

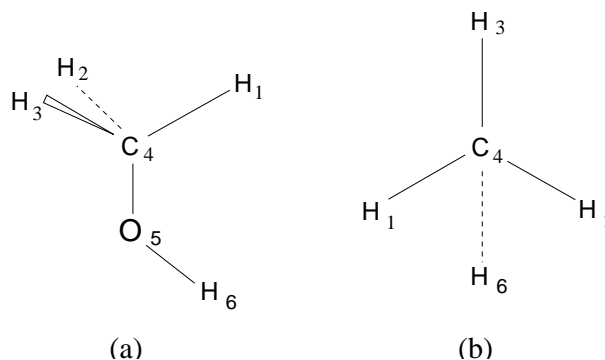
Fundamentals of Molecular Symmetry
Week 8/11

Exercises

8.1 Consider the molecule HSOH. The equilibrium structures of this molecule are analogous to those of HOOH known from the lecture. Determine the MS-group of HSOH

- when there is no “torsional tunneling.”
- when the effects of torsional tunneling can be observed.
- when also the effects of bond breaking and reformation can be observed.

Determine the forward correlation and the reverse correlation between the three groups.



8.2 The displays (a) and (b) show two different views of the molecule methanol $^{12}\text{CH}_3^{16}\text{OH}$. Determine the MS group of $^{12}\text{CH}_3^{16}\text{OH}$

- when there is no torsional tunneling of the OH group relative to the CH_3 group. It is assumed that the molecule has the “staggered” equilibrium configuration in display (b).
- when the effects of torsional tunneling can be observed.

Determine the spin-statistical weight factors in the two cases and derive, taking into account the spin-statistical weight factors, the forward correlation and the reverse correlation between the two groups.