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Important equations for Thermodynamics

The First Law of Thermodynamics $$\Delta U = q_{\mathrm{in}} + w_{\mathrm{on}}$$

ΔU is the change in the internal energy of a thermodynamic system, q_{in} is the heat energy supplied to the thermodynamic system and w_{on} is the mechanical work performed on the thermodynamic system.

Work Done on the System for the Expansion of an Ideal gas $$w_{\mathrm{on}} = -p\Delta V$$

w_{on} is the mechanical work performed on the thermodynamic system, p is the external pressure and ΔV is the change in volume of the gas.

The First Law of Thermodynamics under Isochoric conditions $$\Delta U = q_{\mathrm{V}}$$

ΔU is the internal energy change of a thermodynamic system and q_{V} is the heat energy supplied to the system under isochoric conditions.

Definition of the State Function Enthalpy $$H = U + pV$$

H is the enthalpy of the thermodynamic system, U is the internal energy of the thermodynamic system, p is the pressure of the thermodynamic system and V is the volume of the thermodynamic system.

The First Law of Thermodynamics under Isobaric conditions $$\Delta H = q_{\mathrm{p}}$$

ΔH is the enthalpy change of a thermodynamic system and q_{p} is the heat energy supplied to the system under isobaric conditions.

Work Done on the System for the Reversible Isothermal Expansion of an Ideal gas $$w_{\mathrm{on}} = -nRT \ln \frac{V_{\mathrm{f}}}{V_{\mathrm{i}}}$$

w_{on} is the mechanical work performed on the thermodynamic system, n is the quantity of gas, R is the ideal gas constant = 8.314 J K^{-1} mol^{-1}, T is the temperature in K, V_{f} is the final volume and V_{i} is the initial volume.

Definition of Heat Capacity of a Substance $$C = \frac{q}{\Delta T}$$

C is the heat capacity of the substance, q is the heat energy supplied to the substance and ΔT is the ensuing temperature change of the substance in K.

Definition of Specific Heat Capacity of a Substance $$C_{\mathrm{S}} = \frac{C}{m}$$

C_{S} is the specific heat capacity of the substance, C is the heat capacity of the substance and m is the mass of the substance in kg.

Definition of Molar Heat Capacity of a Substance $$C_{\mathrm{m}} = \frac{C}{n}$$

C_{m} is the molar heat capacity of the substance, C is the heat capacity of the substance and n is the quantity of substance in mol.

Important equations for Thermodynamics

Definition of Isochoric Heat Capacity of a Substance

$$C_{\mathrm{V}} = \frac{q_{\mathrm{V}}}{\Delta T} = \frac{\Delta U}{\Delta T}$$

C_{V} is the isochoric heat capacity of the substance, q_{V} is the heat energy supplied to the substance under isochoric conditions, ΔT is the ensuing temperature change of the substance in K and ΔU is the internal energy change of the substance.

Definition of Isobaric Heat Capacity of a Substance

$$C_{\mathrm{p}} = \frac{q_{\mathrm{p}}}{\Delta T} = \frac{\Delta H}{\Delta T}$$

C_{p} is the isobaric heat capacity of the substance, q_{p} is the heat energy supplied to the substance under isobaric conditions, ΔT is the ensuing temperature change of the substance in K and ΔH is the change in the enthalpy change of the substance.

Relationship Between Molar Isobaric and Isochoric Heat Capacities of a Substance

$$C_{\mathrm{p,m}} - C_{\mathrm{V,m}} = R$$

$C_{\mathrm{p,m}}$ is the molar isobaric heat capacity of the substance, $C_{\mathrm{V,m}}$ is the molar isochoric heat capacity of the substance and R is the ideal gas constant = 8.314 J K^{-1} mol^{-1}.

Entropy Change of a Substance Upon Heating

$$\Delta S = C \ln \frac{T_{\mathrm{f}}}{T_{\mathrm{i}}}$$

ΔS is the entropy change of the substance, C is the heat capacity of the substance, T_{i} and T_{f} are the initial and final temperatures in K.

Definition of Entropy

$$\Delta S = \frac{q_{\mathrm{rev}}}{T}$$

ΔS is the entropy change of the thermodynamic system, q_{rev} is the heat energy reversibly supplied to the system and T is the temperature in K at which the reversible heat transfer to the thermodynamic system occurs.

Definition of Gibbs Energy

$$G = H - TS$$

G is the Gibbs Energy of the thermodynamic system, H is the enthalpy of the thermodynamic system, T is the temperature of the thermodynamic system in K and S is the entropy of the thermodynamic system.

Gibbs Energy Change for an Isothermal Process

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

ΔG is the isothermal Gibbs Energy change of the thermodynamic system, ΔH is the isothermal enthalpy change of the thermodynamic system, T is the temperature of the thermodynamic system in K and ΔS is the isothermal entropy change of the thermodynamic system.

Temperature at Which a Reaction Switches Spontaneity

$$T = \frac{\Delta H}{\Delta S}$$

T is the temperature in K at which the reaction switches spontaneity, ΔH is the enthalpy change of the reaction and ΔS is the entropy change of the reaction.

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Important equations for Thermodynamics

Reaction Gibbs Energy

$$\Delta_r G = (c\mu_C + d\mu_D) - (a\mu_A + b\mu_B)$$

$\Delta_r G$ is the reaction Gibbs Energy, a, b, c and d are the stoichiometric coefficients of a generalised chemical reaction , aA + bB ⇆ cC + dD, and μ_A, μ_B, μ_C and μ_D are the chemical potentials of the reactants A and B and the products C and D, at the composition of the reaction mixture.

Definition of Reaction Gibbs Energy

$$\Delta_r G = \frac{dG}{d\xi}$$

$\Delta_r G$ is the reaction Gibbs Energy, $\frac{dG}{d\xi}$ is the slope of the graph of Gibbs energy G plotted against extent of reaction ξ.

Chemical Potential of a Species i

$$\mu_i = \mu_i^\Theta + RT \ln a_i$$

μ_i is the chemical potential of species i, μ_i^Θ is the standard chemical potential of species i, R is the ideal gas constant = 8.314 J K^{-1} mol^{-1}, T is the temperature in K and a_i is the activity of species i.

Relationship between Reaction Gibbs Energy and Reaction Quotient

$$\Delta_r G = \Delta_r G^\Theta + RT \ln Q$$

$\Delta_r G$ is the reaction Gibbs Energy, $\Delta_r G^\Theta$ is the standard reaction Gibbs , R is the ideal gas constant = 8.314 J K^{-1} mol^{-1}, $T$is the temperature in K and Q is the reaction quotient.

Standard Reaction Gibbs Energy

$$\Delta_r^\Theta G = -RT \ln K$$

$\Delta_r G^\Theta$ is the standard reaction Gibbs Energy, R is the ideal gas constant = 8.314 J K^{-1} mol^{-1}, T is the temperature in K and K is the thermodynamic equilibrium constant.

The Debye T^3 Law for Non-metallic Substances Near Absolute Zero

$$C_{V,m} = aT^3$$

$C_{V,m}$ is the molar isochoric heat capacity of a non-metallic substance at temperature T, a is an empirically determined constant and T is a temperature in K in the vicinity of absolute zero.

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