Crystal Structure of Di-μ-chloro-bis[di-η-cyclopentadienylscandium(III)]

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The crystal and molecular structure of the title compound have been determined from *X*-ray diffractometer data by direct methods. Crystals are monoclinic rods, space group $P2_1/c$, with $Z = 6$ in a cell with $a = 13{\cdot}54(1)$, $b = 16{\cdot}00(1)$, $c = 13{\cdot}40(1)$ Å, $\beta = 93{\cdot}97(5)°$. The structure was refined by least-squares techniques to R 0·072 for 1680 observed reflections. The molecules exist as chlorine-bridged dimers, mean Sc–Cl 2·575 Å. The cyclopentadienyl groups are bonded in a penta-*hapto*-fashion, mean Sc–C 2·46 Å.

THE organometallic chemistry of the lanthanide and actinide elements has recently become the subject of much endeavour,[1,2] in particular the nature of the metal–carbon bond. For the well-known lanthanide cyclopentadienides the covalency of the organometallic bonds has been estimated[3] to be $<2{\cdot}5\%$. However, the crystal structure[4] of $Sm(C_5H_5)_3$ shows a definite preferred orientation of cyclopentadienyl groups, and there is n.m.r. evidence for a covalent bonding mode in the related tetrahydrofuran adduct of tri-indenylsamarium.[5] Since the scandium(III) ion is substantially smaller than the related lanthanide ions, many of the effects noted in rare-earth organometallic chemistry may well be magnified in the scandium compounds. We have described the structure of $Sc(C_5H_5)_3$ and presented a preliminary account of the structure of $[Sc(C_5H_5)_2Cl]_2$;[6,7] we now report the final refinement and the details of the structure analysis of the latter.

EXPERIMENTAL

Yellow-green rod shaped crystals were prepared by the method of ref. 8, and diffraction-quality crystals were grown by slow sublimation.

Crystal Data.—$[Sc(C_5H_5)_2Cl]_2$, $M = 420{\cdot}8$, Monoclinic, $a = 13{\cdot}54(1)$, $b = 16{\cdot}00(1)$, $c = 13{\cdot}40(1)$ Å, $\beta = 93{\cdot}97(5)°$, $U = 2896$ Å^3, $D_c = 1{\cdot}44$ g cm^{-3}, $Z = 6$, $D_m = 1{\cdot}45$ g cm^{-3}, $F(000) = 1296$. Space group $P2_1/c$ from systematic absences. Cu-K_α radiation, $\lambda = 1{\cdot}542$ Å, μ(Cu-K_α) = 85·5 cm^{-1}. Crystal dimensions 0·17 × 0·17 × 0·42 mm.

Crystallographic Measurements.—Preliminary unit-cell

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parameters were determined by precession (Cu-K_α) photographs. Final values of the lattice parameters were obtained by a least-squares refinement of the angular settings of 12 accurately centred reflections. Data were obtained by use of an Enraf–Nonius CAD 4 diffractometer with Ni-filtered copper radiation. The crystal was aligned on the diffractometer such that no symmetry axis was coincident with the ϕ axis of the diffractometer.

TABLE 1

Final fractional co-ordinates and thermal parameters ($\times 10^4$),* with estimated standard deviations in parentheses

Atom	x/a	y/b	z/c
Sc(1)	0·0520(1)	0·7352(1)	0·3488(2)
Sc(2)	0·2511(1)	0·8969(1)	0·4438(2)
Sc(3)	0·4134(1)	0·4134(1)	0·4382(2)
Cl(1)	0·2030(2)	0·8118(2)	0·2842(2)
Cl(2)	0·0963(2)	0·8267(2)	0·5043(2)
Cl(3)	0·4202(2)	0·5729(2)	0·4594(2)
C(1)	−0·0336(9)	0·8097(14)	0·2066(13)
C(2)	−0·0568(11)	0·8507(8)	0·2944(15)
C(3)	−0·1151(10)	0·7983(10)	0·3495(11)
C(4)	−0·1271(7)	0·7291(8)	0·2983(11)
C(5)	−0·0822(9)	0·7322(10)	0·2173(11)
C(6)	0·0206(10)	0·5828(7)	0·3429(13)
C(7)	0·0333(10)	0·6038(8)	0·4416(12)
C(8)	0·1306(14)	0·6274(8)	0·4613(13)
C(9)	0·1750(9)	0·6237(8)	0·3735(16)
C(10)	0·1076(15)	0·5969(9)	0·2980(11)
C(11)	0·3347(9)	0·7838(9)	0·5415(13)
C(12)	0·3852(10)	0·7913(8)	0·4572(11)
C(13)	0·4298(9)	0·8685(8)	0·4602(10)
C(14)	0·4092(8)	0·9076(7)	0·5469(9)
C(15)	0·3509(10)	0·8558(10)	0·5985(9)
C(16)	0·1363(11)	1·0009(10)	0·3770(22)
C(17)	0·1630(16)	1·0269(9)	0·4700(19)
C(18)	0·2560(15)	1·0480(8)	0·4834(13)
C(19)	0·2919(10)	1·0389(7)	0·3899(13)
C(20)	0·2165(15)	1·0149(8)	0·3302(11)
C(21)	0·3736(11)	0·3424(9)	0·2750(10)
C(22)	0·3728(10)	0·4270(11)	0·2576(9)
C(23)	0·4709(13)	0·4534(9)	0·2754(10)
C(24)	0·5252(10)	0·3849(10)	0·3055(10)
C(25)	0·4669(14)	0·3190(9)	0·3074(12)
C(26)	0·2865(22)	0·3125(15)	0·4771(17)
C(27)	0·3537(13)	0·3076(11)	0·5526(16)
C(28)	0·3554(11)	0·3784(15)	0·6016(11)
C(29)	0·2863(18)	0·4303(9)	0·5582(19)
C(30)	0·2475(9)	0·3851(18)	0·4785(17)
H(1) †	0·0038	0·8420	0·1621
H(2)	−0·0447	0·9059	0·3211
H(3)	−0·1374	0·8101	0·4166
H(4)	−0·1640	0·6805	0·3156
H(5)	−0·0742	0·6910	0·1644
H(6)	−0·0372	0·5608	0·3094
H(7)	−0·0190	0·5981	0·4903
H(8)	0·1641	0·6468	0·5227
H(9)	0·2459	0·6374	0·3661
H(10)	0·1173	0·5906	0·2251
H(11)	0·2979	0·7342	0·5585
H(12)	0·3899	0·7466	0·4094
H(13)	0·4653	0·8929	0·4055
H(14)	0·4306	0·9616	0·5676
H(15)	0·3254	0·8647	0·6649
H(16)	0·0734	0·9846	0·3550
H(17)	0·1132	1·0286	0·5258
H(18)	0·2949	1·0637	0·5476
H(19)	0·3600	1·0506	0·3764
H(20)	0·2236	1·0067	0·2548
H(21)	0·3142	0·3071	0·2706
H(22)	0·3210	0·4662	0·2329
H(23)	0·4998	0·5115	0·2713
H(24)	0·5997	0·3864	0·3148
H(25)	0·4934	0·2641	0·3286
H(26)	0·2599	0·2782	0·4171
H(27)	0·3938	0·2545	0·5581
H(28)	0·4019	0·3849	0·6608
H(29)	0·2776	0·4868	0·5907
H(30)	0·1942	0·4182	0·4415

TABLE 1 (*Continued*)

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Sc(1)	35(1)	30(1)	67(2)	2(1)	−19(1)	−5(1)
Sc(2)	41(1)	30(1)	58(2)	2(1)	−14(1)	−4(1)
Sc(3)	36(1)	35(1)	55(2)	−2(1)	−21(1)	4(1)
Cl(1)	47(1)	49(1)	51(2)	−1(1)	−5(2)	−9(1)
Cl(2)	46(2)	47(1)	59(2)	−3(1)	−3(2)	−6(1)
Cl(3)	35(1)	37(1)	69(2)	5(1)	−28(1)	4(1)
C(1)	43(9)	176(18)	113(16)	18(10)	−15(9)	104(13)
C(2)	93(13)	35(7)	193(21)	−4(7)	−83(13)	18(10)
C(3)	73(10)	72(9)	116(15)	32(8)	−35(9)	−40(9)
C(4)	24(7)	75(9)	110(14)	4(6)	−9(7)	7(9)
C(5)	59(10)	96(11)	84(14)	26(8)	−13(8)	−9(9)
C(6)	102(11)	22(6)	164(17)	−9(6)	−71(11)	−11(7)
C(7)	94(11)	55(8)	127(14)	−7(7)	12(10)	15(9)
C(8)	159(17)	38(7)	123(16)	3(8)	−79(12)	12(8)
C(9)	60(9)	52(8)	221(23)	15(7)	−44(12)	30(11)
C(11)	60(10)	65(9)	159(18)	−0(7)	−60(10)	49(10)
C(12)	77(10)	40(7)	135(15)	35(7)	−54(9)	−39(8)
C(13)	72(9)	67(8)	66(12)	3(7)	−16(8)	−10(7)
C(14)	61(8)	31(6)	84(12)	−21(6)	−26(7)	9(6)
C(15)	96(11)	89(10)	37(10)	26(8)	−17(8)	−2(8)
C(16)	66(11)	43(9)	419(42)	−5(9)	−84(18)	51(16)
C(17)	141(19)	33(8)	303(33)	9(10)	126(20)	14(12)
C(18)	191(19)	33(7)	107(16)	8(10)	−70(14)	−18(8)
C(19)	89(10)	29(6)	139(16)	11(6)	14(10)	13(8)
C(20)	226(21)	43(7)	83(13)	−10(11)	−100(14)	8(8)
C(21)	106(12)	73(9)	63(12)	−24(8)	−11(9)	−26(8)
C(22)	107(12)	108(11)	37(11)	54(10)	−37(9)	−1(8)
C(23)	151(15)	60(8)	65(12)	−13(9)	7(11)	−3(7)
C(24)	95(12)	91(11)	77(13)	33(9)	5(9)	−36(9)
C(25)	172(18)	52(8)	105(14)	38(10)	−32(11)	−19(8)
C(26)	249(32)	110(16)	148(25)	−129(18)	39(19)	−33(15)
C(27)	123(16)	68(11)	153(23)	51(11)	40(13)	51(11)
C(28)	76(12)	135(16)	86(14)	−31(11)	−20(10)	13(13)
C(29)	187(23)	38(7)	211(27)	−39(10)	139(19)	−18(11)
C(30)	38(8)	166(19)	177(24)	4(12)	−26(11)	98(17)

* Anisotropic thermal parameters defined by: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$. † Isotropic thermal parameters set at 4·0 Å^2 for all hydrogen atoms. Fractional co-ordinates not refined.

The diffracted intensities were collected by the ω—2θ scan technique with a take-off angle of 1·5°. The scan rate was variable and was determined by a fast (20° min^{-1}) prescan. Calculated speeds based on the net intensity gathered in the prescan ranged from 7 to 1° min^{-1}. Background counts were collected for 25% of the total scan time at each end of the scan range. For each intensity the scan range $= A + B \tan\theta$, where $A = 1{\cdot}0$ and $B = 0{\cdot}5$. Aperture settings were determined in a like manner with $A = 4$ mm and $B = 4$ mm. The crystal-to-source and crystal-to-detector distances were 21·6 and 20·8 cm, respectively. The lower- and upper-level discriminators of the pulse-height analyser were set to obtain a 95% window centred on the Cu-K_α peak. As a check on the stability of the diffractometer and the crystal, a standard peak was measured periodically during data collection. No significant fluctuation was noted.

The standard deviations of the intensities, $\sigma(I)$, were estimated from the formula: $\sigma = \{[C_N + (T_C/2T_B)^2 \,.\, (B_1 + B_2)] + (0{\cdot}03)^2[C_N + (T_C/2T_B)^2 \,.\, (B_1 + B_2)]^2\}^{\frac{1}{2}}$, where C_N is the counts collected during scan time T_C, and B_1 and B_2 are background intensities, each collected during background time T_B. One independent quadrant of data was measured out to $2\theta = 110°$. A total of 1680 reflections were considered observed, having $I > \sigma(I)$.

Intensities were corrected for Lorentz, polarization, and absorption effects.[9]

Fourier calculations were made with the ALFF[10] program. Full-matrix, least-squares refinement was carried out by the program ORFLS.[11] The function $\Sigma w(|F_o| - |F_c|)^2$ was minimized. No corrections were made for extinction or anomalous dispersion. Neutral atom scattering factors were taken from ref. 12. Final bond distances, angles, and errors were computed with the ORFFE[13] program. The crystal structure illustration was obtained with the program ORTEP.[14]

Structure Determination.—Partial structure solution was accomplished by direct methods, and an electron-density map phased on the scandium and chlorine atoms yielded the positions of the remaining non-hydrogen atoms. Several cycles of least-squares refinement with isotropic thermal parameters for all atoms gave R 0·13. Conversion to anisotropic temperature factors, the inclusion of hydrogen atoms in calculated positions, and additional cycles of refinement gave R 0·072 and R' 0·065 $\{R' = [\Sigma w(|F_o| - |F_c|)^2/\Sigma(F_o)^2]^{\frac{1}{2}}\}$. Unit weights were used at all stages of refinement, and no systematic variation of $w(|F_o| - |F_c|)^2$ *vs.* $|F_o|$ or $(\sin\theta)/\lambda$ was observed. The largest parameter shifts in the final cycle of refinement were $<0{\cdot}1\sigma$. A final difference-Fourier map showed no unaccounted electron density. Atomic and thermal parameters are given in Table 1. Observed and calculated structure factor amplitudes are listed in Supplementary Publications No. SUP 20832 (2 pp., 1 microfiche).*

TABLE 2

Molecular geometry

(*a*) Bond distances (Å)

Sc(1)–Sc(2)	3·886(3)	Sc(3)–Sc(3) *	3·922(3)
Sc(1)–Cl(1)	2·585(4)	Sc(1)–Cl(2)	2·583(4)
Sc(2)–Cl(1)	2·580(4)	Sc(2)–Cl(2)	2·559(4)
Sc(3)–Cl(3)	2·568(4)	Sc(3)–Cl(3) *	2·565(4)
Ring A		Ring B	
Sc(1)–C(1)	2·47(1)	Sc(1)–C(6)	2·48(1)
Sc(1)–C(2)	2·44(1)	Sc(1)–C(7)	2·46(1)
Sc(1)–C(3)	2·48(1)	Sc(1)–C(8)	2·48(1)
Sc(1)–C(4)	2·47(1)	Sc(1)–C(9)	2·45(1)
Sc(1)–C(5)	2·44(1)	Sc(1)–C(10)	2·45(1)
C(1)–C(2)	1·40(2)	C(6)–C(7)	1·36(2)
C(2)–C(3)	1·40(2)	C(7)–C(8)	1·38(2)
C(3)–C(4)	1·31(2)	C(8)–C(9)	1·36(2)
C(4)–C(5)	1·28(2)	C(9)–C(10)	1·38(2)
C(5)–C(1)	1·41(2)	C(10)–C(6)	1·38(2)
Ring C		Ring D	
Sc(2)–C(1)	2·46(1)	Sc(2)–C(16)	2·41(1)
Sc(2)–C(12)	2·48(1)	Sc(2)–C(17)	2·44(1)
Sc(2)–C(13)	2·46(1)	Sc(2)–C(18)	2·48(1)
Sc(2)–C(14)	2·47(1)	Sc(2)–C(19)	2·46(1)
Sc(2)–C(15)	2·48(1)	Sc(2)–C(20)	2·45(1)
C(11)–C(12)	1·37(2)	C(16)–C(17)	1·34(2)
C(12)–C(13)	1·37(2)	C(17)–C(18)	1·30(2)
C(13)–C(14)	1·36(2)	C(18)–C(19)	1·38(2)
C(14)–C(15)	1·37(2)	C(19)–C(20)	1·31(2)
C(15)–C(11)	1·39(2)	C(20)–C(16)	1·31(2)
Ring E		Ring F	
Sc(3)–C(21)	2·49(1)	Sc(3)–C(26)	2·44(1)
Sc(3)–C(22)	2·45(1)	Sc(3)–C(27)	2·46(1)
Sc(3)–C(23)	2·45(1)	Sc(3)–C(28)	2·44(1)
Sc(3)–C(24)	2·46(1)	Sc(3)–C(29)	2·45(1)
Sc(3)–C(25)	2·46(1)	Sc(3)–C(30)	2·39(1)
C(21)–C(22)	1·38(2)	C(26)–C(27)	1·32(2)
C(22)–C(23)	1·40(2)	C(27)–C(28)	1·31(2)
C(23)–C(24)	1·36(2)	C(28)–C(29)	1·35(2)
C(24)–C(25)	1·32(2)	C(29)–C(30)	1·37(2)
C(25)–C(21)	1·36(2)	C(30)–C(26)	1·28(2)

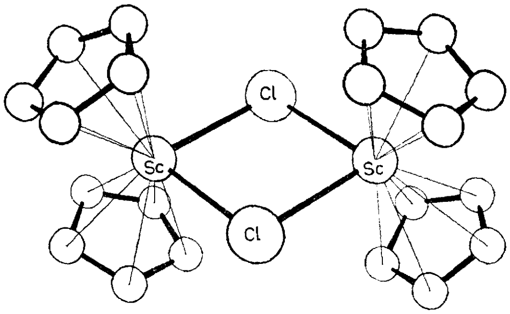
(*b*) Bond angles (°)

Sc(1)–Cl(1)–Sc(2)	97·6(1)	Cl(1)–Sc(1)–Cl(2)	81·8(1)
Sc(1)–Cl(2)–Sc(2)	98·2(1)	Cl(1)–Sc(3)–Cl(2)	82·3(1)
Sc(3)–Cl(3)–Sc(3) *	99·6(1)	Cl(3)–Sc(3)–Cl(3) *	80·4(1)
C(1)–C(2)–C(3)	109·3(13)	C(16)–C(17)–C(18)	113·8(17)
C(2)–C(3)–C(4)	106·5(14)	C(17)–C(18)–C(19)	104·2(14)
C(3)–C(4)–C(5)	111·3(14)	C(18)–C(19)–C(20)	106·0(14)
C(4)–C(5)–C(1)	111·8(15)	C(19)–C(20)–C(16)	113·2(17)
C(5)–C(1)–C(2)	101·1(12)	C(20)–C(16)–C(17)	102·3(13)
C(6)–C(7)–C(8)	107·9(14)	C(21)–C(22)–C(23)	105·8(11)
C(7)–C(8)–C(9)	107·2(13)	C(22)–C(23)–C(24)	107·1(13)
C(8)–C(9)–C(10)	109·8(14)	C(23)–C(24)–C(25)	109·7(14)
C(9)–C(10)–C(6)	105·8(14)	C(24)–C(25)–C(21)	108·6(14)
C(10)–C(6)–C(7)	109·3(12)	C(25)–C(21)–C(22)	108·7(13)
C(11)–C(12)–C(13)	107·3(12)	C(26)–C(27)–C(28)	108·8(15)
C(12)–C(13)–C(14)	108·8(13)	C(27)–C(28)–C(29)	109·1(14)
C(13)–C(14)–C(15)	108·2(11)	C(28)–C(29)–C(30)	103·3(14)
C(14)–C(15)–C(11)	107·4(12)	C(29)–C(30)–C(26)	110·7(15)
C(15)–C(11)–C(12)	108·3(12)	C(30)–C(26)–C(27)	108·1(16)

* Symmetry-related to position given in Table 1 by $(\bar{X}, \bar{Y}, \bar{Z})$ plus a unit translation in X, Y, and Z.

DESCRIPTION OF THE STRUCTURE AND DISCUSSION

In the unit cell there are six chlorine-bridged dimers, of which four lie in general positions and two reside on a centre of symmetry. Although there are two crystallographically different molecules, they do not



Molecular structure

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* For details see Notice to Authors No. 7 in *J.C.S. Dalton*, 1972, Index issue (items less than 10 pp. are supplied as full size copies).

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differ significantly in any respect and the configuration in each case is represented by the Figure. The cyclopentadienyl rings are bonded in a penta-*hapto*-fashion, with the scandium–carbon bond lengths (Table 2) ranging from 2·39 to 2·49, mean 2·46 Å. This value is shorter than that (2·49 Å) in $Sc(C_5H_5)_3$,[7] and could reflect either the greater ability of the chlorine atom to remove electron density from the scandium atom, or the more crowded environment about the scandium atom in $Sc(C_5H_5)_3$.

TABLE 3

Weighted least-squares planes

Plane	Equation
(*A*)	$-0{\cdot}7892X + 0{\cdot}3790Y - 0{\cdot}4832Z - 4{\cdot}0900 = 0$
(*B*)	$-0{\cdot}2495X + 0{\cdot}9472Y - 0{\cdot}2015Z - 7{\cdot}9333 = 0$
(*C*)	$-0{\cdot}7792X + 0{\cdot}4130Y - 0{\cdot}4715Z + 1{\cdot}4367 = 0$
(*D*)	$-0{\cdot}2428X + 0{\cdot}9465Y - 0{\cdot}2123Z - 13{\cdot}7549 = 0$
(*E*)	$0{\cdot}2436X - 0{\cdot}1898Y - 0{\cdot}9511Z + 3{\cdot}3665 = 0$
(*F*)	$0{\cdot}7211X + 0{\cdot}3712Y - 0{\cdot}5849Z - 0{\cdot}6561 = 0$

Deviation (Å) of atoms from planes

Plane (*A*): C(1) 0·00, C(2) −0·00, C(3) −0·00, C(4) 0·00, C(5) −0·00, Sc(1) −2·19

Plane (*B*): C(6) −0·02, C(7) 0·02, C(8) −0·01, C(9) −0·00, C(10) 0·01, Sc(1) 2·17

Plane (*C*): C(1) 0·01, C(12) −0·01, C(13) 0·01, C(14) 0·00, C(15) −0·01, Sc(2) 2·20

Plane (*D*): C(16) −0·03, C(17) 0·02, C(18) −0·01, C(19) −0·01, C(20) 0·03, Sc(2) −2·17

Plane (*E*): C(21) 0·02, C(22) −0·01, C(23) 0·00, C(24) 0·001, C(25) −0·02, Sc(3) −2·17

Plane (*F*): C(26) −0·01, C(27) −0·00, C(28) 0·01, C(29) −0·01, C(30) 0·01, Sc(3) 2·18

If the radius[6,15] of the scandium(III) ion is taken as 0·68 Å, a scandium–carbon bond length of 2·46—2·49 Å agrees very well with the value predicted on the basis of the two known organosamarium structures. The mean samarium–carbon bond distance is 2·78 Å in $(C_5H_5)_3Sm$[4] and 2·75 Å in $(C_9H_7)_3Sm$;[16] the generally accepted radius of the samarium(III) ion is 0·96 Å.[17]

The scandium–chlorine distance (2·575 Å) is quite long compared to that found in $ScCl_3(C_4H_8O)_3$ (2·413 Å).[18] However, the structure of the latter consists of discrete molecules in which each chlorine atom is bonded to only one scandium atom. The lengthening of a bond to a bridging halide ion is quite common: in $[MeAlCl_2]_2$ where there are both bridging and terminal chlorine atoms, the bond lengths are 2·25 and 2·05 Å, respectively.[19]

The scandium atom lies on the average 2·18 Å out of the plane of the cyclopentadienyl groups (Table 3). Within the rings bond distances and angles are as expected.[7]

The packing is typical of a molecular compound: the shortest nonbonded contacts are *ca.* 3·1 Å between carbon atoms on cyclopentadienyl groups bonded to the same scandium atom, and the closest intermolecular carbon–carbon approach is 3·82 Å.

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