

[TP] Ionization energy can be expressed as kJ/mol and as eV/atom. The first ionization energy of Na atom is 5.14 eV. How many kJ are required to ionize one mole of Na atoms? Remember: electron charge is 1.60×10^{-19} C and 1 V = 1 J/C.

11%	1.	300 kJ
60%	2.	500 kJ
26%	3.	700 kJ
3%	4.	900 kJ

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Lecture 5 CH131 Fall 2020

Tuesday, September 22, 2020

Begin ch3: Chemical bonding: The classical description

- Ionization energy: $X(g) \to X^+(g) + e^-$
- Anatomy of electron clouds
- $IE_1 \to$ electron cloud expansion

Next lecture: Electron affinity: $X^-(g) \to X(g) + e^-$; Electronegativity: $EN \sim IE_1 + EA$; Dipole moment and ionic character: $\sim \Delta EN$; Lewis diagrams, shapes, resonance, and polarity of molecules; Begin ch9.1–9.6. The gaseous state ;

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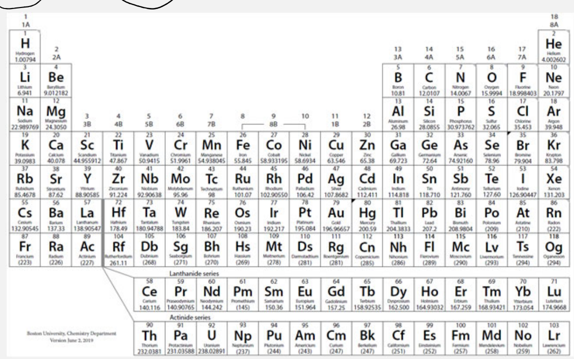
IE, EA, and EN



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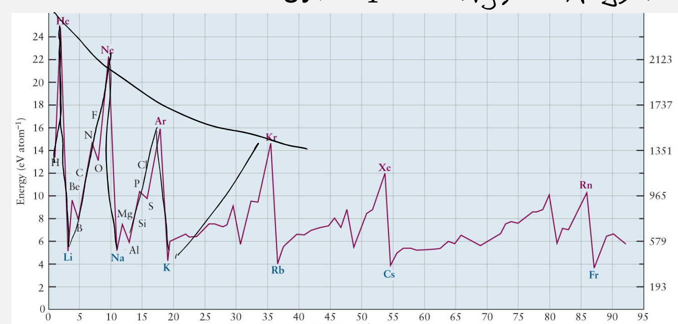
First ionization energy, IE_1

$X(g) \to X^+(g) + e^-(g)$



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eV/atom and kJ/mol

1 eV is the energy of 1 electron charge in a potential of 1 V = I J/C

$e^- = 1.6022 \times 10^{-19}$ C

$1 \text{ eV} = \underbrace{1.6022 \times 10^{-19}\ \cancel{C}}\times \underbrace{1\ \text{J}/\cancel{C}} = 1.6022 \times 10^{-19}$ J

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eV/atom and kJ/mol

For H atom (only; not other atoms),

$$IE_1 = 13.6\ \frac{\text{eV}}{\text{atom}} = 13.6\ \frac{\text{eV}}{\text{atom}} \times 1.6022 \times 10^{-19}\ \frac{\text{J}}{\text{eV}} = 21.8 \times 10^{-19}\ \frac{\text{J}}{\text{atom}}$$

$$IE_1 = 21.8 \times 10^{-19}\ \frac{\text{J}}{\text{atom}} \times \frac{N_A\ \text{atom}}{\text{mol}} = 21.8 \times 10^{-19} \times 6.022 \times 10^{23}\ \text{J/mol}$$

$$= 1.31 \times 10^{6}\ \frac{\text{J}}{\text{mol}} = 1310\ \frac{\text{kJ}}{\text{mol}}$$

$\text{J} \times \frac{1\text{kJ}}{1000\text{J}}$

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$Na(g) \rightarrow Na^+(g) + e^-(g)$ $IE_1 = 5.14\text{eV}$

- 2% 1. 300 kJ
- 90% 2. 500 kJ
- 5% 3. 700 kJ
- 2% 4. 900 kJ

$$\frac{5.14\ \cancel{\text{eV}}}{\text{atom}} \times \boxed{\frac{1.6\times10^{-19}\ \cancel{C}\cdot 1\text{J}/\cancel{C}}{\cancel{\text{eV}}}} \times \frac{6.0\times10^{23}\ \text{atom}}{\text{mol}} \times \frac{\text{kJ}}{1000\text{J}}$$

$= 495$

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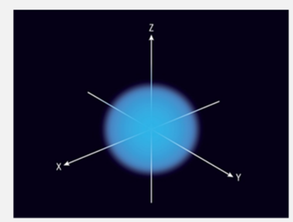
Anatomy of electron clouds

The volume of atoms is due to their electron clouds.

Studying successive ionization energies (how much energy is needed to remove an electron from the cloud) reveals the anatomy of the cloud.



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Anatomy of electron clouds

IE_1 , I_1

Let's do this for the nitrogen atom.

Here is the equation describing removal of one electron from a neutral N atom.

$N(g) \rightarrow N^+(g) + e^-(g), I_1 = 2.32\ \text{aJ} = 2.32 \times 10^{-18}\ \text{J}$

I_1 is called the first ionization energy, and 1 aJ = 1×10^{-18} J (attojoule)

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[TP] The energy required to remove a second electron from nitrogen, $N^+(g) \rightarrow N^{2+}(g) + e^-(g)$, is called the second ionization energy, I_2. Compared to the first ionization energy, I_1, the second ionization energy

28% 1. must be smaller $I_2 < I_1$
8% 2. must be about the same $I_2 \approx I_1$
63% 3. must be larger $I_2 > I_1$
2% 4. Further information required

$N(g) \rightarrow N^+(g) + e^-$ I_1

$N^+(g) \rightarrow N^{2+}(g) + e^-$ I_2

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Anatomy of electron clouds

$I_2 > I_1$

The key in comparing ionization energies, the ionizations

$N(g) \rightarrow N^+(g) + e^-(g), I_1$

$N^+(g) \rightarrow N^{2+}(g) + e^-(g), I_2$

is Coulomb's law,

$E_{\text{Coulomb}} \sim \frac{Q_1 Q_2}{d}$

In words, Coulomb's law says that opposite charges attract, the more so the greater the charges, Q_1 and Q_2, and the more so the closer, d, they are.

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Structure of electron clouds

The key in comparing ionization energies, the ionizations

$N(g) \rightarrow \cancel{N^+(g)} + e^-(g)$ I_1

$\cancel{N^+(g)} \rightarrow N^{2+}(g) + e^-(g)$ I_2

$N(g) \rightarrow N^{2+}(g) + 2e^-$ $I_1 + I_2$

The greater the product of the charges, the more energy required to separate them.

Therefore, I_2 must be larger than I_1, because

for I_2, $Q_1 Q_2 = (+2)(-1) = -2$

for I_1, $Q_1 Q_2 = (+1)(-1) = -1$

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[TP] For the 5th ionization energy of N atom, I_5, what are the values of the Coulomb's law charges Q_1 and Q_2?

4% 1. $Q_1 = +1$ and $Q_2 = -1$
5% 2. $Q_1 = +2$ and $Q_2 = -1$
8% 3. $Q_1 = +4$ and $Q_2 = -1$
73% 4. $Q_1 = +5$ and $Q_2 = -1$
9% 5. $Q_1 = +6$ and $Q_2 = -1$
1% 6. Something else

Q_1 Q_1

1 $N(g) \rightarrow N^+(g) + e^-$ I_1

2 $N^+(g) \rightarrow N^{2+}(g) + e^-$ I_2

⋮

$N^{4+}(g) \rightarrow N^{5+}(g) + e^-$ I_5

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[TP] The energy required to remove a third electron from nitrogen, $N^{2+}(g) \rightarrow N^{3+}(g) + e^-(g)$, is called the third ionization energy, I_3. How do the first three ionization energies compare? Tell your classmates why.

84% 1. $I_1 < I_2 < I_3$
5% 2. $I_1 < I_3 < I_2$
11% 3. $I_3 < I_2 < I_1$

$Q_1 = 1$, $Q_2 = 2$, $Q_3 = 3$

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Successive ionization energies

TABLE 3.1

Successive Ionization Energies of the Elements Hydrogen through Argon (in eV Atom^{-1})

Z	Element	IE_1	IE_2	IE_3	IE_4	IE_5	IE_6	IE_7	IE_8	IE_9	IE_{10}
1	H	13.60									
2	He	24.59	54.42								
3	Li	5.39	75.64	122.45							
4	Be	9.32	18.21	153.89	217.71						
5	B	8.30	25.15	37.93	259.37	340.22					
6	C	11.26	24.38	47.89	64.49	392.08	489.99				
7	N	14.53	29.60	47.45	77.47	97.89	552.06	667.03			
8	O	13.62	35.12	54.93	77.41	113.90	138.12	739.32	871.39		
9	F	17.42	34.97	62.71	87.14	114.24	157.16	185.18	953.89	1103.08	
10	Ne	21.56	40.96	63.45	97.11	126.21	157.93	207.27	239.09	1195.79	1362.16
11	Na	5.14	47.29	71.64	98.91	138.39	172.15	208.47	264.18	299.87	1465.10
12	Mg	7.65	15.04	80.14	109.24	141.26	186.50	224.94	265.90	327.94	367.53
13	Al	5.99	18.83	28.45	119.99	153.71	190.47	241.43	284.59	330.21	398.57
14	Si	8.15	16.35	33.49	45.14	166.77	205.05	246.52	303.17	351.10	401.43
15	P	10.49	19.73	30.18	51.37	65.02	220.43	263.22	309.41	371.73	424.50
16	S	10.36	23.33	34.83	47.30	72.68	88.05	280.93	328.23	379.10	447.10
17	Cl	12.97	23.81	39.61	53.46	67.8	97.03	114.19	348.28	400.03	455.62
18	Ar	15.76	27.63	40.74	59.81	75.02	91.01	124.32	143.46	422.43	478.68
19	K	4.34	31.63	45.72	60.91	82.66	100.0	117.56	154.86	175.82	503.44
20	Ca	6.11	11.87	50.91	67.10	84.41	108.78	127.7	147.24	188.54	211.27
21	Sc	6.54	12.80	24.76	73.47	91.66	111.1	138.0	158.7	180.02	225.32

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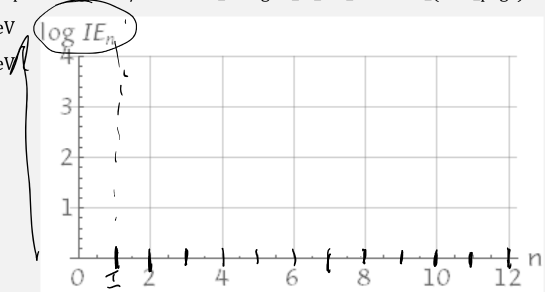
Plot log(IE_n) versus n for Mg

You will need the final two ionization energies, IE_{11} and IE_{12}.

https://en.wikipedia.org/wiki/Ionization_energies_of_the_elements_(data_page)

✓ IE_{11} = 1762 eV

✓ IE_{12} = 1962 eV



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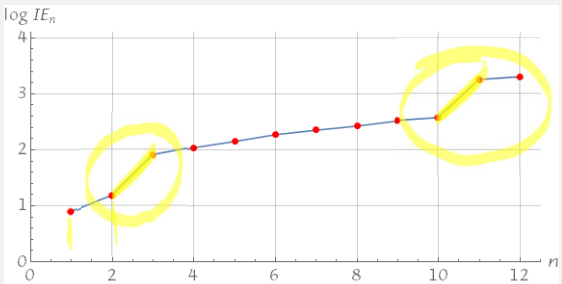
Plot log(IE_n) versus n for Mg

Physically (in terms of Coulomb's law), what accounts for the discontinuity between $n = 2$ and $n = 3$?



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Successive IE_n → electron cloud contraction

$IE_2 > IE_1$: $Mg^{2+} > Mg^{+}$ increase in residual ion charge

$IE_3 \gg IE_2$: $Mg^{3+} \gg Mg^{2+}$ large contraction of electron cloud

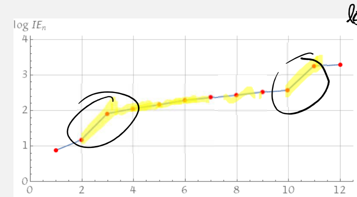
$IE_{10} > IIE_9 > \cdots > IE_3$: increase in residual ion charge

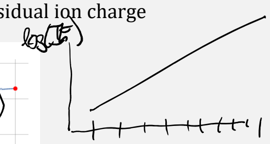
$IE_{11} \gg IE_{10}$: $Mg^{11+} \gg Mg^{10+}$ large contraction of electron cloud

$IE_{12} > IE_{11}$: $Mg^{12+} > Mg^{11+}$ integer increase in residual ion charge

IE_3

$Mg^{2+}(g) \to Mg^{3+}(g) + e^-$





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Structure of electron clouds

Evidence of charge cloud contraction is seen in every element other than H and He. For example,

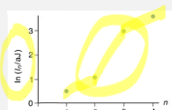

Figure 4.4 The logarithms of the four successive ionization energies (ln I_n/aJ) of a beryllium atom versus the number of electrons removed (n). This graph suggests that the electrons in a beryllium atom are arranged in two shells: an inner shell consisting of two electrons and an outer shell consisting of two electrons.

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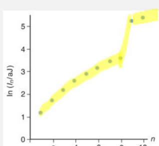

Figure 4.5 The logarithms of the ten successive ionization energies (ln I_n/aJ) of a neon atom versus the number of electrons removed (n). This graph suggests that the electrons in a neon atom are arranged in two shells: an inner shell consisting of two electrons and an outer shell consisting of eight electrons.

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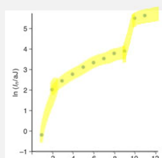

Figure 4.6 The logarithms of the 11 successive ionization energies (ln I_n/aJ) of a sodium atom versus the number of electrons removed (n).

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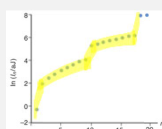

Figure 4.7 The logarithms of the 19 successive ionization energies (ln I_n/aJ) of a potassium atom versus the number of electrons removed (n).

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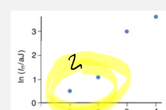
Structure of electron clouds

The "easier to remove" electrons are called valence electrons. The remaining "harder to remove" electrons are called core electrons.

Easy



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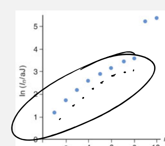

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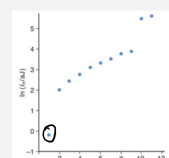

Figure 4.6 The logarithms of the 11 successive ionization energies (ln I_n/aJ) of a sodium atom versus the number of electrons removed (n).

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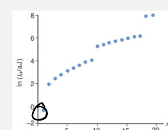

Figure 4.7 The logarithms of the 19 successive ionization energies (ln I_n/aJ) of a potassium atom versus the number of electrons removed (n).

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Structure of electron clouds

The "easy-to-remove" part of electron clouds account for the periodicity of atom properties.

The Lewis electron-dot formula summarizes the number of easily removed (valence) electrons until the much smaller cloud of inner-core electrons remains.

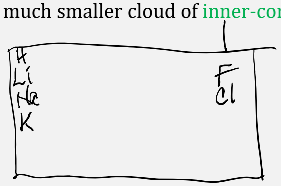

TABLE 4.2 A simple representation of the first 18 elements, indicating their noble-gas-like inner core and their outer electrons

Symbol	Inner-core representation	Lewis electron-dot formula
H	H	H·
He	[He]	He:
Li	[He]·	Li·
Be	[He]:	Be:
B	[He]:	B:
C	·[He]:	·C:
N	·[He]:	·N:
O	·[He]·	·O·
F	:[He]:	:F:
Ne	[Ne]	:Ne:
Na	[Ne]·	Na·
Mg	[Ne]:	Mg:
Al	[Ne]:	Al:
Si	·[Ne]:	·Si:
P	·[Ne]·	·P·
S	·[Ne]·	·S·
Cl	:[Ne]:	:Cl:
Ar	[Ar]	:Ar:
K	[Ar]·	K·
Ca	[Ar]:	Ca:

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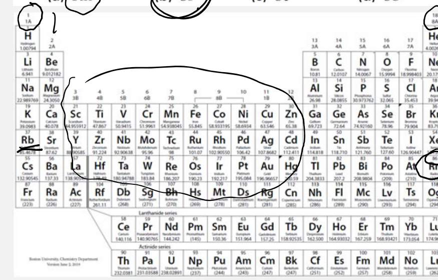
Problem 3.21

Rn
8 valence
86-8=78 core

Sr
2 valence
38-2=36 core
Sr^+ has $37e^-$/38 p
1 valence, 36 core
Rb has 37e/37p

21. For each of the following atoms or ions, state the total number of electrons, the number of valence electrons, and the number of core electrons.
(a) Rn (b) Sr^+ (c) Se^{2-} (d) Sb^-



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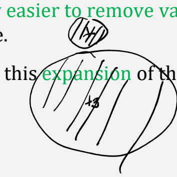
IE_1 → electron cloud expansion

Elements in successive rows of the same column of the periodic table contain the same number of valence electrons but increasing numbers of core electrons.

This means the valence portion of the electron clouds of successive elements in the same column is larger and so farther from the nucleus.

This in turn means it is increasingly easier to remove valence electrons going down a column of the periodic table.

Ionization energies decrease due to this expansion of the valence region of the electron cloud.



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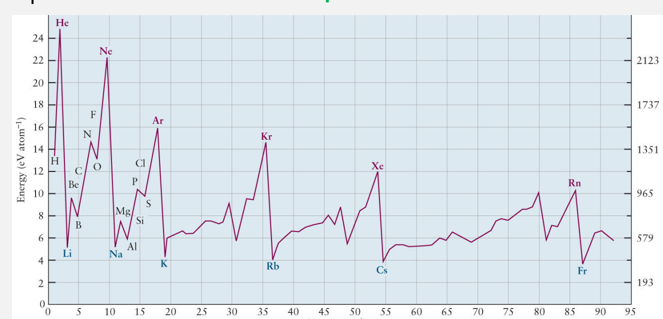
IE_1 → electron cloud expansion



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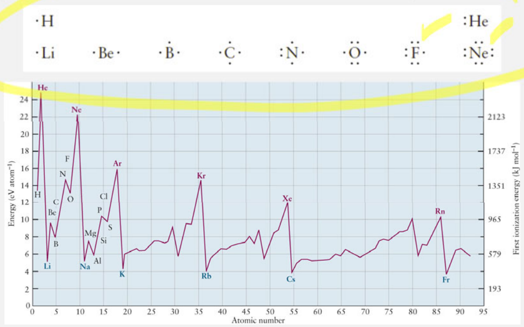
IE_1 → electron cloud expansion

Lewis dot picture summarizes effect of electron cloud expansion.



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