MATHEMATICAL EXPRESSION OF THE COMMUNICATION NUMBERS IN CHEMICAL COMPOUNDS

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Abstract: *article is devoted to the order of mathematical calculation of communication numbers in chemical combinations without using from graphic formulas. Finding of chemical communication numbers by mathematical method in salt and acid molecules is reflected through offered formula. Communication numbers in linoleic acid concerning organic combinations and fat moleculas are determined by mathematical method.*
The article is devoted to finding the total of (σ) sigma bonds used by most elementary school of organic compounds. Finding of π(pi) communication numbers by mathematical method in oil and acid molecules is reflected through offered formula. Exactness of results of mathematical calculations is approved through graphic formulas.
Keywords: *molecule, atom, chemistry teaching, interdisciplinary communication, oil, graphic formula, π(pi) bond, σ(sigma) bond, acid, cubane, fullurene.*

МАТЕМАТИЧЕСКОЕ ВЫРАЖЕНИЕ КОЛИЧЕСТВА СВЯЗЕЙ В ХИМИЧЕСКИХ СОЕДИНЕНИЯХ

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Аннотация: *в статье впервые отображен порядок математического вычисления количества связи в химических соединениях без применения графических форм. С помощью представленной формулы отражено нахождение математическим методом количества химической связи в молекулах соли и кислоты. Математическим методом установлены количества связи в линолевой кислоте и в молекулах масла. В статье впервые решена проблема математического вычисления количества (σ) сигма связей в химических соединениях. С помощью представленной формулы отражено нахождение математическим методом количества π(пи) связи в молекулах масла. Точность результатов математического вычисления утверждена с помощью графических формул.*
Ключевые слова: *молекула, атом, обучения химии, межпредметные связи, масла, графическая формула, π(пи) связь, σ(сигма) связь, кислота, кубан, фуллерен.*

Chemical linkages define the spatial structure of the molecules by forming bond angles, link, join atoms with each other forming chemical compounds. The type of chemical linkages, energy, stability, duration, intensity etc. are one of the basic concepts of the general chemistry [1, 2].

Number of chemical bonds is very important in the calculation of the thermal effect of the reaction, combustion and formation heats, enthalpy and etc.

It is known that the calculation of the communication numbers in chemical compounds is carried out by graphic formulas. Writing graphic formulas of simple chemical compounds is easier, while drawing graphic formulas of complex chemical compounds creates certain difficulties and requires considerable time.

I have conducted research in this direction which has yielded positive results. Thus, all inorganic and organic compounds, became possible to calculate the total amount of sigma *(σ)* and pi *(π)* bonds by mathematical method, without the use of graphic formulas. [3] For this, it is necessary to use the first proposed and the below given formula:

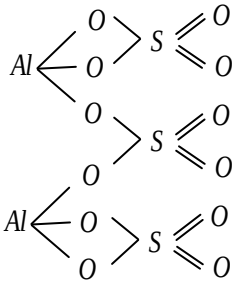
$$A_{(total)} = \frac{a_1e_1 + a_2e_2 + ... + a_ne_n}{2} \qquad (1)$$

$A_{(total)}$ - Here is the total communication numbers in the chemical compound, a_1, a_2 - the amount of different elements in combination, e_1, e_2 - data elements corresponding valence.

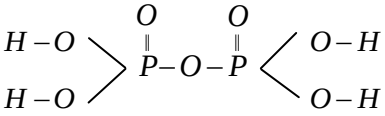
Let's consider the calculation'of the total number of chemical bonds in inorganic compounds $Al_2(SO_4)_3$ and $H_4P_2O_7$. It is known that iron is III, sulfur VI, oxygen is II valent in conjunction.

$$A_{(total)[Al_2(SO_4)_3]} = \frac{a_1e_1 + a_2e_2 + ... + a_ne_n}{2} = \frac{2\cdot 3 + 3\cdot 6 + 12\cdot 2}{2} = \frac{6+18+24}{2} = 24$$

If we write the graphic formula substances, and calculate the total number of links, we obtain the same result.



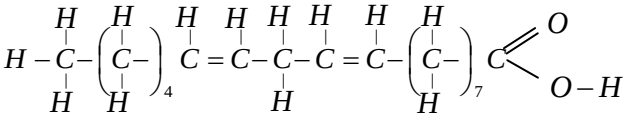
$$A_{(total)[H_4P_2O_7]} = \frac{a_1e_1 + a_2e_2 + ... + a_ne_n}{2} = \frac{4\cdot 1 + 2\cdot 5 + 7\cdot 2}{2} = \frac{4+10+14}{2} = 14$$



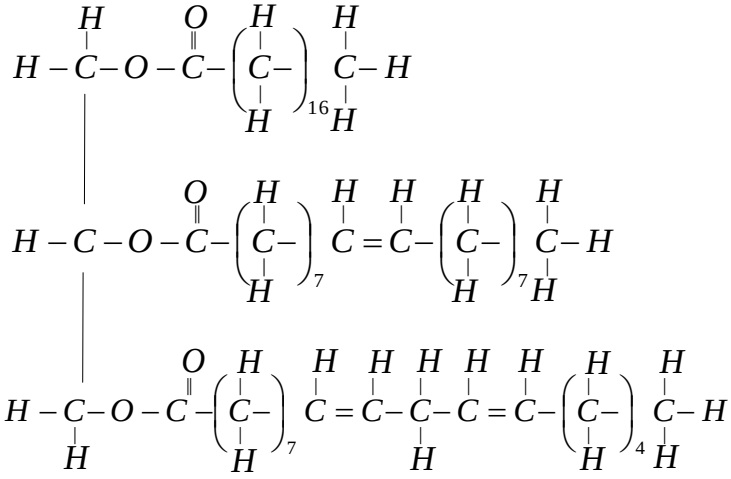
It is clearly seen that in diphosphate acid molecule the total number of connections is 14 in the graphic formula.

Calculation of amounts of chemical bonds in the molecules of organic substances was first proposed by the formula, without the use of graphic formulas ensures accurate results.

$$A_{(total)[C_{17}H_{31}COOH]} = \frac{a_1e_1 + a_2e_2 + ... + a_ne_n}{2} = \frac{18\cdot 4 + 32\cdot 1 + 2\cdot 2}{2} = \frac{72+32+4}{2} = 54$$



$$A_{(общ)}\left[\begin{matrix}CH_2OCOC_{17}H_{35}\\ CHOCOC_{17}H_{33}\\ CH_2OCOC_{17}H_{31}\end{matrix}\right] = \frac{a_1e_1 + a_2e_2 + ... + a_ne_n}{2} = \frac{57\cdot 4 + 104\cdot 1 + 6\cdot 2}{2} = \frac{228+104+12}{2} = \frac{344}{2} = 172$$



Obtaining the same results in graphical formulas, in, the presence of chemical bonds in 54 linoleic acid, and 172 - in the oil molecule demonstrates the importance of the proposed formula.

Using the formula to calculate the total number of chemical compounds in the fullerene molecules with different numbers of carbon atoms is more advantageous. Since fullerene molecules are arranged in a spherical. tubular form, drawing graphic formulas and calculating the amount of chemical bonds creates problems.

However, you can easily and accurately calculate the amount of chemical bonds in the fullerene molecules by the formula without using graphic formulas.

$$A_{(total)[C_{60}]} = \frac{a_1e_1 + a_2e_2 + ... + a_ne_n}{2} = \frac{60 \cdot 4}{2} = 120$$

$$A_{(total)[C_{540}]} = \frac{a_1e_1 + a_2e_2 + ... + a_ne_n}{2} = \frac{540 \cdot 4}{2} = 1080$$

Thus, the fullerene molecule (C_{60}) the number of common connections corresponds to 120, but in the fullerene molecule (C_{540}) - 1080.

Calculation of the numbers of the sigma *(σ)* bonds in chemical compounds.

Calculation of the numbers of sigma *(σ)* bonds in the chemical compounds is performed by graphic formulas as the total number of links. As mentioned above. the composition of graphic formulas of some complex substances creates certain difficulties. As example there can be shown the fullerene molecule in spherical, tubular form. Studies carried out by me in this direction and ended positively. Thus, it firstly became possible to calculate the number of sigma *(σ)* bonds in chemical compounds by mathematical method by proposed formula without using graphic formulas. [4] To do this, it can be used the first proposed and the following formula:

$$A_{(\sigma)} = N_{(total)} + \mathrm{S}\text{-}1 \qquad (2)$$

Here, $A(\sigma)$ - number of sigma *(σ)* connections in the chemical compounds, $N_{(total)}$ - total number of atoms in the compounds, S - the amount of cyclic groups.

It is known that for the calculation of the amounts of sigma *(σ)* connections in certain classes of organic compounds has the inherent formula in each class. However, these formulas do not cover all of the organic compounds. It should be noted that it is impossible to calculate the number of sigma *(σ)* connections with different number of benzene nuclei in automatic compounds belonging to the same class by one formula. If you change quantities benzene nuclei it is necessary to change the formula for calculating the amount of sigma *(σ)* bonds. An example of this can be shown as benzene, naphthalene, anthracene, etc.

However, by the same formula it can be calculated with precision the number of sigma *(σ)* relations in all inorganic and organic compounds.

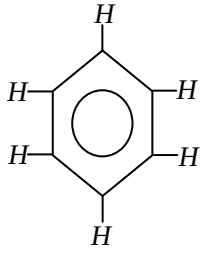
Let's consider the calculation of amounts of sigma *(σ)* bonds in the molecules of benzene (C_6H_6), naphthalene ($C_{10}H_8$) anthracene ($C_{28}H_{14}O_2N_2$). In the molecules of benzene, naphthalene, anthracene and indanthrene there are respective one, two, three, seven cyclic groups.

$$A_{(\sigma)[C_6H_6]} = N_{(total)} + S - 1 = 12 + 1 - 1 = 12 \qquad A_{(\sigma)[C_{10}H_8]} = N_{(total)} + S - 1 = 18 + 2 - 1 = 19$$

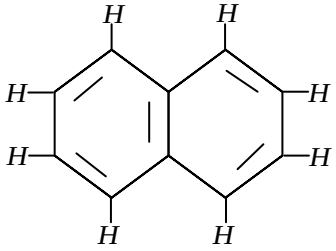
$$A_{(\sigma)[C_{14}H_{10}]} = N_{(total)} + S - 1 = 24 + 3 - 1 = 26$$

$$A_{(\sigma)[C_{28}H_{14}O_4N_2]} = N_{(total)} + S - 1 = 48 + 7 - 1 = 54$$

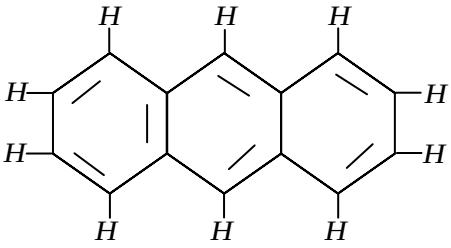
Calculating the number of sigma *(σ)* bonds graphic formulas of substances, we can obtain the same result.



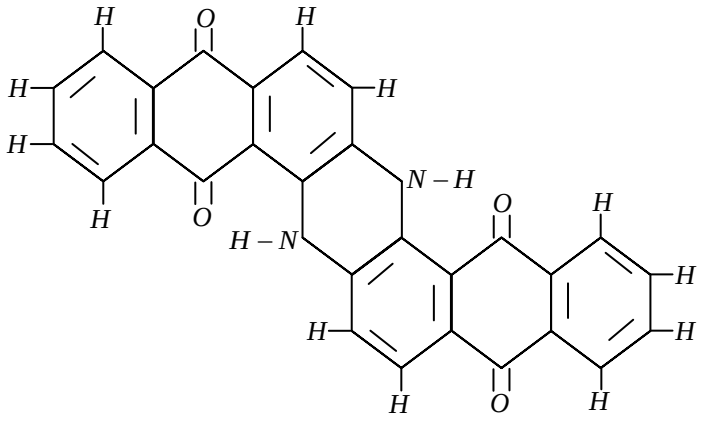
benzene



naphthalene



anthracene



indanthrene

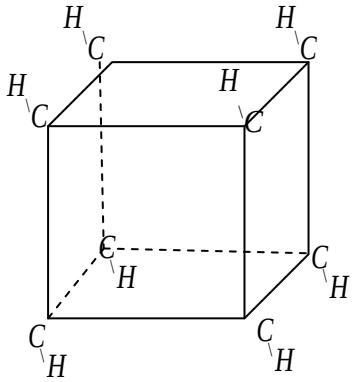
In the presence of polyhedral (tetrahedron, hexahedron, octahedron, dodecahedron, icosahedrons) and rotating bodies in graphic formulas of chemical compounds to calculate amounts of sigma *(σ)* connections to the proposed formula, add the (D) indicating the amount of data geometric shapes.

$$A_{(\sigma)} = N_{(total)} + S - (1 + D) \qquad (3)$$

Let's consider the calculation of the sigma *(σ)* amounts in cubane (C_8H_8) molecule, which contains a multi - faceted (hexahedron or cube).

$$A_{(\sigma)[C_8H_8]} = N_{(total)} + S - (1 + D) = 16 + 6 - (1 + 1) = 20$$

It is clear that the numbers of sigma *(σ)* bonds in the graphic formula is 20.



Through the proposed formula it can be calculated the number of sigma *(σ)* bonds in the molecules of inorganic and organic substances with precision having any spatial structures.

Calculating of the amount of sigma *(σ)* bond in fullurene (C_{60}) molecules with one rotating body, 32 facets (12 five-pointed and 20 six-pointed).

$$A_{(\sigma)[C_{60}]} = N_{(total)} + S - (1 + D) = 60 + 32 - (1 + 1) = 90.$$

References / Список литературы

1. *Abbasov Z.S.* "Kimyevi birleshmelerde rabite saylarının riyazi ifadesi" [Mathematical expression of the communication numbers in chemical compounds] // Elmi Eserler [Scientific Works]. Vol. 85. № 6, 2018. P. 156-158 [in Azerbaijani].
2. *Abbasov M.M., Abbasov Z.S., Zulfigarova A.V., Gunjegori N.A., Abbaszade S.M.* "Matematicheskoye vyrazheniye khimicheskikh svyazey v molekulakh uglevodorodov" [Mathematical expression of chemical bonds in hydrocarbon molecules] // Aspirant i soiskatel [Postgraduate and applicant]. № 1 (103), 2018. P. 9-12 [in Russian].

3. *Abbasov Z.S.* "Matematiyeskiy sposob opredeleniya chisla svyazey v molekulakh" [The mathematical method for determining the number of bonds in molecules] // Khimiya v shkole [Chemistry at school] 1`2015. P. 33-35 [in Russian].
4. *Abbasov M.M., Abbasov Z.S., Zulfigarova A.V., Gunjegori N.A.* "Matematicheskoye vyrazheniye kolichestv σ (sigma) svyazey v khimicheskikh soyedineniyakh" [The mathematical expression of the numbers of σ (sigma) bonds in chemical compounds] // Aspirant i soiskatel [Postgraduate and applicant]. № 4 (100), 2017. P. 18-21 [in Russian].