Grace Kim 1/7/09 class HW Chem Activity 21

Exercise #1-4, 6-10

1) The two main components of dry air are N_2 and O_2. Air does not absorb microwave radiation because N_2 and O_2 are symmetrical homonuclear molecules that do not have a permanent dipole moment, and therefore do not absorb microwaves to produce rotational spectra.
2) BF_3 (trigonal planar) , S_2 (linear), CO_2 (linear), SO_3 (trigonal planar), and $SiCl_4$ (tetrahedral) will not produce rotational spectra because they are very symmetric molecules. [NH_3—trigonal bipyramidal; SO_2—bent are asymmetrical and will produce rotational spectra].
3) The selection rule is that $\Delta J = +1$ or -1. $J=5 \rightarrow J=4$ and $J=4 \rightarrow J=5$ are allowed.
4) $\omega = 3.842\ cm^{-1} = 384.2\ m^{-1}$; $E=hc\ \omega = (6.63 \times 10^{-34}\ J\ s)\ (3.00 \times 10^{8}\ m/s)\ (384.2\ m^{-1}) = 7.64 \times 10^{-23}\ J$
   $\lambda=hc/E = (6.63 \times 10^{-34}\ J\ s)\ (3.00 \times 10^{8}\ m/s)/\ (7.64 \times 10^{-23}\ J) = 0.00260\ m = 2.6\ mm$

   $E\ (J=1 \rightarrow J=0) = 7.64 \times 10^{-23} J$ (the energy for $J=0 \rightarrow J=1$)

   I, moment of inertia for $^{12}C^{16}O$ molecule $= \mu r^2 = (12 \times 15.995)/\ (12 + 15.995) = 6.8562$ g/ mole x (1 mole/ 6.02 x 10^{23} molecules)r^2 =(1.1389×10^{-23}g/ molecule)r^2 = (1.1389×10^{-26}kg/ molecule)r^2

   $E\ (J=0 \rightarrow J=1) = 2B_e = 2h^2/(8\pi^2\mu r^2) = 7.64 \times 10^{-23} J$
   $r = \sqrt{}(2h^2/(8\pi^2(1.1389 \times 10^{-26}kg)(7.64 \times 10^{-23}J))) = \sqrt{}1.28 \times 10^{-20}\ m^2 = 1.13 \times 10^{-10}\ m = 113\ pm$

6) $E\ (J=1 \rightarrow J= 2) = 4B_e = 4h^2/(8\pi^2\mu r^2) =10.19 \times 10^{-24} J$
   μ for $^{39}K^{35}Cl$= (38.96 x 34.97)/ (38.96 +34.97) = 18.43 g/ mole x (1 mole/ 6.02 x 10^{23} molecules)
   = $3.061\ x10^{-23}$ g/ molecule = 3.061×10^{-26} kg/ molecule
   $r=\sqrt{}(4h^2/(8\pi^2(3.061 \times 10^{-26}kg)(10.19 \times 10^{-24}J))) = \sqrt{}7.14 \times 10^{-20}\ m^2 = 2.67 \times 10^{-10}\ m = 267\ pm$
7) $v= 6.350 \times 10^{5}\ MHz = 6.350 \times 10^{11}\ Hz$
   $E=hv = (6.63 \times 10^{-34}\ J\ s)(6.350 \times 10^{11}\ Hz) = 4.210 \times 10^{-22} J$
   μ for $^{1}H^{35}Cl$ = (1.008 x 34.97)/ (1.008 + 34.97) = 0.9798 g/mole x (1 mole/ 6.02 x 10^{23} molecules)
   =1.628×10^{-24} g/ molecule = 1.628×10^{-27} kg/ molecule

   E spacing $(J=0 \rightarrow J=0) = B_e = h^2/(8\pi^2\mu r^2) = 4.210 \times 10^{-22}\ J$
   $r=\sqrt{}(h^2/(8\pi^2(1.628 \times 10^{-27}kg)(4.210 \times 10^{-22}J))) = \sqrt{}8.123 \times 10^{-21}\ m^2 = 9.013 \times 10^{-11}\ m = 90.13\ pm$

   Yes, this bond length makes sense—it is smaller than for KCl and it should be K is in the fourth period and considerably bigger than H.
8) Dry air does not absorb IR radiation because the major components of dry air, N_2 and O_2, are homonuclear diatomic molecules. They cannot increase their vibrational energy by absorption of IR radiation because their dipole moments do not oscillate during vibration. Water, on the other hand, is a bent molecule with 2 H atoms and O atoms. It can absorb IR radiation because it has an oscillating dipole moment associated with its three vibrational modes—its antisymmetrical stretching mode, its symmetric stretching mode, and its bending mode (http://www.lsbu.ac.uk/water/vibrat.html or http://www.atmos.albany.edu/deas/atmclasses/atm335/vib1.htm).
9) The bending mode of CO_2 will be excited by IR radiation because its dipole moment oscillates during the bending motion.
10) The antisymmetrical stretch of CO_2 will also be excited by IR radiation because its dipole moment oscillates during the antisymmetric stretching motion.