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REGULAR ARTICLE

The electronegativity scale of Allred and Rochow: revisited

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Abstract A new scale of electronegativity (χ), based on the view that χ is an atomic property and electronegativity is the force exerted by the screened nucleus on an electron at the periphery of an atom, has been designed and framed. The necessary ansatz used was suggested by Allred and Rochow, $\chi = \text{Force} = e^2\,(Z_{\text{eff}})/r^2$ where e is the electronic charge (esu), Z_{eff} is the effective nuclear charge and r is the absolute (most probable) radius. The electronegativity is calculated in appropriate force unit. We have posited that the absolute (most probable) and not the covalent radii should be the appropriate size descriptor in evaluating electronegativity of atoms. It has been also demonstrated that all previous calculations of electronegativities using Allred and Rochow ansatz suffer from dimension mismatch. We have computed the electronegativities of 103 elements of the periodic table in force (dynes/electron) unit by invoking the electronegativity ansatz of Allred and Rochow, using the absolute radii and effective nuclear charge of Ghosh et al. The new scale of electronegativity satisfies all the sine qua non of a scale of electronegativity.

Keywords Scale of electronegativity · Most probable radii · Electronegativity ansatz of Allred and Rochow · Force field · Effective nuclear charge

1 Introduction

Electronegativity has been one of the most useful theoretical constructs in chemistry from the early days of the history of chemistry. In modern times, the electronegativity concept is widely used by chemists, physicists, biologists and geologists [1, 2]. The electron distribution is fundamental in determining the physico-chemical properties of molecules, and the concept of electronegativity is an important tool in sketching the static distribution and dynamic rearrangement of electronic charge in molecules [3, 4]. The bond energies, bond polarities and the dipole moments, force constants and the inductive effects are some very fundamental descriptors of organic, inorganic and physical chemistry. Such descriptors can only be conceived, rationalized and modeled for evaluation in terms of the concept of electronegativity. The concept of electronegativity finds application in the qualitative understanding and elucidation of quark chemistry [5]. In spite of the fact that the electronegativity has manifold applications and is now an animated field of research addressing its fundamental nature and unit of measurement, the proper definition and evaluation are still at large. Since electronegativity is not physically observable, according to the rules of quantum mechanics, there cannot be any quantum mechanical operator for electronegativity. Thus, electronegativity is not a quantity which can be evaluated quantum theoretically. However, when the fundamental position is straightforward, a group of scientists [6–8] hold that the electronegativity is a quantum mechanical entity. We are led by the postulate that electronegativity is not a quantum theoretical entity. It, therefore, transpires that the electronegativity shall be eluding proper definition and measurement. Thus, according to Kant [9], the exact status of electronegativity is an object knowable by the mind or intellect and not by the senses. Any effort of measurement requires the reification [10] of electronegativity concept so that there can be some mathematical representation leading to its evaluation. However, since there is no uniqueness in the mathematical formulation of a reified noumenon, there is

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enough scope of suggesting multiple scales of measurement of electronegativity.

Tracing the history of measurement of electronegativity we find that it was Pauling [11, 12] who put forward the scientific definition and a scale of measurement of electronegativity for the first time. Pauling's original definition of electronegativity—"the power of an atom in a molecule to attract electrons to it" still remains deeply implanted in the minds of chemists and serves as a guide for designing scale of electronegativity. A good number of workers over a period of 60–70 years have tried to measure that 'electron attracting power', the electronegativity, and have suggested a number of scales to measure it. In the recent review [2] of current scales and concepts of electronegativity, we have pointed out that the efforts to give quantum mechanical status to electronegativity seems not to be convincing, and the idea that electronegativity is not an in situ rather an intrinsic free atom ground state property seems more acceptable. Allen [7] tried to posit that electronegativity is the third dimension of periodic table.

2 Measurement of electronegativity

The oldest scales of measuring electronegativity were due to Pauling [11, 12], Mulliken [13], Gordy [14], and Allred and Rochow's [15]. The scale suggested by Allred and Rochow's [15] has been very popular and profusely cited.

2.1 Scale of Allred and Rochow for measuring electronegativity

In 1958, Allred and Rochow [15] identified the electronegativity of an atom with the electrostatic field and the suggested ansatz for its evaluation. According to them, one measures the electronegativity by measuring this electrostatic force of attraction between the screened nucleus and an electron from the bonded atom

$$\chi = \text{Force} = e^2(Z_{\text{eff}})/r^2 \tag{1}$$

where, χ is the electronegativity, r is the distance between an electron and the nucleus, e is the charge on the electron and $e(Z_{\text{eff}})$ is the charge which is effective at the electron due to the nucleus and its surrounding electrons. In this work [15], the electron was considered to be at the covalent boundary, r, of the atom. It appears that the proposed ansatz was to measure the electronegativity identified as the force of attraction between a nucleus and an electron from a bonded atom. They proposed a more general linear equation to calculate the electronegativity of the atoms invoking the method of least square fitting and using Pauling's electronegativity values as reference. The second ansatz was

$$\chi = 0.359\left(Z_{\text{eff}}/r^2\right) + 0.744 \tag{2}$$

where χ is the electronegativity, Z_{eff} is the effective nuclear charge of the atom and r is the single bond covalent radius. Now an analysis of the ansatz of Pauling's scale reveals that the electronegativity is measured as the square root of energy [2, 7, 16]. Since the numerical parameters of Eq. 2 are least square fitted using Pauling's scale as reference, the dimension of χ is not straightforward when it is evaluated through the ansatz (2). It seems that the ansatz (2) is not computing any force in the real world.

In this report we want to make a critical analysis of the ansatz suggested by Allred and Rochow for measurement of electronegativity. We propose to explore the theoretical justification of the ansatz and also the efficaciousness of the scale in measuring electronegativity. We also propose to explore whether the covalent radii (corresponding to in situ property) or the absolute radii or most probable radii (corresponding to free atom property) is the appropriate size descriptor in computing the electronegativity. A deeper scrutiny of the ansatz used and the results of calculation reveal that the effective nuclear charge was used in atomic units, and the covalent radii were used in angstrom unit. Although the ansatz appears to compute electrostatic force, such a quantity measured by charge in atomic units and distance in angstrom unit really does not represent force in the real world. Little and Jones [17], Mande et al. [18, 19] calculated the electronegativity of the majority of atoms of the periodic table using the ansatz of Allred and Rochow, but none of these workers was concerned about the dimension of the measured quantity vis-à-vis the definition of electrostatic force. Thus, it is transparent that, although Allred and Rochow identified electronegativity with the electrostatic force most justifiably, no attempt has ever been made to measure the electronegativity by invoking the ansatz of Allred and Rochow in appropriate force unit.

2.2 Whether the covalent radius or the absolute radius is a true descriptor of atomic electronegativity

It is widely accepted that electronegativity is an intrinsic free atom ground state property and not an in situ property [5–7, 16]. Ayers [20] seems to have pointed out that, although the electronegativity has not yet been uniquely defined for separated species, it is apparent that electronegativity preserves locality. Atoms approach each other during chemical reaction and form chemical bond by rearrangement of charge. One very important point rationally provided by the concept of electronegativity is the explanation of chemical reaction through charge transfer. The driving force behind the chemical reactivity comes from the tendency of electronegativity equalization of interacting chemical species. In such reactions, one is the donor or base and other is the acceptor or acid. Actually a donor is less electronegative and an acceptor is more electronegative. During chemical reaction the electronegativity (chemical potential) of the two systems becomes equalized. This principle, originally developed by Sanderson [21–23] is now put on sound theoretical background [24–27]. The implication of the electronegativity equalization is that two atoms of different electronegativities (chemical potentials) will form bond by charge transfer. The charge is being transferred from atom of lower electronegativity (higher chemical potential) to the atom of higher electronegativity (lower chemical potential) and the process of charge transfer continues till the electronegativity of both atoms is equal to some intermediate value, and the molecule is represented by a common chemical potential or electronegativity. Assuming the electronegativity equalization principle valid, the atom before molecule formation must have some electronegativity and that value changes (increases or decreases) on molecule formation. Thus, if electronegativity is defined bonded atom is part of the molecule, i.e. covalently bonded; the bonded atoms should have same common electronegativities. Parr et al. [9] observed that “the atom in a molecule” cannot be directly observed by experiment to measure enough property of an atom in a molecule to define it unambiguously. Thus, if the covalent radius is used as size descriptor in computing electronegativity, one computes some in situ property and not the free atom property. Thus, the in situ proposition is self defeating, and the electronegativity of atoms cannot be an in situ property. Moreover, we may point out some obvious disadvantages of in situ property. The in situ electronegativity cannot be transferable. There are some obvious uncertainties about the magnitude of covalent radii. The covalent radii [28] of only 25 elements were known for the long time, and the scientists use such radii profusely in the evaluation of electronegativity and other radial-dependent properties. Pyykkö [29, 30] have recently published the covalent radii of single and multiply bonded atoms. It is well known that covalent radius depends upon the bond strength and degree of covalency. But most important point to note is that covalent radii of atoms are not transferable from one element to other element. Hence such radii cannot be the descriptor of any absolute free atom property. Therefore, we believe that absolute radii should be used to calculate the radial-dependent property like electronegativity.

3 The method of computation

In this venture, we have tried to hold the proper dimension of evaluated electronegativity in force unit. We have also posited that it is not the covalent radius but the absolute (the most probable) radius of the atom is the true size descriptor in evaluating electronegativity. In addition to the resolution of the fundamental problems relating to the proper dimension of the measured quantity and the proper size descriptors of atoms, we have used more reliable set of effective nuclear charge. The ansatz we have used is the Eq. 1, i.e.

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

We have put charge in esu unit and distance in cm unit to compute electronegativity in force (dyne) unit. We have replaced the covalent radius by the most probable radius.

Several workers [31–33] have calculated the screening constants and effective nuclear charge theoretically. In a recent report [34, 35],we have pointed out an interesting fact that effective nuclear charge calculated semi-empirically by Ghosh et al. [33] based on Slater’s [36] suggestion is very much close to the SCF values calculated by Clementi et al. [31, 32]. In view of this finding, we have used the effective nuclear charge from the work of Ghosh et al. [33] in the present calculation. The next input physical quantity is the size of atoms. We have also used atomic radii of Ghosh et al. [34]. It is demonstrated that the relativistic effect is found to be incorporated in the sizes of atoms in such calculation [34] in a distinct way. We have computed the electronegativities of 103 elements of the periodic table using ansatz (1).

The calculated electronegativities in mdynes per electron are presented in Table 1.

4 Results and discussion

The electronegativities of 103 elements are computed in force unit (dynes/electron) through the Eq. 1, and are presented in Table 1. The effective nuclear charge and absolute radii in angstrom unit of 103 elements are also presented in Table 1 along with the electronegativities. In order to test whether electronegativities exhibit periodicity, the evaluated electronegativities are placed in the periodic table of elements (Table 2). The electronegativities of eight metalloid elements are separately presented in Table 3. It is evident from Table 2 that the computed electronegativities reproduce the periodicity of the periods and groups of the periodic table perfectly. Each period begins with a representative element increases monotonically horizontally to be maximum at the noble gas atoms that occur at the top of the curve. The only exception is the electronegativity of Ne. The vertical trend of variation in the inert gas group is deviated from general trend in case of only one element Ne. We note further that:

1. The electronegativity of N is greater than that of Cl.
2. From Table 3, it is distinct that the electronegativity of a group of eight metalloid elements is very close to

Table 1 Computed electronegativities (X mdynes) along with effective nuclear charges and absolute radii (Å) of 103 elements of periodic table

Atomic number	Element	Z_{eff}	Absolute radii	X	Atomic number	Element	Z_{eff}	Absolute radii	X
1	H	1	0.5292	8.22	53	I	7.6	1.1141	14.1
2	He	1.7	0.3113	40.4	54	Xe	8.25	1.0263	18.0
3	Li	1.3	1.6283	1.13	55	Cs	2.2	4.2433	0.281
4	Be	1.95	1.0855	3.81	56	Ba	2.85	3.2753	0.612
5	B	2.6	0.8141	9.04	57	La	3.5	2.6673	1.13
6	C	3.25	0.6513	17.6	58	Ce	4.15	2.2494	1.89
7	N	3.9	0.5428	30.5	59	Pr	4.8	1.9447	2.92
8	O	4.55	0.4652	48.4	60	Nd	5.45	1.7129	4.28
9	F	5.2	0.4071	72.3	61	Pm	6.1	1.5303	6.00
10	Ne	5.7485	0.3676	98.0	62	Sm	6.75	1.383	8.13
11	Na	2.2	2.165	1.08	63	Eu	7.4	1.2615	10.71
12	Mg	2.85	1.6711	2.35	64	Gd	8.05	1.1596	13.8
13	Al	3.5	1.3608	4.35	65	Tb	8.7	1.073	17.4
14	Si	4.15	1.1477	7.26	66	Dy	9.35	0.9984	21.6
15	P	4.8	0.9922	11.2	67	Ho	10	0.9335	26.4
16	S	5.45	0.8739	16.4	68	Er	10.65	0.8765	31.9
17	Cl	6.1	0.7808	23.0	69	Tm	11.3	0.8261	38.1
18	Ar	6.75	0.7056	31.2	70	Yb	11.95	0.7812	45.1
19	K	2.2	3.293	0.467	71	Lu	12.6	0.7409	52.9
20	Ca	2.85	2.5419	1.01	72	Hf	13.25	0.7056	61.3
21	Sc	3	2.4149	1.18	73	Ta	13.9	0.6716	71.0
22	Ti	3.15	2.2998	1.37	74	W	14.55	0.6416	81.4
23	V	3.3	2.1953	1.58	75	Re	15.2	0.6141	92.9
24	Cr	3.45	2.1	1.80	76	Os	15.85	0.589	105.3
25	Mn	3.6	2.0124	2.05	77	Ir	16.5	0.5657	118.8
26	Fe	3.75	1.9319	2.31	78	Pt	17.15	0.5443	133.4
27	Co	3.9	1.8575	2.60	79	Au	17.8	0.5244	149.1
28	Ni	4.05	1.7888	2.92	80	Hg	18.45	0.506	166.0
29	Cu	4.2	1.725	3.25	81	Tl	5	1.867	3.30
30	Zn	4.35	1.6654	3.61	82	Pb	5.65	1.6523	4.77
31	Ga	5	1.4489	5.49	83	Bi	6.3	1.4818	6.61
32	Ge	5.65	1.2823	7.92	84	Po	6.95	1.3431	8.88
33	As	6.3	1.145	11.1	85	At	7.6	1.2283	11.6
34	Se	6.95	1.0424	14.7	86	Rn	8.25	1.1315	14.8
35	Br	7.6	0.9532	19.3	87	Fr	2.2	4.4479	0.256
36	Kr	8.25	0.8782	24.6	88	Ra	2.85	3.4332	0.557
37	Rb	2.2	3.8487	0.342	89	Ac	3	3.2615	0.650
38	Sr	2.85	2.9709	0.744	90	Th	3.15	3.1061	0.752
39	Y	3	2.8224	0.868	91	Pa	4.3	2.2756	1.91
40	Zr	3.15	2.688	1.00	92	U	4.95	1.9767	2.92
41	Nb	3.3	2.5658	1.15	93	Np	5.6	1.7473	4.23
42	Mo	3.45	2.4543	1.32	94	Pu	6.75	1.4496	7.40
43	Tc	3.6	2.352	1.50	95	Am	7.4	1.2915	10.2
44	Ru	3.75	2.2579	1.69	96	Cm	7.55	1.296	10.3
45	Rh	3.9	2.1711	1.91	97	Bk	8.7	1.1247	15.8
46	Pd	4.05	2.0907	2.13	98	Cf	9.35	1.0465	19.7
47	Ag	4.2	2.016	2.38	99	Es	10	0.9785	24.1
48	Cd	4.35	1.9465	2.64	100	Fm	10.65	0.9188	29.1

Table 1 continued

Atomic number	Element	Z_{eff}	Absolute radii	X	Atomic number	Element	Z_{eff}	Absolute radii	X
49	In	5	1.6934	4.02	101	Md	11.3	0.8659	34.7
50	Sn	5.65	1.4986	5.80	102	No	11.95	0.8188	41.1
51	Sb	6.3	1.344	8.04	103	Lr	12.1	0.8086	42.6
52	Te	6.95	1.2183	10.8					

Table 2 Periodic chart of the computed electronegativity values of 103 elements

1 H 8.22	2	Legend Atomic Number Symbol of Element Electronegativity (mdyne)										13	14	15	16	17	2 He 40.4
3 Li 1.13	4 Be 3.81											5 B 9.04	6 C 17.6	7 N 30.5	8 O 48.4	9 F 72.3	10 Ne 98.0
11 Na 1.08	12 Mg 2.35	3	4	5	6	7	8	9	10	11	12	13 Al 4.35	14 Si 7.26	15 P 11.2	16 S 16.4	17 Cl 23.0	18 Ar 31.2
19 K 0.467	20 Ca 1.02	21 Sc 1.18	22 Ti 1.37	23 V 1.58	24 Cr 1.80	25 Mn 2.05	26 Fe 2.31	27 Co 2.60	28 Ni 2.92	29 Cu 3.25	30 Zn 3.61	31 Ga 5.49	32 Ge 7.92	33 As 11.1	34 Se 14.7	35 Br 19.3	36 Kr 24.6
37 Rb 0.342	38 Sr 0.744	39 Y 0.868	40 Zr 1.00	41 Nb 1.15	42 Mo 1.32	43 Tc 1.50	44 Ru 1.69	45 Rh 1.90	46 Pd 2.13	47 Ag 2.38	48 Cd 2.64	49 In 4.02	50 Sn 5.80	51 Sb 8.04	52 Te 10.8	53 I 14.1	54 Xe 18.0
55 Cs 0.281	56 Ba 0.612	57-71	72 Hf 61.3	73 Ta 71.0	74 W 81.4	75 Re 92.9	76 Os 105.3	77 Ir 118.8	78 Pt 133.4	79 Au 149.1	80 Hg 166.0	81 Tl 3.30	82 Pb 4.77	83 Bi 6.61	84 Po 8.88	85 At 11.6	86 Rn 14.8
87 Fr 0.256	88 Ra 0.557	89-103															

57 La 1.13	58 Ce 1.89	59 Pr 2.92	60 Nd 4.28	61 Pm 6.00	62 Sm 8.13	63 Eu 10.7	64 Gd 13.8	65 Tb 17.4	66 Dy 21.6	67 Ho 26.4	68 Er 31.9	69 Tm 38.1	70 Yb 45.1	71 Lu 52.9
89 Ac 0.650	90 Th 0.752	91 Pa 1.91	92 U 2.92	93 Np 4.23	94 Pu 7.40	95 Am 10.2	96 Cm 10.3	97 Bk 15.8	98 Cf 19.7	99 Es 24.1	100 Fm 29.1	101 Md 34.7	102 No 41.1	103 Lr 42.6

Table 3 Verification of silicon rule

Element	Electronegativity (mdyne)
B	9.04
Si	7.26
Ge	7.92
As	11.1
Sb	8.04
Te	10.8
Bi	6.61
Po	8.88

each other. Thus, it is demonstrated that the present scale satisfies the silicon rule reasonably well.

3. The electronegativities of the transition elements are small and close to each other. It is well known that the sizes of the atoms of *d* block and *f* block elements undergo a steady but slow contraction, and the effect is well reproduced in the radii of such elements. It is also well known that the transition elements are soft and easily deformable. This property requires that the electronegativity of the transition elements should be small. From Table 2 it is clear that the electronegativities of the transition metal atoms are small, and increase slowly with increasing atomic number. We

have also observed that the electronegativities of lanthanide elements of present calculation exhibit the expected trend of variation.

4. The identity of the thermodynamic chemical potential with electronegativity [37] implies that the chemical potential is the escaping tendency of electron from an atom, and hence the electronegativity is the holding power of electrons by an atom. The intrinsic inertness of Hg and Au is due to the manifest relativistic effect in such atoms [38, 39]. From Table 1 we see that electronegativity of Hg and Au are 166.0 and 149.1 mdynes, respectively. These high values of electronegativity indicate that such atoms would be holding electrons very tightly, and would be chemically less responsive under small perturbation. This implies that the relativistic effect is incorporated in the computed electronegativities.
5. The difference of electronegativity between Xe and F (54.2 mdynes) and that between O and Xe (30.4 mdynes) and that between Kr and F (47.6 mdynes) suggest that Xe can form compounds with F and O, and Kr can form compounds with F. But the similar possibility of bonding between Cl and Xe is ruled out because the difference between the electronegativities of these two elements is only 5.00 mdynes. It is a fact of chemistry that Cl and Xe never enter into bonding.

Thus, it is transparent that the new scale of electronegativity drawn by identifying electronegativity as electrostatic force of attraction between the nucleus and the valence electron satisfy the essential criteria of a scale of electronegativity. The scale can reasonably correlate the chemical reactivity of elements individually and in a series.

5 Conclusion

We have critically revisited the electronegativity scale of Allred and Rochow, which identifies the electrostatic force field of attraction between the nucleus and valence electron with electronegativity. We have found that, although the model and its physical basis were perfectly alright, the computed electronegativity in terms of the electronegativity ansatz of Allred and Rochow has suffered from dimensionality mismatch. The evaluated electronegativities did not represent any force in the real field. We have taken special care so that no dimensional mismatch occurs between the conceptual structure and the computational procedure. The ansatz we have used is the equation $\chi = \text{Force} = e^2\,(Z_{\text{eff}})/r^2$,where χ is the electronegativity, e is the electronic charge (esu), r is the most probable radius in cm and Z_{eff} is the effective nuclear charge. Thus, electronegativity is computed in proper unit of force. We have also posited that the size input in computing electronegativity cannot be the covalent radius and the proper size descriptor should be the absolute or most probable radius of the atom. Thus, the new scale of electronegativity is based on the view that χ is an atomic property and it relates electronegativity to the force exerted by the screened nucleus on an electron at the periphery of an atom. We have computed the electronegativities of 103 elements of periodic table in force (dynes/electron) unit by invoking the electronegativity ansatz of Allred and Rochow and using the absolute radii [34] and effective nuclear charge of Ghosh et al. [33]. The new scale of electronegativity justifies and correlates the physico-chemical properties of the elements like other existing scales. The cluster of facts like express periodic behavior, correlation of inertness of Hg atom, small variation of electronegativities in the series of d block elements, observance of silicon rule, etc. suggest that a new scale of electronegativity is manifest.

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