

1466
ED

C₄Cl₆

Hexachloro-1,3-butadiene

C₂
Cl₂C=CCl–CCl=CCl₂

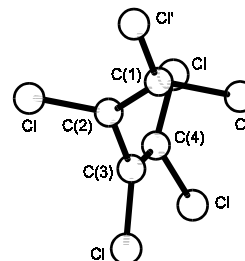
| r_a | Å ^{a)} | θ_α | deg ^{a)} |
|-----------|-----------------|--------------------------------------|-------------------|
| C–Cl | 1.716(3) | C(1)=C(2)–C(3) | 122.6(4) |
| C(1)=C(2) | 1.341(5) | C(3)–C(2)–Cl | 115.8(4) |
| C(2)–C(3) | 1.485(9) | C(2)=C(1)–Cl | 122.50(10) |
| | | $\Delta(C(2)=C(1)–Cl)$ ^{b)} | –0.9(6) |
| | | $\phi(C=C–C=C)$ ^{c)} | 89(3) |

When the root-mean-square amplitude δ for the C=C–C=C torsional angle ϕ was taken into account in a dynamic model, $\delta = 12.0(14)^\circ$ and $\phi = 83.5(19)^\circ$ were obtained. The C–Cl bond lengths were assumed to be equal. The nozzle temperature was 373 K.

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

^{b)} $[C(2)=C(1)–Cl] - [C(2)=C(1)–Cl']$.

^{c)} From *syn* position.



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