1.

a. N=3 for CO_2 and it is linear. So the number of normal modes is 3N-5 = 4 normal modes.
b. I'll use the 6-31G* basis as it is a small molecule and no hydrogens are present, hence no ** or ++ is required.
c. The symmetric stretch (1519cm^{-1}) does not change the dipole mom ent hence it is not IR active. The asymmetric(2585cm^{-1}) is IR active. The wag(746cm^{-1}) is also IR active and degenerate.

2.

R_{HCl}=1.270 A at equilibrium
E(R=1.270) = `-460.0953282 a.u.`

E(R=1.170) = `-460.0875419 a.u.`

E(R=1.370) = `-460.0897602 a.u.`

$$E(x_0 - \Delta x) \cong \frac{1}{2}\frac{d^2U}{dx^2}\bigg|_{x_0}((x_0 - \Delta x) - x_0)^2$$

$$E(x_0 + \Delta x) \cong \frac{1}{2}\frac{d^2U}{dx^2}\bigg|_{x_0}((x_0 + \Delta x) - x_0)^2$$

$$\frac{d^2U}{dx^2}\bigg|_{x_0} \cong 2 \times \frac{E(x_0 - \Delta x) + E(x_0 + \Delta x) - 2 * E(x}{\Delta x^2}$$

$$\mu = \frac{m_H m_{Cl}}{m_H + m_{Cl}}$$
$$= \frac{(1.008)*(35.453)}{1.008 + 35.453} = .9801 g/mol$$
$$\equiv 1.6276e - 27 kg/molecule$$

$$E(x_0 - \Delta x) \cong \frac{1}{2}\frac{d^2U}{dx^2}\bigg|_{x_0}((x_0 - \Delta x) - x_0)^2$$

$$E(x_0 + \Delta x) \cong \frac{1}{2}\frac{d^2U}{dx^2}\bigg|_{x_0}((x_0 + \Delta x) - x_0)^2$$

$$\frac{d^2U}{dx^2}\bigg|_{x_0} \cong \frac{-460.0875419 + -460.0897602 - 2*(-460.0953282)}{.1*.1}$$

$$= 1.33543 au/A^2 \equiv k = 1.33543 au/A^2 * (1J/2.2939e^{17}) * (1A/1e - 10m)^2$$
$$= 5.82166e^2 J/m^2$$

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{5.82166e^{2} J/m^{2}}{1.6276e-27 kg/molecule}} = 5.98067e^{14}/s$$

$$\omega = 1.99156e4 cm^{-1}$$

$$\nu = \frac{\omega}{2\pi} = 3169.67 cm^{-1}$$

$$\nu_{\exp} = 2989.7 cm^{-1}$$

$$\nu_{calc} = 3105 cm^{-1}$$

Calculated value using HF at 6-311G* level. Note the harmonic calculation and computed vaues overestimate the experimental values. Often to correct for the harmonic assumption modelers will multiply the computed values by 5-10%