European Journal of Chemistry

Journal homepage: www.eurjchem.com

Derivation of Gordy's scale and computation of some useful descriptors of chemical reactivity

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ARTICLE INFORMATION

Received: 05 May 2010
Received in revised form: 17 February 2011
Accepted: 17 February 2011
Online: 31 December 2011

KEYWORDS

Electronegativity
Orbital exponent
Mulliken electronegativity scale
Gordy electronegativity scale
Chemical reactivity descriptors
Convergence of Gordy's and Mulliken's scale

ABSTRACT

A new atomic electronegativity scale is proposed by using the essence of electronegativity definitions of Gordy and Mulliken. The new computed atomic electronegativity data is found to satisfy all the sine qua non of a reasonable scale of atomic electronegativity. The electronegativity data is used to compute some useful descriptors of chemical reactivity. Comparative studies reveal that the new approach to derive the Gordy's scale of electronegativity is a successful venture.

1. Introduction

The concept of electronegativity had been a part of chemical thought for nearly about 140 years. Now a day, it is established that the electronegativity is an indispensable tool in every branch (both theoretical and experimental) of chemistry, physics, engineering and biology.

Although the idea of atomic electronegativity was initiated with the work of Jöns Jacob Berzelius [1], the first scientific definition and meaning of atomic electronegativity was given by Pauling [2,3] in 1932. Pauling defined atomic electronegativity as "*the power of an atom in a molecule to attract electrons toward itself*". After the announcement of the definition and the scale of atomic electronegativity, many theoretical concepts were developed. Being a measure of the electron attracting power, atomic electronegativity has been extensively used to study the amount of charge transfer during the heteronuclear molecule formation from its constituent atoms. Thus the atomic electronegativity determines the polarity of the molecule. To explain the process of hetero-nuclear molecule formation, the electronegativity equalization principle was proposed by Sanderson [4].

Despite its manifold usefulness [3-11], a group of scientists [6,12-16] believe that electronegativity is an empirical quantity and there is no experimental as well as quantum mechanical benchmark for electronegativity. It is also opined that electronegativity is very difficult to define [15-17].

1.1. The Gordy's electronegativity ansatz

The concept of screening begins in 1912 with the earlier work of Von Laue [18] and Moseley [19]. In case of H-atom or H-like ions the electrons experience a full attractive force from the nucleus: in a multi-electron atom, the electron in the inner most shell (nearest the nucleus) will experience the whole nuclear charge of Z units; if it is in the outer part of the atom, the electron will feel repulsion from the remaining inner electrons. This repulsion reduces the attraction force of the nucleus on the electron of interest, and is the screening or shielding of the electron from the nucleus.

Slater [18] coined the term "*effective nuclear charge*" (Z_{eff}) to describe the net positive charge which is experienced by an electron in a multi electronic atom.

Thus, Z_{eff} = Nuclear charge - point charge at the nucleus representing the average electron repulsion. i.e.,

$$Z_{eff} = Z - S \qquad (1)$$

where S is the screening constant or shielding constant.

The orbital exponent, ξ is the ratio of the effective nuclear charge (Z_{eff}) and the effective principal quantum number (n^*)

$$\xi = Z_{eff}/n^* \qquad (2)$$

The concept of screening is used by Gordy [20] to define the atomic electronegativity (χ) of an atom as the electrostatic potential felt by the valence electrons at a radial distance equal to atom at the single bond covalent radius (r).

$$\chi = e\,(Z_{eff}/r) \qquad (3)$$

Ghosh and Chakraborty [12] modified the electronegativity scale by suggesting that the atomic electronegativity is not equal but proportional to Z_{eff}/r and also they replaced the covalent radius by the absolute radius in the Gordy's electronegativity ansatz:

$$\chi = a(Z_{eff}/r^{\prime})+b \qquad (4)$$

ISSN 2153-2249 (Print) / ISSN 2153-2257 (Online) © 2011 EURJCHEM
DOI:10.5155/eurjchem.2.4.448-454.94

where $r^{/}$ is the most probable radius of the atom and 'a' and 'b' are constants. They also proposed the value of the constants for each period.

Although the new look (Equation 4) of Gordy's scale satisfies the entire criterion of a reasonable scale of atomic electronegativity and it can successfully explain several chemical facts, we noticed that the atomic electronegativity values of the members of the halogen family and H atom computed by Ghosh and Chakraborty (GC) [12] follow the order: $\chi_F > \chi_H > \chi_{Cl} > \chi_{Br} > \chi_I$. Thus, the use of the GC atomic electronegativity values [12] for the computation of the dipole charge and dipole moment and also the atomic polar tensor of the hydrogen halides is not efficacious. Furthermore, the modified atomic electronegativity value for the alkali metals and alkaline earth metals are in the reverse order than expected. So, the modification of the Gordy's [20] scale is not complete yet and it demands more study.

In a recent work, we [21a,b] have found that the Gordy's electronegativity ansatz can be derived from the Mulliken's definition of electronegativity [22] as well as the density functional definition of electronegativity [23]. In the instant work, to derive the Gordy's electronegativity scale, we proceed as follows-

Classically, the energy E(N) of charging a conducting sphere of radius r with charge q is given by [24-26]

$$E(N)=q^2/2r \text{ (In C.G.S unit)} \quad (5)$$

In Equation 5, E(N) is in ergs, q is in electrostatic unit and r is in cm. Now, for an atom, the change in energy associated with the increase of q, on removal of an electron (of charge e), would be the ionization energy, I. Similarly, the energy evolved on addition of an electron with q would be the electron affinity, A. Hence,

$$I=E(N+1)-E(N)=\{(q+e)^2/2r\}-q^2/2r \quad (6)$$

and,

$$A = E(N)-E(N-1)=[(q^2/2r)-\{(q-e)^2/2r\}] \quad (7)$$

$$\text{Since, } \chi_M = \tfrac{1}{2} (I + A) \quad (8)$$

$$\chi_M = \tfrac{1}{2} [\{\{(q+e)^2/(2r) \}-(q^2/2r)\}+\{ (q^2/2r)-\{(q-e)^2/2r\}] \quad (9)$$

or,

$$\chi_M = qe/r \quad (10)$$

where e is the electronic charge in e.s.u. Now,

$$q= Z_{eff}\, e \quad (11)$$

We can write using the Equations 10 and 11

$$\chi_M = Z_{eff}\, e^2/r \quad (12)$$

In atomic unit Equation 12 looks like

$$\chi_M = Z_{eff}/r = \chi_G \quad (13)$$

2. Method of computation

In a recent work [21b], we have evaluated the orbital exponent values of 118 elements of the periodic table following the rules for light and heaviest elements laid down by Reed [27] with some modifications as under-

We considered Reed's suggestion for s, p and d and extended Reed's rule for f. Electron in the 5f, 6p and higher we have used the contribution of 4f as 1. In the same shell f electrons shield each other by a factor 0.3228. Ghosh *et al.* [28] defined the absolute or most probable radius of atom as:

$$r=n^*/ \xi \text{ (in au)} \quad (14)$$

If we replace the Z_{eff} and r from Equation 13 using the Z_{eff} (Equation 2) and r (Equation 14), the atomic electronegativity definition of Gordy looks like-

$$\chi = \xi^2 \text{ (in au)} \quad (15)$$

At this outset, following Ghosh and Chakraborty's [12] suggestion, we proposed that the atomic electronegativity is not exactly equal but proportional to the orbital exponent of atoms. Thus,

$$\chi \propto \xi^2 \quad (16)$$

The utility of the Equation 16 is that only one atomic parameter, the orbital exponent (ξ) is sufficient to define and also to compute the electronegativity of the atoms. But as there is a proportionality relationship between the two atomic parameter-χ and ξ, to compute the electronegativity of the atoms some constants are required. The linear relation, $\chi=m\,\xi^2+c$ may be adopted for that purpose. Or we may use a very simple relation $\chi = m\, \xi^2$. In each case, to evaluate the proportionality constant (s), we have to compare the ξ^2 with some set of reference data.

In the present work, we consider the simple equation (17) to compute the electronegativity data of atoms.

$$\chi = m\, \xi^2 \text{ (in au)} \quad (17)$$

The constant, m is found to be dependent on the principal quantum number. This implies that it is constant throughout a period.

The values of m for each period were computed by comparing the ξ^2 values with the Ghosh Chakraborty (GC) atomic electronegativity values (in au) [12]. To evaluate the orbital exponent, we have used the values of n* which was evaluated by Slater [18] for n=1 to n=6 and for n=7 we have used the value of n*=4.3 computed by Ghosh and Biswas [25]. Using the newly computed orbital exponents and the m parameters, the atomic electronegativity of 118 elements of the periodic table was computed in this work (Table 1).

Although there is a view [29] that electronegativity is a quantum mechanical observable, we [6,12-14,30] strongly do believe that electronegativity is not a physical observable. Therefore, to perform the validity test of the newly computed electronegativity data, we have computed four very important and useful descriptors of chemical reactivity using the electronegativity values computed by us.

3. Computation of some useful descriptors of chemical reactivity

Pauling [2] evaluated the bond length from the atomic electronegativity, derived from the heats of formation or essentially bond energies. The atomic electronegativity differences between two atoms reflect the strength of the bond to give a quantitative correlation between atomic electronegativity and bond polarity. Using a simple bond charge model (SBC) [31], Ray *et al.* [10] derived the heteropolar bond length, R_{AB}, in terms of the atomic electronegativites, χ_A and χ_B , and covalent radii, $r_A = 1/2R_{AA}$ and $1/2R_{BB}$, of atoms A and B as follows-

$$R_{AB} = (r_A+r_B)-\{(r_Ar_B(\chi^{1/2}{}_A - \chi^{1/2}{}_B)^2\}/(\chi_A\, r_A + \chi_B\, r_B) \quad (18)$$

Table 1. Computed orbital exponent and electronegativity of the present work (χ_{Cal}) along with the electronegativity data computed by Ghosh and Chakraborty (χ_{GC}).

Atom	ξ	χ_{Cal} (eV)	χ_{GC}(eV)	Atom	ξ	χ_{Cal} (eV)	χ_{GC}(eV)	Atom	ξ	χ_{Cal} (eV)	χ_{GC}(eV)
H	1	6.271905	7.17841	Nb	0.81038	1.268716	3.5022	Tl	0.92557	0.710963	4.66107
He	1.6772	17.64287	12.0486	Mo	0.8318	1.336672	3.55471	Pb	1.08681	0.980247	4.73998
Li	0.6634	0.743654	3.22229	Tc	0.85323	1.406433	3.60968	Bi	1.24805	1.292684	4.82978
Be	1.002	1.696507	3.79419	Ru	0.87465	1.477936	3.66682	Po	1.40929	1.648273	4.92773
B	1.3406	3.036817	4.59509	Rh	0.89608	1.551245	3.72614	At	1.56945	2.0442	5.03385
C	1.6792	4.764584	5.62461	Pd	0.9175	1.626294	3.7879	Rn	1.73176	2.488879	5.15085
N	2.0178	6.879809	6.8834	Ag	0.93892	1.703115	3.85212	Fr	0.53656	0.238927	2.72644
O	2.3564	9.382491	8.37031	Cd	0.96035	1.781747	3.91878	Ra	0.69405	0.268698	2.8244
F	2.695	12.27263	10.0854	In	1.12965	2.465328	4.2336	Ac	0.71398	0.284351	2.85161
Ne	3.0336	15.55023	12.0317	Sn	1.29895	3.259656	4.5925	Th	0.73391	0.300447	2.87882
Na	0.76907	0.898038	2.5378	Sb	1.46825	4.164731	4.99521	Pa	1.02895	0.590569	3.13731
Mg	0.9948	1.502569	2.97449	Te	1.63755	5.180552	5.44173	U	1.18644	0.785189	3.3169
Al	1.22053	2.261828	3.5237	I	1.80685	6.30712	5.93178	Np	1.34393	1.007478	3.5237
Si	1.44627	3.175861	4.1852	Xe	1.97615	7.544435	6.46618	Pu	1.63898	1.498407	3.95089
P	1.672	4.244586	4.9591	Cs	0.54933	0.250435	4.43251	Am	1.79647	1.800207	4.26381
S	1.89773	5.468039	5.8458	Ba	0.67714	0.380527	4.46979	Cm	1.95395	2.129655	4.29374
Cl	2.12347	6.846285	6.84459	La	0.73098	0.443445	4.51686	Bk	1.97388	2.173321	4.85699
Ar	2.3492	8.379203	7.9552	Ce	1.03305	0.885668	4.57346	Cf	2.26893	2.871604	5.20799
K	0.62357	0.687721	2.78821	Pr	1.19429	1.183717	4.63958	Es	2.42642	3.284085	5.58621
Ca	0.80659	1.150661	3.0128	Nd	1.35552	1.524896	4.71522	Fm	2.58391	3.724236	5.98892
Sc	0.82976	1.217718	3.0728	Pm	1.51676	1.909247	4.80066	Mv	2.7414	4.192057	6.41884
Ti	0.85292	1.286644	3.1359	Sm	1.678	2.33675	4.89562	No	2.89888	4.687517	6.87325
V	0.87608	1.357467	3.2021	Eu	1.83924	2.807406	5.00011	Lr	2.91881	4.752193	6.98209
Cr	0.89924	1.430188	3.2713	Gd	2.00024	3.320417	5.11412	Rf	2.93874	4.817312	-
Mn	0.92241	1.504839	3.3437	Tb	2.16171	3.878138	5.23793	Db	2.95867	4.882873	-
Fe	0.94557	1.581355	3.41899	Dy	2.32295	4.478248	5.37153	Sg	2.9786	4.948878	-
Co	0.96873	1.659768	3.4976	Ho	2.48419	5.12151	5.51438	Bh	2.99853	5.015326	-
Ni	0.99189	1.740079	3.5791	Er	2.64543	5.807924	5.66703	Hs	3.01847	5.082251	-
Cu	1.01505	1.822287	3.66369	Tm	2.80667	6.537491	5.8292	Mt	3.0384	5.149586	-
Zn	1.03822	1.906429	3.7515	Yb	2.9679	7.31016	6.00089	Uun	3.05833	5.217363	-
Ga	1.22124	2.637813	4.16721	Lu	2.98831	7.411049	6.18238	Uuu	3.07826	5.285584	-
Ge	1.40427	3.487732	4.64061	Hf	3.00871	7.512579	6.37041	Uub	3.09819	5.354248	-
As	1.5873	4.456151	5.172	Ta	3.02912	7.61485	6.57394	Uut	3.10888	5.391261	-
Se	1.77032	5.543007	5.76101	W	3.04952	7.717761	6.784	Uuq	3.26637	5.951318	-
Br	1.95335	6.748419	6.4079	Re	3.06993	7.821415	7.00413	Uup	3.42386	6.539046	-
Kr	2.13638	8.07233	7.11269	Os	3.09033	7.925709	7.23351	Uuh	3.58135	7.154445	-
Rb	0.5768	0.642743	3.1886	Ir	3.11074	8.030744	7.43459	Uus	3.73884	7.797514	-
Sr	0.7461	1.075427	3.3588	Pt	3.13114	8.13642	7.72084	Uuo	3.89633	8.468254	-
Y	0.75178	1.091864	3.4043	Au	3.15155	8.242838	7.97906				
Zr	0.78895	1.202502	3.45211	Hg	3.17195	8.349896	8.24681				

To predict the polarity of a chemical bond, Pauling [2] proceeded to derive an algorithm for the dipole charge, and plotted these percentages against their atomic electronegativity differences to give an equation to calculate the ionic character of a bond (dipole charge) using-

$$q = 1 - \exp\{-(\chi_B - \chi_A)^2/4\} \quad (19)$$

where χ_B and χ_A are the atomic electronegativities of atoms B and A respectively.

A good number of empirical equations were suggested by various workers to evaluate the dipole charge invoking atomic electronegativities of the bonded atoms from various scales. We have invoked three other equations, stated below, for the study of the dipole charge of some heteronuclear diatomics.

Nethercot [32] proposed two formulae to calculate the dipole moment charges as:

$$q = 1 - \exp(-3(\chi_B - \chi_A)^2/2\chi_{AM}^2) \quad (20)$$

and,

$$q = 1 - \exp(-(\chi_B - \chi_A)^{3/2}/\chi_{GM}^{3/2}) \quad (21)$$

where χ_{AM} and χ_{GM} are the arithmetic mean (AM) and the geometric mean (GM) of the two atomic electronegativities.

Barbe [33] proposed another simple equation to calculate the dipole moment charges as follows-

$$q = (\chi_B - \chi_A)/\chi_B \quad (22)$$

Given, $\chi_B > \chi_A$.

Dipole moments μ_d are caused by two opposite charges of magnitude *q* in Coulombs separated by distance r in meters.

$$\mu_d = q \times r \quad (23)$$

The following form defines the molecular dipole moment

$$\mu_d = q \times R_{AB} \quad (24)$$

Here, R_{AB} is the internuclear distance. In Debye,

$$\mu_d = 4.8\, q \times R_{AB} \quad (25)$$

where R_{AB} must be expressed in Å unit.

Kim [11] extended the SBC model [31] to evaluate the atomic polar tensor. The atomic electronegativity and electronegativity equalization can be used to determine the atomic polar tensor for a diatomic molecule.

Kim [11] proposed the algorithm for evaluating the dipole charge as follows:

$$q = \{r_1 r_2/CR_{AB}\}(\chi_B - \chi_A) \quad (26)$$

The centroid of positive charge, r, relative to the point defining the centroid of negative charge was given by Kim [11] as

$$r = \{r_2Z_B - r_1Z_A - (r_1 + r_2)\, q\}/(Z_A + Z_B) \quad (27)$$

Kim 14 defined the dipole moment, μ, as

$$\mu = (Z_A + Z_B)r = -(r_1 + r_2)\, q + (r_1Z_B - r_2Z_A) = -R_{AB}\, q + (r_2Z_B - r_1Z_A)$$
$$= -1/C\, [(r_Ar_B\, \chi_A\, \chi_B) / (r_A\, \chi_A + r_B\, \chi_B)^2][R^2_{AB}\, (\chi_B - \chi_A)] \quad (28)$$

For an AB type diatomic molecule, where the A atom is located at the origin and the B atom is in a positive Cartesian direction and $\chi_B < \chi_A$ the atomic polar tensors (P_x's) for atoms A and B was given by Kim [11] as

$$P_x^B = -P_x^A = (\partial\mu/\partial R)_e \quad (29)$$

where $(\partial\mu/\partial R)_e$ is the dipole moment derivative at geometric equilibrium.

Differentiation of the Equation 28 with respect to R gives the atomic polar tensor of B atom-

$$P_x^B = (\partial\mu/\partial R)_e = -(\chi_B - \chi_A).\, 2R_{AB}r_Ar_B\chi_A\, \chi_B\, /6.9696\, (r_A\chi_A + r_B\, \chi_A)^2 \quad (30)$$

The computed orbital exponent, the atomic electronegativity values and the atomic electronegativity values of Ghosh and Chakrabarty [12] are presented in Table 1. A comparative study of the computed atomic electronegativity data of the present work with Ghosh and Chakrabarty [10] computed atomic electronegativity data and is performed in Figure 1. The computed m parameters for each period are presented in the Table 2.

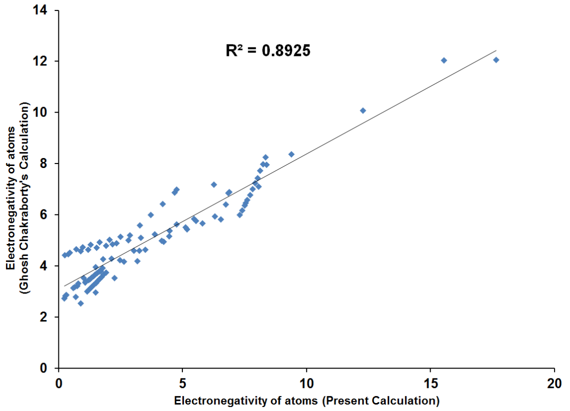

Figure 1. Comparative study of the electronegativity of the present work vis-à-vis the Ghosh and Chakraborty's electronegativity data.

Table 2. Computed m parameters for each period along with effective principal quantum numbers

Period	Effective principal quantum number (n*)	m values
1st	1	0.2305
2nd	2	0.06213
3rd	3	0.05579
4th	3.7	0.065
5th	4	0.071
6th	4.2	0.0305
7th	4.3	0.0205

In Figure 2, the variation of the computed electronegativity data along the groups 13-17 is tested. Figure 3 shows the verification of silicon rule. In Figure 4, the atomic electronegativities of the members of the chalcogen family are presented. In Figure 5, the atomic electronegativity values of the inert gas elements are presented.

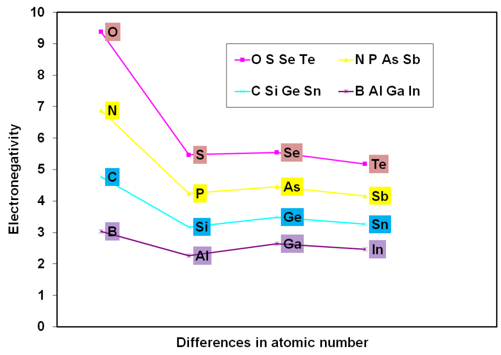

Figure 2. Variation of electronegativity along the groups 13-17.

A comparative study of the computed atomic electronegativity of the H atom and the Halogen family with the electronegativity data of those atom computed by Ghosh and Chakraborty [12], Pearson [35], and Robles and Bartolotti [36] are presented in Figure 6.

The internuclear bond distances of some heteronuclear diatomic molecules computed through the Ray et al formula [10] and using the newly computed atomic electronegativity values along with their spectroscopic counter parts [34] are compared in Figure 7.

The dipole charges of a series of diatomic heteronuclear molecules, computed through the Nethercot arithmetic average formula [29], the Nethercot geometric average formula [29], the Pauling formula [2] and the Barbe formula [30] and using the new atomic electronegativities, and are compared in Figure 8.

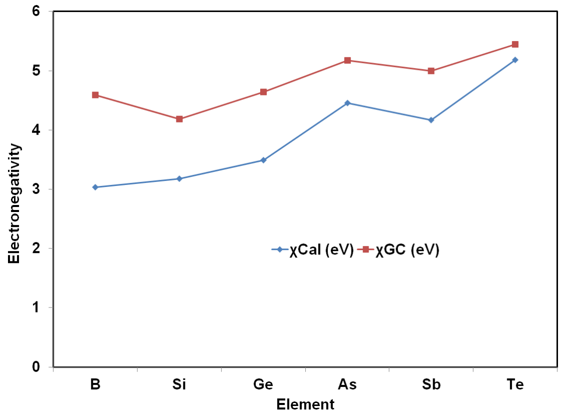

Figure 3. Verification of silicon rule.

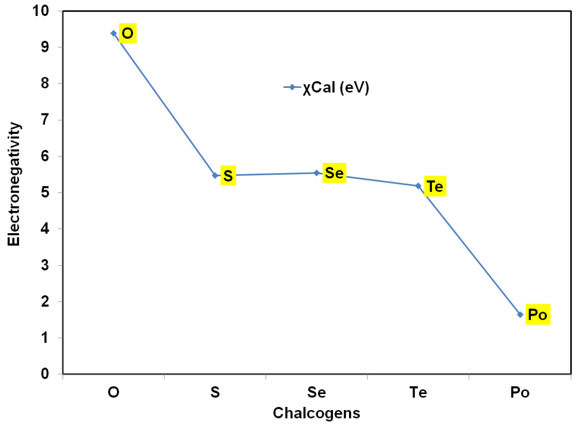

Figure 4. Electronegativity of Chalcogens.

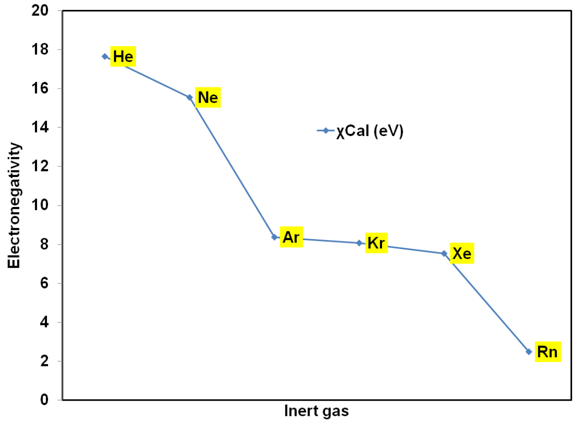

Figure 5. Electronegativity of the inert gas elements.

The dipole moments of some heteronuclear diatomic molecules were computed using the newly computed dipole charges and internuclear distances of the diatomic molecules. The computed dipole moments (in Debye) and experimental results are compared in Figure 9.

We have computed atomic polar tensor (APT) of halogen atoms in hydrogen halide molecules invoking Kim's formula [11] and using the atomic electronegativity values computed by us. We have also computed atomic polar tensor of the halogen atoms in hydrogen halides using Ghosh and Chakraborty [12] atomic electronegativity value. To perform the validity test, two sets of APT values along with their experimental counterparts [11] are compared in Figure 10.

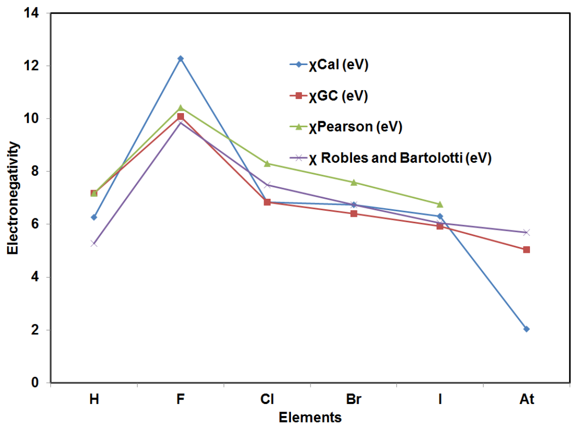

Figure 6. Comparative study of the electronegativity data of H atom along with Halogen family of the present calculation vis-à-vis the data computed by Ghosh and Chakraborty, Pearson, and Robles and Bartolotti.

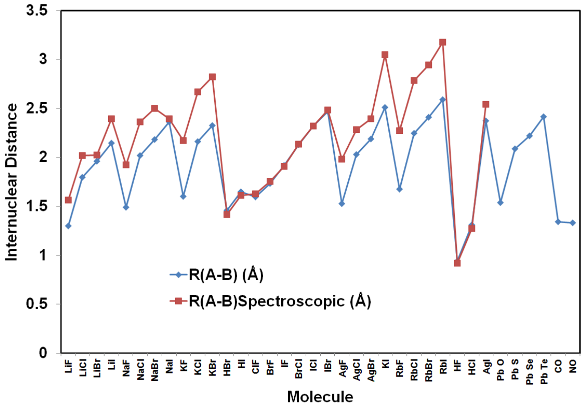

Figure 7. The evaluated inter nuclear distance vis-à-vis the spectroscopic inter nuclear distance of a series of molecules.

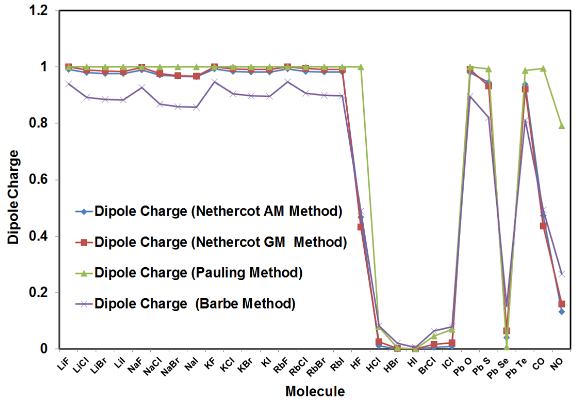

Figure 8. Evaluated Dipole charges using Nethercot arithmetic average (AM) formula, Nethercot geometric average (GM) formula, Pauling formula and Barbe formula of a series of molecules.

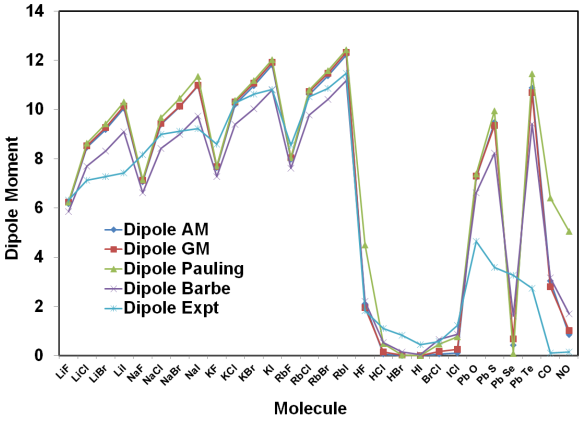

Figure 9. Comparative study of the evaluated Dipole Moment in Debye using the dipole charge of Nethercot arithmetic average (AM) formula, Nethercot geometric average (GM) formula, Pauling formula and Barbe formula and R(A-B) of present calculation vis a vis experimental dipole moment of a series of molecules.

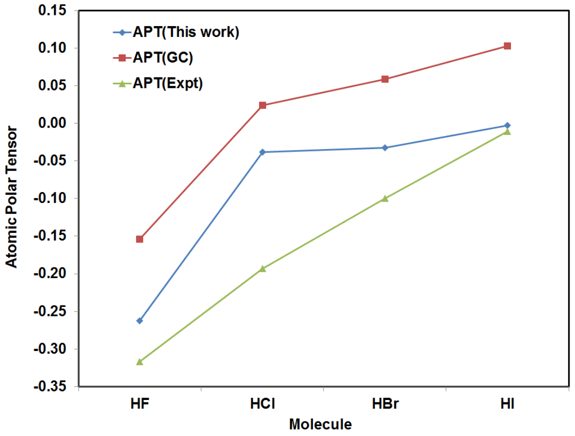

Figure 10. Comparative study of the computed atomic polar tensor (APT) of X atom in hydrogen halides.

4. Results and discussion

It is distinct from Table 1 that the new set of atomic electronegativity data exhibits perfect periodicity of periods and groups. The validity of any theoretical model is its ability to explain and correlate experimental observations. We have listed below the explanations of some interesting experimental observations using the computed electronegativity data.

1. The electronegativity data of N and Cl follow the order- $\chi_N > \chi_{Cl}$. Thus the half shell stability of nitrogen atom is nicely reflected by the electronegativity data of the present calculation.

2. From Table 1, it is obvious that the atomic electronegativities of the transition metal atoms are small and increase slowly with increasing atomic number. Thus the electronegativity data of the said elements of the present calculation exhibit the expected trend.

3. Both set of electronegativity data- the present scale and the GC electronegativity scale, show perfect periodicity of periods and groups and are nicely correlated with each other. The R^2 value of this correlation (Figure 1) is 0.892.

4. The difference of atomic electronegativity between F and Xe and that between O and Xe and also between F and Kr suggest that Xe can form compounds with F and O, and Kr can form compounds with F, but possibility of bonding between Xe and Cl is very difficult.

5. Gyftopoulos and Hatsopoulos [38] identified atomic electronegativity as minus of the thermodynamic chemical potential which implies that atomic electronegativity is the holding power of electron by an atom. The intrinsic inertness and high atomic electronegativity of Hg and Au is well known [39]. A look on the Table 1 reveals that the atomic electronegativity of Hg and Au are very high. These high values of atomic electronegativity indicate that the nuclei of Hg and Au hold their electron cloud very tightly. Hence the intrinsic inertness and high atomic electronegativity of Hg and Au are nicely correlated by the computed electronegativity data for them.

6. It is well known [39] that the actinides are electropositive and reactive. From Table 1, we can see that the atomic electronegativity values of the actinides are accordingly very small.

7. It is well established that the transition within a periodic group from an 8-shell to an 18-shell type of atom gives an increase in atomic electronegativity [40] because the 18 shell atoms are more compact and have a greater tendency to attract electrons expand their electronic spheres toward greater stability. From Figure 2, we see that the present computed electronegativity values of those elements satisfy these observations nicely.

8. A look on the Figure 3 reveals that the computed electronegativity values satisfy the silicon rule.

9. Figure 4 demonstrates that the electronegativity of Chalcogens follows the expected trend.

10. Figure 5 demonstrates that the electronegativities of the inert gas elements are very high.

11. From Figure 6 we can conclude that the atomic electronegativity values of H and halogens of the present work, Pearson's work [32] and Robles and Bartolotti's work [33] follow the expected trend of atomic electronegativity data but the GC atomic electronegativity for H and halogens (except F) show erroneous trend.

12. A look at the Figure 7 reveals that the internuclear distances of the series of heteronuclear diatomic molecules computed through the present atomic electronegativity values are very close to their spectroscopic counterparts.

13. Looking at the Figure 8 we can see that the atomic charge densities of the compounds that are predominantly ionic are nearly equal to unity and that are predominantly covalent are also very small. Thus the dipole charges computed using all of the above mentioned algorithms and the atomic electronegativity values of the present work are consistent with the nature of the bonding and also the chemico-physical features of the compound brought under study.

14. It is distinct from the Figure 9, that the theoretical dipole moments of the ionic compounds show a nice correlation with the experimental dipole moments. But in case of covalent compounds, the computed dipoles, though scattered, fairly correlate with the experimental dipoles. Ghosh and Bhattacharyya [41] opined that because of the lone pair component of the dipoles of such molecules must vectorially couple with the bond moment component. It, therefore, transpires that there can be no good correlation between the experimental dipoles having two contributing components and the bond dipoles of molecules.

From Figure 10, it is transparent that the atomic polar tensors, APTs computed using the atomic electronegativity value of the present work correlate well with the observed value but, except fluorine, the APT's using GC electronegativity show reverse trend with the observed results. The comparison with the observed value also reveals that both the APT of present work and observed show similar trend of variation of the atomic polar tensor.

5. Conclusion

We have derived the electronegativity ansatz of Gordy relying upon the electrostatic definitions of ionization energy and electron affinity and using the electronegativity ansatz of Mulliken. The newly designed scale of atomic electronegativity is found to satisfy entire sine qua non of a reasonable scale of atomic electronegativity. The unique order of atomic electronegativity of H atom and halogen family is nicely correlated in this work.

We have computed four very important and useful descriptors of chemical reactivity using the atomic electronegativity values computed by us and found that in major cases the computed atomic electronegativity data produced results which close to the experimental results.

The periodic behavior of the computed electronegativity data and also the correlation of important physico-chemical properties of elements using the computed electronegativity data suggest that present method of evaluation of the atomic electronegativity of the atoms is quite successful venture.

Acknowledgements

We wish to express our sincere thanks to Professor Dulal Chandra Ghosh, University of Kalyani, India for valuable teaching on this subject.

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