CHEM 4616: Homework #6

Corresponds to the quiz to be given in class on Thursday, March 13th, 2008

Chang, Chapter 17: Problems 17-21, 24-27

17.17 To be IR active, the molecule must have at least one vibrational mode for which the dipole moment changes during the vibration.

(a) N_2 – no (c) CH_4 – yes (e) H_2O_2 – yes

(b) HBr – yes (d) Xe – no (f) NO – yes

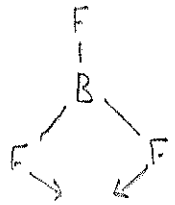
17.18 # vibs = 3N − 6 for non-linear molecules

vibs = 3N − 5 for linear molecules

(a) O_3 : 3 (c) CBr_4 : 9

(b) C_2H_2 : 7 (d) C_6H_6 : 30

17.19

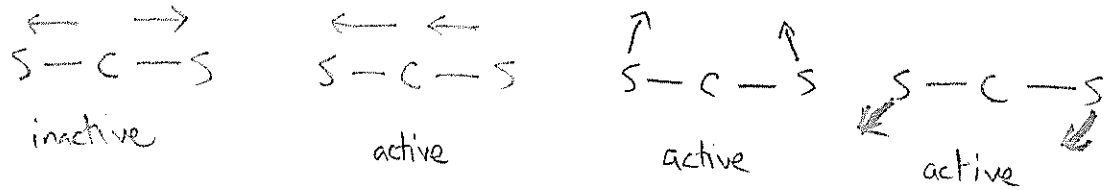


17.21 $\tilde{\nu} = 2143.3\ cm^{-1} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} \rightarrow k = 4\pi^2 c^2 \tilde{\nu}^2 \mu$

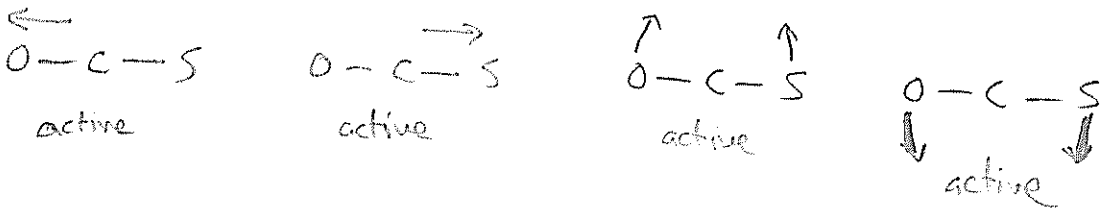
$\frac{1}{\mu} = \frac{1}{m_C} + \frac{1}{m_O} = \frac{1}{12} + \frac{1}{15.9949} \rightarrow \mu = 6.85421\ u = 1139 \times 10^{-26}\ kg$

$\boxed{k = 1856\ N/m}$

17.24 (a)



(b)



17.25 $3N-6 = 3(9272) - 6 = \boxed{27810}$ vibrational modes

17.26 $\bar{\nu} \propto \mu^{-\frac{1}{2}}$. Therefore, the smallest μ gives the largest fundamental frequency. H_2 is lighter than D_2 and HD.

17.27 $\bar{\nu}(D^{35}Cl) = 2081.0\ cm^{-1}$

$$\frac{1}{\mu} = \frac{1}{m_D} + \frac{1}{m_{Cl}} = \frac{1}{(2.014)} + \frac{1}{(34.968)} \rightarrow \mu = 1.9043\ u = 3.163 \times 10^{-27}\ kg$$

$$K = 4\pi^2 c^2 \bar{\nu}^2 \mu = \boxed{486.0\ N/m}$$

This is very similar to the value of 482 N/m computed in example 17.2 for $H^{35}Cl$, which suggest that the force constant is relatively independent of the masses.