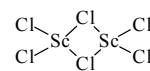
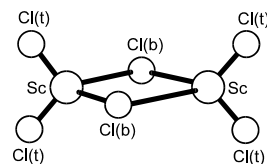


169 **Cl₆Sc₂**ED, DFT
calculations**Di- μ -chloro-bis[dichlorodiscandium(III)]**Di- μ -chloro-tetrachlorodiscandium**D_{2h}** assumed

r_g	\AA^a	θ_α	deg^a
Sc–Cl(t) ^b	2.275(10)	Cl(b)–Sc–Cl(b)	86(2)
Sc–Cl(b)	2.46(2)	Sc–Cl(b)–Sc	94(2)
		Cl(t)–Sc–Cl(t)	114.9 ^c

According to mass spectra recorded simultaneously with ED data, the gas consisted of ScCl₃ (92(2) mol%) and Sc₂Cl₆ (8(2) mol%) molecules.

The nozzle temperature was 900(10) K.



^a) Twice the estimated standard errors including a systematic error.

^b) Difference between the Sc–Cl bond length in the ScCl₃ molecule and the Sc–Cl(t) bond length was assumed at the value from BPW91/LanL2DZ calculations.

^c) Assumed at the value from BPW91/6-311G* calculations.

Haaland, A., Martinsen, K.-G., Shorokhov, D.J., Girichev, G.V., Sokolov, V.I.: J. Chem. Soc., Dalton Trans. (1998) 2787.