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reviewer1@nptel.iitm.ac.in ▾

Unit 8 - Week 7

Course outline

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- Lecture 32 - Diatomic Vibrational Spectra Harmonic Model
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Week 8

Assessment 12

The due date for submitting this assignment has passed. Due on 2017-03-24, 23:59 IST.

Submitted assignment

Chemistry I Introduction to Quantum Chemistry and Molecular Spectroscopy

Week 7: Tutorial 12 by K. Mangala Sunder

Department of Chemistry, Indian Institute of Technology Madras

Assume speed of light to be 3 x 10^8 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 point***

- $\nu_{HF} < \nu_{HCl} < \nu_{HBr} < \nu_{HI}$
- $\nu_{HF} > \nu_{HCl} > \nu_{HBr} > \nu_{HI}$
- $\nu_{HCl} < \nu_{HF} < \nu_{HBr} < \nu_{HI}$
- $\nu_{HF} > \nu_{HCl} > \nu_{HI} > \nu_{HBr}$

No, the answer is incorrect.
Score: 0

Accepted Answers:
$\nu_{HF} > \nu_{HCl} > \nu_{HBr} > \nu_{HI}$

2) The fundamental vibrational frequencies of HCl and DCl have the relation ***1 point***

- $\nu_{HCl} = \nu_{DCl}$
- $\nu_{HCl} \approx 1.395\nu_{DCl}$
- $\nu_{HCl} \approx 0.707\nu_{DCl}$
- $\nu_{HCl} = 2\nu_{DCl}$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$\nu_{HCl} \approx 1.395\nu_{DCl}$

3) The reduced mass of CO is $1.138 \times 10^{-26} kg$ and the force constant is $1902\ Nm^{-1}$. Light required to induce a transition from $n = 2$ to $n = 3$ has the wave number of **1 point**

- $6507\ cm^{-1}$
- $4338\ cm^{-1}$
- $2169\ cm^{-1}$
- $1085\ cm^{-1}$

No, the answer is incorrect.
Score: 0

Accepted Answers:
$2169\ cm^{-1}$

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 `$100K$, the ratio of the number of molecules in the excited vibrational state to those in the ground vibrational state is closest to **1 point**

- 10^{-3}
- 10^{-1}
- 1.2
- 0.9

No, the answer is incorrect.
Score: 0

Accepted Answers:
0.9

5) The Morse potential energy function for a diatomic molecule is given by the formula $D[1 - e^{-\alpha x}]^2$ where x is the vibrational amplitude. The interpretation of D is **1 point**

- It is the force constant
- It is the frequency of fundamental vibration
- It is the energy required to excite the molecule from the ground state to the first excited state
- It is the dissociation energy of molecule from its equilibrium geometry

No, the answer is incorrect.
Score: 0

Accepted Answers:
It is the dissociation energy of molecule from its equilibrium geometry

6) The energy level expression for the Morse oscillator is (x_e is the anharmonicity constant and is $<< 1$) **1 point**

- $E = h\nu_e(n + 1/2)$
- $E = h\nu_e(n + 1/2)^2$
- $E = h\nu_e(1 - x_e)(n + 1/2)$

$E = h\nu_e(n + 1/2) - h\nu_e x_e(n + 1/2)^2$

No, the answer is incorrect.
Score: 0

Accepted Answers:
$E = h\nu_e(n + 1/2) - h\nu_e x_e(n + 1/2)^2$

7) The energy required to raise a Morse oscillator from an energy state with vibrational quantum number $n = 1$ to another state with $n = 3$ is given by **1 point**

- $2h\nu_e - 18h\nu_e x_e$
- $2h\nu_e$
- $2h\nu_e - 10h\nu_e x_e$
- $2h\nu_e - 2h\nu_e x_e$

No, the answer is incorrect.
Score: 0

Accepted Answers:
$2h\nu_e - 10h\nu_e x_e$

8) The approximate formula for the anharmonicity coefficient x_e is (D is the dissociation energy) **1 point**
Hint: Problem 6

- $x_e \approx \sqrt{\frac{1}{D}}$
- $x_e \approx \sqrt{\frac{\nu_e}{D}}$
- $x_e \approx \frac{h\nu_e}{4D}$
- $x_e \approx \frac{\nu_e}{4hD}$

No, the answer is incorrect.
Score: 0

Accepted Answers:
$x_e \approx \frac{h\nu_e}{4D}$

9) The selection rule for transitions in a Morse oscillator is **1 point**

- $\Delta n = \pm 1$
- $\Delta n = \pm 1 \; or \; \pm 2$
- $\Delta n = \pm 2$ only
- Δn can be any integer

No, the answer is incorrect.
Score: 0

Accepted Answers:
Δn can be any integer

10) The parameter α in Morse oscillator is related to the harmonic oscillator frequency. The possible expression is **1 point**

- $\alpha \approx \nu_e$

- $\alpha \approx \sqrt{\frac{m_e \nu_e^2}{2D_e}}$
- $\alpha \approx \frac{1}{\nu_e}$
- $\alpha \approx \nu_e x_e$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$\alpha \approx \sqrt{\frac{m_e \nu_e^2}{2D_e}}$

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