

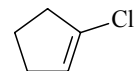
641
MW $\text{C}_5\text{H}_7\text{Cl}$

1-Chlorocyclopentene

 C_1

$r_0^{\text{a})}$	Å
C–Cl	1.723(2)

$\theta_0^{\text{a})}$	deg
$\tau_0^{\text{b})}$	24.4(7)
(C(2)=C(1)–C(5)) ₀ ^{c)}	114.57(9)
(C(1)=C(2)–C(3)) ₀ ^{c)}	111.27(9)



The inversion splittings due to the ring-puckering motion were determined to be 42320(10) and 42270(10) MHz for the ^{35}Cl and ^{37}Cl isotopomers, respectively. The barrier B_0 hindering the ring puckering was evaluated to be 205 cm^{-1} . The flexible model assumes the puckering potential of $V(\tau) = B_0[1 - (\tau/\tau_0)^2]^2$ and the valence angles to vary with τ as $\alpha_i(\tau) = (\alpha_i)_0 + \Delta\alpha_i(\tau/\tau_0)^2$ ($i = 1, 2$).

^{a)} Flexible model parameters derived.

^{b)} Puckering angle, see figure for the definition.

^{c)} Suffix 0 means the equilibrium value.

Caminati, W., Danieli, R., Fantoni, A.C., Lopez, J.C.:
J. Mol. Spectrosc. **181** (1997) 91.

