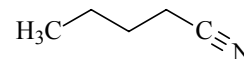
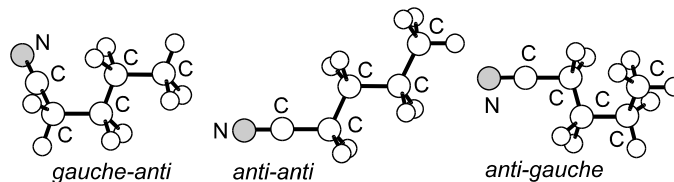


**655**     **C<sub>5</sub>H<sub>9</sub>N**  
MW, *ab initio*  
calculations

**Butyl cyanide**  
Pentanenitrile  
Valeronitrile

**C<sub>s</sub>** (*anti-anti*)  
**C<sub>1</sub>** (*anti-gauche*)  
**C<sub>1</sub>** (*gauche-anti*)

Three conformers, *anti-anti*, *anti-gauche* and *gauche-anti*, were observed. According to the results of HF and MP2 calculations with 6-31G(d,p) and 6-311+G(d,p) basis sets, the differences in their energies are small and the *gauche-anti* conformer is the most stable one.



Atticks, K.A., Bohn, R.K., Michels, H.H.: Int. J. Quant. Chem. **90** (2002) 1440.