A-1 $F = ma$, $F = -k(l - l_0) = -kx$

(10 pts) $F = m\dfrac{d^2x}{dt^2} = -kx$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

A-2 (10 pts)

$$\frac{d^2}{dt^2}(x(t)) = \frac{d^2}{dt^2}(A\sin(\omega t + \phi))$$

$$= A\frac{d}{dt}[\omega\cos(\omega t + \phi)]$$

$$= -A\omega^2\sin(\omega t + \phi)$$

$$= -\omega^2 x(t)$$

substitute into Newton's Equation

$$-\omega^2 x(t) + \frac{k}{m}(x(t)) = 0$$

$$k/m = \omega^2$$

$$\sqrt{\frac{k}{m}} = \omega$$

ω - is the angular frequency of the motion
A - is the amplitude of the motion
ϕ - is a phase shift to match the time variation relative to zero

A-3 (10 pts)

$$-\frac{d}{dx}V(x) = F$$

$$V(x) = -\int F\,dx$$

$$= -\int(-kx)\,dx$$

$$= \frac{1}{2}kx^2 + C$$

but $V(x=0) = 0$ so $C = 0$

$$V(x) = \frac{1}{2}kx^2$$

A-4 $\quad E = KE + V = \frac{1}{2} m v^2 + \frac{1}{2} k x^2$

① $v^2 = \left(\frac{d}{dt} x\right)^2 = \left(\omega\ [\text{scribbled out}]\ A \cos(\omega t + \phi)\right)^2$

$$E = KE + V = \frac{1}{2} m \omega^2 A^2 \cos^2(\omega t + \phi) + \frac{1}{2} k x^2$$

② recall $\omega = \sqrt{\frac{k}{m}}$

$$= \frac{1}{2} \cancel{m} \left(\frac{k}{\cancel{m}}\right) A^2 \cos^2(\omega t + \phi) + \frac{1}{2} k\ x(t)^2$$

③ recall $x(t) = A \sin(\omega t + \phi)$

$$= \frac{1}{2} k \left\{ A^2 \cos^2(\omega t + \phi) + A^2 \sin^2(\omega t + \phi) \right\}$$

$$= \frac{k A^2}{2} \left\{ \cos^2(\omega t + \phi) + \sin^2(\omega t + \phi) \right\}$$

(10 pts) $\quad E = kA^2/2 \ \{ \ 1 \ \}$ $\quad$ (no time dependence)

B Morse Potential

B-1 $\quad V(\ell) = D\left(1 - e^{-\beta(\ell - \ell_0)}\right)^2 \rightarrow V(x) = D\left(1 - e^{-\beta x}\right)^2$

Taylor Series at $x = 0$

(10 pts)

$$V(x) \approx V(x=0) + \left(\left.\frac{dV}{dx}\right|_{x=0}\right) x + \frac{1}{2}\left(\frac{d^2 V}{dx^2}\right)_{x=0} x^2$$

$$= D\left(1 - e^{-0}\right)^2 + \left(\left.(2\beta D \overset{\nearrow 1}{\cancel{e^{-\beta x}}})(1 - \overset{\nearrow 1}{\cancel{e^{-\beta x}}})\right|_{x=0}\right) x + \frac{1}{2}\left(\frac{d^2 V}{dx^2}\right)_{x=0} x^2$$

$$V(x) = 0 + 2\beta D (0) x + \frac{1}{2}\left(\frac{d^2 V}{dx^2}\right)_{x=0} x^2$$

$$V(x) \approx \frac{1}{2}\left[2\beta^2 D \cancelto{1}{e^{-2\beta x}} - \underbrace{2\beta^2 D \cancelto{1}{e^{-\beta x}}(1-\cancelto{1}{e^{-\beta x}})}_{0}\right]\Big|_{x=0} x^2$$

$$\simeq \frac{1}{2}\, 2\beta^2 D\, x^2$$

$$V(x) \simeq \beta^2 D\, x^2 \qquad \text{near } x=0 \quad \text{(parabolic potential)}$$

B-2

(10pts)

$$V(x)_{HO} = +\frac{1}{2} k x^2 = \beta^2 D\, x^2$$

$$k = 2\beta^2 D$$

B-3

(10pts)

$$k = 2\beta^2 D \quad \text{for } H_2$$

$$= 2\left(0.0193 \text{ pm}^{-1}\right)^2 7.61\times 10^{-19}\,\text{J}\left(1\,\frac{\text{N-m}}{\text{J}}\right)$$

$$= 5.67\times 10^{-22}\,\frac{\text{N-m}}{\text{pm}^2}\times\left(10^{+12}\,\frac{\text{pm}}{\text{m}}\right)^2$$

$$= 567.\ \text{N/m}$$

C Small Molecules

C-1

$$\nu = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{k}{m}} = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{567\ \text{N/m}\times N_A\ \cancel{/\text{mole}}}{\left(\frac{1\times 1}{2}\right)\times 10^{-3}\ \text{kg}/\cancel{\text{mole}}}} = \frac{8.26\times 10^{14}}{2\pi}\sqrt{\frac{\text{N}}{\text{kg-m}}}$$

(10 pts)

$$\nu = \frac{8.26\times 10^{14}}{2\pi}\ \text{1/sec}$$

$$\boxed{\tau = \frac{1}{\nu} = 7.60\times 10^{-15}\ \text{sec}}$$

C-2 $\nu = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$ $\mu_{H-H} = \left(\frac{1}{2}\right)$ g/mole

(5 pts) $\mu_{HD} = \left(\frac{2}{3}\right)$ g/mole

$$\nu_{HD} \sim \frac{1}{2\pi}\sqrt{\frac{567 \cdot N_A}{\left(\frac{2}{3}\right) \times 10^{-3}}}$$

$$\sim 1.14 \times 10^{14} /\text{sec}$$

C-3 symmetric molecule $(^2H)_2$ so no change in electric
(5pts) dipole moment under vibration $\Rightarrow$ no absorption

C-4 $$\nu_{CO} \sim \frac{1}{2\pi}\sqrt{\frac{3 \times 567 \times N_A}{\left(\frac{16 \times 12}{28.}\right) \times 10^{-3}}} = 6.15 \times 10^{13} /\text{sec}$$

CO → asymmetric molecule should absorb in IR
$C \equiv O$ (triple bond)
(10pts)

C-5 the potential is asymmetric in that the chemical
bond will "break" if the atoms are stretched
(5pts) too far ... $V(x) \to 0$ when $x \to \infty$