

1575 $\text{C}_4\text{H}_5\text{Cl}$ ED, MW, *ab initio*
calculations (HF/4-21G)

(Z)-1-Chloro-1,3-butadiene

 C_s
 $\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CHCl}$

r_a	\AA^a	θ_a	deg a
C(1)=C(2)	1.342(2)	C(1)=C(2)-C(3)	125.5(2)
C(3)=C(4)	1.345(2)	C(4)=C(3)-C(2)	122.3(4)
C(2)-C(3)	1.466(3)	C(2)=C(1)-Cl	123.9(2)
C-Cl	1.730(2)		
$\Delta(\text{C}=\text{C})^b$	0.0037 c		

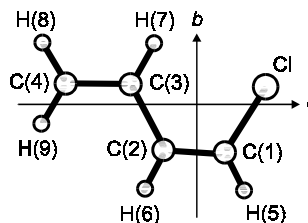
The nozzle temperature was 300 K.

 a) Twice the estimated standard errors including the scale error. b) $[\text{C}(1)=\text{C}(2)] - [\text{C}(3)=\text{C}(4)]$. c) Assumed.Gundersen, G., Thomassen, H.G., Boggs, J.E., Collins, M.L.: J. Mol. Struct. **213** (1989) 1.

MW

r_s	\AA	θ_s	deg
C(1)=C(2)	1.327(6)	C(1)=C(2)-C(3)	126.5(3)
C(3)=C(4)	1.343(2)	C(4)=C(3)-C(2)	123.0(7)
C(2)-C(3)	1.449(13)	C(2)=C(1)-Cl	123.7(3)
C-Cl	1.731(8)	C(2)=C(1)-H(5)	125.5(4)
C(1)-H(5)	1.100(11)	C(1)=C(2)-H(6)	117.9(4)
C(2)-H(6)	1.099(11)	C(4)=C(3)-H(7)	122.3(5)
C(3)-H(7)	1.132(16)	C(3)=C(4)-H(8)	121.0(5)
C(4)-H(8)	1.087(13)	C(3)=C(4)-H(9)	121.7(5)
C(4)-H(9)	1.071(13)		

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$
C(1)	0.6346	-0.9571
C(2)	-0.6883	-0.8552
C(3)	-1.4591	0.3719
C(4)	-2.8015	0.3914
H(5)	1.2032	-1.8992
H(6)	-1.2752	-1.7842
H(7)	-0.8403	1.3196
H(8)	-3.3479	1.3307
H(9)	-3.3778	-0.5110
Cl	1.7023	0.4051

Karlsson, F., Smith, Z.: J. Mol. Spectrosc. **81** (1980) 327.