EJERCICIOS: GUIA 1

UNITS

1- Obtain the equivalence of 1 meV in:

J, K (Kelvin), KJ/mol, Kcal/mol

INTERMOLECULAR INTERACTION

2- Prove that the LJ potential $U_{LJ}(r)$ is minimum at r=1.12 sigma

3- Plot $U_{LJ}(r)$ vs x=r/sigma

4- Plot $U_{LJ}(r)$ vs r for CH_4

5- Plot $U_{LJ}(r)$ between two CO_2 molecules as a function of the distance between the carbons in

   a. parallel orientation
   b. transverse orientation

6- Plot the Coulomb interaction between two CO_2 molecules as a function of the distance between the carbons in

   a. parallel orientation
   b. transverse orientation

   Compare with 5.

SUSTRATE INTERACTION

7- Prove that the minimum of the U93 potential is D at $z_{min}=(2C_3/3D)^{1/3}$

8- Plot U93(z) vs z for CH4 on graphite

9- Plot $U_{93}(z)$ vs z for a CO_2 molecule on graphite as a function of the distance between the carbon atom and the graphite surface

   a. parallel orientation
   b. transverse orientation

Tabla: Parametros de interaction con grafito

	D(Kcal/mol)	Zmin (nm)
CH4	3.10	0.40
C in CO2	1.14	0.31
O in CO2	1.95	0.32