

## Molecular Structures of Methyl(cyclopentadienyl)beryllium and Cyclopentadienylberyllium Chloride by Gas-phase Electron Diffraction

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**Summary** The molecular structures of  $\text{MeBe}(\text{C}_5\text{H}_5)$  and  $(\text{C}_5\text{H}_5)\text{BeCl}$  have been determined by gas-phase electron diffraction.

$\text{CpBeCl}$  is significantly larger than in monomeric beryllium dichloride,<sup>4</sup>  $1.75 \pm 0.02 \text{ \AA}$ .

METHYL(CYCLOPENTADIENYL)BERYLLIUM,  $\text{MeBeCp}$ , and cyclopentadienylberyllium chloride,  $\text{CpBeCl}$ , have been synthesized.<sup>1</sup> Both compounds are monomeric in hydrocarbon solution.<sup>1</sup> We have determined the molecular structures of these compounds by gas-phase electron diffraction. The electron diffraction data show both molecules to be of the "half sandwich" type with approximately  $C_{5v}$  symmetry. The main molecular parameters (estimated standard deviations in parentheses) are given in the Table.

The Be-C(Cp) bond distances are similar to that found [ $1.907(5) \text{ \AA}$ ] between Be and the carbon atoms in the nearest cyclopentadienyl ring in dicyclopentadienylberyllium.<sup>2</sup> The C-C bond distances in the cyclopentadienyl rings in the three compounds are indistinguishable.

The Be-C(Me) bond distance in  $\text{MeBeCp}$  is not significantly different from the Be-C bond distance in dimethylberyllium,<sup>3</sup>  $1.698(5) \text{ \AA}$ , but the Be-Cl bond distance in

TABLE

		$\text{CpBeMe}/\text{\AA}$	$\text{CpBeCl}/\text{\AA}$
C-C	.. ..	1.420(2)	1.424(2)
Be-C(Cp)	.. ..	1.923(3)	1.915(6)
$h^a$	.. ..	1.497(3)	1.484(7)
Be-C(Me)	.. ..	1.706(7)	—
Be-Cl	.. ..	—	1.839(7)

<sup>a</sup>  $h$  is the perpendicular distance from Be to the Cp ring.

It seems reasonable to assume that there is less dative Be-Cl  $\pi$ -bonding in  $\text{CpBeCl}$  than in  $\text{BeCl}_2$ . One possible explanation for this, and for the monomeric nature of the two compounds  $\text{MeBeCp}$  and  $\text{CpBeCl}$ , is that the Be atom, being bonded to the five-electron ligand Cp and having formed  $\sigma$ -bonds to Cl or C(Me), is already surrounded by an octet of electrons.

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<sup>1</sup> D. A. Drew and G. L. Morgan, unpublished results.

<sup>2</sup> A. Haaland, *Acta Chem. Scand.*, 1968, **22**, 3030.

<sup>3</sup> A. Almenningen, A. Haaland, and G. L. Morgan, *Acta Chem. Scand.*, 1969, **23**, 2921.

<sup>4</sup> P. A. Akishin and V. P. Spiridinov, *Kristallografiya*, 1957, **2**, 475.