

# Evaluation of static atomic charges in elementary nanostructures: Boron planar clusters

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**Abstract:** Static atomic charges affect key ground-state parameters of boron quasi-planar clusters  $B_n$ ,  $n \leq 20$ , which serve as building blocks of borophenes and other two-dimensional boron-based materials promising for various advanced applications. Assuming that the outer valence shells partial electron density of the constituent B atoms are shared between them proportionally to their coordination numbers, the static atomic charges in small boron planar clusters in the electrically neutral and positively and negatively singly charged states are estimated to be in the ranges of  $-0.750e$  ( $B_7^0$ ) to  $+0.535e$  ( $B_{20}^0$ ),  $-0.500e$  ( $B_7^+$ ,  $B_8^+$ , and  $B_9^+$ ) to  $+0.556e$  ( $B_{17}^+$ ), and  $-1.000e$  ( $B_7^-$ ) to  $+0.512e$  ( $B_{20}^-$ ), respectively.

**Keywords:** static atomic charge; coordination number; valence electron; cluster; boron

## 1. Introduction

The combination of atoms into a bound structure with subsequent redistribution of the valence electron densities of individual atoms can lead to the appearance of non-zero static atomic charges. Their influence on the polarity of chemical bonds in a substance and the associated physicochemical properties is most significant in chemical compounds with large differences in the electronegativity of the constituent elements. However, static charges of atoms are found even in elementary structures with different coordination of atomic sites. This effect is most noticeable in small clusters with comparable numbers of central and peripheral atoms.

Good examples of such kind are all-boron clusters consisting of up to 20 atoms with quasi-planar ground states. Evaluating static atomic charges in  $B_n$ ,  $n = 1, 2, 3, \dots, 20$ , nanoclusters is not only of academic, but also quite high practical interest, because they are considered as the building blocks of borophenes [1–3], a class of two-dimensional materials promising for nanoelectronics (wiring in nano-IC and nanocapacitor plates) [4–9], radiation protection (from neutron fluxes and accompanying gamma-rays), formation of hard and corrosion-resistant coatings, etc.

In the present work, this problem is solved within the framework of a model approach, which assumes that the partial electron density of the outer valence shells of the constituent B-atoms is redistributed between them in dependence on their coordination.

## 2. Model

To estimate the effective values of the static atomic charges in an elementary

structure, it is natural to assume that the effective number of valence electrons centered on a given atomic site and participating in the electron transfer to/from the nearest neighbors is proportional to its coordination number [10]. This study describes the corresponding simple model of the distribution of static atomic charges in elementary structures.

Let the structure consist of  $n$  identical atoms, each of which gives up  $\nu$  valence electrons participating in the electron transfer to/from the remaining constituent atoms. Then the total number  $N$  of such electrons is:

$$N = n\nu. \quad (1)$$

Denoting the coordination number of the  $i$ th site by  $C_i$  ( $i = 1, 2, 3, \dots, n$ ), the corresponding effective number  $\nu_i$  of localized electrons were found:

$$\nu_i = \frac{NC_i}{\sum_{j=1}^{j=n} C_j} = \frac{n\nu C_i}{\sum_{j=1}^{j=n} C_j}. \quad (2)$$

The difference between  $\nu$  and  $\nu_i$  values give the desired effective charge numbers  $z_i$ :

$$z_i = \nu - \nu_i = \nu \left( 1 - \frac{nC_i}{\sum_{j=1}^{j=n} C_j} \right). \quad (3)$$

An isolated B atom has 3 valence electrons: 2 and 1, respectively, in the inner  $2s$ - and outer  $2p$ -states. The energy level of  $2s$ -electrons is located much deeper than the  $2p$ -level. This means that practically only  $2p$ -electrons are involved in the transfer:  $\nu \approx 1$ . Then, for all-boron structures in the electrically neutral state, the static atomic charge numbers  $z_i^0$  are:

$$z_i^0 \approx 1 - \frac{nC_i}{\sum_{j=1}^{j=n} C_j}. \quad (4)$$

The multiply positively charged atomic structures are metastable due to their high ability to capture electrons from the environment or to annihilate with negatively charged ones, while the multiply negatively charged atomic structures are not stable at all. For this reason, the study considers only singly positively and singly negatively charged all-boron structures with  $N - 1 \approx n - 1$  and  $N + 1 \approx n + 1$  electrons participating in the transfer, respectively. This gives their static atomic charge numbers  $z_i^+$  and  $z_i^-$ :

$$z_i^+ \approx 1 - \frac{(n-1)C_i}{\sum_{j=1}^{j=n} C_j}, \quad (5)$$

$$z_i^- \approx 1 - \frac{(n+1)C_i}{\sum_{j=1}^{j=n} C_j}. \quad (6)$$

Why, despite its simplicity, can the coordination number-based method for estimating static atomic charges be valuable? This is explained by the necessity of representing the bonds polarity in clusters through the interatomic transfer of static point charges, when:

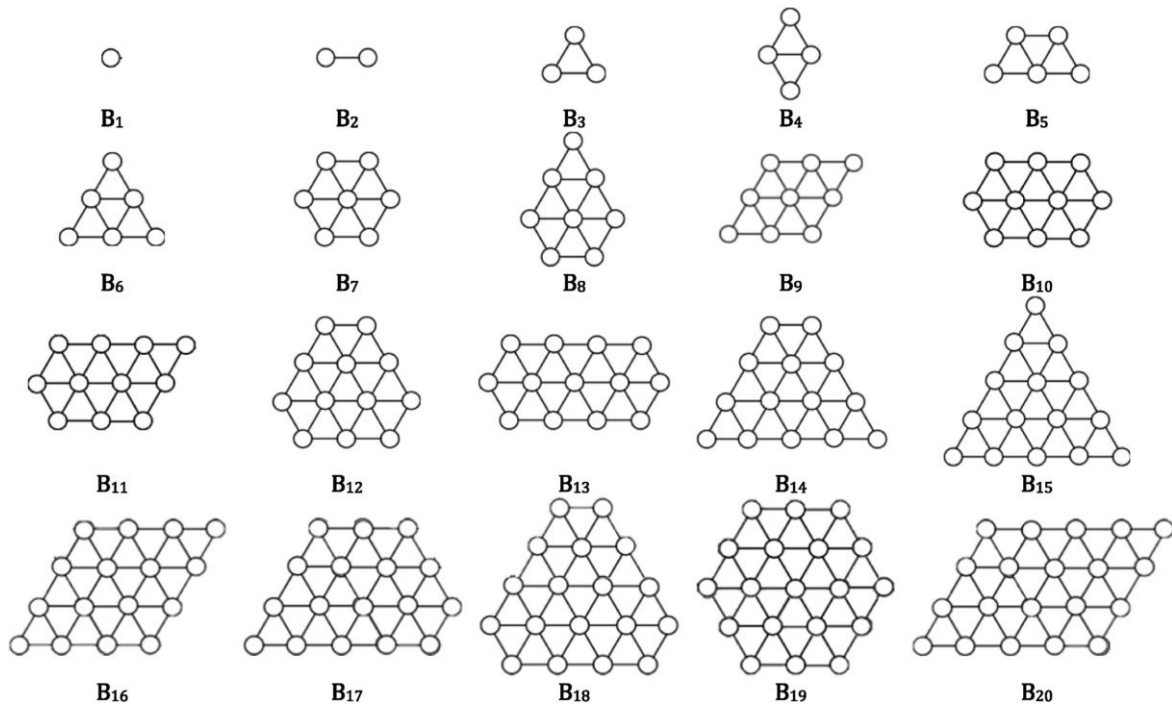
- (1) A diatomic model is used to calculate their binding energy;
- (2) The constituent atoms are identical and, consequently, their non-zero static

charges cannot be attributed to differences in quantum-chemical properties such as ionization energy, electron affinity, and electronegativity;

- (3) For convenience of calculation, the lengths of all bonds between identical atoms are assumed to be the same, which makes the difference in coordination numbers the only cause of interatomic charge transfer.

### 3. Results

**Figure 1** shows the structures of boron small planar clusters  $B_n$ ,  $n = 1, 2, 3, \dots, 20$ , selected for the ground-state isomorphs [11], while **Tables 1–3** present the static atomic charges evaluated using Equations (4)–(6) for electrically neutral, positively and negatively charged clusters, respectively. Note that the charge numbers given in these tables are obtained by rounding the calculated values (to the third decimal place): the charge balance relationships for clusters are only approximately observed.



**Figure 1.** Ground-state isomorphs of boron small planar clusters [11].

**Table 1.** Static atomic charge numbers  $\times$  atomic site numbers in neutral boron small planar clusters.

| Cluster | Coordination number  |                      |                      |                   |                   |                   |
|---------|----------------------|----------------------|----------------------|-------------------|-------------------|-------------------|
|         | 0                    | 1                    | 2                    | 3                 | 4                 | 6                 |
| $B_1^0$ | $\pm 0.000 \times 1$ |                      |                      |                   |                   |                   |
| $B_2^0$ |                      | $\pm 0.000 \times 2$ |                      |                   |                   |                   |
| $B_3^0$ |                      |                      | $\pm 0.000 \times 3$ |                   |                   |                   |
| $B_4^0$ |                      |                      | $+0.200 \times 2$    | $-0.200 \times 2$ |                   |                   |
| $B_5^0$ |                      |                      | $+0.286 \times 2$    | $-0.071 \times 2$ | $-0.429 \times 1$ |                   |
| $B_6^0$ |                      |                      | $+0.333 \times 3$    |                   | $-0.333 \times 3$ |                   |
| $B_7^0$ |                      |                      |                      | $+0.125 \times 6$ |                   | $-0.750 \times 1$ |
| $B_8^0$ |                      |                      | $+0.429 \times 1$    | $+0.143 \times 4$ | $-0.143 \times 2$ | $-0.714 \times 1$ |

|                              |            |            |             |            |
|------------------------------|------------|------------|-------------|------------|
| B <sub>9</sub> <sup>0</sup>  | +0.438 × 2 | +0.156 × 2 | −0.125 × 4  | −0.688 × 1 |
| B <sub>10</sub> <sup>0</sup> |            | +0.211 × 6 | −0.053 × 2  | −0.579 × 2 |
| B <sub>11</sub> <sup>0</sup> | +0.476 × 1 | +0.214 × 4 | −0.048 × 4  | −0.571 × 2 |
| B <sub>12</sub> <sup>0</sup> |            | +0.250 × 6 | ±0.000 × 3  | −0.500 × 3 |
| B <sub>13</sub> <sup>0</sup> |            | +0.250 × 6 | ±0.000 × 4  | −0.500 × 3 |
| B <sub>14</sub> <sup>0</sup> | +0.500 × 2 | +0.250 × 2 | ±0.000 × 7  | −0.500 × 3 |
| B <sub>15</sub> <sup>0</sup> | +0.500 × 3 |            | ±0.000 × 9  | −0.500 × 3 |
| B <sub>16</sub> <sup>0</sup> | +0.515 × 2 | +0.273 × 2 | +0.030 × 8  | −0.454 × 4 |
| B <sub>17</sub> <sup>0</sup> | +0.528 × 1 | +0.292 × 4 | +0.056 × 7  | −0.417 × 5 |
| B <sub>18</sub> <sup>0</sup> |            | +0.308 × 6 | +0.077 × 6  | −0.385 × 6 |
| B <sub>19</sub> <sup>0</sup> |            | +0.321 × 6 | +0.095 × 6  | −0.357 × 7 |
| B <sub>20</sub> <sup>0</sup> | +0.535 × 2 | +0.302 × 2 | +0.070 × 10 | −0.395 × 6 |

**Table 2.** Static atomic charge numbers × atomic site numbers in singly positively charged boron small planar clusters.

| Cluster                      | Coordination number |            |            |            |             |            |
|------------------------------|---------------------|------------|------------|------------|-------------|------------|
|                              | 0                   | 1          | 2          | 3          | 4           | 6          |
| B <sub>1</sub> <sup>+</sup>  | +1.000 × 1          |            |            |            |             |            |
| B <sub>2</sub> <sup>+</sup>  |                     | +0.500 × 2 |            |            |             |            |
| B <sub>3</sub> <sup>+</sup>  |                     |            | +0.333 × 3 |            |             |            |
| B <sub>4</sub> <sup>+</sup>  |                     |            | +0.400 × 2 | +0.100 × 2 |             |            |
| B <sub>5</sub> <sup>+</sup>  |                     |            | +0.429 × 2 | +0.143 × 2 | −0.143 × 1  |            |
| B <sub>6</sub> <sup>+</sup>  |                     |            | +0.444 × 3 |            | −0.111 × 3  |            |
| B <sub>7</sub> <sup>+</sup>  |                     |            |            | +0.250 × 6 |             | −0.500 × 1 |
| B <sub>8</sub> <sup>+</sup>  |                     |            | +0.500 × 1 | +0.250 × 4 | ±0.000 × 2  | −0.500 × 1 |
| B <sub>9</sub> <sup>+</sup>  |                     |            | +0.500 × 2 | +0.250 × 2 | ±0.000 × 4  | −0.500 × 1 |
| B <sub>10</sub> <sup>+</sup> |                     |            |            | +0.282 × 6 | +0.053 × 2  | −0.421 × 2 |
| B <sub>11</sub> <sup>+</sup> |                     |            | +0.524 × 1 | +0.286 × 4 | +0.048 × 4  | −0.429 × 2 |
| B <sub>12</sub> <sup>+</sup> |                     |            |            | +0.313 × 6 | +0.083 × 3  | −0.375 × 3 |
| B <sub>13</sub> <sup>+</sup> |                     |            |            | +0.308 × 6 | +0.077 × 4  | −0.385 × 3 |
| B <sub>14</sub> <sup>+</sup> |                     |            | +0.536 × 2 | +0.304 × 2 | +0.071 × 7  | −0.393 × 3 |
| B <sub>15</sub> <sup>+</sup> |                     |            | +0.533 × 3 |            | +0.067 × 9  | −0.400 × 3 |
| B <sub>16</sub> <sup>+</sup> |                     |            | +0.545 × 2 | +0.318 × 2 | +0.091 × 8  | −0.364 × 4 |
| B <sub>17</sub> <sup>+</sup> |                     |            | +0.556 × 1 | +0.333 × 4 | +0.111 × 7  | −0.333 × 5 |
| B <sub>18</sub> <sup>+</sup> |                     |            |            | +0.346 × 6 | +0.128 × 6  | −0.308 × 6 |
| B <sub>19</sub> <sup>+</sup> |                     |            |            | +0.357 × 6 | +0.143 × 6  | −0.286 × 7 |
| B <sub>20</sub> <sup>+</sup> |                     |            | +0.535 × 2 | +0.302 × 2 | +0.070 × 10 | −0.233 × 6 |

**Table 3.** Static atomic charge numbers × atomic site numbers in singly negatively charged boron small planar clusters.

| Cluster                     | Coordination number |   |   |   |   |   |
|-----------------------------|---------------------|---|---|---|---|---|
|                             | 0                   | 1 | 2 | 3 | 4 | 6 |
| B <sub>1</sub> <sup>−</sup> | −1.000 × 1          |   |   |   |   |   |

|                              |            |            |            |             |
|------------------------------|------------|------------|------------|-------------|
| B <sub>2</sub> <sup>−</sup>  | −0.500 × 2 |            |            |             |
| B <sub>3</sub> <sup>−</sup>  |            | −0.333 × 3 |            |             |
| B <sub>4</sub> <sup>−</sup>  |            | ±0.000 × 2 | −0.500 × 2 |             |
| B <sub>5</sub> <sup>−</sup>  |            | +0.143 × 2 | −0.286 × 2 | −0.714 × 1  |
| B <sub>6</sub> <sup>−</sup>  |            | +0.222 × 3 |            | −0.556 × 3  |
| B <sub>7</sub> <sup>−</sup>  |            |            | ±0.000 × 6 | −1.000 × 1  |
| B <sub>8</sub> <sup>−</sup>  |            | +0.357 × 1 | +0.036 × 4 | −0.286 × 2  |
| B <sub>9</sub> <sup>−</sup>  |            | +0.375 × 2 | +0.063 × 2 | −0.250 × 4  |
| B <sub>10</sub> <sup>−</sup> |            |            | +0.132 × 6 | −0.158 × 2  |
| B <sub>11</sub> <sup>−</sup> |            | +0.429 × 1 | +0.143 × 4 | −0.143 × 4  |
| B <sub>12</sub> <sup>−</sup> |            |            | +0.188 × 6 | −0.083 × 3  |
| B <sub>13</sub> <sup>−</sup> |            |            | +0.192 × 6 | −0.077 × 4  |
| B <sub>14</sub> <sup>−</sup> |            | +0.464 × 2 | +0.196 × 2 | −0.071 × 7  |
| B <sub>15</sub> <sup>−</sup> |            | +0.467 × 3 |            | −0.067 × 9  |
| B <sub>16</sub> <sup>−</sup> |            | +0.485 × 2 | +0.227 × 2 | −0.030 × 8  |
| B <sub>17</sub> <sup>−</sup> |            | +0.500 × 1 | +0.250 × 4 | ±0.000 × 7  |
| B <sub>18</sub> <sup>−</sup> |            |            | +0.269 × 6 | +0.026 × 6  |
| B <sub>19</sub> <sup>−</sup> |            |            | +0.286 × 6 | +0.048 × 6  |
| B <sub>20</sub> <sup>−</sup> |            | +0.512 × 2 | +0.267 × 2 | +0.023 × 10 |
|                              |            |            |            | −0.465 × 6  |

Excluding from consideration the three smallest clusters with identically coordinated atoms, it can be stated that the static atomic charges in small planar B<sub>n</sub> clusters in the electrically neutral and positively and negatively singly charged states are estimated as −0.750e (B<sub>7</sub><sup>0</sup>) to +0.535e (B<sub>20</sub><sup>0</sup>), −0.500e (B<sub>7</sub><sup>+</sup>, B<sub>8</sub><sup>+</sup>, and B<sub>9</sub><sup>+</sup>) to +0.556e (B<sub>17</sub><sup>+</sup>), and −1.000e (B<sub>7</sub><sup>−</sup>) to +0.512e (B<sub>20</sub><sup>−</sup>), respectively. The largest absolute values of the static charge numbers are obtained in B<sub>7</sub><sup>−</sup> and B<sub>20</sub><sup>0</sup>: −1.000 and +0.535, respectively.

#### 4. Conclusion

It has been shown previously that the ground-state parameters of boron small clusters and, consequently, their relative stability and probability of formation can be successfully estimated in the so-called diatomic model or the approximation of pair interatomic potentials [12–15]. In such an approach, replacing the redistributed charge density of valence electrons with point charges does not introduce additional errors, but, on the contrary, taking into account the partial polarity of the bonds increases the reliability. In addition, this allows one to estimate the electric dipole moments of clusters and associated physical interactions with other species, as well as solid surfaces, for example, those that serve as substrates for the borophene growth. The results obtained here for planar boron clusters may have broader applications in future research directions, since nanostructures, clusters, nanoparticles, or structured materials, composed of a single element, such as only carbon atoms or only gold atoms, are materials that exhibit unique properties, often distinct from their bulk counterparts, due to quantum effects and high surface-to-volume ratios.

**Author contributions:** Idea proposed: LC; Calculation: TO; Result summarization: TO & LC; Manuscript writing: LC. Both authors have read and agreed to the published version of the manuscript.

**Conflict of interest:** The authors declare no conflict of interest.

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