

1053  
MW

**C<sub>3</sub>H<sub>2</sub>Cl<sub>2</sub>**

**1,3-Dichloropropyne**

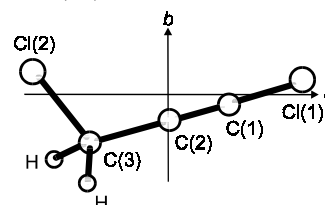
**C<sub>s</sub>**  
ClC≡C–CH<sub>2</sub>Cl

$r_0$	Å <sup>a)</sup>
C(1)≡C(2)	1.201(10)
C(2)–C(3)	1.456(10)
C(3)–H	1.093(15)

$r_s$	Å <sup>b)</sup>
C(1)–Cl(1)	1.6377(50)
C(3)–Cl(2)	1.7787(60)

$\theta_s$	deg <sup>b)</sup>
H–C(3)–H	98.95(100)
H–C(3)–C(2)	108.8(50)
Cl(2)–C(3)–C(2)	112.13(50)

Atom	$ a_s $ [Å]	$ b_s $ [Å]
Cl(1)	2.7100	0.2274
Cl(2)	2.5142	0.4554



<sup>a)</sup> Uncertainties for  $r_0$  parameters were not estimated in the original paper.

<sup>b)</sup> Uncertainties for  $r_s$  parameters are larger than those of the original data.

Günther, H.: Dissertation, Univ. Tübingen 1975.

ED

**C<sub>s</sub> assumed**

$r_\alpha^0$	Å <sup>b)</sup>
C(1)–Cl(1)	1.629(10)
C(1)≡C(2)	1.201(13)
C(2)–C(3)	1.460 <sup>b)</sup>
C(3)–Cl(2)	1.791(6)
C(3)–H	1.093 <sup>b)</sup>

$\theta_\alpha^0$	deg <sup>b)</sup>
C(2)–C(3)–Cl(2)	111.1(10)
H–C(3)–H	98.8(31)
C(2)–C(3)–H	108.7(32)
Cl(1)–C(1)≡C(2)	176.6(11)
C(1)≡C(2)–C(3)	182.7(14)

The nozzle temperature was 80 °C.

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Assumed.

Gleisberg, F., Zeil, W.: J. Mol. Struct. **39** (1977) 115.