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The Aufbau Principle and Energy Level Diagrams

e⁻ "promoted" from 4s to 3d because increase in exchange E

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

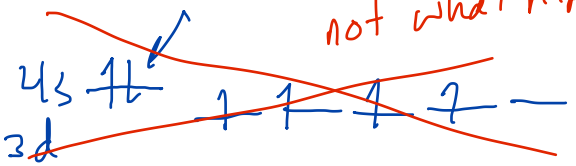
s orbitals penetrate the closest to the nucleus, but to put a 2nd e⁻ in an s orbital, e⁻ have to be paired.

at n=3 3d orbitals became available

e⁻–e⁻ repulsion

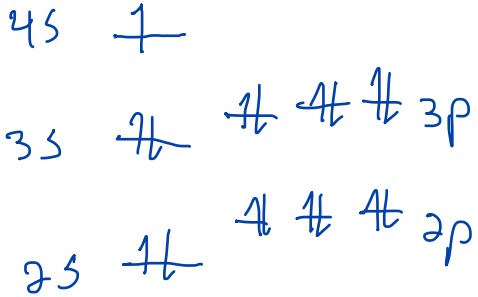
Cr [Ar] 4s¹ 3d⁵

not what happens



this gap + e⁻–e⁻ repulsion + ↓ new exchange interaction

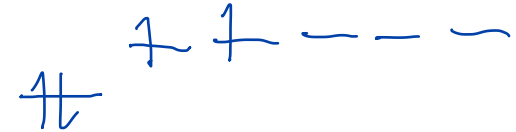
K



Ca [Ar] 4s²

Sc [Ar] 4s² 3d¹

Ti



4s penetrates close so lower in E

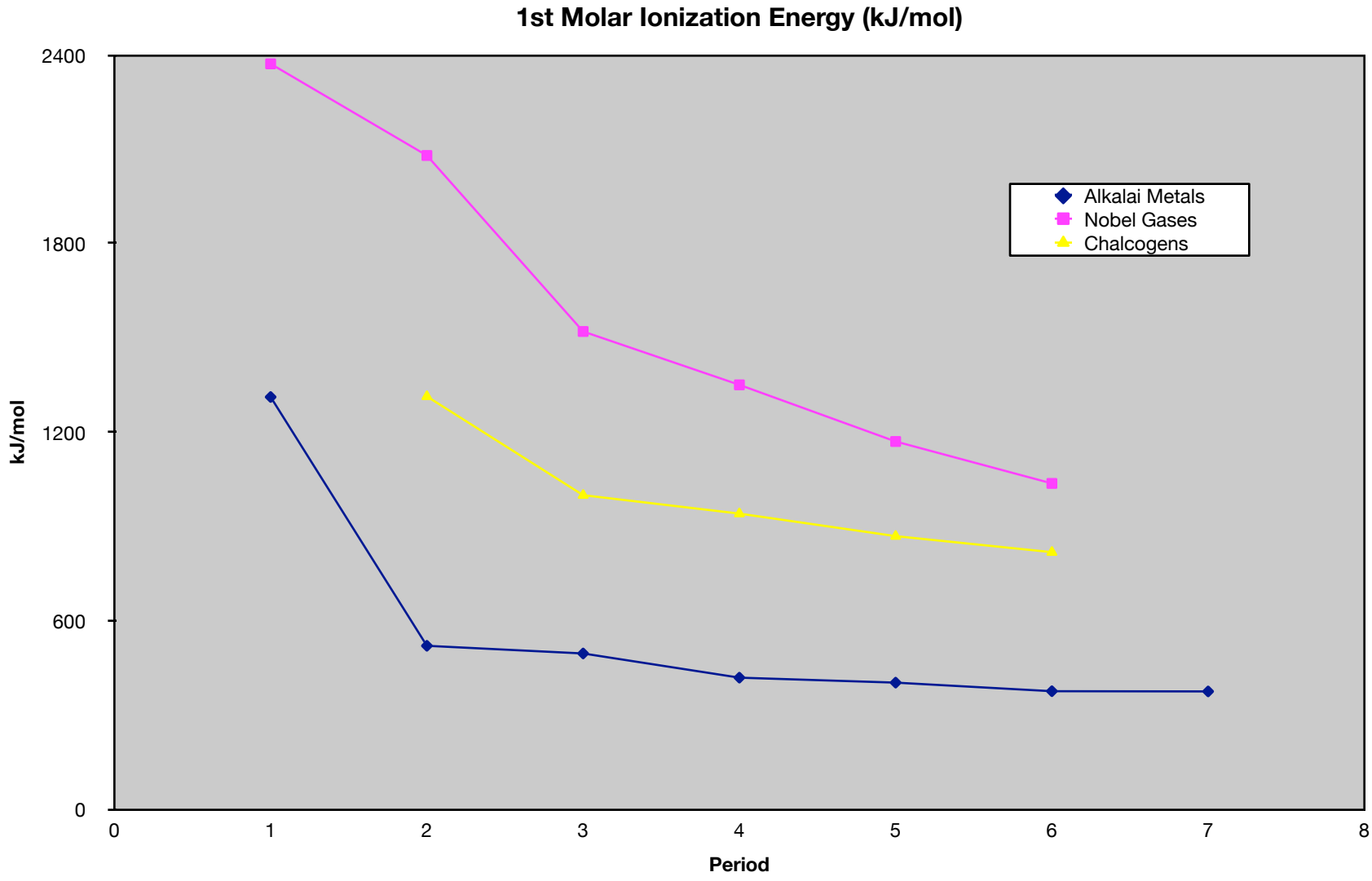
[Ar]

Slater's Rules for Determining Effective Nuclear Charge

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

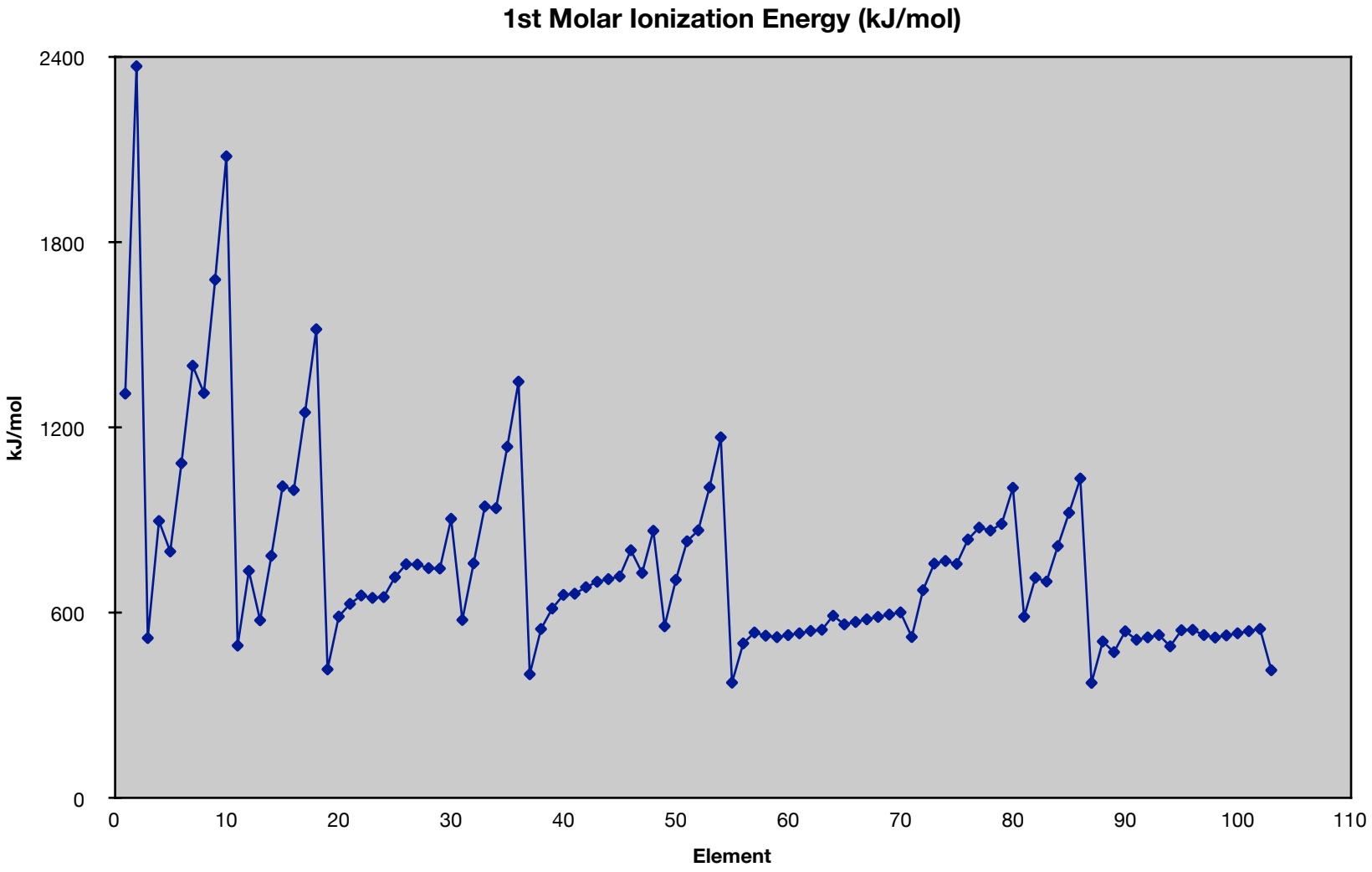
Where Z_{eff} = effective nuclear charge, Z = nuclear charge, and S = shielding constant

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



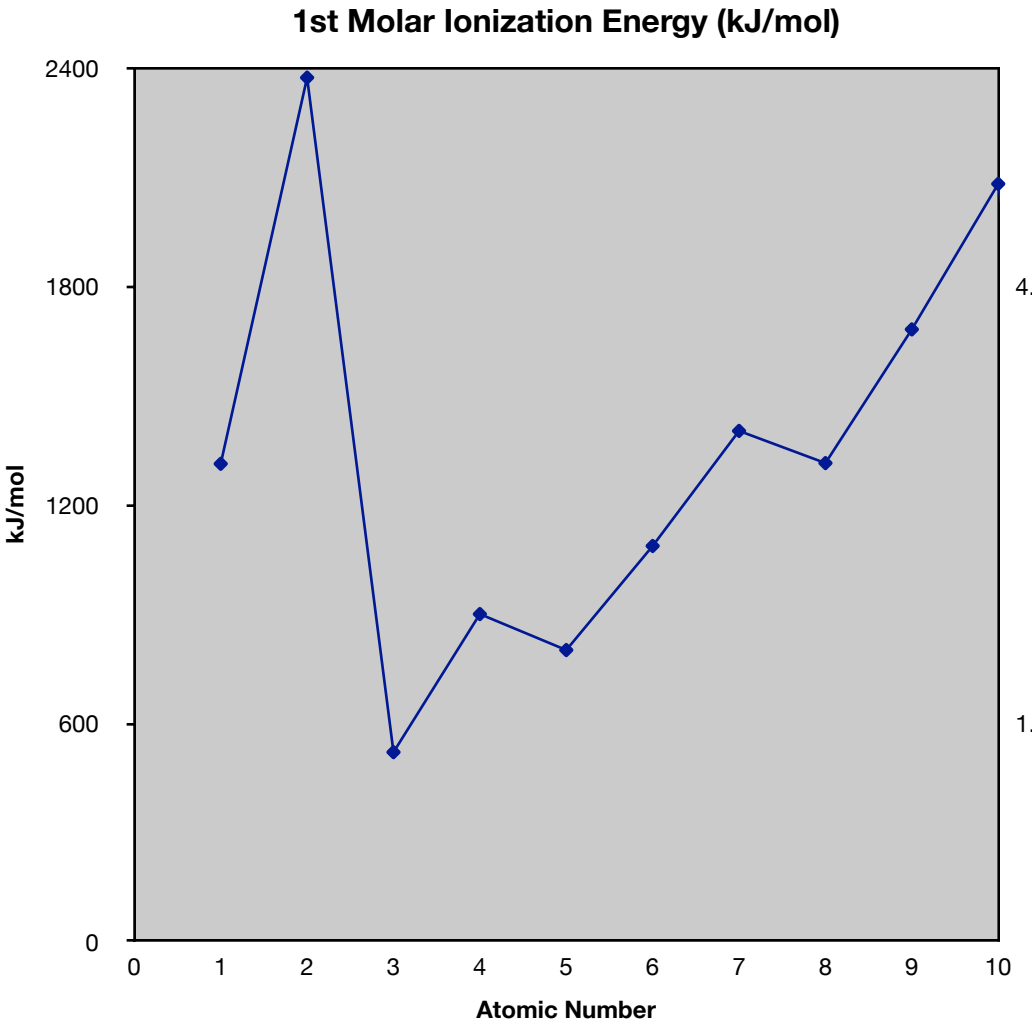
Periodic Trends: Ionization Energy

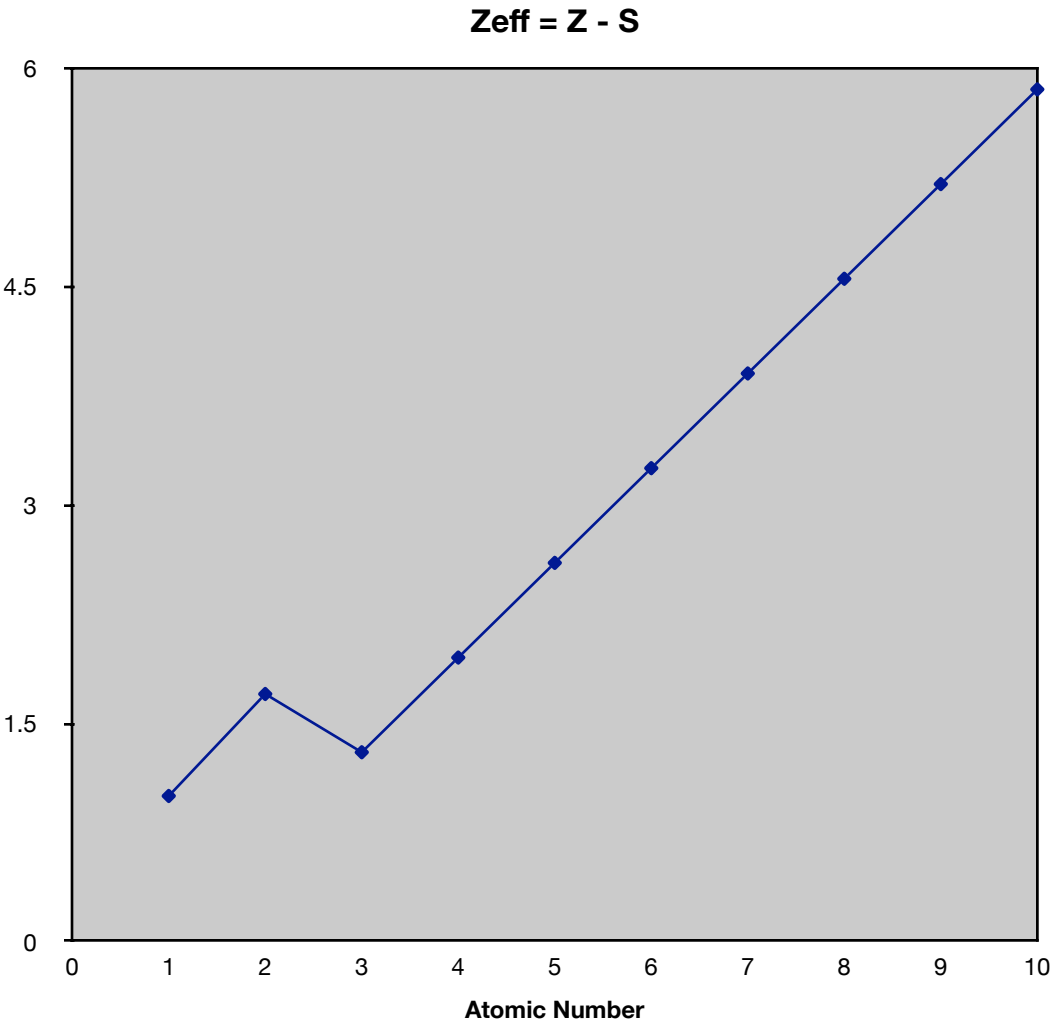
Section 2.3



Periodic Trends: Ionization Energy

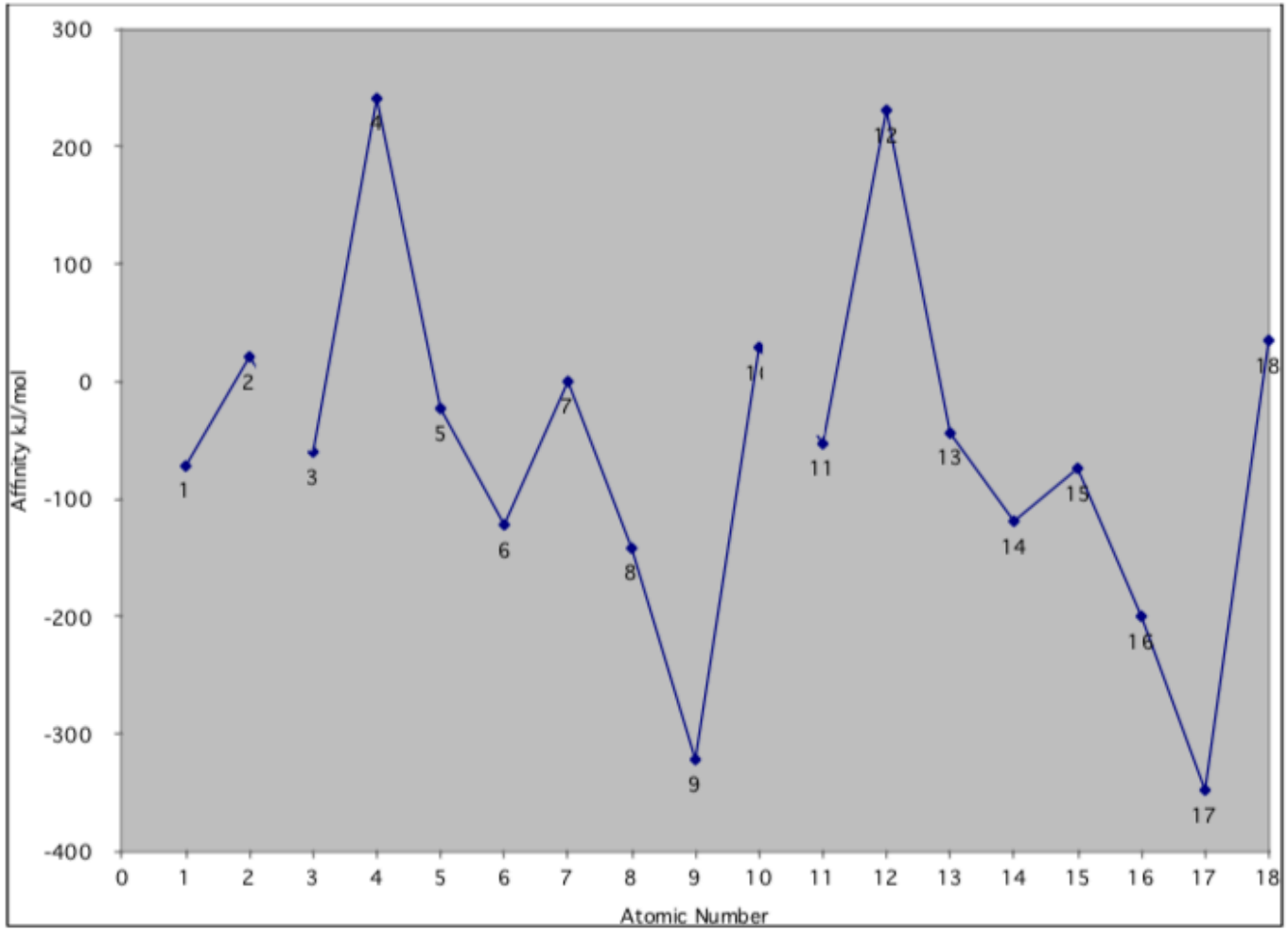
Section 2.3





Periodic Trends: Ionization Energy

Section 2.3


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

$[SCN]^-$ $[OCN]^-$ $[CNO]^-$

$[SCN]^-$ $[OCN]^-$ $[CNO]^-$

$[SCN]^-$ $[OCN]^-$ $[CNO]^-$

$[SCN]^-$ $[OCN]^-$ $[CNO]^-$