

240
MW

C₂H₃Cl₃

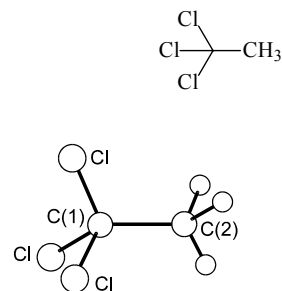
1,1,1-Trichloroethane

C_{3v}

r_s	Å
C–C	1.555(4)

Atom	a_s [Å]
C(1)	0.2671
C(2)	1.8225

When isotope effects: $r(^{12}\text{C}-^{35}\text{Cl}) = r(^{13}\text{C}-^{35}\text{Cl}) + 0.0001\text{Å}$ and $r(^{12}\text{C}-^{12}\text{C}) = r(^{12}\text{C}-^{13}\text{C}) + 0.00008\text{Å}$, were taken into account, the C–C distance was estimated to be 1.516 Å.



Sugie, M., Kato, M., Matsumura, C., Takeo, H.: J. Mol. Struct. **413-414** (1997) 487.

[II/25B\(3, 664\)](#)