

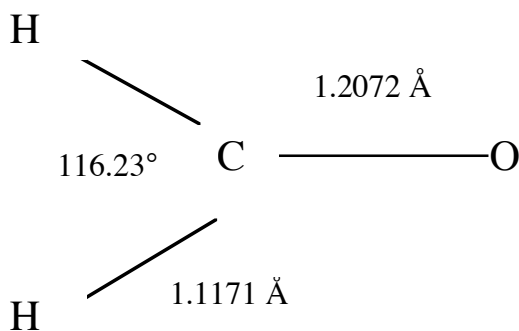
HOMEWORK ASSIGNMENT # 2

*DUE: Wednesday, 19 February*

- Find a relationship among  $A$ ,  $B$ , and  $C$  for a perfectly rigid planar molecule.
- a) Show that, neglecting nuclear spin, for a prolate symmetric top in which  $kT \gg hA$ ,

$$q = \sigma^{1/2} \left\{ \frac{kT}{h} \right\}^{3/2} \{AB^2\}^{1/2}$$

- Determine the fraction of molecules in the lowest five rotational states of the oblate, non-planar symmetric rotor  $\text{PH}_3$  at 300 K.  $B_0 = 133.48015$  GHz,  $C_0 = 117.488$  GHz. Include nuclear spin considerations.
- Determine the exact spectral frequencies for the  $J = 10 \rightarrow 9$  series of absorption lines of  $\text{PH}_3$  if  $D_J = 3950$  kHz and  $D_{JK} = -5180$  kHz. What are the relative intensities of the lines?
  - What are the rotational energy levels and degeneracies for a spherical top ( $A=B=C$ )? Would you expect any dipole-allowed rotational transitions? Why or why not?
  - Determine analytic formulae for the energy levels of a rigid asymmetric top with  $J=2$ .
  - Consider the planar asymmetric top formaldehyde, which possesses the structure



Calculate the principal moments of inertia, the rotational constants in GHz, and the asymmetry parameter  $\sigma$ . For  $J=0-2$ , which levels are ortho and which are para? Determine the allowed transitions and their frequencies (assuming the molecule to be rigid) for all transitions involving  $J = 0$  and/or  $J = 1$ .

- Using a symmetric top basis, determine the non-zero matrix elements for the fourth-order distortion terms of the A-reduced Watson Hamiltonian.