ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Electronegativity and Atomic Number: Linear Isoelectronic Trends.

Dinesh Prakash Upadhyay*, Laxmi Kant Gupta, And Mohan Kumar Sharma.

Department of Chemistry, M.S.J. Govt. (P.G.) College, Bharatpur, Rajasthan 321001, India.

ABSTRACT

Electronegativity originates from the atomic nucleus and electron distribution or shell structure. Here, a linear relationship between the electro negativity and atomic number (Z) has been approached, using isoelectronic series. For the first ten isoelectronic series (H-Ne), it is found that isoelectronic trend of the square root (SQRT) of the electro negativity i.e. $\{(I+A)/2\}^{1/2}$ with atomic number (up to Z=20), is *excellently linear with the determination coefficients (r^2) nearly one*. On this basis it is being inferred that for neutral atomic species, the SQRT electro negativity is proportional to atomic number.
Keywords: Electronegativity, Atomic number, linear relationship.

Corresponding author

ISSN: 0975-8585

INTRODUCTION

Electronegativity [1-2] is one of the most useful theoretical constructs of chemistry. It has become an indispensible tool for chemists to understand physico-chemical properties. The fundamental quantities of inorganic, organic and physical chemistry such as bond energy, polarity, the inductive effect and many more can be visualized in terms of electro negativity. Besides chemistry, the concept finds applications in biology, physics and geology [3-4], nanochemistry, high-temperature superconductors [5-6], spectroscopy [7-8], qualitative understanding of quark atoms [9], for material design [10], drug design [11] etc.

Pauling [1-2] defined electro negativity, "as the power of an atom in a molecule to attract electrons to itself." Several views have been put forth to poke into the electron attracting power of an atom. Various scales of electro negativity have been suggested incorporating different atomic and molecular properties. Pauling [1], Mulliken [12], Gordy [13], Allred and Rochow [14] are some of the pioneering scales of electro negativity. Besides these traditional scales, various attempts have been made to evaluate electro negativity of atoms using other periodic parameters like atomic radius [21], ionization potential [22], polarizability [23-24] etc. Prevalent scenario for electro negativity is based upon density functional theory (DFT). In the DFT [25-26], the electro negativity (χ) is the first derivative of electronic energy (E) with respect to the number of electrons (N) and is defined as follows [27]:

$$\chi = -\left(\frac{\partial E}{\partial N}\right)_{v} \quad (1)$$

Where, v is external nuclear potential and E is the total energy of an N-electron system. Hence, in DFT, electro negativity (χ) is slope of the E *vs.* N plot and represents the change in electronic energy with respect to the number of electrons. The approximate expression for electro negativity can be written in terms of ionization potential **I**, and electron affinity **A** as [28]:

$$\chi \approx \frac{(I + A)}{2} \quad (2)$$

It has been established conclusively that electro negativity is not an in situ property; rather it is an intrinsic ground state property of atom [29-33]. Since electro negativity is an intrinsic atomic property, therefore, it transpires that it has its hidden basis and origin expressed within the electron distribution or shell structure and atomic nucleus or the nuclear charge. Recently, proportionality has been sketched between electro negativity and square of the effective nuclear charge [34]. The sketched relationship also has been justified via isoelectronic series, recently.

Isoelectronic series have been considered as fundamental periodic properties [35]. Isoelectronic species possess equal number of electrons and as per the Slater's theory [36] these have same screening constant. Therefore, in isoelectronic series the change in any property is mainly caused by the atomic number or the nuclear charge. Recently, a potential use of isoelectronic series has been suggested to explore relationship [37]. In isoelectronic series, the electro negativity measure (I+A)/2 have been found to have a quadratic relation with atomic number (Z) recently [38]. Since, there is quadratic relation between the two so, a linear relation is expected between square root (SQRT) of the electro negativity measure i.e. $\{(I+A)/2\}^{1/2}$ and atomic number. In this communication, these correlations have been investigated for the first ten isoelectronic series (H-Ne) upto atomic number 20.

METHODOLOGY

The developed novel methodology [37] is very simple. It is based on the fact from the isoelectronic trend one can predict the relationship. On the basis of the square root (SQRT) of the electro negativity measure i.e. $\{(I+A)/2\}^{1/2}$ vs. atomic number plots, one can predict the interrelation. Here, I and A need not to be the first ionization potential or electron affinities.

ISSN: 0975-8585

RESULTS

The isoelectronic trend of the SQRT of the electro negativity measure i.e. $\{(I+A)/2\}^{1/2}$ with atomic number (up to Z= 20), for the first ten isoelectronic series is presented in Figure 1-3. The Figure 1 involves **H** ($1s^1$), **He** ($1s^2$), **Li** ($1s^2 2s^1$), **N** ($1s^2 2s^2 2p^3$) and **Ne** ($1s^2 2s^2 2p^6$) configuration isoelectronic series. The Figure 2 is for **Be** ($1s^2 2s^2$), **C** ($1s^2 2s^2 2p^2$), and **F** ($1s^2 2s^2 2p^5$) configuration isoelectronic series. The Figure 3 incorporates **B** ($1s^2 2s^2 2p^1$), and **O** ($1s^2 2s^2 2p^4$) configuration isoelectronic series. The plots of Figures 1-3 can be represented by (3)

$$\{(I+A)/2\}^{1/2} = \boldsymbol{s}Z + \boldsymbol{i} \qquad \text{(in eV}^{1/2}\text{)} \qquad (3)$$

In Table **1,** the slopes(***s***), intercepts (***i***) and the determination coefficients (r^2) of the linear trend drawn through the data of Figures 1-3 (Eq. 4) are being listed.

The $\{(I+A)/2\}^{1/2}$ values used in drawing the plots of Figure 1-3 have been presented in Table **2**.

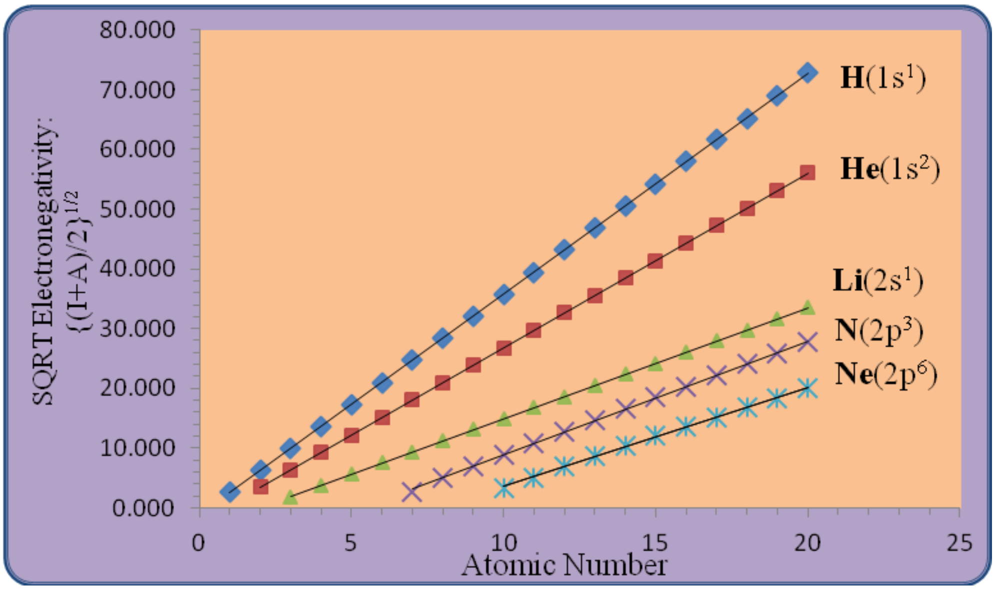

Figure 1: Isoelectronic trend of the SQRT electro negativity measure i.e. $\{(I+A)/2\}^{1/2}$ with atomic number for H ($1s^1$), He ($1s^2$), Li ($1s^2 2s^1$), N ($1s^2 2s^2 2p^3$) and Ne ($1s^2 2s^2 2p^6$) isoelectronic series. The solid lines through the data are the linear trend lines. The $\{(I+A)/2\}^{1/2}$ values obtained using successive ionization potentials given in reference 39.

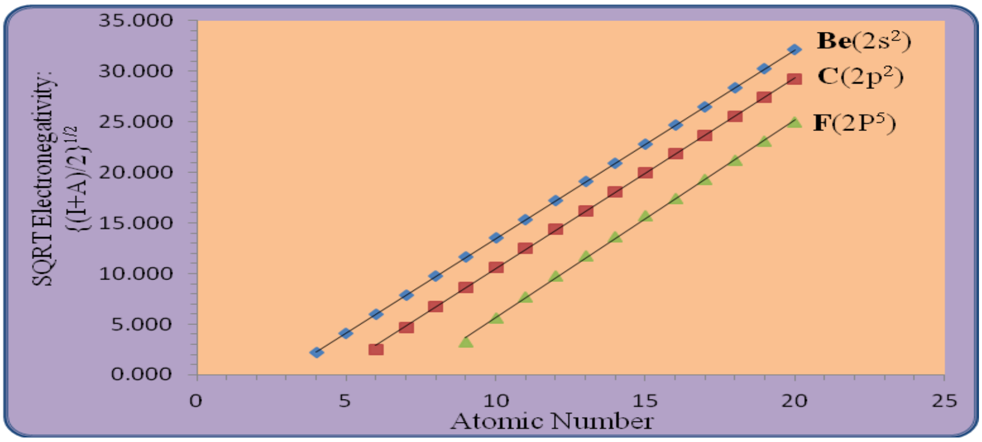

Figure 2: Isoelectronic trend of the SQRT electro negativity measure i.e. $\{(I+A)/2\}^{1/2}$ with atomic number for Be ($1s^2 2s^2$), C ($1s^2 2s^2 2p^2$) and F ($1s^2 2s^2 2p^5$) isoelectronic series. The solid lines through the data are the linear trend lines. The $\{(I+A)/2\}^{1/2}$ values obtained using successive ionization potentials given in reference 39.

Table 1: Slope(*s*), intercept (*i*) and the determination coefficients (r^2) of the linear trend lines drawn in Fig.1-3(Eq. 3).

Isoelectronic series	*S*	*i*	r^2
$H(1s^1)$	3.690	-1.117	1
$He(1s^2)$	2.922	-2.413	1
$Li(1s^2 2s^1)$	1.862	-3.708	1
$Be(1s^2 2s^2)$	1.866	-5.193	1
$B(1s^2 2s^2 2p^1)$	1.885	-7.029	0.999
$C(1s^2 2s^2 2p^2)$	1.893	-8.490	0.999
$N(1s^2 2s^2 2p^3)$	1.910	-10.264	0.999
$O(1s^2 2s^2 2p^4)$	1.937	-12.244	0.999
$F(1s^2 2s^2 2p^5)$	1.954	-13.884	0.999
$Ne(1s^2 2s^2 2p^6)$	1.666	-13.126	0.999

Table 2: The values $\{(I+A)/2\}^{1/2}$ used in isoelectronic plots of Fig. 1-3 and calculating the slope, intercept and the coefficients of table 1. All the successive ionization potentials are from reference [39] and are in electron volts.

		Isoelectronic Series				
		$1s^1$	$1s^2$	$1s^2 2s^1$	$1s^2 2s^2$	$1s^2 2s^2 2p^1$
S.N.	At. No.	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$
1	1	2.679				
2	2	6.285	3.506			
3	3	9.952	6.365	1.733		
4	4	13.631	9.276	3.710	2.159	
5	5	17.315	12.192	5.616	4.090	2.071
6	6	21.001	15.109	7.496	6.011	4.222
7	7	24.689	18.027	9.364	7.903	6.207
8	8	28.379	20.946	11.225	9.780	8.135
9	9	32.070	23.865	13.083	11.649	10.034
10	10	35.763	26.785	14.939	13.513	11.919
11	11	39.457	29.707	16.794	15.373	13.795
12	12	43.153	32.621	18.648	17.232	15.666
13	13	46.851	35.553	20.502	19.089	17.533
14	14	50.551	38.478	22.356	20.946	19.398
15	15	54.253	41.405	24.224	22.803	21.261
16	16	57.957	44.334	26.065	24.660	23.124
17	17	61.663	47.264	27.921	26.518	24.987
18	18	65.096	50.194	29.772	28.377	26.850
19	19	69.083	53.127	31.639	30.247	28.713
20	20	72.797	56.072	33.496	32.101	30.571
		Isoelectronic Series				
		$1s^2 2s^2 2p^2$	$1s^2 2s^2 2p^3$	$1s^2 2s^2 2p^4$	$1s^2 2s^2 2p^5$	$1s^2 2s^2 2p^6$
S.N.	At. No.	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$	$\{(I+A)/2\}^{1/2}$
1	6	2.502				
2	7	4.698	2.696			
3	8	6.710	4.936	2.746		
4	9	8.656	6.988	5.118	3.227	
5	10	10.567	8.960	7.225	5.591	3.284
6	11	12.461	10.893	9.234	7.711	5.120
7	12	14.343	12.802	11.192	9.731	6.898
8	13	16.218	14.695	13.118	11.698	8.615
9	14	18.087	16.578	15.026	13.635	10.293
10	15	19.953	18.455	16.921	15.711	12.154
11	16	21.816	20.325	18.806	17.452	13.583
12	17	23.677	22.191	20.684	19.343	15.206
13	18	25.538	24.054	22.557	21.226	16.821
14	19	27.397	25.914	24.426	23.104	18.429
15	20	29.255	27.773	26.291	24.976	20.031

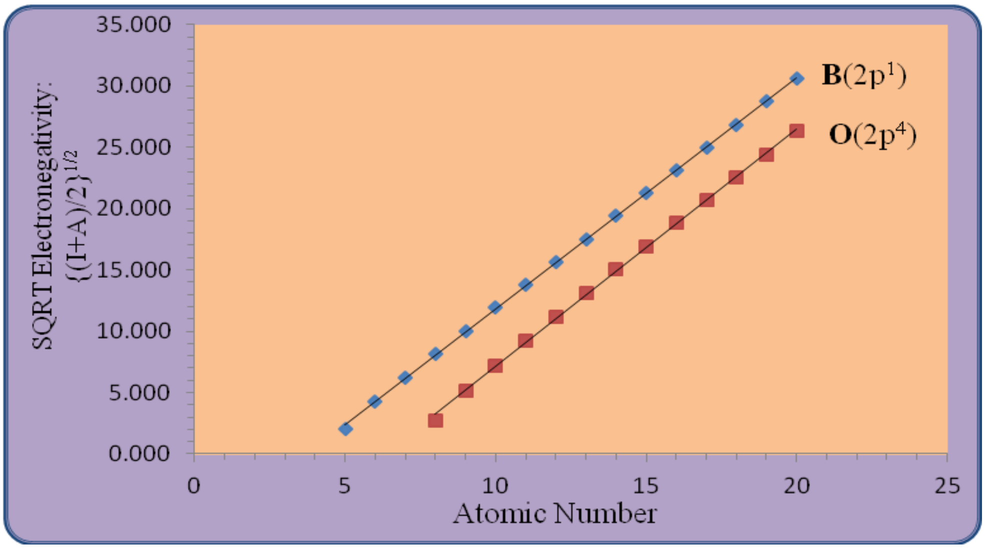

Figure 3: Isoelectronic trend of the SQRT electro negativity measure i.e. $\{(I+A)/2\}^{1/2}$ with atomic number for B ($1s^2 2s^2 2p^1$) and O ($1s^2 2s^2 2p^4$) isoelectronic series. The solid lines through the data are the linear trend lines. The $\{(I+A)/2\}^{1/2}$ values obtained using successive ionization potentials given in reference 39.

DISCUSSION

It is explicit from Figure 1-3 that in isoelectronic series, the square root of the electro negativity measure varies linearly with atomic number. It reveals from the determination coefficients (r^2), listed in Table 1, that the variations are remarkably linear. This justify the presumption regarding a linear isoelectronic trend between SQRT of the electro negativity measure i.e. $\{(I+A)/2\}^{1/2}$ and atomic number. Therefore, *it transpires that, as an atomic neutral species is also a part of an isoelectronic series, the square root of the electro negativity measure (I+A)/2 of neutral atomic species is proportional to atomic number*. Although the present work has been limited to the first ten isoelectronic series upto atomic number 20, if it is extended to other series the similar results might be obtained.

CONCLUSION

The square root of the approximate DFT measure or the Mulliken's electro negativity measure (I+A)/2 follow a linear isoelectronic trend with atomic number. The square root of the electro negativity is proportional to atomic number.

REFERENCES

[1] Pauling L. J Am Chem Soc 1932; 54: 3570-3582.
[2] Pauling L. The nature of the chemical bond, Third ed., Cornell University Press: Ithaca, New York, 1960.
[3] Pritchard HO, Skinner HA. Chem Rev 1955; 55(4): 745-786.
[4] Ghosh DC. J Indian Chem Soc 2003; 80: 527-533.
[5] Reddy RR, Rao TVR, Viswanath R. J Am Chem Soc 1989; 111(8): 2914-2915.
[6] Myers RT. J Chem Educ 1979; 56: 711-718.
[7] Grody W. J Chem Phys 1951; 19: 792-793.
[8] Gutowsky HS, Hoffman CJ. J Chem Phys 1951; 19: 1259-1267.
[9] Lackner KS, Zweig G. Phys Rev D 1983; 28: 1671-1691.
[10] Arroyo-De Dompablo ME, Armand M, Tarascon JM, Amador U. *Solid State Ionics* 2008; 179 : 1758–1762.
[11] Kobayashi S, Hamashima H, Kurihara, Miyata, Tanaka A. Chem Pharm Bull 1998; 46(7) : 1108-1115.
[12] Mulliken RS. J Chem Phys 1934; 2(11): 782-793.
[13] Gordy W. Phys Rev 1946; 69(11-12): 604-607.
[14] Allred AL, Rochow EG. J Inorg Nucl Chem 1958; 5 : 264-268.

ISSN: 0975-8585

[15] Gordy W, Orville Thomas WJ. J Chem Phys 1956; 24: 439-444.
[16] Ghosh DC, Chakraborty T. J Mol Struct (THEOCHEM) 2009; 906: 87-93.
[17] Little EJ, Jones MM. J Chem Educ 1960; 37 : 231-233.
[18] Mande C, Deshmukh P. J Phys B: At Mol Phys 1977; 10: 2293-2300.
[19] Boyd RJ, Markus GE. J Chem Phys 1981; 75: 5385-5388.
[20] Ghosh DC, Chakraborty T, Mandal B. Theor Chem Account 2002; 124: 295–301.
[21] Ghosh DC. J Theoret Comput Chem 2005; 4: 21-33.
[22] Zhang YH. Inorg Chem 1982; 21: 3886-3889.
[23] Nagle JK. J Am Chem Soc 1990; 112: 4741-4747.
[24] Ghosh DC, K. Gupta K. J Theoret Comput Chem 2006; 5: 895-911.
[25] Parr RG, Yang W. Density functional theory of atoms and molecules, Oxford University press, New York, 1989.
[26] Hohenberg P, Kohn W. Phys Rev 1964; 136: B864-B871.
[27] Parr RG, Donnelly RA, Levy M, Palke WE. J Chem Phys 1978;68:3801-3807.
[28] Parr RG, Pearson RG. J Am Chem Soc 1983; 105: 7512-7516.
[29] Iczkowski RP, Margrave JL. J Am Chem Soc 1961; 83: 3547-3551.
[30] Allen LC. J Am Chem Soc 1992; 114(4): 1510-1511.
[31] Allen LC. J Am Chem Soc 1989; 111: 9003-9011.
[32] Mann JB, Meek TL, Knight ET, Capitani JF, Allen LC. J Am Chem Soc 2000; 122(21): 5132-5137.
[33] Murphy LR, Mek TL, Allred AL, Allen LC. J Phys Chem A 2000;104: 5867-5871.
[34] Islam N, Ghosh DC. J Quantum Inform Sci 2011; 1: 133-141.
[35] Geoff Rayner-Canham. Found Chem 2009; 11.2: 123-29.
[36] Slater JC. Phys Rev 1930; 36(1): 57-64.
[37] Upadhyay DP, Sharma MK. International Journal of Advances In Pharmacy, Biology and Chemistry 2013; 2(2): 360-361.
[38] Upadhyay DP, Sharma MK. Res Rev J Chem 2013; 2(2): 4-7.
[39] Lide DR(Ed.), CRC Handbook of Chemistry and Physics, 71st ed.; CRC press: Boca Raton, 1990-1991, pp. 10.210-10.211.