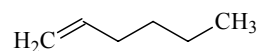


747
MW C_6H_{12}

1-Hexene

 C_1 (conformers 1, 2, 3, 5, 6, 7) C_s (conformer 4)

Seven conformers were detected, and six of them have C_1 symmetry, as verified by the observation of *a*-, *b*- and *c*-type electric-dipole transitions. The remaining conformer has C_s symmetry, consistent with its small inertial defect $\Delta = -12.65 \text{ u \AA}^2$ and the observation of only *a*- and *b*-type transitions. The energy differences between the conformers *n* and 1 are 130(140), 840(140), 520(140), 570(140), 530(140) and 480(130) in cm^{-1} for *n* = 2, 3, 4, 5, 6, 7, respectively. The dihedral angles estimated by MP2/6-31G* calculations are listed.

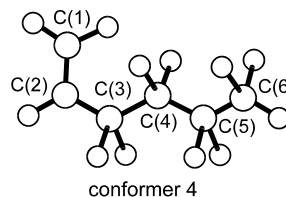
Conformer <i>n</i>	τ_1 [deg] ^{a)}	τ_2 [deg] ^{b)}	τ_3 [deg] ^{c)}	τ_4 [deg] ^{d)}
1	-116.8	-178.6	-179.8	179.9
2	118.6	-64.2	-179.3	-60.0
3	-110.7	-62.7	-176.2	-59.6
4	0.0	180.0	180.0	-59.8
5	116.5	-177.8	-64.5	-175.7
6	120.9	-58.6	-61.0	66.0
7	116.6	174.4	63.1	-64.5

^{a)} The C(1)–C(2)–C(3)–C(4) dihedral angle.

^{b)} The C(2)–C(3)–C(4)–C(5) dihedral angle.

^{c)} The C(3)–C(4)–C(5)–C(6) dihedral angle.

^{d)} The C(4)–C(5)–C(6)–H dihedral angle.



Fraser, G.T., Suenram, R.D., Lugez, C.L.: J. Phys. Chem. A **104** (2000) 1141.