Elementos matemáticos

Potencias y logaritmos.

$$x^a x^b = x^{a+b} \qquad \frac{x^a}{x^b} = x^{a-b} \qquad \left(x^a\right)^b = x^{ab}$$

$$\ln(xy) = \ln x + \ln y \qquad \ln(x/y) = \ln x - \ln y \qquad \ln x^b = b \ln x$$

Derivadas y diferenciales.

$$(cu)' = cu' \qquad (u+v)' = u' + v' \qquad \frac{d(u(v(x)))}{dx} = \frac{d(u(v))}{dv}\frac{dv}{dx}$$

$$(uv)' = u'v + uv' \qquad \left(\frac{u}{v}\right)' = \frac{u'v - uv'}{v^2}$$

$$d(f(x,y,z...)) = \left(\frac{\partial f}{\partial x}\right)_{y,z...} dx + \left(\frac{\partial f}{\partial y}\right)_{x,z...} dy + \left(\frac{\partial f}{\partial z}\right)_{x,y...} dz + ...$$

$$\frac{d}{dx}\left(x^n\right) = nx^{n-1} \qquad \frac{d}{dx}\left(\frac{1}{x^n}\right) = -\frac{n}{x^{n+1}} \qquad \frac{d}{dx}\left(\sqrt[n]{x}\right) = \frac{1}{n\sqrt[n]{x^{n-1}}}$$

$$\frac{d}{dx}\left(e^x\right) = e^x \qquad \frac{d}{dx}\left(a^x\right) = a^x \ln a$$

$$\frac{d}{dx}(\ln x) = \frac{1}{x} \qquad \frac{d}{dx}\left(\log_a x\right) = \frac{1}{x \ln a}$$

$$\frac{d}{dx}(\operatorname{sen} x) = \cos x \qquad \frac{d}{dx}(\cos x) = -\operatorname{sen} x \qquad \frac{d}{dx}(\operatorname{tg} x) = \frac{1}{\cos^2 x}$$

Integrales.

$$\int af(x)dx = a\int f(x)dx \qquad \int (u+v)dx = \int udx + \int vdx$$

$$\int x^n dx = \frac{x^{n+1}}{n+1} + C(n \neq -1) \qquad \int \frac{dx}{x} = \ln|x| + C$$

$$\int e^x dx = e^x + C \qquad \int a^x dx = \frac{a^x}{\ln a} + C$$

$$\left.\begin{array}{ll} \int_{-\infty}^{+\infty} x^{2n} e^{-ax^2} dx = 2\int_0^{\infty} x^{2n} e^{-ax^2} dx & \int_{-\infty}^{+\infty} x^{2n+1} e^{-ax^2} dx = 0 \\ \int_0^{\infty} e^{-ax^2} dx = \frac{\pi^{\frac{1}{2}}}{2a^{\frac{1}{2}}} & \int_0^{\infty} x e^{-ax^2} dx = \frac{1}{2a} \\ \int_0^{\infty} x^{2n} e^{-ax^2} dx = \frac{(2n)!\,\pi^{\frac{1}{2}}}{2^{2n+1} n!\, a^{n+\frac{1}{2}}} & \int_0^{\infty} x^{2n+1} e^{-ax^2} dx = \frac{n!}{2a^{n+1}} \end{array}\right\} \begin{array}{l} a > 0 \\ n = 1,2,... \end{array}$$

$$Erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-x^2} dx \qquad Erf(0) = 0; Erf(\infty) = 1$$

$$\int_0^x e^{-at^2} dt = \frac{\sqrt{\pi}}{2a^{\frac{1}{2}}} Erf\left(\sqrt{a}x\right); \qquad \int_0^x t^2 e^{-at^2} dt = \frac{\sqrt{\pi}}{4a^{\frac{3}{2}}} Erf\left(\sqrt{a}x\right) - \frac{x}{2a} e^{-ax^2}$$

Aproximaciones:

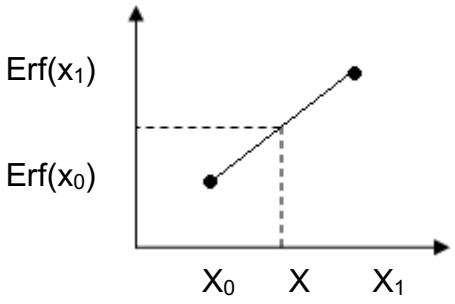
$$Stirling \rightarrow \ln N! \approx N \ln N - N (\text{para N grande})$$

$$e^{-x} \approx 1 - x (si\ |x| << 1) \qquad e^x \approx 1 + x (si\ |x| << 1)$$

FUNCIÓN DE ERROR										
	0	1	2	3	4	5	6	7	8	9
0.0	0.	0.0112834	0.0225646	0.0338412	0.0451111	0.056372	0.0676216	0.0788577	0.0900781	0.101281
0.1	0.112463	0.123623	0.134758	0.145867	0.156947	0.167996	0.179012	0.189992	0.200936	0.21184
0.2	0.222703	0.233522	0.244296	0.255023	0.2657	0.276326	0.2869	0.297418	0.30788	0.318283
0.3	0.328627	0.338908	0.349126	0.359279	0.369365	0.379382	0.38933	0.399206	0.409009	0.418739
0.4	0.428392	0.437969	0.447468	0.456887	0.466225	0.475482	0.484655	0.493745	0.50275	0.511668
0.5	0.5205	0.529244	0.537899	0.546464	0.554939	0.563323	0.571616	0.579816	0.587923	0.595936
0.6	0.603856	0.611681	0.619411	0.627046	0.634586	0.642029	0.649377	0.656628	0.663782	0.67084
0.7	0.677801	0.684666	0.691433	0.698104	0.704678	0.711156	0.717537	0.723822	0.73001	0.736103
0.8	0.742101	0.748003	0.753811	0.759524	0.765143	0.770668	0.7761	0.78144	0.786687	0.791843
0.9	0.796908	0.801883	0.806768	0.811564	0.816271	0.820891	0.825424	0.82987	0.834232	0.838508
1.0	0.842701	0.84681	0.850838	0.854784	0.85865	0.862436	0.866144	0.869773	0.873326	0.876803
1.1	0.880205	0.883533	0.886788	0.889971	0.893082	0.896124	0.899096	0.902	0.904837	0.907608
1.2	0.910314	0.912956	0.915534	0.91805	0.920505	0.9229	0.925236	0.927514	0.929734	0.931899
1.3	0.934008	0.936063	0.938065	0.940015	0.941914	0.943762	0.945561	0.947312	0.949016	0.950673
1.4	0.952285	0.953852	0.955376	0.956857	0.958297	0.959695	0.961054	0.962373	0.963654	0.964898
1.5	0.966105	0.967277	0.968413	0.969516	0.970586	0.971623	0.972628	0.973603	0.974547	0.975462
1.6	0.976348	0.977207	0.978038	0.978843	0.979622	0.980376	0.981105	0.98181	0.982493	0.983153
1.7	0.98379	0.984407	0.985003	0.985578	0.986135	0.986672	0.98719	0.987691	0.988174	0.988641
1.8	0.989091	0.989525	0.989943	0.990347	0.990736	0.991111	0.991472	0.991821	0.992156	0.992479
1.9	0.99279	0.99309	0.993378	0.993656	0.993923	0.994179	0.994426	0.994664	0.994892	0.995111
2.0	0.995322	0.995525	0.995719	0.995906	0.996086	0.996258	0.996423	0.996582	0.996734	0.99688
2.1	0.997021	0.997155	0.997284	0.997407	0.997525	0.997639	0.997747	0.997851	0.997951	0.998046
2.2	0.998137	0.998224	0.998308	0.998388	0.998464	0.998537	0.998607	0.998674	0.998738	0.998799
2.3	0.998857	0.998912	0.998966	0.999016	0.999065	0.999111	0.999155	0.999197	0.999237	0.999275
2.4	0.999311	0.999346	0.999379	0.999411	0.999441	0.999469	0.999497	0.999523	0.999547	0.999571
2.5	0.999593	0.999614	0.999635	0.999654	0.999672	0.999689	0.999706	0.999722	0.999736	0.999751
2.6	0.999764	0.999777	0.999789	0.9998	0.999811	0.999822	0.999831	0.999841	0.999849	0.999858
2.7	0.999866	0.999873	0.99988	0.999887	0.999893	0.999899	0.999905	0.99991	0.999916	0.99992
2.8	0.999925	0.999929	0.999933	0.999937	0.999941	0.999944	0.999948	0.999951	0.999954	0.999956
2.9	0.999959	0.999961	0.999964	0.999966	0.999968	0.99997	0.999972	0.999973	0.999975	0.999976

Interpolación lineal:

$$erf(x) = erf(x_0) + \frac{erf(x_1) - erf(x_0)}{x_1 - x_0}(x - x_0)$$



$$\rightarrow \frac{y - y_1}{y_2 - y_1} = \frac{x - x_1}{x_2 - x_1}$$

CONSTANTES FUNDAMENTALES				
Nombre	**Símbolo**	**Valor**		**Unidades**
Velocidad de la luz	c	2.997 924 58	$10^{8(*)}$	m s^{-1}
Carga elemental	e	1.602 177	10^{-19}	C
Constante de Faraday	$F=N_Ae$	9.648 53	10^{4}	C mol^{-1}
Constante de Boltzmann	k	1.380 66	10^{-23}	J K^{-1}
Constante de los gases	$R=N_Ak$	8.314 51		J K^{-1} mol^{-1}
		0.083 145 1		L bar K^{-1} mol^{-1}
		0.082 057 8		L atm K^{-1} mol^{-1}
Constante de Planck	h	6.626 08	10^{-34}	J s
	$\hbar=h/2\pi$	1.054 57	10^{-34}	Js
Número de Avogadro	N_A	6.022 14	10^{23}	mol^{-1}
Unidad de masa atómica	uma	1.66054	10^{-27}	kg
Masa electrón	m_e	9.109 39	10^{-31}	kg
Masa protón.	m_p	1.672 62	10^{-27}	kg
Masa neutrón	m_n	1.674 93	10^{-27}	kg
Permitividad en el vacío	$\varepsilon_0=1/c^2\mu_0$	8.854 19	10^{-12}	$J^{-1}C^2m^{-1}$
	$4\pi\varepsilon_0$	1.112 65	10^{-10}	$J^{-1}C^2m^{-1}$
Permeabilidad en el vacío.	μ_0	4π	$10^{-7(*)}$	$Js^2C^{-2}m^{-1}(=T^2J^{-1}m^3)$
Magnetón Bohr	$\mu_B=e\hbar/2m_e$	9.274 02	10^{-24}	JT^{-1}
Magnetón nuclear	$\mu_N=e\hbar/2m_p$	5.050 79	10^{-27}	JT^{-1}
Constante de Rydberg	$R=m_ee^4/8h^3\ c\varepsilon^2{}_0$	1.097 377	10^{5}	cm^{-1}
Aceleración en caída libre	g	9.806 65$^{(*)}$		ms^{-2}
Constante gravitatoria	G	6.672 59	10^{-11}	Nm^2kg^{-2}

$^{(*)}$ Valor exacto

FACTORES DE CONVERSIÓN
1 cal = 4.184 J(*)
1 cm^{-1} = 1.9864 10^{-23} J
1 ev = 1.60218 10^{-19} J
1 atm = 1.01325 10^5 Pa
1 atm = 760 Torr
1 bar = 10^5 Pa
1 D = 3.335 64 10^{-30} C m
1 Å = 10^{-10} m(*)
1 P = 0.1 Pa·s
1 J = 10^7 erg
1 N = 10^5 dina
1 erg = 1 dina·cm
1 J = 1 N·m

Submúltiplo	Prefijo	Símbolo	Múltiplo	Prefijo	Símbolo
10^{-1}	deci	d	10	deca	da
10^{-2}	centi	c	10^2	hecto	h
10^{-3}	mili	m	10^3	kilo	k
10^{-6}	micro	μ	10^6	mega	M
10^{-9}	nano	n	10^9	giga	G
10^{-12}	pico	p	10^{12}	tera	T
10^{-15}	femto	f	10^{15}	peta	P
10^{-18}	atto	a	10^{18}	exa	E

Tema 1

$$Q=\sum_j e^{-\frac{E_j}{kT}} \qquad p_j=\frac{e^{-\frac{E_j}{kT}}}{Q} \qquad U=U(0)+kT^2\left(\frac{\partial lnQ}{\partial T}\right)_{N,V} \qquad P=kT\left(\frac{\partial lnQ}{\partial V}\right)_{N,T} \qquad S=\frac{U-U(0)}{T}+klnQ$$

$$A=U(0)-kT\,lnQ \qquad G=U(0)-kT\,lnQ+kTV\left(\frac{\partial lnQ}{\partial V}\right)_{N,T} \qquad \mu_B=\mu_B(0)-RT\left(\frac{\partial lnQ}{\partial N_B}\right)_{T,V,N_c\neq N_B}$$

$$\Lambda=\frac{h}{(2\pi mkT)^{\frac{1}{2}}} \qquad q_t=\frac{V}{\Lambda^3} \qquad \Theta_r=\frac{h^2}{8\pi^2 Ik}=\frac{hB}{k}=\frac{hc\overline{B}}{k} \qquad q_r=\frac{T}{\sigma\Theta_r}; \qquad q_r=\frac{\sqrt{\pi}T^{\frac{3}{2}}}{\sigma\sqrt{\Theta_A\Theta_B\Theta_C}}$$

$$\Theta_v=\frac{h\nu}{k} \qquad q_v=\prod_{s=1}^{3N-5\,(3N-6)}\frac{1}{1-e^{-\frac{\Theta_{v,s}}{T}}} \qquad K_p=e^{-\frac{\Delta U_m(0)}{RT}}\prod_i\left(\frac{q^{\theta}_{m,i}}{N_A}\right)^{\nu_i} \qquad \Delta U_m(0)=-N_A\sum_i \nu_i D_{0,i}$$

Tema 2

$$g(v_x)=\left(\frac{m}{2\pi kT}\right)^{\frac{1}{2}}e^{-\frac{mv_x^2}{2kT}} \qquad \phi(v)=\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}e^{-\frac{mv^2}{2kT}} \qquad G(v)=4\pi v^2\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}e^{-\frac{mv^2}{2kT}} \qquad G(\varepsilon)=2\pi\left(\frac{1}{\pi kT}\right)^{\frac{3}{2}}\varepsilon^{\frac{1}{2}}e^{-\frac{\varepsilon}{kT}}$$

$$v_{rms}=\left\langle v^2\right\rangle^{1/2}=\left(\frac{3kT}{m}\right)^{1/2} \qquad v_p=\left(\frac{2kT}{m}\right)^{1/2}$$

$$<v>=\left(\frac{8kT}{\pi m}\right)^{\frac{1}{2}} \qquad z_w=\frac{1}{4}\frac{N}{V}<v> \qquad z_{(1)2}=\pi d_{12}^2\left(\frac{8kT}{\pi\mu}\right)^{\frac{1}{2}}\frac{N_2}{V} \qquad Z_{12}=z_{(1)2}\frac{N_1}{V}$$

$$z_{(1)1}=\sqrt{2}\pi d^2\left(\frac{8kT}{\pi m}\right)^{\frac{1}{2}}\frac{N_1}{V} \qquad Z_{11}=\frac{1}{2}z_{(1)1}\frac{N_1}{V} \qquad \lambda=\frac{1}{\sqrt{2}\pi d^2}\frac{V}{N}$$

$$k_r=A\exp\left(-\frac{E_a}{RT}\right) \;;\; E_a=-R\frac{d\ln k_r}{d(1/T)}=RT^2\frac{d\ln k_r}{dT} \qquad ; \quad k_r=\left(\frac{8kT}{\pi\mu}\right)^{1/2}N_A\pi d_{BC}^2\exp\left(-\frac{\varepsilon_0}{kT}\right)$$

$$E_a=\frac{1}{2}RT+E_0 \;; \qquad k_r=\frac{kT}{h}\frac{\bar{q}^{\ddagger}/N_AV}{q_B/N_AV\;\;q_C/N_AV}\exp\left(-\frac{\Delta\varepsilon_0^{\ddagger}}{kT}\right) \;;\; k_r=\frac{kT}{h}\left(\frac{1}{C^0}\right)^{n-1}\exp\left(-\frac{\Delta G_C^{0\ddagger}}{RT}\right);$$

$$k_r=\frac{kT}{h}\left(\frac{RT}{P^0}\right)^{n-1}\exp\left(-\frac{\Delta G_P^{0\ddagger}}{RT}\right);\; E_a=nRT+\Delta H_p^{0\ddagger}; \qquad A=\frac{kT}{h}\left(\frac{RT}{p^0}\right)^{n-1}e^n e^{\frac{\Delta S_p^{0\ddagger}}{R}}$$

Tema 3

$$J_z = -\kappa \frac{dT}{dz}; \qquad J_z = -\eta \frac{dv_x}{dz}; \qquad \frac{dV}{dt} = -\frac{\pi r^4}{8\eta}\left(\frac{dP}{dz}\right); \qquad J_j = -\left(\frac{c_j D_{jk}}{RT}\right)\nabla \mu_j; \quad J_j = -D_{jk}\nabla c_j;$$

$$J_{D_{jk},z} = -D_{jk}\frac{dc_j}{dz};$$

$$J_z = \frac{I}{A} = -\sigma\frac{d\phi}{dz} = \sigma E_z; \quad R = \rho\frac{\ell}{A}; \quad I = \sum_j I_j = FA\frac{\Delta\phi}{\ell}\sum_j |z_j| u_j c_j;$$

$$\kappa = \frac{25\pi}{64} < v > \lambda\rho\frac{C_{v,m}}{N_A}; \eta = \frac{5\pi}{32} < v > \lambda\rho\frac{M}{N_A}; D_{jj} = \frac{3\pi}{16} < v > \lambda; \quad \sigma = F\sum_j |z_j| u_j c_j; \quad t_j = \frac{|z_j| u_j c_j}{\sum_k |z_k| u_k c_k};$$

$$\boldsymbol{J}_j = -\left(\frac{c_j D_{jk}}{RT}\right)\nabla\overline{\mu}_j + c_j\boldsymbol{v}; \quad \Lambda_m = \Lambda_m^0 - \Re\sqrt{c}; \quad \Lambda_m^0 = \nu_+\lambda_+^0 + \nu_-\lambda_-^0; \quad \langle u_j \rangle = \frac{\langle v_j \rangle}{|\boldsymbol{E}|} = \frac{q}{f} = \frac{qD}{k_B T};$$

$$u_{j,disolvente}^{\infty} = \frac{|z_j| e}{6\pi\eta_{disolvente} r_j}; \quad D = \frac{k_B T}{6\pi\eta r_p} \; ; \; \boldsymbol{F}_\eta = -f\cdot\boldsymbol{v} = -6\pi\eta r_p \boldsymbol{v}$$

Tema 4

$$p_{in} = p_{ex} + \frac{2\gamma}{r} \qquad ln\left(\frac{p}{p^*}\right) = \frac{V_m^L}{RT}\left[(p - p^*) + \frac{2\gamma}{r}\right] \qquad h = \frac{2\gamma\cos\theta}{(\rho^L - \rho^V)gR}$$

$$d\gamma = -\sum_i \Gamma_i^\sigma d\mu_i \qquad \Gamma_{2(1)} = -\frac{C_2^\beta}{RT}\left(\frac{\partial\gamma}{\partial C_2^\beta}\right)_T$$

$$\theta = \frac{Kp}{1+Kp} \qquad \theta = \frac{(Kp)^{1/2}}{1+(Kp)^{1/2}} \qquad \left(\frac{\partial \ln p}{\partial 1/T}\right)_\theta = \frac{\Delta H°_{ads}}{R}$$

$$\frac{\mathrm{V}}{\mathrm{V_{mon}}} = \frac{\mathrm{cx}}{(1-\mathrm{x})(1-\mathrm{x}+\mathrm{cx})} \qquad c=K/K^* \qquad x=p/p^* \qquad \theta = kp^{1/n} \qquad \theta = A\ln(Bp)$$

$$d\gamma = -\sum_i \Gamma_i d\mu_i - \sigma^\alpha d(\Delta\phi) \qquad \left(\frac{\partial\gamma}{\partial V}\right)_{T,\mu} = -\sigma \qquad C = \frac{d\sigma}{dV} = -\left(\frac{\partial^2\gamma}{\partial V^2}\right)_{T,\mu}$$

$$\gamma = \gamma^{max} - \frac{\varepsilon}{2d}\phi_e^2 \qquad x_D = \left(\frac{\varepsilon RT}{2F^2 I}\right)^{1/2} \qquad \gamma = \gamma^{max} - \frac{\varepsilon}{2x_D}\phi_e^2$$

Tema 5

$$v = \frac{k_1 k_2 [S][C]}{k_1[S] + k_{-1} + k_2}; \qquad v_0 = \frac{k_2 [S]_0 [C]_0}{[C]_0 + [S]_0 + K_m}$$

$$i = nFAv_{total} = nFAk^0 \left(e^{\frac{(1-\alpha)nF(E-E^{0\prime})}{RT}} [R] - e^{-\frac{\alpha nF(E-E^{0\prime})}{RT}} [O] \right)$$

$$i_0 = i_{a,eq} = nFAk^0 \cdot e^{\frac{(1-\alpha)nF(E_{eq}-E^{0\prime})}{RT}} [R]$$

$$i_0 = -i_{c,eq} = nFAk^0 \cdot e^{-\frac{\alpha nF(E_{eq}-E^{0\prime})}{RT}} [O]$$

$$i = i_0 \left(e^{\frac{(1-\alpha)nF\eta}{RT}} - e^{-\left(\frac{\alpha nF\eta}{RT}\right)} \right) \quad ; \quad j = j_0 \left(e^{\frac{(1-\alpha)nF\eta}{RT}} - e^{-\left(\frac{\alpha nF\eta}{RT}\right)} \right)$$

Tema 6

$$\bar{x}_{\mathrm{n}} = \frac{\sum_{i=1}^{i=\infty} x_i N_i}{\sum_{i=1}^{i=\infty} N_i} = \sum x_i n_i; \qquad \bar{x}_{\mathrm{w}} = \frac{\sum_{i=1}^{i=\infty} x_i^2 N_i}{\sum_{i=1}^{i=\infty} x_i N_i} = \frac{\sum_{i=1}^{i=\infty} x_i^2 n_i}{\sum_{i=1}^{i=\infty} x_i n_i}; \qquad \bar{x}_{\mathrm{z}} = \frac{\sum_{i=1}^{i=\infty} x_i^3 N_i}{\sum_{i=1}^{i=\infty} x_i^2 N_i} = \frac{\sum_{i=1}^{i=\infty} x_i^3 n_i}{\sum_{i=1}^{i=\infty} x_i^2 n_i}$$

$$\bar{x}_{\mathrm{n}} = \frac{1}{\sum \frac{w_i}{x_i}}; \qquad \bar{x}_{\mathrm{w}} = \sum w_i x_i; \qquad \bar{x}_{\mathrm{z}} = \frac{\sum x_i^2 w_i}{\sum x_i w_i}$$

$$\bar{x}_{\mathrm{v}} = \left(\frac{\sum x_i^{1+a} n_i}{\sum x_i n_i} \right)^{1/a} = \left(\sum x_i^a w_i \right)^{1/a}; \qquad \Delta G_{\mathrm{M}} = kT\chi_1 n_1 \phi_2 + kT\left(n_1 \ln \phi_1 + n_2 \ln \phi_2 \right)$$