63 (2)	55 (3)	70 (3)
C₁	152 (14)	142 (13)	201 (20)	53 (11)	77 (14)	68 (15)
C₂	156 (14)	154 (15)	160 (17)	49 (11)	49 (12)	55 (14)
C₃	154 (14)	134 (13)	159 (18)	41 (11)	55 (13)	42 (13)
C₄	160 (14)	116 (11)	215 (21)	56 (10)	83 (14)	58 (14)
C₅	292 (19)	193 (13)	282 (21)	96 (13)	154 (17)	120 (14)
C₆	261 (17)	164 (12)	243 (20)	51 (12)	130 (16)	29 (14)
O₁	271 (16)	256 (13)	726 (28)	148 (13)	180 (18)	219 (16)
O₂	222 (17)	311 (17)	1089 (42)	114 (15)	31 (20)	301 (22)
O₃	183 (14)	194 (11)	782 (28)	55 (11)	126 (16)	17 (15)
C₇	397 (28)	249 (20)	828 (47)	177 (21)	290 (32)	244 (25)
C₈	400 (36)	328 (27)	890 (56)	211 (27)	144 (38)	318 (33)
C₉	253 (28)	380 (30)	727 (47)	185 (25)	31 (29)	164 (34)
C₁₀	225 (28)	390 (37)	798 (51)	123 (29)	115 (30)	52 (40)
C₁₁	194 (28)	325 (31)	977 (64)	18 (25)	47 (33)	112 (38)
C₁₂	287 (24)	247 (21)	757 (45)	48 (19)	203 (26)	55 (27)

ᵃ The standard deviation of the least significant figure is given in parentheses. ᵇ The form of the anisotropic thermal ellipsoid is $\exp[-10^{-4}(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.

Figure 3. A stereoscopic view of the unit cell for [K((CH₃OCH₂CH₂)₂O)]₂[C₈H₄(CH₃)₄]. The a axis is horizontal, the c axis is vertical, and the b axis goes nto the drawing. Thermal ellipsoids enclose 20% of the electron distribution. Only the molecules on the back face are shown. Hydrogens have been omitted.

shorter than the average K–C distance of 3.16 (3) Å observed in [K((CH₃OCH₂CH₂)₂O)][Ce(C₈H₈)₂].⁹ The normal to the plane of the ring is nearly parallel to the K–K vector; the angle between them is 0.9°.

The eight carbon atoms of the ring form a regular octagon. The average C–C bond length is 1.407 (6) Å. The average alternate bond lengths, 1.398 (7) and 1.416 (7) Å, are equal within experimental error. The planarity of the ring and the C–C bond lengths show that the free dianion is truly an aromatic π system. The puckering of the ring is minimal; one methyl group is bent out of the plane of the ring 0.5° and the other 2.6°. The geometry of this free dianion thus

compares very closely with the dianion in its metal complexes.

The diglyme is coordinated to the potassium through all three oxygen atoms; the average K–O distance of 2.385 (14) Å is slightly longer than that observed in [K((CH₃OCH₂CH₂)₂O)]₂[Ce(C₈H₈)₂].⁹ The bond lengths within the diglyme molecule are artificially short due to the effect of the large thermal motion of that part of the structure. As can be seen in Figure 3, the thermal motion increases within each [K((CH₃OCH₂CH₂)₂O)]₂-[C₈H₄(CH₃)₄] trimeric unit on going outward from the center of the cyclooctatetraene ring. The ring itself is packed quite firmly in its position while the

diglyme rings occupy relatively large holes in the structure.[26] When corrected for thermal motion, the bond lengths in the diglyme molecule approach or exceed expected C–C and C–O bond lengths, depending upon the model chosen.[27]

(26) The potassium atom and the center of the triangle of oxygens are almost in the xz plane. The molecules pack on a layer structure. The dihedral angles between the ring and the xy, xz, and yz planes are 70.5, 87.3, and 22.5°, respectively. The ring axis forms angles of 19.8, 111.7, and 92.8° with the x, y, and z axes, respectively.
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Magnetic Circular Dichroism Spectra of Some Tetrahedral Cobalt(II) Complexes

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Abstract: Magnetic circular dichroism (MCD) spectra of tetrahedral cobalt(II) ions, $Co(NCS)_4{}^{2-}$, $Co(TBPO)_4{}^{2+}$, $Co(Ph_3PO)_4{}^{2+}$, $Co(Ph_3P)_2X_2$, and $Co(Ph_3PO)_2X_2$ (X = Cl, Br, I, SCN), have been measured in solution. A clear assignment of almost all bands of $Co(Ph_3PO)_2Br_2$ is made by analysis based on the assumption that the cobalt(II) ion is in the tetrahedral ligand field whose properties are a numerical average of those of the actual ligands. The temperature-dependence experiments have proved that the major contribution to MCD is derived from the C term. This is consistent with the previous studies on the MCD of tetrahalide cobalt(II) ions and also with the present assignment. It seems that the effect of low symmetry components in the ligand field upon the MCD is smaller than the effect of the spin–orbit coupling upon the MCD. We extend the assignment to the other cobalt(II) complexes.

The magnetic circular dichroism (MCD) spectra of a number of transition metal complexes have been measured and analyzed, and the MCD technique has been found useful in clarifying spectroscopic assignment and characterizing the symmetry of transitions.[1–5] The MCD of tetrahalide complexes of cobalt(II) has been studied in detail by many investigators.[6–13] The signs and magnitudes of the MCD were used to make

a clear assignment of bands. The source of the MCD was found to be the temperature-dependent C term whose origin lies in the Zeeman splitting of the ground state.[10,13] At the present time it appears that the application of the MCD studies to the other tetrahedral complexes of cobalt(II) would be of great interest.

Absorption spectra and magnetic susceptibilities have been reported for some tetrahedral and pseudo-tetrahedral complexes of cobalt(II) of the type CoL_4, CoL_2X_2, $CoLX_3$, and CoX_4, and the analyses and interpretations of these data have been discussed.[14–23] The

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