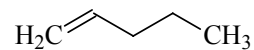


660
MW C_5H_{10}

1-Pentene

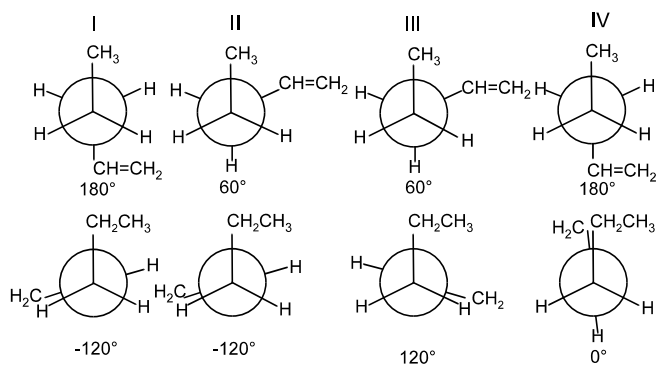
 C_s (conformer IV)
 C_1 (conformers I, II, III)

θ_0	$\tau(1,2,3,4)$ [deg] ^{a) b)}	$\tau(2,3,4,5)$ [deg] ^{a) b)}
conformer I	-119.3(10)	-178.2(10)
conformer II	-119.9(10)	66.5(10)
conformer III	117.2(10)	64.7(10)
conformer IV	13.5(10)	180.0(10)

Four of the five expected conformers, I – IV, have been detected.

^{a)} Dihedral angle. Other structural parameters were assumed at the values from MP2/6-31G* calculations.

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



Newman projections for the conformers I, II, III, and IV.
The approximate values for the dihedral angles $\tau(2,3,4,5)$ (top) and $\tau(1,2,3,4)$ (bottom) are shown.

Fraser, G.T., Xu, L.-H., Suenram, R.D., Lugez, C.L.: J. Chem. Phys. **112** (2000) 6209.