

Lecture 7 January 2019

Electronegativity Scales

Electric Dipole Moments

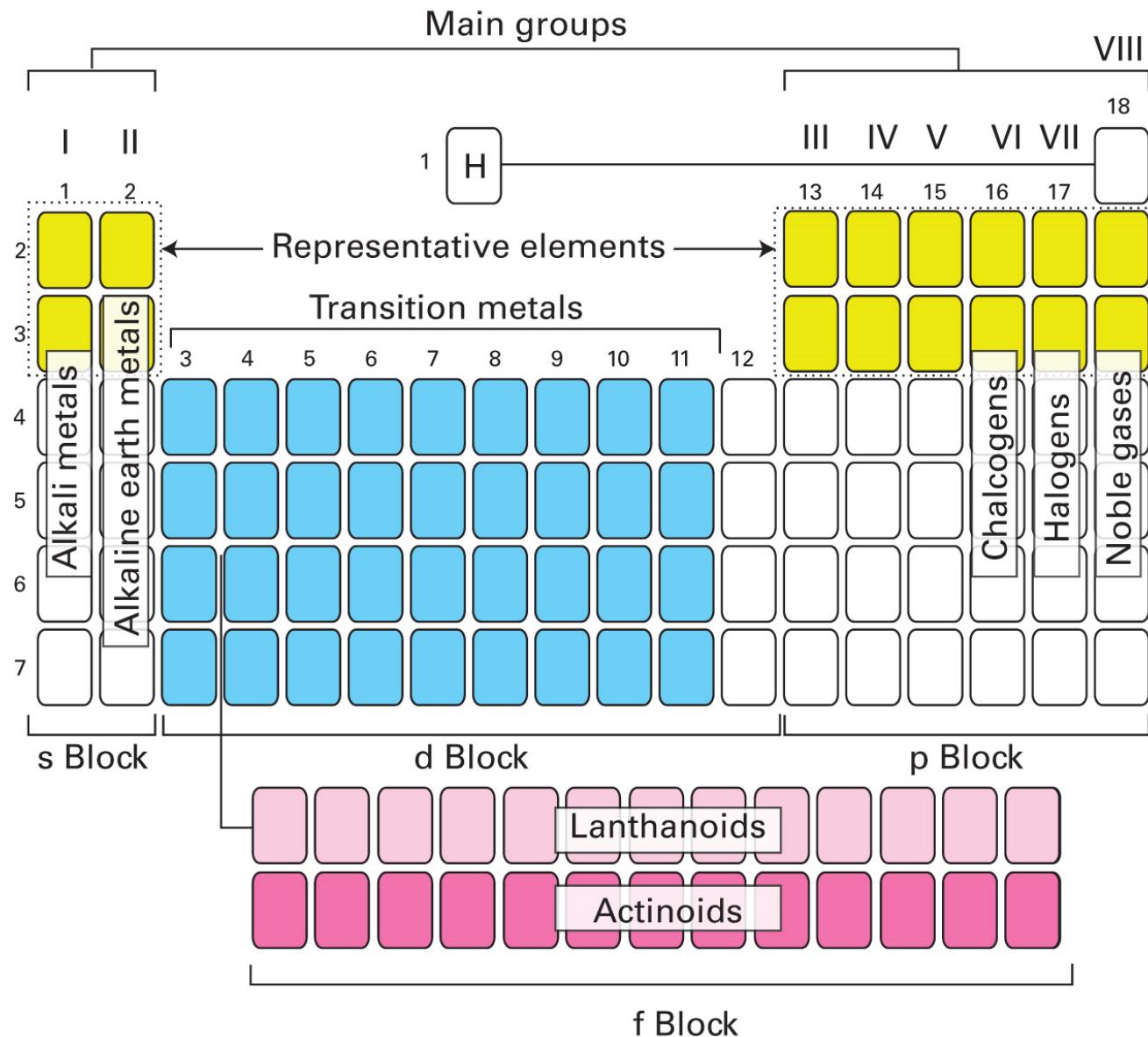
Lewis Structures;

Oxidation States;

Formal Charges

Inorganic Chemistry Chapter 1: Figure 1.22

W.H.
FREEMAN



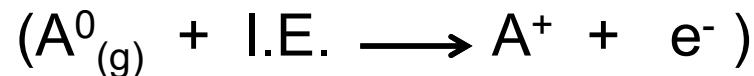
Trends in Atomic Properties

- Size (atomic, ionic, covalent, van der Waals radii)
- Ionization Potential ($A^0_{(g)} + I.E. \longrightarrow A^+ + e^-$)
- Electron Affinity Energies ($A^0_{(g)} + e^- \rightarrow A^- + E.A.E.$)
- Electronegativity: Ability of an atom, within a molecule to attract electrons to itself.

Trends in Atomic Properties

- Size (atomic, ionic, covalent, van der Waals radii)

- Ionization Potential energy



- Electron Affinity Energy ($A^0_{(g)} + e^- \rightarrow A^- + \text{E.A.E.}$)

- Electronegativity: Ability of an atom, within a molecule to attract electrons to itself.

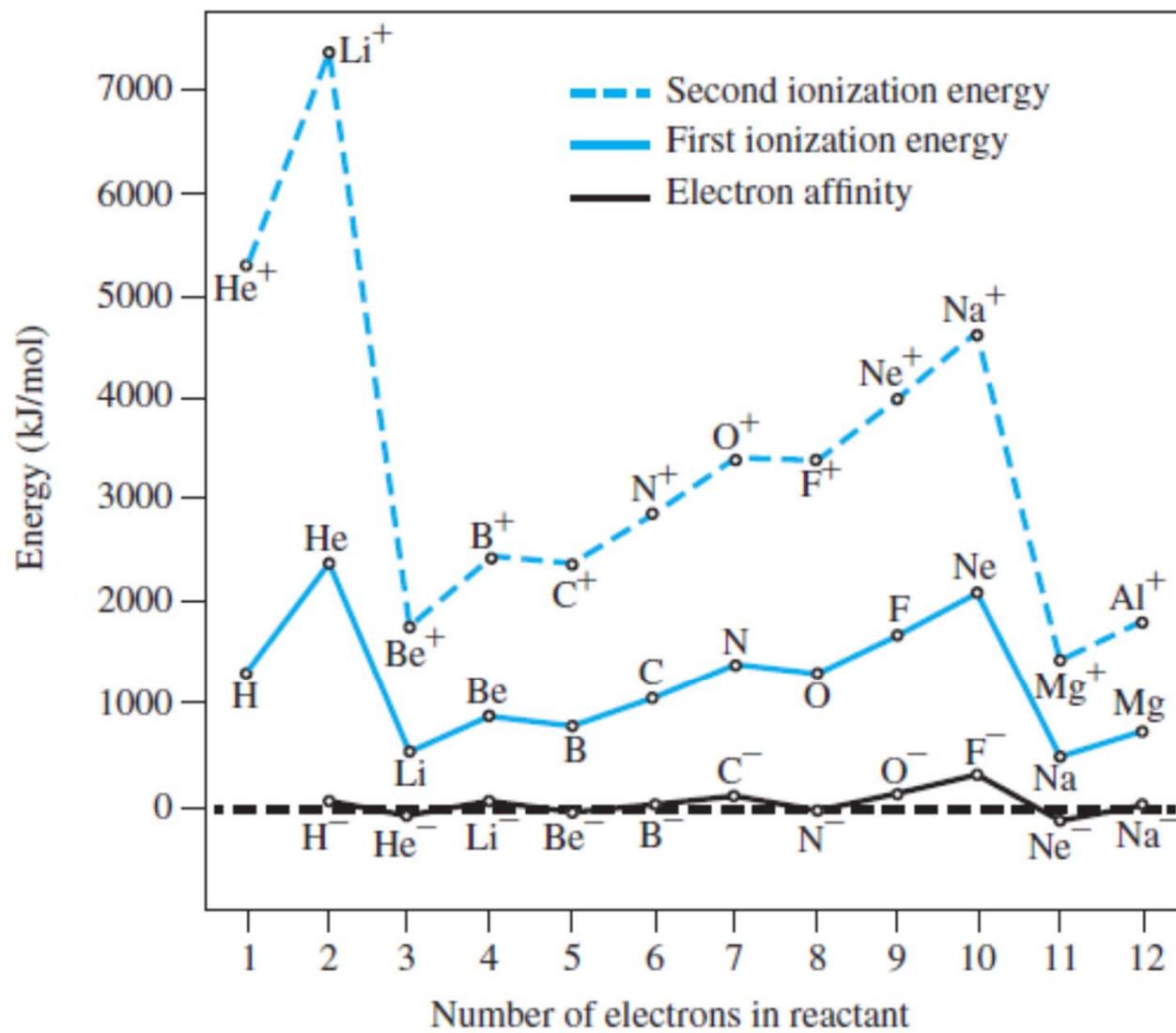
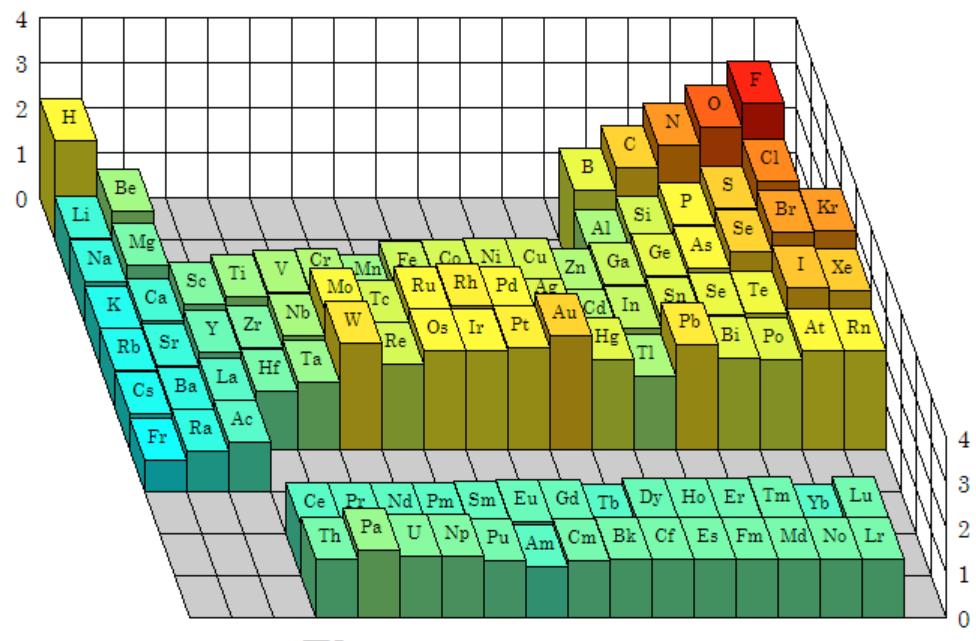


Table 1.6 First electron affinities of the main-group elements, $E_a/(kJ\ mol^{-1})^*$

H								He
72								-48
Li	Be	B	C	N	O	F	Ne	
60	≤ 0	27	122	-8	141	328	-116	
					-780			
Na	Mg	Al	Si	P	S	Cl	Ar	
53	≤ 0	43	134	72	200	349	-96	
					-492			
K	Ca	Ga	Ge	As	Se	Br	Kr	
48	2	29	116	78	195	325	-96	
Rb	Sr	In	Sn	Sb	Te	I	Xe	
47	5	29	116	103	190	295	-77	

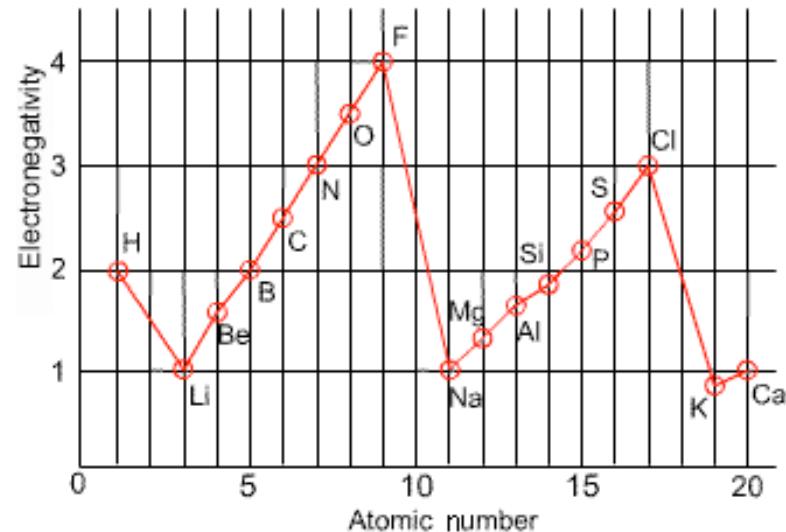
* The first values refer to the formation of the ion X^- from the neutral atom; the second value to the formation of X^{2-} from X^- .



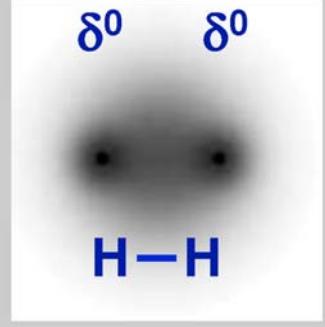
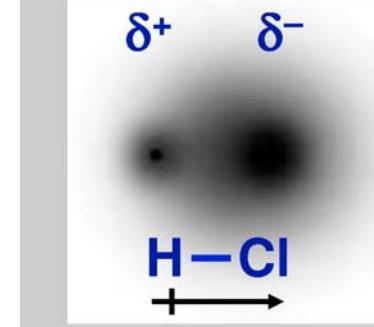
Electronegativity

1 H 1.0079	2	10 He 4.0016
3 Li 6.941	4 Be 9.0111	11 Na 12.990
12 Mg 14.025	13 Al 14.007	13 Al 14.007
19 K 39.098	20 Ca 40.078	14 Si 40.078
31 Sc 44.956	22 Ti 47.957	15 P 50.940
32 Ti 47.957	23 V 50.940	16 Cr 51.996
33 V 50.940	24 Cr 51.996	17 Mn 54.938
34 Cr 51.996	25 Fe 55.845	18 Co 55.935
35 Mn 54.938	26 Co 55.935	19 Ni 58.693
36 Fe 55.845	27 Ni 58.693	20 Cu 58.746
37 Co 55.935	28 Cu 58.746	21 Zn 63.546
38 Ni 58.693	29 Zn 63.546	22 Ga 69.723
39 Cu 63.546	30 Ga 69.723	23 Ge 72.64
40 Zn 69.723	31 Ge 72.64	24 As 74.921
41 Ga 72.64	32 As 74.921	25 Se 78.95
42 Ge 74.921	33 Se 78.95	26 Br 79.904
43 As 78.95	34 Br 83.798	27 Kr 83.798
44 Se 83.798	35 Kr 83.798	19 F 10.811
45 Br 83.798	36 Kr 83.798	10 Ne 10.810
46 Kr 83.798	37 Ne 11.011	11 Ne 11.011
47 Kr 83.798	38 Ne 11.011	12 Ar 14.007
48 Kr 83.798	39 Ar 14.007	13 Ar 14.007
49 Kr 83.798	40 Ar 15.200	14 Ar 15.200
50 Kr 83.798	41 Ar 15.200	15 Ar 15.200
51 Kr 83.798	42 Ar 15.200	16 Ar 15.200
52 Kr 83.798	43 Ar 15.200	17 Ar 15.200
53 Kr 83.798	44 Ar 15.200	18 Ar 15.200
54 Kr 83.798	45 Ar 15.200	19 Ar 15.200
55 Cs 132.91	56 Ba 137.33	56 Kr 83.798
56 Ba 137.33	57 La 139.91	57 Kr 83.798
57 La 139.91	58 Hf 139.49	58 Kr 83.798
58 Hf 139.49	59 Ta 140.95	59 Kr 83.798
59 Ta 140.95	60 W 143.84	60 Kr 83.798
60 W 143.84	61 Re 144.14	61 Kr 83.798
61 Re 144.14	62 Os (145)	62 Kr 83.798
62 Os (145)	63 Pt (146)	63 Kr 83.798
63 Pt (146)	64 Rh (147)	64 Kr 83.798
64 Rh (147)	65 Ir (148)	65 Kr 83.798
65 Ir (148)	66 Au (149)	66 Kr 83.798
66 Au (149)	67 Tb (150)	67 Kr 83.798
67 Tb (150)	68 Dy (151)	68 Kr 83.798
68 Dy (151)	69 Ho (152)	69 Kr 83.798
69 Ho (152)	70 Er (153)	70 Kr 83.798
70 Er (153)	71 Tm (154)	71 Kr 83.798
71 Tm (154)	72 Yb (155)	72 Kr 83.798
72 Yb (155)	73 Lu (156)	73 Kr 83.798

increasing



Electronegativity



BDE: 427

436 kJ/mol

Electronegativity-

- Pauling

$$|\chi_A - \chi_B| = 0.208 \sqrt{E_{A-B} - 1/2(E_{A-A} + E_{B-B})}$$

arithmetic mean

$$|\chi_A - \chi_B| = 0.208 \sqrt{E_{A-B} - (E_{A-A} \cdot E_{B-B})^{1/2}}$$

geometric mean

- Mulliken

$$\chi_m = \frac{1}{2}(I + E_{ea})$$

Allred and Rochow Scale

This scale considers electronegativity as the force acting on electrons at a distance of the covalent radius.

$$\chi = 0.744 + \frac{0.359 Z_{\text{eff}}}{r_{\text{cov}}^2}$$

Z_{eff} = Effective nuclear charge

r_{cov} = Covalent radius of the atom in Angstroms.

- Rochow

Linus Pauling

Le Pr Linus Pauling est le seul homme
a avoir reçu 2 Prix Nobel non partagés



The Nobel Prize
in Chemistry 1954



The Nobel
Peace Prize 1962



Photos: Copyright © The Nobel Foundation

$$\text{BDE H}_2 = 436 \text{ kJ/mol}$$

$$\text{BDE Cl}_2 = 239$$

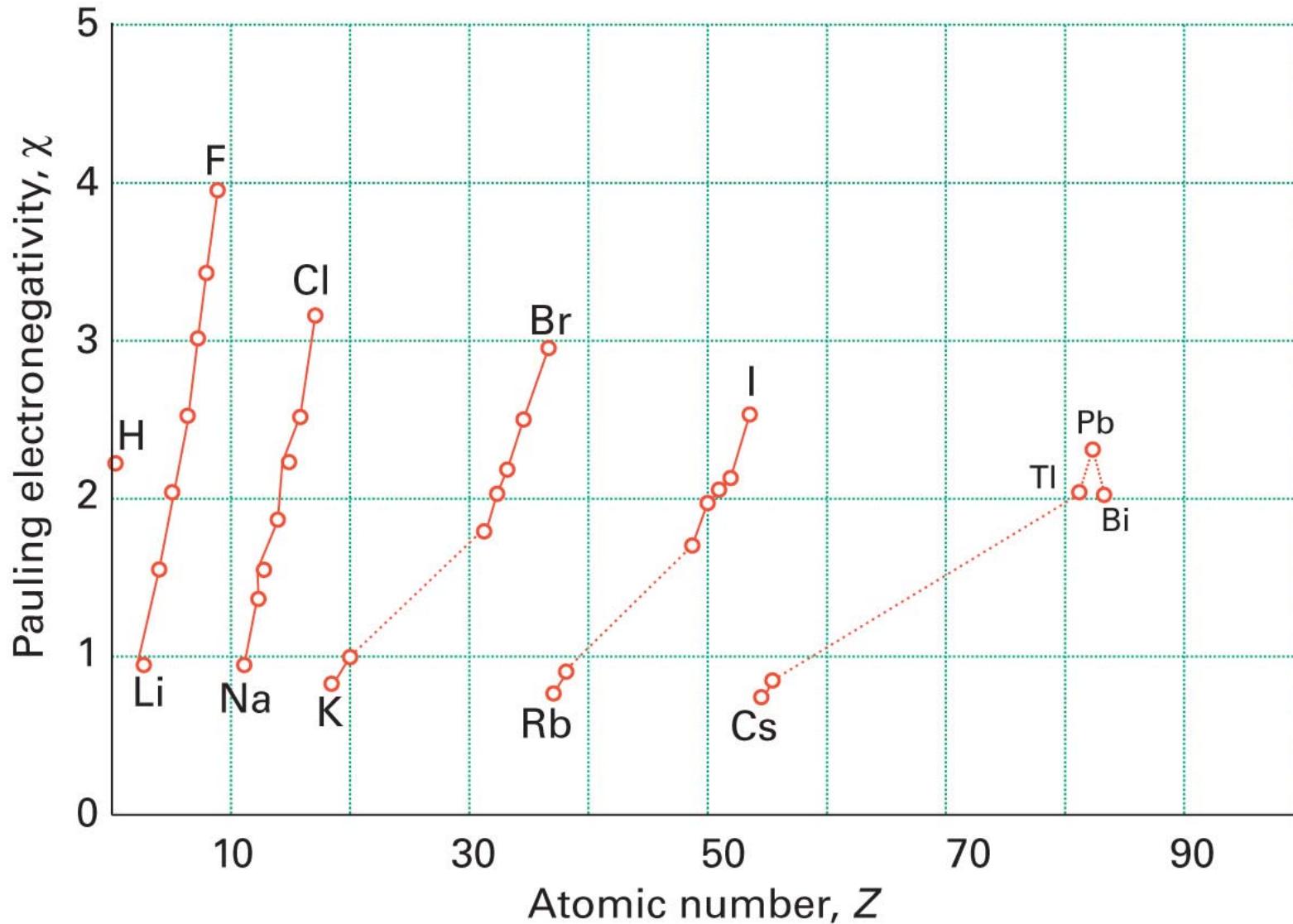
$$\text{BDE HCl} = 427$$

Pauling: If strictly covalent: BDE HCl should be average of H₂ and Cl₂

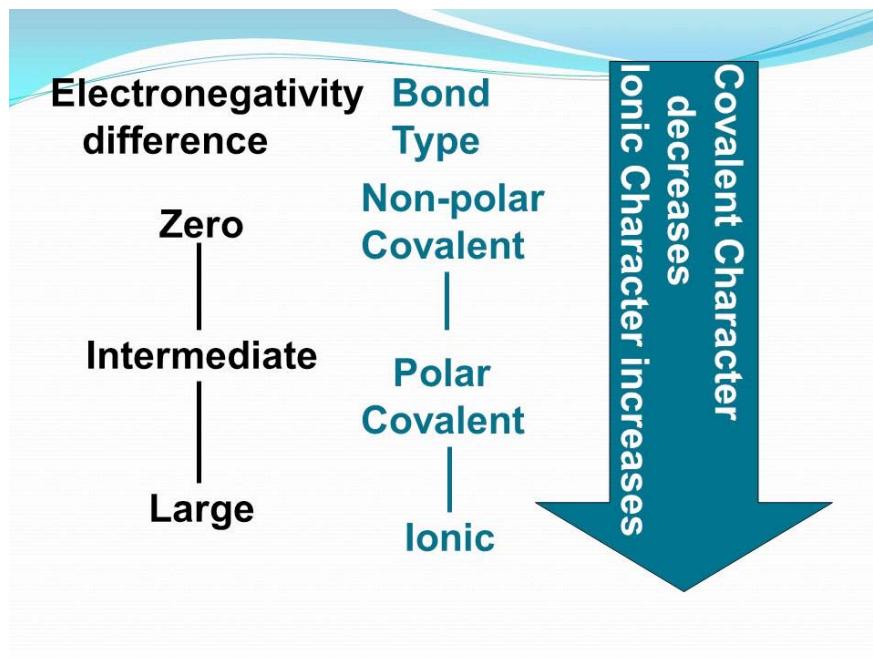
Which would be $\frac{1}{2} (436 + 239) = 338 \text{ kJ/mol}$. The extra stability is Due to electronegativity difference, and **electrostatic attraction**. That is, this Bond is polar covalent.

Table 1.7 Pauling χ_p , Mulliken, χ_m , and Allred–Rochow, χ_{AR} , electronegativities

H							He
2.20							5.5
3.06							
2.20							
Li	Be	B	C	N	O	F	Ne
0.98	1.57	2.04	2.55	3.04	3.44	3.98	
1.28	1.99	1.83	2.67	3.08	3.22	4.43	4.60
0.97	1.47	2.01	2.50	3.07	3.50	4.10	5.10
Na	Mg	Al	Si	P	S	Cl	Ar
0.93	1.31	1.61	1.90	2.19	2.58	3.16	
1.21	1.63	1.37	2.03	2.39	2.65	3.54	3.36
1.01	1.23	1.47	1.74	2.06	2.44	2.83	3.30
K	Ca	Ga	Ge	As	Se	Br	Kr
0.82	1.00	1.81	2.01	2.18	2.55	2.96	3.0
1.03	1.30	1.34	1.95	2.26	2.51	3.24	2.98
0.91	1.04	1.82	2.02	2.20	2.48	2.74	3.10
Rb	Sr	In	Sn	Sb	Te	I	Xe
0.82	0.95	1.78	1.96	2.05	2.10	2.66	2.6
0.99	1.21	1.30	1.83	2.06	2.34	2.88	2.59
0.89	0.99	1.49	1.72	1.82	2.01	2.21	2.40
Cs	Ba	Tl	Pb	Bi			
0.79	0.89	2.04	2.33	2.02			
0.70	0.90	1.80	1.90	1.90			
0.86	0.97	1.44	1.55	1.67			



Significance: Bond type



en = electronegativity

en > 1.7 = **ionic bond**

en < 1.7 = **Polar covalent bond**

en = 0
is non-polar covalent bond

Properties of Hydrogen Halides: polar covalent bonds, bond dipoles, electric dipole moments,

$$\mu = q \times r$$

Hydrogen Fluoride (HF)

m.p. -83.1°C, b.p. 19.9°C

pKa (aq) 3.17

r(H-F) = 0.92 Å; dipole moment = 1.8D

Hydrogen Chloride (HCl)

m.p. -114.2°C, b.p. -85.0 deg.C

pKa (aq) -7

r(H-Cl) = 1.28 Å; dipole moment = 1.1D

Hydrogen Bromide (HBr)

m.p. -86.8°C, b.p. -66.7°C

pKa (aq) -9

r(H-Br) = 1.41 Å; dipole moment = 0.8D

Hydrogen Iodide (HI)

m.p. -50.8°C, b.p. -35.35°C

pKa (aq) -10

r(H-I) = 1.60 Å; dipole moment = 0.4D

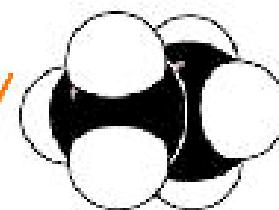
Why??? Electric dipole moment is the product of magnitude of charges and the distance of separation between the charges. Magnitude of charges will depend on difference in electronegativity of the atoms. Now in this case, F has highest electronegativity hence HF will have highest magnitude of charges. But, as we go down the group, the atomic radii increases, hence the distance of separation (bond length) will increase. So, we would expect the two factors to balance each other. Here, it seems the difference in electronegativity out weighs the distance (bond length) and that is why Dipole moment decreases,

Covalent bond types

- Polar molecules
 - Electrons are not equally shared
 - One part of molecule is more negative than the another part of the molecule
 - Molecule thus has negative and positive 'poles' like a battery
 - Hydrophilic ('water loving')
- Nonpolar molecules
 - Electrons are equally shared
 - No one part of molecule is distinctly negative or positive; no 'poles'
 - Hydrophobic 'water fearing'



Water, a polar molecule



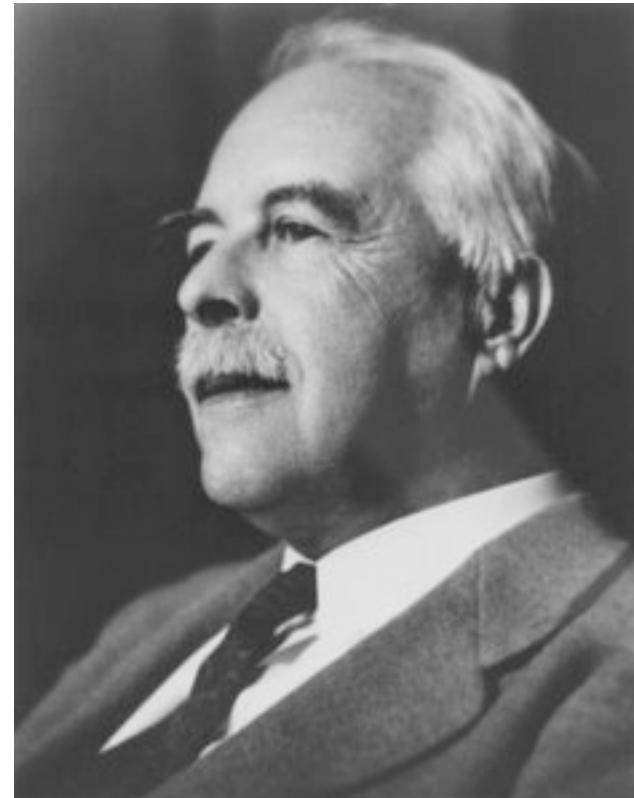
Ethane, a nonpolar molecule

Figure 1
Potential Energy Changes that Accompany
Changes in the Internuclear Separation of Two
Hydrogen Atoms

Two Electrons Shared between Two Atoms Make a Bond! G.N. Lewis

(G. = Gilbert
N. = Newton
Lewis as in Lewis Structures!)

Lewis Structures and VSEPR:
Workshop Study



Simple Review videos
<https://www.youtube.com/watch?v=1ZlnzyHahvo>
https://www.youtube.com/watch?v=xNYiB_2u8J4