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Title of the Unit: Periodicity of elements

Module Name: Allred and Rochow scale of electronegativity

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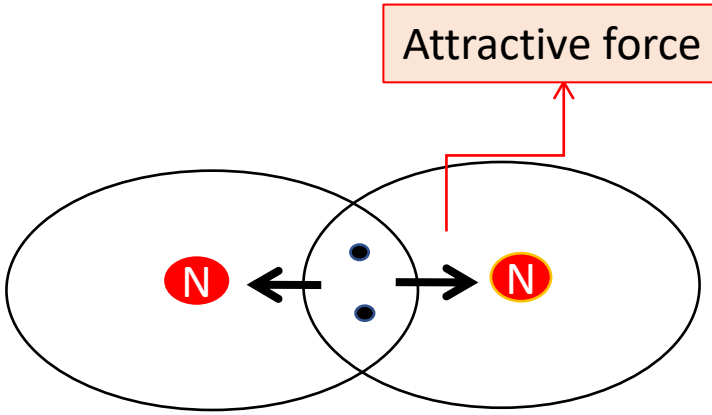
ALLRED AND ROCHOW ELECTRONEGATIVITY

What is electronegativity (χ)?

Elecronegativity is the property of an ATOM in the MOLECULES

"The power of an atom in a molecule to attract electrons to itself"
.....Linus Pauling



H_2 molecule

As in the atom, shared electron in the molecules are attracted by proton's in the nucleus of an atom

Hence , electronegativity can be also define as a measure of an atom's ability to attract the bonding/ shared electrons of a covalent bond to itself.

Electronegativity (χ) α Attractive force (F)

Electronegativity cannot be measured directly.

METHODS OF DETERMINING ELECTRONEGATIVITY

PAULING's METHOD (1931): Most common method

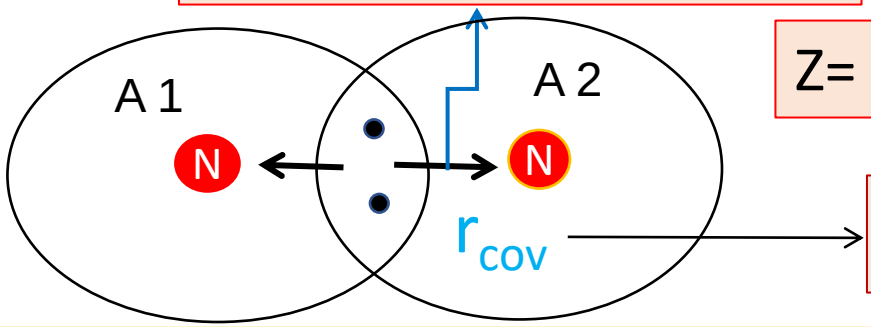
MULLIKEN METHOD (1934)

ALLRED AND ROCHOW METHOD (1958)

Allred and Rochow (1958) define electronegativity as:

Attractive force between a nucleus and valence shared electron at a distance equal to the covalent radius

Attractive force (F) α Z

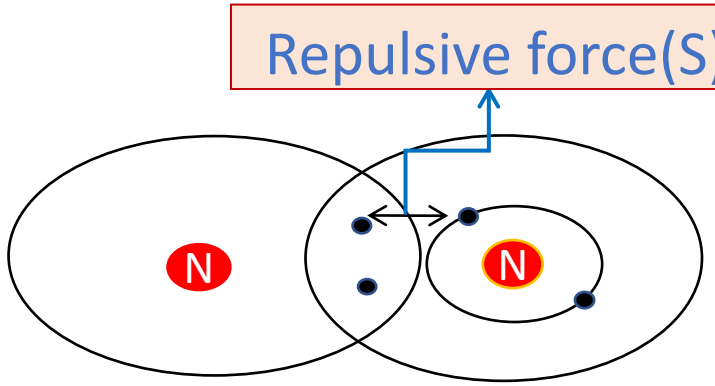


Z= Number of protons=Atomic number

Covalent radius (r_{cov})

It shows that, Electronegativity depends on atomic number (Z) and the distance between the shared electrons and the positively charged nucleus (r_{cov})

However, the shared electron in the valence shell of molecules are attracted by proton's in the nucleus and at the same time repelled by other electrons in the atoms



These cumulative effect of attractive and repulsive forces on the shared electron is called EFFECTIVE NUCLEAR CHARGE (Z_{eff})

∴ The extent of **attractive nuclear force** on the shared electrons is proportional to

Effective nuclear charge ($Z_{eff} = Z_{actual} - S$) or Net nuclear charge.

Where , the effective nuclear charge(, Z_{eff})is the reduced nuclear charge felt by the shared electrons due to repulsive forces

$$F \alpha Z_{effective} \quad ...1$$

Allred and Rochow, identified the electronegativity of an atom with the electrostatic field. Thus attractive Force (F) is electrostatic in nature and is given by Coulomb's law:

$$F \alpha \frac{e^2}{r^2} \qquad ..2$$

Where , **e** is the charge on an electrons
r is the covalent radius (Å)

Combining equations 1 & 2,

$$F \alpha \frac{e^2 Z_{effective}}{r^2}$$

Accordingly, one measures the electronegativity by measuring this electrostatic force of attraction between the nucleus and an shared electron from the bonded atom.

Electronegativity (χ) α Attractive force (F)

$\chi \alpha$ Force = $e^2(Z_{eff})/r^2$

Where , e is the charge on the electron

$e(Z_{eff})$ is the charge which is effective at the electron due to the nucleus and its surrounding electrons.

Thus Allred and Rochow converted this attractive force (F) values in to electronegativity values by choosing the numericals to give the values comparable to Pauling's elctronegativities by using an empirical relationship.

$$\chi_{AR} = \left(\frac{0.359\, Z_{effective}}{r_{cov}^2}\right) + 0.744$$

The value of Z_{eff} is determined from Slater's rules

Allred and Rochow obtained this numerical by adding certain parameters so that it would more closely corresponding to Pauling's electronegativity scale.

Examples: The covalent radii of carbon atom is 0.77Å. Calculate the electronegativity of carbon atom following Allred-Rochow's approach.

Solution:

$$\chi_{AR} = \left(\frac{0.359\, Z_{effective}}{r_{cov}^2}\right) + 0.744$$

Given: r_{cov} = 0.77Å

Z_{eff}=?

χ_{AR}=?

$Z_{effective} = Z_{actual} - S$

$= 6 - (0.35 * 4 + 0.85*2)$

$= 2.90$

Z_{actual} =6

E.C of C =$(1s^2)(2s^2\ 2p^2)$

$\mathbf{S}_C$= (0.35 * 4 + 0.85*2)

χ_{AR}= $0.359*2.90/(0.77)^2 + 0.744$

=2.50

Comparison between Allred and Rochow electronegativity values with Pauling's electronegativity values.

Element	Pauling (χ_p)	Allred-Rochow(χ_{AR})
H	2.1	2.20
Li	1.0	0.97
Be	1.5	1.58
B	2.0	2.05
C	2.5	2.50
N	3.0	3.07
O	3.5	3.61
F	4.0	4.10

The electronegativity values so obtained are in good agreement with those obtained by Pauling (1931)

SIGNIFICANCE

- Possible to make a reasonable guess at the electronegativity values for the element

- Predict the nature of bonds formed

The atoms with similar electronegativity values will form non-polar bond (covalent)

The atoms with large electronegativity difference will form polar bond (Ionic)

References:

1. *Inorganic Chemistry, Principles of Structure and Reactivity;* J E Huheey, E A Keiter, R. L. Keiter, 4th Edtn, Harper Collins College Publishers, 1993, 186-190
2. *Inorganic Chemistry;* P Atkins, T Overton, J Rourke, M Weller, F Armstrong, Oxford University Press,4th Edtn,32,
3. *Concise Inorganic Chemistry;* J. D, Lee, Wiley India Edition, 5th Edtn, 2003, 162-163
4. *Principles of Inorganic Chemistry;* B R Puri, L.R. Sharma, K.C. Kalia, Milestone Publisher, 31st Edtn, 94-96.
5. *Inorganic chemistry;* A G Sharpe, Pearson Education, 2008, 65-66
6. The electronegativity scale of Allred and Rochow: revisited D.C. Ghosh T. Chakraborty,B. Mandal, *Theor Chem Acc.,* 2009, 124:295–301
7. https://en.wikipedia.org/wiki/Electronegativity