The Energy Of A Transition From The 2 To The 3 State In CO Is 0.00143 Ev (a) Compute The Rotational Inertia

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Understanding the fundamental properties of molecular energy transitions is crucial in fields such as quantum chemistry, spectroscopy, and molecular physics. When a molecule undergoes a transition between energy states, it provides insights into its structure, rotational dynamics, and bonding characteristics. In this article, we focus on a specific transition in carbon monoxide (CO): from the second to the third vibrational or rotational state, with an energy change of 0.00143 eV. We will explore how to compute the rotational inertia associated with this transition, delving into the underlying physics, relevant formulas, and step-by-step calculations.

Introduction to Molecular Energy Transitions

Molecular energy states are quantized, meaning molecules can only occupy specific energy levels. Transitions between these levels involve the absorption or emission of discrete energy quanta, often observed through spectroscopic techniques such as infrared (IR), microwave, or Raman spectroscopy.

Types of molecular transitions include:

- Vibrational transitions: involving changes in vibrational energy levels.
- Rotational transitions: involving changes in rotational energy states.
- Electronic transitions: involving changes in electronic energy levels.

In the case of CO, a diatomic molecule, the rotational and vibrational energy levels are often well-resolved and can be analyzed using quantum mechanical models.

The Significance of Rotational Inertia

Rotational inertia, or the moment of inertia, is a measure of an object's resistance to rotational acceleration about an axis. For diatomic molecules like CO, the moment of inertia is directly related to the molecule's bond length and atomic masses:

Formula for the moment of inertia (I):

$$ I = \mu r^2 $$

where:

- μ = reduced mass of the molecule
- r = bond length between the two atoms

Understanding and calculating the rotational inertia is essential for interpreting spectroscopic data, as it influences the rotational energy levels and transition frequencies.

Given Data and Objective

The problem states:

> The energy of a transition from the 2 to the 3 state in CO is 0.00143 eV.
> Compute the rotational inertia (I).

Our goal is to determine the rotational inertia based on this energy transition.

Converting Energy Units for Calculations

Spectroscopic calculations often require energies in SI units (joules). Since the given energy is in electronvolts (eV), we need to convert it:

Conversion factor:

$$ 1\, \text{eV} = 1.602 \times 10^{-19}\, \text{J} $$

Calculation:

$$ E = 0.00143\, \text{eV} \times 1.602 \times 10^{-19}\, \text{J/eV} $$
$$ E \approx 2.290 \times 10^{-22}\, \text{J} $$

Understanding Rotational Energy Levels in Diatomic Molecules

The rotational energy levels of a diatomic molecule are given by the quantum mechanical relation:

$$ E_J = B J (J + 1) $$

where:

- J = rotational quantum number
- B = rotational constant, related to the moment of inertia by:

$$ B = \frac{\hbar^2}{2 I} $$

- $\hbar$ = reduced Planck's constant $(1.055 \times 10^{-34}\, \text{Js})$

Energy difference between rotational levels:

For a transition from level J to $J + 1$:

$$ \Delta E = E_{J+1} - E_J = 2 B (J + 1) $$

In our case, the transition is from the $J=2$ to $J=3$ level:

$$ \Delta E_{2 \to 3} = 2 B (3) = 6 B $$

Relating the Transition Energy to the Rotational Constant

Given:

$$ \Delta E_{2 \to 3} = 0.00143\, \text{eV} = 2.290 \times 10^{-22}\, \text{J} $$

and the relation:

$$ \Delta E_{2 \to 3} = 6 B $$

we can solve for B:

$$ B = \frac{\Delta E_{2 \to 3}}{6} $$
$$ B = \frac{2.290 \times 10^{-22}}{6} $$
$$ B \approx 3.817 \times 10^{-23}\, \text{J} $$

Calculating the Moment of Inertia (I)

Recall the relation between B and I:

$$ B = \frac{\hbar^2}{2 I} $$

Rearranged to solve for I:

$$ I = \frac{\hbar^2}{2 B} $$

Substituting known values:

$$ I = \frac{(1.055 \times 10^{-34})^2}{2 \times 3.817 \times 10^{-23}} $$
$$ I = \frac{1.113 \times 10^{-68}}{7.634 \times 10^{-23}} $$
$$ I \approx 1.457 \times 10^{-46}\, \text{kg} \cdot \text{m}^2 $$

This value represents the rotational inertia of the CO molecule corresponding to the transition from the 2 to the 3 state.

Understanding the Results and Implications

The calculated rotational inertia offers insights into the molecular structure:

- Bond length estimation: Using $I = \mu r^2$, where μ is the reduced mass, we can estimate the bond length.

- Comparison with known data: The typical bond length in CO is approximately 1.128 Å (or 1.128×10^{-10} meters). Our calculated I aligns with this value, confirming the consistency of the calculation.

Determining the Reduced Mass of CO

To further analyze, we compute the reduced mass:

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

where:

- m_1 and m_2 are the masses of carbon and oxygen atoms.

Atomic masses:

- Carbon (C): 12.01 u
- Oxygen (O): 16.00 u

Converting atomic mass units to kilograms:

$$1\, \text{u} = 1.6605 \times 10^{-27}\, \text{kg}$$

Calculating:

$$m_C = 12.01 \times 1.6605 \times 10^{-27} \approx 1.996 \times 10^{-26}\, \text{kg}$$
$$m_O = 16.00 \times 1.6605 \times 10^{-27} \approx 2.6568 \times 10^{-26}\, \text{kg}$$

Then,

$$\mu = \frac{(1.996 \times 10^{-26})(2.6568 \times 10^{-26})}{1.996 \times 10^{-26} + 2.6568 \times 10^{-26}}$$
$$\mu \approx \frac{5.308 \times 10^{-52}}{4.6528 \times 10^{-26}}$$
$$\mu \approx 1.141 \times 10^{-26}\, \text{kg}$$

Estimating the Bond Length (r)

Using $I = \mu r^2$:

$$r = \sqrt{\frac{I}{\mu}}$$

Plugging in the values:

$$r = \sqrt{\frac{1.457 \times 10^{-46}}{1.141 \times 10^{-26}}}$$
$$r = \sqrt{1.277 \times 10^{-20}}$$
$$r \approx 1.13 \times 10^{-10}\, \text{m}$$

which aligns with the known bond length in CO (about 1.128 Å).

Conclusion and Significance

Calculating the rotational inertia from spectroscopic data allows scientists to infer detailed molecular structure information, including bond lengths and atomic arrangements. The process involves understanding the relationship between energy transitions, rotational constants, and molecular moments of inertia.

In our case, the transition energy of 0.00143 eV from the 2 to the 3 rotational state in CO led to a rotational inertia estimate consistent with known molecular data. This exemplifies how quantum mechanical principles underpin spectroscopic analysis and molecular characterization.

Key takeaways:

- Transition energies in molecules are directly related to their rotational and vibrational properties.
- Spectroscopic data can be used to calculate molecular parameters such as bond length and inertia.
- Understanding these calculations is essential for fields like molecular physics, materials science, and chemical analysis.

Frequently Asked Questions

What is the significance of the energy transition from the 2 to the 3 state in CO being 0.00143 eV?

This energy value indicates the energy difference between rotational energy levels in CO, which is essential for calculating properties like rotational inertia and understanding molecular spectra.

How do you convert the given energy of 0.00143 eV into SI units for calculating rotational inertia?

Multiply 0.00143 eV by 1.602 x 10^-19 Joules per eV to convert it into Joules, which is necessary for applying physics formulas to compute rotational inertia.

What is the formula to compute the rotational inertia (I) from the energy difference between rotational states?

The rotational energy difference $\Delta E = B h c (J+1) - J$, where B is the rotational constant. Rearranged, I can be calculated using $\Delta E = (h^2) / (8\pi^2 I) [J(J+1) - (J-1)J]$, depending on the specific transition.

How does the rotational inertia relate to the moment of inertia in molecular rotation?

The rotational inertia (I) is the moment of inertia of the molecule concerning its rotation axis, determining the energy levels; it can be derived from the observed energy transitions between rotational states.

What assumptions are typically made when calculating rotational inertia from spectral data like the 0.00143 eV transition?

Assumptions include that the molecule behaves as a rigid rotor, the transition is between adjacent rotational levels, and effects like centrifugal distortion are negligible at this energy scale.

Can the rotational inertia be used to determine the bond length of CO? If so, how?

Yes, by calculating the moment of inertia I from the transition energy and knowing the reduced mass of CO, the bond length can be derived since $I = \mu r^2$, where μ is the reduced mass and r is the bond length.

Additional Resources

Understanding the Energy of Transition from the 2 to the 3 State in CO: A Deep Dive into Rotational Inertia

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Introduction

The transition of a carbon monoxide (CO) molecule from its second to third rotational energy level, characterized by an energy change of approximately 0.00143 eV, offers profound insights into molecular rotational dynamics and the underlying physics governing diatomic molecules. This energy difference, although seemingly minute, encapsulates essential information about the molecule's rotational inertia, moments of inertia, and the quantum mechanical principles that describe molecular energy states.

In this comprehensive review, we will explore the significance of this transition, delve into the methodology for calculating the rotational inertia of CO, and understand the broader implications of these calculations in molecular physics and spectroscopy.

Significance of the Transition Energy in Molecular Physics

Quantum Mechanical Foundations

Diatomic molecules like CO are quintessential systems in molecular physics, providing a testing ground for quantum theory. Their rotational energy levels are quantized and can be described accurately using quantum numbers:

- Rotational quantum number (J): An integer (0, 1, 2, ...) denoting the rotational state.
- Energy of a rotational level (E_J): Given by the rigid rotor model as:

$$
E_J = B J (J + 1)
$$

where B is the rotational constant in energy units, related to the molecule's moment of inertia I by:

$$
B = \frac{\hbar^2}{2I}
$$

with $\hbar$ being the reduced Planck's constant.

The transition from the J=2 to J=3 state involves an energy change ΔE that can be precisely measured via spectroscopic techniques, providing a direct link to the molecule's moments of inertia.

Relevance of the 0.00143 eV Transition

- Spectroscopic measurements: The small energy value (~1.43 meV) corresponds to microwave or far-infrared regions, typical of rotational transitions.
- Molecular characterization: Knowing this energy allows for the calculation of the rotational constant B, and subsequently, the moment of inertia I, which reveals information about bond length and molecular mass distribution.

Conversion and Contextualization of Transition Energy

Before proceeding to calculations, it's crucial to convert the given energy into SI units for consistency:

$$

$$
1\, \mathrm{eV} = 1.60218 \times 10^{-19}\, \mathrm{J}
$$

Thus,

$$
\Delta E = 0.00143\, \mathrm{eV} = 0.00143 \times 1.60218 \times 10^{-19}\, \mathrm{J} \approx 2.29 \times 10^{-22}\, \mathrm{J}
$$

This energy corresponds to the difference between the $J=2$ and $J=3$ rotational levels, which we will relate to the rotational constant B.

Calculating the Rotational Constant (B)

Theoretical Framework

The energy difference between adjacent rotational levels in a rigid rotor is:

$$
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$$
E_{J+1} - E_J = 2B (J + 1)
$$

Specifically, for the $J=2 \rightarrow 3$ transition:

$$
\Delta E = E_3 - E_2 = 2B (3) = 6B
$$

Rearranged, the rotational constant B is:

$$
B = \frac{\Delta E}{6}
$$

Using the calculated ΔE:

$$
B = \frac{2.29 \times 10^{-22}\, \mathrm{J}}{6} \approx 3.82 \times 10^{-23}\, \mathrm{J}
$$

Determining the Moment of Inertia (I)

Given B in energy units, and knowing:

$$
B = \frac{\hbar^2}{2I}
$$

we can solve for I:

$$
I = \frac{\hbar^2}{2B}
$$

Where:

$$
\hbar = \frac{h}{2\pi} = 1.0545718 \times 10^{-34}\, \mathrm{Js}
$$

Plugging in the values:

$$
I = \frac{(1.0545718 \times 10^{-34})^2}{2 \times 3.82 \times 10^{-23}}
$$

Calculations:

$$
I = \frac{1.112 \times 10^{-68}}{7.64 \times 10^{-23}} \approx 1.45 \times 10^{-46}\, \mathrm{kg \cdot m^2}
$$

This is the rotational inertia of the CO molecule in its ground state, corresponding to the bond length and atomic masses.

Interpreting the Rotational Inertia of CO

Atomic Contributions

Carbon monoxide (CO) consists of:

- Carbon atom with atomic mass $\approx 12.01\, \mathrm{amu}$
- Oxygen atom with atomic mass $\approx 16.00\, \mathrm{amu}$

Expressed in kilograms:

$$
1\, \mathrm{amu} = 1.66054 \times 10^{-27}\, \mathrm{kg}
$$

So,

$$
m_C = 12.01 \times 1.66054 \times 10^{-27} \approx 1.994 \times 10^{-26}\, \mathrm{kg}
$$

$$
m_O = 16.00 \times 1.66054 \times 10^{-27} \approx 2.657 \times 10^{-26}\, \mathrm{kg}
$$

Calculating the Bond Length

Assuming the molecule behaves as a rigid rotor with point masses:

$$
I = \mu r^2
$$

where:

- μ is the reduced mass:

$$
\mu = \frac{m_C m_O}{m_C + m_O}
$$

Calculating:

$$
\mu = \frac{(1.994 \times 10^{-26})(2.657 \times 10^{-26})}{1.994 \times 10^{-26} + 2.657 \times 10^{-26}} \approx 1.095 \times 10^{-26}\, \mathrm{kg}
$$

Rearranging for bond length r:

$$
r = \sqrt{\frac{I}{\mu}}
$$

Plugging in:

$$
r = \sqrt{\frac{1.45 \times 10^{-46}}{1.095 \times 10^{-26}}} \approx \sqrt{1.324 \times 10^{-20}} \approx 1.15 \times
$$

$$
10^{-10}\, \mathrm{m}
$$

which is approximately:

$$
r \approx 115\, \mathrm{pm}
$$

This value aligns well with experimentally known bond lengths for CO (~112-115 pm), validating the calculation's accuracy.

Broader Implications and Applications

Spectroscopic Significance

Understanding the rotational inertia and the associated rotational constant B allows spectroscopists to:

- Identify molecular species in various environments (e.g., interstellar space).
- Determine molecular bond lengths with high precision.
- Study isotopic substitutions, as replacing atoms affects the

moment of inertia and spectral lines.

Molecular Dynamics and Material Science

Knowledge of rotational inertia informs:

- Molecular rotational temperature distributions.
- Collisional dynamics in gases.
- Insights into molecular bonding and structure.

Astrophysics and Astrochemistry

Rotational spectra of molecules like CO are pivotal in:

- Tracing molecular clouds.
- Understanding star formation processes.
- Analyzing the chemical composition of distant celestial objects.

Limitations and Considerations

While the calculations above provide a good approximation, real-world molecules are not perfect rigid rotors:

- Centrifugal distortion: At higher rotational levels, bond lengths stretch, affecting inertia.
- Vibrational coupling: Vibrational motion influences rotational levels.
- Electronic states: The molecule's electronic environment can modulate rotational constants.

Advanced models incorporate these factors, utilizing spectroscopic data to refine the molecular parameters.

Conclusion

The transition from the J=2 to J=3 state in CO, with an energy change of approximately 0.00143 eV, serves as a window into the molecule's rotational characteristics. Through meticulous calculation, we deduce that the rotational inertia I is approximately $1.45 \times 10^{-46}\, \mathrm{kg \cdot m^2}$, consistent with known bond lengths and molecular structure.

This analysis underscores the profound connection between quantum mechanical principles and observable spectroscopic phenomena. It exemplifies how a tiny energy shift can reveal detailed molecular insights, contributing significantly to fields

like chemical physics, spectroscopy, and astrochemistry. The **precision and depth of these calculations continue to enhance our understanding of molecular behavior, enabling scientists to decode the complexities of matter at the quantum level.**

References

- **Herzberg, G. (1950). Molecular Spectra and Molecular Structure: Spectra of Diatomic Molecules. Van Nostrand Reinhold.**
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