

FORMULAIRE “Matériaux: de la Chimie aux Propriétés » / FORMULARY “Materials : from Chemistry to Properties”

CONSTANTES ET VALEURS

Vitesse de la lumière
Accélération terrestre
Constante de Planck
Constante de Boltzmann
Nombre d’Avogadro
Charge fondamentale
Constante des gaz parfaits

Volume molaire des gaz parfaits
Masse atomique unitaire
Constante de Faraday
Constante de Rydberg
Masse du proton
Masse du neutron
Masse de l’électron
Constante diélectrique du vide
Perméabilité magnétique du vide

CONSTANTS and VALUES

Speed of light
Acceleration due to gravity
Planck’s constant
Boltzmann’s constant
Avogadro’s constant
Fundamental Charge
Gas constant

Molar Volume of a perfect gas
Atomic mass unit
Faraday constant
Rydberg constant
Mass of the proton
Mass of the neutron
Mass of the electron
Permittivity of vacuum
Permeability of vacuum

c 3×10^8 m/s
 g 9.8 m/s²
 h $6,626 \times 10^{-34}$ J s
 k ou k_B $1,38 \times 10^{-23}$ J/K
 N_A $6,022 \times 10^{23}$ particules mol⁻¹
 e (ou $-q_e$) $1,6 \times 10^{-19}$ C ou As
 $R = N_A k$ $8,314$ J K⁻¹ mol⁻¹ / $0,08205$ L atm mol⁻¹ K⁻¹
 $8,3145$ kPa L mol⁻¹ K⁻¹ / $8,314 \times 10^{-2}$ L bar K⁻¹ mol⁻¹
 $V_{mol} = R \times 273,15 / p_0$ $22,7$ L mol⁻¹, $p_0 = 1$ bar, $T = 0^\circ\text{C}$
 $\underline{u} = 10^{-3} / N_A$ $1,66 \times 10^{-27}$ kg
 $F = N_A e$ $96\,485$ C mol⁻¹
 $R_\infty = m_e \mu_0^2 e^4 c^3 / (8 h^3)$ $1,097 \times 10^7$ m⁻¹
 m_p $1,672 \times 10^{-27}$ kg = 1 u
 m_n $1,674 \times 10^{-27}$ kg = 1 u
 m_e $9,1 \times 10^{-31}$ kg = $5,485 \times 10^{-4}$ u
 ϵ_0 $8,85 \times 10^{-12}$ A s V⁻¹ m⁻¹
 μ_0 $4\pi \times 10^{-7}$ V s (Am)⁻¹

CONVERSION D’UNITÉS /

$1 \text{ \AA} = 10^{-10} \text{ m}$ $1 \text{ eV} = 1,6021 \times 10^{-19} \text{ J}$

CONVERSION OF UNITS

$1 \text{ N} = \text{kg m s}^{-2}$ $1 \text{ Pa} = 1 \text{ N m}^{-2} = 1 \text{ kg m}^{-1} \text{ s}^{-2}$ $1 \text{ F} = 1 \text{ As V}^{-1}$ $1 \text{ J} = 1 \text{ kg m}^2 \text{ s}^{-2} = 1 \text{ Ws}$ $1 \text{ T} = \text{Vs m}^{-2}$

STRUCTURE ATOMIQUE /

Niveaux d’énergie de l’atome H
Energie de Rydberg
Spectre longueur d’ondes pour H
Energie d’un photon
Principe d’exclusion de Pauli : un jeu (n, ℓ, m_ℓ, m_s) correspond à un seul électron
Règle de Hund: sur une orbitale (n, ℓ) , on fixe d’abord m_s et m_ℓ varie
Potentiel de Lennard-Jones
Loi des gaz parfaits

ATOMIC STRUCTURE

Energy levels of the H-atom:
Rydberg energy
Wavelength of the spectra of H:
Energy of a photon
Principle of Pauli : one set (n, ℓ, m_ℓ, m_s) corresponds to one single electron
Hund’s Rule : for a (n, ℓ) orbital, m_s is fixed first while m_ℓ is varied
Lennard-Jones Potential
Gas law

$E_n = -13,6 \text{ eV } n^{-2}$ ($n = 1, 2, 3, \dots$)
 $R_H = hcR_\infty = (Ry)$ $13,6 \text{ eV}$
 $\frac{1}{\lambda} = R_\infty \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$ $n_2 > n_1$; λ : longueur d’onde / **wavelength**
 $E = hc/\lambda = h\nu$ [J]
Principle of Pauli : one set (n, ℓ, m_ℓ, m_s) corresponds to one single electron
Hund’s Rule : for a (n, ℓ) orbital, m_s is fixed first while m_ℓ is varied
 $V = \epsilon_0 \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^6 \right]$ $F(r) = -\frac{dV}{dr}$
 $pV = nRT$

THERMODYNAMIQUE

+ apporté au système, - enlevé du système

Enthalpie (U : énergie interne, p : pression, V : volume)

Entropie (classiquement)

Variation d'entropie de l'Univers

Chaleur spécifique à p constant

Variation d'énergie libre de Gibbs à T constant

Variation standard de / **Standard Variation of**

- Entropie de réaction / **reaction entropy**

$$\Delta S_r^0 = \sum_{i=1}^p \nu_i S_i^0 (\text{products}) - \sum_{j=1}^r \nu_j S_j^0 (\text{reactants})$$

- Enthalpie ΔH ou énergie libre de Gibbs ΔG de réaction

Reaction enthalpy ΔH and Gibbs free energy ΔG : ($X = H, G$)

$$\Delta X_r^0 = \sum_{i=1}^p \nu_i \Delta_f X_i^0 (\text{products}) - \sum_{j=1}^r \nu_j \Delta_f X_j^0 (\text{reactants})$$

Variation de l'énergie libre de Gibbs de réaction avec la composition **Variation of Gibbs free energy of reaction with composition:**

avec Q le quotient de réaction / **with Q reaction Quotient**

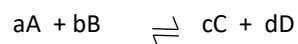
Relation entre ΔG_r^0 et K (constante d'équilibre)

Relation between ΔG_r^0 and K (equilibrium constant):

Règle des phases de Gibbs (C : nombre de composants, P : nombre de phases, V : nombre de degrés de liberté)

Gibbs Phase rule (C : number of components, P : number of phases, V : number of variations)

EQUILIBRE



constante d'équilibre / **equilibrium constant**

$$K = \frac{[C]^c [D]^d}{[A]^a [B]^b} \quad (\text{concentrations à l'équilibre / } \text{concentrations at equilibrium})$$

Quotient de réaction / **reaction Quotient**

$$Q = \frac{[C]^c [D]^d}{[A]^a [B]^b} \quad (\text{concentrations à tout instant / } \text{concentrations at any moment})$$

Solubilité / **solubility**: $aA_{(s)} \rightleftharpoons bB_{(aq)} + cC_{(aq)}$

Constante de solubilité / **solubility constant**: $K_s = [B]^b [C]^c$

ACIDES ET BASES



Constante de dissociation de l'eau

Echelle des pH et pOH

THERMODYNAMICS

+ on the system, - from the system

Enthalpy (U : internal energy, p : pressure, V : volume):

$$H = U + pV \quad [\text{kJ mol}^{-1}]$$

Entropy (classically):

$$\Delta S = \frac{Q_{rev}}{T} \quad [\text{J K}^{-1} \text{mol}^{-1}]$$

Variation of the entropy of the universe:

$$\Delta S_{universe} = \Delta S_{sys} + \Delta S_{env} = \Delta S_r^0 + \frac{-\Delta H_r^0}{T}$$

Specific heat capacity, $p = \text{const.}$:

$$c_p = \frac{1}{m} \frac{dH}{dT} \quad [\text{J K}^{-1} \text{g}^{-1}]$$

Variation of Gibbs free energy at constant temperature:

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

- $\Delta G_f^0, \Delta H_f^0$ et S^0 mesurés aux conditions standards (et tabulés)

measured at standard conditions (and tabulated)

- avec ν_i, ν_j les coefficients stoechiométriques des produits et réactants

with ν_i, ν_j stoichiometric coefficients of the products and reactants

$$\Delta G_r = \Delta G_r^0 + RT \ln Q$$

$$\Delta G_r^0 = -RT \ln K$$

$$2 + C = V + P$$

EQUILIBRIUM

ACIDS AND BASES

Dissociation constant of water: $K_e = [H_3O^+][OH^-] M^{-2} = 1.0 \times 10^{-14} (@25^\circ C)$

Scale of pH and pOH: $pH = -\log[H_3O^+] \quad pOH = -\log[OH^-]$

Relation entre pH et pOH

Constante d'acidité K_a

Constante basique K_b

Relation entre K_a et K_b pour une paire conjuguée acide-base

pH d'une solution acide forte ($K_a \gg 1$)

pH d'une solution aqueuse diluée d'un acide fort

pH d'une solution acide faible ($K_a \ll 1$) (general)

Si $[HA]_0 > 100K_a$

pOH d'une solution basique forte ($K_b \gg 1$)

pOH d'une solution aqueuse diluée d'une base forte

pH of a weak base solution (general) ($K_b \ll 1$)

Si $[B]_0 > 100K_b$

ELECTROCHIMIE

Potentiel standard d'une batterie

Relation entre ΔG_r^0 et ΔE_{pile}^0

Potentiel standard et constante d'équilibre

Equation de Nernst

Loi de Faraday (F : constante de Faraday)

Avec: n : nombre de moles produit / number of moles of products ;

z : nombre d'électrons transférés / number of transferred electrons

Relation between pH and pOH :

Acidity Constant K_a :

Basicity Constant K_b :

Relation between K_a and K_b of a conjugate acid-base pair : $K_a K_b = K_e$

pH of a strong acid solution ($K_a \gg 1$) :

pH of a diluted aqueous solution of a strong acid :

pH of a weak acid solution ($K_a \ll 1$) (general):

If $[HA]_0 > 100 K_a$:

pOH of a strong base solution ($K_b \gg 1$) :

pOH of a diluted aqueous solution of a strong base :

pH of a weak base solution (general) ($K_b \ll 1$) :

If $[B]_0 > 100K_b$: $x = [OH^-] = \sqrt{K_b c_b}$

ELECTROCHEMISTRY

Standard potential of a battery :

Relation between ΔG_r^0 and ΔE_{pile}^0 :

Standard Potential and equilibrium constant :

Nernst equation :

Faraday's law (F : Faraday constant) :

I : intensité du courant / current intensity

t : temps / time

pH + pOH = 14.00 (@ 25°C)

$$K_a = \frac{[H_3O^+][A^-]}{[HA]}$$

$$K_b = \frac{[BH^+][OH^-]}{[B]}$$

$$pH = -\log\left(\frac{[H^+]}{1M}\right) = -\log\left(\frac{c_a}{1M}\right)$$

$$c_a = [HA]_0 = [H^+] \quad [\text{mol L}^{-1}]$$

$$[H^+] = \frac{c_a + \sqrt{c_a^2 + 4K_e}}{2} \quad c_a < 10^{-6}$$

$$[H^+] = x = \frac{-K_a + \sqrt{K_a^2 + 4K_a c_a}}{2}$$
$$x = [H^+] = \sqrt{K_a c_a} \quad pH = 1/2 (pK_a - \log[HA]_0)$$

$$pOH = -\log(c_b/1M) \quad c_b = [B]_0$$

$$[OH]^- = \frac{c_b + \sqrt{c_b^2 + 4K_e}}{2} \quad c_b < 10^{-6}$$

$$x = [OH^-] = \frac{-K_b + \sqrt{K_b^2 + 4K_b c_b}}{2}$$
$$pH = 1/2 (14 + pK_a + \log[B]_0)$$

$$\Delta E_{pile}^0 = E^0 (\text{cathode}) - E^0 (\text{anode}) \quad [V]$$

$$\Delta G_r^0 = -zF\Delta E_{pile}^0$$

$$\ln K = zF\Delta E^0 / (RT)$$

$$\Delta E = \Delta E^0 - \frac{[RT]}{zF} \ln Q$$

$$n = IT / (zF)$$

Standard Electrode Potentials at 25 °C

Reduction Half-Reaction	E° (V)
$F_2(g) + 2 e^- \longrightarrow 2 F^-(aq)$	2.87
$H_2O_2(aq) + 2 H^+(aq) + 2 e^- \longrightarrow 2 H_2O(l)$	1.78
$PbO_2(s) + 4 H^+(aq) + SO_4^{2-}(aq) + 2 e^- \longrightarrow PbSO_4(s) + 2 H_2O(l)$	1.69
$MnO_4^-(aq) + 4 H^+(aq) + 3 e^- \longrightarrow MnO_2(s) + 2 H_2O(l)$	1.68
$MnO_4^-(aq) + 8 H^+(aq) + 5 e^- \longrightarrow Mn^{2+}(aq) + 4 H_2O(l)$	1.51
$Au^{3+}(aq) + 3 e^- \longrightarrow Au(s)$	1.50
$PbO_2(s) + 4 H^+(aq) + 2 e^- \longrightarrow Pb^{2+}(aq) + 2 H_2O(l)$	1.46
$Cl_2(g) + 2 e^- \longrightarrow 2 Cl^-(aq)$	1.36
$Cr_2O_7^{2-}(aq) + 14 H^+(aq) + 6 e^- \longrightarrow 2 Cr^{3+}(aq) + 7 H_2O(l)$	1.33
$O_2(g) + 4 H^+(aq) + 4 e^- \longrightarrow 2 H_2O(l)$	1.23
$MnO_2(s) + 4 H^+(aq) + 2 e^- \longrightarrow Mn^{2+}(aq) + 2 H_2O(l)$	1.21
$IO_3^-(aq) + 6 H^+(aq) + 5 e^- \longrightarrow \frac{1}{2} I_2(aq) + 3 H_2O(l)$	1.20
$Br_2(l) + 2 e^- \longrightarrow 2 Br^-(aq)$	1.09
$VO_2^+(aq) + 2 H^+(aq) + e^- \longrightarrow VO^{2+}(aq) + H_2O(l)$	1.00
$NO_3^-(aq) + 4 H^+(aq) + 3 e^- \longrightarrow NO(g) + 2 H_2O(l)$	0.96
$ClO_2(g) + e^- \longrightarrow ClO_2^-(aq)$	0.95
$Ag^+(aq) + e^- \longrightarrow Ag(s)$	0.80
$Fe^{3+}(aq) + e^- \longrightarrow Fe^{2+}(aq)$	0.77
$O_2(g) + 2 H^+(aq) + 2 e^- \longrightarrow H_2O_2(aq)$	0.70
$MnO_4^-(aq) + e^- \longrightarrow MnO_4^{2-}(aq)$	0.56
$I_2(s) + 2 e^- \longrightarrow 2 I^-(aq)$	0.54
$Cu^+(aq) + e^- \longrightarrow Cu(s)$	0.52
$O_2(g) + 2 H_2O(l) + 4 e^- \longrightarrow 4 OH^-(aq)$	0.40
$Cu^{2+}(aq) + 2 e^- \longrightarrow Cu(s)$	0.34
$SO_4^{2-}(aq) + 4 H^+(aq) + 2 e^- \longrightarrow H_2SO_3(aq) + H_2O(l)$	0.20
$Cu^+(aq) + e^- \longrightarrow Cu^0(aq)$	0.16
$Sn^{4+}(aq) + 2 e^- \longrightarrow Sn^{2+}(aq)$	0.15
$2 H^+(aq) + 2 e^- \longrightarrow H_2(g)$	0
$Fe^{3+}(aq) + 3 e^- \longrightarrow Fe(s)$	-0.036
$Pb^{2+}(aq) + 2 e^- \longrightarrow Pb(s)$	-0.13
$Sn^{2+}(aq) + 2 e^- \longrightarrow Sn(s)$	-0.14
$Ni^{2+}(aq) + 2 e^- \longrightarrow Ni(s)$	-0.23
$Cd^{2+}(aq) + 2 e^- \longrightarrow Cd(s)$	-0.40
$Fe^{2+}(aq) + 2 e^- \longrightarrow Fe(s)$	-0.45
$Cr^{3+}(aq) + e^- \longrightarrow Cr^{2+}(aq)$	-0.50
$Cr^{3+}(aq) + 3 e^- \longrightarrow Cr(s)$	-0.73
$Zn^{2+}(aq) + 2 e^- \longrightarrow Zn(s)$	-0.76
$2 H_2O(l) + 2 e^- \longrightarrow H_2(g) + 2 OH^-(aq)$	-0.83
$Mn^{2+}(aq) + 2 e^- \longrightarrow Mn(s)$	-1.18
$Al^{3+}(aq) + 3 e^- \longrightarrow Al(s)$	-1.66
$Mg^{2+}(aq) + 2 e^- \longrightarrow Mg(s)$	-2.37
$Na^+(aq) + e^- \longrightarrow Na(s)$	-2.71
$Ca^{2+}(aq) + 2 e^- \longrightarrow Ca(s)$	-2.76
$Ba^{2+}(aq) + 2 e^- \longrightarrow Ba(s)$	-2.90
$K^+(aq) + e^- \longrightarrow K(s)$	-2.92
$Li^+(aq) + e^- \longrightarrow Li(s)$	-3.04

Stronger
oxidizing agent

Weaker
reducing agent

Weaker
oxidizing agent

Stronger
reducing agent

PERIODIC TABLE OF THE ELEMENTS

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11.0079 H Hydrogen 2.1 g 36.941 49.0122 Li Be Lithium Beryllium 1.0 a 1.5 b 22.990 24.305 Na Mg Sodium Magnesium 0.9 a 1.2 b Atomic number 5 10.811 Atomic mass B Symbol Boron Name Electronegativity 2.0 f Group a Alkali metal b Alkaline earth metal c Metal d Transition metal e Lanthanide f Metalloid g Non-metal h Halogen i Noble gas j Actinide 13 14 15 16 17 5 10.811 B Boron 2.0 f 6 12.011 C Carbon 2.5 g 7 14.007 N Nitrogen 3.0 g 8 15.999 O Oxygen 3.5 g 9 18.998 F Fluorine 4.0 h 10 20.180 Ne Neon -- i 13 26.982 Al Aluminium 1.5 e 14 28.086 Si Silicon 1.8 f 15 30.974 P Phosphorus 2.1 g 16 32.065 S Sulfur 2.5 g 17 35.543 Cl Chlorine 3.0 h 18 39.948 Ar Argon -- i <tr><td colspan="18">3</td><td colspan="18">4</td><td colspan="18">5</td><td colspan="18">6</td><td colspan="18">7</td><td colspan="18">8</td><td colspan="18">9</td><td colspan="18">10</td><td colspan="18">11</td><td colspan="18">12</td></tr> <tr><td colspan="18">19</td><td colspan="18">20</td><td colspan="18">21</td><td 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<tr><td colspan="18">La</td><td colspan="18">Lanthanum</td><td colspan="18">Ce</td><td colspan="18">Cerium</td><td colspan="18">Pr</td><td colspan="18">Praseodymium</td><td colspan="18">Nd</td><td colspan="18">Neodymium</td><td colspan="18">Pm</td><td colspan="18">Promethium</td><td colspan="18">Sm</td><td colspan="18">Samarium</td><td colspan="18">Eu</td><td colspan="18">Europium</td><td colspan="18">Gd</td><td colspan="18">Gadolinium</td><td colspan="18">Tb</td><td colspan="18">Terbium</td><td colspan="18">Dy</td><td colspan="18">Dysprosium</td><td colspan="18">Ho</td><td colspan="18">Holmium</td><td colspan="18">Er</td><td colspan="18">Erbium</td><td colspan="18">Tm</td><td colspan="18">Thulium</td><td colspan="18">Yb</td><td colspan="18">Ytterbium</td><td colspan="18">Lu</td><td colspan="18">Lutetium</td></tr> <tr><td colspan="18">89</td><td colspan="18">(227)</td><td colspan="18">90</td><td colspan="18">232.04</td><td colspan="18">91</td><td colspan="18">231.04</td><td 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