Assessment 15

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 15 by K. Mangala Sunder

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Assume speed of light to be $3 \times 10^8$ m.s$^{-1}$; Planck's constant $\hbar = 6.626 \times 10^{-34}$

J.S. Boltzmann constant $k_B = 1.38 \times 10^{-23}$ J.K$^{-1}$. 1 amu = $1.661 \times 10^{-27}$ kg.

1.1) The microwave spectrum of BF species has the following spectral data: $J = 5$ to $J = 6$, 576257.28 MHz for $^{10}$B$^{19}$F. (Reference Source: NIST Tables.) The non-zero moment of inertia is $0.175 \times 10^{-49}$ kg m$^2$.

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

$0.175 \times 10^{-47}$ kgm$^2$

1.2) The rotational spectrum of a symmetric top molecule is given by lines which are separated from the neighboring ones by a spacing of $BJ(J + 1)$ $\frac{2B}{BJ(J + 1) - AK^2}$ $B(2J + 1)$

No, the answer is incorrect.
Score: 0
Accepted Answers:
2B

1.3) Rotational levels of a symmetric top are degenerate and

the degeneracy is one for all values of $K$
the degeneracy is $(2J + 1)$
the degeneracy increases as $K^2$ for each $K$

$K = 0$ state is nondegenerate and all others are doubly degenerate

No, the answer is incorrect.
Score: 0

Accepted Answers:
$K = 0$ state is nondegenerate and all others are doubly degenerate

1.4) Only one of the following four tables is correct with respect to all entries. Identify the correct table.

<table>
<thead>
<tr>
<th>CH₄, CCl₄, Octahedron</th>
<th>Symmetric top</th>
</tr>
</thead>
<tbody>
<tr>
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<td>Spherical top</td>
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<td>Asymmetric top</td>
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No, the answer is incorrect.
Score: 0

Accepted Answers:

1.5) The microwave spectrum of $^{12}$C$^{16}$O has a rotational splitting (between adjacent lines) of 115260 MHz. The carbon-oxygen interatomic distance is

1.301 Angstrom
1.403 Angstrom
1.131 Angstrom
1.6) The spacing between adjacent microwave lines for the molecule $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ is 12.16 GHz. The transition frequency corresponding to the transition between $J = 20$ and $J = 21$ is

- 276.52 GHz
- 255.36 GHz
- 243.20 GHz
- 222.04 GHz

No, the answer is incorrect. Score: 0

Accepted Answers:
- 1.131 Å

1.7) The spacing between adjacent microwave lines for the molecule $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ is 11.86 GHz. The ratio of the number of molecules in the $J = 2$ to $J = 3$ state at 300 K, $N_2/N_3$, is

- \( \frac{N_2}{N_3} = 1.50 \)
- \( \frac{N_2}{N_3} = 0.847 \)
- \( \frac{N_2}{N_3} = 1.26 \)
- \( \frac{N_2}{N_3} = 0.718 \)

No, the answer is incorrect. Score: 0

Accepted Answers:
- \( \frac{N_2}{N_3} = 0.718 \)

8) Using the figure 1 given below, the moment of inertia of water molecule about the z-axis is obtained as

- \( m_H r^2 \sin^2 \theta \)
- \( 2m_H r^2 \sin^2 \frac{\theta}{2} \)
- \( m_H r^2 \sin^2 \frac{\theta}{2} \)
The rotational J value for which the intensity of transition will be maximum is given by the value:

\[ J = 1 \text{, the first non-trivial rotational state} \]

\[ J = \sqrt{\frac{K_B T}{2hcB}} - \frac{1}{2} \text{ or the nearest integer} \]

\[ J = \frac{hcB}{K_B T} \text{ or the nearest integer} \]

The rotational constant of \( ^{12}\text{C}^{16}\text{O} \) is 3.842 cm\(^{-1} \) and that of \( ^{13}\text{C}^{16}\text{O} \) is 3.673 cm\(^{-1} \). The ratio of these constants, given by 1.046, is consistent with the ratio:

\[ \left( \frac{\mu_{^{13}\text{C}^{16}\text{O}}}{\mu_{^{12}\text{C}^{16}\text{O}}} \right)^2 \]

\[ \left( \frac{\mu_{^{12}\text{C}^{16}\text{O}}}{\mu_{^{13}\text{C}^{16}\text{O}}} \right)^2 \]