

1777  
MW

**C<sub>4</sub>H<sub>9</sub>Cl**

***t*-Butyl chloride**  
2-Chloro-2-methylpropane

**C<sub>3v</sub>**  
ClC(CH<sub>3</sub>)<sub>3</sub>

[1]

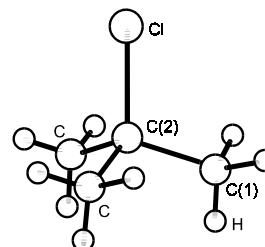
$r_s$	Å
C–Cl	1.8031(20)
C–C	1.530(2)

$\theta_s$	deg
C–C–C	110.9(2)
C–C–H	110.8 <sup>a)</sup>

[2]

$r_0$	Å
C–H	1.078(10)

Atom	$a_s$ [Å]	$b_s$ [Å]
C(1)	–0.9110	1.4554
C(2)	–0.4389	0.0
Cl	1.3642	0.0



<sup>a)</sup> Assumed.

[1] Lide, D.R., Jen, M.: J. Chem. Phys. **38** (1963) 1504.

[2] Hilderbrandt, R.L., Wieser, J.D.: J. Chem. Phys. **56** (1972) 1143.

ED, MW

[1]

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–C	1.528(2)	Cl–C–C	107.3(3)
C–Cl	1.828(5)	C–C–H	110.8(9)
C–H	1.102(7)	C–C–D	110.7(9)
C–D	1.099(5)	C–C–C	111.6(2)
(C–H) – (C–D) <sup>b)</sup>	0.0035(19)	H–C–H	108.1(12)
$\Delta$ (C–C) <sup>b)</sup>	0.0010(7)	D–C–D	108.2(10)
$\Delta$ (C–Cl) <sup>b)</sup>	0.0010(15)		

[2]

$r_{av}$	Å <sup>a)</sup>	$\theta_z$	deg <sup>a)</sup>
C–C	1.525(3)	Cl–C–C	107.3(3)
C–Cl	1.827(5)	C–C–H	110.8(9)
C–H	1.082(8)		

The nozzle was at room temperature [1].

<sup>a)</sup> Estimated limits of error.

<sup>b)</sup> Difference of the parameters in (CH<sub>3</sub>)<sub>3</sub>CCl and (CD<sub>3</sub>)<sub>3</sub>CCl.

[1] Hilderbrandt, R.L., Wieser, J.D.: J. Chem. Phys. **55** (1971) 4648.

[2] See [2] above.

See also: Momany, F.A., Bonham, R.A., Druelinger, M.L.: J. Am. Chem. Soc. **85** (1963) 3075.