Assessment 14

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
Tutorial 14 by K. Mangala Sunder
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Assume speed of light to be 3 x 10^8 m.s^{-1}; Planck’s constant \( \hbar = 6.626 \times 10^{-34} \) J.s.
J.S. Boltzmann constant \( k_B = 1.38 \times 10^{-23} \) J.K^{-1}. 1 amu = 1.661 \times 10^{-27} \) kg.

1) The SI unit for the moment of inertia of a diatomic molecule is

- \( kg \)
- \( N \ m^{-1} \)
- \( kg \ m^2 \)
- \( Joule \)

No, the answer is incorrect.
Score: 0

Accepted Answers:
- \( kg \ m^2 \)

2) The rotational constant for a diatomic molecule is given by the formula ( I is the moment of inertia about an axis passing through the centre of mass and perpendicular to the bond axis )

- \( \hbar^2 \ / 8\pi^2Ic \)
- \( \hbar \ / 8\pi^2IC \)
- \( \hbar IC \ / 8\pi^2 \)
- \( \hbar^2C \ / 8\pi^2I \)

No, the answer is incorrect.
Score: 0

Accepted Answers:
3) A symmetric top molecule has the following relation between its moment of inertia about the three principal axes which are mutually perpendicular to each other

- $I_x \neq I_y \neq I_z$
- $I_x = I_y \neq I_z$
- $I_x = I_z, I_z = 0$
- $I_x = I_y = I_z$

No, the answer is incorrect.
Score: 0
Accepted Answers:
$I_x = I_y \neq I_z$

4) Only one of the statements below is incorrect. Please identify.

- For a diatomic molecule there are two mutually perpendicular axes about which the moments of inertia is nonzero.
- For a diatomic molecule two of the three moments of inertia are equal and the third is very large.
- All three moments of inertia of a symmetric top molecule are nonzero.
- For a planar molecule, the sum of two of the moments of inertia is equal to the third.

No, the answer is incorrect.
Score: 0
Accepted Answers:
For a diatomic molecule two of the three moments of inertia are equal and the third is very large.

5) The molecule $BF_3$ is planar. The following statement is the correct statement.

- The sum of two moments of inertia about the principle axes is equal to the moment of inertia about the perpendicular axis.
- One of the moment of inertia is zero.
- All three moments of inertia are unequal.
- All three moments of inertia are equal.

No, the answer is incorrect.
Score: 0
Accepted Answers:
The sum of two moments of inertia about the principle axes is equal to the moment of inertia about the perpendicular axis.

6) The energy difference between successive rotational levels ($J$ and $J+1$) in a rigid diatomic molecule (in terms of its rotational constant $B$) is

- $hcB(2J + 1)$
- $2hcBJ$
- $2hcB(J + 1)$
- $hcB(J + 1)$

No, the answer is incorrect.
Score: 0
Accepted Answers:
$2hcB(J + 1)$

7) The rotational levels of a rigid diatomic molecule with the quantum number $J$ are
8) The rotational constants of the two molecules HCl and DCl (Deuterium chloride) are in the ratio, (assuming the equilibrium bond lengths to be the same)  

\[
\frac{B_{H\text{Cl}}}{B_{D\text{Cl}}} = \frac{\mu_{H\text{Cl}}^2}{\mu_{D\text{Cl}}^2}
\]

\[
\frac{B_{H\text{Cl}}}{B_{D\text{Cl}}} = \frac{\mu_{D\text{Cl}}}{\mu_{H\text{Cl}}}
\]

\[
\frac{B_{H\text{Cl}}}{B_{D\text{Cl}}} = \frac{\mu_{H\text{Cl}}^2}{\mu_{D\text{Cl}}^2}
\]

\[
\frac{B_{H\text{Cl}}}{B_{D\text{Cl}}} = \frac{\mu_{D\text{Cl}}}{\mu_{H\text{Cl}}}
\]

No, the answer is incorrect.  
Score: 0 
Accepted Answers:  
(2J+1) - fold degenerate 
J- fold degenerate 
Doubly degenerate except for the quantum number \( K \), projection of \( J \) onto an axis, equal to zero 
nondegenerate

9) The rotational constant for a certain molecule is 1 cm\(^{-1}\). The ratio of the number of molecule in \( J=1 \) to \( J=2 \) states at 1K, \( \frac{N_2}{N_1} \) is 

- 1  
- 0.5  
- 0.05  
- 0.005

No, the answer is incorrect.  
Score: 0 
Accepted Answers:  
0.005

10) A molecule with the formula \( AB_2 \) has a microwave spectrum with lines which are equidistant. The structure of the molecule is, 

- Linear A-A-B  
- Linear A-B-A  
- Bent A-B-B  
- Bent B-A-B

No, the answer is incorrect.  
Score: 0 
Accepted Answers:  
Linear A-A-B