

group of a neighbouring ligand. The chain is built by repetition of tributyltin(IV) 1-uracilacetate units along twofold screw axes. The carboxylate group bonds to tin through only one O atom [Sn—O(1) 2.124 (5) Å] and is monodentate. The Sn—O(4') bond [2.669 (6) Å] involving the uracil group is significantly shorter than the sum of the appropriate van der Waals radii (3.70 Å). Bridging by a uracil O atom is probably sterically less demanding than bridging by a carbonyl O atom. The difference in length between the Sn—O(acyl) and Sn—O(uracil) bonds is greater than 0.22 Å, the difference found in triphenyltin(IV) 8-quinolyloxyacetate hydrate (Kumar Das, Chen, Ng & Mak, 1987) where the molecules are linked by hydrogen bonding through coordinated water molecules. In a triphenyltin(IV) 3-pyridinecarboxylate (Ng, Kumar Das, van Meurs, Schagen & Straver, 1989) the corresponding difference is 0.431 Å and molecules are linked by intermolecular Sn←:N bridges.

The three C atoms C(1), C(5) and C(9) define the equatorial plane of the trigonal bipyramid, with the Sn atom located 0.292 (2) Å above this plane. The Sn—C distances are 2.126 (14), 2.154 (11) and 2.140 (10) Å and the sum of the C—Sn—C angles is

354.4 (13)°. The O—Sn—O skeleton is nearly linear [172.8 (2)°]; similar angles in polymeric triorgano-tin(IV) carboxylates range from 170 to 174°.

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Synthesis and Structure of 3-Fluorenyl-3-cobalta-1,2-dicarbocloso-nonaborane(11), 3-(η^5 -C₁₃H₉)-3,1,2-closo-CoC₂B₉H₁₁

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Abstract. C₁₅H₂₀B₉Co, $M_r = 356.55$, orthorhombic, $P2_12_12_1$, $a = 8.759$ (3), $b = 13.037$ (3), $c = 15.366$ (4) Å, $V = 1754.7$ (8) Å³, $Z = 4$, $D_x = 1.349$ Mg m⁻³, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 0.94$ mm⁻¹, $F(000) = 728$, $T = 291$ (1) K, $R = 0.0793$ for 1930 independent observed reflections. The (staggered) conformation of the fluorenyl ligand relative to the metal-bonded C₂B₃ face of the carbaborane is such that one pair of junction C atoms is *trans* to a B—B connectivity, the other being *trans* to a B—C connectivity. This conformation is shown to be the optimum by analysis of the results from molecular orbital calculations on a model compound.

Introduction. The synthesis and structural properties of carbametallaboranes in which the indenyl ligand

(C₉H₇) is η^5 -bonded (exopolyhedrally) to the cluster metal atom are of interest since (i) electronically controlled conformational possibilities exist that are not possible in analogous cyclopentadienyl carbametallaboranes and (ii) slipping distortions are well known both in carbametallaboranes and in indenyl transition-metal compounds separately, and it is instructive to devise molecules in which either or both distortions are present, possibly in competition.

To these ends we have already reported the compound 3-(η^5 -C₉H₇)-3,1,2-closo-CoC₂B₉H₁₁ and its 1e⁻ and 2e⁻ reduced forms (Smith & Welch, 1986). The conformation of, and slipping distortions in, the neutral compound are rationalized (*via* frontier molecular orbital analysis) in terms of the influence of the six-carbon ring fused to the side of the η^5 -

pentagon. Recently (Lewis, Reed & Welch, 1991) we have extended this initial study by probing the consequences on structure of introducing ether (—CH₂OCH₃) and phenyl groups as substituents to the cage C atoms.

The fluorenyl ligand (C₁₃H₉) is to indenyl as indenyl is to cyclopentadienyl, *i.e.* it comprises *two* pseudo-aromatic six-carbon rings fused to the central C₅ unit. Clearly it was of interest to determine the key structural features of a molecule containing both fluorenyl and carbaborane ligands, and accordingly the studies described herein were undertaken.

Experimental. The title compound was prepared by dropwise addition of a tetrahydrofuran (THF) solution of lithium fluorenyl (1.079 mmol) to a cooled (273 K), stirred suspension of Ti[TiC₂B₉H₁₁] (0.583 g, 1.079 mmol) and Co(acac)₃ (0.384 g, 1.079 mmol) (acac = acetylacetonate) in THF (20 cm³). After 3 h the mixture was filtered and the filtrate evaporated *in vacuo*. CH₂Cl₂ was added to the resulting brown solid, the product filtered, and the filtrate concentrated to a small volume. TLC (CH₂Cl₂:hexane, 1:1) on silica plates afforded the product as an amber band (*R_f* 0.45) in low yield (< 5%). Dark red needles were grown by diffusion of hexane into a CH₂Cl₂ solution at 263 K. Crystal, 0.1 × 0.1 × 0.5 mm, mounted in a Lindemann capillary and set on an Enraf-Nonius CAD-4 diffractometer (Mo K α X-radiation, graphite monochromator); cell parameters and orientation matrix from least-squares refinement of the setting angles ($5 < \theta < 12^\circ$) of 25 centred reflections; data collection by ω -2 θ scans in 96 steps with ω -scan width ($0.8 + 0.34 \tan \theta$) $^\circ$; two octants of data (*h*: 0 to 10, *k*: 0 to 15, *l*: -18 to 18) measured for $1 \leq \theta \leq 25^\circ$ over 113 X-ray hours with no appreciable decay or movement; corrections for Lorentz and polarization effects applied (Gould & Smith, 1986); of 3505 data measured, 2182 [$F \geq 2.0\sigma(F)$] used to solve (direct methods; Sheldrick, 1986) and refine (Sheldrick, 1976) the structure to isotropic convergence; cage C atoms identified by a combination of intercage distances and refined (as B) cage atom thermal parameters; absolute configuration established by parallel refinement of both enantiomers; empirical absorption correction (Walker & Stuart, 1983) applied (correction factors 0.767–1.191); equivalent reflections (*h*0*l* and *h*0 \bar{l} ; 0*k**l* and 0*k* \bar{l} ; 00*l* and 00 \bar{l}) merged ($R_{\text{merge}} = 0.032$) to afford a final set of 1930 reflections; all non-H atoms refined with anisotropic thermal parameters; cage H atoms allowed positional refinement subject to a single X—H distance of 1.05 (1) Å; fluorenyl H atoms set in idealized positions with C—H 1.08 Å; cage and fluorenyl H atoms refined with separate group thermal parameters, 0.039 (8) and 0.103 (12) Å² respectively at convergence; weights

assigned according to $w^{-1} = [\sigma^2(F) + 0.000473F^2]$. Model refined by least squares on *F* in two blocks (fluorenyl ligand and carbacobaltaborane, 121 and 145 parameters respectively) to convergence; $R = 0.0793$, $wR = 0.0605$, $S = 1.16$ (relatively high residuals attributed to crystal quality); maximum shift/e.s.d. in final cycle < 0.06; maximum and minimum residues in final ΔF synthesis 0.86 and -1.36 e Å⁻³ respectively; scattering factors for C, H and B inlaid in *SHELX76*. Those for Co from *International Tables for X-ray Crystallography* (1974, Vol. IV); figures drawn using *EASYORTEP* (Mallinson & Muir, 1985); molecular geometry calculations *via CALC* (Gould & Taylor, 1986).

Discussion. Table 1 lists coordinates of refined non-H atoms and equivalent isotropic thermal parameters,* and Table 2 details internuclear distances and selected interbond angles. Fig. 1 shows a perspective view of a single molecule and demonstrates the atomic numbering scheme adopted.

The study confirms that the title compound (1), which was produced in yields too low for spectroscopic analysis, is 3-(η^5 -C₁₃H₉)-3,1,2-*closo*-CoC₂B₉H₁₁. To the best of our knowledge (1), which has been synthesized (albeit in low yield) by an analogous route to that which has previously afforded 3-(η^5 -C₅H₅)-3,1,2-*closo*-CoC₂B₉H₁₁ (2) (Jones & Hawthorne, 1973) and 3-(η^5 -C₉H₇)-3,1,2-*closo*-CoC₂B₉H₁₁ (3) (Smith & Welch, 1986), is the first reported fluorenyl carbametallaborane. Moreover, it is one of relatively few fluorenyl transition-metal compounds to have been structurally characterized; other examples include (η^5 -C₁₃H₉)(η^3 -C₁₃H₉)ZrCl₂ (4) (Kowala & Wunderlich, 1976) and (η^5 -C₁₃H₉)Cr(CO)₂(NO) (5) (Atwood, Shakir, Malito, Herberhold, Kremnitz, Bernhagen & Alt, 1979).

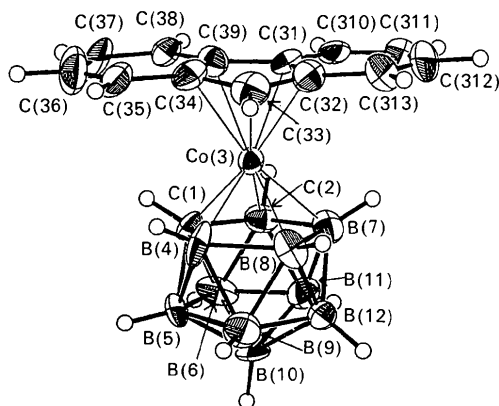
Compound (1) crystallizes with no important intermolecular contacts. The lengths of the Co-cage atom connectivities in (1) compare well with those of the equivalent connectivities in (2) and (3) (Smith & Welch, 1986). The metal-bonded C₂B₃ face is, as usual, folded into an envelope conformation about B(4)···B(7), with fold angles (Mingos, Forsyth & Welch, 1978; Smith & Welch, 1986) $\theta^p = 2.69$ and $\varphi^p = 1.37^\circ$. The slip parameter Δp that defines any lateral movement of the metal atom across the polyhedral face is zero to within experimental error.

The fluorenyl ligand in (1) is η^5 bonded to cobalt (η^6 -fluorenyl bonding is known; Johnson & Triechel,

* Lists of structure factors, H-atom positions, additional interbond angles and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54570 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference MU0270]

Table 1. Fractional coordinates and equivalent isotropic thermal parameters (\AA^2)
$$U_{eq} = (\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j) / 3.$$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Co(3)	0.32496 (14)	0.07999 (9)	1.10255 (8)	0.0281 (5)
C(1)	0.2923 (9)	0.0570 (6)	1.2277 (6)	0.030 (6)
B(4)	0.2404 (14)	0.1767 (11)	1.1933 (10)	0.049 (9)
C(2)	0.4649 (12)	0.0293 (7)	1.1976 (6)	0.040 (7)
B(8)	0.4007 (14)	0.2266 (9)	1.1367 (7)	0.041 (8)
B(7)	0.5410 (13)	0.1253 (10)	1.1362 (7)	0.042 (8)
B(11)	0.5957 (14)	0.1033 (10)	1.2473 (9)	0.045 (9)
B(12)	0.5527 (14)	0.2298 (9)	1.2102 (8)	0.037 (8)
B(6)	0.4378 (16)	0.0584 (9)	1.3046 (7)	0.044 (8)
B(5)	0.2956 (14)	0.1527 (10)	1.3036 (7)	0.044 (8)
B(10)	0.4906 (14)	0.1845 (10)	1.3132 (7)	0.042 (8)
B(9)	0.3709 (15)	0.2604 (10)	1.2495 (10)	0.054 (9)
C(32)	0.3426 (12)	0.0788 (8)	0.9664 (5)	0.041 (5)
C(31)	0.3627 (10)	-0.0272 (8)	0.9991 (6)	0.042 (7)
C(39)	0.2214 (11)	-0.0536 (7)	1.0438 (6)	0.038 (6)
C(33)	0.2047 (11)	0.1180 (8)	0.9947 (6)	0.051 (7)
C(38)	0.1737 (13)	-0.1422 (7)	1.0881 (6)	0.047 (6)
C(34)	0.1237 (11)	0.0330 (8)	1.0374 (7)	0.048 (7)
C(35)	-0.0250 (11)	0.0336 (8)	1.0774 (7)	0.052 (7)
C(36)	-0.0653 (12)	-0.0519 (10)	1.1200 (8)	0.070 (9)
C(37)	0.0299 (13)	-0.1385 (10)	1.1269 (7)	0.071 (9)
C(310)	0.5019 (10)	-0.0845 (10)	0.9858 (6)	0.053 (7)
C(313)	0.4634 (13)	0.1186 (9)	0.9136 (6)	0.060 (8)
C(312)	0.5872 (13)	0.0633 (10)	0.9002 (7)	0.064 (8)
C(311)	0.6130 (13)	-0.0367 (10)	0.9368 (7)	0.066 (8)

Fig. 1. Perspective view of 3-(η^5 -C₁₃H₅)-3,1,2-closo-CoC₂B₃H₁₁ (1) (50% thermal ellipsoids, except for H atoms which have an artificial radius of 0.1 Å for clarity).

1977) and the metal atom is substantially slipped ($\Delta^h = 0.095 \text{ \AA}$) across the C₅ ring towards C(33), resulting in a spread of Co—C_{fluorenyl} distances of 0.134 Å. We note that both smaller [compound (5), $\Delta^h = 0.011 \text{ \AA}$] and larger [compound (4), $\Delta^h = 0.244 \text{ \AA}$] slip distortions are observed for formally η^5 -fluorenyl ligands [cf. $\Delta^h = 0.474 \text{ \AA}$ for a formally η^3 -fluorenyl ligand in compound (4)]. The C₅ ring in (1) is also folded towards Co(3) in an envelope conformation, by 6.87° across the C(32)⋯C(34) vector. However, because the best (least-squares) plane through the C₅ ring is not parallel with that through the B(5)—B(6)—B(11)—B(12)—B(9) pentagon (dihedral angle 2.16°), it is not possible to quantify accurately θ^h and φ^h as it was for (2) and (3)

Table 2. Interatomic distances (Å) and selected inter-bond angles (°)

Co(3)—C(1)	1.967 (8)	B(11)—B(12)	1.785 (18)
Co(3)—B(4)	2.021 (14)	B(11)—B(6)	1.741 (18)
Co(3)—C(2)	2.018 (10)	B(11)—B(10)	1.730 (18)
Co(3)—B(8)	2.090 (12)	B(12)—B(10)	1.775 (17)
Co(3)—B(7)	2.049 (12)	B(12)—B(9)	1.749 (18)
Co(3)—C(32)	2.098 (10)	B(6)—B(5)	1.750 (17)
Co(3)—C(31)	2.142 (10)	B(6)—B(10)	1.713 (17)
Co(3)—C(39)	2.160 (9)	B(5)—B(10)	1.764 (17)
Co(3)—C(33)	2.026 (10)	B(5)—B(9)	1.761 (18)
Co(3)—C(34)	2.118 (10)	B(10)—B(9)	1.743 (18)
C(1)—B(4)	1.709 (16)	C(32)—C(31)	1.481 (14)
C(1)—C(2)	1.621 (13)	C(32)—C(33)	1.382 (14)
C(1)—B(6)	1.738 (15)	C(32)—C(313)	1.430 (15)
C(1)—B(5)	1.708 (15)	C(31)—C(39)	1.456 (13)
B(4)—B(8)	1.775 (18)	C(31)—C(310)	1.444 (14)
B(4)—B(5)	1.790 (18)	C(39)—C(38)	1.405 (14)
B(4)—B(9)	1.801 (19)	C(39)—C(34)	1.420 (14)
C(2)—B(7)	1.703 (16)	C(33)—C(34)	1.471 (14)
C(2)—B(11)	1.682 (16)	C(38)—C(37)	1.395 (15)
C(2)—B(6)	1.704 (16)	C(34)—C(35)	1.440 (15)
B(8)—B(7)	1.803 (17)	C(35)—C(36)	1.340 (16)
B(8)—B(12)	1.747 (17)	C(36)—C(37)	1.408 (17)
B(8)—B(9)	1.808 (18)	C(310)—C(311)	1.379 (16)
B(7)—B(11)	1.796 (18)	C(313)—C(312)	1.318 (16)
B(7)—B(12)	1.777 (17)	C(312)—C(311)	1.439 (16)
C(1)—Co(3)—B(4)	50.7 (5)	B(11)—B(12)—B(10)	58.1 (7)
C(1)—Co(3)—C(2)	48.0 (4)	B(10)—B(12)—B(9)	59.3 (7)
B(4)—Co(3)—B(8)	51.1 (5)	C(1)—B(6)—C(2)	56.2 (6)
C(2)—Co(3)—B(7)	49.5 (4)	C(1)—B(6)—B(5)	58.6 (6)
B(8)—Co(3)—B(7)	51.7 (5)	C(2)—B(6)—B(11)	58.4 (7)
C(32)—Co(3)—C(31)	40.9 (4)	B(11)—B(6)—B(10)	60.1 (7)
C(32)—Co(3)—C(33)	39.1 (4)	B(5)—B(6)—B(10)	61.2 (7)
C(31)—Co(3)—C(39)	39.6 (4)	C(1)—B(5)—B(4)	58.4 (6)
C(39)—Co(3)—C(34)	38.7 (4)	C(1)—B(5)—B(6)	60.3 (6)
C(33)—Co(3)—C(34)	41.5 (4)	B(4)—B(5)—B(9)	61.0 (7)
Co(3)—C(1)—B(4)	66.3 (5)	B(6)—B(5)—B(10)	58.3 (7)
Co(3)—C(1)—C(2)	67.6 (5)	B(10)—B(5)—B(9)	59.3 (7)
B(4)—C(1)—B(5)	63.2 (7)	B(11)—B(10)—B(12)	61.2 (7)
C(2)—C(1)—B(6)	60.9 (6)	B(11)—B(10)—B(6)	60.8 (7)
B(6)—C(1)—B(5)	61.1 (6)	B(12)—B(10)—B(9)	59.6 (7)
Co(3)—B(4)—C(1)	63.0 (5)	B(6)—B(10)—B(5)	60.4 (7)
Co(3)—B(4)—B(8)	66.4 (6)	B(5)—B(10)—B(9)	60.3 (7)
C(1)—B(4)—B(5)	58.4 (6)	B(4)—B(9)—B(8)	58.9 (7)
B(8)—B(4)—B(9)	60.7 (7)	B(4)—B(9)—B(5)	60.3 (7)
B(5)—B(4)—B(9)	58.7 (7)	B(8)—B(9)—B(12)	58.8 (7)
Co(3)—C(2)—C(1)	64.4 (5)	B(12)—B(9)—B(10)	61.1 (7)
Co(3)—C(2)—B(7)	66.2 (5)	B(5)—B(9)—B(10)	60.4 (7)
C(1)—C(2)—B(6)	63.0 (6)	C(31)—C(32)—C(33)	110.0 (8)
B(7)—C(2)—B(11)	64.1 (7)	C(31)—C(32)—C(313)	116.3 (9)
B(11)—C(2)—B(6)	61.9 (7)	C(33)—C(32)—C(313)	133.7 (9)
Co(3)—B(8)—B(4)	62.4 (6)	C(32)—C(31)—C(39)	106.2 (8)
Co(3)—B(8)—B(7)	63.0 (5)	C(32)—C(31)—C(310)	122.3 (9)
B(4)—B(8)—B(9)	60.3 (7)	C(39)—C(31)—C(310)	131.4 (9)
B(7)—B(8)—B(12)	60.0 (7)	C(31)—C(39)—C(38)	132.5 (9)
B(12)—B(8)—B(9)	58.9 (7)	C(31)—C(39)—C(34)	107.0 (8)
Co(3)—B(7)—C(2)	64.3 (5)	C(38)—C(39)—C(34)	120.5 (9)
Co(3)—B(7)—B(8)	65.3 (5)	C(32)—C(33)—C(34)	106.5 (9)
C(2)—B(7)—B(11)	57.4 (7)	C(39)—C(38)—C(37)	116.6 (9)
B(8)—B(7)—B(12)	58.4 (7)	C(39)—C(34)—C(33)	109.8 (9)
B(11)—B(7)—B(12)	59.9 (7)	C(39)—C(34)—C(35)	102.4 (9)
C(2)—B(11)—B(7)	58.5 (7)	C(33)—C(34)—C(35)	128.5 (9)
C(2)—B(11)—B(6)	59.7 (7)	C(34)—C(35)—C(36)	116.2 (10)
B(7)—B(11)—B(12)	59.5 (7)	C(35)—C(36)—C(37)	123.3 (11)
B(12)—B(11)—B(10)	60.6 (7)	C(38)—C(37)—C(36)	122.0 (11)
B(6)—B(11)—B(10)	59.1 (7)	C(31)—C(310)—C(311)	116.1 (9)
B(8)—B(12)—B(7)	61.5 (7)	C(32)—C(313)—C(312)	119.1 (10)
B(8)—B(12)—B(9)	62.3 (7)	C(313)—C(312)—C(311)	124.3 (11)
B(7)—B(12)—B(11)	60.6 (7)	C(310)—C(311)—C(312)	120.8 (10)

(Smith & Welch, 1986). Indeed, the fluorenyl ligand as a whole is tilted such that C(37) is *ca* 0.25 Å closer to the B₅ plane than is C(313).

As previously stated, an important feature of the structure of (1) is the conformation of the fluorenyl ligand relative to the metal-bonded C₂B₃ face. A previous study of (3) has shown that the preferred conformation of the indenyl ligand is such that its six-membered ring lies *cisoid* with respect to the cage C atoms. In this (staggered) conformation (staggered conformations are always observed in compounds of the [*nido*-C₂B₉H₁₁]²⁻ ligand since H atoms *exo* to the metal-bonded cage atoms are inclined towards the metal) the relatively weak metal-C_{ring junction} bonding can best be compensated by strong metal-B bonding, the frontier molecular orbitals of the carborane ligand having been shown to be localized on the B atoms of the C₂B₃ face (Mingos, Forsyth & Welch, 1978). Extending this argument to (1), in which there are two pairs of ring-junction C atoms in the carbocyclic ligand, of the three possible staggered conformations (I-III, Scheme 1) (I) is clearly expected to be preferred and is, indeed, the conformation observed in (1) (Fig. 2). The electronic preference for (I) has been confirmed by the results of a

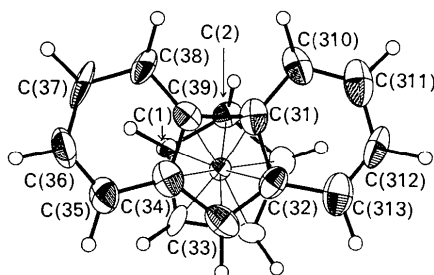


Fig. 2. Plan view of (1) illustrating the orientation of the fluorenyl ligand to the carbaborane ligand. For clarity only the metal-bonded C₂B₃ face of the carbaborane ligand is shown, and B atoms are drawn as plain ellipsoids.

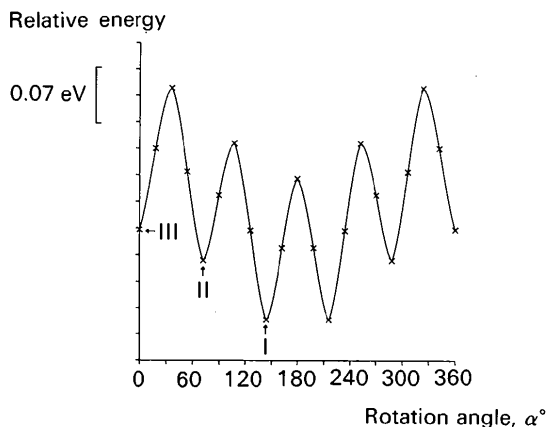
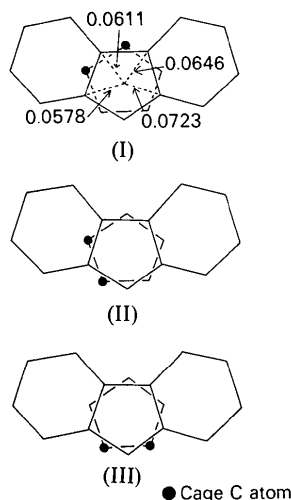


Fig. 3. Plot of relative energy (eV) versus α , the angle of rotation of the fluorenyl ligand about the Co(3)···B(10) axis, for an idealized model of (1) as given by extended Huckel molecular orbital calculations.

series of extended Huckel molecular orbital calculations (Howell, Rossi, Wallace, Haraki & Hoffmann, 1977) performed on idealized models of (1). Fig. 3 plots the sum of $1e^-$ energy as a function of α , the angle of rotation of the fluorenyl ligand about the Co(3)···B(10) axis. $\alpha = 0^\circ$ corresponds to (III). Local minima occur at $\alpha = 0, 72$ and 144° (staggered conformations) and local maxima at $\alpha = 36, 108$ and 180° (eclipsed conformations). Note that all staggered forms are more stable than all eclipsed forms, the best eclipsed form being that in which C(1)—C(2) is eclipsed by C(39)—C(31) corresponding to both pairs of junction C atoms lying *trans* to B atoms. The global minimum, however, ($\alpha = 144^\circ$) corresponds to the conformation of the structure of (1) determined crystallographically.



In conformation (I) the ring-junction atoms C(34) and C(39) are *trans* to two B atoms, whereas C(31) and C(32) are *trans* to one B and one cage C atom. Since, as outlined above, metal-boron bonding is expected to be somewhat stronger than metal-cage carbon bonding, we would expect weaker interactions between Co(3) and C(34,39) than between Co(3) and C(31,32). This expectation is in agreement with the measured distances, and although the differences involved [$\Delta_{\text{Co}(3)-\text{C}(31)/\text{Co}(3)-\text{C}(39)} = 0.018$ (13), $\Delta_{\text{Co}(3)-\text{C}(32)/\text{Co}(3)-\text{C}(34)} = 0.020$ (14) Å] are not statistically significant, they are nevertheless consistent with the calculated atom-atom overlap populations shown in (I).

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Metal–Betaine Interactions. XI.* Structure of *catena*-[μ -Dichloro-(triethylammonioacetato)cadmium(II)]

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Abstract. A new cadmium(II) complex of triethylammonioacetate [(C₂H₅)₃N⁺CH₂COO⁻, designated Et₃BET] has been prepared and characterized. [Cd{(C₂H₅)₃NCH₂COO}{ μ -Cl)}₂]_n, $M_r = 342.55$, monoclinic, $C2/c$, $a = 18.097$ (4), $b = 9.714$ (2), $c = 13.845$ (1) Å, $\beta = 92.46$ (1)°, $U = 2431.1$ (7) Å³, $Z = 8$, $D_m = 1.862$, $D_x = 1.871$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 22.1$ cm⁻¹, $F(000) = 1360$, $T = 298$ (1) K, $R = 0.024$ for 2875 unique Mo $K\alpha$ observed data. Each Cd^{II} atom is in a distorted octahedral environment, surrounded by an uncommon symmetrical bidentate chelating carboxylato group and two pairs of bridging chloro ligands. Successive octahedra related by the c -glide share edges to generate a one-dimensional polymeric structure.

Introduction. Although the carboxylate group exhibits a number of coordination modes in the extensively studied crystal structures of its metal complexes, the symmetrical bidentate chelating mode is rarely observed. This has been correlated to the relief of steric constraints induced by the coordina-

tion mode resulting in the more appreciable unsymmetrical form of chelation (Oldham, 1987).

In our ongoing systematic investigation on the ligating properties of betaines, considered as neutral structural analogues of carboxylato ligands, we have found that the prototype betaine, Me₃N⁺CH₂COO⁻ (abbreviated as BET), and its derivatives exhibit a rich variety of bonding modes in their metal complexes (Huang, Lü, Chen & Mak, 1991), including the common bidentate *syn-syn* and *syn-anti* bridging modes and the tridentate bridging mode. Two very interesting variations have also been found, with pyridine betaine (C₅H₅N⁺CH₂COO⁻, pyBET) acting as an unusual *syn*-skew bridging ligand in [Cd₃(pyBET)₄Cl₆] (Mak & Chen, 1991), and BET acting as an uncommon skew-skew bridging ligand in [Mn(BET)₃]_n.*n*MnCl₄ (Chen & Mak, 1991a). Owing to the fact that the O—C—O bond angle in betaine ligands is usually larger in comparison to that of the common carboxylates, the bidentate chelating mode is rarely observed in metal complexes of betaines. Even for zinc complexes, in which most carboxylates behave as bidentate chelates, the betaines still function as unidentate ligands in [Zn(BET)₂Cl₂].H₂O and two other related zinc(II) complexes (Chen & Mak, 1991b). Hitherto the only example of an unsymmetrical chelating betaine

* For Part X on silver(I) complexes of triethylammonioacetate, see Huang, Lü, Chen & Mak (1991).

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