

1504
ED

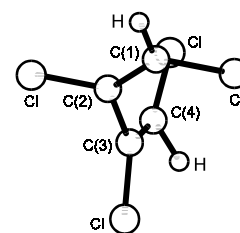
C₄H₂Cl₄

(*E,E*)-1,2,3,4-Tetrachloro-1,3-butadiene

C₂

ClHC=CCl-CCl=CHCl

r_a	Å ^{a)}	θ_α	deg ^{a)}
C-H	1.100 ^{b)}	C(1)=C(2)-C(3)	125.7(4)
C(1)=C(2)	1.343(5)	C(3)-C(2)-Cl	115.6(4)
C(2)-C(3)	1.481(8)	C(2)=C(1)-Cl	122.4(5)
C-Cl	1.725(3)	C(2)=C(1)-H	124.0 ^{b)}
		$\phi(\text{C}=\text{C}-\text{C}=\text{C})$ ^{c)}	76.6(23)



When the root-mean-square amplitude δ of the C=C-C=C torsional angle ϕ was taken into account in a dynamic model, $\delta = 16.3(16)^\circ$ and $\phi = 77.8(20)^\circ$ were obtained. The C-Cl bond lengths were assumed to be equal. The nozzle temperature was 363 K.

^{a)} 1.4 times the estimated standard errors including the scale error.

^{b)} Assumed.

^{c)} From the *syn* position.

Gundersen, G., Nielsen, C.J., Thomassen, H.G., Becher, G.: J. Mol. Struct. **176** (1988) 33.