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5.80 Small-Molecule Spectroscopy and Dynamics
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MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Chemistry 5.76
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Problem Set #4

Some problems [indicated] were taken from various chapters of Molecules and Radiation by J. I. Steinfeld, Harper & Row, 1974

1. [Steinfeld, Ch. 7, #1]
2. [Steinfeld, Ch. 8, # 2]
3. [Steinfeld, Ch. 8, # 4]
4. [Steinfeld, Ch. 8, # 6]
5. [Steinfeld, Ch. 8, # 8]
6. $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ is a linear molecule. The bond lengths are

$$r_{\text{CO}} = 1.16\text{\AA}$$

$$r_{\text{CS}} = 1.56\text{\AA}$$

and the observed fundamental vibrational frequencies are

$$\nu_1 = 858.9 \text{ cm}^{-1} \text{ stretch}$$

$$\nu_2 = 520.4 \text{ cm}^{-1} \text{ bend}$$

$$\nu_3 = 2062.2 \text{ cm}^{-1} \text{ stretch.}$$

- (a) Obtain k_{CS} , k_{CO} , and $k_{\theta}[r_{\text{CO}}r_{\text{CS}}]^{-1}$ in dynes/cm.
 - (b) What are the amplitudes for C-O and C-S stretch in the ν_1 fundamental level?
 - (c) What are the vibrational frequencies for $^{18}\text{O}^{12}\text{C}^{32}\text{S}$?
7. [Steinfeld, Ch. 9, #1]