LECTURE 17/35 OCT-16-02

ATOMIC STRUCTURE

IONIZATION ENERGY

ELECTRON AFFINITY

ELECTRONEGATIVITY

COVALENT BONDING

READ TODAY GRAY CH 2 42-58
NEXT LEC GRAY CH 2 58-67

6-19. ELEMENTS IN THE SAME COLUMN OF THE PERIODIC TABLE HAVE SIMILAR VALENCE-ELECTRON CONFIGURATIONS

Figure 6-30 is a periodic table indicating the orbitals that are used in building up the electron configuration of each element. Note that after neon we must go to the $3s$ and $3p$ orbitals to obtain the next row of the periodic table:

Element	Ground-state configuration	Abbreviated form of ground-state configuration
sodium	$1s^2 2s^2 2p^6 3s^1$	$[Ne]3s^1$
magnesium	$1s^2 2s^2 2p^6 3s^2$	$[Ne]3s^2$
aluminum	$1s^2 2s^2 2p^6 3s^2 3p^1$	$[Ne]3s^2 3p^1$
silicon	$1s^2 2s^2 2p^6 3s^2 3p^2$	$[Ne]3s^2 3p^2$
phosphorus	$1s^2 2s^2 2p^6 3s^2 3p^3$	$[Ne]3s^2 3p^3$
sulfur	$1s^2 2s^2 2p^6 3s^2 3p^4$	$[Ne]3s^2 3p^4$
chlorine	$1s^2 2s^2 2p^6 3s^2 3p^5$	$[Ne]3s^2 3p^5$
argon	$1s^2 2s^2 2p^6 3s^2 3p^6$	$[Ne]3s^2 3p^6$ or [Ar]

- ATOMIC PROPETIES AND VALENCE ORBITAL STRUCTURE
- ONLY THE OUTER ELECTRONS ARE IMPORTANT IN CHEMICAL RXN
- VALENCE e^- ARE e^- BEYOND THE CLOSED-SHELL CONFIGURATIONS
- EFFECTIVE ATOMIC RADIUS
  ONE HALF THE DISTANCE BETWEEN TWO NUCLEI OF THE ELEMENT THAT ARE HELD TOGETHER BY A PURELY COVALENT SINGLE BOND
- COVALENT BOND = PAIR OF ELECTRONS SHARED BETWEEN TWO ATOMS

H_2 — 0.74 Å

ATOMIC RADIUS H = 0.37 Å

TREND — EFFECTIVE SIZE ~ ATOMIC #

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TABLE 6.5 Atomic Radii of the First 36 Elements [a]

Z	Element Symbol	r (Å)
1	H	0.37
2	He	(0.5)[b]
3	Li	1.52
4	Be	1.11
5	B	0.80
6	C	0.77
7	N	0.74
8	O	0.74
9	F	0.71
10	Ne	(0.65)[b]
11	Na	1.86
12	Mg	1.60
13	Al	1.43
14	Si	1.18
15	P	1.10
16	S	1.03
17	Cl	0.99
18	Ar	(0.95)[b]
19	K	2.27
20	Ca	1.97
21	Sc	1.61
22	Ti	1.45
23	V	1.31
24	Cr	1.25
25	Mn	1.37
26	Fe	1.24
27	Co	1.25
28	Ni	1.25
29	Cu	1.28
30	Zn	1.33
31	Ga	1.22
32	Ge	1.23
33	As	1.25
34	Se	1.16
35	Br	1.14
36	Kr	(1.10)[b]

[a]The values are based on measurements of interatomic distances in either metallic or covalently bonded elements.

[b]Estimated values.

IONIZATION ENERGY

$$\text{ATOM}(g) + h\nu_1 \longrightarrow \text{ION}^+(g) + e^-$$

$$h\nu_1 = IE_1$$

ELECTRON AFFINITY

$$\text{ATOM}(g) + e^- \longrightarrow \text{ION}^-(g) + \text{ENERGY}$$

$$\text{ION}^-(g) + h\nu_{EA} \longrightarrow \text{ATOM}(g) + e^-$$

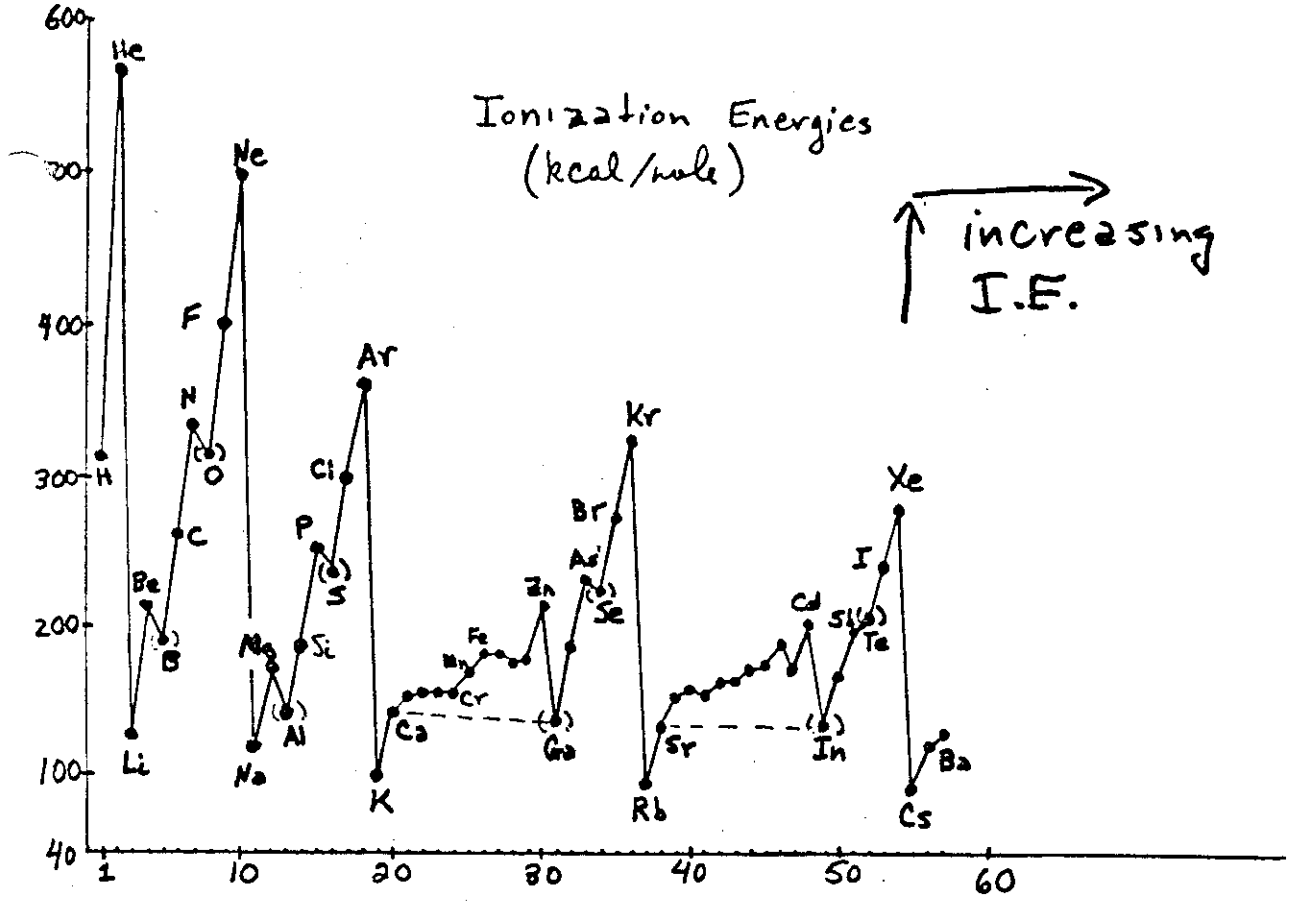
$$h\nu_{EA} = EA$$

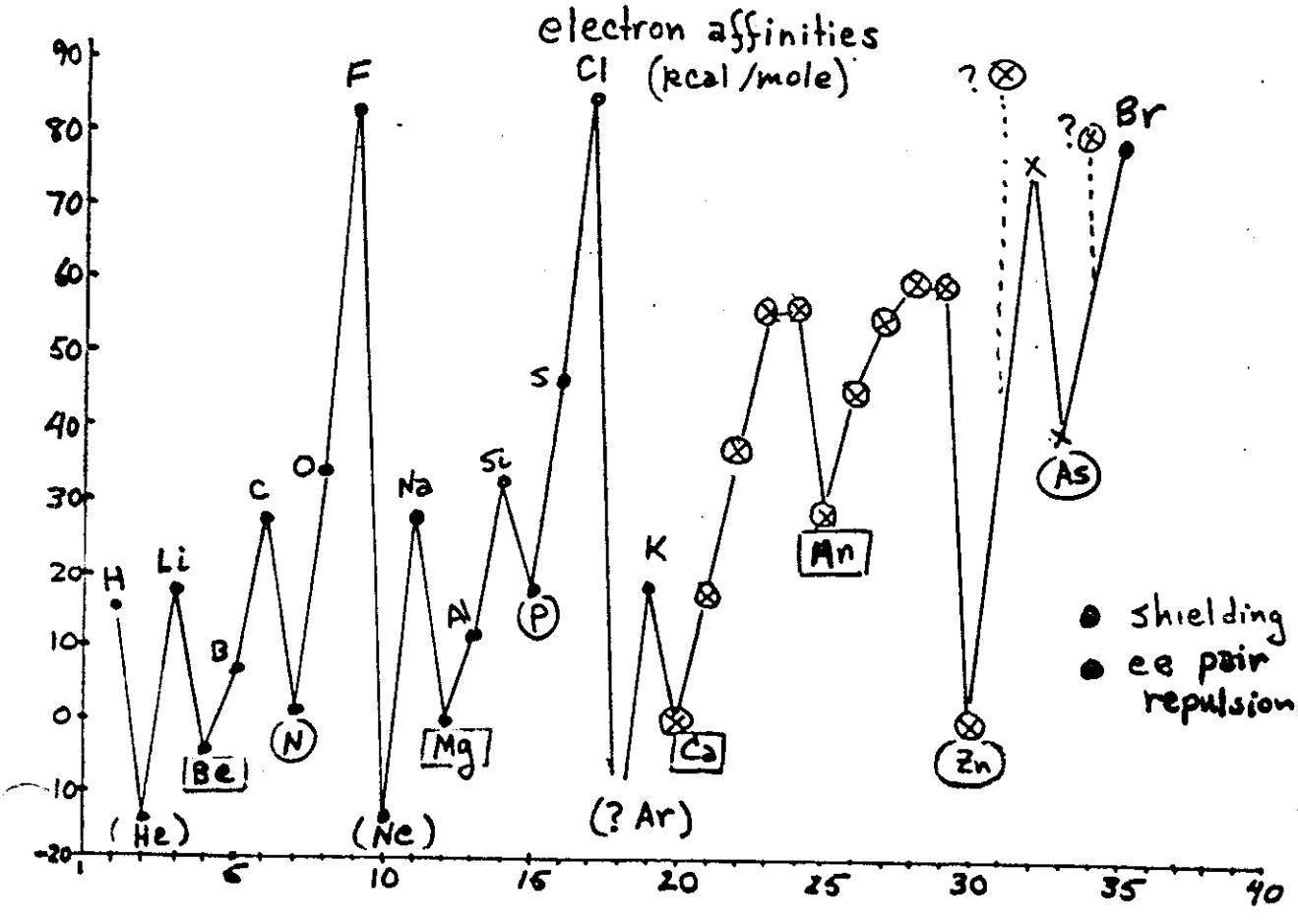
ELECTRONEGATIVITY (EN)

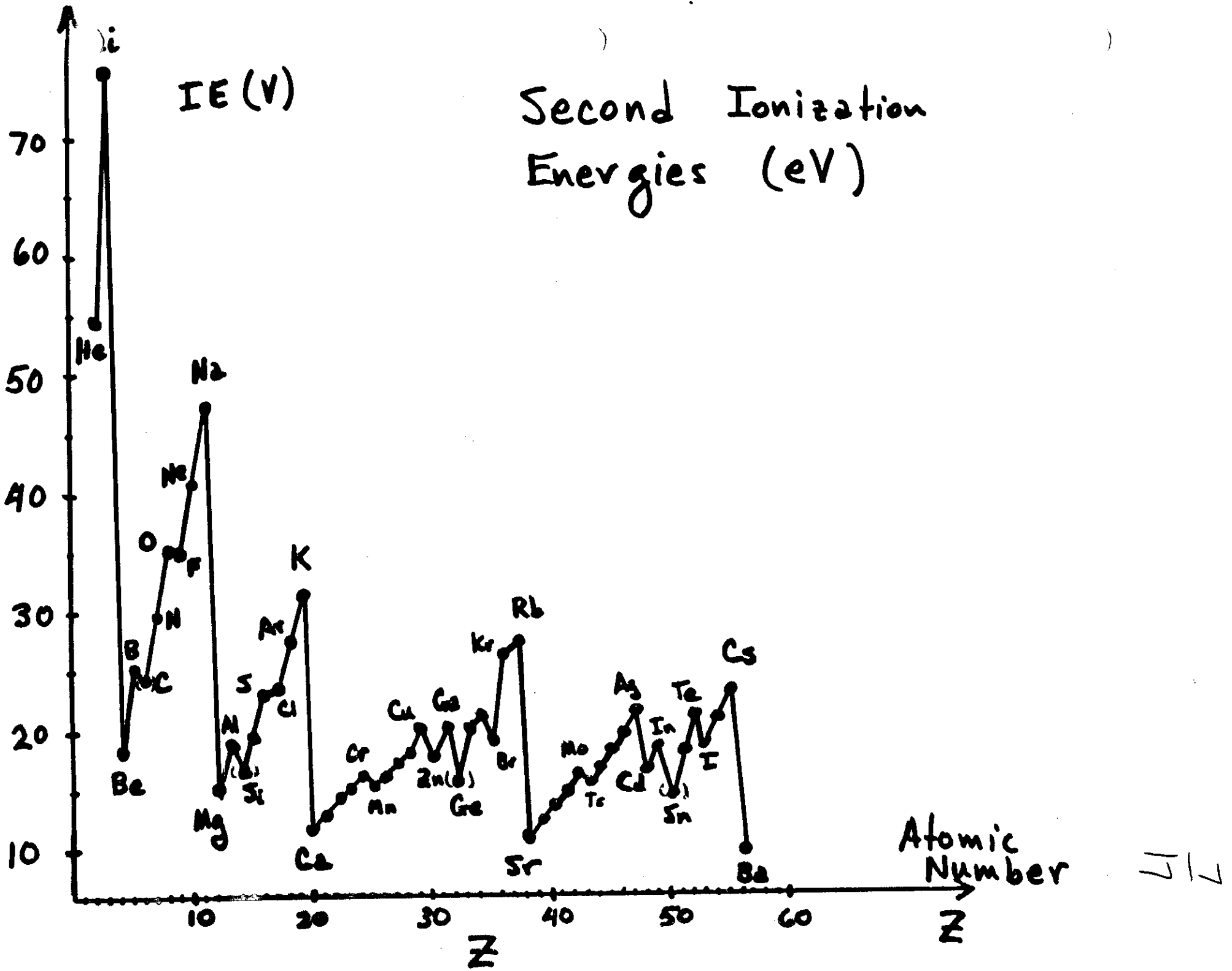
RELATIVE ABILITY OF AN ATOM TO ATTRACT e^- TO ITSELF IN A CHEMICAL BOND

$$EN \propto (IE + EA) \quad \text{MULIKEN}$$

NOT ENOUGH EA


Ionization Energies
(kcal/mole)
increasing I.E.
600
400
300
200
100
40
1
10
20
30
40
50
60
He
H
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Cr
Mn
Fe
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
In
Cd
Sn
Sb
Te
I
Xe
Cs
Ba


electron affinities
(kcal/mole)
90
80
70
60
50
40
30
20
10
0
-10
-20
5
10
15
20
25
30
35
40
H
Li
Be
B
C
O
F
Na
Mg
Al
Si
P
S
Cl
K
Ca
Mn
Zn
As
Br
(He)
(Ne)
(? Ar)
shielding
ee pair repulsion


Second Ionization Energies (eV)
IE (V)
70
60
50
40
30
20
10
Li
He
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
Y
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Ag
Cd
In
Sn
Sb
Te
I
Xe
Cs
Ba
10
20
30
40
50
60
Z
Z
Atomic Number

PAULING (1930's)

EN — COMPARING BOND ENERGIES OF DIFFERENT MOLECULES CONTAINING THAT ATOM

H_2 — 103 Kcal/mol

F_2 — 33 Kcal/mol

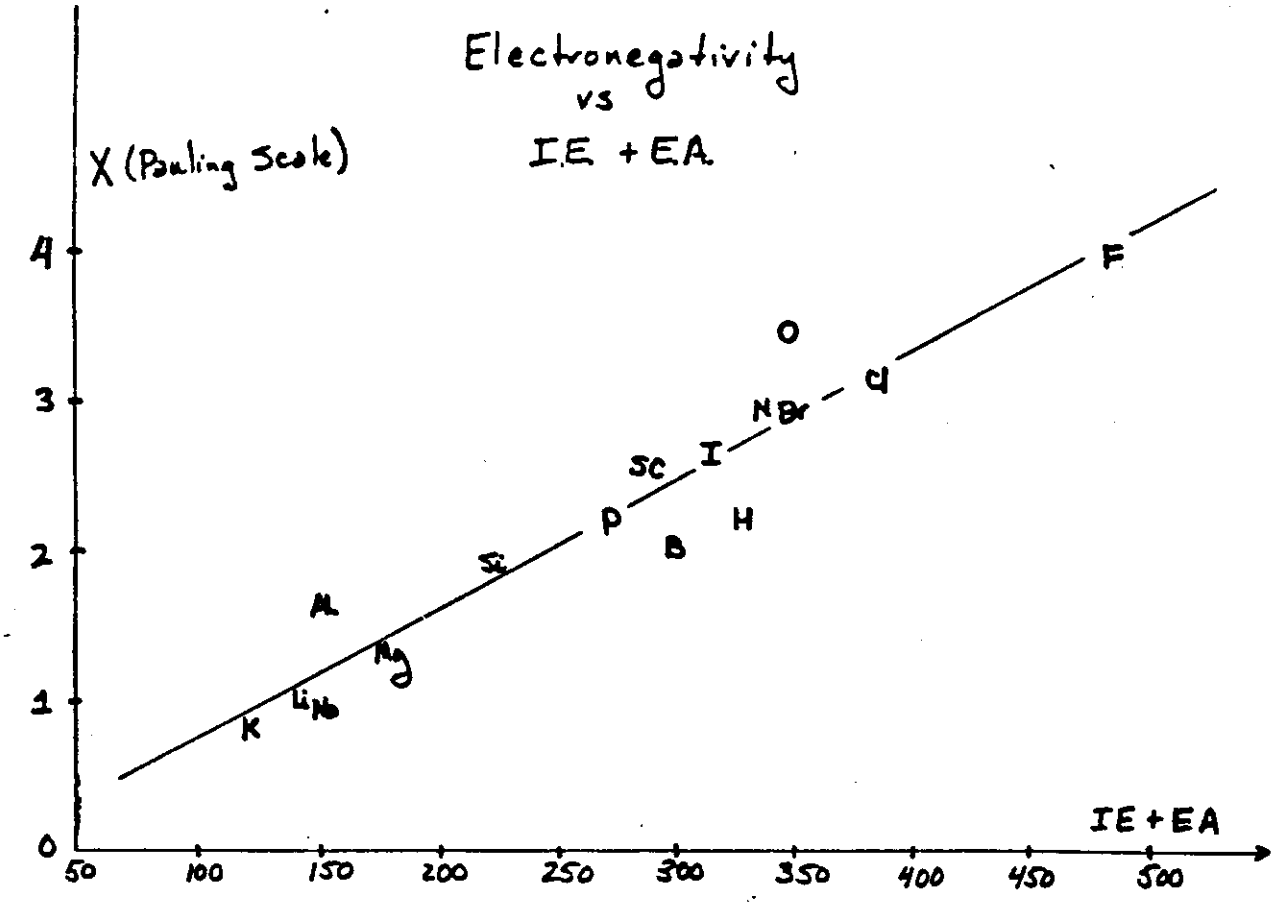
HF — 135 Kcal/mol

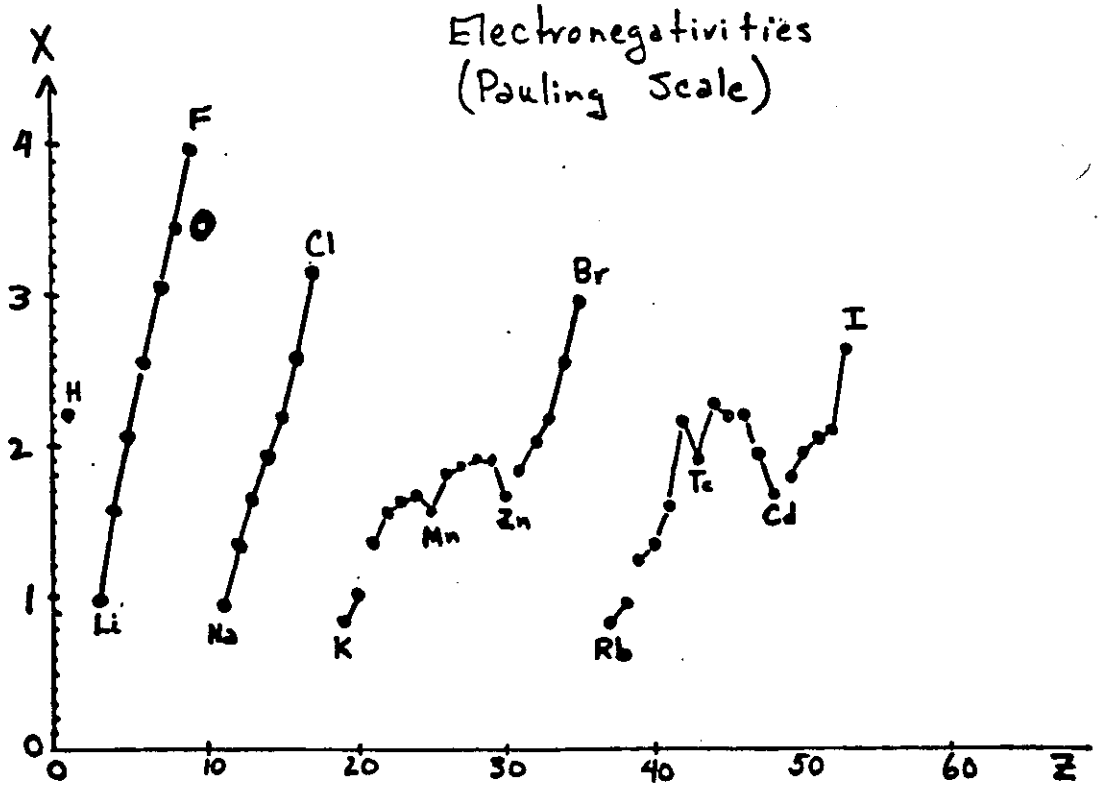
EN ~ GEOMETRIC MEAN

$\sqrt{33 + 103} = 58$

EXTRA BOND ENERGY

$$EN_A - EN_B \propto \Delta^{1/2}$$


Electronegativity
vs
I.E + E.A.
X (Pauling Scale)
IE + EA
0
1
2
3
4
50
100
150
200
250
300
350
400
450
500
F
O
Cl
N
Br
I
Sc
P
H
B
Si
Al
Mg
Li
Na
K


Electronegativities
(Pauling Scale)
X
0
1
2
3
4
0
10
20
30
40
50
60
Z
F
O
Cl
Br
I
H
Li
Na
K
Mn
Zn
Rb
Tc
Cd

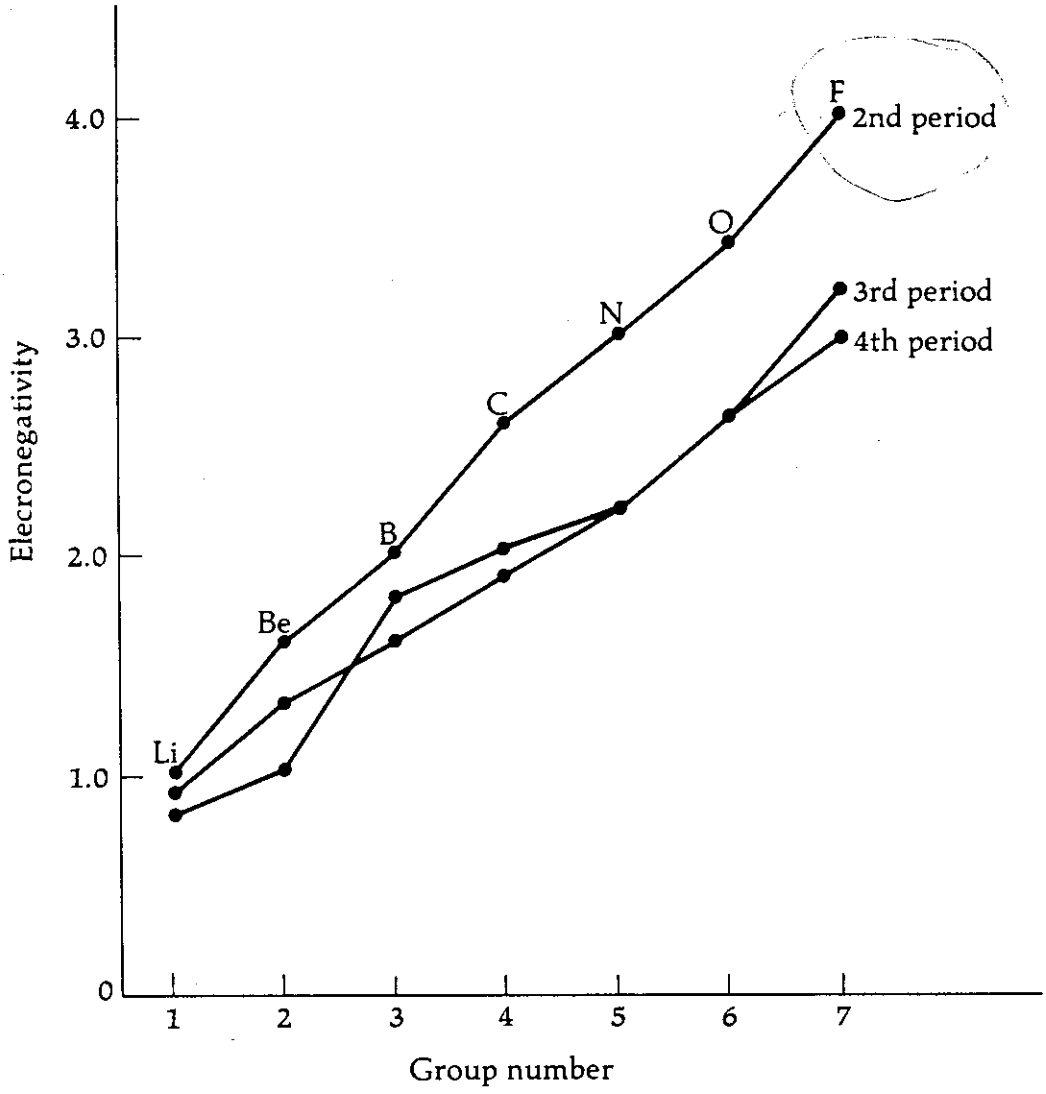


FIGURE 6.20 Electronegativities of the representative elements.

6.7 Using the data in Table 6.4, determine the electronegativity of sodium.

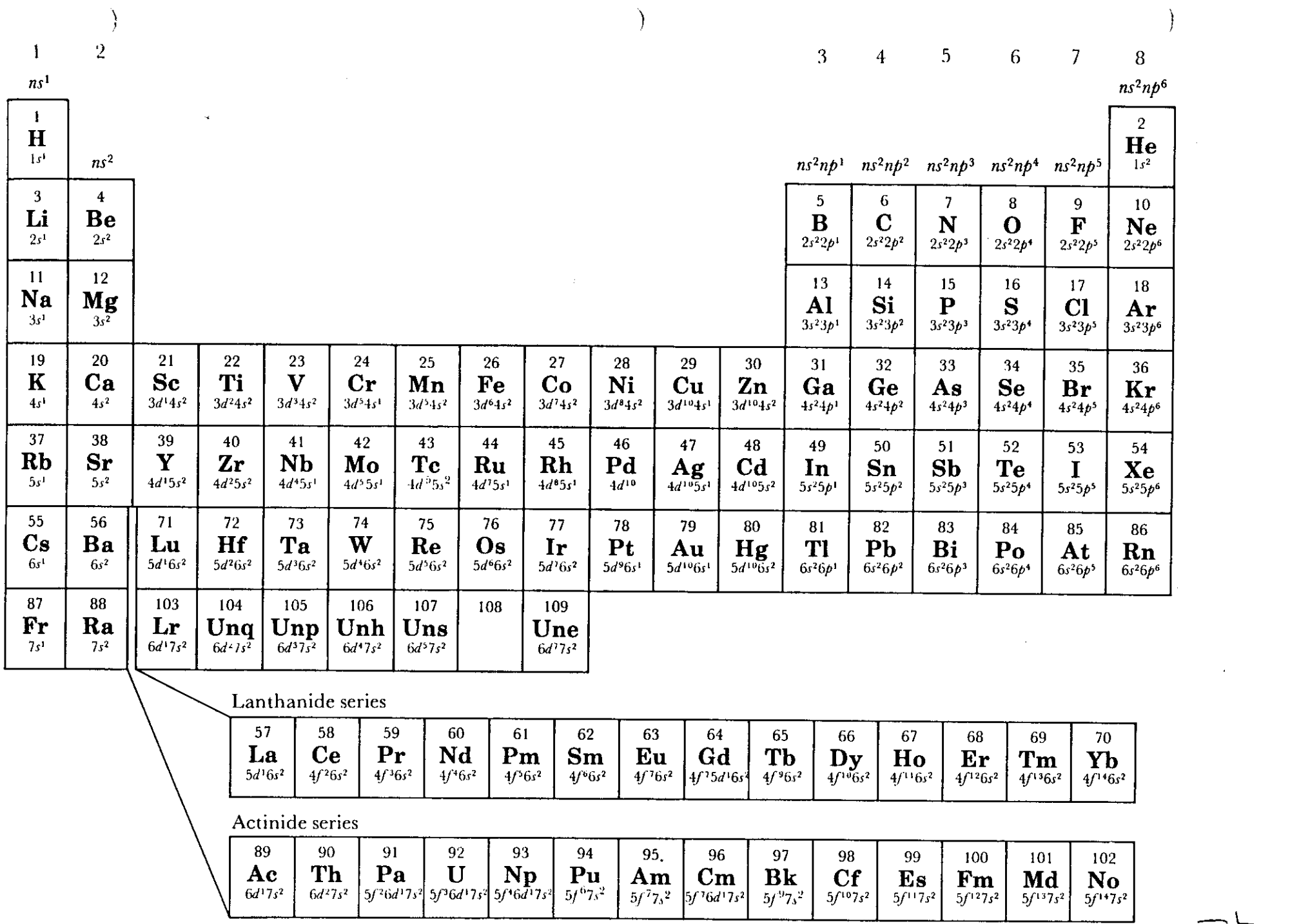
The value of χ can be obtained by means of the tabulated first ionization energy and electron affinity, scaled to a value of 4.0 for fluorine. Applying Equation 6.5 to fluorine we have

$$\chi_F = \frac{I_F + \varepsilon_F}{2}$$

$$= \frac{1681 \text{ kJ mol}^{-1} + 328.0 \text{ kJ mol}^{-1}}{2}$$

$$= 1005 \text{ kJ mol}^{-1}$$

Adjusting this value to 4.0 yields a scaling factor of


1
2
3
4
5
6
7
8
ns^1
ns^2
ns^2np^1
ns^2np^2
ns^2np^3
ns^2np^4
ns^2np^5
ns^2np^6
1 H $1s^1$
2 He $1s^2$
3 Li $2s^1$
4 Be $2s^2$
5 B $2s^22p^1$
6 C $2s^22p^2$
7 N $2s^22p^3$
8 O $2s^22p^4$
9 F $2s^22p^5$
10 Ne $2s^22p^6$
11 Na $3s^1$
12 Mg $3s^2$
13 Al $3s^23p^1$
14 Si $3s^23p^2$
15 P $3s^23p^3$
16 S $3s^23p^4$
17 Cl $3s^23p^5$
18 Ar $3s^23p^6$
19 K $4s^1$
20 Ca $4s^2$
21 Sc $3d^14s^2$
22 Ti $3d^24s^2$
23 V $3d^34s^2$
24 Cr $3d^54s^1$
25 Mn $3d^54s^2$
26 Fe $3d^64s^2$
27 Co $3d^74s^2$
28 Ni $3d^84s^2$
29 Cu $3d^{10}4s^1$
30 Zn $3d^{10}4s^2$
31 Ga $4s^24p^1$
32 Ge $4s^24p^2$
33 As $4s^24p^3$
34 Se $4s^24p^4$
35 Br $4s^24p^5$
36 Kr $4s^24p^6$
37 Rb $5s^1$
38 Sr $5s^2$
39 Y $4d^15s^2$
40 Zr $4d^25s^2$
41 Nb $4d^45s^1$
42 Mo $4d^55s^1$
43 Tc $4d^55s^2$
44 Ru $4d^75s^1$
45 Rh $4d^85s^1$
46 Pd $4d^{10}$
47 Ag $4d^{10}5s^1$
48 Cd $4d^{10}5s^2$
49 In $5s^25p^1$
50 Sn $5s^25p^2$
51 Sb $5s^25p^3$
52 Te $5s^25p^4$
53 I $5s^25p^5$
54 Xe $5s^25p^6$
55 Cs $6s^1$
56 Ba $6s^2$
71 Lu $5d^16s^2$
72 Hf $5d^26s^2$
73 Ta $5d^36s^2$
74 W $5d^46s^2$
75 Re $5d^56s^2$
76 Os $5d^66s^2$
77 Ir $5d^76s^2$
78 Pt $5d^96s^1$
79 Au $5d^{10}6s^1$
80 Hg $5d^{10}6s^2$
81 Tl $6s^26p^1$
82 Pb $6s^26p^2$
83 Bi $6s^26p^3$
84 Po $6s^26p^4$
85 At $6s^26p^5$
86 Rn $6s^26p^6$
87 Fr $7s^1$
88 Ra $7s^2$
103 Lr $6d^17s^2$
104 Unq $6d^27s^2$
105 Unp $6d^37s^2$
106 Unh $6d^47s^2$
107 Uns $6d^57s^2$
108
109 Une $6d^77s^2$
Lanthanide series
57 La $5d^16s^2$
58 Ce $4f^26s^2$
59 Pr $4f^36s^2$
60 Nd $4f^46s^2$
61 Pm $4f^56s^2$
62 Sm $4f^66s^2$
63 Eu $4f^76s^2$
64 Gd $4f^75d^16s^2$
65 Tb $4f^96s^2$
66 Dy $4f^{10}6s^2$
67 Ho $4f^{11}6s^2$
68 Er $4f^{12}6s^2$
69 Tm $4f^{13}6s^2$
70 Yb $4f^{14}6s^2$
Actinide series
89 Ac $6d^17s^2$
90 Th $6d^27s^2$
91 Pa $5f^26d^17s^2$
92 U $5f^36d^17s^2$
93 Np $5f^46d^17s^2$
94 Pu $5f^67s^2$
95 Am $5f^77s^2$
96 Cm $5f^76d^17s^2$
97 Bk $5f^97s^2$
98 Cf $5f^{10}7s^2$
99 Es $5f^{11}7s^2$
100 Fm $5f^{12}7s^2$
101 Md $5f^{13}7s^2$
102 No $5f^{14}7s^2$