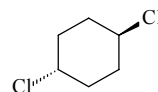


740 **C₆H₁₀Cl₂**
ED, *ab initio* and DFT
calculations

trans-1,4-Dichlorocyclohexane**C_{2h} (ee)****C_{2h} (aa)**

r_g	\AA^a		θ_α	deg^a	
	ee	aa		ee	aa
C–H ^{b)}	1.115(4)	1.113 ^{c)}	C(2)–C(1)–C(6)	109.9(14)	110.1 ^{c)}
C–C ^{b)}	1.531(2)	1.530 ^{c)}	C–C–Cl	109.7(4)	109.8 ^{c)}
$\Delta(\text{C–C})^d)$	–0.017(19)	–0.008 ^{c)}	C(2)–C(1)–H	109.5(32)	109.7 ^{c)}
C(1)–C(2)	1.525(6)	1.527	C(3)–C(2)–H(2)	111.1(33)	112.9 ^{c)}
C(2)–C(3)	1.542(13)	1.535	C(3)–C(2)–H(2')	110.9(33)	110.6 ^{c)}
C–Cl	1.799(3)	1.812 ^{c)}	C(1)–C(2)–C(3) ^{e)}	110.9(10)	112.9
			$\phi[\text{H}(2)]^f)$	92.0(73)	151.6 ^{c)}
			$\phi[\text{H}(2')]^g)$	207.9(59)	267.4 ^{c)}
			$\varphi^h)$	–51.7(19)	47.2(12)

The molecule exists as a mixture of the ee and aa conformers (equatorially and axially disposed chlorine atoms, respectively) with mole fractions of $x_{ee} = 0.46(6)$ and $x_{aa} = 0.54(6)$. These experimental compositions agreed with those predicted by MP2/6-311G* and QCISD/6-311+G(2df,p) calculations, $x_{ee} = 0.43$, derived from the conformational energy difference ΔE of 0.28 kcal mol^{–1} with corrections for zero-point energy and entropy differences.

The nozzle temperature was 105 °C.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Average value.

^{c)} Differences between the r_α parameters of the ee and aa conformers were assumed at the values from HF/6-31G* calculations.

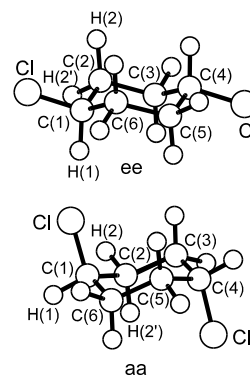
^{d)} $[\text{C}(1)–\text{C}(2)] – [\text{C}(2)–\text{C}(3)]$.

^{e)} Dependent parameter.

^{f)} Dihedral angle between the C(3)C(2)H(2) and C(2)C(3)C(5)C(6) planes.

^{g)} Dihedral angle between the C(3)C(2)H(2') and C(2)C(3)C(5)C(6) planes.

^{h)} Dihedral angle between the C(1)C(2)C(6) and C(2)C(6)C(5)C(3) planes.



Richardson, A.D., Hedberg, K., Wiberg, K.B.: J. Phys. Chem. A. **103** (1999) 7709.

See also: Atkinson, V.A., Hassel, O.: Acta Chem. Scand. **13** (1959) 1737.