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Research Article

A Theoretical Framework for the Calculation of the Number of Covalent Bonds in Unsaturated Organic Compounds

Vlad Cristian Gavrilă*, Teodor Octavian Nicolescu

Department of Organic Chemistry, Faculty of Pharmacy, University of Medicine and Pharmacy "Carol Davila", Bucharest, Romania

Abstract

Theoretical frameworks are important structures that provide novel ways of understanding unique and complex ideas related to many fields of science. Therefore, in this manuscript we try to present a theoretical framework with new general equations that share a similar structure with the index of hydrogen deficiency and can be used to calculate the number of covalent bonds for numerous unsaturated organic molecules. Our mathematical model is based on graph theory combined with classical organic chemistry concepts, and the variables that made up all the general equations are represented by the number of atoms and the valence of those atoms that correspond to unsaturated organic compounds which contain only simple covalent bonds. The main scope of this model is to be used manually by scientists that are interested in performing an easy and fast calculation of bonds and rings for various classes of molecules in order to deduce more information about their possible chemical structures. Other objectives include the possibility for future implementation of computer programs based on IHD like equations similar with the ones that will be presented in this manuscript to help researchers speed up the process of identification and calculation of multiple chemical variables. In essence, our study represents a novel comprehensive methodology for finding the number of covalent bonds and rings in specific chemical compounds.

Keywords

Covalent Bonds, Theoretical Framework, Organic Compounds, Graph Theory, Equalities, Index of Hydrogen Deficiency

1. Introduction

In order to present our new mathematical equations for the calculation of covalent bonds in unsaturated organic compounds, we have established a general model that will be shown in this manuscript for five categories of organic molecules. Our model is based on graph theory principles [1], Lewis theory of chemical bonding [2], and valence bond theory [3]. However, algebraic calculations and a fixed structure which is similar with the general formula of the hydrogen deficiency index [4], were also required to achieve a simple and effective mathematical model for unsaturated organic molecules that fulfill certain structural conditions.

Besides the hydrogen deficiency index, another equation that uses only the number of atoms within a molecule for the calculation of σ-bonds exists [5]. However, this equation only works for acyclic organic compounds, because for the cyclic ones we also need to know the number of rings within a molecule and not just the number of atoms in order to calculate the number of σ-bonds. Additionally, there are particular

*Corresponding author: vlad.cristian.gavrila@gmail.com (Vlad Cristian Gavrilă)

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models with certain equations for the calculation of covalent bonds in Aliphatic Unsaturated Open Chain and Cycloalkynes [6], and for the calculation of covalent bonds in Open Chain Alcohols and Cycloamines [7].

Nevertheless, right now there isn't published any other methodology that has general equations for the calculation of the number of all the simple covalent bonds in specific unsaturated organic compounds which utilize only the molecular formula and respectively the number of atoms and the valence of those atoms for a given molecule. Therefore, in this article we try to present a simple and accessible theoretical framework that include eleven novel examples of general equations and two equations that already existed for five cases of equalities between chemical variables such as the number of π-bonds, double bonds, triple bonds and rings.

2. Materials and Methods

For this research, we have developed and applied a new methodology [8] which utilize the general structure of the equation for index of hydrogen deficiency (also known as the degree of unsaturation [9]) for unsaturated organic compounds. Our results include calculations performed on numerous theoretical molecular formulas, and they will be presented in the form of five tables that are rigorously verified with computer programs [10, 11]. Additionally, all the equations were also verified on many organic compounds using other methods such as manual calculations and comparisons between large sets of unsaturated molecules [12]. Therefore, the novel model that will be shown in this article consists of thirteen unique equations, eleven of them were deduced by us, and two of them already existed:

The general equations labeled with (3), (6), (9), (10), (12), (13), (16), (17) for σ and single bonds were made by precisely finding the value of specific numerical constants. In order to achieve this, we used graph theory principles and comparisons between large sets of molecules.

The general equations labeled with (7), (8), (11), (14), (15), (18) for π-bonds, double, triple bonds and rings were made by integrating various calculations from the index of hydrogen deficiency with our own ideas [2] and applying them on different classes of unsaturated molecules.

The equations labeled with (1), (2), (4), (5) for σ-bonds and π-bonds already existed, and we introduced them into our model to validate and solidify our claims.

Finally, our novel mathematical model for unsaturated organic compounds consist of eleven unique and new equations (3), (6), (7), (8), (9), (10), (11), (12), (13), (14), (15), (16), (17), (18) and two unique equations that already existed (1), (2), (4), (5) which taken together allow researchers who are working in the fields of organic chemistry, physical chemistry and analytical chemistry to perform a manual or automatic rapid calculation of covalent bonds and rings for certain molecules, and also to create tables based on their molecular formulas [13, 14].

3. Results and Discussion

For starters, all the equations that will be presented throughout this section are made up of multiple general variables. The meanings of those variables are as follows:

n_σ = the number of sigma bonds in a molecule n_π = the number of pi bonds in a molecule. n_r = the number of rings in a molecule. n_i = the number of atoms that correspond to a chemical element. v_i = the valence of a chemical element. n_s = the number of single bonds in a molecule. n_d = the number of double bonds in a molecule. n_t = the number of triple bonds in a molecule. i = the number of chemical elements in a molecule.

Additionally, in this manuscript we will show examples of molecules that have four types of chemical elements (C, N, O, H) so they can be easier to understand, however any atom who can participate in the formation of covalent bonds can be integrated into the upcoming general equations in a similar fashion with the index of hydrogen deficiency (IHD).

$$IHD = 1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right)$$

3.1. Unsaturated Acyclic Organic Compounds with Double Bonds

In order to calculate the number of covalent bonds for unsaturated acyclic organic compounds with double bonds we must choose a fixed valence for every chemical element that is present in our molecule. Also, the number of π-bonds is equal with the number of double bonds.

$$v_C = 4; \quad v_N = 3; \quad v_O = 2; \quad v_H = 1$$

3.1.1. Calculation of π-bonds ($n_\pi = n_d$)

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated acyclic organic molecule with double bonds. When this step is finished, the number of π-bonds will be calculated for the case in which we have one or more than one double bond present in our chosen unsaturated acyclic compound.

$$n_\pi = 1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right) \quad (1)$$

Example for : $C_7H_{14}N_2O_2$

$$n_\pi = 1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right)$$

$$n_\pi = 1 + \frac{2}{2}n_C + \frac{1}{2}n_N + \frac{0}{2}n_O - \frac{1}{2}n_H$$

$$n_\pi = 1 + 7 + 1 + 0 - 7$$

$$n_\pi = 2$$

3.1.2. Calculation of σ-bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated acyclic organic molecule with double bonds. When this step is finished, the number of σ-bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one double bond present in our chosen unsaturated acyclic compound.

$$n_\sigma = n_i - 1 \quad (2)$$

Example for : $C_7H_{14}N_2O_2$

$$n_\sigma = n_i - 1$$

$$n_\sigma = n_C + n_N + n_O + n_H - 1$$

$$n_\sigma = 7 + 2 + 2 + 14 - 1$$

$$n_\sigma = 24$$

3.1.3. Calculation of Single Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated acyclic organic molecule with double bonds. When this step is finished, the number of single bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one double bond present in our chosen unsaturated acyclic compound.

$$n_s = \left|2 + \tfrac{1}{2}\left(\sum_i n_i(v_i - 4)\right)\right| \quad (3)$$

Example for: $C_7H_{14}N_2O_2$

$$n_s = \left|2 + \tfrac{1}{2}\left(\sum_i n_i(v_i - 4)\right)\right|$$

$$n_s = \left|2 + \tfrac{0}{2}n_C - \tfrac{1}{2}n_N - \tfrac{2}{2}n_O - \tfrac{3}{2}n_H\right|$$

$$n_s = |2 + 0 - 1 - 2 - 21|$$

$$n_s = 22$$

Some theoretical examples of molecular structures for unsaturated acyclic organic compounds that contain only π-bonds, σ-bonds, single bonds and a double bond or multiple double bonds are:

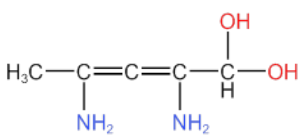

Figure 1. *First example of acyclic molecular structure with double bonds.*

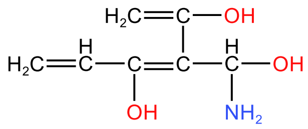

Figure 2. *Second example of acyclic molecular structure with double bonds.*

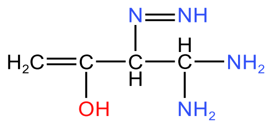

Figure 3. *Third example of acyclic molecular structure with double bonds.*

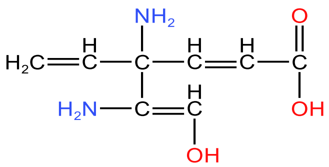

Figure 4. *Fourth example of acyclic molecular structure with double bonds.*

3.2. Unsaturated Acyclic Organic Compounds with Triple Bonds

In order to calculate the number of covalent bonds for unsaturated acyclic organic compounds with triple bonds we must choose a fixed valence for every chemical element that is present in our molecule. Also, the number of π-bonds is not equal with the number of triple bonds.

$$v_C = 4;\quad v_N = 3;\quad v_O = 2;\quad v_H = 1$$

3.2.1. Calculation of π-bonds ($n_\pi \neq n_t$)

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated acyclic organic molecule with triple bonds. When this step is finished, the number of π-bonds will be calculated for the case in which we have one or more than one triple bond present in our chosen unsaturated acyclic compound.

$$n_\pi = 1 + \tfrac{1}{2}\left(\sum_i n_i(v_i - 2)\right) \quad (4)$$

Example for : $C_8H_7NO_3$

$$n_\pi = 1 + \tfrac{1}{2}\left(\sum_i n_i(v_i - 2)\right)$$

$$n_\pi = 1 + \tfrac{2}{2}n_C + \tfrac{1}{2}n_N + \tfrac{0}{2}n_O - \tfrac{1}{2}n_H$$

$$n_\pi = 1 + 8 + 0.5 + 0 - 3.5$$

$$n_\pi = 6$$

3.2.2. Calculation of σ-bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated acyclic organic molecule with triple bonds. When this step is finished, the number of σ-bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one triple bond present in our chosen unsaturated acyclic compound.

$$n_\sigma = n_i - 1 \quad (5)$$

Example for: $C_8H_7NO_3$

$$n_\sigma = n_i - 1$$

$$n_\sigma = n_C + n_N + n_O + n_H - 1$$

$$n_\sigma = 8 + 1 + 3 + 7 - 1 \quad n_\sigma = 18$$

3.2.3. Calculation of Single Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated acyclic organic molecule with triple bonds. When this step is finished, the number of single bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one triple bond present in our chosen unsaturated acyclic compound.

$$n_s = \left|\frac{3}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 6)\right)\right| \quad (6)$$

Example for: $C_8H_7NO_3$

$$n_s = \left|\frac{3}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 6)\right)\right|$$

$$n_s = \left|\frac{3}{2} - \frac{2}{4}n_C - \frac{3}{4}n_N - \frac{4}{4}n_O - \frac{5}{4}n_H\right|$$

$$n_s = |1.5 - 4 - 0.75 - 3 - 8.75|$$

$$n_s = 15$$

3.2.4. Calculation of Triple Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated acyclic organic molecule. When this step is finished, the number of triple bonds will be calculated.

$$n_t = \frac{1}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 2)\right) \quad (7)$$

Example for: $C_8H_7NO_3$

$$n_t = \frac{1}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 2)\right)$$

$$n_t = \frac{1}{2} + \frac{2}{4}n_C + \frac{1}{4}n_N + \frac{0}{4}n_O - \frac{1}{4}n_H$$

$$n_t = 0.5 + 4 + 0.25 + 0 - 1.75$$

$$n_t = 3$$

Some theoretical examples of molecular structures for unsaturated acyclic organic compounds that contain only π-bonds, σ-bonds, single bonds and a triple bond or multiple triple bonds are:

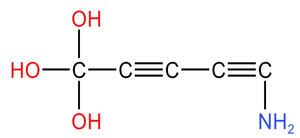

Figure 5. First example of acyclic molecular structure with triple bonds.

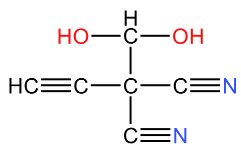

Figure 6. Second example of acyclic molecular structure with triple bonds.

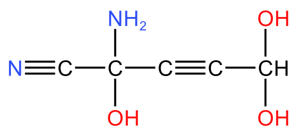

Figure 7. Third example of acyclic molecular structure with triple bonds.

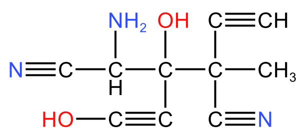

Figure 8. Fourth example of acyclic molecular structure with triple bonds.

3.3. Unsaturated Cyclic Organic Compounds with Double Bonds

In order to calculate the number of covalent bonds for unsaturated cyclic organic compounds with double bonds we must choose a fixed valence for every chemical element that is present in our molecule. Also, the number of π-bonds is equal with the number of double bonds and the number of rings.

$$v_C = 4; \quad v_N = 3; \quad v_O = 2; \quad v_H = 1$$

3.3.1. Calculation of π-bonds ($n_\pi = n_d = n_r$)

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with double bonds. When this step is finished, the number of π-bonds will be calculated for the case in which we have one or more than one double bond present in our chosen unsaturated cyclic compound.

$$n_\pi = \frac{1}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 2)\right) \tag{8}$$

Example for: $C_6H_{13}N_3O$

$$n_\pi = \frac{1}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 2)\right)$$

$$n_\pi = \frac{1}{2} + \frac{2}{4}n_C + \frac{1}{4}n_N + \frac{0}{4}n_O - \frac{1}{4}n_H$$

$$n_\pi = 0.5 + 3 + 0.75 + 0 - 3.25$$

$$n_\pi = 1$$

3.3.2. Calculation of σ-bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with double bonds. When this step is finished, the number of σ-bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one double bond present in our chosen unsaturated cyclic compound.

$$n_\sigma = -\frac{1}{2} + \frac{1}{4}\left(\sum_i n_i(v_i + 2)\right) \tag{9}$$

Example for : $C_6H_{13}N_3O$

$$n_\sigma = -\frac{1}{2} + \frac{1}{4}\left(\sum_i n_i(v_i + 2)\right)$$

$$n_\sigma = -\frac{1}{2} + \frac{6}{4}n_C + \frac{5}{4}n_N + \frac{4}{4}n_O + \frac{3}{4}n_H$$

$$n_\sigma = -0.5 + 9 + 3.75 + 1 + 9.75$$

$$n_\sigma = 23$$

3.3.3. Calculation of Single Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with double bonds. When this step is finished, the number of single bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one double bond present in our chosen unsaturated cyclic compound.

$$n_s = n_i - 1 \tag{10}$$

Example for : $C_6H_{13}N_3O$

$$n_s = n_i - 1$$

$$n_s = n_C + n_N + n_O + n_H - 1$$

$$n_s = 6 + 3 + 1 + 13 - 1 \quad n_s = 22$$

Some theoretical examples of molecular structures for unsaturated cyclic organic compounds that contain only π-bonds, σ-bonds, single bonds and a double bond or multiple double bonds are:

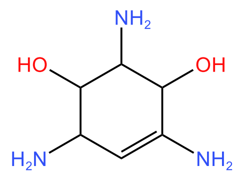

Figure 9. First example of cyclic molecular structure with a double bond.

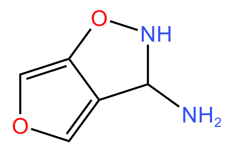

Figure 10. Second example of cyclic molecular structure with double bonds.

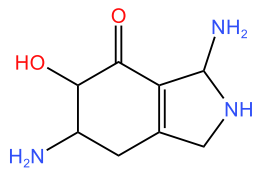

Figure 11. Third example of cyclic molecular structure with double bonds.

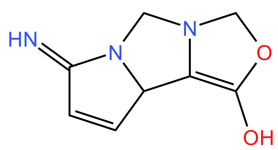

Figure 12. Fourth example of cyclic molecular structure with double bonds.

3.4. Unsaturated Cyclic Organic Compounds with Triple Bonds

In order to calculate the number of covalent bonds for unsaturated cyclic organic compounds with triple bonds we must choose a fixed valence for every chemical element that is present in our molecule. Also, the number of π-bonds is not equal with the number of triple bonds. However, the number of π-bonds is equal with the number of rings.

$$v_C = 4; \quad v_N = 3; \quad v_O = 2; \quad v_H = 1$$

3.4.1. Calculation of π-bonds ($n_\pi \neq n_t; \quad n_\pi = n_r$)

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with triple bonds. When this step is finished, the number of π-bonds will be calculated for the case in which we have one or more than one triple bond present in our chosen unsaturated cyclic compound.

$$n_\pi = \frac{1}{2} + \frac{1}{4}\left(\sum_i n_i (v_i - 2)\right) \quad (11)$$

Example for : $C_9H_{14}N_2O_4$

$$n_\pi = \frac{1}{2} + \frac{1}{4}\left(\sum_i n_i (v_i - 2)\right)$$

$$n_\pi = \frac{1}{2} + \frac{2}{4}n_C + \frac{1}{4}n_N + \frac{0}{4}n_O - \frac{1}{4}n_H$$

$$n_\pi = 0.5 + 4.5 + 0.5 + 0 - 3.5$$

$$n_\pi = 2$$

3.4.2. Calculation of σ-bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with triple bonds. When this step is finished, the number of σ-bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one triple bond present in our chosen unsaturated cyclic compound.

$$n_\sigma = -\frac{1}{2} + \frac{1}{4}\left(\sum_i n_i (v_i + 2)\right) \quad (12)$$

Example for: $C_9H_{14}N_2O_4$

$$n_\sigma = -\frac{1}{2} + \frac{1}{4}\left(\sum_i n_i (v_i + 2)\right)$$

$$n_\sigma = -\frac{1}{2} + \frac{6}{4}n_C + \frac{5}{4}n_N + \frac{4}{4}n_O + \frac{3}{4}n_H$$

$$n_\sigma = -0.5 + 13.5 + 2.5 + 4 + 10.5$$

$$n_\sigma = 30$$

3.4.3. Calculation of Single Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with triple bonds. When this step is finished, the number of single bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one triple bond present in our chosen unsaturated cyclic compound.

$$n_s = -\frac{3}{4} + \frac{1}{8}\left(\sum_i n_i (v_i + 6)\right) \quad (13)$$

Example for: $C_9H_{14}N_2O_4$

$$n_s = -\frac{3}{4} + \frac{1}{8}\left(\sum_i n_i (v_i + 6)\right)$$

$$n_s = -\frac{3}{4} + \frac{10}{8}n_C + \frac{9}{8}n_N + \frac{8}{8}n_O + \frac{7}{8}n_H$$

$$n_s = -0.75 + 11.25 + 2.25 + 4 + 12.25$$

$$n_s = 29$$

3.4.4. Calculation of Triple Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule. When this step is finished, the number of triple bonds will be calculated.

$$n_t = \frac{1}{4} + \frac{1}{8}\left(\sum_i n_i (v_i - 2)\right) \quad (14)$$

Example for: $C_9H_{14}N_2O_4$

$$n_t = \frac{1}{4} + \frac{1}{8}\left(\sum_i n_i (v_i - 2)\right)$$

$$n_t = \frac{1}{4} + \frac{2}{8}n_C + \frac{1}{8}n_N + \frac{0}{8}n_O - \frac{1}{8}n_H$$

$$n_t = 0.25 + 2.25 + 0.25 + 0 - 1.75$$

$$n_t = 1$$

Some theoretical examples of molecular structures for unsaturated cyclic organic compounds that contain only π-bonds, σ-bonds, single bonds and a triple bond or multiple triple bonds are:

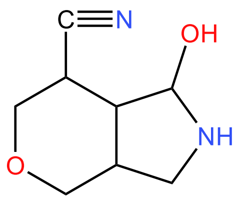

Figure 13. *First example of cyclic molecular structure with a triple bond.*

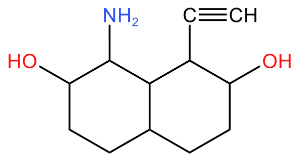

Figure 14. *Second example of cyclic molecular structure with a triple bond.*

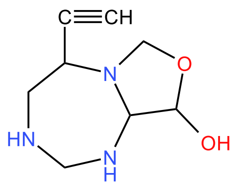

Figure 15. *Third example of cyclic molecular structure with a triple bond.*

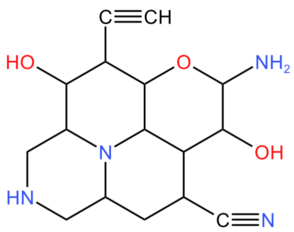

Figure 16. *Fourth example of cyclic molecular structure with triple bonds.*

3.5. Unsaturated Cyclic Organic Compounds with Double and Triple Bonds

In order to calculate the number of covalent bonds for unsaturated cyclic organic compounds with double and triple bonds we must choose a fixed valence for every chemical element that is present in our molecule. Also, the number of π-bonds is not equal with the number of triple bonds. However, the number of double bonds, triple bonds and rings are equal.

$$v_C = 4;\quad v_N = 3;\quad v_O = 2;\quad v_H = 1$$

3.5.1. Calculation of π-bonds ($n_d = n_t = n_r$)

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with double and triple bonds. When this step is finished, the number of π-bonds will be calculated for the case in which we have one or more than one double bond and one or more than one triple bond that are present in our chosen unsaturated cyclic compound.

$$n_\pi = \frac{3}{4} + \frac{3}{8}\left(\sum_i n_i(v_i - 2)\right) \tag{15}$$

Example for: $C_6H_9N_3O_3$

$$n_\pi = \frac{3}{4} + \frac{3}{8}\left(\sum_i n_i(v_i - 2)\right)$$

$$n_\pi = \frac{3}{4} + \frac{6}{8}n_C + \frac{3}{8}n_N + \frac{0}{8}n_O - \frac{3}{8}n_H$$

$$n_\pi = 0.75 + 4.5 + 1.125 + 0 - 3.375$$

$$n_\pi = 3$$

3.5.2. Calculation of σ-bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with double and triple bonds. When this step is finished, the number of σ-bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one double and triple bonds that are present in our chosen unsaturated cyclic compound.

$$n_\sigma = -\frac{3}{4} + \frac{1}{8}\left(\sum_i n_i(v_i + 6)\right) \tag{16}$$

Example for: $C_6H_9N_3O_3$

$$n_\sigma = -\frac{3}{4} + \frac{1}{8}\left(\sum_i n_i(v_i + 6)\right)$$

$$n_\sigma = -\frac{3}{4} + \frac{10}{8}n_C + \frac{9}{8}n_N + \frac{8}{8}n_O + \frac{7}{8}n_H$$

$$n_\sigma = -0.75 + 7.5 + 3.375 + 3 + 7.875$$

$$n_\sigma = 21$$

3.5.3. Calculation of Single Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule with double and triple bonds. When this step is finished, the number of single bonds will be calculated for the case in which we have a π-bond or multiple π-bonds and one or more than one double and triple bonds that are present in our chosen unsaturated cyclic compound.

$$n_s = \left|\frac{5}{4} + \frac{1}{8}\left(\sum_i n_i(v_i - 10)\right)\right| \tag{17}$$

Example for: $C_6H_9N_3O_3$

$$n_s = \left|\frac{5}{4} + \frac{1}{8}\left(\sum_i n_i(v_i - 10)\right)\right|$$

$$n_s = \left|\frac{5}{4} - \frac{6}{8}n_C - \frac{7}{8}n_N - \frac{8}{8}n_O - \frac{9}{8}n_H\right|$$

$$n_s = |1.25 - 4.5 - 2.625 - 3 - 10.125|$$

$$n_s = 19$$

3.5.4. Calculation of Triple Bonds

Initially, we have to count the number of atoms for every chemical element that is found in an unsaturated cyclic organic molecule that also contains double bonds. When this step is finished, the number of triple bonds will be calculated.

$$n_t = \frac{1}{4} + \frac{1}{8}\left(\sum_i n_i(v_i - 2)\right) \quad (18)$$

Example for: $C_6H_9N_3O_3$

$$n_t = \frac{1}{4} + \frac{1}{8}\left(\sum_i n_i(v_i - 2)\right)$$

$$n_t = \frac{1}{4} + \frac{2}{8}n_C + \frac{1}{8}n_N + \frac{0}{8}n_O - \frac{1}{8}n_H$$

$$n_t = 0.25 + 1.5 + 0.375 + 0 - 1.125$$

$$n_t = 1$$

Table 1. *Calculation of covalent bonds for Unsaturated Acyclic Organic Compounds with double bonds ($n_\pi = n_d$).*

Examples of Unsaturated Acyclic Organic Compounds with double bonds	**σ-bonds** $n_i - 1$	**Single bonds** $\left|2 + \frac{1}{2}\left(\sum_i n_i(v_i - 4)\right)\right|$	**π-bond/bonds** $1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right)$	**Double bond/bonds** $1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right)$
$C_5H_{10}N_2O_2$	18	16	2	2
$C_7H_{11}NO_3$	21	18	3	3
$C_4H_{10}N_4O$	18	16	2	2
$C_8H_{12}N_2O_3$	24	20	4	4
$C_9H_{15}N_3O_4$	30	26	4	4
$C_{14}H_{28}N_4O_4$	49	46	3	3
$C_{19}H_{32}N_6O_7$	63	56	7	7
$C_{25}H_{43}N_7O_6$	80	72	8	8
$C_{30}H_{50}N_8O_8$	95	85	10	10

Table 2. *Calculation of covalent bonds for Unsaturated Acyclic Organic Compounds with triple bonds ($n_\pi \neq n_t$).*

Examples of Unsaturated Acyclic Organic Compounds with triple bonds	**σ-bonds** $n_i - 1$	**Single bonds** $\left|\frac{3}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 6)\right)\right|$	**π-bonds** $1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right)$	**Triple bond/bonds** $\frac{1}{2} + \frac{1}{4}\left(\sum_i n_i(v_i - 2)\right)$
$C_5H_5NO_3$	13	11	4	2
$C_6H_4N_2O_2$	13	10	6	3
$C_5H_6N_2O_3$	15	13	4	2
$C_{10}H_9N_3O_2$	23	19	8	4
$C_{15}H_{16}N_4O_3$	37	32	10	5
$C_{18}H_{20}N_6O_2$	45	39	12	6
$C_{26}H_{27}N_5O_6$	63	55	16	8
$C_{29}H_{31}N_7O_9$	75	66	18	9
$C_{33}H_{33}N_9O_{10}$	84	73	22	11

Table 3. *Calculation of covalent bonds for Unsaturated Cyclic Organic Compounds with double bonds ($n_\pi = n_d = n_r$).*

Examples of Unsaturated Cyclic Organic Compounds with double bonds	**σ-bonds** $-\frac{1}{2}+\frac{1}{4}(\sum_i n_i(v_i+2))$	**Single bonds** $n_i - 1$	**π-bond/bonds** $\frac{1}{2}+\frac{1}{4}(\sum_i n_i(v_i-2))$	**Double bond/bonds and Ring/Rings** $\frac{1}{2}+\frac{1}{4}(\sum_i n_i(v_i-2))$
$C_6H_{13}N_3O_2$	24	23	1	1 n_d; 1 n_r
$C_5H_6N_2O_2$	16	14	2	2 n_d; 2 n_r
$C_8H_{13}N_3O_2$	27	25	2	2 n_d; 2 n_r
$C_8H_9N_3O_2$	24	21	3	3 n_d; 3 n_r
$C_{10}H_{14}N_4O_5$	35	32	3	3 n_d; 3 n_r
$C_{13}H_{17}N_5O_5$	43	39	4	4 n_d; 4 n_r
$C_{25}H_{32}N_8O_4$	75	68	7	7 n_d; 7 n_r
$C_{28}H_{33}N_7O_9$	84	76	8	8 n_d; 8 n_r
$C_{32}H_{30}N_4O_6$	81	71	10	10 n_d; 10 n_r

Table 4. *Calculation of covalent bonds for Unsaturated Cyclic Organic Compounds with triple bonds ($n_\pi \neq n_t$; $n_\pi = n_r$).*

Examples of Unsaturated Cyclic Organic Compounds with triple bonds	**σ-bonds** $-\frac{1}{2}+\frac{1}{4}(\sum_i n_i(v_i+2))$	**Single bonds** $-\frac{3}{4}+\frac{1}{8}(\sum_i n_i(v_i+6))$	**π-bonds and Ring/Rings** $\frac{1}{2}+\frac{1}{4}(\sum_i n_i(v_i-2))$	**Triple bond/bonds** $\frac{1}{4}+\frac{1}{8}(\sum_i n_i(v_i-2))$
$C_8H_{12}N_2O_2$	25	24	2 n_π; 2 n_r	1
$C_{12}H_{19}NO_2$	35	34	2 n_π; 2 n_r	1
$C_8H_{13}N_3O_2$	27	26	2 n_π; 2 n_r	1
$C_{16}H_{22}N_4O_3$	48	46	4 n_π; 4 n_r	2
$C_{20}H_{26}N_8O_5$	64	61	6 n_π; 6 n_r	3
$C_{27}H_{34}N_{10}O_9$	87	83	8 n_π; 8 n_r	4
$C_{30}H_{33}N_{11}O_{12}$	95	90	10 n_π; 10 n_r	5
$C_{34}H_{34}N_{12}O_{12}$	103	97	12 n_π; 12 n_r	6
$C_{40}H_{39}N_{13}O_{15}$	120	113	14 n_π; 14 n_r	7

Some theoretical examples of molecular structures for unsaturated cyclic organic compounds that contain π-bonds, σ-bonds, single bonds, double and triple bonds are the following ones:

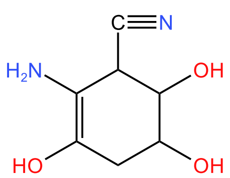

Figure 17. *First example of cyclic molecular structure with a double and a triple bond.*

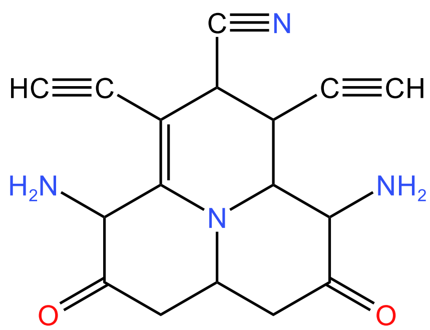

Figure 18. *Second example of cyclic molecular structure with double and triple bonds.*

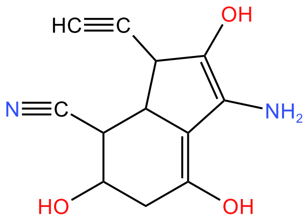

Figure 19. *Third example of cyclic molecular structure with double and triple bonds.*

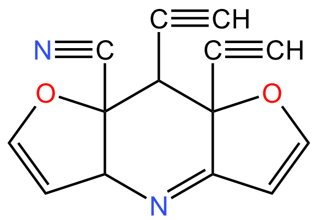

Figure 20. *Fourth example of cyclic molecular structure with double and triple bonds.*

Table 5. *Calculation of covalent bonds for Unsaturated Cyclic Organic Compounds with double and triple bonds ($n_d = n_t = n_r$).*

Examples of Unsaturated Cyclic Organic Compounds with double and triple bonds	**σ-bonds** $-\frac{3}{4}+\frac{1}{8}(\sum_i n_i(v_i+6))$	**Single bonds** $\left\lvert\frac{5}{4}+\frac{1}{8}(\sum_i n_i(v_i-10))\right\rvert$	**π-bonds** $\frac{3}{4}+\frac{3}{8}(\sum_i n_i(v_i-2))$	**Double bond/bonds, Triple bond/bonds and Ring/Rings** $\frac{1}{4}+\frac{1}{8}(\sum_i n_i(v_i-2))$
$C_7H_{10}N_2O_3$	22	20	3	1 n_d; 1 n_t; 1 n_r
$C_{17}H_{16}N_4O_2$	41	35	9	3 n_d; 3 n_t; 3 n_r
$C_{12}H_{12}N_2O_3$	30	26	6	2 n_d; 2 n_t; 2 n_r
$C_{14}H_8N_2O_2$	27	23	6	2 n_d; 2 n_t; 2 n_r
$C_{19}H_{13}N_5O_5$	45	37	12	4 n_d; 4 n_t; 4 n_r
$C_{26}H_{20}N_6O_8$	64	54	15	5 n_d; 5 n_t; 5 n_r
$C_{31}H_{25}N_9O_6$	76	64	18	6 n_d; 6 n_t; 6 n_r
$C_{36}H_{20}N_{10}O_7$	80	64	24	8 n_d; 8 n_t; 8 n_r
$C_{40}H_{18}N_8O_{11}$	85	67	27	9 n_d; 9 n_t; 9 n_r

4. Conclusions

In this study, a mathematical model for the calculation of covalent bonds in specific unsaturated organic compounds was presented. The model is based on Lewis theory of chemical bonding and valence bond theory and does not include molecular orbital theory [15], therefore at this moment it has limited practical applications.

However, the equations that were shown in this article can be used by organic, physical and analytical chemists alongside with the index of hydrogen deficiency to perform calculations for covalent bonds, and to potentially aid by speeding up the process of structural identification for specific unsaturated molecules [16, 17]. Additionally, the theoretical impact of this methodology may be seen as potentially significant due to the fact that we have demonstrated how to calculate all the simple covalent bonds within certain unsaturated compounds using equations that share many similarities with the index of hydrogen deficiency, therefore for future research studies this type of equations may have a chance to show their significance in measurement techniques such as NMR spectroscopy [18] and mass spectrometry [19] for chemical compounds.

Finally, the novel theoretical framework of this manuscript offers a new perspective on graph theory applications for well-known organic chemistry principles [20, 21] and can open the path to other similar mathematical models [22].

Abbreviations

IHD Index of Hydrogen Deficiency

Author Contributions

Vlad Cristian Gavrila: Conceptualization, Formal Analysis, Investigation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing.

Teodor Octavian Nicolescu: Investigation, Validation, Visualization, Writing – review & editing.

Conflicts of Interest

The authors declare no conflicts of interest.

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