Crystal and Molecular Structure of 2-(η-cyclopentadienyl)-2-cobalta-*nido*-pentaborane(9)

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Summary An *X*-ray structural determination of the title compound $(\eta\text{-}C_5H_5)Co(B_4H_8)$, revealed that the metalloborane fragment has a square-pyramidal structure in which the cobalt occupies a basal position.

The recent interest in metalloborane chemistry[1] has been due in part to the recognition of the versatility of boron cage systems for forming a variety of structurally novel complexes. Of special interest has been the recent synthesis[2,3] of several complexes employing the borane fragment, B_4H_8 (isoelectronic with cyclobutadiene, C_4H_4) as a ligand. In particular, two isomeric cobaltaboranes having the formula $(B_4H_8)Co(C_5H_5)$ were synthesized[2] by the reaction of NaB_5H_8 with an excess of $CoCl_2$ and NaC_5H_5 in tetrahydrofuran. Based on the spectroscopic data, one of these complexes was assigned a structure with the cobalt occupying a basal position in a square-based pyramid formed by the cobalt and the four boron atoms. We now report the *X*-ray structural determination of this complex which confirms the proposed structure.

Table. Selected interatomic distances and angles

Distances/Å			
Co–B(1)	2·007(10)	Co–H(1)	1·429(47)
Co–B(2)	2·135(8)	B(2)–H(1)	1·434(54)
B(1)–B(3)	1·660(16)	B(2)–H(2)	1·300(64)
B(1)–B(2)	1·685(11)	B(3)–H2)	1·092(60)
B(2)–B(3)	1·757(2)		
Angles/degrees			
B(2)–Co–B(2′)	74·40(51)	H(1)–Co–H(1′)	77·87(3·65)
B(2)–B3–B(2′)	94·55(73)	Co–B(1)–B(3)	103·71(68)
Co–B(2)–B(3)	95·47(47)		

The complex crystallizes as red plates in the orthohombic space group *Pnma*, $a = 12{\cdot}014(21)$, $b = 9{\cdot}635(17)$, $c = 7{\cdot}588(14)$, $Z = 4$. Diffraction data to $2\theta = 55°$ (Mo-K_α radiation) were collected on a Picker FACS I diffractometer and the structure was solved by conventional Patterson, Fourier and full-matrix least-squares refinement techniques, using 738 observed reflections to a conventional R of 0·053.

The molecular structure is shown in the Figure and consists of a cobalt atom sandwiched between C_5H_5 and B_4H_8 units, the borane fragment being formally trihapto to the cobalt. A similar tridentate bonding of a borane fragment has previously been found[4] in $Mn(CO)_3[B_9H_{12}$(tetrahydrofuran)]. The metalloborane fragment can best be described as an analogue of pentaborane(9) in which one basal BH group has been replaced by a $Co(C_5H_5)$ unit. A selected list of bond distances and angles are in the Table.

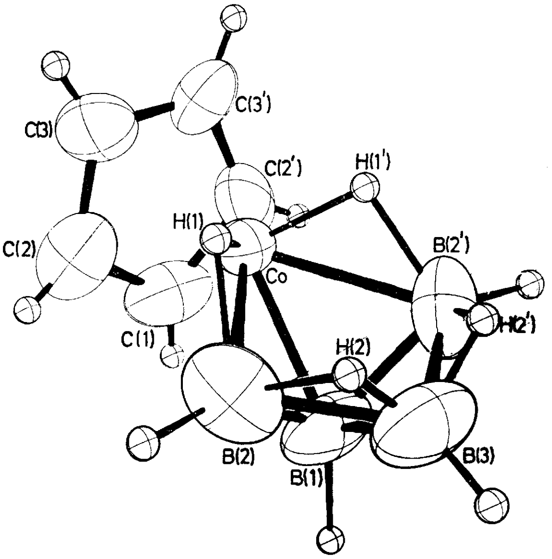

Figure. The molecular structure of 2-(η-cyclopentadienyl)-2-cobalta-*nido*-pentaborane(9).

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