A novel method for the calculation of bond stretching force constants of diatomic molecules

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ABSTRACT

Chemical hardness is one of the chemical reactivity descriptors of chemical species and this concept has widely benefited from the development of Density Functional Theory (DFT). In the present report, chemical hardness values for approximately fifty diatomic molecules have been calculated using a new molecular hardness (η_M) equation derived by us in recent times. Then, correlation between force constant (k) and chemical hardness for the above mentioned diatomic molecules that situate hydrides, halides, oxides and sulfides among them has been investigated. Consequently, a relation that can be presented by a simple equation between chemical hardness with bond stretching force constants has been found.

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1. Introduction

A primary goal of theoretical chemists is to predict the structure, stability, and chemical reactivity of molecules that are difficult to investigate by experimental means. Several models based on simplifications and assumptions, are available to provide new insights into the properties of molecules. It is unfortunate that the atoms and molecules are invisible only we can observe some radiation signals coming out the atom and molecule. The signals bear the signature of all the energetic effects including the effects of relativity present in the complex electronic structure of the species. The electron correlation, relaxation and relativity are the actual features of the inner plenum of electron constitution of atom and molecule. The actual features of the plenum of electron constitution are incorporated into the signals coming out of inner world of the atoms. Ghosh and Islam [1,2] rightly pointed out that any calculation of atomic property entailing spectroscopic data, the electron correlation, relaxation and relativity are automatically subsumed in such calculated property.

The present exercise investigates force constants in diatomic molecules, a measure of the stiffness of the bond. Bond stretching force constants of diatomic molecules are generally used to predict equilibrium geometries, electron correlation or basis set effects and harmonic vibrational frequencies of the molecules. Bond stretching force constants also have important applications in vibrational spectroscopy (IR and Raman

spectroscopies) and in molecular mechanics force fields. If a bond is distorted (stretched or contracted) from its equilibrium length, the molecule's energy increases and, as a result, there is a force on each atom in the direction that reduces the bond energy. Stronger the bond, larger will be the force constant. Thus the force constant is linearly related to bond order. Bond force constants of molecules can be easily determined by means of the data of IR or Raman spectroscopy [3,4]. Using these spectroscopic methods, bond vibrational frequencies of molecules are easily determined and for diatomic molecules, considering the following equation, bond force constants of diatomic molecules are calculated [5].

$$\overline{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}} \tag{1}$$

where c, k and μ are light speed, bond force constant and reduced mass, respectively.

Conceptual Density Functional Theory (CDFT) [6,7] provides great conveniences to chemists for understanding of chemical reactivity. Chemical reactivity descriptors such as chemical hardness (η) [8–11], chemical potential (μ) [12] and electronegativity (χ) [13,14] are defined as the derivatives of the electronic energy (E) of a system with respect to number of electrons (N) at a constant external potential, $\upsilon(r)$ and can be calculated considering ionization energy (I) and electron affinity (A) values of chemical species through the contributions to quantum

chemistry of this theory [15].

$$\mu = -\chi = \left(\frac{\partial E}{\partial N}\right)_{v(r)} \tag{2}$$

$$\eta = \left(\frac{\partial^2 E}{\partial N^2}\right)_{v(r)} = \left(\frac{\partial \mu}{\partial N}\right)_{v(r)}. \tag{3}$$

Pearson and Parr put forward the operational definitions of chemical hardness, chemical potential and electronegativity as follows by applying the finite differences approximation to Eq. (2) and Eq. (3) [16,17].

$$-\mu = \chi = \frac{I+A}{2} \tag{4}$$

$$\eta = I - A \tag{5}$$

where I is the ionization energy and A is the electron affinity of the chemical species.

In recent times, a new and useful method for calculation of chemical hardness of molecules (η_M) has been presented by us [18].

$$\eta_M = \frac{2\sum_{i=1}^{N}\frac{b_i}{a_i} + q_M}{\sum_{i=1}^{N}\frac{1}{a_i}}. \tag{6}$$

In this equation, q_M is the charge of molecule, N is the number of atoms in molecule, and a_i and b_i are the correlation parameters. These correlation parameters are defined as:

$$a_i = \frac{I+A}{2} \tag{7}$$

$$b_i = \frac{I-A}{2}. \tag{8}$$

Badger [19] put forwarded the empirical relation between bond lengths, force constants and bond dissociation energies as:

$$k = \frac{1.86 \times 10^5}{(r_e - d_{ij})^3} \tag{9}$$

where, k is bond stretching force constant in *dyn cm^{-1}* units. r_e represents the internuclear distance in Angstrom (Å) units and d_{ij} is a function of the position of bonded atoms in the periodic table.

A relation between bond force constants, bond orders, bond lengths and the electronegativities of bonded atoms has been demonstrated by Gordy as follows [20,21]

$$k = aN\left(\chi_A\chi_B/d^2\right)^{3/4} + b \tag{10}$$

where k is the bond force constant, d is the bond length, N is the bond order and, χ_A and χ_B are electronegativities of bonded atoms. a and b have different numerical values for different molecules/groups.

In 1993, T. Ghanty and S. K. Ghosh [22] demonstrated the interesting correlations between the hardness, polarizability and size of molecules. It has been proved that the softness of a molecule (σ) is proportional to bond length (r_e). Pearson who introduced chemical hardness and softness concepts has studied some diatomic hydride molecules (HX) and reached to the conclusion that there is a correlation between the dissociation energy and $k^{1/2}$ (k is force constant). In addition to this correlation, Pearson deduced a new equation regarding the calculation of force constants of diatomic covalent molecules. The equation is given

as follows [23].

$$kr_e = 77\chi_A^2 + 117. \tag{11}$$

In the equation, k is force constant, r_e is bond length, and χ_A is atomic electronegativity value which belongs to atom that is different from hydrogen in any diatomic hydride in Pauling units.

Towards the end of the twentieth century, K. Ohwada published some important theoretical studies relating to the calculation of bond force constants of diatomic molecules. In one of these, Ohwada derived a new formula under several reasonable assumptions to calculate the heteronuclear diatomic force constants (K_{AB}) based on homonuclear diatomic force constants (K_{AA} and K_{BB}) as [24]:

$$K_{AB} = (K_{AA}.K_{BB})^{1/2}. \tag{12}$$

Following this work, he improved the Eq. (12) through the second-order perturbation theory and presented the equation given below for the calculation of bond force constants of heteronuclear diatomic molecules [25].

$$K_{AB} = \xi^3 (K_{AA}.K_{BB})^{1/2} \tag{13}$$

where ξ is correction factor and it is defined as $\xi = (R_{AA}.R_{BB})^{1/2}/R_{AB}$ based on R_{AA}, R_{BB} and R_{AB}, the internuclear distances of diatomic molecules AA, BB and AB, respectively.

Despite the vast prospective of quantum chemical methods, there is still a need to understand the properties and behavior of molecules on the basis of simple empirical models that require no sophisticated calculations. The present work provides a simple empirical model for calculation of bond stretching frequencies of diatomic molecules. The present work is focused on investigating whether molecular hardness is useful to predict the force constants of some diatomic molecule groups. The goal is to present a new equation based on the relation between molecular hardness and bond length with force constant.

2. Theoretical model

From the above discussions it seems that the bond-stretching force constant k has some connection with the density functional theoretical parameters. Now let us ponder over the concepts of the bond stretching force constants, hardness and bond distance of diatomic molecules. It is unequivocal that the bond stretching force constant is intimately connected to the hardness and bond distance of the diatomic molecules. By definition, the chemical hardness is a measure of the resistance power of the chemical species towards electron cloud polarization or deformation. In 1997, S. Arulmozhıraja and P. Kolandaıvel [26] pointed out that "*With increasing chemical hardness in diatomic molecules, either the force constants or binding energies of molecules increase*" and "*The chemical hardness is a better pointer of stability of the molecules that is the chemical potential*". Thus it is expected that the bond stretching force constants is proportional to the hardness of diatomic molecules. Considering the definitions of bond stretching force constants and hardness of diatomic molecules, we can safely assume that $k \propto \eta_M$ when r_e and other parameters related to the bond stretching are constant. It is well known that k decreases with bond distance. Thus we can safely assume that $k \propto (1/r_e^2)$ when r_e and other parameters related to the bond stretching are constant. It is well known that k varies with all the quantities like electronegativity, hardness, bond order, bond distances etc. Now, Ghosh and Islam [27–30] based on the fundamental identity of the basic concept and the origin of the electronegativity and the hardness posited the conceptual commonality between the electronegativity and the hardness. There are several reports where k of diatomic molecules are expressed as a function of electronegativity we here consider the hardness of the molecule to compute the k.

It should be possible, therefore, to express k as a combined function

$$k = f(\eta_M, r_e). \qquad (14)$$

In the study, it is envisaged that η_M/r_e^2 parameter is proportional to the bond stretching force constants of diatomic molecules. In order to compute the bond force constants of diatomic molecules the following equations (Eq. (15) and Eq. (16)) are presented.

$$k = \frac{a\eta_M}{r_e^2} + b. \qquad (15)$$

In the equation, k is bond force constant in N/m unit; η_M is molecular hardness in eV unit. r_e represents the bond length of diatomic molecules. a and b are the correlation parameters that can subsume the effect of anharmonicity.

The number of electrons in the valence shell is considered for binary covalent or nearly covalent compounds of hydrogen atoms. Hence, $\eta_M V_e/r_e^2$ parameter is considered instead of η_M/r_e^2 parameter to obtain a linear graph (Fig. 3) for those molecules. Here V_e represents the number of electrons in the valence shell of atom that is different from hydrogen for any binary compound of hydrogen. As is known, according to Allen electronegativity definition [31], "Electronegativity is the average one-electron energy of the valence-shell electrons in ground-state free atoms". For this reason, V_e parameter given in Eq. (16) is closely related to the electronegativity of atom that is different from hydrogen for any binary compound of hydrogen. Already, we mentioned above that Pearson presented an equation based on the electronegativity of atom that is different from hydrogen to calculate the bond force constants of diatomic hydrides.

$$k = \frac{aV_e\eta_M}{r_e^2} + b \qquad (16)$$

Anharmonicity is the deviation of a system from being a harmonic oscillator. The effect of anharmonicity is usually calculated using perturbation theory. If the anharmonicity is large, then several numerical techniques have to be used. It is well known that the hybrid functional B3LYP [32,33] within the framework of density functional theory, DFT, can provide nearly accurate anharmonic force fields. Miani et al. [34] pointed out that the B3LYP spectroscopic constants are significantly more accurate than the Hartree–Fock results. In this study, to subsume the effect of anharmonicity in the proposed Eqs. (15) and (16) very simple correlation technique is used. The proposed parameter is first
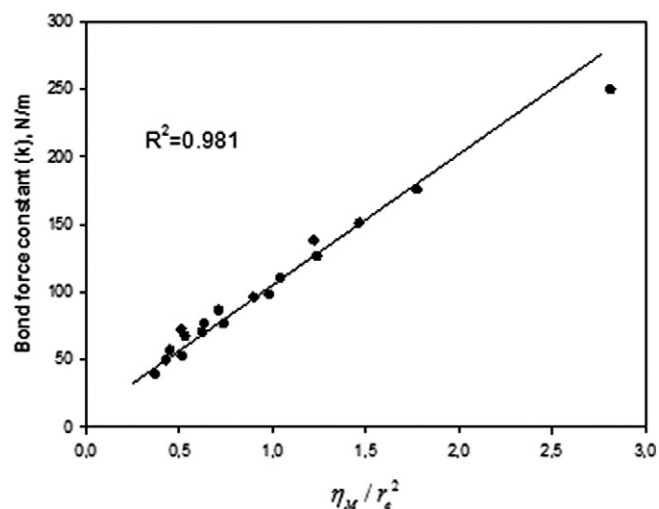

Fig. 1. Variation with ηM/re 2 parameter of bond force constants for alkali halides.

correlated with the experimental force constant values of the different sets of diatomic molecule invoked in the present work to generate the anharmonicity correlation coefficients 'a' and 'b'.

It is important to mention here that η_M values are calculated using the molecular hardness formula (Eq. (5)) proposed by us. For alkali halides, molecular hardness, bond length and observed bond force constants data are presented in Table 1. The plot in Fig. 1 supports our assumption that bond force constants are proportional to η_M/r_e^2.

Table 1
Molecular hardness, bond length and bond force constant values for alkali halides.

Alkali halide	η_M (eV)	r_e (Å)	k (N m^{-1})
LiF	6.85	1.56	249.5
LiCl	5.99	2.02	150.8
LiBr	5.85	2.17	126.4
LiI	5.56	2.38	98.17
NaF	6.62	1.93	175.4
NaCl	5.81	2.36	110.12
NaBr	5.63	2.50	95.82
NaI	5.43	2.71	76.4
KF	5.76	2.17	137.84
KCl	5.08	2.67	86.32
KBr	4.95	2.82	70.05
KI	4.77	3.04	52.58
RbF	5.59	2.27	130.84
RbCl	4.94	2.79	76.57
RbBr	4.82	3.01	67.09
RbI	4.65	3.29	49.31
CsF	5.26	2.47	124.85
CsCl	4.66	3.02	71.94
CsBr	4.54	3.17	56.85
CsI	4.39	3.45	39.06

Table 2
Molecular hardness, bond length and bond force constant values for some binary compounds of hydrogen atom and some A$_2$ type molecules have different bond orders.

| Molecule	η_M (eV)	r_e (Å)	k (N m^{-1})
LiH	7.16	1.595	102.6
NaH	6.95	1.887	78.62
KH	6.12	2.224	55.78
RbH	5.94	2.367	52.00
CsH	5.62	2.494	47.23
HF	13.28	0.92	965.7
HCl	11.23	1.28	517.6
HBr	10.71	1.41	415.04
HI	10.04	1.61	314.93
NH	13.65	1.04	596.7
PH	11.10	1.42	322.4
GeH	9.07	1.59	197.53
SnH	8.68	1.78	170.56
AsH	10.62	1.53	269.26
OH	12.51	0.97	783.36
SH	10.40	1.34	425.69
SeH	10.03	1.48	338.31
CH	11.32	1.12	447.6
SiH	9.19	1.52	240.0
H$_2$	12.84	0.74	573
Li$_2$	4.774	2.67	25.5
Na$_2$	4.590	3.08	17.2
K$_2$	3.84	3.92	9.9
Rb$_2$	3.69	4.50	8.2
C$_2$	9.99	1.242	1220
B$_2$	8.00	1.590	358
Si$_2$	6.76	2.246	215
Sn$_2$	6.23	2.746	121
N$_2$	14.46	1.098	2300
P$_2$	9.74	1.893	558
As$_2$	8.97	2.103	409
Sb$_2$	7.56	2.342	262
S$_2$	8.28	1.889	499
O$_2$	12.16	1.21	1177
Se$_2$	7.73	2.166	345
Te$_2$	7.04	2.557	230
Br$_2$	8.45	2.281	249
I$_2$	7.39	2.666	172
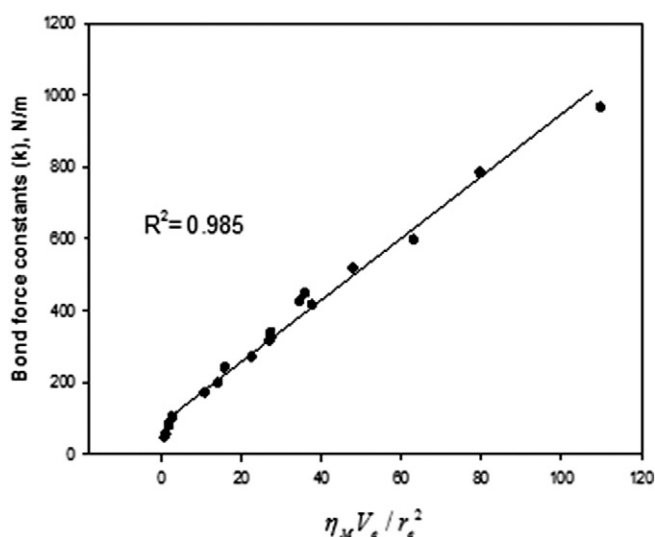
Fig. 2. Variation with $\eta_M V_e/r_e^2$ parameter of bond force constants for binary compounds of hydrogen in Table 2.

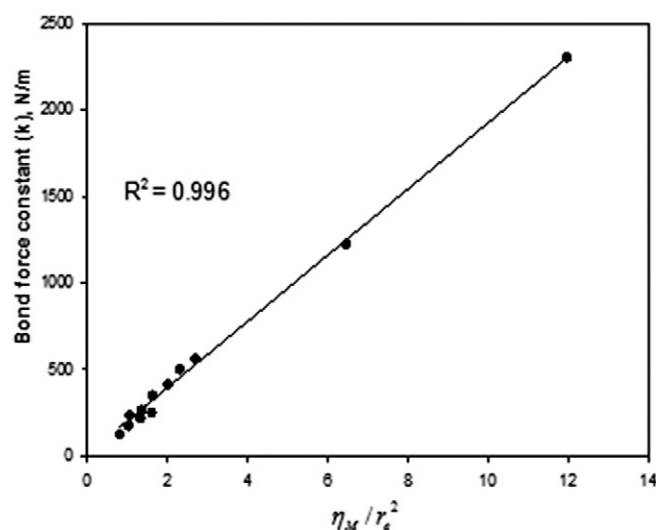**Fig. 3.** Variation with η_M/r_e^2 parameter with bond force constants for A_2 type molecules in Table 2.

In order to justify our assumption "bond force constants are proportional to η_M/r_e^2", some binary compounds of hydrogen atoms and some A_2 type diatomic molecules are taken for study (Table 2). It should be noted that as the number of electrons in valence shell of atom increases, the bond force constant of binary compound of hydrogen also increases. Fig. 2 provides the relation between $\eta_M V_e/r_e^2$ parameter with bond force constants of binary compounds of hydrogen. Numerical values of a and b parameters for different set of molecules are computed using correlation method. The computed a and b data are presented in Table 3.

Figs. 2 and 3 which associate with molecules in Table 2 show that there is a linear correlation between η_M/r_e^2 values with bond force constants of some groups of molecules. In Fig. 3 variation of bond force constants with η_M/r_e^2 parameter for some A_2 type molecules are investigated.

3. Results and discussion

Chemical hardness concept introduced by Pearson, has been associated with several topics and has been considered in many theoretical and experimental studies. In this study, we associated with their force constants the molecular hardness values calculated via our molecular hardness equation for diatomic molecules. Besides, we proposed that η_M/r_e^2 parameter will provide convenience for comparison of bond force constants of diatomic molecules.

The calculated bond force constants using Eqs. (15)–(16) and bond force constant values observed experimentally regarding molecules studied in this study are presented in Table 4. The percentage deviations between calculated and observed bond stretching force constants were determined considering the following equation.

$$Percentage\ deviation = \frac{|k_{obs} - k_{cal}|}{k_{obs}} \times 100 \qquad (17)$$

The agreement between observed (k_{obs}) and calculated (k_{cal}) bond stretching force constants values are understood from percentage

Table 3
Numerical values of a and b parameters for different molecule groups.

Molecules	a (N m^{-1} (Å)^2/eV)	b (N m^{-1})
Alkali halides	85.72	18.63
Binary compounds of hydrogen	8.6	78.77
A_2 type molecules	199.2	−4.119

Table 4
Observed and calculated bond stretching bond force constants for some selected molecules (N m^{-1}).

Molecule	k_{obs}	k_{cal}	Deviation (%)
LiF	249.5	259.91	4.17
LiCl	150.8	144.46	4.20
LiBr	126.4	125.12	1.01
LiI	98.17	102.77	4.68
NaF	175.4	170.97	2.52
NaCl	110.12	108.04	1.88
NaBr	95.82	95.84	0.02
NaI	76.40	82.00	7.32
KF	137.84	123.48	10.41
KCl	86.32	79.71	7.65
KBr	70.05	71.98	2.75
KI	52.58	62.87	19.57
RbCl	76.57	73.03	4.62
RbBr	67.09	64.23	4.26
RbI	49.31	55.45	12.45
CsCl	71.94	62.42	13.23
CsBr	56.85	57.35	0.87
CsI	39.06	50.24	28.62
LiH	102.6	102.97	0.360
NaH	78.62	95.55	21.53
HF	965.7	1023.30	5.96
HCl	517.6	491.39	5.06
HBr	415.04	403.07	2.88
HI	314.93	311.94	0.94
NH	596.7	621.43	4.14
PH	322.4	315.47	2.14
GeH	197.53	202.18	2.35
SnH	170.56	173.01	1.43
AsH	269.26	273.84	1.700
OH	783.36	764.83	2.36
SH	425.69	377.63	11.28
SeH	338.31	315.05	6.87
CH	447.6	389.20	13.04
SiH	240.0	215.60	10.16
C_2	1220	1286.97	5.48
Si_2	215	262.90	22.27
Sn_2	121	160.46	32.61
N_2	2300	2385.08	3.69
P_2	558	537.31	3.70
As_2	409	400.08	2.18
Sb_2	262	270.44	3.22
S_2	499	458.22	8.17
O_2	1117	1650	47.0
Se_2	345	324	6.08
Te_2	230	210	8.69

Table 5
Experimental and calculated force constants for some diatomic hydrides.

Molecule	Present work	Eq. (13)	Eq. 12	Ab-initio	Experimental
OH	798	760	821	881	773
NH	654	749	1147	710	587
CH	407	524	835	547	445
SH	377	359	533	448	416
PH	309	319	564	351	323
LiH	102.9	83.2	121	143	102
NaH	95.5	51	99.3	95.1	77.6
KH	89.22	33.1	75.3	77.6	55.7
AlH	155	138	245	191	161
FH	1023	717	504	1047	965
ClH	491	370	428	579	516
BrH	403	292	375	462	412
IH	311.9	214	318	356	312

Note: Ab-initio results were taken from Ref. 25.

deviation values given for all molecules considered in the study. Moreover, it has been demonstrated that there is a remarkable relation between molecular hardness and bond force constants. At this stage, it should be stated that the present results obtained by us support the past predictions related to the work of S. Arulmozhıraja and P. Kolandaıvel. Finally, we would like to state again that η_M/r_e^2 parameter for diatomic molecules is quite useful for comparison of the bond stretching force constants of diatomic molecules.

It is well-known that ab-initio methods have been extensively used to predict the many properties such as molecular orbitals, molecular energies and structures, force constants, and vibrational frequencies of molecules. However, it is important to note that the selecting of basis set and method for systematic calculations made using ab-initio methods such as Gaussian is quite important. To support the reliability of the Equations proposed in this study, we also compared with the force constants obtained using Eq. (12), Eq. (13) and ab-initio quantum chemical methods (Gaussian 98W; 6-31G, 6-311G, CEP-121G, LanL2DZ). Ab-initio data for bond force constants were taken from Ref. 25. Experimental force constant values and force constant values calculated with the help of some theoretical models for some heteronuclear diatomic molecules are presented in Table 5. The results given in this table indicate that the presented method will be useful in terms of the prediction of bond force constants of diatomic molecules.

4. Conclusions

In the present paper, we investigated the relation between molecular hardness with bond stretching force constants for some molecule groups and obtained a considerable correlation between mentioned chemical properties. Consequently, we presented new equations to calculate the bond force constants of molecule groups considered in the study and saw that there is an agreement between observed and calculated bond stretching force constants. The following conclusions could be drawn from this study.

(1) There is an important correlation between their bond force constants and chemical hardnesses of diatomic molecules.

(2) η_M/r_e^2 ratio will be a useful tool to compare the bond force constants of diatomic molecules.

(3) The number of electrons in the valence shell of atom that is different from hydrogen for any binary compound of hydrogen should be considered to calculate the bond force constant of said compound.

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