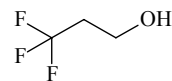
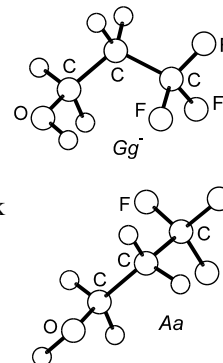


378  
MW $\text{C}_3\text{H}_5\text{F}_3\text{O}$ 

3,3,3-Trifluoro-1-propanol

 $\text{C}_1 (Gg^-)$  $\text{C}_s (Aa)$ 

Two of five possible conformers,  $Gg^-$  and  $Aa$ , were assigned: The former is stabilized by a six membered intramolecular hydrogen bond formed between one of the fluorine atoms and the hydrogen atom of the hydroxyl group. No such interaction is possible in  $Aa$ , in which both the  $\text{O}-\text{C}-\text{C}-\text{C}$  and  $\text{H}-\text{O}-\text{C}-\text{C}$  chains of atoms are in the *anti* conformation. The internal hydrogen bond is weak, since the  $Gg^-$  form is only  $3.5(10) \text{ kJ mol}^{-1}$  more stable than  $Aa$ . The weak intramolecular hydrogen bond is also evident from the gas-phase IR spectrum of the  $\text{O}-\text{H}$  stretching vibration.



Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand. **53** (1999) 202.