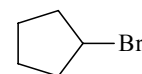


650
MW C_5H_9Br **Bromocyclopentane**
Cyclopentyl bromide C_s (axial)
 C_s (equatorial)

r_0	$\text{\AA}^a)$		θ_0	$\text{deg}^a)$	
	axial	equatorial		axial	equatorial
C–Br	1.966(5)	1.948(5)	C(β')–C(α)–C(β)	103.1(5)	103.5(5)
C(α)–C(β)	1.524(5)	1.523(5)	C(α)–C(β)–C(γ)	104.2(5)	102.6(5)
C(β)–C(γ)	1.543(5)	1.543(5)	C(β)–C(γ)–C(γ')	105.6(5)	105.7(5)
C(γ)–C(γ')	1.558(5)	1.559(5)	Br–C–H	104.1(5)	105.7(5)
C(α)–H	1.090(10)	1.094(10)	H–C(β)–H' ^{b)}	107.5(10)	108.4(10)
C(β)–H	1.098(10)	1.092(10)	H–C(γ)–H' ^{b)}	106.9(10)	107.5(10)
C(β)–H' ^{b)}	1.092(10)	1.095(10)	Br–C(α)–C(β)	110.7(5)	113.2(5)
C(γ)–H	1.093(10)	1.093(10)	H–C(α)–C(β)	114.3(10)	110.7(10)
C(γ)–H' ^{b)}	1.092(10)	1.092(10)	H–C(β)–C(α)	107.2(10)	113.2(10)
			H'–C(β)–C(α) ^{b)}	113.6(10)	107.9(10)
			H–C(β)–C(γ)	110.9(10)	113.8(10)
			H'–C(β)–C(γ) ^{b)}	113.3(10)	110.8(10)
			H–C(γ)–C(β)	111.2(10)	110.2(10)
			H'–C(γ)–C(β) ^{b)}	110.3(10)	111.8(10)
			H–C(γ)–C(γ')	112.8(10)	110.3(10)
			H'–C(γ)–C(γ') ^{b)}	110.1(10)	111.5(10)
			C(β')–C(α)–C(β)–C(γ') ^{c)}	40.0(10)	43.1(10)
			C(β)–C(γ)–C(γ')–C(β') ^{c)}	0.0 ^{d)}	0.0 ^{d)}
			$\phi^e)$	40.2(10)	44.0(10)

Two conformers, axial and equatorial, were observed.
The structural parameters from MP2/6-31G** and
MP2/6-311++G** calculations with full electron correlation
were adjusted to fit the experimental rotational constants.

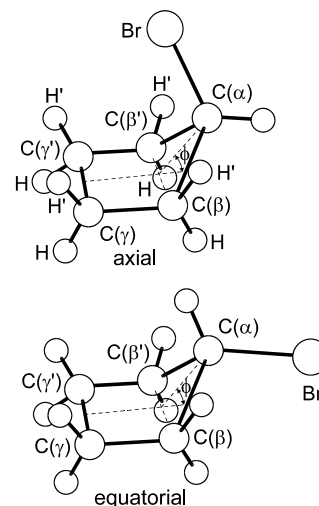
^{a)} Uncertainties were not estimated in the original paper.

^{b)} H atoms with a prime and Br atom are in the same side
of the ring.

^{c)} Dihedral angle.

^{d)} Assumed.

^{e)} Puckering angle.



Durig, J.R., Zhao, W., Zhu, X.: J. Mol. Struct. **521** (2000) 25.

ED, *ab initio*
calculations

r_g	$\text{\AA}^a)$	θ_α	$\text{deg}^a)$
C–H (average)	1.093(7)	Br–C–C (axial)	110.2(6) ^{b)}
C–Br (axial)	1.974(7) ^{b)}	Br–C–C (equatorial)	112.9(6) ^{b)}
C–Br (equatorial)	1.954(7) ^{b)}	H–C–C	111.9(11)
C–C (average)	1.540(2)		
C(α)–C(β)	1.527 ^{b)}		
C(β)–C(γ)	1.546 ^{b)}		
C(γ)–C(γ')	1.553 ^{b)}		
$\rho^c)$	0.37(2)		

A pseudorotational potential function of the form $V(\phi) = (V_1/2)(1 + \cos\phi) + (V_2/2)(1 + \cos 2\phi)$, where ϕ is the phase angle, and $V_1 = 0.74(40) \text{ kcal mol}^{-1}$ and $V_2 = 0.42(85) \text{ kcal mol}^{-1}$ gave the best agreement with the experimental data. The conformer with the ring in the envelope form and with the bromine atom in the axial position is more stable than the conformer with the bromine atom in the equatorial position by $0.74(40) \text{ kcal mol}^{-1}$.

The nozzle temperature was 333 K.

^{a)} Uncertainties were unidentified, possibly estimated total errors.

^{b)} Differences in the C–Br, C–C and Br–C–C parameters were assumed at the values from MP2/6-311++G** calculations.

^{c)} Thermal averaged puckering amplitude, by which the perpendicular displacement of the C_i atom from the ring plane is given by $z_i = (2/5)^{1/2} \rho \cos [4\pi(i-1)/5 + \phi]$, ($i = 1 \dots 5$).

Bickford, C., Shen, Q.: J. Mol. Struct. **567-568** (2001) 269.