Lecture 3 CH131 Summer 1
Tuesday, May 26, 2020

- Limiting reagent recipe

Begin ch3: Chemical bonding: The classical description
- Ionization energy: X (g) → X^+(g) + e−, electron cloud shell structure
- Electron affinity: X^-(g) → X(g) + e−

Next lecture: Electronegativity: $EN \sim IE_1 + EA$; Dipole moment and ionic character: $\sim \Delta EN$; Complete ch3: Lewis diagrams, shapes, resonance, and polarity of molecules; begin ch9.1–9.6. The gaseous state

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Problem: 7e 2.49, 8e 2.37

49. The iron oxide Fe_2O_3 reacts with carbon monoxide (CO) to give iron and carbon dioxide:

$$Fe_2O_3 + 3\ CO \longrightarrow 2\ Fe + 3\ CO_2$$

The reaction of 433.2 g Fe_2O_3 with excess CO yields 254.3 g iron. Calculate the theoretical yield of iron (assuming complete reaction) and its percentage yield.

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General limiting reagent recipe

2 A + 3 B → C + 2 D, 7.00 mol of A and 10.00 mol of B react with 52% yield. How much A, B, C, and D at the end of the reaction?

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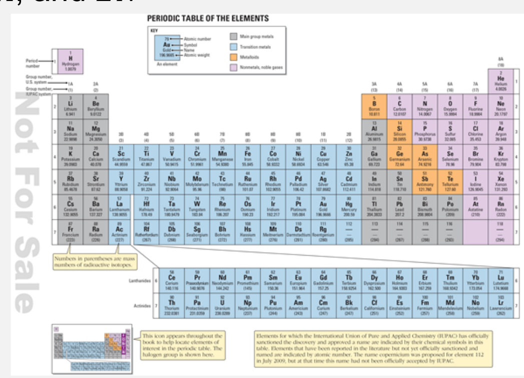
IE, EA, and EN



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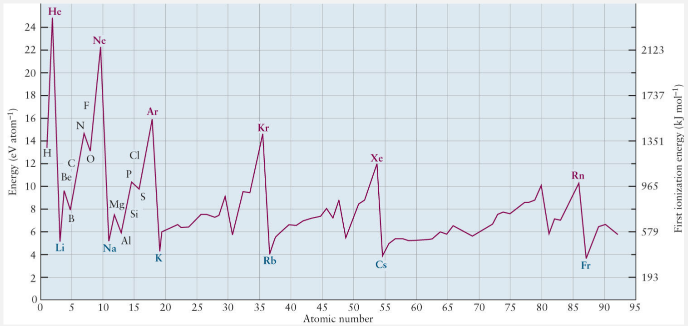
First ionization energy, IE_1



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

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eV/atom and kJ/mol

For H atoms,

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

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

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

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[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 I V = 1 J/C.

$5.14\ eV \quad Na \to Na^+ + e^-$

0%	1.	300 kJ
94%	2.	500 kJ
6%	3.	700 kJ
0%	4.	900 kJ

$1.6 \times 10^{-19}\,\frac{C * J}{C} = 1\ eV$

$1.6 \times 10^{-19}\,\frac{J}{\cancel{eV}} * 5.14\,\frac{\cancel{eV}}{\cancel{atom}} * \frac{6.0 \times 10^{23}\ \cancel{atoms}}{mol}$

$\frac{1.6 * 10^{4}\ \cancel{J} * 5.14 * 6 * kJ}{mol\ 10^{3}\ \cancel{J}}$

$16 * 5 * 6\ \frac{kJ}{mol}$

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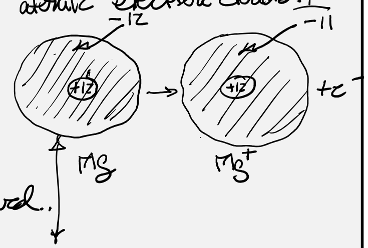
Successive ionization energies

Insight into the internal structure of atomic electron clouds.

Ionization energy = energy required to remove an electron from an atom

$_{12}Mg \to {}_{12}Mg^{+} + e^{-}$

$_{12}Mg^{+} \to {}_{12}Mg^{2+} + e^{-}$



Expect the cloud to get smoothly smaller as more and units of electron charge are removed.

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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

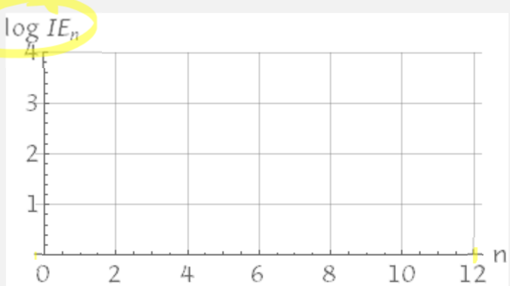
You will need the final two ionization energies, IE_{11} and IE_{12}.

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

$IE_{11} = 1762$ eV

$IE_{12} = 1962$ eV

log(1962) = 3.29



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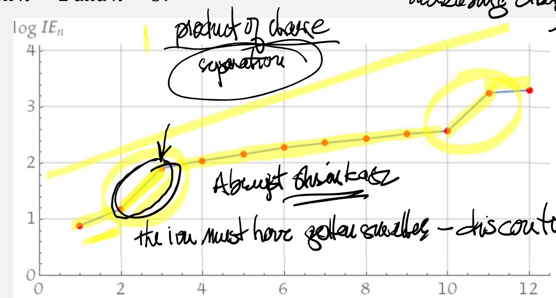
Plot log(IE_n) versus n for Mg

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

increasing charge on the ion left behind.



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Successive IE_n → electron cloud contraction

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

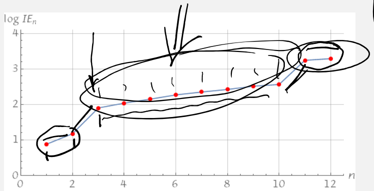
$IE_3 \gg IE_2$: $Mg^{3+} \gg Mg^{2+}$ large contraction of electron cloud

$IE_{10} > IE_9 > \cdots > IE_3$: 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

$1s^2 (2s^2 2p^6) 3s^2$



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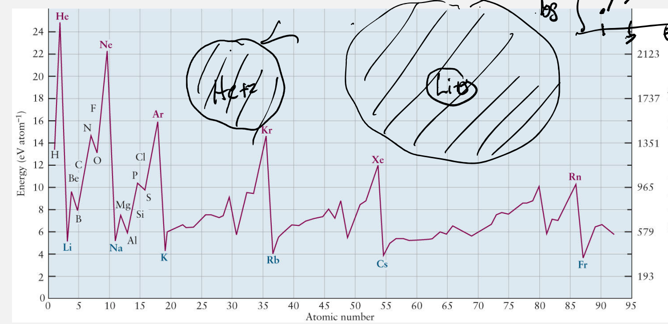
IE_1 → electron cloud expansion



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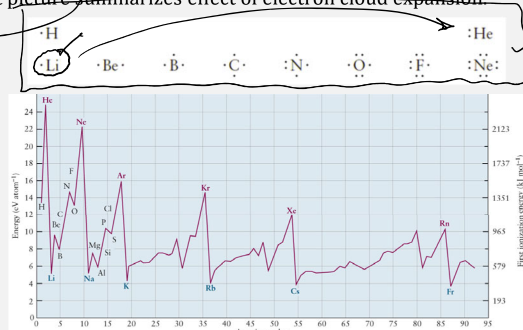
IE_1 → electron cloud expansion

Valence electrons

Lewis dot picture summarizes effect of electron cloud expansion.



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Electron affinity, EA

Electronegativity, EN

Ionic character

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Electron affinity, EA: $X^- \rightarrow X + e^-$

$IE_1: X \rightarrow X^+ + e^-$

TABLE 3.2

Electron Affinity of Selected Atoms (in kJ mol^{-1})

H 73							He *
Li 60	Be *	B 27	C 122	N *	O 141	F 328	Ne *
Na 53	Mg *	Al 42	Si 134	P 72	S 200	Cl 349	Ar *
K 48	Ca 2	Ga 41	Ge 119	As 79	Se 195	Br 325	Kr *
Rb 47	Sr 5	In 29	Sn 107	Sb 101	Te 190	I 295	Xe *
Cs 46	Ba 14	Tl 19	Pb 35	Bi 91	Po 183	At 270	Rn *

*No stable anion A$^-$ exists for this element in the gas phase.

He:

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Problem 3.23a

$Cl^- \rightarrow Cl + e^-$

3.7 $IE_1(K) = 4.34$ eV/atom

$IE_1(Cl) = 12.97$ eV/atom

3.2 $EA(K) = 48$ kJ/mol

$EA(Cl) = 349$ kJ/mol

23 Use the data in Figure 3.7 and Table 3.2 to calculate the energy changes (ΔE) for the following pairs of reactions:

(a) $K(g) + Cl(g) \longrightarrow K^+(g) + Cl^-(g)$

$\boxed{K(g) + Cl(g) \longrightarrow K^-(g) + Cl^+(g)}$

(b) $Na(g) + Cl(g) \longrightarrow Na^+(g) + Cl^-(g)$

$Na(g) + Cl(g) \longrightarrow Na^-(g) + Cl^+(g)$

Explain why K^+Cl^- and Na^+Cl^- form in preference to K^-Cl^+ and Na^-Cl^+.

$K(g) + Cl(g) \rightarrow K^+(g) + Cl^-(g)$

$K \rightarrow K^+ + \cancel{e^-}$ 4.34 eV/atom IE_1

$Cl + \cancel{e^-} \rightarrow Cl^-$ $\boxed{-349 \text{ kJ/mol}}$ $-EA$

$K + Cl \rightarrow K^+ + Cl^-$

$\frac{4.34 \text{ eV}}{\text{atom}} * \frac{1.6 \times 10^{-19} \text{ J}}{\text{eV}} * \frac{6 \times 10^{23} \text{ atom}}{\text{mol}} * \frac{\text{kJ}}{10^3 \text{ J}}$

$43.4 * 1.6 * 6$ kJ/mol. = 416 kJ/mol

416 kJ/mol

− 349 kJ/mol

~ 70 kJ/mol

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