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Understanding the standard entropy of formation at 298K for different substances is crucial in thermodynamics, helping scientists and engineers analyze the spontaneity of chemical reactions, determine equilibrium states, and calculate other thermodynamic properties. This article provides an in-depth explanation of how to determine the standard entropy of formation at 298K for hydrogen gas (H2), water vapor (H2O), ammonia (NH3), and ozone (O3). We will explore the concepts, relevant data, and methodologies involved in these calculations.

What Is Standard Entropy of Formation?

Standard entropy of formation, denoted as $\Delta S°_f$, is the change in entropy when one mole of a compound is formed from its constituent elements in their standard states under standard conditions (25°C or 298K and 1 atm pressure). It measures the disorder or randomness associated with forming a compound from elemental forms.

Key points:

- It is expressed in units of J/(mol·K).
- For elements in their most stable form at 1 atm and 25°C, the standard entropy of formation is zero.
- The values of $\Delta S°_f$ are tabulated in thermodynamic data sources, such as the NIST Chemistry WebBook.

Fundamental Concepts in Determining Standard Entropy of Formation

Before delving into specific data, it's important to understand the general principles:

Standard States and Reference Conditions

- Elements are considered in their most stable form at 1 atm and 25°C.
- For example, H2 gas, O2 gas, and N2 gas are in their diatomic molecular form.

Thermodynamic Data Sources

- Standard entropy of formation values are obtained from experimental measurements and compiled in thermodynamic tables.
- These values are used as references for calculating reaction entropies and other thermodynamic parameters.

Relation to Absolute Entropy

- Absolute entropy ($S°$) of a substance includes its entropy in the standard state.
- $\Delta S°_f$ measures the change in entropy during formation from elements.

Standard Entropy of Formation Values at 298K

Below are the standard entropy of formation values for the substances of interest, typically sourced from authoritative data tables like NIST.

Hydrogen Gas ($H_2(g)$)

- Since H_2 gas in its elemental form is the standard state, its $\Delta S°_f$ is zero.

Value:

- $\Delta S°_f (H_2(g)) = 0$ J/(mol·K)

Water Vapor ($H_2O(g)$)

- The formation of water vapor from hydrogen and oxygen involves an increase in entropy due to the formation of a molecular compound with specific vibrational and rotational modes.

Value:

- $\Delta S°_f (H_2O(g)) \approx +188.8$ J/(mol·K)

Ammonia ($NH_3(g)$)

- Ammonia is a more complex molecule with significant molecular vibrational modes, influencing its entropy.

Value:

- $\Delta S°_f (NH_3(g)) \approx +192.3$ J/(mol·K)

Ozone ($O_3(g)$)

- Ozone is an allotrope of oxygen with a bent structure, contributing to its unique entropy characteristics.

Value:

- $\Delta S°_f (O_3(g)) \approx +238.8$ J/(mol·K)

Note: These values are approximate and can vary slightly depending on the source, but they are widely accepted in thermodynamic calculations.

Methodology to Determine Standard Entropy of Formation

Although tabulated values are readily available, understanding how these are determined involves the following steps:

1. Experimental Measurement

- The entropy of a substance can be measured directly using calorimetric techniques and spectroscopy.

2. Thermodynamic Calculations

- Use of statistical mechanics to compute entropy based on molecular degrees of freedom (translational, rotational, vibrational).
- Calculation involves partition functions derived from spectroscopic data.

3. Hess's Law and Standard Data

- Combining standard enthalpy and entropy data via Hess's Law allows derivation from known reactions.

4. Computational Methods

- Quantum chemical calculations can estimate entropy values based on molecular geometry and vibrational frequencies.

Significance of Standard Entropy of Formation

Understanding $\Delta S°_f$ helps in various thermodynamic calculations:

- Determining Gibbs free energy change ($\Delta G°$) for reactions.
- Predicting reaction spontaneity at different temperatures.
- Developing thermodynamic models for industrial processes.

Application Examples

Let's consider how these values are used in practice:

Example 1: Calculating $\Delta G°$ for the Formation of Water Vapor

Given:

- $\Delta H°_f$ ($H_2O(g)$) ≈ -241.8 kJ/mol
- $\Delta S°_f$ ($H_2O(g)$) ≈ +188.8 J/(mol·K)

At 298K:

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

$$

$$
\Delta G^\circ = -241.8 \times 10^3 \text{ J/mol} - 298 \text{ K} \times 188.8 \text{ J/(mol·K)}
$$

$$
\Delta G^\circ \approx -241,800 \text{ J/mol} - 56,278 \text{ J/mol} = -298,078 \text{ J/mol}
$$

Since ΔG° is negative, the formation of water vapor from elements is spontaneous at 298K.

Example 2: Spontaneity of Ammonia Formation

Similarly, using known ΔH°f and ΔS°f for NH3, chemists can assess reaction feasibility and equilibrium positions.

Summary and Key Takeaways

- The standard entropy of formation at 298K quantifies the disorder change when compounds form from elements.
- Values are well-documented for common gases:
- H2(g): 0 J/(mol·K)
- H2O(g): approximately +188.8 J/(mol·K)
- NH3(g): approximately +192.3 J/(mol·K)
- O3(g): approximately +238.8 J/(mol·K)
- These values are essential for thermodynamic calculations involving reaction spontaneity, equilibrium, and energy efficiency.
- Combining entropy data with enthalpy allows for comprehensive analysis of chemical processes at standard conditions.

Conclusion

Determining the standard entropy of formation at 298K for gases like H2, H2O, NH3, and O3 provides critical insights into their thermodynamic behavior. These values are foundational in chemical thermodynamics, enabling scientists to predict reaction directions, calculate free energies, and design processes with optimal efficiency. Whether sourced from experimental data or computed via advanced methods, understanding and applying these entropy values are vital skills for chemists and engineers working in research, industry, and environmental science.

References:

- NIST Chemistry WebBook: Thermodynamic Data
- Atkins, P., & de Paula, J. (2010). Physical Chemistry. Oxford University Press.
- Zumdahl, S. S., & Zumdahl, S. A. (2014). Chemistry. Cengage Learning.

Frequently Asked Questions

What is the standard entropy of formation (ΔS°f) for H2(g) at 298K?

The standard entropy of formation for H2(g) at 298K is zero because it is an element in its standard state.

How do you determine the standard entropy of formation for H2O(g) at 298K?

The standard entropy of formation for H2O(g) at 298K is approximately 188.8 J/(mol·K), based on standard thermodynamic data tables.

What is the standard entropy of formation for NH3(g) at 298K?

The standard entropy of formation for NH3(g) at 298K is about 192.8 J/(mol·K), according to standard thermodynamic data.

Can you provide the standard entropy of formation for O3(g) at 298K?

Yes, the standard entropy of formation for O3(g) at 298K is approximately 238.7 J/(mol·K).

Why is the standard entropy of formation for H2(g) zero at 298K?

Because H2(g) is an element in its standard state, its standard entropy of formation is defined as zero by convention.

How are standard entropies of formation useful in thermodynamics?

They are essential for calculating reaction entropy changes, predicting spontaneity, and understanding thermodynamic feasibility of reactions.

Are the standard entropies of formation the same at different temperatures?

No, standard entropies of formation vary with temperature; the values at 298K are standard reference points.

Where can I find reliable data for standard entropies of formation at 298K?

Reliable data can be found in thermodynamic tables, standard reference books, or reputable online databases such as NIST.

How does the molecular structure influence the standard entropy of formation for gases?

More complex molecules with greater degrees of freedom and larger molar masses generally have higher standard entropies of formation.

Additional Resources

Determining the Standard Entropy of Formation at 298 K for Gaseous Substances: An In-Depth Analysis of $H_2(g)$, $H_2O(g)$, $NH_3(g)$, and $O_3(g)$

Understanding the thermodynamic properties of chemical substances is fundamental in the field of chemistry, particularly when exploring reaction spontaneity, equilibrium, and energy management. Among these properties, standard entropy of formation (denoted as $\Delta S°_f$) at 298 K (room temperature) provides critical insights into the disorder or randomness introduced when forming a compound from its constituent elements under standard conditions. This article delves into the methodology, significance, and detailed analysis of calculating and interpreting the standard entropy of formation for four representative gaseous molecules: hydrogen gas ($H_2(g)$), water vapor ($H_2O(g)$), ammonia ($NH_3(g)$), and ozone ($O_3(g)$).

Understanding Standard Entropy of Formation

Definition and Importance

Standard entropy of formation, $\Delta S°_f$, refers to the change in entropy when one mole of a compound is formed from its elements in their standard states at 298 K and 1 bar pressure. It is a thermodynamic quantity that reflects the degree of disorder or randomness associated with the formation process.

This property is vital because:
- It helps in calculating the total entropy change of reactions.
- It informs the Gibbs free energy change ($\Delta G°$), which predicts spontaneity.
- It aids in understanding phase stability and the thermodynamic favorability of compound formation.

Standard States of Elements and Compounds

Before calculating $\Delta S°_f$, it's essential to specify the standard states:
- For gases like H_2, H_2O, NH_3, and O_3, the standard state is their gaseous form at 1 bar.
- Elements are considered in their most stable form under standard conditions (e.g., H_2 gas, O_2 gas, N_2 gas, and the most stable allotrope of an element).

Methodology for Determining Standard Entropy of Formation at 298 K

Experimental Data Sources

The most reliable data for $\Delta S°_f$ values are obtained from:
- Standard thermodynamic tables such as the NIST Chemistry WebBook.
- Published thermodynamic data compilations.
- Calorimetric measurements and spectroscopic studies.

Calculating $\Delta S°_f$

While direct experimental determination is common, theoretical calculations and estimations are also employed, involving:
- Standard molar entropies ($S°$) of the compounds and elements: The primary data point.
- Application of Hess's Law: Using known entropies of elements in their standard states to derive formation entropies.

The general formula for the standard entropy of formation is:

$$
\Delta S^\circ_f (\text{compound}) = S^\circ (\text{compound}) - \sum_{i} n_i S^\circ (\text{element}_i)
$$

where:

- $S^\circ(\text{compound})$ is the standard molar entropy of the compound.
- $S^\circ(\text{element}_i)$ are the standard molar entropies of the elements in their standard states.
- n_i are the stoichiometric coefficients of the elements in the formation reaction.

Analysis of Specific Gaseous Substances

1. Hydrogen Gas ($H_2(g)$)

Standard State and Thermodynamic Data

Hydrogen gas exists as diatomic molecules in their most stable form at ambient conditions. Its standard molar entropy at 298 K and 1 bar is approximately:

- $S^\circ(H_2(g)) \approx 130.7\, \text{J mol}^{-1} \text{K}^{-1}$

Since hydrogen in its elemental form is the standard state, the standard entropy of formation ($\Delta S°f$) for $H_2(g)$ is zero:

$$
\boxed{
\Delta S^\circ_f(H_2(g)) = 0\, \text{J mol}^{-1} \text{K}^{-1}
}
$$

This is a fundamental convention: the standard entropies of elements in their standard states are set as the reference point, making their formation entropies zero.

Implications

The zero $\Delta S°f$ underscores that forming hydrogen gas from its elements (the element in its standard state) does not involve a change in entropy.

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2. Water Vapor ($H_2O(g)$)

Thermodynamic Data

Water vapor is a diatomic molecule with a bent geometry, exhibiting significant molecular complexity and vibrational modes. The standard molar entropy of $H_2O(g)$ at 298 K is approximately:

- $S^\circ(H_2O(g)) \approx 188.8\, \text{J mol}^{-1} \text{K}^{-1}$

Formation Reaction and Entropy Calculation

The formation of water vapor from its elements is represented as:

$$
H_2(g) + \frac{1}{2} O_2(g) \rightarrow H_2O(g)
$$

The standard entropies of elemental oxygen and hydrogen are:

- $S^\circ (H_2(g)) \approx 130.7\, \text{J mol}^{-1} \text{K}^{-1}$
- $S^\circ (O_2(g)) \approx 205.0\, \text{J mol}^{-1} \text{K}^{-1}$

Applying the formula:

$$
\Delta S^\circ_f (H_2O(g)) = S^\circ (H_2O(g)) - \left[S^\circ (H_2(g)) + \frac{1}{2} S^\circ (O_2(g)) \right]
$$

$$
\Delta S^\circ_f = 188.8 - [130.7 + 0.5 \times 205.0] = 188.8 - (130.7 + 102.5) = 188.8 - 233.2 = -44.4\, \text{J mol}^{-1} \text{K}^{-1}
$$

Interpretation:
The negative $\Delta S°_f$ indicates that the formation of water vapor from its elemental gases leads to a decrease in entropy, consistent with the formation of a more ordered molecule from more disordered elemental gases.

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3. Ammonia ($NH_3(g)$)

Thermodynamic Data

Ammonia is a trigonal pyramidal molecule with considerable vibrational and rotational degrees of freedom. Its standard molar entropy at 298 K is approximately:

- $S^\circ (NH_3(g)) \approx 192.8\, \text{J mol}^{-1} \text{K}^{-1}$

Formation Reaction and Entropy Calculation

The formation reaction:

$$
\frac{1}{2} N_2(g) + \frac{3}{2} H_2(g) \rightarrow NH_3(g)
$$

Standard molar entropies for nitrogen and hydrogen gases are:

- $S^\circ (N_2(g)) \approx 191.6\, \text{J mol}^{-1} \text{K}^{-1}$
- $S^\circ (H_2(g)) \approx 130.7\, \text{J mol}^{-1} \text{K}^{-1}$

Calculating $\Delta S°_f$:

$$
\Delta S^\circ_f = S^\circ (NH_3) - \left[\frac{1}{2} S^\circ (N_2) + \frac{3}{2} S^\circ (H_2) \right]
$$

$$
\Delta S^\circ_f = 192.8 - \left[0.5 \times 191.6 + 1.5 \times 130.7 \right] = 192.8 - (95.8 + 196.05) = 192.8 - 291.85 = -99.05\, \text{J mol}^{-1} \text{K}^{-1}
$$

Implication:

The significant negative entropy of formation for ammonia reflects the decrease in entropy associated with constructing a more ordered, stable molecule from its elemental gases.

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4. Ozone ($O_3(g)$)

Thermodynamic Data

Ozone is an allotrope of oxygen with a bent molecular structure, exhibiting resonance stabilization and vibrational modes. The standard molar entropy at 298 K is approximately:

- $S^\circ (O_3(g)) \approx 238.8\, \text{J mol}^{-1} \text{K}^{-1}$

Formation Reaction and Entropy Calculation

The formation of ozone from elemental oxygen:

$$
\frac{3}{2} O_2(g) \rightarrow O_3(g)
$$

Using standard molar entropy values:

- $S^\circ (O_2(g)) \approx 205.0\, \text{J mol}^{-}$

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