What Percentage Of Na Atoms Are In The Lowest Excited State In An Acetylene-air Flame At 2 500 K? The

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Understanding the behavior of sodium (Na) atoms in high-temperature combustion environments, such as acetylene-air flames, is crucial for applications ranging from spectroscopy to flame diagnostics. A key aspect of this is determining what proportion of sodium atoms occupy the lowest excited state at a given temperature—in this case, 2,500 K. This article explores the factors influencing atomic excitation, the theoretical basis for calculating the percentage of Na atoms in the lowest excited state, and the practical implications of these calculations.

Introduction to Sodium Atom Excitation in Flames

Sodium atoms are commonly studied in flame spectroscopy due to their prominent emission lines, notably the D-line doublet at approximately 589 nm. The intensity of these lines depends heavily on the population distribution of sodium atoms across various energy states, governed by thermodynamic principles and plasma conditions.

In a high-temperature flame like an acetylene-air mixture at 2,500 K, sodium atoms experience frequent collisions, leading to a distribution of atoms across different energy levels, as described by statistical mechanics. The key question is: what fraction of sodium atoms remains in the lowest excited state under these conditions?

Fundamental Concepts for Atomic Population Distribution

1. Boltzmann Distribution

The population of atoms in a specific energy state within a thermal equilibrium is described by the Boltzmann distribution:

$$ \frac{N_i}{N} = \frac{g_i e^{-E_i / (k T)}}{Z} $$

Where:
- N_i: number of atoms in energy level i
- N: total number of atoms
- g_i: degeneracy (statistical weight) of level i
- E_i: energy of level i above the ground state
- k: Boltzmann constant ($1.380649 \times 10^{-23} \, \mathrm{J\,K^{-1}}$)
- T: temperature in Kelvin
- Z: partition function, sum over all states

This relation indicates that the relative population of an energy level depends exponentially on the energy difference and inversely on temperature.

2. Partition Function Z

The partition function sums contributions from all energy states:

$$ Z = \sum_{i} g_i e^{-E_i / (k T)} $$

At high temperatures, higher energy levels become thermally accessible, increasing the partition function.

Energy Levels and Degeneracies of Sodium Atoms

To determine the population in the lowest excited state, we need specific information about sodium’s energy levels.

1. Ground State of Sodium

- Electronic configuration: $ [Ne] 3s^1 $
- Term symbol: $ ^2S_{1/2} $
- Energy: Reference zero (0 eV)

2. First Excited State

- State: $3p$
- Term: $^2P_{1/2}$ and $^2P_{3/2}$
- Energy difference: approximately 2.10 eV above ground

The D-line transitions correspond to electrons transitioning from the $3p$ state to the $3s$ state, resulting in strong emission at 589 nm.

3. Degeneracies g_i

- For $^2S_{1/2}$: $g_0 = 2 \times 1/2 + 1 = 2$
- For $^2P_{1/2}$: $g_1 = 2 \times 1/2 + 1 = 2$
- For $^2P_{3/2}$: $g_2 = 2 \times 3/2 + 1 = 4$

Given the focus on the lowest excited state, we consider the $3p$ states collectively, with a total degeneracy of 6.

Calculating the Population of Sodium in the Lowest Excited State at 2,500 K

1. Energy Difference Between Ground and First Excited State

- $\Delta E = 2.10 \, \mathrm{eV}$

Converting to Joules:

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

$$\Delta E = 2.10 \times 1.60218 \times 10^{-19} \approx 3.3648 \times 10^{-19} \, \mathrm{J}$$

2. Boltzmann Factor Calculation

Using the Boltzmann distribution:

$$\frac{N_1}{N_0} = \frac{g_1}{g_0} e^{-\Delta E / (k T)}$$

Where:
- g_1: degeneracy of excited state (sum over $^2P_{1/2}$ and $^2P_{3/2}$), total $g_{excited} = 6$
- $g_0 = 2$ (ground state)

Note: For simplicity, we consider the combined excited states as a single level with degeneracy 6.

Calculating the exponential term:

$$\frac{\Delta E}{k T} = \frac{3.3648 \times 10^{-19}}{1.380649 \times 10^{-23} \times 2500}$$

$$= \frac{3.3648 \times 10^{-19}}{3.45162 \times 10^{-20}} \approx 9.74$$

Then,

$$e^{-9.74} \approx 5.88 \times 10^{-5}$$

Now, the ratio:

$$\frac{N_{excited}}{N_{ground}} = \frac{6}{2} \times 5.88 \times 10^{-5} = 3 \times 5.88 \times 10^{-5} \approx 1.76 \times 10^{-4}$$

Determining the Percentage of Na Atoms in the Lowest Excited State

The total population of sodium atoms in the relevant states:

$$N_{total} = N_{ground} + N_{excited}$$

Given the ratio $N_{excited} / N_{ground}$:

$$N_{excited} \approx 1.76 \times 10^{-4} \times N_{ground}$$

So,

$$N_{total} \approx N_{ground} \times (1 + 1.76 \times 10^{-4})$$

The fraction of atoms in the lowest excited state:

$$\text{Percentage} = \left(\frac{N_{excited}}{N_{total}} \right) \times 100 \%$$

$$\approx \left(\frac{1.76 \times 10^{-4} \times N_{ground}}{N_{ground} \times (1 + 1.76 \times 10^{-4})} \right) \times 100 \%$$

$$ \approx \frac{1.76 \times 10^{-4}}{1 + 1.76 \times 10^{-4}} \times 100 \% $$

Since 1.76×10^{-4} is very small,

$$ \approx 1.76 \times 10^{-4} \times 100 \% \approx 0.0176 \% $$

Therefore, approximately 0.018% of sodium atoms are in the lowest excited state at 2,500 K in an acetylene-air flame.

Implications for Flame Spectroscopy and Diagnostics

Understanding this low excitation percentage is vital for interpreting sodium emission lines accurately. The weak population in excited states at this temperature explains why sodium emission intensity is sensitive to temperature and plasma conditions.

Practical considerations include:

- Emission intensity dependence: Since only a tiny fraction of sodium atoms are in the excited state, emission intensity scales with temperature and excitation conditions.
- Flame diagnostics: Accurate temperature measurements require knowledge of the population distribution.
- Spectroscopic techniques: Such calculations inform the calibration of atomic emission and absorption measurements.

Conclusion

In summary, at a temperature of 2,500 K, only a minute fraction—roughly 0.018%—of sodium atoms in an acetylene-air flame occupy the lowest excited state. This low population reflects the high energy gap and thermal equilibrium distribution governed by the Boltzmann law. These insights are essential for scientists and engineers working in flame spectroscopy, combustion diagnostics, and related fields to accurately interpret emission spectra and understand plasma behaviors.

References and Further Reading

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- Atkins, P., & de Paula, J. (2014). Physical Chemistry. Oxford University Press.
- NIST Atomic Spectra Database. (2023

Frequently Asked Questions

What is the approximate percentage of sodium (Na) atoms in the lowest excited state in an acetylene-air flame at 2500 K?

Typically, around 1-5% of sodium atoms are in the lowest excited state at 2500 K in such flames, depending on conditions like pressure and flame composition.

How does temperature influence the population of sodium atoms in the lowest excited state in a flame?

Higher temperatures increase the thermal energy, promoting more sodium atoms into excited states; at 2500 K, a notable fraction populates the lowest excited state, but it remains a small percentage relative to the total sodium atoms.

What factors affect the percentage of Na atoms in the lowest excited state in a combustion flame?

Factors include temperature, pressure, flame composition, and collisional deactivation processes, all of which influence the excitation and de-excitation dynamics of sodium atoms.

Why is sodium's emission in flames primarily due to transitions from the lowest excited state?

Because the lowest excited state is easily populated at high temperatures, and transitions from this state produce the characteristic bright yellow emission used in flame tests.

Can the percentage of sodium atoms in the excited state be directly measured experimentally in a

flame?

Yes, using spectroscopic techniques like emission spectroscopy, the relative populations of excited states can be estimated based on emission intensities and Boltzmann distributions.

How does the Boltzmann distribution help determine the population of Na atoms in the lowest excited state at 2500 K?

The Boltzmann distribution relates the population of excited states to temperature, allowing calculation of the fraction of atoms in the lowest excited state based on energy differences and temperature.

Is the percentage of sodium atoms in the lowest excited state significant enough to influence the flame's emission spectrum at 2500 K?

Yes, even a small percentage in the lowest excited state can produce strong emission lines, especially since transitions from this state are responsible for characteristic sodium flame colors.

Additional Resources

What Percentage Of Na Atoms Are In The Lowest Excited State In An Acetylene-air Flame At 2,500 K?

Introduction

The study of atomic excitation states within combustion environments provides critical insights into flame chemistry, spectral emissions, and the underlying physical processes. Among the myriad elements analyzed in such contexts, sodium (Na) stands out due to its prominent spectral lines and relevance in flame diagnostics. When sodium atoms are introduced into high-temperature flames, their excitation and ionization states influence both the radiative properties and the chemical dynamics of the system.

In particular, understanding what percentage of Na atoms are in the lowest excited state within an acetylene-air flame at 2,500 K offers valuable data for spectroscopic diagnostics, modeling of combustion processes, and the development of analytical techniques. This article aims to thoroughly evaluate this question by exploring the thermodynamic principles, atomic physics, and experimental considerations involved.

Background and Significance

Sodium's spectral signature, especially the prominent D-lines at approximately 589.0 nm and 589.6 nm, corresponds to electronic transitions from the first excited state (the 3p state) to the ground state (3s). The population distribution among sodium's atomic energy levels directly affects the intensity of these lines, which are often used in flame photometry and atomic absorption spectroscopy.

In combustion environments, especially in flames generated by acetylene-air mixtures, several factors influence atomic excitation:

- Temperature: Governs the distribution of atoms across energy states via Boltzmann statistics.
- Electron density: Affects collisional excitation and de-excitation processes.
- Chemical environment: Influences ionization and atomization efficiency.
- Radiative processes: Determine emission intensities based on population distributions.

Acetylene-air flames are characterized by high temperatures (~2,500 K), which promote significant atomic excitation but generally do not reach ionization equilibrium for sodium at this temperature. To estimate the percentage of Na atoms in the lowest excited state, a rigorous understanding of thermodynamic population distributions is essential.

Atomic Structure and Energy Levels of Sodium

Sodium (Na, atomic number 11) has a relatively simple electronic structure:

- Ground state: 3s (2S1/2)
- First excited state: 3p (2P1/2 and 2P3/2)

The primary spectral lines arise from the 3p → 3s transition, known as the D-lines.

Key energy parameters:

Level	Term	Energy (cm^{-1})	Approximate Energy (eV)
3s	2S1/2	0	0.000
3p	2P1/2	~17,200	~2.13
3p	2P3/2	~17,300	~2.14

The energy difference between the ground and first excited state (~2.1 eV) is significant relative to thermal energies at 2,500 K.

Thermodynamic Population Distribution: Boltzmann Equation

The fractional population of atoms in a particular energy level is described by the Boltzmann distribution:

$$
\frac{N_i}{N} = \frac{g_i e^{-E_i / (k_B T)}}{Z}
$$

where:

- N_i: number of atoms in state i
- N: total number of atoms
- g_i: degeneracy of level i
- E_i: energy of level i
- k_B: Boltzmann's constant ($8.617 \times 10^{-5}\, \mathrm{eV/K}$)
- T: temperature in Kelvin
- Z: partition function

Degeneracy g_i: For the 3p state, considering fine structure:

- 2P1/2: $g = 2J + 1 = 2$
- 2P3/2: $g = 4$

For simplicity, the total 3p state degeneracy is $g_{3p} = 2 + 4 = 6$.

Calculation of Population Fractions at 2,500 K

To determine the percentage of Na atoms in the lowest excited state, we focus on the dominant 3p state (averaging over fine structure). The key steps involve:

1. Estimate the Boltzmann factor:

$$
e^{-E_{3p} / (k_B T)} = e^{-\frac{2.1\, \mathrm{eV}}{8.617 \times 10^{-5} \times 2500}}
$$

Calculating the denominator:

$$
8.617 \times 10^{-5} \times 2500 \approx 0.2154\, \mathrm{eV}
$$

Thus,

$$
e^{-2.1 / 0.2154} \approx e^{-9.75} \approx 5.8 \times 10^{-5}

\]

2. Estimate the partition function Z:

At high temperatures, the partition function includes contributions from various states, but for sodium at 2,500 K, the dominant populations are:

- Ground state 3s
- First excited states (3p)
- Higher states are negligible at this temperature

Assuming the ground state degeneracy $g_{ground} = 2$ (for 2S1/2), and the excited state degeneracy $g_{3p} = 6$:

$$
Z \approx g_{ground} + g_{3p} \times e^{-E_{3p} / (k_B T)} \approx 2 + 6 \times 5.8 \times 10^{-5} \approx 2 + 3.5 \times 10^{-4} \approx 2.00035
$$

3. Calculate the fraction in the excited state:

$$
\frac{N_{3p}}{N} \approx \frac{6 \times 5.8 \times 10^{-5}}{2 + 3.5 \times 10^{-4}} \approx \frac{3.48 \times 10^{-4}}{2.00035} \approx 1.74 \times 10^{-4}
$$

Expressed as a percentage:

$$
\approx 0.0174\%
$$

This indicates that less than 0.02% of sodium atoms are in the lowest excited state at 2,500 K under thermal equilibrium.

Considerations Beyond Pure Thermodynamics

While the Boltzmann distribution provides a baseline estimate, real combustion environments involve additional factors:

- Collisional excitation and de-excitation: Collisions with electrons and molecules can alter populations, often increasing excited state populations relative to LTE predictions.
- Radiative decay rates: The lifetime of the 3p states (~16 ns) influences steady-state populations.
- Ionization: Sodium tends to ionize at high temperatures, reducing the neutral atom population.

In laboratory flames, measurements often show that the excited state populations are higher than predicted by LTE models at comparable temperatures, owing to non-thermal excitation mechanisms.

However, at 2,500 K, the temperature is typically insufficient to cause significant non-thermal excitation of sodium atoms, especially in a relatively stable acetylene-air flame, which favors thermodynamic equilibrium.

Experimental Diagnostics and Validation

Spectroscopic measurements, such as emission line intensities, enable indirect estimation of excited state populations. Using the Einstein coefficients and emission intensities, researchers can back-calculate the level populations.

Typical experimental findings:

- The relative intensity of the sodium D-lines correlates with the excited state population.
- In flames at similar temperatures, the excited state population of Na is often a tiny fraction—on the order of 10^{-4} to 10^{-3}—consistent with thermodynamic calculations.

Implications and Conclusions

Based on thermodynamic principles and typical spectral data:

- Less than 0.02% of sodium atoms are in the lowest excited state (3p) in an acetylene-air flame at 2,500 K.
- The dominant sodium population remains in the ground state, with a minuscule fraction thermally excited.
- Non-thermal effects, such as electron bombardment or laser excitation, can significantly increase the excited state population, but under typical flame conditions, thermal equilibrium dominates.

This small population fraction underscores the importance of sensitive spectroscopic techniques for sodium detection in combustion diagnostics. Furthermore, the negligible excited state population at 2,500 K suggests that sodium emission intensity is primarily driven by the ground state atom abundance and excitation mechanisms.

Future Directions and Research Opportunities

While the thermodynamic estimate provides a solid foundation, further experimental studies are necessary to:

- Quantify non-equilibrium effects in real flames.
- Investigate the influence of varying flame compositions and temperatures.
- Model collisional-radiative processes to refine population estimates.

Understanding these nuances will enhance the accuracy of spectroscopic diagnostics and improve models of flame chemistry.

Summary

In conclusion, less than 0.02% of Na atoms are in the lowest excited state (3p) in an acetylene-air flame at 2,500 K under thermal equilibrium conditions. This tiny fraction reflects the high energy gap and the relatively moderate temperature, emphasizing the need for sensitive detection methods when analyzing sodium

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