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# New Equations for Rapid Calculation of π-bonds, σ-bonds, Single, Double and Triple Bonds in Open Chain Alcohols and Cycloamines

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***Abstract***— *Molecules are chemical structures composed of atoms, and in order to improve the understanding of the classical organic chemistry concepts it is necessary to have accessible mathematical models that contain all the important structural elements of a molecule. An interesting tool for organic chemistry is represented by the prediction of the number of π-bonds, σ-bonds, single, double and triple bonds for organic compounds based on their molecular formulas in order to solve different kinds of problems regarding the representation of molecules. In this manuscript we try to present a simple method comprised of multiple empirical equations for two important classes of organic molecules that can have a significant impact on their rapid calculation of chemical bonds. Therefore, our new mathematical model that will be presented enable an easy calculation of the number of π-bonds, σ-bonds, single, double and triple bonds for graphical representations of the molecular structures that corresponds to open chain alcohols and cycloamines using their molecular formulas.*

***Keywords***— ***Calculations, Cycloamines, New equations, Open chain alcohols, Rapid***

## I. INTRODUCTION

Calculating the number of covalent bonds in open chain alcohols and cycloamines with simple equations based on their molecular formula is a difficult challenge that requires innovative ideas. Therefore, we propose in this manuscript an easy method for the calculation of π-bonds, σ-bonds, single, double and triple bonds with the help of eight new equations and two equations that already existed for open chain alcohols. In the past, many new innovative methods including: "A novel formalism to characterize the degree of unsaturation of organic molecules" [1], "Rapid Calculation of the Number of π-bonds, σ-bonds, Single and Triple Bonds in Aliphatic Unsaturated Open Chain and Cycloalkynes" [2], and certain types of equations for covalent bonds which emerge from graph theory using Euler's characteristic [3] were published.

We chose to begin with these two types of molecules because alcohols [4] and cycloamines [5] are used in multiple research studies, and a rapid method to calculate the number of bonds for their structural representations can sometimes speed up some parts of the research process. Additionally, all the equations were made based on empirical methods such as comparisons between large samples of molecules, calculations and multiple sets of rules. Afterwards, the equations were tested using computer programs for multiple types of theoretical molecular formulas [6] and those results will be presented in four different tables throughout the results and discussion section.

## II. MATERIALS AND METHODS

In this study, we merged different mathematical fields such as graph theory [7], [8] and algebra [9] with organic chemistry in order to obtain new expressions for open chain alcohols and cycloamines. All of our methods are based on logical deductions, comparisons and observations which taken together establish a new empirical model that contains carbon, hydrogen, oxygen and nitrogen atoms and is easy to apply manually or with the help of a computer by chemists and mathematicians.

## III. RESULTS AND DISCUSSION

### 3.1. Open Chain Alcohols With Double Bonds

The equations that will be presented for open chain alcohols are appliable when an alcohol only has π-bonds, σ-bonds, single bonds and one or more than one double bonds. Therefore our molecules must have zero triple bonds and no rings. Additionally the number of π-bonds will be equal with the number of double bonds.

3.1.1. Calculation of π-bonds

First thing that we have to do, is to count the carbon and hydrogen atoms for an open chain alcohol. Afterwards, the number of π-bonds will be calculated for the case in which we have one or more than one double bonds that are present in our chosen alcohol.

A = the number of carbon atoms
B = the number of hydrogen atoms

$$P_d = (2A - B + 2) / 2 \quad (1)$$

Example for : $C_{10}H_{16}O$ ; $A = 10$ , $B = 16$

$P_d = (2A - B + 2) / 2$

$P_d = (2\times10 - 16 + 2) / 2$

$P_d = 3$ π-bonds

3.1.2. Calculation of σ-bonds

First thing that we have to do, is to count the carbon, hydrogen and oxygen atoms for an open chain alcohol. Afterwards, the number of σ-bonds will be calculated for the case in which our chosen alcohol contains a π-bond or multiple π-bonds and one or more than one double bonds.

A = the number of carbon atoms
B = the number of hydrogen atoms
C = the number of oxygen atoms

$$S_d = (A + B + C - 1) \quad (2)$$

Example for : $C_{10}H_{16}O$ ; $A = 10$ , $B = 16$ , $C = 1$

$S_d = (A + B + C - 1)$
$S_d = (10 + 16 + 1 - 1)$
$S_d = 26$ σ-bonds

3.1.3. Calculation of single bonds

First thing that we have to do, is to count the hydrogen and oxygen atoms for an open chain alcohol. Afterwards, the number of single bonds will be calculated for the case in which our chosen alcohol contains a π-bond or multiple π-bonds and one or more than one double bonds.

B = the number of hydrogen atoms
C = the number of oxygen atoms

$$E_d = (3B + 2C - 4) / 2 \quad (3)$$

Example for : $C_{10}H_{16}O$ ; $B = 16$ , $C = 1$

$E_d = (3B + 2C - 4) / 2$

$E_d = (3\times16 + 2\times1 - 4) / 2$

$E_d = 23$ single bonds

Some theoretical examples of molecular structures for open chain alcohols that contain only π-bonds, σ-bonds, single bonds and a double bond or multiple double bonds are:

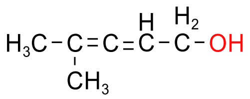

*Fig. 1*

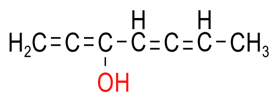

*Fig. 2*

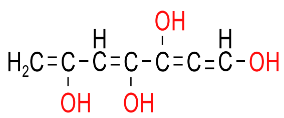

*Fig. 3*

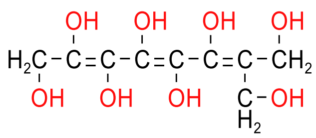

*Fig. 4*

### 3.2. Open Chain Alcohols with Triple Bonds

The equations that will be presented for open chain alcohols are appliable when an alcohol only has π-bonds, σ-bonds, single bonds and one or more than one triple bonds. Therefore our molecules must have zero double bonds and no rings. Additionally the number of π-bonds is not equal with the number of triple bonds.

3.2.1. Calculation of π-bonds

First thing that we have to do, is to count the carbon and hydrogen atoms for an open chain alcohol. Afterwards, the number of π-bonds will be calculated for the case in which we have one or more than one triple bonds that are present in our chosen alcohol.

A = the number of carbon atoms
B = the number of hydrogen atoms

$$P_t = (2A - B + 2) / 2 \quad (1)$$

Example for : $C_{17}H_{20}O_4$ ; $A = 17$ , $B = 20$

$P_t = (2A - B + 2) / 2$

$P_t = (2\times17 - 20 + 2) / 2$

$P_t = 8$ π-bonds

3.2.2. Calculation of σ-bonds

First thing that we have to do, is to count the carbon, hydrogen and oxygen atoms for an open chain alcohol. Afterwards, the number of σ-bonds will be calculated for the case in which our chosen alcohol contains π-bonds and one or more than one triple bonds.

A = the number of carbon atoms
B = the number of hydrogen atoms
C = the number of oxygen atoms

**$S_t$ = (A + B + C – 1)** **(2)**

Example for : $C_{17}H_{20}O_4$ ; A = 17 , B = 20 , C = 4
$S_t$ = (A + B + C – 1)
$S_t$ = (17 + 20 + 4 – 1)
$S_t$ = 40 σ-bonds

3.2.3. Calculation of single bonds

First thing that we have to do, is to count the carbon, hydrogen and oxygen atoms for an open chain alcohol. Afterwards, the number of single bonds will be calculated for the case in which our chosen alcohol contains π-bonds and one or more than one triple bonds.

A = the number of carbon atoms
B = the number of hydrogen atoms
C = the number of oxygen atoms

**$E_t$ = (2A + 5B + 4C – 6) / 4** **(4)**

Example for : $C_{17}H_{20}O_4$ ; A = 17 , B = 20 , C = 4
$E_t$ = (2A + 5B + 4C – 6) / 4
$E_t$ = (2×17 + 5×20 + 4×4 – 6) / 4
$E_t$ = 36 single bonds

3.2.4. Calculation of triple bonds

First thing that we have to do, is to count the carbon and hydrogen atoms for an open chain alcohol. Afterwards, the number of triple bonds will be calculated.

A = the number of carbon atoms
B = the number of hydrogen atoms

**T = (2A – B + 2) / 4** **(5)**

Example for : $C_{17}H_{20}O_4$ ; A = 17 , B = 20

T = (2A – B + 2) / 4

T = (2×17 – 20 + 2) / 4

T = 4 triple bonds

Some theoretical examples of molecular structures for open chain alcohols that contain only π-bonds, σ-bonds, single bonds and a triple bond or multiple triple bonds are:

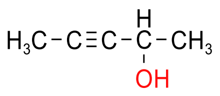

*Fig. 5*

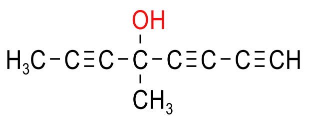

*Fig. 6*

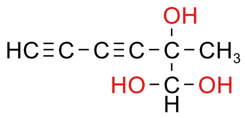

*Fig. 7*

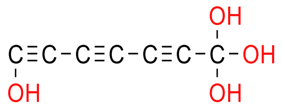

*Fig. 8*

### 3.3. Monocyclic and Polycyclic Amines With Double Bonds

The equations that will be presented for cycloamines are appliable when a cycloamine only has π-bonds, σ-bonds, single bonds and one or more than one double bonds. Therefore our molecules must have zero triple bonds. However in order for the equations to work, the number of rings must be equal with the number of π-bonds. Additionally the number of π-bonds will also be equal with the number of double bonds.

3.3.1. Calculation of π-bonds

First thing that we have to do, is to count the carbon, hydrogen and nitrogen atoms for a monocyclic or polycyclic amine. Afterwards, the number of π-bonds will be calculated for the case in which we have one or more than one double bonds that are present in our chosen monocyclic or polycyclic amine.

A = the number of carbon atoms
B = the number of hydrogen atoms
D = the number of nitrogen atoms

**$P_d$ = (2A – B + D + 2) / 4** **(6)**

Example for $C_{16}H_{25}N_3$: ; A = 16 , B = 25 , D = 3
$P_d$ = (2A – B + D + 2) / 4
$P_d$ = (2×16 – 25 + 3 + 2) / 4
$P_d$ = 3 π-bonds

3.3.2. Calculation of σ-bonds

First thing that we have to do, is to count the carbon, hydrogen and nitrogen atoms for a monocyclic or polycyclic amine. Afterwards, the number of σ-bonds will be calculated for the case in which our chosen monocyclic or polycyclic amine contains a π-bond or multiple π-bonds and one or more than one double bonds.

A = the number of carbon atoms
B = the number of hydrogen atoms
D = the number of nitrogen atoms

**$S_d$ = (6A + 3B + 5D – 2) / 4** **(7)**

Example for $C_{16}H_{25}N_3$: ; A = 16 , B = 25 , D = 3
$S_d$ = (6A + 3B + 5D – 2) / 4
$S_d$ = (6×16 + 3×25 + 5×3 – 2) / 4
$S_d$ = 46 σ-bonds

3.3.3. Calculation of single bonds

First thing that we have to do, is to count the carbon, hydrogen and nitrogen atoms for a monocyclic or polycyclic amine. Afterwards, the number of single bonds will be calculated for the case in which our chosen monocyclic or polycyclic amine contains a π-bond or multiple π-bonds and one or more than one double bonds.

A = the number of carbon atoms
B = the number of hydrogen atoms
D = the number of nitrogen atoms

**$E_d = (A + B + D - 1)$ (8)**

Example for $C_{16}H_{25}N_3$: ; A = 16 , B = 25 , D = 3
$E_d = (A + B + D - 1)$
$E_d = (16 + 25 + 3 - 1)$
$E_d = 43$ single bonds

Some theoretical examples of molecular structures for monocyclic and polycyclic amines that contain only π-bonds, σ-bonds, single bonds and a double bond or multiple double bonds are:

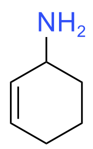

Fig. 9

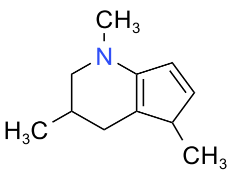

Fig.10

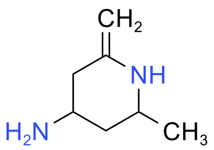

Fig. 11

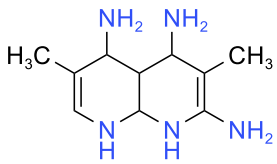

Fig. 12

## 3.4. Polycyclic Amines With Triple Bonds

The equations that will be presented for cycloamines are appliable when a cycloamine only has π-bonds, σ-bonds, single bonds and one or more than one triple bonds. Therefore our molecules must have zero double bonds. However in order for the equations to work, the number of rings must be equal with the number of π-bonds. Additionally the number of π-bonds is not equal with the number of triple bonds.

3.4.1. Calculation of π-bonds

First thing that we have to do, is to count the carbon, hydrogen and nitrogen atoms for a polycyclic amine. Afterwards, the number of π-bonds will be calculated for the case in which we have one or more than one triple bonds that are present in our chosen polycyclic amine.

A = the number of carbon atoms
B = the number of hydrogen atoms
D = the number of nitrogen atoms

**$P_t = (2A - B + D + 2) / 4$ (6)**

Example for $C_{13}H_{21}N$: ; A = 13 , B = 21 , D = 1
$P_t = (2A - B + D + 2) / 4$
$P_t = (2\times13 - 21 + 1 + 2) / 4$
$P_t = 2$ π-bonds

3.4.2. Calculation of σ-bonds

First thing that we have to do, is to count the carbon, hydrogen and nitrogen atoms for a polycyclic amine. Afterwards, the number of σ-bonds will be calculated for the case in which our chosen polycyclic amine contains π-bonds and one or more than one triple bonds.

A = the number of carbon atoms
B = the number of hydrogen atoms
D = the number of nitrogen atoms

**$S_t = (6A + 3B + 5D - 2) / 4$ (7)**

Example for $C_{13}H_{21}N$: ; A = 13 , B = 21 , D = 1
$S_t = (6A + 3B + 5D - 2) / 4$
$S_t = (6\times13 + 3\times21 + 5\times1 - 2) / 4$
$S_t = 36$ σ-bonds

3.4.3. Calculation of single bonds

First thing that we have to do, is to count the carbon, hydrogen and nitrogen atoms for a polycyclic amine. Afterwards, the number of single bonds will be calculated for the case in which our chosen polycyclic amine contains π-bonds and one or more than one triple bonds.

A = the number of carbon atoms
B = the number of hydrogen atoms
D = the number of nitrogen atoms

**$E_t = (10A + 7B + 9D - 6) / 8$ (9)**

Example for $C_{13}H_{21}N$: ; A = 13 , B = 21 , D = 1
$E_t = (10A + 7B + 9D - 6) / 8$
$E_t = (10\times13 + 7\times21 + 9\times1 - 6) / 8$
$E_t = 35$ single bonds

3.4.4. Calculation of triple bonds

First thing that we have to do, is to count the carbon, hydrogen and nitrogen atoms for a polycyclic amine. Afterwards, the number of triple bonds will be calculated.

A = the number of carbon atoms
B = the number of hydrogen atoms
D = the number of nitrogen atoms

**$T = (2A - B + D + 2) / 8$ (10)**

Example for $C_{13}H_{21}N$: ; A = 13 , B = 21 , D = 1
$T = (2A - B + D + 2) / 8$

T = (2×13 – 21 + 1 + 2) / 8
T = 1 triple bond

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

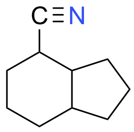


*Fig. 13*

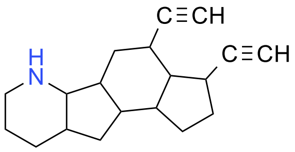


*Fig. 14*

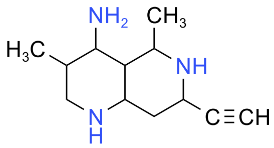


*Fig. 15*

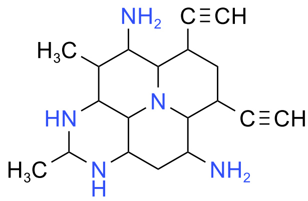


*Fig. 16*

*Table 1*

| Examples for Open Chain Alcohols With Double Bonds | π-bond/bonds $\left(\frac{2A-B+2}{2}\right)$ | σ-bonds $(A+B+C-1)$ | Single Bonds $\left(\frac{3B+2C-4}{2}\right)$ | Double bond/bonds $\left(\frac{2A-B+2}{2}\right)$ |
|---|---|---|---|---|
| $C_6H_{10}O$ | 2 | 16 | 14 | 2 |
| $C_7H_8O$ | 4 | 15 | 11 | 4 |
| $C_7H_8O_4$ | 4 | 18 | 14 | 4 |
| $C_9H_{14}O_8$ | 3 | 30 | 27 | 3 |
| $C_{20}H_{30}O$ | 6 | 50 | 44 | 6 |
| $C_{35}H_{66}O$ | 3 | 101 | 98 | 3 |
| $C_{23}H_{32}O_{12}$ | 8 | 66 | 58 | 8 |
| $C_{42}H_{74}O_{10}$ | 6 | 125 | 119 | 6 |
| $C_{55}H_{90}O_{20}$ | 11 | 164 | 153 | 11 |

*Table 2*

| Examples for Open Chain Alcohols With Triple Bonds | π-bonds $\left(\frac{2A-B+2}{2}\right)$ | σ-bonds $(A+B+C-1)$ | Single Bonds $\left(\frac{2A+5B+4C-6}{4}\right)$ | Triple bond/bonds $\left(\frac{2A-B+2}{4}\right)$ |
|---|---|---|---|---|
| $C_5H_8O$ | 2 | 13 | 12 | 1 |
| $C_9H_8O$ | 6 | 17 | 14 | 3 |
| $C_7H_8O_3$ | 4 | 17 | 15 | 2 |
| $C_7H_4O_4$ | 6 | 14 | 11 | 3 |
| $C_{26}H_{34}O$ | 10 | 60 | 55 | 5 |
| $C_{40}H_{54}O$ | 14 | 94 | 87 | 7 |
| $C_{57}H_{76}O$ | 20 | 133 | 123 | 10 |
| $C_{23}H_{16}O_8$ | 16 | 46 | 38 | 8 |
| $C_{44}H_{54}O_{13}$ | 18 | 110 | 101 | 9 |

*Table 3*

| Examples for Monocyclic and Polycyclic Amines With Double Bonds | π-bond/bonds $\left(\frac{2A-B+D+2}{4}\right)$ | σ-bonds $\left(\frac{6A+3B+5D-2}{4}\right)$ | Single bonds $(A+B+D-1)$ | Double bond/bonds $\left(\frac{2A-B+D+2}{4}\right)$ | Ring/Rings $\left(\frac{2A-B+D+2}{4}\right)$ |
|---|---|---|---|---|---|
| $C_6H_{11}N$ | 1 | 18 | 17 | 1 | 1 |
| $C_{11}H_{17}N$ | 2 | 30 | 28 | 2 | 2 |
| $C_7H_{14}N_2$ | 1 | 23 | 22 | 1 | 1 |
| $C_{10}H_{19}N_5$ | 2 | 35 | 33 | 2 | 2 |
| $C_{20}H_{27}N$ | 4 | 51 | 47 | 4 | 4 |
| $C_{33}H_{49}N$ | 5 | 87 | 82 | 5 | 5 |
| $C_{54}H_{83}N$ | 7 | 144 | 137 | 7 | 7 |
| $C_{35}H_{53}N_{13}$ | 8 | 108 | 100 | 8 | 8 |
| $C_{56}H_{95}N_{17}$ | 9 | 176 | 167 | 9 | 9 |

*Table 4*

| Examples for Polycyclic Amines With Triple Bonds | π-bonds $\left(\frac{2A-B+D+2}{4}\right)$ | σ-bonds $\left(\frac{6A+3B+5D-2}{4}\right)$ | Single bonds $\left(\frac{10A+7B+9D-6}{8}\right)$ | Triple bond/bonds $\left(\frac{2A-B+D+2}{8}\right)$ | Rings $\left(\frac{2A-B+D+2}{4}\right)$ |
|---|---|---|---|---|---|
| $C_{10}H_{15}N$ | 2 | 27 | 26 | 1 | 2 |
| $C_{19}H_{25}N$ | 4 | 48 | 46 | 2 | 4 |
| $C_{12}H_{21}N_3$ | 2 | 37 | 36 | 1 | 2 |
| $C_{19}H_{29}N_5$ | 4 | 56 | 54 | 2 | 4 |
| $C_{34}H_{39}N$ | 8 | 81 | 77 | 4 | 8 |
| $C_{50}H_{63}N$ | 10 | 123 | 118 | 5 | 10 |
| $C_{37}H_{61}N_9$ | 6 | 112 | 109 | 3 | 6 |
| $C_{50}H_{66}N_{12}$ | 12 | 139 | 133 | 6 | 12 |
| $C_{67}H_{85}N_{21}$ | 18 | 190 | 181 | 9 | 18 |

The new mathematical model that was presented in this manuscript for open chain alcohols and cycloamines consist of ten different equations that were verified and tested with computer programs [10], [11] and can be classified as follows:

- The equations for σ-bonds and single bonds labeled with the numbers **(3)**, **(4)**, **(7)**, **(8)**, **(9)** were made by combining the number of carbon, hydrogen, oxygen and nitrogen atoms together after we compared a large sample of molecules for open chain alcohols and cycloamines in order to precisely multiply, divide, add or subtract the numerical values of atoms with numerical constants to discover completely new equations for specific organic molecules.
- The equation labeled with **(2)** for σ-bonds was made by applying another equation that already exists for hydrocarbons [2], [3] on open chain

alcohols after integrating the number of oxygen atoms, thus resulting a unique equation.

- The equations labeled with **(1)** and **(5)** for π-bonds, double and triple bonds are the same equations from the article referenced with [2], however we applied them to organic compounds that also have oxygen atoms.
- The equations labeled with **(6)** and **(10)** for π-bonds, double and triple bonds were deduced using the degree of unsaturation [1], and other new types of mathematical calculations for chemical compounds with nitrogen atoms.

Therefore, our novel model for open chain alcohols and cycloamines consist of eight new equations **(2)**, **(3)**, **(4)**, **(6)**, **(7)**, **(8)**, **(9)**, **(10)** and two equations that already existed **(1)**, **(5)** which taken together allow researchers to perform a manual or automatic rapid calculation of π-bonds, σ-bonds, single, double and triple bonds and to create tables based on their molecular formulas.

## IV. CONCLUSION

In conclusion the equations for chemical bonds are represented by a novel type of mathematical model that can provide useful calculations and representations for some types of organic compounds. Theoretically speaking we combined algebra and graph theory concepts with organic chemistry theories such as Lewis theory of chemical bonding [12] and valence bond theory [13], in order to obtain simple equations that have multiple purposes. Finally, the presented model does not reflect on the real nature of molecular bonds [14], but rather represents a mathematical abstraction based on molecular graphs [15] that can be used by researchers to calculate the number of bonds and generate tables based on theoretical molecular formulas for organic compounds in a rapid fashion with a computer.

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