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Introduction

Understanding the entropy change during phase transitions is fundamental in thermodynamics and chemical engineering. Specifically, calculating the entropy change (ΔS) when a substance undergoes a phase change from solid to liquid provides insights into the disorder and energy dispersal in the system. In this article, we will explore how to determine the entropy change for 1.74 moles of naphthalene as it melts at 80.3°C, given the enthalpy of fusion (h) as 18.8 kJ/mol.

Fundamentals of Entropy and Phase Change

What is Entropy?

Entropy (S) is a thermodynamic property that quantifies the degree of disorder or randomness in a system. During a phase change, such as melting or vaporization, entropy typically increases because molecules become more disordered.

Phase Change and Enthalpy of Fusion

When a solid melts into a liquid, the system absorbs energy known as the enthalpy of fusion (ΔH_{fus}). This energy facilitates the transition from an ordered solid to a more disordered liquid without changing temperature. The enthalpy of fusion is expressed in units of energy per mole, commonly kJ/mol.

Calculating the Entropy Change (ΔS)

The fundamental relation connecting the entropy change during a phase change to the enthalpy of fusion is:

$$\Delta S = \Delta H / T$$

Where:
- ΔS = entropy change (J/K)
- ΔH = enthalpy of fusion (J)
- T = absolute temperature in Kelvin (K)

Since the enthalpy of fusion is given per mole, the total entropy change for a given number of moles (n) is:

$$\Delta S_{total} = n \times (\Delta H_{fus} / T)$$

Step-by-Step Calculation

1. Convert Enthalpy of Fusion to Correct Units

Given:
- Enthalpy of fusion, h = 18.8 kJ/mol

Convert to joules per mole:

$$h = 18.8 \text{ kJ/mol} \times 1000 \text{ J/kJ} = 18{,}800 \text{ J/mol}$$

2. Convert Temperature to Kelvin

Given temperature:
- T = 80.3°C

Convert to Kelvin:

$$T = 80.3 + 273.15 = 353.45 \text{ K}$$

3. Calculate Entropy Change per Mole

Using the formula:

ΔS per mol = $\Delta H_{fus} / T$ = 18,800 J/mol / 353.45 K ≈ 53.2 J/(mol·K)

4. Calculate Total Entropy Change for 1.74 Moles

Multiply by the number of moles:

ΔS_{total} = 1.74 mol × 53.2 J/(mol·K) ≈ 92.6 J/K

Final Result

The entropy change associated with the melting of 1.74 moles of naphthalene at 80.3°C is approximately 92.6 Joules per Kelvin.

Additional Considerations

Temperature Dependence

While the calculation assumes the entropy change at the melting point, real systems may experience slight variations if the temperature differs from the melting point due to supercooling or superheating. However, for standard thermodynamic calculations, using the melting temperature provides a reliable estimate.

Impact of Pressure

The enthalpy of fusion and entropy change are typically considered at atmospheric pressure unless specified otherwise. Changes in pressure can influence melting points and enthalpy values.

Application in Industrial Processes

Understanding the entropy change during melting helps in designing processes such as crystallization, material synthesis, and thermal management. In the case of naphthalene, which is used in mothballs and chemical manufacturing, controlling phase transitions is vital for storage and processing.

Summary

- The entropy change during the melting of naphthalene can be calculated using the relation $\Delta S = \Delta H / T$.
- Given the enthalpy of fusion (18.8 kJ/mol) and temperature (80.3°C), the calculation yields approximately 53.2 J/(mol·K) per mole.
- For 1.74 moles, the total entropy change is approximately 92.6 J/K.
- This process highlights the increase in disorder as naphthalene transitions from solid to liquid.

Conclusion

Determining the entropy change during phase transitions is essential for thermodynamic analysis and process optimization. By understanding the principles of entropy and utilizing the appropriate formulas, engineers and scientists can accurately quantify the disorder introduced during melting. In the specific case of naphthalene, the entropy increase is significant, reflecting the molecular disorder introduced as the solid melts into a liquid at its melting temperature. Such calculations are indispensable in material science, chemical engineering, and thermodynamics for designing efficient and safe industrial processes.

References

- Atkins, P., & de Paula, J. (2010). Physical Chemistry. Oxford University Press.
- Smith, J. M., Van Ness, H. C., & Abbott, M. M. (2005). Introduction to Chemical Engineering Thermodynamics. McGraw-Hill.
- Naphthalene data sheet, Chemical Safety Data Sheets (CSDS), 2023.

Note: Always ensure to use the most recent and accurate thermodynamic data for precise calculations, especially in professional or research settings.

Frequently Asked Questions

What is the significance of the molar enthalpy of fusion (h) in calculating the heat required for the phase change of naphthalene?

The molar enthalpy of fusion (h) represents the amount of energy needed to convert one mole of naphthalene from solid to liquid at its melting point. It is used to calculate the total heat (S) required for the phase change by multiplying it with the number of moles.

How do you calculate the heat (S) required to melt 1.74 moles of naphthalene at 80.3°C?

Since the molar enthalpy of fusion is given as 18.8 kJ/mol, the heat required is $S = n \times h = 1.74 \text{ mol} \times 18.8 \text{ kJ/mol} = 32.712 \text{ kJ}$.

Is the temperature of 80.3°C above or below naphthalene's melting point, and how does this affect the calculation of S?

Naphthalene's melting point is approximately 80.2°C, so 80.3°C is just above it. Since the phase change occurs at the melting point, the calculation of S considers the heat needed at that temperature. If the temperature is above or below, additional considerations for temperature change would be necessary.

What units should be used for the enthalpy of fusion (h) and the resulting S value in calculations?

The enthalpy of fusion (h) should be in kilojoules per mole (kJ/mol), and the total heat (S) will be in kilojoules (kJ) when multiplied by the number of moles.

Can the formula for determining S be applied directly without considering temperature differences in this case?

Yes, because the calculation involves the heat required to change the phase at the melting temperature. If the temperature differs significantly from the melting point, additional heat calculations for heating or cooling would be necessary.

What is the approximate value of the heat S required for the phase change of 1.74 moles of naphthalene from solid to liquid at 80.3°C?

Using $S = n \times h$, the approximate heat required is 32.712 kJ.

Additional Resources

Determining the entropy change (ΔS) for the phase transition of naphthalene from solid to liquid at 80.3°C involves understanding thermodynamic principles, phase transition phenomena, and the application of specific heat and enthalpy data. This process is fundamental in physical chemistry, providing insights into the molecular disorder and energy transformations during melting. In this comprehensive review, we will explore the theoretical foundations, detailed calculations, and broader implications of such a determination, exemplified by the given data: 1.74 moles of naphthalene, melting point at 80.3°C, and an enthalpy of fusion (h) equal to 18.8 kJ/mol.>

Understanding Phase Changes and Thermodynamics

Phase Changes in Substances

Phase transitions, such as melting, boiling, or sublimation, are physical processes where a substance changes its state—solid, liquid, or gas—without altering its chemical composition. Melting, or fusion, specifically refers to the transition from solid to liquid. For naphthalene, this process occurs at a precise temperature of 80.3°C under standard atmospheric pressure, marking its melting point.

This transition involves an energy input to overcome intermolecular forces holding the molecules in a crystalline lattice. The energy required per mole to effect this change is termed the enthalpy of fusion (ΔH_{fus} or h). For naphthalene, this is given as 18.8 kJ/mol, representing the molar energy needed to convert solid naphthalene at its melting point into liquid at the same temperature.

Thermodynamic Quantities in Phase Changes

Key thermodynamic parameters associated with phase changes include:

- Enthalpy of Fusion (ΔH_{fus}): The energy absorbed per mole during melting at constant pressure.
- Entropy of Fusion (ΔS_{fus}): The change in entropy associated with melting, indicating increased molecular disorder.
- Gibbs Free Energy (ΔG): Determines the spontaneity of the phase change; at equilibrium (melting point), $\Delta G = 0$.

The fundamental thermodynamic relationship connecting these quantities is:

$$
\Delta G = \Delta H - T \Delta S
$$

At the melting point (T_m), the phase change occurs at equilibrium, so:

$$
\Delta G_{fusion} = 0 \Rightarrow \Delta H_{fusion} = T_m \Delta S_{fusion}
$$

This relationship allows us to calculate the entropy change directly from the enthalpy of fusion and the melting temperature.

Calculating the Entropy Change (ΔS) During Melting

Basic Formula for ΔS

Given the relationship at equilibrium:

$$
\Delta S_{fusion} = \frac{\Delta H_{fusion}}{T_m}
$$

where:

- ΔH_{fusion} is the molar enthalpy of fusion,
- T_m is the melting temperature in Kelvin.

For naphthalene:

$$
T_m = 80.3^\circ C = 80.3 + 273.15 = 353.45\, K
$$

Thus, the molar entropy change for melting is:

$$
\Delta S_{fusion} = \frac{18.8\, \text{kJ/mol}}{353.45\, \text{K}}
$$

Note: Convert kJ to J for consistency:

$$
18.8\, \text{kJ/mol} = 18800\, \text{J/mol}
$$

So,

$$
\Delta S_{fusion} = \frac{18800\, \text{J/mol}}{353.45\, \text{K}} \approx 53.2\, \text{J/(mol·K)}
$$

This value indicates the increase in disorder per mole as naphthalene melts.

Calculating Total Entropy Change for 1.74 Moles

The total entropy change (ΔS_{total}) for the specified amount of substance is:

$$
\Delta S_{total} = n \times \Delta S_{fusion}
$$

where:

- $n = 1.74\, \text{moles}$,
- $\Delta S_{fusion} \approx 53.2\, \text{J/(mol·K)}$.

Thus,

$$
\Delta S_{total} = 1.74 \times 53.2 \approx 92.6\, \text{J/K}
$$

This value reflects the overall increase in entropy associated with melting 1.74 moles of naphthalene at its melting point.

Incorporating Specific Heat and Other Thermodynamic Considerations

Role of Specific Heat (c) and Heat Capacity

While the primary calculation of ΔS at the melting point is straightforward, in practical scenarios, the temperature may not be exactly at the melting point, or the heating process may involve temperature gradients. Specific heat capacity (c) influences the energy required to raise the temperature of the substance, and thus, the entropy change associated with heating or cooling processes.

Given the specific heat c (not provided explicitly here but often available in thermodynamic tables), the entropy change when heating a substance from temperature T_1 to T_2 is:

$$
\Delta S = n c \ln \frac{T_2}{T_1}
$$

However, in the context of melting at the melting point, this consideration is secondary unless the temperature deviates from T_m.

Impact of Enthalpy of Fusion (h) and Latent Heat

The enthalpy of fusion (h = 18.8 kJ/mol) is a measure of the latent heat required for melting. This energy input doesn't change the temperature until the phase transition completes. The total energy input for 1.74 moles of naphthalene is:

$$
Q = n \times h = 1.74 \times 18.8\, \text{kJ} \approx 32.7\, \text{kJ}
$$

While this energy primarily affects the enthalpy change, it also correlates with the entropy change, as shown earlier, emphasizing the link between energy absorption and increased molecular disorder.

Broader Implications and Applications

Understanding Material Properties and Stability

Determining ΔS for phase transitions like melting provides critical insights into the thermodynamic stability of substances. A higher entropy change indicates a more substantial increase in disorder, which can influence melting behavior, solubility, and reactivity.

For naphthalene, knowing the entropy change helps in:

- Predicting melting behavior under different conditions.
- Designing processes involving melting and solidification.
- Understanding thermodynamic cycles involving naphthalene.

Relevance in Chemical Engineering and Material Science

Accurate thermodynamic data underpin the design of industrial processes such as:

- Crystallization and purification.
- Thermal storage systems.
- Material synthesis and processing.

Quantitative knowledge of entropy changes aids in optimizing energy efficiency and safety.

Environmental and Safety Considerations

Since naphthalene is a volatile aromatic hydrocarbon, understanding its phase behavior is essential for:

- Safe storage and handling.
- Environmental impact assessments.
- Regulatory compliance.

Knowledge of the thermodynamics involved in melting and vaporization helps in developing safety protocols and containment strategies.

Conclusion

Determining the entropy change (\(\Delta S\)) for the phase transition of 1.74 moles of naphthalene from solid to liquid at 80.3°C encapsulates fundamental thermodynamic principles. By leveraging the molar enthalpy of fusion and the melting temperature, we find that the entropy increases by approximately 92.6 J/K during this process. This analysis not only underscores the importance of thermodynamic parameters in understanding phase transitions but also highlights their practical relevance in scientific and industrial contexts.

The process exemplifies how detailed calculations, grounded in thermodynamic theory, enable scientists and engineers to predict and manipulate material behaviors. As we deepen our understanding of such fundamental phenomena, we pave the way for innovations in material design, energy management, and safety protocols—integral components of advancing science and technology.

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