



Bond dissociation energies from a new electronegativity scale

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ABSTRACT

The bond dissociation energies of some diatomic molecules (in both covalent and ionic forms) are estimated from different formulas and using a new scale of electronegativity. The calculated bond dissociation energies are compared with those which are obtained from the other commonly used electronegativity scales such as Pauling and Allred–Rochow. The best linear correlation is observed between the obtained bond dissociation energies from new electronegativity scale and experimental data. Comparison between the corrected results, which are calculated from the linear relationship equations for different scales, shows that in both covalent and ionic bonds the new scale of electronegativity represents a better correlation with the experimental data than the others. This indicates the reliability of the obtained results from the new scale.

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1. Introduction

Recently it is shown that the obtained atomic electrophilicities from a Morse-like function for electronic energies, $E(N)$, are strongly linked with Pauling [1] and Allred–Rochow [2] electronegativity scales [3]. Therefore these electrophilicities are introduced as a new scale for atomic electronegativity. This scale obeys all of the fundamental rules [4] which are required for an acceptable scale of electronegativity and successfully determines the bond character of diatomic molecules [3]. The reliability of a given electronegativity scale is supported by its ability in predicting different molecular properties such as bond dissociation energy, heat of formation, bond character etc. Among these parameters, Bond Dissociation Energy (BDE) has unique and valuable applications to the interpretation of a vast area of chemistry and is an important concept in understanding the nature of chemical bonds. In fact knowledge of BDEs of chemical bonds in molecules is essential for understanding chemical process [5]. Dissociation energy of a given A–B bond is defined as the energy needed to separate the radicals A and B to infinity; each species being in its ground state. A consensus has developed that energy per electron is the appropriate dimension for electronegativity [6]. Therefore it is suggested that electronegativity should enter the heteronuclear single BDE (D_{A-B}) expression as $|\Delta\chi|$ [4]; where $\Delta\chi$ is defined as the difference between the electronegativities of constituent atoms ($\chi_A - \chi_B$). According to the Pauling's bond energy equation [7], D_{A-B} can be simply related to the corresponding homonuclear terms D_{A-A} and D_{B-B} as

$$D_{A-B} = \frac{1}{2}(D_{A-A} + D_{B-B}) + 23\Delta\chi^2 \quad (1)$$

Twenty-three is a conversion factor when all the energies are expressed in kcal mol^{−1}. The more familiar form of Pauling equation is [7]

$$D_{A-B} = \overline{D_{A-B}} + 30\Delta\chi^2 \quad (2)$$

where $\overline{D_{A-B}}$ is the geometric mean of the corresponding homonuclear diatomic dissociation energies, $(D_{A-A}D_{B-B})^{1/2}$. Clearly the equation using the arithmetic mean (Eq. (1)) is conceptually superior since bond energies combine additively in their contribution to heats of reaction [4]. Both of these equations state that the extra ionic energy of a bond is proportional to the square electronegativity difference, $(\Delta\chi)^2$. It is shown that Eq. (2) is valid only for a small number of bonds with low polarity [4]. Some efforts have been also made to remove this difficulty and improve the accuracy of the mentioned equations by adding other factors [8–14]. For example, Matcha [15] proposed a formula for BDE in the basis of simple quantum mechanical theory to model the interaction potential between two atoms A and B. This formula relates bond energy to bond polarity and has the following form:

$$D_{A-B} = \overline{D_{A-B}} + 103[1 - \exp(-0.29\Delta\chi^2)] \quad (3)$$

It is shown that the above relation gives more accurate estimation for the energies of both ionic and covalent bonds, and also it relates electronegativity differences and bond energies to each other better than the Pauling equations [15].

Another formula which correlates electronegativity differences to bond energies is proposed by Reddy et al. [16] and has the following form:

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$$D_{A-B} = \overline{D_{A-B}} + 32.058\Delta\chi \quad (4)$$

It is appeared that this simple relation can successfully predict the energies of both ionic and covalent bonds. The estimated bond energies with this formula are in good agreement with the Matcha results; but it is found to be superior to the Pauling equations [16]. In fact the reliability of the estimated BDE from a formula is depended to the accuracy of the electronegativity scale, which is used for the calculation of $\Delta\chi$. According to this fact many attempts have been made, theoretically and experimentally, to determine the BDEs of different bonds [17–26]. A new approach to the relationship between bond energy and electronegativity is also given by Smith [27].

In the present article the ability of a new electronegativity scale in predicting the BDEs of some ionic and covalent bonds with different equations is checked. Also a comparison is made with those results which are obtained from the other electronegativity scales such as Pauling and Allred–Rochow.

2. Results and discussion

It is known that the reliability of a given electronegativity scale is supported by its ability in predicting different molecular properties. It is also shown that the calculated ionicities of some diatomic molecules using a new scale of electronegativity are in good agreement with the experimental data [3]. Now it is attempted to compute the BDEs of some diatomic molecules using this scale of electronegativity. Notice that diatomic molecules have gained increased interest over the past years in both experimental and theoretical studies; because of their importance in astrophysical process and many chemical reactions. Since bond dissociation energy is a prime factor in astrophysics, we have evaluated these energies for some diatomic molecules observed or suspected to be present in astrophysical environment. The selected species are divided into covalent and ionic categories, which will be discussed separately. The values of new electronegativities for some elements, which are used in this study, and BDEs of the corresponding homonuclear diatomic molecules are collected in Table 1. The Pauling and Allred–Rochow electronegativity values of these elements are also given in this table for comparison.

To check the ability of new scale in predicting dissociation energy of a covalent bond, 35 diatomic molecules are selected,

Table 1
Homonuclear bond dissociation energies and Pauling, Allred–Rochow and new electronegativity values for the considered atoms in this study.

Atom	D_{A-A}^a	χ_P	χ_{A-R}	χ_ω
H	104.2	2.20	2.20	1.687
Li	26.5	0.98	0.97	0.676
Na	18.0	0.93	1.01	0.689
K	13.2	0.82	0.91	0.656
Be	45.7	1.57	1.47	1.113
Mg	36.6	1.31	1.23	0.900
Ca	31.6	1.00	1.04	0.779
C	83.1	2.55	2.50	1.954
Si	42.2	1.90	1.74	1.430
N	38.4	3.04	3.07	2.528
P	51.3	2.00	2.06	1.611
As	32.1	2.18	2.20	1.673
O	33.2	3.44	3.50	2.841
S	50.9	2.58	2.44	2.131
F	36.6	3.98	4.10	3.505
Cl	58.0	3.16	2.83	2.390
Br	46.1	2.74	2.74	2.262
Cu	37.43	1.74	1.75	1.481

^a From Ref. [7] and all in kcal mol^{−1}.

which are shown in Table 2. BDEs of these species are calculated from Eqs. (2)–(4) and using new scale of electronegativity. The results (D_ω) are summarized in Table 2. The obtained values from Pauling and Allred–Rochow electronegativity scales (D_P and D_{A-L} , respectively) and the corresponding experimental values (D_{Exptl}) are also given for comparison in this table. Least-squares fit for all of the 35 systems are performed between the experimental dissociation energies and each set of these computed values from different electronegativity scales.

The correlation coefficients (R^2) are presented in the last row of this table. It is clear that the Matcha equation Eq. (3) is more successful in predicting the BDEs than the other relations. It does not depend on the electronegativity scale which is used in calculations. Also the best correlation is observed for the energies which are calculated from this formula and new electronegativity scale ($R^2 = 0.976$).

The obtained linear correlation relationships from Matcha formula for Pauling, Allred–Rochow and new electronegativity scales are

$$D_{\text{corr}}^P = 1.2243D_P - 13.536 \quad (5)$$

$$D_{\text{corr}}^{\text{AR}} = 1.1507D_{\text{AR}} - 7.2377 \quad (6)$$

$$D_{\text{corr}}^\omega = 1.2144D_\omega - 9.6736 \quad (7)$$

These relations are used to compute the corrected BDEs from Matcha formula. The corrected energies for the considered covalent bonds by using Matcha equation and different electronegativity scales Eqs. (5)–(7) are gathered in Table 3. The mean absolute deviation (MAD) for each scale is also calculated, which are presented in the last row of this table. It is found that the least MAD is observed for the new electronegativity scale (4.38). Therefore it is claimed that, by utilizing new electronegativity scale in Matcha relation, the BDEs for covalent bonds are superior estimated.

Now we consider the ionic bonds. The BDE values of 18 ionic diatomic molecules, which are shown in Table 4 have been calculated. Different electronegativity scales and using Eqs. (2)–(4) are used for this purpose and the results are gathered in Table 4 along with the experimental values. Again least-squares fit for each electronegativity scale and formula is performed for all of the 18 systems. The obtained correlation coefficients are also given in the last row of this table for comparison. It is clear that the least correlation coefficient ($R^2 = 0.548$) belongs to the Pauling electronegativity scale and Eq. (2), which is one of the Pauling relations. It is not unexpected; because the Pauling equation is successful in predicting the BDEs of covalent bonds and differs considerably from the experimental data for ionic molecules. Although the Pauling relation is not successful in predicting BDEs of ionic bonds but by using new electronegativity values in this relation, the results show a better correlation with the experiment ($R^2 = 0.687$) than those which are obtained from Pauling ($R^2 = 0.549$) or Allred–Rochow ($R^2 = 0.662$) electronegativity values. By comparison of correlation coefficients in Table 4, it is found that the best results are achieved when Matcha formula is used; as in the covalent case. The obtained linear correlation relationships with this formula for Pauling, Allred–Rochow and new electronegativity scales are

$$D_{\text{corr}}^P = 1.2243D_P - 5.5135 \quad (8)$$

$$D_{\text{corr}}^{\text{AR}} = 1.3834D_{\text{AR}} - 47.737 \quad (9)$$

$$D_{\text{corr}}^\omega = 1.0094D_\omega + 7.6152 \quad (10)$$

Corrected BDEs are calculated using these Eqs. (8)–(10), which are listed in Table 5. Mean absolute deviations for these data are also

Table 2Calculated bond dissociation energies for covalent bonds using different equations and electronegativity scales. All in Kcal mol⁻¹.

Molecule	Eq. (2)			Eq. (3)			Eq. (4)			D_{Exptl}^a
	D_P	D_{A-L}	D_{ω}	D_P	D_{A-L}	D_{ω}	D_P	D_{A-L}	D_{ω}	
HF	156.81	170.06	160.91	123.66	128.60	125.26	118.82	122.67	120.04	134.6
HCl	105.39	89.65	92.57	101.9	88.94	91.49	108.52	97.94	100.28	103.2
HBr	86.64	78.06	79.23	85.19	77.66	78.73	93.67	86.62	87.74	87.5
CH	96.73	95.75	95.19	96.65	95.71	95.16	104.27	102.67	101.61	98.8
CN	63.69	66.24	66.37	63.42	65.75	65.88	72.20	74.76	74.89	69.7
CP	134.40	136.53	134.25	134.32	136.35	134.18	141.95	144.83	141.72	159.1b
CO	76.29	82.53	76.13	73.66	78.45	73.54	81.06	84.58	80.96	84.0
CS	65.06	65.14	65.98	65.06	65.14	65.97	65.99	63.11	70.71	62.0
CCl	80.59	72.69	75.13	79.96	72.63	74.95	88.98	80.00	83.40	78.5
CBr	66.94	63.62	64.74	66.80	63.60	64.69	75.04	69.59	71.77	69.9
SiH	69.01	72.66	68.29	68.97	72.44	68.26	75.93	81.06	74.55	70.4
SiC	71.89	76.55	67.46	71.10	75.10	67.10	80.06	83.58	76.02	69.3
SiO	108.58	130.36	97.16	88.65	98.47	82.61	86.80	93.85	82.66	88.2
SiF	169.09	206.39	168.47	112.93	121.82	112.75	105.98	114.96	105.82	129.3
SiCl	97.10	85.11	77.12	87.48	79.49	73.63	89.87	84.42	80.24	85.7
SiBr	77.81	74.11	64.87	72.75	70.04	62.84	78.08	76.16	70.78	69.1
NH	84.40	85.96	84.47	82.32	83.55	82.36	90.18	91.15	90.22	93.4
NF	63.99	69.32	66.13	60.77	64.77	62.40	67.62	70.51	68.81	64.5
NCl	47.63	48.92	47.77	47.62	48.90	47.76	43.35	54.88	51.62	47.7
PH	73.11	73.70	73.29	73.11	73.69	73.29	73.11	77.60	75.55	76.4
PS	112.10	112.10	115.88	111.94	111.99	115.54	119.95	119.95	124.44	129.4
PCI	82.20	72.33	72.75	78.70	70.81	71.17	85.32	79.23	79.52	79.1
PBr	65.96	62.50	61.35	64.52	61.56	60.54	72.99	70.43	69.50	65.4
OH	104.94	109.52	98.77	95.87	98.72	91.81	98.57	100.49	95.81	110.6
OF	43.61	45.66	48.09	43.21	45.07	47.22	52.17	54.09	56.15	44.2
OCI	46.23	57.35	49.98	46.20	56.45	49.78	52.86	65.36	58.34	48.5
SH	77.16	74.56	78.74	77.05	74.53	78.55	85.01	80.52	87.06	81.1
SCI	64.43	58.90	56.35	63.91	58.78	56.32	72.93	66.84	62.64	59.7
SBr	52.77	51.14	48.96	52.66	51.09	48.95	60.62	58.06	52.64	50.7
AsH	57.85	57.83	57.84	57.85	57.83	57.84	58.48	57.83	58.28	58.6
AsF	131.48	142.58	134.96	97.03	101.12	98.36	91.98	95.19	93.01	111.3
AsCl	71.96	55.06	58.57	68.19	54.35	57.41	74.57	63.36	66.13	68.9
AsBr	56.72	47.22	48.88	55.13	46.82	48.33	63.47	55.78	57.35	56.5
BrCl	52.91	51.95	52.20	52.90	51.95	52.20	58.12	54.59	55.81	52.3
CuH	68.80	68.53	63.73	68.58	68.33	63.71	77.20	76.88	69.06	66.0b
R^2	0.864	0.751	0.861	0.968	0.949	0.976	0.919	0.9501	0.9522	
Slope	0.84 ± 0.06	0.63 ± 0.07	0.83 ± 0.06	1.22 ± 0.04	1.15 ± 0.05	1.21 ± 0.03	1.25 ± 0.06	1.25 ± 0.05	1.27 ± 0.05	
Inter.	11.1 ± 5.1	25.9 ± 6.0	15.1 ± 4.9	-13.5 ± 3.1	-7.2 ± 3.7	-9.7 ± 2.3	-21.4 ± 5.4	-21.2 ± 4.2	-21.0 ± 4.1	

^a From Ref. [28].^b From Ref. [26].**Table 3**Corrected bond dissociation energies for the selected covalent bonds using Matcha equation and different electronegativity scales. All in Kcal mol⁻¹.

Molecule	D_{corr}^P	D_{corr}^{AR}	D_{corr}^{ω}	$D_{\text{Exptl.}}$	Molecule	D_{corr}^P	D_{corr}^{AR}	D_{corr}^{ω}	$D_{\text{Exptl.}}^b$
HF	137.86	140.74	142.44	134.6	NCl	44.77	49.03	48.33	47.7
HCl	111.22	95.10	101.44	103.2	PH	75.98	77.56	79.32	76.4
HBr	90.77	82.13	85.93	87.5	PS	123.58	121.63	130.64	129.4
CH	104.79	102.89	105.89	98.8	PCI	82.82	74.25	76.75	79.1
CN	64.11	68.42	70.33	69.7	PBr	65.45	63.60	63.85	65.4
CP	150.91	149.66	153.27	159.1	OH	103.84	106.36	101.83	110.6
CO	76.65	83.04	79.63	84.0	OF	39.37	44.62	47.67	44.2
CS	66.12	67.72	70.44	62.0	OCI	43.02	57.72	50.78	48.5
CCl	84.36	76.33	81.34	78.5	SH	80.80	78.53	85.72	81.1
CBr	68.24	65.95	68.89	65.9	SCI	64.71	60.40	58.72	59.7
SiH	70.90	76.12	73.23	70.4	SBr	50.94	51.56	49.77	50.7
SiC	73.51	79.18	71.82	69.3	AsH	57.29	59.31	60.57	58.6
SiO	95.00	106.09	90.65	88.2	AsF	105.25	109.12	109.77	111.3
SiF	124.72	132.94	127.25	129.3	AsCl	69.95	55.30	60.05	68.9
SiCl	93.56	84.23	79.74	85.7	AsBr	53.96	46.64	49.01	56.5
SiBr	75.53	73.35	66.64	69.1	BrCl	51.23	52.54	53.71	52.3
NH	87.24	88.91	90.34	93.4	CuH	70.43	71.39	67.70	66.0
NF	60.87	67.29	66.10	64.5	MAD	5.27	5.83	4.38	

calculated, which are presented in the last row of this table. Again the MADs show that the corrected BDEs which are obtained from new electronegativity values (MAD = 4.96) are to some extent better than those which are obtained from Pauling (MAD = 6.63) and

Allred–Rochow (MAD = 5.10) electronegativity scales. Therefore the obtained dissociation energies from the new scale are much better correlates with the experimental data than those which calculated using the other scales. Hence it seems that the new

Table 4Calculated bond dissociation energies for ionic bonds using different equations and electronegativity scales. All in Kcal mol⁻¹.

Molecule	Eq. (2)			Eq. (3)			Eq. (4)			<i>D</i> _{Exptl.}
	<i>D</i> _P	<i>D</i> _{A-L}	<i>D</i> _ω	<i>D</i> _P	<i>D</i> _{A-L}	<i>D</i> _ω	<i>D</i> _P	<i>D</i> _{A-L}	<i>D</i> _ω	
LiF	301.14	325.05	271.24	126.57	128.13	124.03	127.32	131.48	121.84	136.2
LiCl	181.78	142.99	127.34	116.25	104.43	98.27	109.09	98.83	94.15	111.6
LiBr	152.56	128.94	110.41	104.91	96.43	88.29	98.42	91.69	85.80	99.8
NaF	304.74	312.11	263.56	121.73	122.21	118.34	123.44	124.73	115.94	122.9
NaCl	181.50	131.68	119.11	110.96	95.90	90.80	103.80	90.66	86.84	97.5
NaBr	152.43	118.59	103.04	100.63	88.57	81.55	93.88	84.27	79.23	86.2
KF	321.55	327.26	265.48	119.29	119.60	115.20	123.28	124.25	113.31	116.9
KCl	191.94	138.26	117.87	109.62	95.31	87.60	102.69	89.22	83.26	100.1
KBr	162.06	125.14	102.05	100.38	88.67	78.92	93.27	83.33	76.15	90.1
BeF	215.12	248.39	212.53	124.77	130.02	124.28	118.14	125.19	117.56	151
BeCl	127.30	106.95	100.38	104.98	94.22	90.27	102.43	95.06	92.40	110
BeBr	103.84	94.27	85.48	90.06	84.36	78.64	90.44	86.59	82.71	89
MgF	303.02	283.72	240.19	131.77	130.16	125.22	132.15	128.62	120.12	123
MgCl	148.76	122.89	112.69	110.91	100.06	94.99	105.40	97.38	93.86	97
MgBr	122.77	109.49	96.74	97.32	90.92	83.94	93.99	89.50	84.75	81
CaF	300.40	314.90	256.92	129.15	130.18	125.05	129.52	132.09	121.38	132
CaCl	182.76	138.91	120.65	119.17	105.12	97.27	112.04	100.17	94.44	103
CaBr	153.40	124.85	104.13	107.34	96.60	86.72	100.98	92.65	85.69	96
<i>R</i> ²	0.548	0.662	0.687	0.732	0.851	0.853	0.728	0.808	0.823	
Slope	0.19 ± 0.04	0.17 ± 0.03	0.22 ± 0.04	1.38 ± 0.19	1.07 ± 0.11	1.01 ± 0.10	1.20 ± 0.18	0.949 ± 0.12	1.06 ± 0.12	
Inter.	68.9 ± 9.4	77 ± 6.3	73.3 ± 6.4	-47.7 ± 23.7	-5.5 ± 12.0	7.6 ± 10.6	-22.3 ± 20.1	10.2 ± 12.1	4.5 ± 12.15	

*From Ref [28].

Table 5Corrected bond dissociation energies for the selected ionic bonds using Matcha equation and different electronegativity scales. All in Kcal mol⁻¹.

Molecule	<i>D</i> _{Corr} ^P	<i>D</i> _{Corr} ^{AR}	<i>D</i> _{Corr} ^ω	<i>D</i> _{Exptl.}
LiF	127.36	132.16	132.81	136.2
LiCl	113.08	106.70	106.81	111.6
LiBr	97.39	98.10	96.73	99.8
NaF	120.66	125.80	127.06	122.9
NaCl	105.76	97.53	99.27	97.5
NaBr	91.47	89.65	89.93	86.2
KF	117.29	122.99	123.89	116.9
KCl	103.91	96.89	96.04	100.1
KBr	91.12	89.76	87.27	90.1
BeF	124.86	134.19	133.06	151
BeCl	97.49	95.73	98.74	110
BeBr	76.85	85.13	87.00	89.0
MgF	134.56	134.35	134.01	123
MgCl	105.70	102.01	103.49	97.0
MgBr	86.90	92.18	92.35	81.0
CaF	130.93	134.36	133.85	132
CaCl	117.12	107.44	104.80	103
CaBr	100.76	98.28	95.15	96.0
<i>MAD</i>	6.63	5.10	4.96	

electronegativity scale is comparatively superior to Pauling and Allred–Rochow electronegativity scales for estimating BDEs of both ionic and covalent bonds.

3. Conclusion

The ability of a new electronegativity scale in predicting the bond dissociation energies of diatomic molecules (in both ionic and covalent forms) is checked with different formulas. It is found that by utilizing the new electronegativity scale and Matcha formula, the best results are obtained for both ionic and covalent bonds. Comparison between the estimated dissociation energies, which are obtained from different electronegativity scales (Pauling, Allred–Rochow and new scales), shows that the new scale is more successful than the others. Then it supports the idea that new electronegativity values represent a proper scale for such correlation.

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