## PROBLEMS

Problems marked with an icon may be more conveniently solved on a personal computer with a mathematical program.

**13.1** Since the energy of a molecular quantum state is divided by $kT$ in the Boltzmann distribution, it is of interest to calculate the temperature at which $kT$ is equal to the energy of photons of different wavelengths. Calculate the temperature at which $kT$ is equal to the energy of photons of wavelength $10^3$ cm, $10^{-1}$ cm, $10^{-3}$ cm, and $10^{-5}$ cm.

**13.2** Most chemical reactions require activation energies ranging between 40 and 400 kJ mol$^{-1}$. What are the equivalents of 40 and 400 kJ mol$^{-1}$ in terms of (*a*) nm, (*b*) wavenumbers, and (*c*) electron volts?

**13.3** (*a*) What vibrational frequency in wavenumbers corresponds to a thermal energy of $kT$ at 25 °C? (*b*) What is the wavelength of this radiation?

**13.4** Show that equation 13.17 is a solution of equation 13.9 by differentiating equation 13.17 and substituting it into equation 13.9.

**13.5** Calculate the reduced mass and the moment of inertia of $D^{35}Cl$, given that $R_e = 127.5$ pm.

**13.6** The H—O—H bond angle for $^1H_2O$ is 104.5°, and the H—O bond length is 95.72 pm. What is the moment of inertia of $H_2O$ about its $C_2$ axis?

**13.7** Some of the following gas molecules have pure microwave absorption spectra and some do not: $N_2$, HBr, $CCl_4$, $CH_3CH_3$, $CH_3CH_2OH$, $H_2O$, $CO_2$, $O_2$. What is the gross selection rule for rotational spectra, and which molecules satisfy it?

**13.8** Calculate the frequency in wavenumbers and the wavelength in cm of the first rotational transition ($J = 0 \rightarrow 1$) for $D^{35}Cl$.

**13.9** The pure rotational spectrum of $^{12}C^{16}O$ has transitions at 3.863 and 7.725 cm$^{-1}$. Calculate the internuclear distance in $^{12}C^{16}O$. Predict the positions, in cm$^{-1}$, of the next two lines.

**13.10** Assume the bond distances in $^{13}C^{16}O$, $^{13}C^{17}O$, and $^{12}C^{17}O$ are the same as in $^{12}C^{16}O$. Calculate the position, in