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.

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

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

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

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

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

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

$$\frac{d}{dx}\left(\text{sen}x\right) = \cos x \qquad \frac{d}{dx}\left(\cos x\right) = -\text{sen}x \qquad \frac{d}{dx}\left(\text{tg}\, x\right) = \frac{1}{\cos^2 x}$$

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:

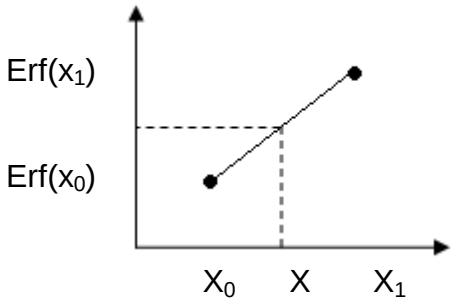
$$Stirling \rightarrow \ln N! \approx N \ln N - N (\text{para N grande})$$

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

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 átomica	u	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

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

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

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

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

Tema 2

$$V_{c-c} = \frac{q_1 q_2}{4\pi\varepsilon_0 r} \qquad V_{c-d} = -\frac{q^2\mu^2}{6(4\pi\varepsilon_0)^2 kTr^4} \qquad V_{d-d} = -\frac{2\mu_1^2\mu_2^2}{3(4\pi\varepsilon_0)^2 kTr^6} \qquad V_{c-di} = -\frac{q^2\alpha}{2(4\pi\varepsilon_0)^2 r^4}$$

$$V_{d-di} = -\frac{\mu^2\alpha}{(4\pi\varepsilon_0)^2 r^6} \qquad V_{di-di} = -\frac{3}{2}\frac{I_1 I_2}{I_1 + I_2}\frac{\alpha_1\alpha_2}{(4\pi\varepsilon_0)^2 r^6} \qquad \alpha' = \frac{\alpha}{4\pi\varepsilon_0}$$

$$V_{LJ} = \frac{B}{r^{12}} - \frac{C}{r^6} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] = \varepsilon\left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^6\right]$$

$$\left(P + \frac{a}{V_m^2}\right)(V_m - b) = RT; \qquad \frac{PV_m}{RT} = 1 + \frac{B(T)}{V_m} + \frac{C(T)}{V_m^2} + \ldots \qquad B(T) = 2\pi N_A \int_0^{\infty}\left(1 - e^{-\frac{V(r)}{kT}}\right) r^2 dr$$

$$dN_r = 4\pi r^2 \rho g(r) dr; \qquad g(r) = e^{-\frac{w}{kT}} \qquad U = \frac{3}{2}NkT + 2\pi\rho N\int_0^{\infty} V(r)g(r)r^2 dr$$

Tema 3

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

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

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

Tema 4

$$J_{Q,z} = -\kappa\frac{dT}{dz} \qquad J_{p_x,z} = -\eta\frac{dv_x}{dz} \qquad J_{D_{jk},z} = -D_{jk}\frac{dc_j}{dz} \qquad \frac{dV}{dt} = -\frac{\pi r^4}{8\eta}\frac{dp}{dz}$$

$$\kappa = \frac{25\pi}{64} < v > \lambda\rho\frac{C_{v,m}}{N_A} \qquad \eta = \frac{5\pi}{32} < v > \lambda\rho\frac{M}{N_A} \qquad D_{jj} = \frac{3\pi}{16} < v > \lambda \qquad \rho = \frac{N}{V}$$

Tema 5

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

$$k_r = \frac{kT}{h}\frac{\bar{q}^{\ddagger}/N_A V}{q_B/N_A V \; q_C/N_A V}\exp\left(-\frac{\Delta\varepsilon_0^{\ddagger}}{kT}\right) \qquad k_r = \frac{kT}{h}\left(\frac{1}{C^0}\right)^{n-1}\exp\left(-\frac{\Delta G_C^{0\ddagger}}{RT}\right) \qquad k_r = \frac{kT}{h}\left(\frac{RT}{P^0}\right)^{n-1}\exp\left(-\frac{\Delta G_P^{0\ddagger}}{RT}\right)$$

Tema 6

$$P_{in} = P_{ex} + \frac{2\gamma}{r} \qquad P = P^* exp(2\gamma V_m^L/(rRT)) \qquad h = \frac{2\gamma\cos\theta}{(\rho^L - \rho^V)gR}$$

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

Tema 7

$$\theta = \frac{KP}{1+KP} \qquad \theta = \frac{(KP)^{1/2}}{1+(KP)^{1/2}} \qquad \theta = kP^{1/n} \qquad \theta = A\ln(BP) \qquad \left(\frac{\partial \ln P}{\partial 1/T}\right)_{\theta} = \frac{\Delta H^{\circ}_{ads}}{R}$$

$$\frac{V}{V_{mon}} = \frac{KP}{(1-K*P)(1-K*P+KP)} \qquad v = \frac{k_1 k_2 [S][C]}{k_{-1}+k_2} \qquad v_0 = \frac{k_1 k_2 [C]_0 [S]_0}{k_1([C]_0+[S]_0)+k_{-1}+k_2}$$

Tema 8

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

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

Tema 9

$$\overline{M}_n = \frac{\sum N_i M_i}{\sum N_i} = \sum x_i M_i \qquad \overline{M}_w = \frac{\sum W_i M_i}{\sum W_i} = \frac{\sum N_i M_i^2}{\sum N_i M_i} \qquad \overline{M}_z = \frac{\sum N_i M_i^3}{\sum N_i M_i^2}$$

$$\overline{M}_v = \left(\frac{\sum N_i M_i^{a+1}}{\sum N_i M_i}\right)^{1/a} \qquad \Delta G_M = k_B T \chi_1 n_1 \phi_2 + T k_B (n_1 \ln\phi_1 + n_2 \ln\phi_2)$$

$$\Delta\mu_1 = RT\left(\ln\phi_1 + \left(1-\frac{1}{r}\right)\phi_2 + \chi_1\phi_2^2\right) \qquad \phi_{1c} = \frac{1}{1+1/\sqrt{r_n}} \qquad \chi_{1c} = \frac{1}{2}\left(1+\frac{1}{\sqrt{r_n}}\right)^2$$