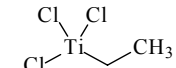
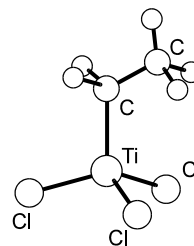


282	C₂H₅Cl₃Ti	Trichloroethyltitanium(IV)	C_s (staggered)																		
ED, DFT calculations		Ethyltitanium trichloride																			
	<table><tr><th><i>r</i>_a</th><th>Å ^{a)}</th></tr><tr><td>Ti–C</td><td>2.090(15)</td></tr><tr><td>C–C</td><td>1.526(11)</td></tr><tr><td>Ti–Cl</td><td>2.195(3)</td></tr><tr><td>C–H</td><td>1.104(10)</td></tr></table>	<i>r</i> _a	Å ^{a)}	Ti–C	2.090(15)	C–C	1.526(11)	Ti–Cl	2.195(3)	C–H	1.104(10)	<table><tr><th><i>θ</i>_α</th><th>deg ^{a)}</th></tr><tr><td>Ti–C–C</td><td>116.6(11)</td></tr><tr><td>Cl–Ti–C</td><td>104.6(4)</td></tr><tr><td>C–C–H(methyl)</td><td>109 ^{b)}</td></tr></table>	<i>θ</i> _α	deg ^{a)}	Ti–C–C	116.6(11)	Cl–Ti–C	104.6(4)	C–C–H(methyl)	109 ^{b)}	
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Two molecular models with staggered and eclipsed positions of CH₃ group with respect to the Ti–C bond described the experimental data equally well. According to DFT calculations [1], the eclipsed conformation is 1.7 kcal mol^{–1} higher than the staggered conformation, corresponding to a saddle point on the potential energy surface. Local C_{3v} symmetry was assumed for the TiCl₃ and CH₃ groups. Identical H–C–H angles were assumed in the CH₃ and CH₂ groups. The nozzle was at room temperature.

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

^{b)} Assumed.



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[1] Haaland, A., Scherer, W., Ruud, K., McGrady, G.S., Downs, A.J., Swang, O.: *J. Am. Chem. Soc.* **120** (1998) 3762.