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

**Tutorial 12 by K. Mangala Sunder**

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**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 vibrational normal mode(s) that is (are) infrared active in SO2 molecule is (are)
   1. Symmetric stretch mode only
   2. Asymmetric stretch mode only
   3. Bending mode only
   4. All three modes Answer: d
2. The number of genuine vibrational modes in the molecule is
   1. 30
   2. 29
   3. 31
   4. 33 Answer: c
3. The infrared inactive mode(s) in CO2 in molecule is (are)
   1. Symmetric stretch mode only
   2. Degenerate bending modes only
   3. Asymmetric and degenerate bending modes
   4. Symmetric and asymmetric stretching modes Answer: a
4. The zero point vibrational energy of carbon dioxide is given as
   1. 
   2. 
   3. 
   4.  Answer: c
5. NH3 has two degenerate normal vibrational modes each having the same frequency . The two modes are denoted by quantum numbers v1 and v2. When one quantum of radiation with the frequency  is absorbed by the molecule from its ground state, the quantum numbers of the excited states are
   1. (v1=0, v2=1) and (v1=1, v2=0)
   2. v1=1, v2=0 only
   3. v1=0, v2=1 only
   4. (v1=1, v2=1) Answer: a
6. The normal vibrational modes of CS2 have two degenerate bending modes each with a frequency corresponding to 397 cm-1. If a light of frequency corresponding to 794 cm-1 is used to excite ground state CS2, it will result in
   1. Exciting one degenerate vibration by two quanta to v=2 level
   2. Exciting each mode of CS2 by one quantum to v=1 level
   3. Exciting both bending modes to v=2 level
   4. Will not result in any absorption in the limit of harmonic oscillator model. Answer: d
7. The fundamental frequencies of vibrations of the diatomic molecule are given in brackets in the following reaction scheme,

HCl (2989 cm-1) + D2 (3119 cm-1)  DCl (2119 cm-1) + HD (3817 cm-1).

The enthalpy for the reaction in wave number units is

* 1. 147 cm-1
  2. -147 cm-1
  3. -73.5 cm-1
  4. 73.5 cm-1 Answer: c

1. The number of translational (T), rotational (R) and vibrational (V) degrees of the freedom of the molecule are
   1. 3 (T), 3 (R) and 6n+12 (V)
   2. 3 (T), 2 (R) and 6n+13 (V)
   3. 2 (T), 2 (R) and 6n+14 (V)
   4. 2 (T), 3 (R) and 6n+5 (V) Answer: b
2. A linear molecule AB2 may have either of the two possible structures A-B-B and B-A-B. The number of infrared active modes for each of them, are, respectively,
   1. 3 and 3
   2. 4 and 2
   3. 4 and 3
   4. 4 and 4 Answer: c
3. A linear molecule A2B2 has been assigned one of the possible structures, A-B-B-A, A-B-A-B, B-A-A-B or B-A-B-A. The molecule has two bending modes which are degenerate and all the seven modes are IR active. The correct structure is likely to be
   1. A-B-B-A only
   2. B-A-A-B only
   3. Both A-B-A-B and B-A-B-A
   4. Both A-B-A-B and B-A-A-B Answer: c