**Chemistry I Introduction to Quantum Chemistry and Molecular Spectroscopy**

**Tutorial 12 by K. Mangala Sunder**

**Department of Chemistry, Indian Institute of Technology Madras**

**Assume speed of light to be 3 x 108 m.s-1; Planck’s constant *h* = 6.626 x 10-34 J.s**

1. The force constants of HI, HBr, HCl and HF are given as 314, 412, 516 and 966 Nm-1, respectively. The fundamental (or harmonic) vibrational frequencies are in the order
   1. 
   2. 
   3. 
   4.  Answer: a
2. The fundamental vibrational frequencies of HCl and DCl have the relation
   1. 
   2. 
   3. 
   4.  Answer: b
3. The reduced mass of CO is 1.138 x 10-26 kg and the force constant is 1902 Nm-1. Light required to induce a transition from  has a wave number of
   1. 6507 cm-1
   2. 4338 cm-1
   3. 2169 cm-1
   4. 1085 cm-1 Answer: c
4. The energy required to excite a molecule from its ground state to the first excited state corresponds to a wave number of 10 cm-1 both states being non-degenerate. In thermal equilibrium, at a temperature of 100 K, the ratio of the number of molecules in the excited vibrational state to those in the ground vibrational state is closest to
   1. 10-3
   2. 10-1
   3. 1.2
   4. 0.9 Answer : d
5. The Morse potential energy function for a diatomic molecule is given by the formula  where  is the vibrational amplitude. The interpretation of  is
   1. It is the force constant
   2. It is the frequency of fundamental vibration
   3. It is the energy required to excite the molecule from the ground state to the first excited state
   4. It is the dissociation energy of molecule from its equilibrium geometry Answer: d
6. The energy level expression for the Morse oscillator is ( is the anharmonicity constant and is << 1)
   1. 
   2. 
   3. 
   4.  Answer: d
7. The energy required to raise a Morse oscillator from an energy state with vibrational quantum number  to another state with  is given as
   1. 
   2. 
   3. 
   4.  Answer : c
8. The approximate formula for the anharmonicity coefficient  is ( id the dissociation energy; hint: problem 6)
   1. 
   2. 
   3. 
   4.  Answer: c
9. The selection rule for transitions in a Morse oscillator is
   1. 
   2. 
   3. 
   4.  can be of any integer. Answer: d
10. The parameter  in Morse oscillator is related to the harmonic oscillator frequency. The possible expression is
    1. 
    2. 
    3. 
    4.  Answer: b