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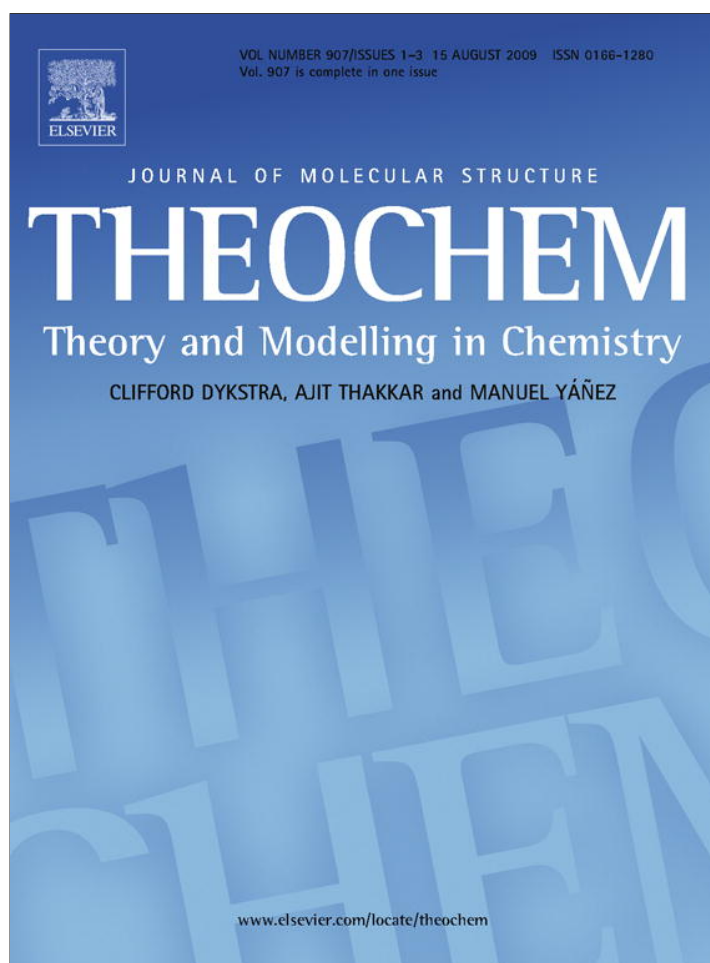


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# Estimation of atomic correlation energies from the electron density at the nucleus and atomic additivity of the correlation energy in molecules

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## ABSTRACT

A new method based on electron density at the nucleus is presented to determine electron correlation energy in atomic species. Using the nuclear-electron coalescence cusp condition, we have shown that the atomic correlation energy can be well represented by different power of atomic number for different isoelectronic series. The computed correlation energies have been achieved chemical accuracy with average absolute deviation in the order of 1 kcal/mol for 17 isoelectronic series. Also it is shown that the correlation energy for a molecule can be expressed in terms of the correlation energies of its constituent atoms and its number of electrons. The proposed formula confirms that in a molecule the electron correlation is larger than the sum over electron correlations of its corresponding constituent atoms.

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## 1. Introduction

The problem of determining electron correlation energy is of great importance in quantum chemistry and solid state physics. The origin of this problem can be traced to the Hartree–Fock approximation. It is an independent electron approximation in which the instantaneous electron–electron repulsion is replaced by an averaged electron–electron interaction in the Hamiltonian. Consequently, the Hartree–Fock ground state has a higher energy than the true ground state and the difference is defined as the correlation energy. This problem was recognized very early in the development of quantum mechanics as applied to atoms and molecules.

Historically, after Wigner's finding [1] that the atomic correlation energy is a function of atomic number, many attempts have been made to evaluate correlation energy contribution from measurable properties in an approximation manner. Clementi [2] estimated correlation energy of atoms by subtracting from the experimental ground state energies obtained from Moore's tabulation [3] the values of the corresponding Hartree–Fock energy and relativistic corrections [4] from Breit–Pauli perturbation theory. That work has been complemented by analysis of the degeneracy effect in the isoelectronic series of the second row atoms [5]. More recently, Clementi and Corongiu [6] obtained equation of the form

$$E_{\text{corr}} = -0.0170N^{1.31}(e^2/a_0) \quad (1)$$

for neutral atoms, where  $N$  is a number of electrons and  $a_0$  is the Bohr radius.

Davidson and co-workers have improved the correlation energy of the ground state atomic ions with 3–10 electrons and  $Z$  up to 20 by combining experimental data and improved ab-initio calculations [7]. They used experimental estimate of correlation energy contribution to ionization energy to fit the low- $Z$  data for  $N = 3$ –5 satisfactorily to a three-term series in  $Z^{-1}$  of the form

$$\Delta E_{\text{corr}}(N, Z) = a + b/Z + c/Z^2 \quad (2)$$

This approach was then extended to atomic ions with 11–18 electrons [8].

Alonso and Cordero have noticed that the empirical correlation energy of atoms and singly charged positive and negative ions show a roughly linear dependence with respect to the number of electrons. Thus, they suggested that the correlation energy of atom is proportional to the number of pairing  $N_{\uparrow\downarrow}$  between antiparallel-spin electrons in the same main shell [9],

$$E_{\text{corr}} = -\alpha N_{\uparrow\downarrow} \quad (3)$$

where the empirical constant  $\alpha$  has the meaning of a general pairing energy. They substantially improved the relation between  $E_{\text{corr}}$  and  $N_{\uparrow\downarrow}$  by considering separate linear relation that is different slope  $\alpha$  for different groups of atoms, related to electronic subshell filling [10].

Silva et al. [11] used the backpropagation neural network to estimate the correlation energy of diatomic molecules and neutral atoms up to radon (Rn). The advantage of using the neural network is that the correlation energy of many electron systems can be generated without prohibiting computational implications.

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In the present study, a simple method based on the electron density at the nucleus has been proposed to estimate the electron correlation for atomic species. The additivity scheme has been also used to determine the molecular correlation energy for 35 closed-shell polyatomic molecules composed of H, C, N, O and F atoms.

## 2. Computational details

Recently, Parr and Liu have shown that the ground state atomic correlation energies can be well represented by empirical formula of the form

$$E_{\text{corr}} = CN\rho(0)Z^{-\gamma} \quad (4)$$

where  $C$  and  $\gamma$  are constants,  $N$  is the number of electrons and  $\rho(0)$  is the electron density at the nucleus [12].

Here, we use the nuclear-electron cusp condition on  $\rho(r)$  which results

$$\rho(0) = AZ^B \quad (5)$$

where  $A$  and  $B$  are determinable parameters [13].

Inserting  $\rho(0)$  from Eq. (5) into Eq. (4) and considering the number of electrons as a variable of the order of  $\alpha$ , ( $N^\alpha$ ), the new form of the correlation energy can be written as;

$$E_{\text{corr}} = \lambda N^\alpha Z^\beta \quad (6)$$

where  $\alpha$ ,  $\beta$  and  $\lambda$  are constants that can be determined within a sets of atomic and ionic species.

To test the proposed formula, we used a set including atoms from He through Ar as well as their singly charged positive ions. Accurate values of correlation energy of the species were taken from Ref. [8] to determine the constants  $\alpha$ ,  $\beta$  and  $\lambda$  by multiple linear regressions on the following equation which is equivalent to Eq. (6),

$$\ln E_{\text{corr}} = \ln \lambda + \alpha \ln N + \beta \ln Z \quad (7)$$

All over our work, the correlation energies are taken as positive quantities for simplicity.

## 3. Results and discussion

### 3.1. Atomic correlation energy

The fitting values for  $\lambda$ ,  $\alpha$  and  $\beta$  were found to be 0.0133, 1.116 and 0.278, respectively. These fitted parameters were used to calculate the correlation energies for the species included in our data set using the following equation,

$$E_{\text{corr}} = 0.0133 N^{1.116} Z^{0.278} \quad (8)$$

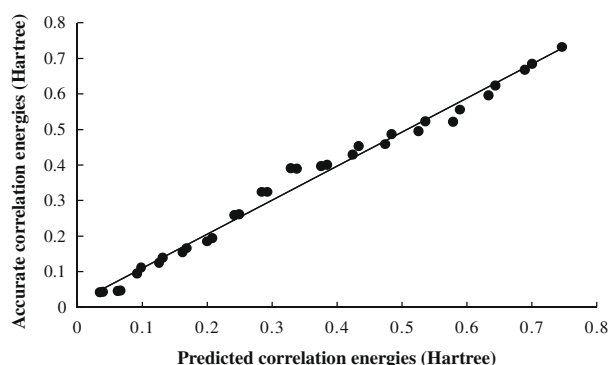


Fig. 1. Accurate versus predicted correlation energies for 33 species including He through Ar as well as their singly charged positive ions.

The accurate values of correlation energies versus the predicted values are shown in Fig. 1 for 33 neutral and charged atoms. Although the regression coefficient  $R^2 = 0.983$  indicates a rather satisfactory comparability between our results and the accurate values, the absolute deviations are some times more than 6 kcal/mol which are far from chemical accuracy. This deviation is due to different behavior of the correlation energy in species with different number of electrons.

To approach a higher accuracy we relax the restriction that  $N$  is variable and let  $\lambda$  and  $\beta$  to be separately determined for isoelectronic series. Thus, the Eq. (6) can be rewritten as

$$\frac{E_{\text{corr}}}{N} = \lambda Z^\beta \quad (9)$$

We simply do a linear regression fit of the following equation and determine the best values of  $\lambda$  and  $\beta$  for each series with  $N = 4-18$

$$\ln \frac{E_{\text{corr}}}{N} = \ln \lambda + \beta \ln Z \quad (10)$$

The computed values for  $\lambda$ , and  $\beta$ , regression coefficients ( $R^2$ ) and the average absolute deviation (AAD) for 15 isoelectronic series are summarized in Table 1.

In Figs. 2–5 we plot the correlation energy versus atomic number for the ground state of isoelectronic series with  $N = 2-18$ . The plots confirm again that the correlation energy takes a different power of  $Z$  for different isoelectronic series. More specifically, for  $N = 7-11$  (Fig. 2) the correlation energies take almost the same trend and  $\beta$  parameters have similar order. This similarity has been also observed for  $N = 6, 12-18$  (Fig. 3), where the correlation energies follow a well defined trend. The reported values of  $\lambda$  and  $\beta$  parameters for  $N = 4, 5$  show that the correlation energy depends on  $Z$  with completely different slope (Fig. 4).

A close look at the deviations reveals that the Eq. (9) is accurate enough for computing the correlation energy in isoelectronic series ( $N = 4-18$ ) and a proper accordance, within chemical accuracy, has been observed between the predicted and accurate correlation energies.

A comparison between Figs. 2–4 and Fig. 5 shows that for isoelectronic series with  $N = 2, 3$  the correlation energy is not a linear function of atomic number. However, for  $N = 2, 3$  the correlation energies are poorly fitted to the Eq. (10) and the regression coefficients are in the order of 0.690. Therefore, for isoelectronic series with  $N = 2, 3$  a quadratic fit of the below form has been used.

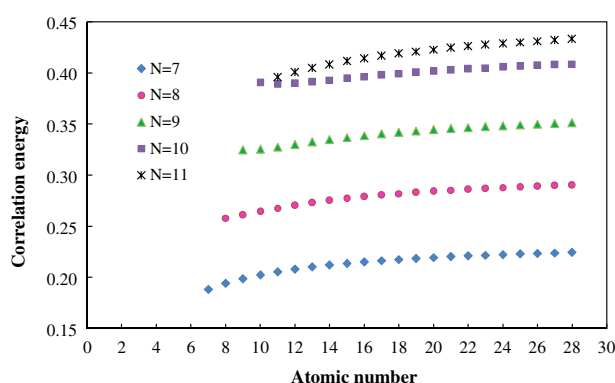
$$\ln \frac{E_{\text{corr}}}{N} = \ln \lambda + \beta \ln Z + \gamma (\ln Z)^2 \quad (11)$$

The accurate correlation energies of species with  $N = 2, 3$  from Ref. [7] are then used to find the best fit for parameters  $\lambda$ ,  $\beta$  and  $\gamma$ . The

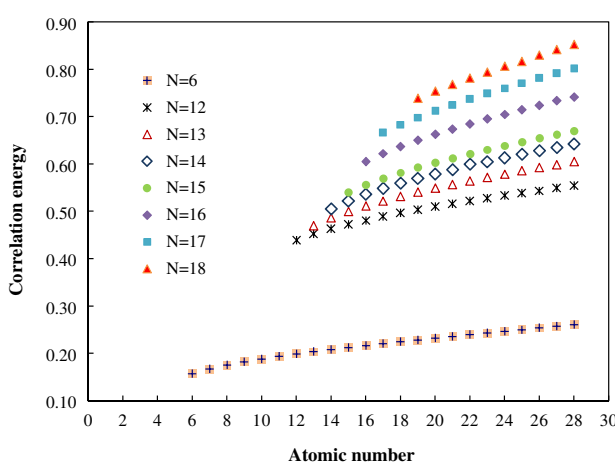
Table 1

Fitting parameters, regression coefficients and average absolute deviations (kcal/mol) of Eq. (10) for isoelectronic series with  $N = 4-18$ .

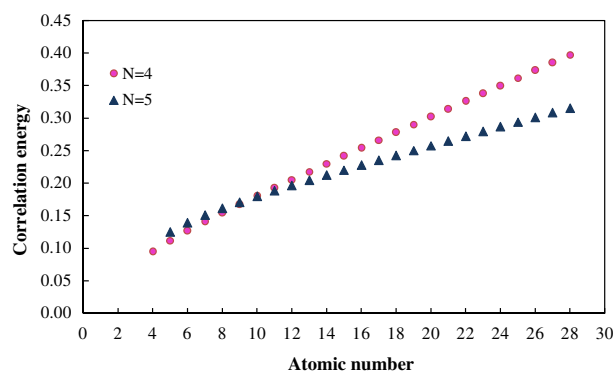
| $N$ | $\beta$ | $\lambda$ | $R^2$ | Number of data points | AAD  |
|-----|---------|-----------|-------|-----------------------|------|
| 4   | 0.736   | 0.008     | 0.999 | 25                    | 1.74 |
| 5   | 0.528   | 0.011     | 0.998 | 24                    | 1.20 |
| 6   | 0.317   | 0.015     | 0.999 | 23                    | 0.49 |
| 7   | 0.116   | 0.022     | 0.957 | 22                    | 1.08 |
| 8   | 0.094   | 0.027     | 0.984 | 21                    | 0.70 |
| 9   | 0.074   | 0.031     | 0.992 | 20                    | 0.54 |
| 10  | 0.052   | 0.034     | 0.976 | 19                    | 0.47 |
| 11  | 0.094   | 0.029     | 0.985 | 18                    | 0.70 |
| 12  | 0.266   | 0.019     | 0.996 | 17                    | 0.95 |
| 13  | 0.318   | 0.016     | 0.995 | 16                    | 1.34 |
| 14  | 0.335   | 0.015     | 0.995 | 15                    | 1.61 |
| 15  | 0.335   | 0.015     | 0.997 | 14                    | 1.06 |
| 16  | 0.357   | 0.014     | 0.997 | 13                    | 1.07 |
| 17  | 0.365   | 0.014     | 0.998 | 12                    | 0.98 |
| 18  | 0.371   | 0.014     | 0.999 | 11                    | 0.90 |



**Fig. 2.** Correlation energy (Hartree) versus atomic number for isoelectronic series,  $N = 7–11$ .



**Fig. 3.** Correlation energy (Hartree) versus atomic number for isoelectronic series,  $N = 6, 12–18$ .

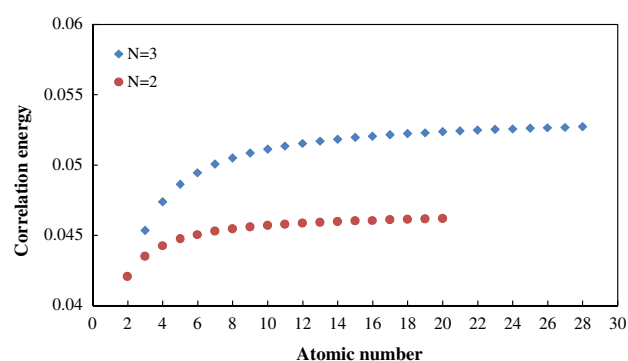


**Fig. 4.** Correlation energy (Hartree) versus atomic number for isoelectronic series,  $N = 4, 5$ .

values of fitting parameters and the regression coefficients are reported in Table 2. The regression coefficients and the AAD values indicate the reliability of the proposed formula to predict the correlation energies for 2- and 3-electron species.

### 3.2. Molecular correlation energy

Important efforts have been made to provide new methods for calculation of molecular correlation energy. These calculations have various problems such as large disc space demand, slow con-



**Fig. 5.** Correlation energy (Hartree) versus atomic number for isoelectronic series,  $N = 2, 3$ .

**Table 2**

Fitting parameters, regression coefficients and average absolute deviations (kcal/mol) of Eq. (11) for isoelectronic series with  $N = 2, 3$ .

| $N$ | $\gamma$ | $\beta$ | $\lambda$ | $R^2$ | Number of data points | AAD  |
|-----|----------|---------|-----------|-------|-----------------------|------|
| 2   | −0.017   | 0.121   | 0.020     | 0.996 | 19                    | 0.03 |
| 3   | −0.03    | 0.197   | 0.013     | 0.995 | 26                    | 0.07 |

vergence and restricted applicability [14–16]. However, there still remains the need to develop more efficient methods which allow extension of the electron correlation calculations to large systems.

Here, we checked the additivity of atomic correlation energies to obtain the correlation energy for closed-shell molecules. Clementi has pointed out there is a more or less extra correlation energy in a molecule for each chemical bond that is formed [17]. However, some studies demonstrate that the molecular correlation energies are additive in view of the fact that chemical bond energies are very small fraction of the total energies [18–20].

In this work, our main goal is to show that the correlation energy of closed-shell polyatomic molecules in their ground state can be computed in terms of the correlation energies of the constituent atoms. For developing and testing the proposed method we construct a set of molecules composed of H, C, N, O, and F atoms. The molecular correlation energy is expressed in terms of atomic correlation energies and total number of electrons in the molecule ( $N$ )

$$E_{\text{corr}}(\text{Molecule}) = a \sum_i E_{\text{corr}}(i) + bN + c \quad (12)$$

where the sum is extended over the exact correlation energy of all atoms in the molecule. To evaluate the parameters  $a$ ,  $b$  and  $c$  we use the molecular correlation energies reported at G2 level [20]. Despite the G2 correlation energy is not certainly the best possible choice for the correlation energy, yet provides near chemical accuracy energies, we have chosen the G2 method because it is well tested on a large set of molecules where CI calculations are not readily available.

We used a set including 35 closed-shell molecules composed of H, C, N, O, and F atoms to obtain the fitting parameters  $a$ ,  $b$  and  $c$  by multiple linear regression. The parameters  $a$ ,  $b$  and  $c$  are determined to be, respectively, 0.393, 0.018 and 0.012 for reproducing best the G2 correlation energies in our molecular data set. Table 3 collects the calculated molecular correlation energy and the corresponding values reported at G2 level,  $E_{\text{corr}}(\text{G2})$ , as well as the percent of errors. The results show how good is the agreement between the  $E_{\text{corr}}(\text{G2})$  and the calculated correlation energies in this work. The linear regression coefficient of  $R^2 = 0.999$  indicates the reliability of the present method.

**Table 3**

Correlation energies of 35 molecules obtained in this work and G2 values (Hartree) as well as the percent of errors.

| Molecule   | $E_{\text{corr}}$ (this work) | $E_{\text{corr}}$ (G2) | Error (%) |
|--|-------------------------------|------------------------|-----------|
| Methane (CH <sub>4</sub> )   | 0.2532                        | 0.2433                 | 4.06      |
| Water (H <sub>2</sub> O)   | 0.2933                        | 0.2998                 | −2.18     |
| Hydrogen fluoride (HF)   | 0.3196                        | 0.3063                 | 4.34      |
| Carbon monoxide (CO)   | 0.4264                        | 0.4125                 | 3.37      |
| Nitrogen (N <sub>2</sub> )   | 0.4201                        | 0.4302                 | −2.34     |
| Formaldehyde (H <sub>2</sub> CO)                                     | 0.4623                        | 0.4616                 | 0.16      |
| Fluorine (F <sub>2</sub> )   | 0.5910                        | 0.5885                 | 0.42      |
| Carbondioxide (CO <sub>2</sub> )                                     | 0.6715                        | 0.6835                 | −1.76     |
| Hydrogen cyanide (HCN)   | 0.4032                        | 0.4031                 | 0.03      |
| Ethane (C <sub>2</sub> H <sub>6</sub> )                              | 0.4582                        | 0.4480                 | 2.27      |
| Methylamine (CH <sub>3</sub> NH <sub>2</sub> )                       | 0.4751                        | 0.4811                 | −1.25     |
| Isobutene (C <sub>4</sub> H <sub>8</sub> )                           | 0.8323                        | 0.8219                 | 1.26      |
| Methanol (CH <sub>3</sub> OH)  | 0.4983                        | 0.5028                 | −0.90     |
| Formic acid (HCO <sub>2</sub> H)                                     | 0.7074                        | 0.7230                 | −2.16     |
| Acetonitrile (CH <sub>3</sub> CN)                                    | 0.6082                        | 0.6062                 | 0.33      |
| Dimethylether (CH <sub>3</sub> OCH <sub>3</sub> )                    | 0.7033                        | 0.7088                 | −0.78     |
| Oxirane (C <sub>2</sub> H <sub>4</sub> O)                            | 0.6673                        | 0.6748                 | −1.11     |
| Carboxyfluoride (COF <sub>2</sub> )                                  | 1.0051                        | 0.9954                 | 0.98      |
| Aziridine (C <sub>2</sub> H <sub>4</sub> NH)                         | 0.6442                        | 0.6519                 | −1.19     |
| Acrylonitrile (CH <sub>2</sub> CHCN)                                 | 0.7773                        | 0.7733                 | 0.52      |
| Acetyl fluoride (CH <sub>3</sub> COF)                                | 0.9387                        | 0.9340                 | 0.51      |
| Acetic acid (CH <sub>3</sub> CO <sub>2</sub> H)                      | 0.9124                        | 0.9276                 | −1.64     |
| Acetaldehyde (CH <sub>3</sub> CHO)                                   | 0.6673                        | 0.6665                 | 0.13      |
| Ethanol (C <sub>2</sub> H <sub>5</sub> OH)                           | 0.7033                        | 0.7091                 | −0.82     |
| Glyoxal (HCOCOH)   | 0.8765                        | 0.8878                 | −1.27     |
| Dimethylamine ((CH <sub>3</sub> ) <sub>2</sub> NH)                   | 0.6801                        | 0.6882                 | −1.18     |
| Cyclobutane (C <sub>4</sub> H <sub>8</sub> )                         | 0.8323                        | 0.8257                 | 0.79      |
| Acetone ((CH <sub>3</sub> ) <sub>2</sub> CO)                         | 0.8723                        | 0.8731                 | −0.09     |
| Trans-butane (C <sub>4</sub> H <sub>10</sub> )                       | 0.8682                        | 0.8626                 | 0.65      |
| Methyl ethyl ether (C <sub>2</sub> H <sub>5</sub> OCH <sub>3</sub> ) | 0.9083                        | 0.9154                 | −0.78     |
| Furan (C <sub>4</sub> H <sub>4</sub> O)                              | 1.0055                        | 1.0114                 | −0.59     |
| Trifluoroacetonitrile (CF <sub>3</sub> CN)                           | 1.4224                        | 1.4111                 | 0.80      |
| Propane (C <sub>3</sub> H <sub>8</sub> )                             | 0.6632                        | 0.6551                 | 1.23      |
| Pyridine (C <sub>5</sub> H <sub>5</sub> N)                           | 1.1514                        | 1.1468                 | 0.40      |
| Cyclopropene (C <sub>3</sub> H <sub>4</sub> )                        | 0.5913                        | 0.5800                 | 1.95      |

**Table 4**

Correlation energies obtained in this work and G2 values (Hartree) as well as the percent of errors for the prediction set of 12 molecules.

| Molecule   | $E_{\text{corr}}$ (this work) | $E_{\text{corr}}$ (G2) | Error (%) |
|--|-------------------------------|------------------------|-----------|
| Trans-butadiene (C <sub>4</sub> H <sub>6</sub> )     | 0.7972                        | 0.7793                 | 2.30      |
| Tetrafluoromethane (CF <sub>4</sub> )                | 1.2789                        | 1.3054                 | −2.03     |
| Trifluoromethane (CF <sub>3</sub> H)                 | 1.0685                        | 1.0393                 | 2.81      |
| Difluoromethane (CF <sub>2</sub> H <sub>2</sub> )    | 0.7968                        | 0.7722                 | 3.18      |
| Acetamide (CH <sub>3</sub> CONH <sub>2</sub> )       | 0.8902                        | 0.9055                 | −1.69     |
| Tetrafluoroethylene (C <sub>2</sub> F <sub>4</sub> ) | 1.5095                        | 1.4763                 | 2.25      |
| Ethylene (C <sub>2</sub> H <sub>4</sub> )            | 0.4226                        | 0.4064                 | 3.99      |
| Hydrazine (N <sub>2</sub> H <sub>4</sub> )           | 0.4924                        | 0.5149                 | −4.37     |
| Ethanedinitrile (NCCN)                               | 0.7590                        | 0.7785                 | −2.50     |
| Acetylene (C <sub>2</sub> H <sub>2</sub> )           | 0.3866                        | 0.3699                 | 4.52      |
| 2-Butyne (C <sub>4</sub> H <sub>6</sub> )            | 0.7972                        | 0.7795                 | 2.27      |
| Propylene (C <sub>3</sub> H <sub>6</sub> )           | 0.6279                        | 0.6132                 | 2.40      |

The prediction ability of our proposed method for calculation of molecular correlation energy was confirmed by calculation of the correlation energies for 12 molecules which no included in our fitting data set. Indeed, the prediction ability of our model has been checked by random splitting of the data into calibration (35 mole-

cules) and prediction (12 molecules) sets. Using the fitting parameters ( $a$ ,  $b$  and  $c$ ) and the Eq. (12), the correlation energies were computed for the prediction set of molecules. The computed correlation energies in Table 4 reveal that not only the correct trend is well reproduced but also the calculated correlation energies are quantitatively in very good agreement with those reported by G2 method. Therefore, it could be concluded that the introduced method in this work offers an economical procedure which is easily available to estimate the correlation energies of closed-shell polyatomic molecules.

#### 4. Conclusions

In the present work, a good performance of electron density at the nucleus has been developed to estimate atomic correlation energy. Starting from the empirical formula of  $E_{\text{corr}} = CN\rho(0)Z^{-\gamma}$ , we use the nuclear-electron coalescence cusp condition which implies that  $\rho(0)$  is a function of atomic number. First, we try to estimate the atomic correlation energy as a bilinear function of atomic number and number of electrons. The large deviation of the calculated correlation energies from accurate ones indicate that the correlation energy takes different behavior in species with different number of electrons. Therefore, we defined  $\frac{E_{\text{corr}}}{N} = \lambda Z^{\beta}$ , where  $\lambda$  and  $\beta$  are constants that are largely invariant within an isoelectronic series. We found that the proposed formula can achieve chemical accuracy (average absolute deviation in the order of 1 kcal/mol) for various isoelectronic series with  $N = 4$ –18. For  $N = 2, 3$  a quadratic expression in terms of  $\ln Z$  would result the best fit of correlation energy with deviation less than 0.1 kcal/mol.

Also the additivity scheme has been used to obtain molecular correlation energy in terms of correlation energies of the constituent atoms and number of electrons. The calculated correlation energies are in good agreement with those obtained by G2 method. In addition, the proposed formula confirms that in a molecule the electron correlation is larger than the sum over electron correlations of its corresponding constituent atoms.

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