*__Ionization Energy (IE):-__ also known as the ***ionization potential***, **Is the energy required to remove an electron from a gaseous atom or ion**. The losing of an electron is an ***Endothermic*** process (require energy).

$$A^{n+}(g) \longrightarrow A^{(n+1)+}(g) + e^- \qquad \text{ionization energy } (IE) = \Delta U$$

*Where n = 0 (first ionization energy), n = 1 (second ionization energy), and so on. As would be expected from the effects of shielding, the ionization energy varies with different nuclei and different numbers of electrons.

* Depends on:

a- Size of the atom - IE decreases as the size of the atom increases, thus IE decreases down the group.

b- IE increase from left to right in every period because of the increasing Z_{eff}.

* The following table shows the first, second and (some higher) ionization energies of the elements from Na to Ar in KJ/mol unit.

Element	I_1	I_2	I_3	I_4	I_5	I_6	I_7
Na	496	4560					
Mg	738	1450	7730		(Inner-shell electrons)		
Al	578	1820	2750	11,600			
Si	786	1580	3230	4360	16,100		
P	1012	1900	2910	4960	6270	22,200	
S	1000	2250	3360	4560	7010	8500	27,100
Cl	1251	2300	3820	5160	6540	9460	11,000
Ar	1521	2670	3930	5770	7240	8780	12,000

* First ionization energies vary systematically through the periodic table (Table below), being smallest at the lower left (near **Cs**) and greatest near

the upper right (near **He**). The variation follows the pattern of effective nuclear charge, and (as Z_{eff} itself shows) there are some subtle modulations arising from the effect of electron–electron repulsions within the same subshell. A useful approximation is that for an electron from a shell with principal quantum number ***n***

$$IE \propto \frac{Z_{eff}^2}{n^2}$$

$$\mathbf{I.E = 13.6\ e.v * [(Z^*)^2 / n^2]}$$

Z^* = Effective nuclear charge

n = principle quantum number

13.6 e.v= the ionization energy of the H atom is 13.6 eV, so to remove an electron from an H atom is equivalent to dragging the electron through a potential difference of 13.6 V.

Ex: Calculate the first ionization energy or (potential) of $_3$**Li**

Ans:

First we must calculate Effective nuclear charge (Z_{eff} or Z^*)

$_3Li\ 1S^2\ 2S^1$

$\sigma = (0 * .35) + (2 * 0.85) = 1.7$

$Z_{eff} = Z - \sigma = 3 - 1.7 = 1.3$

So I.E = 13.6 e.v $*[(Z^*)^2 / n^2]$

= 13.6 e.v * $[(1.3)^2 / (2)^2]$

= 13.6 e.v * [0.4225]

= 5.746 e.v

So IE of $_3$Li in KJ/ mol = [5.746] * [96.485]

= 554.4 KJ/ mol

Table First, second, and third (and some fourth) ionization energies of the elements, $I/(\mathrm{kJ\ mol^{-1}})$

H							**He**
1312							2373
							5259
Li	**Be**	**B**	**C**	**N**	**O**	**F**	**Ne**
513	899	801	1086	1402	1314	1681	2080
7297	1757	2426	2352	2855	3386	3375	3952
11809	14844	3660	4619	4577	5300	6050	6122
		25018					
Na	**Mg**	**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
495	737	577	786	1011	1000	1251	1520
4562	1476	1816	1577	1903	2251	2296	2665
6911	7732	2744	3231	2911	3361	3826	3928
		11574					
K	**Ca**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
419	589	579	762	947	941	1139	1351
3051	1145	1979	1537	1798	2044	2103	3314
4410	4910	2963	3302	2734	2974	3500	3565
Rb	**Sr**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
403	549	558	708	834	869	1008	1170
2632	1064	1821	1412	1794	1795	1846	2045
3900	4210	2704	2943	2443	2698	3197	3097
Cs	**Ba**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
375	502	590	716	704	812	926	1036
2420	965	1971	1450	1610	1800	1600	
3400	3619	2878	3080	2466	2700	2900	

***** Ionization energies also correlate strongly with atomic radii, and elements that have small atomic radii generally have high ionization energies. The explanation of the correlation is that in a small atom an electron is close to the nucleus and experiences a strong Coulombic attraction, making it difficult to remove. Therefore, as the atomic radius increases down a group, the ionization energy decreases, and the decrease in radius across a period is accompanied by a gradual increase in ionization energy

* The tables below represent the first three ionization energy and electron affinity of elements in ev unit.

Atom			Ionization energy (eV) I_1	I_2	I_3	Electron affinity E_{ea} (eV)
1	H	$1s^1$	13.60			+0.754
2	He	$1s^2$	24.59	54.51		−0.5
3	Li	$[He]2s^1$	5.320	75.63	122.4	+0.618
4	Be	$[He]2s^2$	9.321	18.21	153.85	≤0
5	B	$[He]2s^22p^1$	8.297	25.15	37.93	+0.277
6	C	$[He]2s^22p^2$	11.257	24.38	47.88	+1.263
7	N	$[He]2s^22p^3$	14.53	29.60	47.44	−0.07
8	O	$[He]2s^22p^4$	13.62	35.11	54.93	+1.461
9	F	$[He]2s^22p^5$	17.42	34.97	62.70	+3.399
10	Ne	$[He]2s^22p^6$	21.56	40.96	63.45	−1.2
11	Na	$[Ne]3s^1$	5.138	47.28	71.63	+0.548
12	Mg	$[Ne]3s^2$	7.642	15.03	80.14	≤0
13	Al	$[Ne]3s^23p^1$	5.984	18.83	28.44	+0.441
14	Si	$[Ne]3s^23p^2$	8.151	16.34	33.49	+1.385
15	P	$[Ne]3s^23p^3$	10.485	19.72	30.18	+0.747
16	S	$[Ne]3s^23p^4$	10.360	23.33	34.83	+2.077
17	Cl	$[Ne]3s^23p^5$	12.966	23.80	39.65	+3.617
18	Ar	$[Ne]3s^23p^6$	15.76	27.62	40.71	−1.0
19	K	$[Ar]4s^1$	4.340	31.62	45.71	+0.502
20	Ca	$[Ar]4s^2$	6.111	11.87	50.89	+0.02

Atom			Ionization energy (eV) I_1	I_2	I_3	Electron affinity E_{ea} (eV)
21	Sc	$[Ar]3d^14s^2$	6.54	12.80	24.76	
22	Ti	$[Ar]3d^24s^2$	6.82	13.58	27.48	
23	V	$[Ar]3d^34s^2$	6.74	14.65	29.31	
24	Cr	$[Ar]3d^54s^1$	6.764	16.50	30.96	
25	Mn	$[Ar]3d^54s^2$	7.435	15.64	33.67	
26	Fe	$[Ar]3d^64s^2$	7.869	16.18	30.65	
27	Co	$[Ar]3d^74s^2$	7.876	17.06	33.50	
28	Ni	$[Ar]3d^84s^2$	7.635	18.17	35.16	
29	Cu	$[Ar]3d^{10}4s^1$	7.725	20.29	36.84	
30	Zn	$[Ar]3d^{10}4s^2$	9.393	17.96	39.72	
31	Ga	$[Ar]3d^{10}4s^24p^1$	5.998	20.51	30.71	+0.30
32	Ge	$[Ar]3d^{10}4s^24p^2$	7.898	15.93	34.22	+1.2
33	As	$[Ar]3d^{10}4s^24p^3$	9.814	18.63	28.34	+0.81
34	Se	$[Ar]3d^{10}4s^24p^4$	9.751	21.18	30.82	+2.021
35	Br	$[Ar]3d^{10}4s^24p^5$	11.814	21.80	36.27	+3.365
36	Kr	$[Ar]3d^{10}4s^24p^6$	13.998	24.35	36.95	−1.0
37	Rb	$[Kr]5s^1$	4.177	27.28	40.42	+0.486
38	Sr	$[Kr]5s^2$	5.695	11.03	43.63	+0.05
39	Y	$[Kr]4d^15s^2$	6.38	12.24	20.52	
40	Zr	$[Kr]4d^15s^2$	6.84	13.13	22.99	

Atom			Ionization energy (eV) I_1	I_2	I_3	Electron affinity E_{ea}(eV)
41	Nb	[Kr]$4d^4 5s^1$	6.88	14.32	25.04	
42	Mo	[Kr]$4d^5 5s^1$	7.099	16.15	27.16	
43	Tc	[Kr]$4d^5 5s^2$	7.28	15.25	29.54	
44	Ru	[Kr]$4d^7 5s^1$	7.37	16.76	28.47	
45	Rh	[Kr]$4d^8 5s^1$	7.46	18.07	31.06	
46	Pd	[Kr]$4d^{10}$	8.34	19.43	32.92	
47	Ag	[Kr]$4d^{10} 5s^1$	7.576	21.48	34.83	
48	Cd	[Kr]$4d^{10} 5s^2$	8.992	16.90	37.47	
49	In	[Kr]$4d^{10} 5s^2 5p^1$	5.786	18.87	28.02	+0.3
50	Sn	[Kr]$4d^{10} 5s^2 5p^2$	7.344	14.63	30.50	+1.2
51	Sb	[Kr]$4d^{10} 5s^2 5p^3$	8.640	18.59	25.32	+1.07
52	Te	[Kr]$4d^{10} 5s^2 5p^4$	9.008	18.60	27.96	+1.971
53	I	[Kr]$4d^{10} 5s^2 5p^5$	10.45	19.13	33.16	+3.059
54	Xe	[Kr]$4d^{10} 5s^2 5p^6$	12.130	21.20	32.10	−0.8
55	Cs	[Xe]$6s^1$	3.894	25.08	35.24	
56	Ba	[Xe]$6s^2$	5.211	10.00	37.51	
57	La	[Xe]$5d^1 6s^2$	5.577	11.06	19.17	
58	Ce	[Xe]$4f^1 5d^1 6s^2$	5.466	10.85	20.20	
59	Pr	[Xe]$4f^3 6s^2$	5.421	10.55	21.62	
60	Nd	[Xe]$4f^4 6s^2$	5.489	10.73	20.07	
61	Pm	[Xe]$4f^5 6s^2$	5.554	10.90	22.28	
62	Sm	[Xe]$4f^6 6s^2$	5.631	11.07	23.42	
63	Eu	[Xe]$4f^7 6s^2$	5.666	11.24	24.91	
64	Gd	[Xe]$4f^7 5d^1 6s^2$	6.140	12.09	20.62	
65	Tb	[Xe]$4f^9 6s^2$	5.851	11.52	21.91	
66	Dy	[Xe]$4f^{10} 6s^2$	5.927	11.67	22.80	
67	Ho	[Xe]$4f^{11} 6s^2$	6.018	11.80	22.84	
68	Er	[Xe]$4f^{12} 6s^2$	6.101	11.93	22.74	
69	Tm	[Xe]$4f^{13} 6s^2$	6.184	12.05	23.68	
70	Yb	[Xe]$4f^{14} 6s^2$	6.254	12.19	25.03	
71	Lu	[Xe]$4f^{14} 5d^1 6s^2$	5.425	13.89	20.96	
72	Hf	[Xe]$4f^{14} 5d^2 6s^2$	6.65	14.92	23.32	

Atom			Ionization energy (eV) I_1	I_2	I_3	Electron affinity E_{ea}(eV)
73	Ta	[Xe]$4f^{14} 5d^3 6s^2$	7.89	15.55	21.76	
74	W	[Xe]$4f^{14} 5d^4 6s^2$	7.89	17.62	23.84	
75	Re	[Xe]$4f^{14} 5d^5 6s^2$	7.88	13.06	26.01	
76	Os	[Xe]$4f^{14} 5d^6 6s^2$	8.71	16.58	24.87	
77	Ir	[Xe]$4f^{14} 5d^7 6s^2$	9.12	17.41	26.95	
78	Pt	[Xe]$4f^{14} 5d^9 6s^1$	9.02	18.56	29.02	
79	Au	[Xe]$4f^{14} 5d^{10} 6s^1$	9.22	20.52	30.05	
80	Hg	[Xe]$4f^{14} 5d^{10} 6s^2$	10.44	18.76	34.20	
81	Tl	[Xe]$4f^{14} 5d^{10} 6s^2 6p^1$	6.107	20.43	29.83	
82	Pb	[Xe]$4f^{14} 5d^{10} 6s^2 6p^2$	7.415	15.03	31.94	
83	Bi	[Xe]$4f^{14} 5d^{10} 6s^2 6p^3$	7.289	16.69	25.56	
84	Po	[Xe]$4f^{14} 5d^{10} 6s^2 6p^4$	8.42	18.66	27.98	
85	At	[Xe]$4f^{14} 5d^{10} 6s^2 6p^5$	9.64	16.58	30.06	
86	Rn	[Xe]$4f^{14} 5d^{10} 6s^2 6p^6$	10.75			
87	Fr	[Rn]$7s^1$	4.15	21.76	32.13	
88	Ra	[Rn]$7s^2$	5.278	10.15	34.20	
89	Ac	[Rn]$6d^1 7s^2$	5.17	11.87	19.69	
90	Th	[Rn]$6d^2 7s^2$	6.08	11.89	20.50	
91	Pa	[Rn]$5f^2 6d^1 7s^2$	5.89	11.7	18.8	
92	U	[Rn]$5f^3 6d^1 7s^2$	6.19	14.9	19.1	
93	Np	[Rn]$5f^4 6d^1 7s^2$	6.27	11.7	19.4	
94	Pu	[Rn]$5f^6 7s^2$	6.06	11.7	21.8	
95	Am	[Rn]$5f^7 7s^2$	5.99	12.0	22.4	
96	Cm	[Rn]$5f^7 6d^1 7s^2$	6.02	12.4	21.2	
97	Bk	[Rn]$5f^9 7s^2$	6.23	12.3	22.3	
98	Cf	[Rn]$5f^{10} 7s^2$	6.30	12.5	23.6	
99	Es	[Rn]$5f^{11} 7s^2$	6.42	12.6	24.1	
100	Fm	[Rn]$5f^{12} 7s^2$	6.50	12.7	24.4	
101	Md	[Rn]$5f^{13} 7s^2$	6.58	12.8	25.4	
102	No	[Rn]$5f^{14} 7s^2$	6.65	13.0	27.0	
103	Lr	[Rn]$5f^{14} 6d^1 7s^2$	4.6	14.8	23.0	

*<u>**Electron Affinity (EA)**</u>

Electron affinity: ***Is defined as the energy released when an electron is added to an atom***. The gaining of an electron is an ***exothermic*** process (releasing energy).

$$\mathbf{X(g) + e^- \rightarrow X^- (g) + Energy}$$

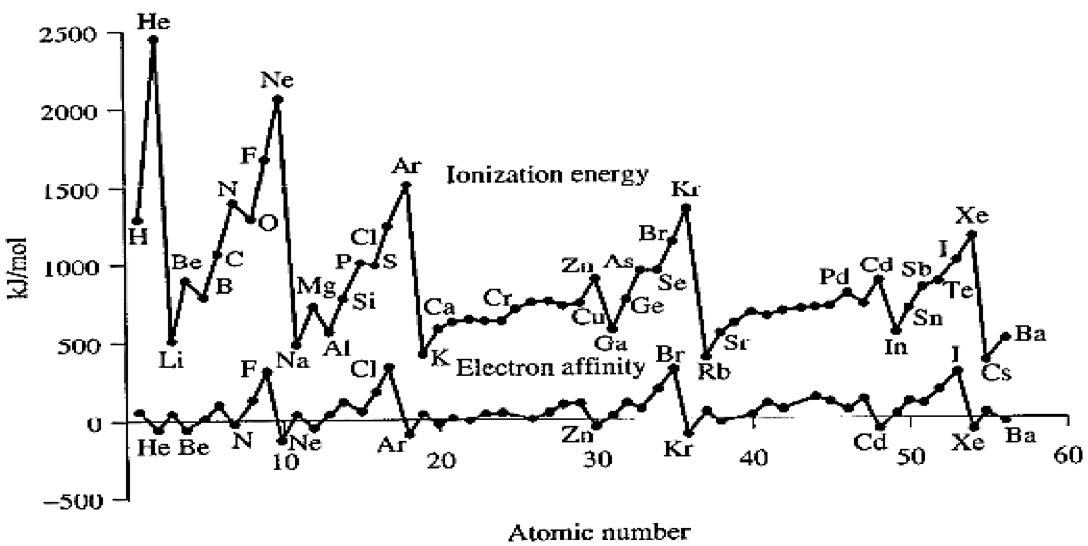
*Electron affinity can be also defined as; ***the energy required to remove an electron from a negative ion***.

$$A^-(g) \longrightarrow A(g) + e^- \qquad \text{electron affinity } (EA) = \Delta U$$

*Because of the similarity of this reaction to the ionization for an atom, electron affinity is sometimes described as the ***zeroth ionization energy***. This reaction is endothermic (positive *U*) except for the noble gases and the alkaline earth elements.

*The EA of an atom measures the tightness with which it binds an additional electron to itself.

*The next figure shows the ionization energies and electron affinities of elements.



***On moving across a period**, the atomic size decreases and hence the force of attraction exerted by the nucleus on the electrons increases. Consequently, the atom has a greater tendency to attract additional electron i.e., its electron affinity increases.

* EA values of metals are low while those of non-metals are high. *Halogens have high electron affinities. This is due to their strong tendency to gain an additional electron to change into the stable ns^2np^6 configuration.

***On moving down a group**, the atomic size increases and therefore, the effective nuclear attraction decreases and thus electron affinity decreases.

* The next table represents the affinities values of main group elements in KJ/mol.

H 72							**He** −48
Li 60	**Be** ≤0	**B** 27	**C** 122	**N** −8	**O** 141 −780	**F** 328	**Ne** −116
Na 53	**Mg** ≤0	**Al** 43	**Si** 134	**P** 72	**S** 200 −492	**Cl** 349	**Ar** −96
K 48	**Ca** 2	**Ga** 29	**Ge** 116	**As** 78	**Se** 195	**Br** 325	**Kr** −96
Rb 47	**Sr** 5	**In** 29	**Sn** 116	**Sb** 103	**Te** 190	**I** 295	**Xe** −77

*<u>**Electronegativity**</u>;- Pauling defined electronegativity as ***the power of an atom in a molecule to attract shared electrons to itself***.

*Others definitions;

** Electronegativity ***is a measure of an atom's ability to attract electrons from a neighboring atom to which it is bonded***.

** Electronegativity ***is the ability of an atom to win the competition to attract shared electrons***.

* This relative attraction for bonding electron pairs really reflects the comparative $\mathbf{Z_{eff}}$ of the two atoms on the shared electrons. Thus, the values increase from left to right across a period and decrease down a group in the same way as ionization energies do.

*Some useful electronegativity values are shown in Figure below:

H 2.1			
C 2.5	N 3.0	O 3.5	F 4.0
Si 1.8	P 2.1	S 2.5	Cl 3.0
Ge 1.8	As 2.0	Se 2.4	Br 2.8

*In most cases the different methods give similar electronegativity values, sometimes with the exception of the transition metals. We choose to use the values reported by Linus Pauling, Mann, Meek, Allen, and others.

Electronegativity Scales

Principal Authors	Method of Calculation or Description
Pauling	Bond energies
Mulliken	Average of electron affinity and ionization energy
Allred & Rochow	Electrostatic attraction proportional to Z^*/r^2
Sanderson	Electron densities of atoms
Pearson	Average of electron affinity and ionization energy
Allen	Average energy of valence shell electrons, configuration energies
Jaffé	Orbital electronegativities