CHEM442-001
College of Charleston
Spring 1999
Exam V
1(25). For ${ }^{12} \mathrm{C} \equiv{ }^{16} \mathrm{O}\left(\mu=1.138518 \times 10^{-26} \mathrm{~kg}\right)$ the microwave rotational spectrum consists of a series of evenly spaced lines at $3.8604 \mathrm{~cm}^{-1}, 7.7208 \mathrm{~cm}^{-1}, 11.5812 \mathrm{~cm}^{-1}, 15.4416 \mathrm{~cm}^{-1}$, etc.

Calculate the bond length of this molecule.
The IR spectrum of ${ }^{12} \mathrm{C} \equiv{ }^{16} \mathrm{O}$ has an absorption peak centered at $\omega_{\mathrm{e}}=2142.61 \mathrm{~cm}^{-1}$.
Calculate the force constant of this molecule.
Predict the location of the IR spectrum absorption peak for ${ }^{12} \mathrm{C} \equiv{ }^{18} \mathrm{O}\left(\mu=1.19538 \times 10^{-26}\right.$ kg ).

2(20). The polarizability of $\mathrm{CO}(\mathrm{g})$ is $2.20 \times 10^{-40} \mathrm{C}^{2} \mathrm{~N}^{-1} \mathrm{~m}$ and the dipole moment is $3.90 \times 10^{-31}$ C m (interestingly, the negative end is the C atom). Calculate the fraction of intermolecular forces potential energy resulting from the dipole interactions, $\left(U_{\mathrm{d} / \mathrm{d}}+\right.$ $\left.U_{\mathrm{d} / \mathrm{ind}}\right) /\left(U_{\mathrm{d} / \mathrm{d}}+U_{\mathrm{d} / \mathrm{ind}}+U_{\mathrm{L}}\right)$, at $25^{\circ} \mathrm{C}$.

3(20). Consider the following proposed mechanism for the decomposition of ozone

$$
2 \mathrm{O}_{3}(\mathrm{~g}) \rightarrow 3 \mathrm{O}_{2}(\mathrm{~g})
$$

given by
$\mathrm{O}_{3}+\underset{\substack{k_{-2} \\ \mathrm{M}_{2}}}{\stackrel{k_{2}}{\prime}} \mathrm{O}+\mathrm{O}+\mathrm{M}$
$\mathrm{O}+\mathrm{O}_{3}{ }_{2} 2 \mathrm{O}_{2}$
Apply the steady state approximation for $C\left(\mathrm{O}^{\cdot}\right)$ and find $-\mathrm{d} C\left(\mathrm{O}_{3}\right) / \mathrm{d} t$.
4(15). The rate constant for

$$
\mathrm{COCl}_{2}(\mathrm{~g}) \rightarrow \mathrm{CO}(\mathrm{~g})+\mathrm{Cl}_{2}(\mathrm{~g}) \quad \Delta_{\mathrm{r}} U_{700}=103.1 \mathrm{~kJ}
$$

is given by

$$
\ln \left[k /(\min )^{-1}\right]=\frac{-26296}{[T /(\mathrm{K})]}+34.893
$$

Prepare a reaction coordinate diagram (label properly) for this reaction.
$5(20)$. The following data were obtained for the reaction

$$
2 \mathrm{H}_{2} \mathrm{O}_{2}(\mathrm{aq}) \rightarrow 2 \mathrm{H}_{2} \mathrm{O}(\mathrm{l})+\mathrm{O}_{2}(\mathrm{~g})
$$

| $t /(\mathrm{s})$ | 0 | 300 | 600 | 900 | 1500 | 2100 | 2700 | $\infty$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $V\left(\mathrm{O}_{2}\right) /\left(\mathrm{cm}^{3}\right)$ | 0.00 | 7.50 | 14.00 | 19.65 | 28.80 | 35.80 | 41.20 | 57.90 |

Determine graphically (graph paper attached) the order of reaction with respect to $C\left(\mathrm{H}_{2} \mathrm{O}_{2}\right)$.

