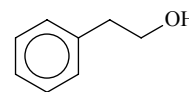
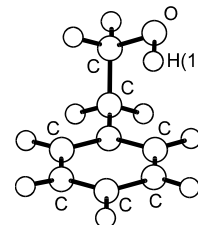


848  
MW**C<sub>8</sub>H<sub>10</sub>O****2-Phenylethanol**  
Phenethyl alcohol  
Benzeneethanol**C<sub>1</sub> (*gauche*)**

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
H(1)	1.540	1.094	1.108

By comparing observed and *ab initio* predicted spectroscopic rotational constants and hydroxyl-deuteration isotopic substitution coordinates, the species has been identified with a *gauche* conformer in which the hydroxyl hydrogen atom is involved in an intramolecular hydrogen bond with the  $\pi$ -electron cloud of the aromatic ring. *Ab initio* calculations with electron correlation at the MP2/6-31G(d,p) level show that the *gauche* conformer is *ca.* 8 kJ mol<sup>-1</sup> lower in energy than all the other possible conformers.

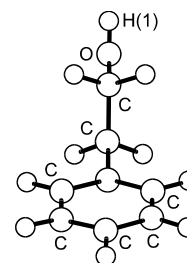


Godfrey, P.D., Jorissen, R.N., Brown, R.D.: J. Phys. Chem. A **103** (1999) 7621; Erratum: J. Phys. Chem. A **104** (2000) 2144.

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
Hydroxyl H	4.15	0.08	0.94

The *anti* conformer was detected.

Brown, R.D., Godfrey, P.D.: J. Phys. Chem. A **104** (2000) 5742.

**C<sub>s</sub> (*anti*)**