The Nature of the Scandium–Carbon Bond. The Crystal and Molecular Structure of $[(C_5H_5)_2ScCl]_2$

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Summary The first view of the stereochemistry of an organoscandium complex is provided by the *X*-ray structure analysis of the dicyclopentadienylscandium chloride dimer.

TRICYCLOPENTADIENYLSCANDIUM,[1] triphenyl- and triphenylethynyl-scandium,[2] and dicyclopentadienylscandium chloride and derivatives[3] have been prepared, but no structural data have been presented. We report the *X*-ray crystallographic structure of $[(C_5H_5)_2ScCl]_2$, and a study of the nature of the scandium–carbon bond.

Yellow-green rod shaped crystals of dicyclopentadienylscandium chloride, prepared by the method of Coutts and Wailes,[3] were grown by sublimation.

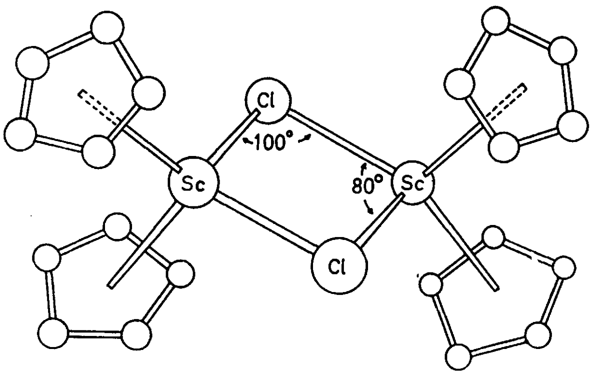
Crystal data: monoclinic, space group $P2_1/c$, $a = 13{\cdot}54(1)$, $b = 16{\cdot}00(1)$, $c = 13{\cdot}40(1)$Å, $\beta = 93{\cdot}97(5)°$, and $D_c = 1{\cdot}44$ g cm^{-3}. Cu-K_α data were collected up to $2\theta = 120°$ on an Enraf-Nonius CAD-4 automated diffractometer. Absorption corrections were not made. A total of 1680 independent observed reflections were measured and used in the structure determination.

The structure was solved by direct methods and refined by full-matrix anisotropic least-squares methods to a conventional R value of 8·1%. No attempt was made to locate the hydrogen atoms. There are six chlorine-bridged dimers in the unit cell, of which four lie in general positions and two in special positions ($\bar{1}$) in the space group $P2_1/c$. Thus the occurrence of one and one-half dimers in the asymmetric unit allows several independent determinations of each structural parameter. Those reported here are in all cases average values. The standard deviation in the bond lengths is 0·01 Å and in the bond angles, 0·5°.

TABLE

Comparison of metal–cyclopentadienyl carbon bond distances and metal ion radii

Compound	M–C Distance (Å)	M^{n+} Radius (Å)	$\lvert Sc^{3+}-M^{n+}\rvert$	$\lvert(Sc–C) - (M–C)\rvert$	Ref.
$[(C_5H_5)_2ScCl]_2$	2·48	0·68	—	—	
$(C_5H_5)_2Ti(C_6H_5)_2$	2·31	0·60	0·08	0·17	4
$[C_5H_5TiCl_2]_2O$	2·35	0·60	0·08	0·13	5
$(C_5H_5)_3Sm$	2·78	0·96	0·28	0·30	6
$(C_9H_7)_3Sm$	2·75	0·96	0·28	0·27	7



The Figure shows that in the dimeric molecule the cyclopentadienyl rings exhibit penta-*hapto*-co-ordination, with the scandium atom 2·17 Å from the plane of the rings. Since this is the first organoscandium structure to be determined crystallographically, the average Sc–Sc distance (3·91 Å), Sc–Cl distance (2·57 Å), and Sc–C distance (2·48 Å) have no real basis for comparison. However, as seen in the Table, the relation of the metal-carbon bond distances and metal ion radii in cyclopentadienyl compounds of titanium and samarium shows the scandium–carbon bond distance to be reasonable.

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