

1779
MW

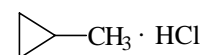
$\text{C}_4\text{H}_9\text{Cl}$

Methylcyclopropane – hydrogen chloride (1/1)
(weakly bound complex)

C_1

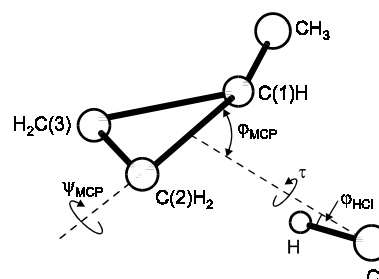
r_0	\AA
$\text{Cl}\cdots\text{X}^{\text{a}}$	3.554(5)

θ_0	deg
$\phi_{\text{HCl}}^{\text{b}}$	5.0 ^c
$\phi_{\text{MCP}}^{\text{d}}$	94(1)
$\psi_{\text{MCP}}^{\text{e}}$	8(2)
τ^{f}	0.0 ^c



	N m^{-1}
k_{s}	9.4

A structure in which the HCl interacts with the C–C bond of the methylcyclopropane ring that is adjacent to the methyl-substituted carbon.



^a) X is the midpoint of the C(1)–C(2) bond.

^b) The angle between $r(\text{X}\cdots\text{Cl})$ and HCl bond axis.

^c) Fixed.

^d) The angle between $r(\text{Cl}\cdots\text{X})$ and C(2)–C(1) bond axis; obtuse values imply a twist of the CHCH_3 end away from $r(\text{Cl}\cdots\text{X})$.

^e) Torsional angle about the C(2)–C(1) bond, *i.e.*, the tilt angle of the C–C–C plane from coplanar with the $\text{X}\cdots\text{Cl}$ line ($\psi_{\text{MCP}} = 0^\circ$ for coplanarity).

^f) Torsional angle $\text{H}-\text{Cl}\cdots\text{X}-\text{C}(2)$.

Forest, S.E., Andrews, A.M., Kuczkowski, R.L.: J. Phys. Chem. **98** (1994) 2050.