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

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Assume speed of light to be $3 \times 10^8$ m.s$^{-1}$; Planck’s constant $h = 6.626 \times 10^{-34}$ 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 $\nu_{HF} < \nu_{HCl} < \nu_{HBr} < \nu_{HI}$

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

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

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

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 $\nu_{HCl} = \nu_{DCl}$

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

$\nu_{HCl} \approx 0.707 \nu_{DCl}$

$\nu_{HCl} = 2 \nu_{DCl}$

No, the answer is incorrect.

Score: 0

Accepted Answers:
\[ \nu_{HCl} \approx 1.395 \nu_{DCl} \]

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

- \(6507 \text{ cm}^{-1}\)
- \(4338 \text{ cm}^{-1}\)
- \(2169 \text{ cm}^{-1}\)
- \(1085 \text{ cm}^{-1}\)

No, the answer is incorrect.
Score: 0
Accepted Answers:

2169 \text{ 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 \(10 \text{ cm}^{-1}\) 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

- \(10^{-3}\)
- \(10^{-1}\)
- 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

- 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 \(<< 1\))

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

\[
E = \hbar \nu_e (n + 1/2) - \hbar \nu_e x_e (n + 1/2)^2
\]

No, the answer is incorrect.
Score: 0
Accepted Answers:
\[
E = \hbar \nu_e (n + 1/2) - \hbar \nu_e x_e (n + 1/2)^2
\]

8) The approximate formula for the anharmonicity coefficient \( x_e \) is (\( D \) is the dissociation energy)

Hint: Problem 6

\[
x_e \approx \sqrt{\frac{1}{D}}
\]
\[
x_e \approx \sqrt{\frac{\nu_e}{D}}
\]
\[
x_e \approx \frac{\hbar \nu_e}{4D}
\]
\[
x_e \approx \frac{\nu_e}{4D}
\]

No, the answer is incorrect.
Score: 0
Accepted Answers:
\[
x_e \approx \sqrt{\frac{1}{D}}
\]

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

\[
\Delta n = \pm 1
\]
\[
\Delta n = \pm 1 \text{ or } \pm 2
\]
\[
\Delta n = \pm 2 \text{ only}
\]
\[
\Delta n \text{ can be any integer}
\]

No, the answer is incorrect.
Score: 0
Accepted Answers:
\[
\Delta n = \pm 1 \text{ or } \pm 2
\]

10) The parameter \( \alpha \) in Morse oscillator is related to the harmonic oscillator frequency. The possible expression is

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

\[ \alpha \approx \frac{1}{\nu_e} \]

\[ \alpha \approx \nu_e x_e \]

No, the answer is incorrect.
Score: 0
Accepted Answers:
\[ \alpha \approx \sqrt{\frac{m_e \nu_e^2}{2D_e}} \]