Calculate G At 298 K For The ReactionCS2(l)+3O2(g)CO2(g)+2SO2(g)CS2(l)+3O2(g)CO2(g)+2SO2(g)based On These

Calculate G At 298 K For The Reaction $CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$ Based On These

Understanding how to calculate the Gibbs free energy change (ΔG) at a specific temperature, such as 298 K, is fundamental in thermodynamics, especially when analyzing chemical reactions. The reaction:

$CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$

involves both gaseous and liquid reactants and products, and determining ΔG at 298 K helps predict whether the reaction is spontaneous under standard conditions. This comprehensive guide will walk you through the necessary steps, concepts, and calculations involved in determining ΔG for this reaction at 298 K.

Introduction to Gibbs Free Energy (ΔG)

What is Gibbs Free Energy?

Gibbs free energy (G) is a thermodynamic potential that measures the maximum reversible work obtainable from a thermodynamic system at constant temperature and pressure. It is expressed as:

$$ G = H - TS $$

where:
- H is enthalpy,
- T is temperature (in Kelvin),
- S is entropy.

The change in Gibbs free energy (ΔG) during a reaction indicates whether the process is spontaneous:
- $\Delta G < 0$: reaction is spontaneous,
- $\Delta G = 0$: reaction is at equilibrium,
- $\Delta G > 0$: reaction is non-spontaneous.

Why Calculate ΔG at 298 K?

298 K (about 25°C) is standard room temperature, making it a common reference point for thermodynamic calculations. Calculating ΔG at this temperature helps determine if the reaction occurs naturally under standard conditions.

Gathering Necessary Data

Standard Thermodynamic Data

To calculate ΔG at 298 K, you need standard thermodynamic data for each species involved:

- Standard Gibbs free energy of formation (ΔG°f)
- Standard enthalpy of formation (ΔH°f)
- Standard entropy (S°)

These values are typically tabulated in thermodynamic data tables.

Data for Reactants and Products

Species	ΔG°f (kJ/mol)	ΔH°f (kJ/mol)	S° (J/mol·K)
$CS_2(l)$	–119.0	–89.4	213.8
$O_2(g)$	0	0	205.0
$CO_2(g)$	–394.4	–393.5	213.7
$SO_2(g)$	–300.2	–296.8	248.0

Note: These are approximate standard values; actual values may vary slightly depending on the source.

Calculating ΔG° for the Reaction

Step 1: Write the Reaction in Terms of Standard Data

The reaction:

$CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$

requires calculating the standard Gibbs free energy change (ΔG°) using:

$$\Delta G^\circ_{\text{reaction}} = \sum \nu_i \Delta G^\circ_{f,i}$$

where:
- νi is the stoichiometric coefficient (positive for products, negative for reactants),
- ΔG°f,i is the standard Gibbs free energy of formation for each species.

Step 2: Apply the Formula

$$ \Delta G^\circ_{\text{reaction}} = [\Delta G^\circ_{f,\mathrm{CO}_2} + 2 \times \Delta G^\circ_{f,\mathrm{SO}_2}] - [\Delta G^\circ_{f,\mathrm{CS}_2} + 3 \times \Delta G^\circ_{f,\mathrm{O}_2}] $$

Plugging in the numbers:

$$ \Delta G^\circ_{\text{reaction}} = [(-394.4) + 2 \times (-300.2)] - [(-119.0) + 3 \times 0] $$

Calculations:

$$ \Delta G^\circ_{\text{reaction}} = (-394.4 - 600.4) - (-119.0) $$
$$ \Delta G^\circ_{\text{reaction}} = -994.8 + 119.0 $$
$$ \Delta G^\circ_{\text{reaction}} = -875.8\, \text{kJ/mol} $$

This indicates the reaction is thermodynamically favorable under standard conditions.

Calculating ΔH° for the Reaction

Similarly, to find the enthalpy change:

$$ \Delta H^\circ_{\text{reaction}} = \sum \nu_i \Delta H^\circ_{f,i} $$

Using the data:

$$ \Delta H^\circ_{\text{reaction}} = [–393.5 + 2 \times (–296.8)] - [–89.4 + 3 \times 0] $$
$$ \Delta H^\circ_{\text{reaction}} = (–393.5 – 593.6) – (–89.4) $$
$$ \Delta H^\circ_{\text{reaction}} = –987.1 + 89.4 $$
$$ \Delta H^\circ_{\text{reaction}} = –897.7\, \text{kJ/mol} $$

Calculating ΔS° for the Reaction

The standard entropy change:

$$ \Delta S^\circ_{\text{reaction}} = \sum \nu_i S^\circ_i $$

Calculations:

$$ \Delta S^\circ_{\text{reaction}} = [S^\circ_{\mathrm{CO}_2} + 2 \times S^\circ_{\mathrm{SO}_2}] - [S^\circ_{\mathrm{CS}_2} + 3 \times S^\circ_{\mathrm{O}_2}] $$

$$ \Delta S^\circ_{\text{reaction}} = (213.7 + 2 \times 248.0) - (213.8 + 3 \times 205.0) $$

$$ \Delta S^\circ_{\text{reaction}} = (213.7 + 496.0) - (213.8 + 615.0) $$
$$ \Delta S^\circ_{\text{reaction}} = 709.7 – 828.8 $$
$$ \Delta S^\circ_{\text{reaction}} = -119.1\, \text{J/mol·K} $$

Calculating ΔG at 298 K

Step 1: Convert ΔS° to kJ/mol·K

Since ΔG°, ΔH°, and ΔS° are in different units, convert entropy to kJ:

$$ \Delta S^\circ = -119.1\, \text{J/mol·K} = -0.1191\, \text{kJ/mol·K} $$

Step 2: Use the Gibbs Free Energy Equation

The temperature (T) is 298 K. Apply:

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

$$ \Delta G_{298\,K} = –897.7\, \text{kJ/mol} – 298\, \text{K} \times (–0.1191\, \text{kJ/mol·K}) $$

$$ \Delta G_{298\,K} = –897.7 + 35.5 $$
$$ \Delta G_{298\,K} = –862.2\, \text{kJ/mol} $$

This negative value confirms that the reaction proceeds spontaneously at 298 K under standard conditions.

Interpreting the Results

The calculated ΔG at 298 K is approximately –862.2 kJ/mol, indicating a highly spontaneous reaction. The negative Gibbs free energy change confirms that, under standard conditions, the reaction between CS_2 and oxygen produces CO_2 and SO_2 gases spontaneously at room temperature.

Additionally, the large magnitude of ΔG suggests the reaction is thermodynamically favorable and will likely proceed readily without requiring external energy input.

Additional Considerations and Practical Applications

Factors Influencing ΔG

While thermodynamic calculations predict spontaneity, actual reaction rates depend on kinetics and other factors such as:
- Temperature variations,
- Pressure conditions,
- Catalysts,
- Concentrations.

Industrial Relevance

Understanding ΔG for this reaction is essential in:
- Sulfur compound processing,
- Combustion analysis,
- Environmental impact assessments, especially regarding sulfur dioxide emissions.

Environmental Implications

The formation of SO_2 is a concern due to its role in acid rain. Calculations confirming the spontaneity can aid in designing better pollution control strategies.

Summary

Calculating Gibbs free energy change at 298 K involves:
- Collecting standard thermodynamic data for all species involved,
- Calculating ΔG°, ΔH°, and ΔS° for the reaction,
- Applying the Gibbs free energy equation at the

Frequently Asked Questions

What is the standard Gibbs free energy change (ΔG°) for the reaction $CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$ at 298 K?

To calculate ΔG° at 298 K, use the equation $\Delta G° = \Delta H° - T\Delta S°$, where ΔH° and ΔS° are the standard enthalpy and entropy changes for the reaction. You need to find these values from standard data tables and then substitute T = 298 K.

How do you determine the standard enthalpy change (ΔH°) for the reaction involving CS_2 and oxygen?

The standard enthalpy change (ΔH°) is calculated using standard enthalpies of formation (ΔHf°) for the reactants and products: $\Delta H^\circ = [\Delta H_f^\circ(CO_2) + 2\times\Delta H_f^\circ(SO_2)] - [\Delta H_f^\circ(CS_2)]$. Use values from thermodynamic data tables.

What is the role of entropy change (ΔS°) in calculating G at 298 K for this reaction?

The entropy change (ΔS°) accounts for the disorder change during the reaction. It is calculated using standard molar entropies (S°) of all reactants and products: $\Delta S^\circ = [S^\circ(CO_2) + 2\times S^\circ(SO_2)] - [S^\circ(CS_2)]$. This value influences the spontaneity and free energy calculation.

Where can I find the standard enthalpy and entropy values needed to compute ΔG at 298 K for this reaction?

These values are available in standard thermodynamic data tables, such as those provided in chemistry textbooks, reference books, or reputable online databases like NIST Chemistry WebBook.

What is the significance of calculating ΔG at 298 K for the reaction $CS_2 + 3O_2$?

Calculating ΔG at 298 K helps determine whether the reaction is spontaneous under standard conditions. A negative ΔG indicates a spontaneous process, while a positive value suggests non-spontaneity.

How can I interpret the calculated G at 298 K for this reaction?

The value of G (Gibbs free energy) indicates the thermodynamic favorability of the reaction at 298 K. Negative G suggests the reaction proceeds spontaneously, whereas positive G suggests it is non-spontaneous under standard conditions.

Are there any assumptions or approximations involved in calculating ΔG° at 298 K for this reaction?

Yes, calculations typically assume standard conditions (1 atm, 25°C), pure substances in their standard states, and neglect activity coefficients. Also, enthalpy and entropy values are often taken as constant near standard conditions.

Can I use Hess's Law to simplify the calculation of ΔG° for this reaction?

Hess's Law is useful for calculating ΔH° and ΔS°, which are then used to find ΔG°. It allows you to sum known reactions to derive the thermodynamic parameters for the target reaction, simplifying the

process when direct data is unavailable.

Additional Resources

Calculate G at 298 K for the reaction $CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$

Introduction

Understanding the thermodynamic parameters that govern chemical reactions is fundamental in the fields of chemistry and chemical engineering. Among these parameters, the Gibbs free energy change (ΔG) is pivotal because it indicates whether a reaction is spontaneous under specific conditions. When ΔG is negative, the reaction proceeds spontaneously; when positive, it is non-spontaneous; and when zero, the system is at equilibrium. Accurate calculation of ΔG at a given temperature, particularly at standard conditions such as 298 K, provides essential insights into the thermodynamic feasibility of reactions.

In this article, we focus on calculating the Gibbs free energy change (ΔG) at 298 K for the reaction:

$CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$

This reaction involves the oxidation of carbon disulfide (CS_2) to produce carbon dioxide and sulfur dioxide. The calculation of ΔG involves thermodynamic data such as standard Gibbs free energies of formation ($\Delta G°f$) for all reactants and products, as well as understanding how to appropriately combine these data for the overall reaction.

Thermodynamic Foundations

Gibbs Free Energy and Its Significance

Gibbs free energy (G) is a thermodynamic potential that combines enthalpy (H), entropy (S), and temperature (T):

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

The change in Gibbs free energy (ΔG) during a reaction determines its spontaneity:

- $\Delta G < 0$: Reaction is spontaneous
- $\Delta G = 0$: Reaction at equilibrium
- $\Delta G > 0$: Reaction is non-spontaneous

At constant temperature and pressure, ΔG can be calculated from standard Gibbs free energies of formation:

$$\Delta G^\circ_{reaction} = \sum \nu_i \Delta G^\circ_{f,products} - \sum \nu_j \Delta G^\circ_{f,reactants}$$

where ν_i and ν_j are the stoichiometric coefficients.

Standard Gibbs Free Energies of Formation ($\Delta G°_f$)

These are tabulated values representing the Gibbs free energy change when one mole of a compound forms from its elements in their standard states at 1 atm and 298 K. They are essential for calculating ΔG for reactions.

Gathering Essential Data

To perform the calculation, accurate thermodynamic data are necessary. Here are typical values for ΔG°f at 298 K (these are approximate and should be verified from thermodynamic tables):

Compound	ΔG°f (kJ/mol)	Notes
CS2(l)	+94.0	Standard state: liquid
O2(g)	0.0	Elemental form in standard state
CO2(g)	-394.4	From thermodynamic tables
SO2(g)	-300.2	Standard Gibbs free energy of formation

Note: The values can vary slightly depending on the source; for precise calculations, consult the latest thermodynamic data.

Calculating ΔG at 298 K

Step 1: Write the Overall Reaction

The reaction:

$$CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$$

From the balanced equation, the stoichiometric coefficients are:

- Reactants: 1 $CS_2(l)$, 3 $O_2(g)$
- Products: 1 $CO_2(g)$, 2 $SO_2(g)$

Step 2: Apply the ΔG° Formula

Using:

$$\Delta G^\circ_{reaction} = \sum \nu_i \Delta G^\circ_{f,products} - \sum \nu_j \Delta G^\circ_{f,reactants}$$

Plugging in the data:

$$\Delta G^\circ_{reaction} = [(1)(-394.4) + (2)(-300.2)] - [(1)(94.0) + (3)(0)]$$

Calculations:

- Sum of products:

$$-394.4 + 2 \times (-300.2) = -394.4 - 600.4 = -994.8 \text{ kJ/mol}$$

- Sum of reactants:

$$94.0 + 3 \times 0 = 94.0 \text{ kJ/mol}$$

- Overall ΔG°:

$$-994.8 - 94.0 = -1088.8 \text{ kJ/mol}$$

Result:

$$\boxed{\Delta G^\circ_{298K} \approx -1088.8 \text{ kJ/mol}}$$

This highly negative value indicates that, under standard conditions, the oxidation of CS_2 by oxygen is thermodynamically spontaneous at 298 K.

Discussion and Analytical Insights

Implications of the ΔG Calculation

The calculated ΔG of approximately -1088.8 kJ/mol signifies a strong thermodynamic driving force favoring the formation of carbon dioxide and sulfur dioxide from carbon disulfide and oxygen. This aligns with the understanding that combustion and oxidation reactions are typically exergonic and spontaneous at room temperature, provided the reactants are available in sufficient quantities.

Such a negative ΔG underscores the energy release potential when CS2 is oxidized, which is relevant in industrial processes involving the combustion of CS2 or its use as a chemical intermediate.

Thermodynamic Considerations Beyond Standard Conditions

While the calculation above assumes standard conditions, real-world applications may involve variations in temperature and pressure. To account for such variations, the Gibbs free energy change can be adjusted using the following thermodynamic relation:

$$ \Delta G = \Delta G^\circ + RT \ln Q $$

where:

- $ R $ is the universal gas constant (8.314 J/mol·K),
- $ T $ is the temperature in Kelvin,
- $ Q $ is the reaction quotient based on activities or partial pressures.

At 298 K, the standard free energy provides a baseline; deviations from standard conditions require correction factors.

Additional Thermodynamic Parameters and Their Roles

While ΔG is the primary focus, other thermodynamic quantities provide a more comprehensive understanding:

- Standard Enthalpy Change (ΔH°): Indicates heat absorbed or released during the reaction.
- Standard Entropy Change (ΔS°): Reflects the change in disorder or randomness.
- Gibbs Free Energy of Reaction (ΔG): Combines enthalpy and entropy to assess spontaneity.

Knowledge of ΔH° and ΔS° allows for the calculation of ΔG at any temperature via:

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

Environmental and Industrial Relevance

Understanding the thermodynamics of CS2 oxidation is crucial in several contexts:

- Environmental Impact: CS2 is a toxic compound; its combustion leads to emissions of CO2 and SO2, both of which have environmental implications.
- Industrial Processes: The exergonic nature of the reaction suggests its utility in energy generation or material processing, provided that reaction conditions are optimized for safety and efficiency.
- Chemical Safety: Knowledge of the thermodynamics helps in designing safe handling and disposal strategies for CS2 and related compounds.

Conclusion

The calculation of Gibbs free energy change at 298 K for the oxidation of carbon disulfide provides clear evidence of the reaction's spontaneity under standard conditions. With a ΔG° of approximately -1088.8 kJ/mol, the reaction is highly thermodynamically favored, reinforcing the understanding of CS2 oxidation as a exergonic process. Such thermodynamic insights are vital for industrial applications, environmental management, and advancing our fundamental understanding of chemical reactivity.

Further research could explore kinetic factors, reaction mechanisms, and the impact of varying conditions on the reaction's feasibility, ensuring safe and efficient utilization of these chemical transformations.

References

1. Atkins, P., & de Paula, J. (2010). Physical Chemistry (9

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