CHEM-E6100 FUNDAMENTALS OF CHEMICAL THERMODYNAMICS

EXAMINATION 4.12.2023, 14:00-18:00

All relevant calculation steps should be included in the responses. An equation sheet is provided at the end of the document. All questions give a maximum 5 points each, maximum score is 30 points.

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Questions

1. The reduction of iron oxide in the blast furnace proceeds according to the following reactions

i) $3\ Fe_2O_3 + CO \rightarrow 2\ Fe_3O_4 + CO_2$; $\Delta H°_{298} = -53.1$ kJ

ii) $Fe_3O_4 + CO \rightarrow 3\ FeO + CO_2$ $\Delta H°_{298} = +41.0$ kJ

iii) $FeO + CO \rightarrow Fe + CO_2$ $\Delta H°_{298} = -18.4$ kJ

Calculate $\Delta H°_{298}$ for the reaction

iv) $Fe_2O_3 + 3\ CO \rightarrow 2\ Fe + 3\ CO_2$ $\Delta H°_{298} = ?$

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2. Calculate the enthalpy change of 1 mol of iodine (I_2) when it is heated from 298.15 K to 473.15 K at 1 bar from the following data:

Heat capacity of solid iodine:
$C_p(s)$ (J/ (mol·K)) = 54.28 + 0.001343 **(T/K);** /

Heat capacity of liquid iodine:
$C_p(s)$ (J/ (mol·K)) = 80.33;

Heat capacity of gaseous iodine:
$C_p(s)$ (J/ (mol·K)) = 37.20;

Enthalpy of melting: 15774 J/mol; melting point: 114 °C
Enthalpy of vaporization: 41714 J/mol; boiling point: 183 °C

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3. The enthalpy of formation of Ag_2O at 298.15 K is -30543 J/mol. Calculate the approximate temperature at which Ag_2O begins to decompose to Ag and O_2 on heating, (a) in pure oxygen, $P(O_2)$= 1 bar, and (b) in air, $P(O_2)$=0.21 bar.

Use the following data:

	$S°_{298.15}$ (J/ mol·K)	C_p/ (J/ mol·K)
Ag_2O	121.75	65.7
O_2	205.0	29.3
Ag	42.7	25.5

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4. 20 tons of molten copper is cooled from 1350 °C to 1200 °C by adding solid copper (T = 25 °C). (Pure) copper has a melting point of 1083 °C.

We know the following properties:

Cu(s)	$c_p = 22.64 + 0.0063 \times T$	J/mol K
Cu(l)	$c_p = 31.38$	J/mol K
$\Delta H_{Cu}(s \rightarrow l, 1083\ °C) = 13.054$		kJ/mol.

How much coolant (Cu) is needed? The heat losses are assumed as negligible.

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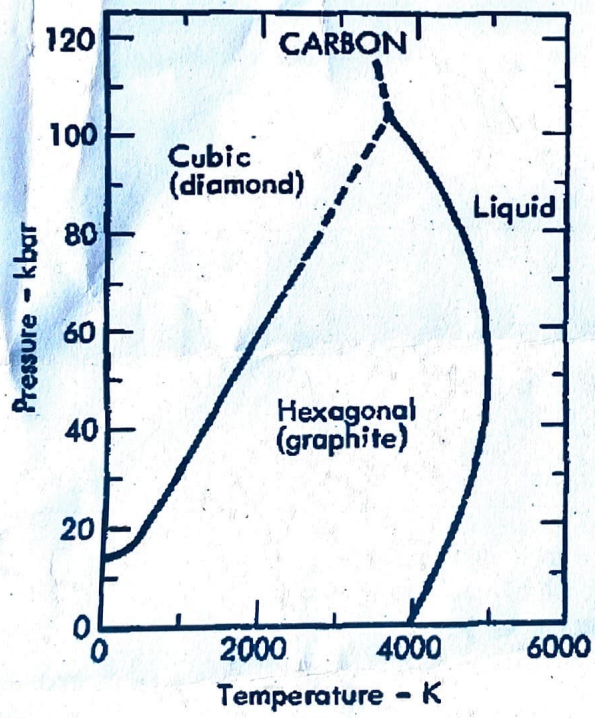
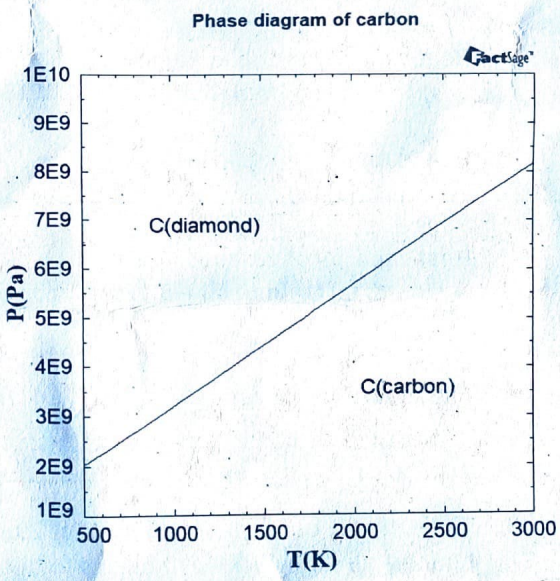
5. a) What is the Gibbs phase rule and the meaning of its variables?

b) Identify the P-T-coordinate for the invariant point in the P-T phase diagram of carbon below (Left figure), and identify the stable phases at these invariant points.

c) Estimate the change in molar volume for the reaction C(diamond) -> C(graphite), based on the phase equilibria (right Figure) and the Clausius-Clapeyron relations.

ΔS(diamond->graphite) is 4.7 J/(mol K).





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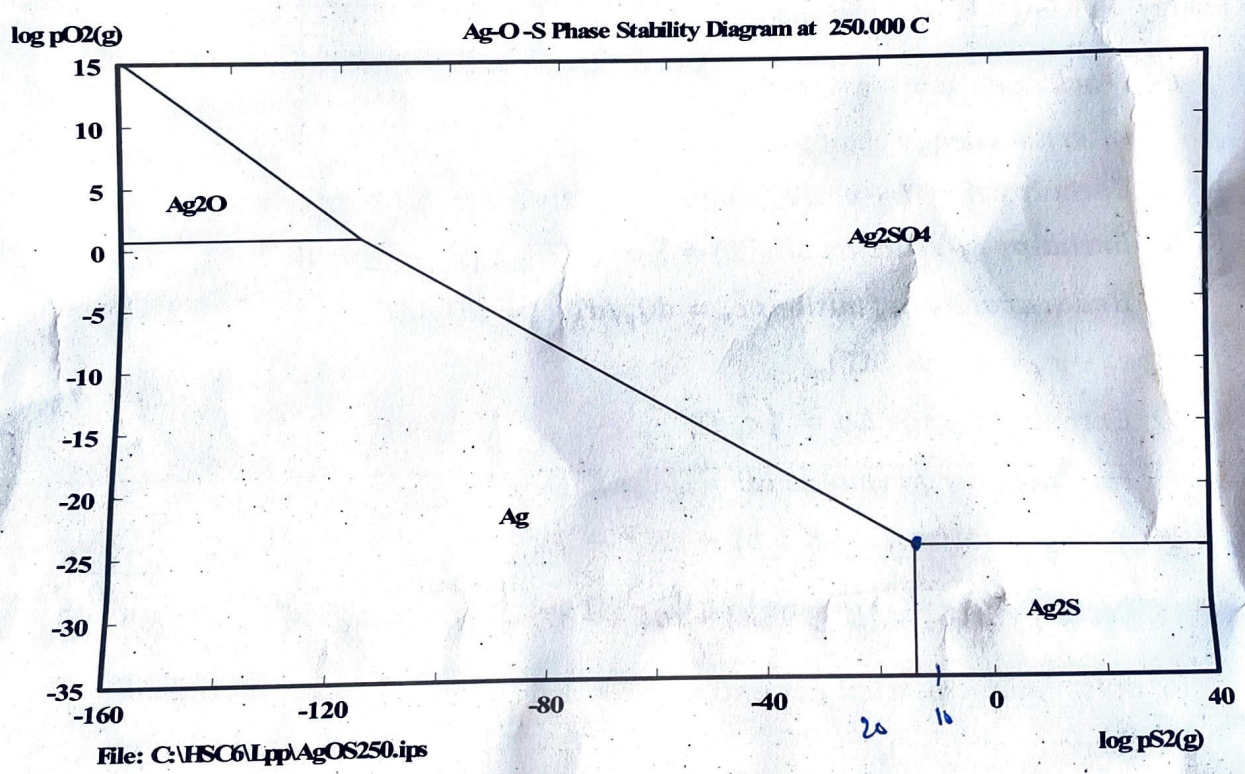
6. The included Kellogg diagram shows equilibria and the phase boundaries between pure substances and gas (limited to S_2 and O_2) at a constant temperature in system Ag-S-O.

a) Write the equilibrium reaction and the Gibbs energy of the reaction for the equilibrium between silver oxide and silver sulphate.

b) Calculate the equilibrium pressure of sulfur at the metallic silver / silver sulfide phase boundary using the Gibbs energy values given below.

c) At which partial pressures of S_2 and O_2 can three solid phases occur in equilibrium simultaneously? Which three phases are stable together at these conditions?

Reactions T = 523.15 K	ΔG° / J/mol
$2Ag + ½O_2(g) = Ag_2O$	3622
$2Ag + ½S_2(g) = Ag_2S$	-68903
$2Ag + ½S_2(g) + 2O_2(g) = Ag_2SO_4$	-567736



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