(6) **Today**

2.2.4 Shielding

2.3 Periodic Properties

Next Class (7)

2.3 Periodic Properties

3.1 Lewis Structures

(8) **Second Class from Today**

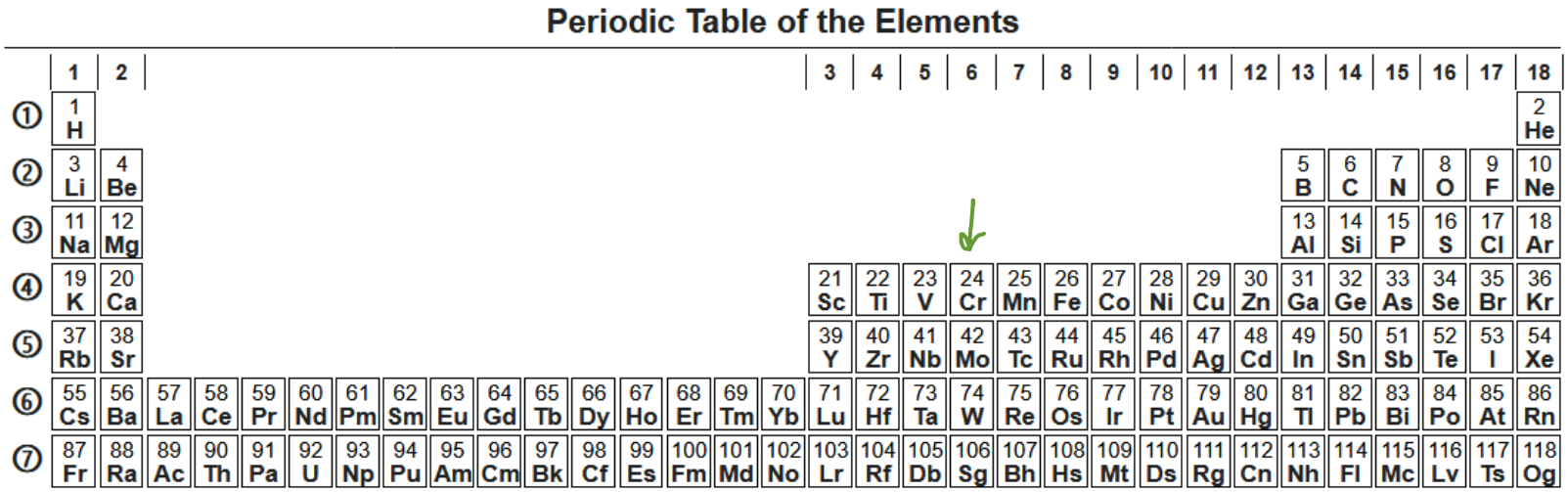
3.1 Lewis Structures

3.2 VSEPR

Third Class from Today (9)

3.2 VSEPR

3.3 Molecular Polarity



Cr [Ar] $4s^2$ $3d^4$

3d ↑ ↑ ↑ ↑
4s ↑↓ ↑

exchange interaction lowers E enough such that it would require more E to pair the e⁻'s in the 4s

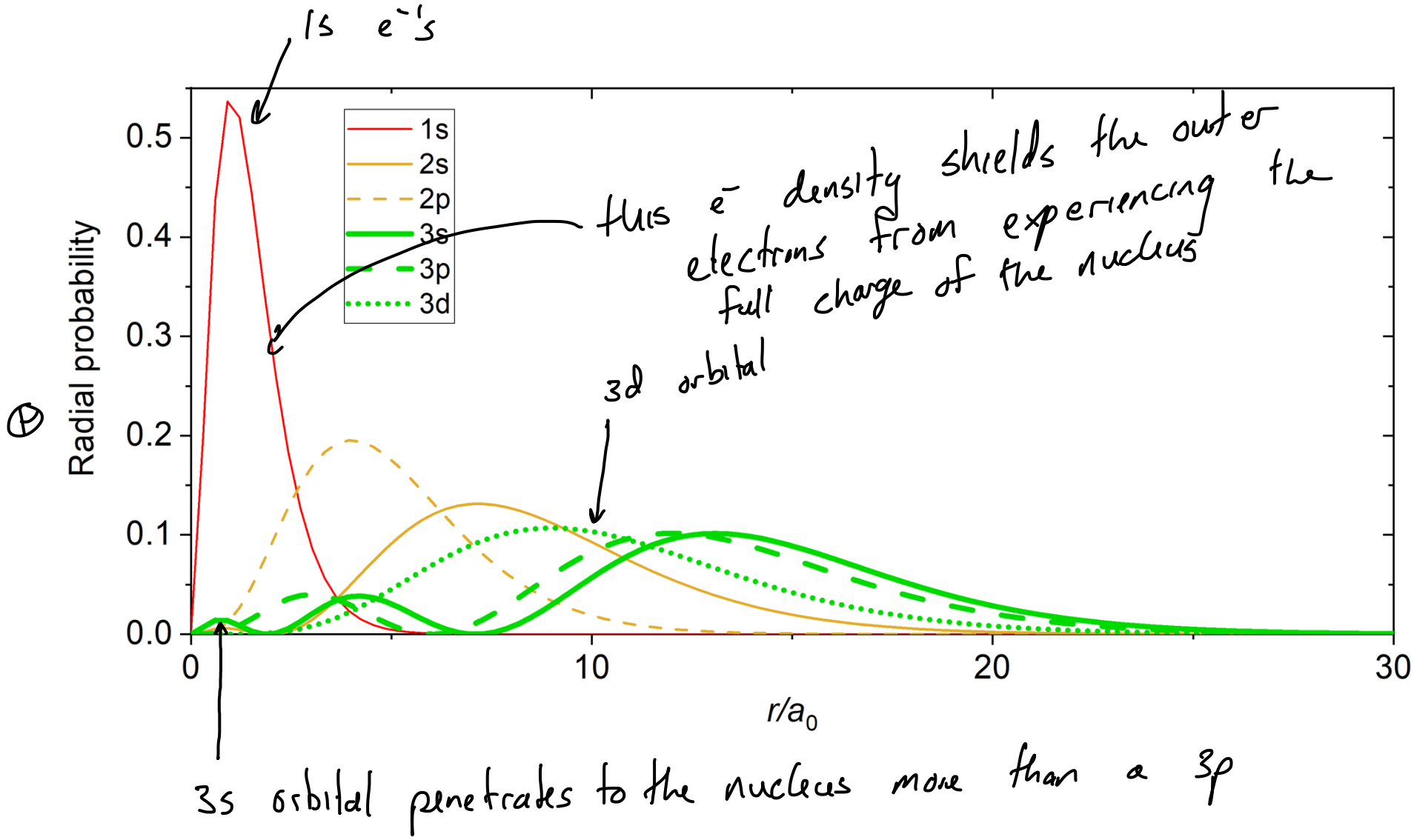
Mn [Ar]

3d ↑ ↑ ↑ ↑ ↑
4s ↑↓

↑ 7th e⁻ goes here

4s orbital is bigger than 3d orbitals

3d orbitals have 2 nodal planes


1s e⁻'s
1s
2s
2p
3s
3p
3d
thus e⁻ density shields the outer electrons from experiencing the full charge of the nucleus
3d orbital
Radial probability
0.0
0.1
0.2
0.3
0.4
0.5
0
10
20
30
r/a0
3s orbital penetrates to the nucleus more than a 3p

nuclear charge

Slater's Rules for Approximating Effective Nuclear Charge

$Z_{eff} = Z - S$ ← some of that charged is blocked by the other e⁻'s

Where Z_{eff} = effective nuclear charge, Z = nuclear charge, and S = shielding constant

1. group orbitals by n and l
   (1s) (2s,2p) (3s,3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) (5d) (etc)
2. electrons in groups to the right do not shield electrons to their left
3. S can be determined for *ns* and *np* electrons
   a. each electron in the same group contributes 0.35 to the value of S for other electrons in the same group
      exception, 1s electron contributes 0.30
   b. each electron in n - 1 groups contribute 0.85 to S
   c. each electron in n - 2 groups contribute 1.00 to S
4. for *nd* and *nf*
   a. each electron in the same group contributes 0.35 to the value of S (same as 3a)
   b. each electron in a group to the left contributes 1.00 to S

H

$1s^1$

$Z_{eff} = Z - S$

$= 1 - (0 \times 0.3)$

$Z_{eff} = 1$

He

$1s^2$

$Z_{eff} = 2 - (1 \times 0.3)$

1 e⁻ shields the other e⁻

$Z_{eff} = 1.7$

F $1s^2\ 2s^2 2p^5$

Z_{eff} for 1s

$Z_{eff} = 9 - (1 \times 0.3)$

$= 8.7$

Z_{eff} for 2s+2p

shielding constant for neighbors

$Z_{eff} = 9 - (2 \times 0.85 + 6 \times 0.35)$

both 1s e⁻'s shield e⁻'s in n=2 shell

shielding constant for n-1 shell

$Z_{eff} = 9 - 3.8$

$= 5.2$

Slater's Rules for Determining Effective Nuclear Charge

$$Z_{eff} = Z - S$$

Where Z_{eff} = effective nuclear charge, Z = nuclear charge, and S = shielding constant

2 8 8 6 2

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Z_{eff} for iron's 3d e^-'s + 4s e^-'s $\quad 1s^2\ 2s^2 2p^6\ 3s^2 3p^6\ 4s^2 3d^6$

$Z_{eff} = 26 - S$

$= 26 - (5 \times 0.35 + 18)$

$= 26 - 19.75$

$= 6.25$

3d e^-'s are more strongly attracted to the nucleus

$Z_{eff} = 26 - S$

$= 26 - (1 \times 0.35 + (6+8) \times 0.85 + 10)$

$= 3.75$

for 3d 1s, 2s+2p, 3s+3p are shielding

for 4s 3d + 3s+3p are n-1
2s+2p are n-2
1s are n-3

$H \rightarrow H^+ + e^- \quad \Delta E$

Ionization energy decreases as we go down a family

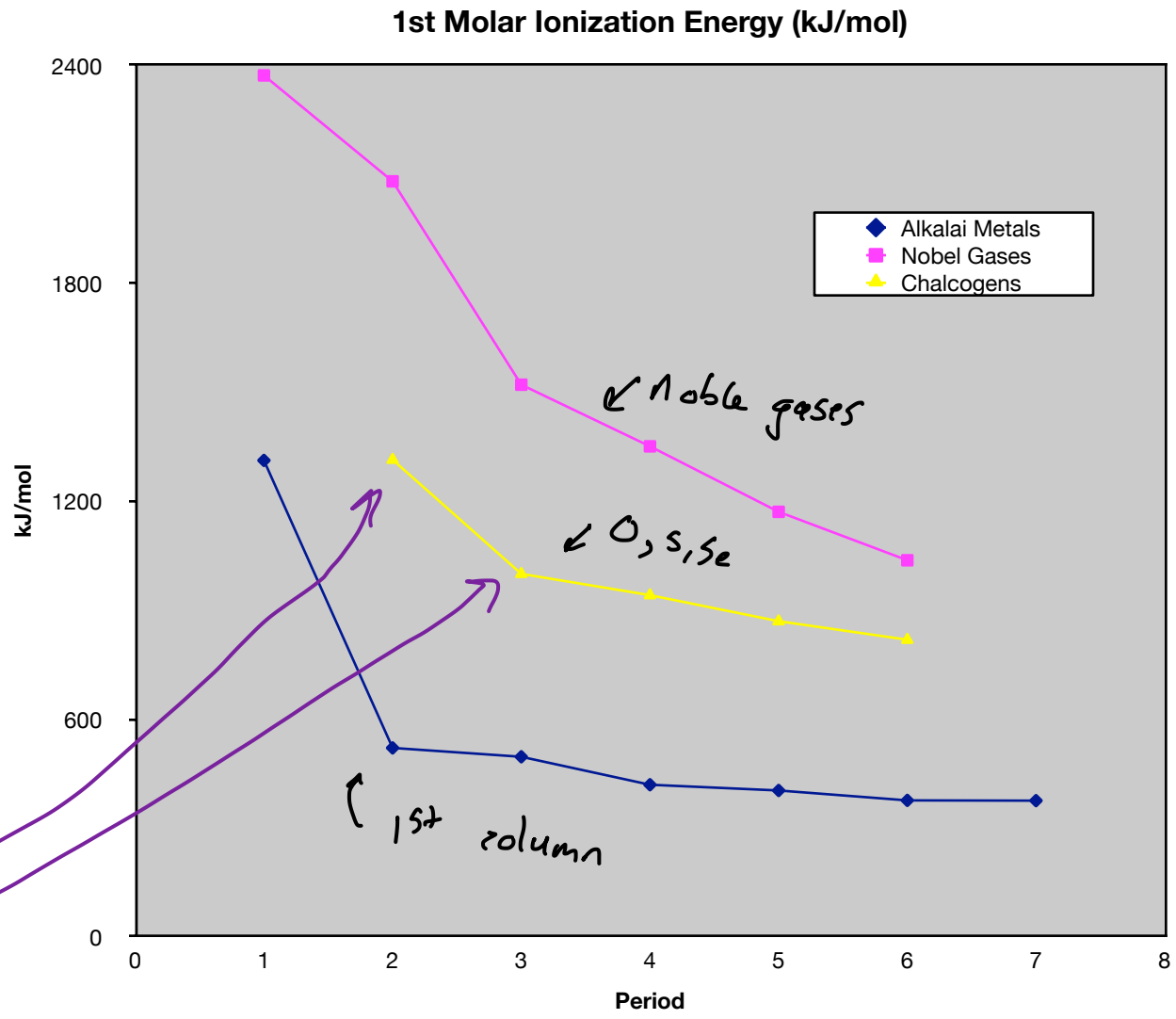
Why...

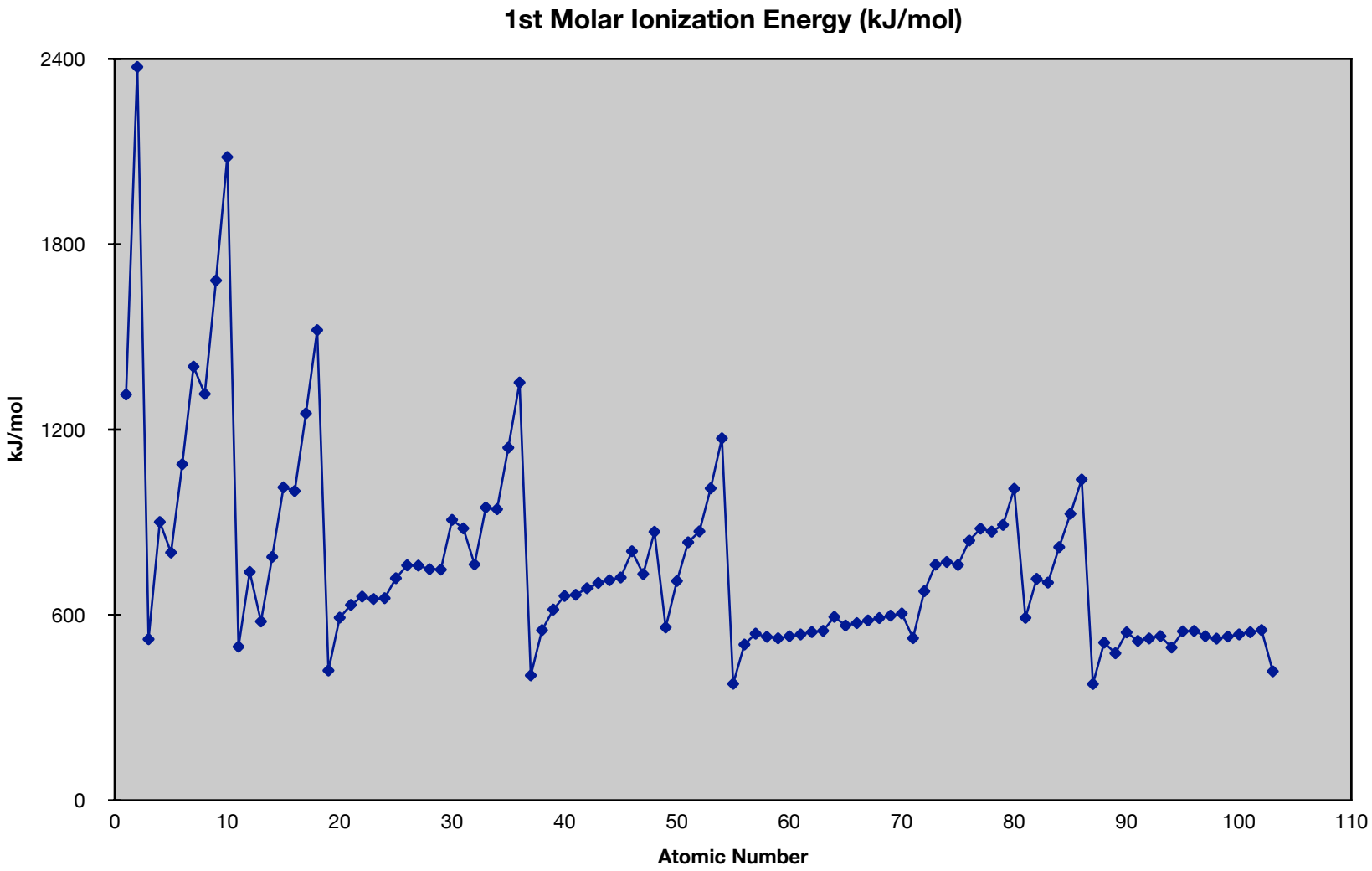
$$\frac{q_1 q_2}{r}$$

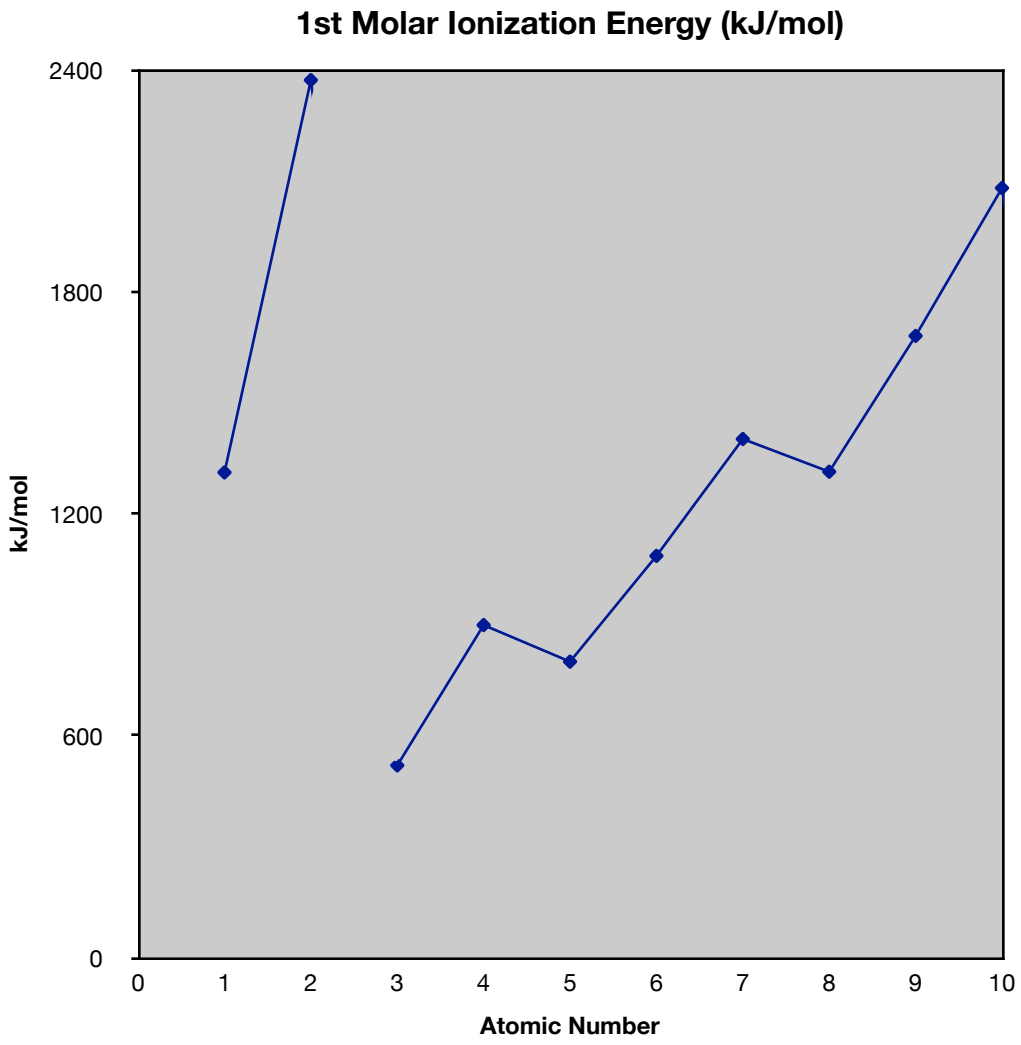
charge goes up a bit (Z_{eff})

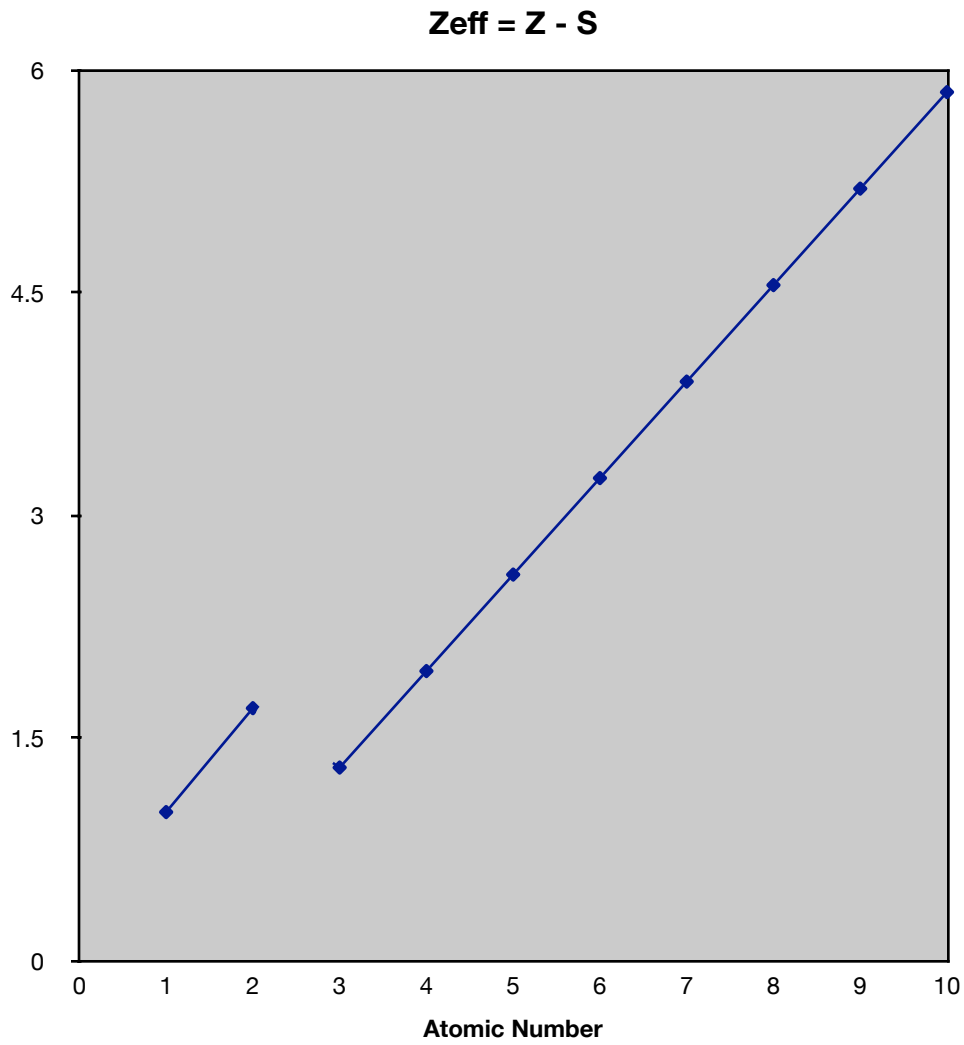
r goes up a bunch

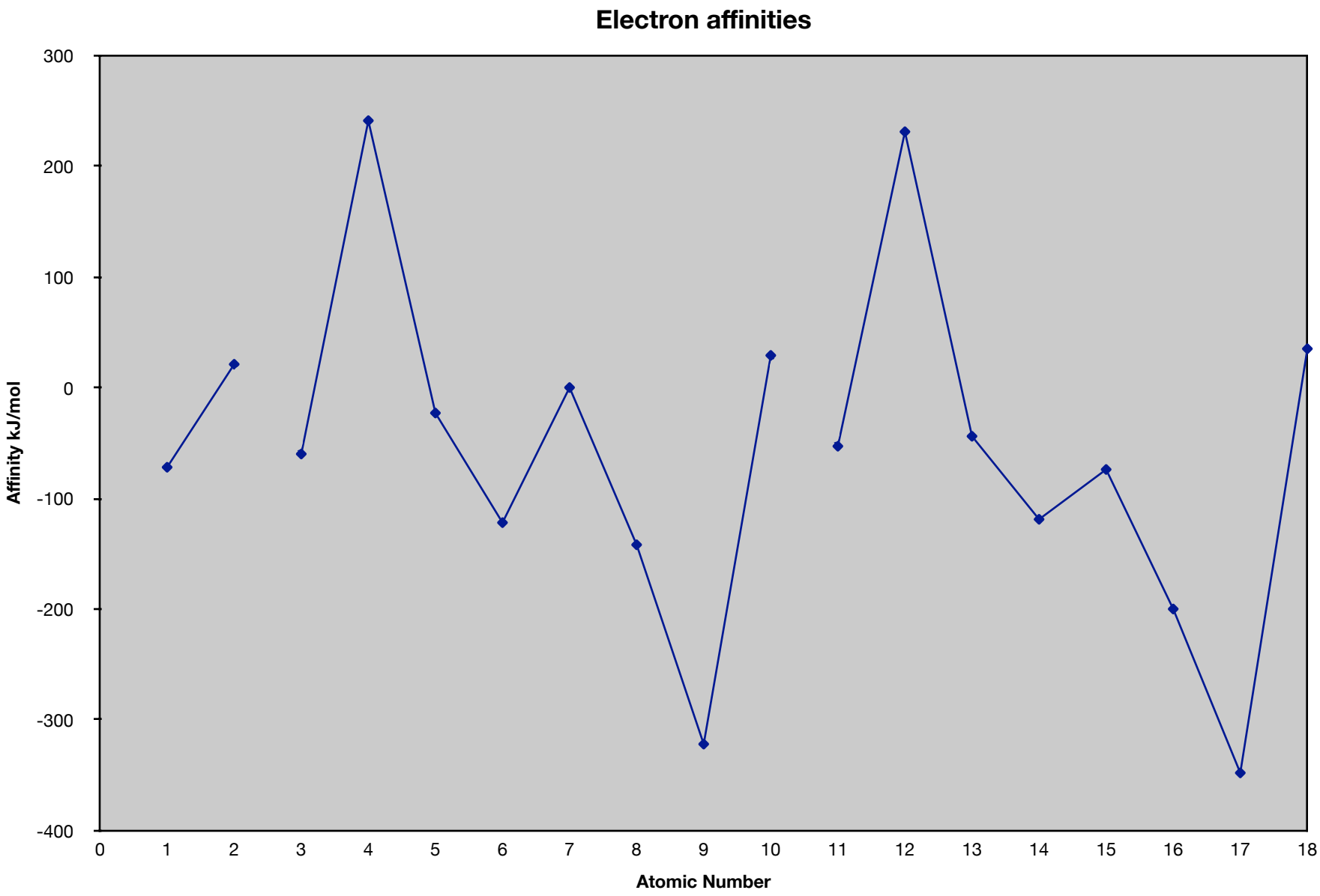
n=2 shell to n=3 shell




1st Molar Ionization Energy (kJ/mol)
kJ/mol
2400
1800
1200
600
0
0
10
20
30
40
50
60
70
80
90
100
110
Atomic Number


1st Molar Ionization Energy (kJ/mol)
kJ/mol
2400
1800
1200
600
0
0 1 2 3 4 5 6 7 8 9 10
Atomic Number

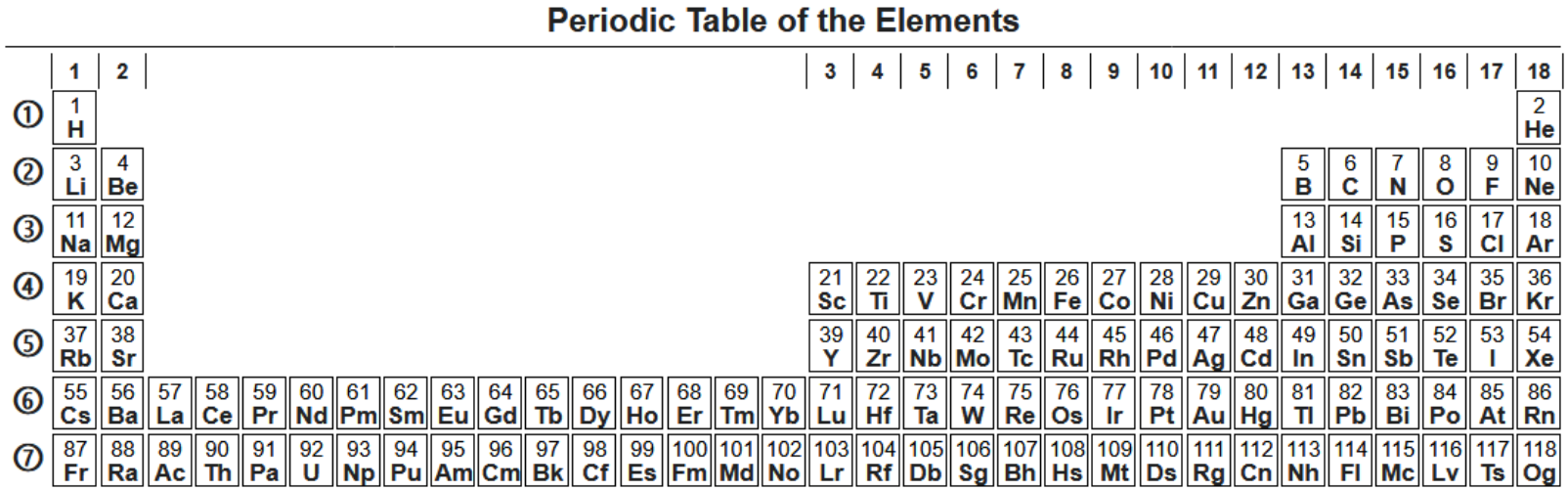

Zeff = Z - S
6
4.5
3
1.5
0
0 1 2 3 4 5 6 7 8 9 10
Atomic Number


Electron affinities
Affinity kJ/mol
300
200
100
0
-100
-200
-300
-400
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
Atomic Number

Nonpolar atomic radii: The radius of an atom is derived from the bond lengths within nonpolar molecules; one-half the distance between the nuclei of two atoms within a covalent bond.

van der Waals radius: The radius of an atom is determined by collision with other atoms.

Crystal radii: The atomic or ionic radius is determined using electron density maps from X-ray data.[1]



[1] Quoted from https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Inorganic_Chemistry_(LibreTexts)/02%3A_Atomic_Structure/2.03%3A_Periodic_Properties_of_Atoms/2.3.03%3A_Covalent_and_Ionic_Radii