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Understanding how to calculate the Gibbs free energy (G) at a specific temperature is fundamental in thermodynamics, especially when analyzing chemical reactions. In this article, we will explore the process of calculating the Gibbs free energy (G) at 298 K for a particular reaction involving calcium, carbon dioxide, oxygen, and calcium carbonate. This detailed guide aims to clarify the concepts, formulas, and step-by-step procedures necessary for accurate computation, making it useful for students, educators, and professionals working in chemistry and related fields.

Introduction to 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 a vital concept because it helps predict the spontaneity of a chemical reaction:

- If $\Delta G < 0$, the reaction is spontaneous.
- If $\Delta G = 0$, the reaction is at equilibrium.
- If $\Delta G > 0$, the reaction is non-spontaneous.

The calculation of G at a given temperature involves understanding the relationship between enthalpy (H), entropy (S), and temperature (T). The fundamental equation is:

$$ G = H - TS $$

where:
- G = Gibbs free energy
- H = Enthalpy
- T = Temperature in Kelvin
- S = Entropy

Understanding the Reaction

The reaction in question involves calcium, carbon dioxide, oxygen, and calcium carbonate. Based on the provided reactants and products, the likely reaction is the formation of calcium carbonate from calcium and carbon dioxide, possibly involving oxygen:

$$
\text{Part A Reaction:} \quad \mathrm{Ca(s)} + \mathrm{CO_2(g)} + \frac{1}{2} \mathrm{O_2(g)} \rightarrow \mathrm{CaCO_3(s)}
$$

This reaction signifies the synthesis of calcium carbonate, a common mineral found in limestone and marble, from elemental calcium, carbon dioxide, and oxygen.

Key points:

- Reactants: calcium (Ca), carbon dioxide (CO_2), oxygen (O_2)
- Product: calcium carbonate ($CaCO_3$)
- States: solids (s), gases (g)

Thermodynamic Data Needed

To calculate ΔG at 298 K, we need standard thermodynamic data for each species involved. These include:

- Standard Gibbs free energy of formation (ΔG_f°)
- Standard enthalpy of formation (ΔH_f°)
- Standard entropy (S°)

The standard thermodynamic data are typically available in thermodynamic tables or reputable chemical data sources.

Sample Thermodynamic Data at 298 K:

Species	ΔG_f° (kJ/mol)	ΔH_f° (kJ/mol)	S° (J/mol·K)
Ca(s)	0	0	32.2
CO_2(g)	-394.4	-393.5	213.7
O_2(g)	0	0	205.0
$CaCO_3$(s)	-1128.8	-1206.9	93.7

Note: Values are approximate and can vary based on sources. Always verify

with the latest data.

Step-by-Step Calculation of ΔG at 298 K

The calculation involves several steps:

1. Write the Balanced Chemical Equation

Ensure the reaction is balanced:

$$
\mathrm{Ca(s)} + \mathrm{CO_2(g)} + \frac{1}{2} \mathrm{O_2(g)} \rightarrow \mathrm{CaCO_3(s)}
$$

Balances as written, with one calcium atom, one carbon atom, and 1.5 oxygen atoms on each side.

2. Calculate Standard Gibbs Free Energy Change (ΔG°) for the Reaction

Using the standard Gibbs free energies of formation:

$$
\Delta G^\circ_{reaction} = \sum \nu_i \Delta G_f^\circ (products) - \sum \nu_j \Delta G_f^\circ (reactants)
$$

where:
- ν_i and ν_j are the stoichiometric coefficients.

Applying the data:

$$
\Delta G^\circ_{reaction} = [1 \times (-1128.8)] - [1 \times 0 + 1 \times (-394.4) + 0.5 \times 0]
$$

$$
\Delta G^\circ_{reaction} = -1128.8 - (0 - 394.4 + 0) = -1128.8 + 394.4 = -734.4\, \text{kJ/mol}
$$

This is the standard Gibbs free energy change at 298 K.

3. Calculate the Entropy Change (ΔS°) for the Reaction

Similarly, using standard molar entropies:

$$
\Delta S^\circ_{reaction} = \sum \nu_i S^\circ (\text{products}) - \sum \nu_j S^\circ (\text{reactants})
$$

$$
\Delta S^\circ_{reaction} = [1 \times 93.7] - [1 \times 32.2 + 1 \times 213.7 + 0.5 \times 205.0]
$$

$$
\Delta S^\circ_{reaction} = 93.7 - (32.2 + 213.7 + 102.5) = 93.7 - 348.4 = -254.7\, \text{J/(mol·K)}
$$

Note: Convert J to kJ for consistency: $-254.7\, \text{J/(mol·K)} = -0.2547\, \text{kJ/(mol·K)}$.

4. Calculate the Gibbs Free Energy at 298 K

Using the relation:

$$
\Delta G^\circ_{reaction} = \Delta H^\circ_{reaction} - T \Delta S^\circ_{reaction}
$$

Alternatively, since we have $\Delta G^\circ_{reaction}$ directly, this step confirms the calculation.

If needed, the free energy at 298 K can be calculated directly:

$$
G_{products} = \sum \nu_i G^\circ_i
$$
$$
G_{reactants} = \sum \nu_j G^\circ_j
$$
$$
\Rightarrow \Delta G^\circ_{reaction} = G_{products} - G_{reactants}
$$

\]

which matches the previous calculation.

Understanding Spontaneity and Equilibrium

The negative value of \(\Delta G^\circ_{reaction} \) indicates that the formation of calcium carbonate from calcium, carbon dioxide, and oxygen at 298 K is spontaneous under standard conditions. This aligns with real-world observations where calcium carbonate readily forms in natural settings.

Implications:

- The reaction favors the formation of $CaCO_3$.
- The process releases free energy, which can be harnessed in various industrial applications such as cement manufacturing.

Additional Considerations in G Calculations

While the above approach provides a fundamental calculation, several factors can influence the accuracy:

- Temperature dependence: Thermodynamic properties vary with temperature; data at 298 K are standard but may differ at other temperatures.
- Non-standard conditions: Actual conditions may deviate from standard states, requiring correction factors.
- Activity corrections: For pure solids and liquids, activity is typically 1; for gases, partial pressures are considered.

Conclusion and Summary

Calculating the Gibbs free energy at 298 K for a chemical reaction involves understanding the reaction's thermodynamics, gathering accurate standard data, and applying the fundamental relations between enthalpy, entropy, and free energy. For the specific reaction of calcium reacting with carbon dioxide and oxygen to produce calcium carbonate, the process is thermodynamically favorable at standard conditions, with a significant negative ΔG.

Key steps summarized:

1. Write and balance the chemical reaction.
2. Obtain thermodynamic data (ΔG_f°, ΔH_f°, S°) for all species.
3. Calculate $\Delta G^\circ_{reaction}$ using standard formation energies.
4. Find the entropy change ΔS°.
5. Confirm the spontaneity and calculate the free energy change at 298 K.

This methodology is applicable to a broad array of reactions, and mastering it enhances your ability to analyze chemical processes thermodynamically.

References:

- Atkins, P., & de Paula, J. (2010). Physical Chemistry. Oxford University Press.
- Linstrom, P. J., & Mallard, W. G. (Eds.). (2001). NIST Chemistry WebBook. NIST Standard Reference Database Number 69.

Note: Always verify thermodynamic data from reputable sources for precise

Frequently Asked Questions

What is the standard Gibbs free energy change (ΔG°) for the reaction Ca(s) + CO_2(g) → $CaCO_3$(s) at 298 K?

The standard Gibbs free energy change (ΔG°) at 298 K can be calculated using ΔG° = ΔH° - TΔS°. Using standard thermodynamic data for each substance, ΔG° for the reaction is approximately -394 kJ/mol, indicating the reaction is spontaneous under standard conditions.

How do you determine the standard Gibbs free energy change (ΔG°) for the reaction at 298 K?

To determine ΔG° at 298 K, sum the standard Gibbs free energies of formation (ΔGf°) for products and reactants: ΔG° = Σ ΔGf°(products) - Σ ΔGf°(reactants). For $CaCO_3$, Ca, and CO_2, use their tabulated ΔGf° values and perform the calculation accordingly.

What are the standard Gibbs free energies of formation (ΔGf°) for Ca(s), CO_2(g), and $CaCO_3$(s) at

298 K?

At 298 K, approximate values are: $\Delta G_f^\circ(Ca(s)) = 0$ kJ/mol, $\Delta G_f^\circ(CO_2(g)) = -394.4$ kJ/mol, and $\Delta G_f^\circ(CaCO_3(s)) = -1128.8$ kJ/mol.

Using the standard formation energies, what is the calculated ΔG° for the reaction at 298 K?

Applying the values: $\Delta G^\circ = [\Delta G_f^\circ(CaCO_3)] - [\Delta G_f^\circ(Ca) + \Delta G_f^\circ(CO_2)] = -1128.8 - (0 + -394.4) = -1128.8 + 394.4 = -734.4$ kJ/mol. This indicates a spontaneous reaction under standard conditions.

What does a negative ΔG° value imply about the spontaneity of the reaction at 298 K?

A negative ΔG° value indicates that the reaction is thermodynamically spontaneous at 298 K under standard conditions.

How does temperature influence the calculation of ΔG for this reaction?

Temperature impacts the TΔS° term in $\Delta G = \Delta H^\circ - T\Delta S^\circ$. Changes in temperature can shift the reaction's spontaneity, but at 298 K, using standard thermodynamic data provides a reliable estimate of ΔG°.

Can the reaction $Ca(s) + CO_2(g) \rightarrow CaCO_3(s)$ occur spontaneously at room temperature based on the calculated ΔG°?

Yes, since the calculated ΔG° is negative (~ -734.4 kJ/mol), the reaction is thermodynamically spontaneous at 298 K under standard conditions.

Additional Resources

Calculating Standard Gibbs Free Energy Change (ΔG°) at 298 K for the Reaction: $Ca(s) + Co_2(g) + 12O_2(g) \rightarrow CaCO_3(s)$

Introduction

Understanding the thermodynamics of chemical reactions is fundamental in predicting whether a reaction will proceed spontaneously under given conditions. Among various thermodynamic parameters, the Gibbs free energy change (ΔG) plays a pivotal role because it directly indicates the spontaneity of a reaction at constant temperature and pressure. This review

delves into the detailed process of calculating ΔG° at 298 K for the reaction between calcium metal and oxygen, with the involvement of carbon dioxide, leading to the formation of calcium carbonate.

Overview of the Reaction

The reaction under consideration is:

$$
\text{Ca(s)} + \text{Co}_2(g) + 12 \text{O}_2(g) \rightarrow \text{CaCO}_3(s)
$$

This reaction involves:

- A solid metal (calcium)
- Gaseous carbon dioxide (CO_2)
- Gaseous oxygen (O_2)
- Solid calcium carbonate ($CaCO_3$)

The overall energy change hinges on the thermodynamic properties of all reactants and products at 298 K, notably their standard Gibbs free energies of formation ($\Delta G°_f$).

Step 1: Understanding the Significance of ΔG° in Thermodynamics

1.1 Definition of ΔG°

The standard Gibbs free energy change (ΔG°) for a reaction at a specified temperature (here, 298 K) is given by:

$$
\Delta G° = \sum \Delta G°_{f,\text{products}} - \sum \Delta G°_{f,\text{reactants}}
$$

where $\Delta G°_f$ is the standard Gibbs free energy of formation for each substance.

1.2 Spontaneity and ΔG°

- If $\Delta G° < 0$, the reaction occurs spontaneously.
- If $\Delta G° > 0$, the reaction is non-spontaneous under standard conditions.
- If $\Delta G° = 0$, the system is at equilibrium.

1.3 Relationship with Equilibrium Constant

The link between ΔG° and the equilibrium constant (K) at temperature T is:

$$
\Delta G^\circ = -RT \ln K
$$

where R is the universal gas constant (8.314 J mol^{-1} K^{-1}).

Step 2: Gathering Thermodynamic Data

Accurate calculation of ΔG° requires the standard Gibbs free energies of formation for all reactants and products at 298 K.

2.1 Standard Gibbs Free Energies of Formation (ΔG°_f)

Substance	State	ΔG°_f (kJ/mol)	Source/Comments
Ca(s)	Solid	0 (by definition)	Element in its standard state
Co_2(g)	Gas	-197.4	Standard thermodynamic data
O_2(g)	Gas	0 (by definition)	Element in its standard state
$CaCO_3$(s)	Solid	-1128.8	Commonly tabulated value

Note: The ΔG°_f values are typically obtained from thermodynamic tables or standard references like the JANAF Thermochemical Tables.

Step 3: Calculating ΔG° for the Reaction

Applying the formula:

$$
\Delta G^\circ_{reaction} = \left[\Delta G^\circ_f (\text{CaCO}_3)\right] - \left[\Delta G^\circ_f (\text{Ca}) + \Delta G^\circ_f (\text{Co}_2) + 12 \times \Delta G^\circ_f (\text{O}_2)\right]
$$

Plugging in the known values:

$$
\Delta G^\circ_{reaction} = (-1128.8\, \text{kJ/mol}) - \left[0 + (-197.4\, \text{kJ/mol}) + 12 \times 0\right]
$$

$$
\Delta G^\circ_{reaction} = -1128.8\, \text{kJ/mol} - (-197.4\, \text{kJ/mol}) = -1128.8\, \text{kJ/mol} + 197.4\, \text{kJ/mol}
$$

$$
\Delta G^\circ_{reaction} = -931.4\, \text{kJ/mol}
$$

\]

This negative value indicates that, under standard conditions, the formation of calcium carbonate from calcium, carbon dioxide, and oxygen is thermodynamically favorable.

Step 4: Interpreting the Results

4.1 Spontaneity

Since ΔG° is significantly negative (-931.4 kJ/mol), the reaction is highly spontaneous at 298 K. This aligns with the observed natural formation of calcium carbonate as a common mineral and sediment.

4.2 Implications in Geochemistry and Industry

- The formation of calcium carbonate is a key process in sedimentology, limestone formation, and biomineralization.
- Industrially, calcium carbonate is a major raw material in cement production, paper, and plastics.

Step 5: Additional Thermodynamic Considerations

While the ΔG° calculation provides a thermodynamic perspective, real-world conditions may differ due to factors such as:

- Activity coefficients and non-ideal behavior
- Partial pressures of gases
- Temperature variations (beyond 298 K)
- Kinetic barriers that could prevent the reaction despite thermodynamic favorability

---

Step 6: Computing the Equilibrium Constant (K)

Using the ΔG° value, the equilibrium constant at 298 K can be calculated:

\[
K = e^{-\frac{ΔG°}{RT}}
\]

Converting ΔG° to Joules:

\[
ΔG° = -931.4\, \text{kJ/mol} = -931,400\, \text{J/mol}
\]

Calculating K:

$$
K = e^{-\frac{-931,400}{8.314 \times 298}} = e^{\frac{931,400}{2477.572}} \approx e^{375.7}
$$

Since $e^{375.7}$ is an astronomically large number, this indicates the reaction strongly favors products, consistent with the negative ΔG°.

Step 7: Limitations and Assumptions

7.1 Standard Conditions

- The calculation assumes standard conditions (1 bar pressure, pure substances).
- Actual partial pressures, especially of gases, can influence the reaction's direction.

7.2 Data Accuracy

- Thermodynamic data are subject to experimental uncertainties.
- The chosen $\Delta G°_f$ values are representative; slight variations in data sources could alter the result.

7.3 Reaction Pathway and Kinetics

- Thermodynamics predicts the feasibility but not the rate.
- Kinetic barriers might slow down or prevent the reaction, despite thermodynamic favorability.

Conclusion

Calculating the standard Gibbs free energy change (ΔG°) for the reaction:

$$
\text{Ca(s)} + \text{Co}_2(g) + 12 \text{O}_2(g) \rightarrow \text{CaCO}_3(s)
$$

at 298 K reveals a highly negative value (~ -931.4 kJ/mol), confirming the thermodynamic spontaneity of calcium carbonate formation under standard conditions. This reinforces the understanding that calcium carbonate is thermodynamically stable and naturally forms in environments rich in calcium and oxygen, especially with available CO_2.

This detailed thermodynamic analysis underscores the importance of ΔG° calculations in predicting reaction behavior, guiding industrial processes,

and understanding natural mineral formation. It exemplifies how fundamental thermodynamic data, combined with precise calculations, can offer profound insights into chemical systems.

References

- L. M. Robie, R. E. Hemingway, and R. L. Fisher, "Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 bar," U.S. Geological Survey Bulletin 1452, 1979.
- NIST Chemistry WebBook, National Institute of Standards and Technology.
- Atkins, P., & de Paula, J., Physical Chemistry, 10th Edition, Oxford University Press, 2014.
- JANAF Thermochemical Tables, 3rd Edition.

In essence, the calculation of ΔG° at 298 K for this reaction not only provides insights into its spontaneity but also illustrates the broader application of thermodynamic principles in chemistry and geochemistry.

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