Article

Not peer-reviewed version

Deduction and Application of Novel IHD-Like Equations for the Calculation of Covalent Bonds in Cyclic Unsaturated Molecules

Vlad Cristian Gavrilă * and Teodor Octavian Nicolescu

Posted Date: 4 March 2025

doi: 10.20944/preprints202503.0108.v1

Keywords: Chemical graph theory; Bonds; Molecules; Novel equations; Inequalities

doi:10.20944/preprints202503.0108.v1

Article

Deduction and Application of Novel IHD-Like Equations for the Calculation of Covalent Bonds in Cyclic Unsaturated Molecules

Vlad Cristian Gavrilă *, Teodor Octavian Nicolescu

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

* Correspondence: vlad.cristian.gavrila@gmail.com

Abstract: Currently in order to calculate the number of covalent bonds for cyclic unsaturated organic molecules there are equations that include the index of hydrogen deficiency (IHD), a σ-bonds derivation from the Euler characteristic for planar graphs and other empirical formulations. However the IHD which is also known as the degree of unsaturation (DOU) requires to assign a numerical value for the pi(π) bonds and rings without knowing their precise number in a molecule, and all the other equations that are used to determine the numerical value of sigma(σ) and single bonds are made up of variables such as the number of rings, double and triple bonds. In this manuscript we present a novel type of mathematical model that was deduced by using chemical graph theory and can be applied to calculate the value of covalent bonds and rings for cyclic organic molecules with double or triple bonds only knowing the number of atoms, their corresponding valences and a new chemical concept which we called total unsaturation (TU) that represents the degree of unsaturation expressed as a percentage. The objective of this study is to highlight a deeper mathematical relationship formed by multiple structural elements of a molecule in order to enhance the correlations between graph theory and organic chemistry from a different perspective that is primarly focused on the number of bonds.

Keywords: Chemical graph theory; Bonds; Molecules; Novel equations; Inequalities

---

1. Introduction

For decades now, chemical graph theory [1–4] is used to deepen our understanding of molecular structures, chemical reactions, stereochemistry mechanisms, and many other chemical phenomena that take place at both microscopic and macroscopic levels. This study aims to present a novel mathematical model that utilizes chemical graph theory for the calculation of the number of covalent bonds and rings for the vast majority of cyclic unsaturated molecules. First of all, our model is based on Lewis theory of chemical bonding [5] and valence bond theory [6], and can only be applied to neutral molecules that are made up by non-metallic elements. The current formalisms that are used in order to calculate the number of bonds and rings for organic compounds which adheres to the previous enumerated chemical restraints include: the index of hydrogen deficiency also known as the degree of unsaturation [7], an equation to calculate the number of sigma(σ) bonds based on the number of atoms and rings within a molecule [8], a theoretical framework for the calculation of the number of covalent bonds in unsaturated organic compounds [9], and two particular models for the calculation of covalent bonds in aliphatic unsaturated open chain and cycloalkynes [10], and for the calculation of covalent bonds in open chain alcohols and cycloamines [11]. In our last publication that treated this subject [9], we have presented original equations for all acyclic unsaturated molecules with double or triple bonds and a few specific general equations for cyclic molecules with double or triple bonds where the number of pi(π) bonds is equal to the number of rings. However for the vast majority of organic molecules the number of pi(π) bonds is not equal to the number of rings, therefore in this manuscript we will show thirteen novel equations that were used to deduce more than thirty new specific general equations for multiple cases of inequalities between pi (π) bonds and rings. Additionally our equations can potentially offer novel insights in areas such as computational chemistry applications [12] for: IR spectroscopy [13,14], NMR spectroscopy [15,16], mass spectrometry [17,18] and aromaticity predictions [19,20] by integrating them with the currently existing techniques.

2. Materials and Methods

At present all the existing equations that include the IHD [7] and any other formulas for sigma(σ) [8] or single bonds have multiple downsides both chemically and mathematically speaking.

$$\mathrm{IHD} = 1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right) \ \text{ and } \ n_\pi + n_r = 1 + \frac{1}{2}\left(\sum_i n_i(v_i - 2)\right)$$

$$n_\sigma = n_i + n_r - 1 \ \text{ and } \ n_s = n_i + n_r - n_d - 1 \ \text{ or } \ n_s = n_i + n_r - n_t - 1$$

Every single equation from above has two particular downsides and they share a common general one. First the index of hydrogen deficiency equation cannot be used to differentiate between the number of pi(π) bonds and the number of rings, moreover, it doesn't work for sigma(σ) and single bonds. Second the equations for sigma(σ) and single bonds do not include the valences of the chemical elements of a molecule and also they require to exactly know the number of rings, double or triple bonds in order to be applied. The general downside is represented by the fact that these equations have different kind of structures and do not share the same variables between all of them. However in this manuscript we have managed to solve these five problems by inventing 12 novel equations for covalent bonds and rings alongside a new chemical concept which we called total unsaturation. The total unsaturation is the index of hydrogen deficiency expressed as a percentage where TU is always equal with 100% and the sum between the percentage of pi(π) bonds and the percentage of rings is equal with TU. In the upcoming section of this article, all of these equations will be applied to deduce 36 new specific general equations for sigma(σ) bonds, pi(π) bonds, single bonds, double bonds, triple bonds and rings. Furthermore, to validate and verify our equations we used computer programs [21,22] alongside manual calculations [23,24] and both of these methods were applied on many molecular formulas that correspond to real and theoretical cyclic unsaturated organic compounds. Therefore in this research we will present a total of 49 original equations in a simple and elegant manner that can unlock novel ideas related to molecular structures [25].

3. Results and Discussion

Firstly, this section will contain many variables that have the following meanings and notations: the number of sigma bonds in a molecule ($\mathbf{n_\sigma}$), the number of single bonds in a molecule ($\mathbf{n_s}$), the number of pi bonds in a molecule ($\mathbf{n_\pi}$), the number of double bonds in a molecule ($\mathbf{n_d}$), the number of triple bonds in a molecule ($\mathbf{n_t}$), the number of chemical elements in a molecule ($\mathbf{i}$), the number of atoms that correspond to a chemical element ($\mathbf{n_i}$), the valence of a chemical element ($\mathbf{v_i}$), the number of rings in a molecule ($\mathbf{n_r}$), the percentage of pi bonds from TU in a molecule ($\mathbf{p_\pi}$), the percentage of rings from TU in a molecule ($\mathbf{p_r}$). Also, all the molecular formulas will have two (C, H are mandatory), or more of the following chemical elements: S, P, C, N, O, H, Cl. For each element we chose a fixed valence in order to keep our calculations as simple as possible:

$$v_S = 6 \ ; \ v_P = 5 \ ; \ v_C = 4 \ ; \ v_N = 3 \ ; \ v_O = 2 \ ; \ v_H = 1 \ ; \ v_{Cl} = 1$$

Additionally, thirteen novel mathematical equations (including the total unsaturation) that we used to calculate the number of covalent bonds and rings for cyclic molecules with double or triple bonds by deducing thirty-six specific general equations which have as variables the number of atoms

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

and their valences will be presented in four cases throghout this section with two solved examples for each one of them and a total of eight tables, one for every ratio established between p_π and p_r from TU.

1) For cyclic unsaturated molecules with double bonds in which $p_\pi > p_r$
   $p_\pi + p_r = TU$ and $p_\pi + p_r = 100\%$
   $0\% < p_r < 50\%$ and $50\% < p_\pi < 100\%$
2) For cyclic unsaturated molecules with double bonds in which $p_r > p_\pi$
   $p_\pi + p_r = TU$ and $p_\pi + p_r = 100\%$
   $0\% < p_\pi < 50\%$ and $50\% < p_r < 100\%$
3) For cyclic unsaturated molecules with triple bonds in which $p_\pi > p_r$
   $p_\pi + p_r = TU$ and $p_\pi + p_r = 100\%$
   $0\% < p_r < 50\%$ and $50\% < p_\pi < 100\%$
4) For cyclic unsaturated molecules with triple bonds in which $p_r > p_\pi$
   $p_\pi + p_r = TU$ and $p_\pi + p_r = 100\%$
   $0\% < p_\pi < 50\%$ and $50\% < p_r < 100\%$

3.1. Cyclic unsaturated molecules with double bonds in which $p_\pi > p_r$

For all the cyclic unsaturated molecules that contain σ-bonds, π-bonds, single bonds and double bonds where the number of π-bonds is always greater than the number of rings, we have invented four mathematical equations to be able to deduce many other specific general equations for covalent bonds and rings:

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

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

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + \left(\frac{p_\pi}{p_r} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{p_\pi}{p_r} - 1\right)} \quad (3)$$

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

In order to find any percentages for π-bonds and rings that correspond to cyclic unsaturated molecules with double bonds in which $p_\pi > p_r$; $0\% < p_r < 50\%$ and $50\% < p_\pi < 100\%$, we can start by choosing a molecular structure where $n_\pi > n_r$, write it's molecular formula and calculate the correlated degree of unsaturation. Afterwards, the number of π-bonds and rings will be converted into percentages using the rule of three, and those numerical values will be substituted into the main mathematical equations to deduce other specific general equations that have as variables only the number of atoms and their valences, and work for molecules that share the same values of p_π and p_r as our chosen molecular structure.

 doi:10.20944/preprints202503.0108.v1

3.1.1. First example

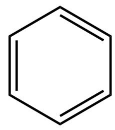


Figure 1. 1,3,5-Cyclohexatriene $\mathbf{C_6H_6}$

$$n_\pi + n_r = \mathrm{DOU} \quad \text{and} \quad n_\pi + n_r = 1 + \tfrac{1}{2}\textstyle\sum_i n_i(v_i - 2)$$

$$n_\pi + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}n_H(1-2) \;\; => \;\; n_\pi + n_r = 4 \;\; \text{and} \;\; n_\pi = 3 \;\; ; \;\; n_r = 1$$

$$p_\pi + p_r = \mathrm{TU} \quad \text{and} \quad p_\pi + p_r = 100\% \tag{5}$$

$$p_\pi = \frac{3 \cdot 100\%}{4} = 75\% \;\; \text{and} \;\; p_r = \frac{1 \cdot 100\%}{4} = 25\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 75\%$ of TU and $p_r = 25\%$ of TU.

$$p_\pi + p_r = \mathrm{TU} \tag{5}$$

$$p_\pi + p_r = 100\% \quad ; \quad 75\% + 25\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 2\left(\frac{75\%}{25\%} - 1\right)(n_i - 1) - 2}{4 + 2\left(\frac{75\%}{25\%} - 1\right)}$$

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

$$\mathbf{n_\sigma = \frac{\sum_i n_i(v_i + 6) - 6}{8}} \tag{6}$$

$$n_s = \frac{4(n_i - 1) - \left(\frac{75\%}{25\%} - 1\right)\left(\sum_i n_i(v_i - 4) + 4\right)}{4 + 2\left(\frac{75\%}{25\%} - 1\right)}$$

$$n_s = \frac{4n_i - 4 - 2\sum_i n_i(v_i - 4) - 8}{4 + 2 \cdot 2}$$

$$n_s = \frac{-2\sum_i n_i(v_i - 6) - 12}{8} \;\; => \;\; \mathbf{n_s = \frac{-\sum_i n_i(v_i - 6) - 6}{4}} \tag{7}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + \left(\frac{75\%}{25\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{75\%}{25\%} - 1\right)}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2\sum_i n_i(v_i - 2) + 4 + 2}{4 + 2 \cdot 2}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$\mathrm{n_\pi = n_d = \frac{3\sum_i n_i(v_i - 2) + 6}{8}} \Rightarrow \mathbf{n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{2.666666667}} \quad (8)$$

$$\mathrm{n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{75\%}{25\%} - 1\right)}}$$

$$\mathrm{n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2 \cdot 2}}$$

$$\mathbf{n_r = \frac{\sum_i n_i(v_i - 2) + 2}{8}} \quad (9)$$

After deducing the specific general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with double bonds where $p_\pi = 75\%$ and $p_r = 25\%$, we will apply them on a molecular formula as an example: $C_{12}H_{12}N_2O_3$

$$\mathrm{n_\sigma = \frac{\sum_i n_i(v_i + 6) - 6}{8}} \quad (6)$$

$$\mathrm{n_\sigma = \frac{n_C(4+6) + n_N(3+6) + n_O(2+6) + n_H(1+6) - 6}{8}}$$

$$\mathrm{n_\sigma = \frac{120 + 18 + 24 + 84 - 6}{8}} \Rightarrow \mathbf{n_\sigma = 30}$$

$$\mathrm{n_s = \frac{-\sum_i n_i(v_i - 6) - 6}{4}} \quad (7)$$

$$\mathrm{n_s = \frac{-n_C(4-6) - n_N(3-6) - n_O(2-6) - n_H(1-6) - 6}{4}}$$

$$\mathrm{n_s = \frac{24 + 6 + 12 + 60 - 6}{4}} \Rightarrow \mathbf{n_s = 24}$$

$$\mathrm{n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{2.666666667}} \quad (8)$$

$$\mathrm{n_\pi = n_d = \frac{n_C(4-2) + n_N(3-2) + n_O(2-2) + n_H(1-2) + 2}{2.666666667}}$$

$$\mathrm{n_\pi = n_d = \frac{24 + 2 + 0 - 12 + 2}{2.666666667}} \Rightarrow \mathbf{n_\pi = n_d = 6}$$

$$\mathrm{n_r = \frac{\sum_i n_i(v_i - 2) + 2}{8}} \quad (9)$$

$$\mathrm{n_r = \frac{n_C(4-2) + n_N(3-2) + n_O(2-2) + n_H(1-2) + 2}{8}}$$

$$\mathrm{n_r = \frac{24 + 2 + 0 - 12 + 2}{8}} \Rightarrow \mathbf{n_r = 2}$$

Other molecular formulas where their corresponding molecules can have $p_\pi = 75\%$ of TU and $p_r = 25\%$ of TU, will be presented in the following table:

Table 1. Calculation of covalent bonds and rings for unsaturated cyclic molecules with double bonds

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$p_{\pi} = 75\% \;\; and \; p_r = 25\%$$

Examples of Unsaturated Cyclic Molecules with double bonds	**σ-bonds** $-\frac{3}{4}+\frac{1}{8}(\sum_i \mathbf{n_i}(\mathbf{v_i}+\mathbf{6}))$	**Single bonds** $\left\lvert\frac{3}{2}+\frac{1}{4}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{6}))\right\rvert$	**π-bonds and double bonds** $\frac{2}{2.6}+\frac{1}{2.6}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{2}))$	**Ring/Rings** $\frac{1}{4}+\frac{1}{8}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{2}))$
C_6H_6	12	9	$3\ n_{\pi}$; $3\ n_d$	1
$C_{12}H_{12}N_2O_3$	30	24	$6\ n_{\pi}$; $6\ n_d$	2
$C_{12}H_{13}N_3$	29	23	$6\ n_{\pi}$; $6\ n_d$	2
$C_{14}H_{10}S_2O_6Cl_4$	38	29	$9\ n_{\pi}$; $9\ n_d$	3
$C_{16}H_{10}O_5$	33	24	$9\ n_{\pi}$; $9\ n_d$	3
$C_{22}H_{12}N_3O_3Cl_5$	48	36	$12\ n_{\pi}$; $12\ n_d$	4
$C_{20}H_{22}P_4O_8$	57	45	$12\ n_{\pi}$; $12\ n_d$	4
$C_{24}H_{26}S_4O_9$	67	52	$15\ n_{\pi}$; $15\ n_d$	5
$C_{27}H_{16}O_{10}$	57	42	$15\ n_{\pi}$; $15\ n_d$	5

Some examples of molecular structures for cyclic unsaturated molecules with double bonds where $p_{\pi} > p_r$ and $p_{\pi} = 75\%$; $p_r = 25\%$ from the total unsaturation are the following ones:

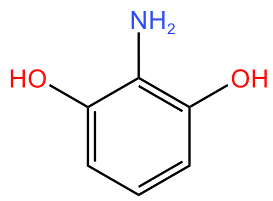


Figure 2. 2-amino benzene-1,3-diol.

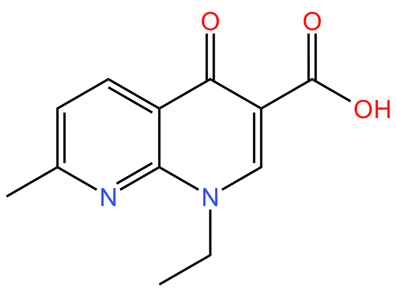


Figure 3. 1-Ethyl-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid.

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

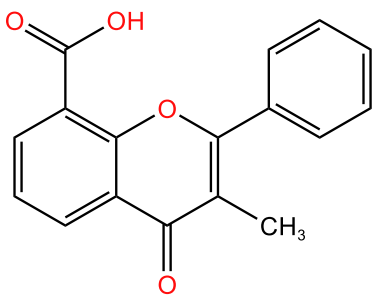


Figure 4. 3-Methyl-4-oxo-2-phenyl-4H-chromene-8-carboxylic acid.

3.1.2. Second example

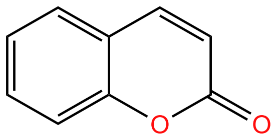


Figure 5. 2H-Chromen-2-one $\mathbf{C_9H_6O_2}$.

$$n_\pi + n_r = DOU \quad \text{and} \quad n_\pi + n_r = 1 + \tfrac{1}{2}\sum_i n_i(v_i - 2)$$

$$n_\pi + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}\,n_O(2-2) + \frac{1}{2}n_H(1-2) \Rightarrow \ n_\pi + n_r = 7 \ \text{ and } \ n_\pi = 5 \ ; \ n_r = 2$$

$$p_\pi + p_r = TU \quad \text{and} \quad p_\pi + p_r = 100\% \tag{5}$$

$$p_\pi = \frac{5 \cdot 100\%}{7} = 71.42857143\% \ \text{ and } \ p_r = \frac{2 \cdot 100\%}{7} = 28{,}57142857\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 71.42857143\%$ of TU and $p_r = 28.57142857\%$ of TU.

$$p_\pi + p_r = TU \tag{5}$$

$$p_\pi + p_r = 100\% \quad ; \quad 71.42857143\% + 28.57142857\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 2\left(\frac{71.42857143\%}{28.57142857\%} - 1\right)(n_i - 1) - 2}{4 + 2\left(\frac{71.42857143\%}{28.57142857\%} - 1\right)}$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 3n_i - 3 - 2}{4 + 2 \cdot 1.5}$$

$$\mathbf{n_\sigma = \frac{\sum_i n_i(v_i + 5) - 5}{7}} \tag{10}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_s = \frac{4(n_i - 1) - \left(\frac{71.42857143\%}{28.57142857\%} - 1\right)\left(\sum_i n_i(v_i - 4) + 4\right)}{4 + 2\left(\frac{71.42857143\%}{28.57142857\%} - 1\right)}$$

$$n_s = \frac{4n_i - 4 - 1.5\sum_i n_i(v_i - 4) - 6}{4 + 2 \cdot 1.5}$$

$$n_s = \frac{-1.5\sum_i n_i(v_i - 6.666666667) - 10}{7} \Rightarrow \mathbf{n_s} = \frac{-\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{6.666666667}) - \mathbf{6.6666666}}{\mathbf{4.666666667}} \quad (11)$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + \left(\frac{71.42857143\%}{28.57142857\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{71.42857143\%}{28.57142857\%} - 1\right)}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 1.5\sum_i n_i(v_i - 2) + 3 + 2}{4 + 2 \cdot 1.5}$$

$$n_\pi = n_d = \frac{2.5\sum_i n_i(v_i - 2) + 5}{7} \Rightarrow \mathbf{n_\pi} = \mathbf{n_d} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{2.8}} \quad (12)$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{71.42857143\%}{28.57142857\%} - 1\right)}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2 \cdot 1.5}$$

$$\mathbf{n_r} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{7}} \quad (13)$$

After deducing the general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with double bonds where $p_\pi = 71.42857143\%$ and $p_r = 28.57142857\%$, we will apply them on a molecular formula as an example: $C_8H_4O_3$

$$n_\sigma = \frac{\sum_i n_i(v_i + 5) - 5}{7} \quad (10)$$

$$n_\sigma = \frac{n_C(4 + 5) + n_O(2 + 5) + n_H(1 + 5) - 5}{7}$$

$$n_\sigma = \frac{72 + +21 + 24 - 5}{7} \Rightarrow \mathbf{n_\sigma} = \mathbf{16}$$

$$n_s = \frac{-\sum_i n_i(v_i - 6.666666667) - 6.666666667}{4.666666667} \quad (11)$$

$$n_s = \frac{-n_C(4 - 6.666666667) - n_O(2 - 6.666666667) - n_H(1 - 6.666666667) - 6.6666666}{4.666666667}$$

$$n_s = \frac{21.33333334 + 14 + 22.66666667 - 6.666666667}{4.666666667} \Rightarrow \mathbf{n_s} = \mathbf{11}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{2.8} \tag{12}$$

$$n_\pi = n_d = \frac{n_C(4-2) + n_O(2-2) + n_H(1-2) + 2}{2.8}$$

$$n_\pi = n_d = \frac{16 + 0 - 4 + 2}{2.8} \quad => \ \mathbf{n_\pi = n_d = 5}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{7} \tag{13}$$

$$n_r = \frac{n_C(4-2) + n_O(2-2) + n_H(1-2) + 2}{7}$$

$$n_r = \frac{16 + 0 - 4 + 2}{7} \quad => \ \mathbf{n_r = 2}$$

Other molecular formulas where their corresponding molecules can have $p_\pi = 71.42857143\%$ of TU and $p_r = 28.57142857\%$ of TU, will be presented in the following table:

Table 2. Calculation of covalent bonds and rings for unsaturated cyclic molecules with double bonds $p_\pi = 71.42857143\% \ \ and \ \ p_r = 28.57142857\%$

Examples of Unsaturated Cyclic Molecules with double bonds	σ-bonds $-\frac{5}{7}+\frac{1}{7}(\sum_i \mathbf{n_i}(\mathbf{v_i}+\mathbf{5}))$	Single bonds $\left\lvert\frac{6.\bar{6}}{4.\bar{6}}+\frac{1}{4.\bar{6}}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{6.\bar{6}}))\right\rvert$	π-bonds and double bonds $\frac{2}{2.8}+\frac{1}{2.8}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{2}))$	Ring/Rings $\frac{2}{7}+\frac{1}{7}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{2}))$
$C_9H_5NOCl_2$	19	14	5 n_π ; 5 n_d	2
$C_{19}H_{12}O_4$	38	28	10 n_π ; 10 n_d	4
$C_{16}H_{10}N_4O_3$	36	26	10 n_π ; 10 n_d	4
$C_{30}H_{10}Cl_{10}$	55	40	15 n_π ; 15 n_d	6
$C_{33}H_{42}S_4O_9$	93	78	15 n_π ; 15 n_d	6
$C_{33}H_{29}P_4N_5O_8$	86	66	20 n_π ; 20 n_d	8
$C_{37}H_{32}N_{12}$	88	68	20 n_π ; 20 n_d	8
$C_{46}H_{46}P_8O_{13}$	122	97	25 n_π ; 25 n_d	10
$C_{54}H_{32}O_7Cl_8$	110	85	25 n_π ; 25 n_d	10

Some examples of molecular structures for cyclic unsaturated molecules with double bonds where $p_\pi > p_r$ and $p_\pi = 71.42857143\%$; $p_r = 28.57142857\%$ from the total unsaturation are the following ones:

 doi:10.20944/preprints202503.0108.v1

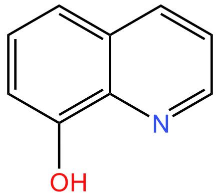


Figure 6. 8-quinolinol.

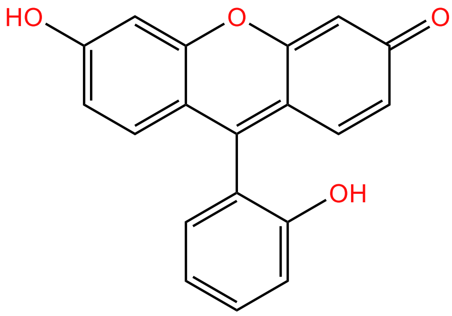


Figure 7. 6-hydroxy-9-(2-hydroxyphenyl)xanthen-3-one.

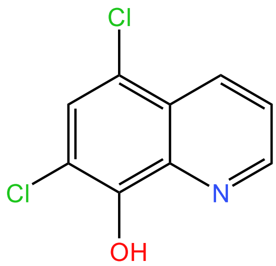


Figure 8. 5,7-dichloro-8-quinolinol.

3.2. Cyclic unsaturated molecules with double bonds in which $p_r > p_\pi$

For all the cyclic unsaturated molecules that contain σ-bonds, π-bonds, single bonds and double bonds where the number of rings is always greater than the number of π-bonds, we have invented four mathematical equations to be able to deduce many other specific general equations for covalent bonds and rings:

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + \left(\frac{p_r}{p_\pi} - 1\right)\sum_i n_i v_i - 2}{4 + 2\left(\frac{p_r}{p_\pi} - 1\right)} \quad (14)$$

$$n_s = \frac{4(n_i - 1) + \left(\frac{p_r}{p_\pi} - 1\right)\sum_i n_i v_i}{4 + 2\left(\frac{p_r}{p_\pi} - 1\right)} \quad (15)$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{p_r}{p_\pi} - 1\right)} \quad (16)$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + \left(\frac{p_r}{p_\pi} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{p_r}{p_\pi} - 1\right)} \quad (17)$$

In order to find any percentages for π-bonds and rings that correspond to cyclic unsaturated molecules with double bonds in which $p_r > p_\pi$; $0\% < p_\pi < 50\%$ and $50\% < p_r < 100\%$, we can start

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

by choosing a molecular structure where $n_r > n_\pi$, write it's molecular formula and calculate the correlated degree of unsaturation. Afterwards, the number of π-bonds and rings will be converted into percentages using the rule of three, and those numerical values will be substituted into the main mathematical equations to deduce other specific general equations that have as variables only the number of atoms and their valences, and work for molecules that share the same values of p_π and p_r as our chosen molecular structure.

3.2.1. First example

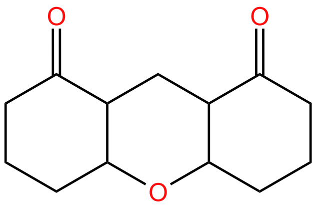


Figure 9. 3,4,4a,5,6,7,8a,9,9a,10a-decahydro-2H-xanthene-1,8-dione $\mathbf{C_{13}H_{18}O_3}$.

$$n_\pi + n_r = \mathrm{DOU} \quad \text{and} \quad n_\pi + n_r = 1 + \tfrac{1}{2}\textstyle\sum_i n_i(v_i - 2)$$

$$n_\pi + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}n_O(2-2) + \frac{1}{2}n_H(1-2) \Rightarrow n_\pi + n_r = 5 \text{ and } n_\pi = 2\ ;\ n_r = 3$$

$$p_\pi + p_r = \mathrm{TU} \quad \text{and} \quad p_\pi + p_r = 100\% \tag{5}$$

$$p_\pi = \frac{2 \cdot 100\%}{5} = 40\% \text{ and } p_r = \frac{3 \cdot 100\%}{5} = 60\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 40\%$ of TU and $p_r = 60\%$ of TU.

$$p_\pi + p_r = \mathrm{TU} \tag{5}$$

$$p_\pi + p_r = 100\% \quad ; \quad 40\% + 60\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + \left(\frac{60\%}{40\%} - 1\right)\sum_i n_i v_i - 2}{4 + 2\left(\frac{60\%}{40\%} - 1\right)}$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 0.5\sum_i n_i v_i - 2}{4 + 2 \cdot 0.5}$$

$$\mathbf{n_\sigma = \frac{\sum_i n_i(1.5v_i + 2) - 2}{5}} \tag{18}$$

$$n_s = \frac{4(n_i - 1) + \left(\frac{60\%}{40\%} - 1\right)\sum_i n_i v_i}{4 + 2\left(\frac{60\%}{40\%} - 1\right)}$$

$$n_s = \frac{4n_i - 4 + 0.5\sum_i n_i v_i}{4 + 2 \cdot 0.5}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_s = \frac{0.5\sum_i n_i(v_i + 8) - 4}{5} \Rightarrow \mathbf{n_s} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} + \mathbf{8}) - \mathbf{8}}{\mathbf{10}} \tag{19}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{60\%}{40\%} - 1\right)}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2 \cdot 0.5}$$

$$\mathbf{n_\pi} = \mathbf{n_d} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{5}} \tag{20}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + \left(\frac{60\%}{40\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{60\%}{40\%} - 1\right)}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 0.5\sum_i n_i(v_i - 2) + 1 + 2}{4 + 2 \cdot 0.5}$$

$$n_r = \frac{1.5\sum_i n_i(v_i - 2) + 3}{5} \Rightarrow \mathbf{n_r} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{3.333333333}} \tag{21}$$

After deducing the general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with double bonds where $p_\pi = 40\%$ and $p_r = 60\%$, we will apply them on a molecular formula as an example: $C_{14}H_{20}O_2$

$$n_\sigma = \frac{\sum_i n_i(1.5v_i + 2) - 2}{5} \tag{18}$$

$$n_\sigma = \frac{n_C(1.5 \cdot 4 + 2) + n_O(1.5 \cdot 2 + 2) + n_H(1.5 \cdot 1 + 2) - 2}{5}$$

$$n_\sigma = \frac{112 + 10 + 70 - 2}{5} \Rightarrow \mathbf{n_\sigma} = \mathbf{38}$$

$$n_s = \frac{\sum_i n_i(v_i + 8) - 8}{10} \tag{19}$$

$$n_s = \frac{n_C(4 + 8) + n_O(2 + 8) + n_H(1 + 8) - 8}{10}$$

$$n_s = \frac{168 + 20 + 180 - 8}{10} \Rightarrow \mathbf{n_s} = \mathbf{36}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{5} \tag{20}$$

$$n_\pi = n_d = \frac{n_C(4 - 2) + n_O(2 - 2) + n_H(1 - 2) + 2}{5}$$

$$n_\pi = n_d = \frac{28 + 0 - 20 + 2}{5} \Rightarrow \mathbf{n_\pi} = \mathbf{n_d} = \mathbf{2}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{3.333333333} \tag{21}$$

 doi:10.20944/preprints202503.0108.v1

$$n_r = \frac{n_C(4-2) + n_O(2-2) + n_H(1-2) + 2}{3.333333333}$$

$$n_r = \frac{28 + 0 - 20 + 2}{3.333333333} \quad => \quad \mathbf{n_r = 3}$$

Other molecular formulas where their corresponding molecules can have $p_\pi = 40\%$ of TU and $p_r = 60\%$ of TU, will be presented in the following table:

Table 3. Calculation of covalent bonds and rings for unsaturated cyclic molecules with double bonds

$p_\pi = 40\% \quad and \quad p_r = 60\%$

Examples of Unsaturated Cyclic Molecules with double bonds	σ-bonds $-\frac{2}{5} + \frac{1}{5}(\sum_i \mathbf{n_i}(\mathbf{1.5v_i + 2}))$	Single bonds $-\frac{4}{5} + \frac{1}{10}(\sum_i \mathbf{n_i}(\mathbf{v_i + 8}))$	π-bonds and double bonds $\frac{2}{5} + \frac{1}{5}(\sum_i \mathbf{n_i}(\mathbf{v_i - 2}))$	Ring/Rings $\frac{2}{3.3} + \frac{1}{3.3}(\sum_i \mathbf{n_i}(\mathbf{v_i - 2}))$
$C_{14}H_{20}O_2$	38	36	$2\ n_\pi$; $2\ n_d$	3
$C_{14}H_{20}$	36	34	$2\ n_\pi$; $2\ n_d$	3
$C_{13}H_{19}NO_2$	37	35	$2\ n_\pi$; $2\ n_d$	3
$C_{25}H_{28}O_5Cl_4$	67	63	$4\ n_\pi$; $4\ n_d$	6
$C_{24}H_{36}N_6$	71	67	$4\ n_\pi$; $4\ n_d$	6
$C_{38}H_{68}S_5O_{14}$	133	127	$6\ n_\pi$; $6\ n_d$	9
$C_{32}H_{57}P_5N_6O_{17}$	125	119	$6\ n_\pi$; $6\ n_d$	9
$C_{50}H_{86}P_8O_{16}$	171	163	$8\ n_\pi$; $8\ n_d$	12
$C_{46}H_{79}S_9O_{19}Cl_{11}$	175	167	$8\ n_\pi$; $8\ n_d$	12

Some examples of molecular structures for cyclic unsaturated molecules with double bonds where $p_r > p_\pi$ and $p_\pi = 40\%$; $p_r = 60\%$ from the total unsaturation are the following ones:

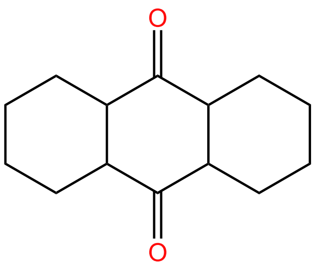


Figure 10. 1,2,3,4,4a,5,6,7,8,8a,9a,10a-dodecahydroanthracene-9,10-dione.

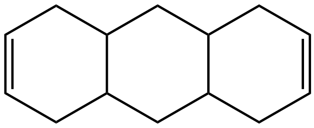


Figure 11. 1,4,4a,5,8,8a,9,9a,10,10a-decahydroanthracene.

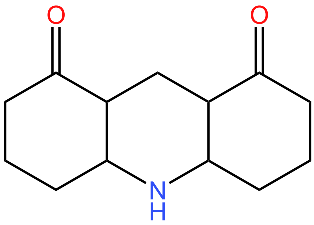


Figure 12. 2,3,4,4a,5,6,7,8a,9,9a,10,10a-dodecahydroacridine-1,8-dione.

3.2.2. Second example

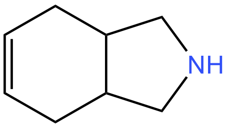


Figure 13. 2,3,3a,4,7,7a-hexahydro-1H-isoindole $\mathbf{C_8H_{13}N}$.

$$n_\pi + n_r = DOU \text{ and } n_\pi + n_r = 1 + \frac{1}{2}\sum_i n_i(v_i - 2)$$

$$n_\pi + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}n_O(2-2) + \frac{1}{2}n_H(1-2) \Rightarrow n_\pi + n_r = 3 \text{ and } n_\pi = 1 \; ; \; n_r = 2$$

$$p_\pi + p_r = TU \text{ and } p_\pi + p_r = 100\% \quad (5)$$

$$p_\pi = \frac{1 \cdot 100\%}{3} = 33.33333333\% \text{ and } p_r = \frac{2 \cdot 100\%}{3} = 66.66666667\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 33.33333333\%$ of TU and $p_r = 66.66666667\%$ of TU.

$$p_\pi + p_r = TU \quad (5)$$

$$p_\pi + p_r = 100\% \; ; \; 33.33333333\% + 66.66666667\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + \left(\frac{66.66666667\%}{33.33333333\%} - 1\right)\sum_i n_i v_i - 2}{4 + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

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

$$n_\sigma = \frac{2\sum_i n_i(v_i + 1) - 2}{6} \Rightarrow \mathbf{n_\sigma = \frac{\sum_i n_i(v_i + 1) - 1}{3}} \quad (22)$$

$$n_s = \frac{4(n_i - 1) + \left(\frac{66.66666667\%}{33.33333333\%} - 1\right)\sum_i n_i v_i}{4 + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

$$n_s = \frac{4n_i - 4 + \sum_i n_i v_i}{4 + 2 \cdot 1}$$

$$\mathbf{n_s} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} + \mathbf{4}) - \mathbf{4}}{\mathbf{6}} \tag{23}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

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

$$\mathbf{n_\pi} = \mathbf{n_d} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{6}} \tag{24}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + \left(\frac{66.66666667\%}{33.33333333\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + \sum_i n_i(v_i - 2) + 2 + 2}{4 + 2 \cdot 1}$$

$$n_r = \frac{2\sum_i n_i(v_i - 2) + 4}{6} => \mathbf{n_r} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{3}} \tag{25}$$

After deducing the general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with double bonds where $p_\pi = 33.33333333\%$ and $p_r = 66.66666667\%$, we will apply them on a molecular formula as an example: $C_9H_{16}N_2$

$$n_\sigma = \frac{\sum_i n_i(v_i + 1) - 1}{3} \tag{22}$$

$$n_\sigma = \frac{n_C(4 + 1) + n_N(3 + 1) + n_H(1 + 1) - 1}{3}$$

$$n_\sigma = \frac{45 + 8 + 32 - 1}{3} \quad => \mathbf{n_\sigma} = \mathbf{28}$$

$$n_s = \frac{\sum_i n_i(v_i + 4) - 4}{6} \tag{23}$$

$$n_s = \frac{n_C(4 + 4) + n_N(3 + 4) + n_H(1 + 4) - 4}{6}$$

$$n_s = \frac{72 + 14 + 80 - 4}{6} \quad => \mathbf{n_s} = \mathbf{27}$$

$$n_\pi = n_d = \frac{\sum_i n_i(v_i - 2) + 2}{6} \tag{24}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_\pi = n_d = \frac{n_C(4-2) + n_N(3-2) + n_H(1-2) + 2}{6}$$

$$n_\pi = n_d = \frac{18 + 2 - 16 + 2}{6} \quad => \; \mathbf{n_\pi = n_d = 1}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{3} \tag{25}$$

$$n_r = \frac{n_C(4-2) + n_N(3-2) + n_H(1-2) + 2}{3}$$

$$n_r = \frac{18 + 2 - 16 + 2}{3} \quad => \; \mathbf{n_r = 2}$$

Other molecular formulas where their corresponding molecules can have $p_\pi = 33.33333333\%$ of TU and $p_r = 66.66666667\%$ of TU, will be presented in the following table:

Table 4. Calculation of covalent bonds and rings for unsaturated cyclic molecules with double bonds $p_\pi = 33.33333333\% \;\; and \;\; p_r = 66.66666667\%$

Examples of Unsaturated Cyclic Molecules with double bonds	σ-bonds $-\frac{1}{3}+\frac{1}{3}(\sum_i \mathbf{n_i}(\mathbf{v_i}+\mathbf{1}))$	Single bonds $-\frac{2}{3}+\frac{1}{6}(\sum_i \mathbf{n_i}(\mathbf{v_i}+\mathbf{4}))$	π-bonds and double bonds $\frac{1}{3}+\frac{1}{6}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{2}))$	Ring/Rings $\frac{2}{3}+\frac{1}{3}(\sum_i \mathbf{n_i}(\mathbf{v_i}-\mathbf{2}))$
$C_8H_{12}O$	22	21	$1\ n_\pi$; $1\ n_d$	2
$C_{11}H_{18}O_2$	32	31	$1\ n_\pi$; $1\ n_d$	2
$C_9H_{14}O_2$	26	25	$1\ n_\pi$; $1\ n_d$	2
$C_{15}H_{29}P_2N_3O_4$	56	54	$2\ n_\pi$; $2\ n_d$	4
$C_{18}H_{32}S_2O_6Cl_2$	63	61	$2\ n_\pi$; $2\ n_d$	4
$C_{24}H_{37}N_5$	71	68	$3\ n_\pi$; $3\ n_d$	6
$C_{26}H_{48}P_4O_{12}$	95	92	$3\ n_\pi$; $3\ n_d$	6
$C_{34}H_{38}Cl_8$	87	83	$4\ n_\pi$; $4\ n_d$	8
$C_{30}H_{42}N_4O_7$	90	86	$4\ n_\pi$; $4\ n_d$	8

Some examples of molecular structures for cyclic unsaturated molecules with double bonds where $p_r > p_\pi$ and $p_\pi = 33.33333333\%$; $p_r = 66.66666667\%$ from the total unsaturation are the following ones:

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

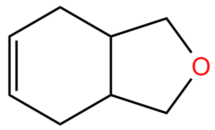


Figure 14. 1,3,3a,4,7,7a-hexahydro-2-benzofuran.

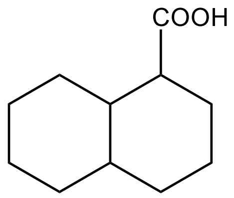


Figure 15. 1,2,3,4,4a,5,6,7,8,8a-decahydronaphthalene-1-carboxylic acid.

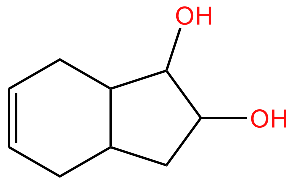


Figure 16. 2,3,3a,4,7,7a-hexahydro-1H-indene-1,2-diol.

3.3. Cyclic unsaturated molecules with triple bonds in which $p_\pi > p_r$

For all the cyclic unsaturated molecules that contain σ-bonds, π-bonds, single bonds and triple bonds where the number of π-bonds is always greater than the number of rings, we used two newly invented mathematical equations and another three previously shown for cyclic unsaturated molecules with double bonds ($p_\pi > p_r$) to deduce many other specific general equations for covalent bonds and rings:

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

$$n_s = \frac{\sum_i n_i(v_i + 6) + \left(\frac{p_\pi}{p_r} - 1\right)\left(\sum_i n_i(6 - v_i) - 6\right) - 6}{8 + 4\left(\frac{p_\pi}{p_r} - 1\right)} \tag{26}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + \left(\frac{p_\pi}{p_r} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{p_\pi}{p_r} - 1\right)} \tag{3}$$

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

$$n_t = \frac{\sum_i n_i(v_i - 2) + \left(\frac{p_\pi}{p_r} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{8 + 4\left(\frac{p_\pi}{p_r} - 1\right)} \tag{27}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

In order to find any percentages for π-bonds and rings that correspond to cyclic unsaturated molecules with triple bonds in which $p_\pi > p_r$; $0\% < p_r < 50\%$ and $50\% < p_\pi < 100\%$, we can start by choosing a molecular structure where $n_\pi > n_r$, write it's molecular formula and calculate the correlated degree of unsaturation. Afterwards, the number of π-bonds and rings will be converted into percentages using the rule of three, and those numerical values will be substituted into the main mathematical equations to deduce other specific general equations that have as variables only the number of atoms and their valences, and work for molecules that share the same values of p_π and p_r as our chosen molecular structure.

3.3.1. First example

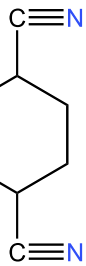


Figure 17. cyclohexane-1,4-dicarbonitrile $\mathbf{C_8H_{10}N_2}$

$$n_\pi + n_r = \text{DOU} \quad \text{and} \quad n_\pi + n_r = 1 + \tfrac{1}{2}\textstyle\sum_i n_i(v_i - 2)$$

$$n_\pi + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}n_H(1-2) \;\Rightarrow\; n_\pi + n_r = 5 \;\text{ and }\; n_\pi = 4 \;;\; n_r = 1$$

$$p_\pi + p_r = \text{TU} \quad \text{and} \quad p_\pi + p_r = 100\% \tag{5}$$

$$p_\pi = \frac{4 \cdot 100\%}{5} = 80\% \;\text{ and }\; p_r = \frac{1 \cdot 100\%}{5} = 20\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 80\%$ of TU and $p_r = 20\%$ of TU.

$$p_\pi + p_r = \text{TU} \tag{5}$$

$$p_\pi + p_r = 100\% \quad ; \quad 80\% + 20\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 2\left(\frac{80\%}{20\%} - 1\right)(n_i - 1) - 2}{4 + 2\left(\frac{80\%}{20\%} - 1\right)}$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 6n_i - 6 - 2}{4 + 2 \cdot 3}$$

$$\mathbf{n_\sigma = \frac{\sum_i n_i(v_i + 8) - 8}{10}} \tag{28}$$

$$n_s = \frac{\sum_i n_i(v_i + 6) + \left(\frac{80\%}{20\%} - 1\right)\left(\sum_i n_i(6 - v_i) - 6\right) - 6}{8 + 4\left(\frac{80\%}{20\%} - 1\right)}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_s = \frac{\sum_i n_i(v_i + 6) + 3\sum_i n_i(6 - v_i) - 18 - 6}{8 + 4 \cdot 3}$$

$$n_s = \frac{2\sum_i n_i(12 - v_i) - 24}{20} => \mathbf{n_s} = \frac{\sum_i \mathbf{n_i}(\mathbf{12} - \mathbf{v_i}) - \mathbf{12}}{\mathbf{10}} \quad (29)$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + \left(\frac{80\%}{20\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{80\%}{20\%} - 1\right)}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 3\sum_i n_i(v_i - 2) + 6 + 2}{4 + 2 \cdot 3}$$

$$n_\pi = \frac{4\sum_i n_i(v_i - 2) + 8}{10} => \mathbf{n_\pi} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{2.5}} \quad (30)$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{80\%}{20\%} - 1\right)}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2 \cdot 3}$$

$$\mathbf{n_r} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{10}} \quad (31)$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + \left(\frac{80\%}{20\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{8 + 4\left(\frac{80\%}{20\%} - 1\right)}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 3\sum_i n_i(v_i - 2) + 6 + 2}{8 + 4 \cdot 3}$$

$$n_t = \frac{4\sum_i n_i(v_i - 2) + 8}{20} => \mathbf{n_t} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{5}} \quad (32)$$

After deducing the specific general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with triple bonds where $p_\pi = 80\%$ and $p_r = 20\%$, we will apply them on a molecular formula as an example: $C_8H_{10}N_2$

$$n_\sigma = \frac{\sum_i n_i(v_i + 8) - 8}{10} \quad (28)$$

$$n_\sigma = \frac{n_C(4 + 8) + n_N(3 + 8) + n_H(1 + 8) - 8}{10}$$

$$n_\sigma = \frac{96 + 22 + 90 - 8}{10} => \mathbf{n_\sigma} = \mathbf{20}$$

$$n_s = \frac{\sum_i n_i(12 - v_i) - 12}{10} \quad (29)$$

$$n_s = \frac{n_C(12 - 4) + n_N(12 - 3) + n_H(12 - 1) - 12}{10}$$

$$n_s = \frac{64 + 18 + 110 - 12}{10} \quad => \quad \mathbf{n_s = 18}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{2.5} \tag{30}$$

$$n_\pi = \frac{n_C(4-2) + n_N(3-2) + n_H(1-2) + 2}{2.5}$$

$$n_\pi = \frac{16 + 2 - 10 + 2}{2.5} \quad => \quad \mathbf{n_\pi = 4}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{10} \tag{31}$$

$$n_r = \frac{n_C(4-2) + n_N(3-2) + n_H(1-2) + 2}{10}$$

$$n_r = \frac{16 + 2 - 10 + 2}{10} \quad => \quad \mathbf{n_r = 1}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{5} \tag{32}$$

$$n_t = \frac{n_C(4-2) + n_N(3-2) + n_H(1-2) + 2}{5}$$

$$n_t = \frac{16 + 2 - 10 + 2}{5} \quad => \quad \mathbf{n_t = 2}$$

Other molecular formulas where their corresponding molecules can have $p_\pi = 80\%$ of TU and $p_r = 20\%$ of TU, will be presented in the following table:

Table 5. Calculation of covalent bonds and rings for unsaturated cyclic molecules with triple bonds

$$p_\pi = 80\% \quad and \quad p_r = 20\%$$

Examples of Unsaturated Cyclic Molecules with triple bonds	σ-bonds $-\frac{4}{5} + \frac{1}{10}(\sum_i \mathbf{n_i}(\mathbf{v_i} + \mathbf{8}))$	Single bonds $-\frac{6}{5} + \frac{1}{10}(\sum_i \mathbf{n_i}(\mathbf{12} - \mathbf{v_i}))$	π-bonds and triple bonds $\frac{2}{2.5} + \frac{1}{2.5}(\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}))$ $\frac{2}{5} + \frac{1}{5}(\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}))$	Ring/Rings $\frac{2}{10} + \frac{1}{10}(\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}))$
$C_9H_{12}N_2$	23	21	$4\ n_\pi$; $2\ n_t$	1
C_6H_4	10	8	$4\ n_\pi$; $2\ n_t$	1
C_7H_7N	15	13	$4\ n_\pi$; $2\ n_t$	1
$C_{12}H_8N_2O_2$	25	21	$8\ n_\pi$; $4\ n_t$	2
$C_{14}H_7O_2Cl_3$	27	23	$8\ n_\pi$; $4\ n_t$	2

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$C_{18}H_{24}S_4O_8$	56	50	12 n_{π} ; 6 n_t	3
$C_{20}H_{16}N_4O_5$	47	41	12 n_{π} ; 6 n_t	3
$C_{30}H_{16}Cl_6$	55	47	16 n_{π} ; 8 n_t	4
$C_{36}H_{34}O_{11}$	84	76	16 n_{π} ; 8 n_t	4

Some examples of molecular structures for cyclic unsaturated molecules with triple bonds where $p_{\pi} > p_r$ and $p_{\pi} = 80\%$; $p_r = 20\%$ from the total unsaturation are the following ones:

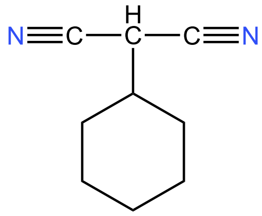


Figure 18. 2-cyclohexyl propanedinitrile.

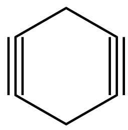


Figure19. cyclohexa-1,4-diyne.

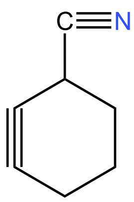


Figure 20. cyclohex2-yne-1-carbonitrile.

3.3.2. Second example

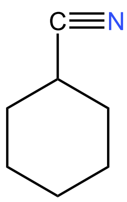


Figure 21. cyclohexanecarbonitrile $\mathbf{C_7H_{11}N}$

$$n_{\pi} + n_r = DOU \text{ and } n_{\pi} + n_r = 1 + \frac{1}{2}\sum_i n_i(v_i - 2)$$

$$n_{\pi} + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}n_N(3-2) + \frac{1}{2}n_H(1-2) \Rightarrow n_{\pi} + n_r = 3 \text{ and } n_{\pi} = 2 \; ; \; n_r = 1$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$p_\pi + p_r = TU \quad \text{and} \quad p_\pi + p_r = 100\% \tag{5}$$

$$p_\pi = \frac{2 \cdot 100\%}{3} = 66.66666667\% \text{ and } p_r = \frac{1 \cdot 100\%}{3} = 33.33333333\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 66.66666667\%$ of TU and $p_r = 33.33333333\%$ of TU.

$$p_\pi + p_r = TU \tag{5}$$

$$p_\pi + p_r = 100\% \quad ; \quad 66.66666667\% + 33.33333333\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)(n_i - 1) - 2}{4 + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

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

$$\mathbf{n_\sigma} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} + \mathbf{4}) - \mathbf{4}}{\mathbf{6}}$$

$$n_s = \frac{\sum_i n_i(v_i + 6) + \left(\frac{66.66666667\%}{33.33333333\%} - 1\right)\left(\sum_i n_i(6 - v_i) - 6\right) - 6}{8 + 4\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

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

$$n_s = \frac{12n_i - 12}{12} \Rightarrow \mathbf{n_s} = \mathbf{n_i} - \mathbf{1} \tag{34}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + \left(\frac{66.66666667\%}{33.33333333\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

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

$$n_\pi = \frac{2\sum_i n_i(v_i - 2) + 4}{6} \Rightarrow \mathbf{n_\pi} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{3}} \tag{35}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2 \cdot 1}$$

$$\mathbf{n_r} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{6}} \tag{36}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + \left(\frac{66.66666667\%}{33.33333333\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{8 + 4\left(\frac{66.66666667\%}{33.33333333\%} - 1\right)}$$

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

$$n_t = \frac{2\sum_i n_i(v_i - 2) + 4}{12} => \mathbf{n_t} = \frac{\sum_i \mathbf{n_i}(\mathbf{v_i} - \mathbf{2}) + \mathbf{2}}{\mathbf{6}} \quad (37)$$

After deducing the general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with triple bonds where $p_\pi = 66.66666667\%$ and $p_r = 33.33333333\%$, we will apply them on a molecular formula as an example: $C_6H_{12}O_3S$

$$n_\sigma = \frac{\sum_i n_i(v_i + 4) - 4}{6} \quad (33)$$

$$n_\sigma = \frac{n_S(6+4) + n_C(4+4) + n_O(2+4) + n_H(1+4) - 4}{6}$$

$$n_\sigma = \frac{10 + 48 + 18 + 60 - 4}{6} \quad => \ \mathbf{n_\sigma} = \mathbf{22}$$

$$n_s = n_i - 1 \quad (34)$$

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

$$n_s = 1 + 6 + 3 + 12 - 1 => \mathbf{n_s} = \mathbf{21}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{3} \quad (35)$$

$$n_\pi = \frac{n_S(6-2) + n_C(4-2) + n_O(2-2) + n_H(1-2) + 2}{3}$$

$$n_\pi = \frac{4 + 12 + 0 - 12 + 2}{3} \quad => \ \mathbf{n_\pi} = \mathbf{2}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{6} \quad (36)$$

$$n_r = \frac{n_S(6-2) + n_C(4-2) + n_O(2-2) + n_H(1-2) + 2}{6}$$

$$n_r = \frac{4 + 12 + 0 - 12 + 2}{6} \quad => \ \mathbf{n_r} = \mathbf{1}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{6} \quad (37)$$

$$n_t = \frac{n_S(6-2) + n_C(4-2) + n_O(2-2) + n_H(1-2) + 2}{6}$$

$$n_t = \frac{4 + 12 + 0 - 12 + 2}{6} \quad => \ \mathbf{n_t} = \mathbf{1}$$

Other molecular formulas where their corresponding molecules can have $p_\pi = 66.66666667\%$ of TU and $p_r = 33.33333333\%$ of TU, will be presented in the following table:

Table 6. Calculation of covalent bonds and rings for unsaturated cyclic molecules with triple bonds

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$p_\pi = 66.66666667\% \quad and \quad p_r = 33.33333333\%$$

Examples of Unsaturated Cyclic Molecules with triple bonds	σ-bonds $-\frac{2}{3}+\frac{1}{6}(\sum_i \mathbf{n_i}(\mathbf{v_i}+4))$	Single bonds $\mathbf{n_i}-\mathbf{1}$	π-bonds and triple bonds $\frac{2}{3}+\frac{1}{3}(\sum_i \mathbf{n_i}(\mathbf{v_i}-2))$ $\frac{1}{3}+\frac{1}{6}(\sum_i \mathbf{n_i}(\mathbf{v_i}-2))$	Ring/Rings $\frac{1}{3}+\frac{1}{6}(\sum_i \mathbf{n_i}(\mathbf{v_i}-2))$
$C_6H_8O_2$	16	15	$2\ n_\pi\ ;1\ n_t$	1
$C_7H_9NCl_2$	19	18	$2\ n_\pi\ ;1\ n_t$	1
$C_7H_{10}O$	18	17	$2\ n_\pi\ ;1\ n_t$	1
$C_{11}H_{15}N_3O_2$	32	30	$4\ n_\pi\ ;2\ n_t$	2
$C_{14}H_{14}Cl_4$	33	31	$4\ n_\pi\ ;2\ n_t$	2
$C_{16}H_{22}P_2O_2$	44	41	$6\ n_\pi\ ;3\ n_t$	3
$C_{18}H_{28}S_2O_5$	55	52	$6\ n_\pi\ ;3\ n_t$	3
$C_{21}H_{23}N_3$	50	46	$8\ n_\pi\ ;4\ n_t$	4
$C_{21}H_{23}N_3O_8$	58	54	$8\ n_\pi\ ;4\ n_t$	4

Some examples of molecular structures for cyclic unsaturated molecules with triple bonds where $p_\pi > p_r$ and $p_\pi = 66.66666667\%$; $p_r = 33.33333333\%$ from the total unsaturation are the following ones:

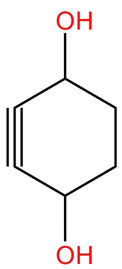


Figure 22. cyclohex-2-yne-1,4-diol.

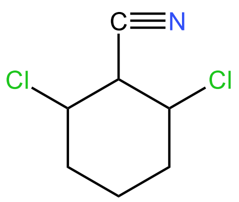
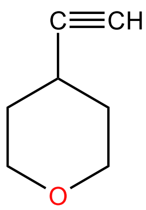


Figure 23. 2,6-dichloro cyclohexane-1-carbonitrile.



Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

Figure 24. 4-ethynyloxane

3.4. Cyclic unsaturated molecules with triple bonds in which $p_r > p_\pi$

For all the cyclic unsaturated molecules that contain σ-bonds, π-bonds, single bonds and triple bonds where the number of rings is always greater than the number of π-bonds, we used two newly invented mathematical equations and another three previously shown for cyclic unsaturated molecules with double bonds ($p_r > p_\pi$) to deduce many other specific general equations for covalent bonds and rings:

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + \left(\frac{p_r}{p_\pi} - 1\right)\sum_i n_i v_i - 2}{4 + 2\left(\frac{p_r}{p_\pi} - 1\right)} \tag{14}$$

$$n_s = \frac{\sum_i n_i(v_i + 6) + 2\left(\frac{p_r}{p_\pi} - 1\right)\sum_i n_i v_i - 6}{8 + 4\left(\frac{p_r}{p_\pi} - 1\right)} \tag{38}$$

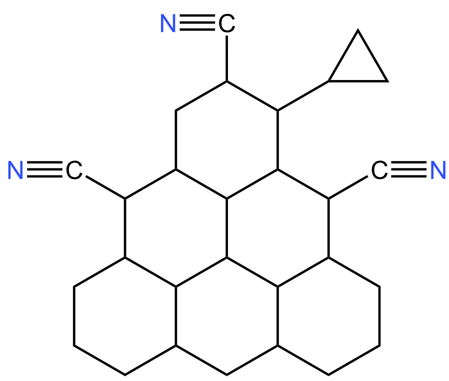
$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{p_r}{p_\pi} - 1\right)} \tag{16}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + \left(\frac{p_r}{p_\pi} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{p_r}{p_\pi} - 1\right)} \tag{17}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{8 + 4\left(\frac{p_r}{p_\pi} - 1\right)} \tag{39}$$

In order to find any percentages for π-bonds and rings that correspond to cyclic unsaturated molecules with triple bonds in which $p_r > p_\pi$; $0\% < p_\pi < 50\%$ and $50\% < p_r < 100\%$, we can start by choosing a molecular structure where $n_r > n_\pi$, write it's molecular formula and calculate the correlated degree of unsaturation. Afterwards, the number of π-bonds and rings will be converted into percentages using the rule of three, and those numerical values will be substituted into the main mathematical equations to deduce other specific general equations that have as variables only the number of atoms and their valences, and work for molecules that share the same values of p_π and p_r as our chosen molecular structure. Additionally, because cyclic unsaturated molecules with triple bonds where $n_r > n_\pi$ are less common, we will be using theoretical molecular structures as examples instead of real organic compounds.

3.4.1. First example



Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

Figure 25. First theoretical molecular structure with rings and triple bonds $\mathbf{C_{28}H_{35}N_3}$.

$$n_\pi + n_r = DOU \text{ and } n_\pi + n_r = 1 + \frac{1}{2}\sum_i n_i(v_i - 2)$$

$$n_\pi + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}n_N(3-2) + \frac{1}{2}n_H(1-2) \Rightarrow n_\pi + n_r = 13 \text{ and } n_\pi = 6 \ ; \ n_r = 7$$

$$p_\pi + p_r = TU \text{ and } p_\pi + p_r = 100\% \quad (5)$$

$$p_\pi = \frac{6 \cdot 100\%}{13} = 46.15384615\% \text{ and } p_r = \frac{7 \cdot 100\%}{13} = 53.84615385\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 46.15384615\%$ of TU and $p_r = 53.84615385\%$ of TU.

$$p_\pi + p_r = TU \quad (5)$$

$$p_\pi + p_r = 100\% \ ; \ 46.15384615\% + 53.84615385\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + \left(\frac{53.84615385\%}{46.15384615\%} - 1\right)\sum_i n_i v_i - 2}{4 + 2\left(\frac{53.84615385\%}{46.15384615\%} - 1\right)}$$

$$n_\sigma = \frac{\sum_i n_i(v_i + 2) + 0.166666667\sum_i n_i v_i - 2}{4 + 2 \cdot 0.166666667}$$

$$\mathbf{n_\sigma = \frac{\sum_i n_i(1.166666667 v_i + 2) - 2}{4.333333334}} \quad (40)$$

$$n_s = \frac{\sum_i n_i(v_i + 6) + 2\left(\frac{53.84615385\%}{46.15384615\%} - 1\right)\sum_i n_i v_i - 6}{8 + 4\left(\frac{53.84615385\%}{46.15384615\%} - 1\right)}$$

$$n_s = \frac{\sum_i n_i(v_i + 6) + 0.333333334\sum_i n_i v_i - 6}{8 + 4 \cdot 0.166666667}$$

$$\mathbf{n_s = \frac{\sum_i n_i(1.333333334 v_i + 6) - 6}{8.666666668}} \quad (41)$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{53.84615385\%}{46.15384615\%} - 1\right)}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2 \cdot 0.166666667}$$

$$\mathbf{n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4.333333334}} \quad (42)$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + \left(\frac{53.84615385\%}{46.15384615\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{53.84615385\%}{46.15384615\%} - 1\right)}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_r = \frac{\sum_i n_i(v_i - 2) + 0.166666667\sum_i n_i(v_i - 2) + 0.333333334 + 2}{4 + 2 \cdot 0.166666667}$$

$$n_r = \frac{1.166666667\sum_i n_i(v_i - 2) + 2.333333334}{4.333333334} => \mathbf{n_r} = \frac{\boldsymbol{\sum_i n_i(v_i - 2) + 2}}{\mathbf{3.714285714}} \tag{43}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{8 + 4\left(\frac{53.84615385\%}{46.15384615\%} - 1\right)}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{8 + 4 \cdot 0.166666667}$$

$$\mathbf{n_t} = \frac{\boldsymbol{\sum_i n_i(v_i - 2) + 2}}{\mathbf{8.666666668}} \tag{44}$$

After deducing the general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with triple bonds where $p_\pi = 46.15384615\%$ and $p_r = 53.84615385\%$, we will apply them on a molecular formula as an example: $C_{28}H_{35}N_3$

$$n_\sigma = \frac{\sum_i n_i(1.166666667v_i + 2) - 2}{4.333333334} \tag{40}$$

$$n_\sigma = \frac{n_C(1.166666667 \cdot 4 + 2) + n_N(1.166666667 \cdot 3 + 2) + n_H(1.166666667 \cdot 1 + 2) - 2}{4.333333334}$$

$$n_\sigma = \frac{186.6666667 + 16.500000003 + 110.8333333 - 2}{4.333333334} \quad => \mathbf{n_\sigma} = \mathbf{72}$$

$$n_s = \frac{\sum_i n_i(1.333333334v_i + 6) - 6}{8.666666668} \tag{41}$$

$$n_s = \frac{n_C(1.333333334 \cdot 4 + 6) + n_N(1.333333334 \cdot 3 + 6) + n_H(1.333333334 \cdot 1 + 6) - 6}{8.666666668}$$

$$n_s = \frac{317.3333334 + 30.00000001 + 256.6666667 - 6}{8.666666668} \quad => \mathbf{n_s} = \mathbf{69}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4.333333334} \tag{42}$$

$$n_\pi = \frac{n_C(4 - 2) + n_N(3 - 2) + n_H(1 - 2) + 2}{4.333333334}$$

$$n_\pi = \frac{56 + 3 - 35 + 2}{4.333333334} \quad => \mathbf{n_\pi} = \mathbf{6}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{3.714285714} \tag{43}$$

$$n_r = \frac{n_C(4 - 2) + n_N(3 - 2) + n_H(1 - 2) + 2}{3.714285714}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_r = \frac{56+3-35+2}{3.714285714} \quad => \quad \mathbf{n_r = 7}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{8.666666668} \tag{44}$$

$$n_t = \frac{n_C(4-2) + n_N(3-2) + n_H(1-2) + 2}{8.666666668}$$

$$n_t = \frac{56+3-35+2}{8.666666668} \quad => \quad \mathbf{n_t = 3}$$

Other molecular formulas where their corresponding molecules can have $p_\pi = 46.15384615\%$ of TU and $p_r = 53.84615385\%$ of TU, will be presented in the following table:

Table 7. Calculation of covalent bonds and rings for unsaturated cyclic molecules with triple bonds

$p_\pi = 46.15384615\% \;\; and \;\; p_r = 53.84615385\%$

Examples of Unsaturated Cyclic Molecules with triple bonds	**σ-bonds** $\frac{-2}{4.\overline{3}} + \frac{1}{4.\overline{3}}(\sum_i n_i(1.1\overline{6}v_i + 2))$	**Single bonds** $\frac{-6}{8.\overline{6}} + \frac{1}{8.\overline{6}}(\sum_i n_i(1.\overline{3}v_i + 6))$	**π-bonds and triple bonds** $\frac{2}{4.\overline{3}} + \frac{1}{4.\overline{3}}(\sum_i n_i(v_i - 2))$ $\frac{2}{8.\overline{6}} + \frac{1}{8.\overline{6}}(\sum_i n_i(v_i - 2))$	**Ring/Rings** $\frac{2.\overline{3}}{4.\overline{3}} + \frac{1.1\overline{6}}{4.\overline{3}}(\sum_i n_i(v_i - 2))$
$C_{24}H_{31}N_7$	68	65	$6\ n_\pi$; $3\ n_t$	7
$C_{62}H_{83}P_3O_8$	169	163	$12\ n_\pi$; $6\ n_t$	14
$C_{58}H_{75}N_9O_6$	161	155	$12\ n_\pi$; $6\ n_t$	14
$C_{63}H_{53}S_2Cl_5$	143	134	$18\ n_\pi$; $9\ n_t$	21
$C_{57}H_{39}N_4Cl_3$	123	114	$18\ n_\pi$; $9\ n_t$	21
$C_{110}H_{118}O_{12}$	267	255	$24\ n_\pi$; $12\ n_t$	28
$C_{114}H_{118}Cl_8$	267	255	$24\ n_\pi$; $12\ n_t$	28
$C_{135}H_{163}P_7$	339	324	$30\ n_\pi$; $15\ n_t$	35
$C_{142}H_{192}S_9$	377	362	$30\ n_\pi$; $15\ n_t$	35

Some examples of molecular structures for cyclic unsaturated molecules with triple bonds where $p_r > p_\pi$ and $p_\pi = 46.15384615\%$; $p_r = 53.84615385\%$ from the total unsaturation are the following ones:

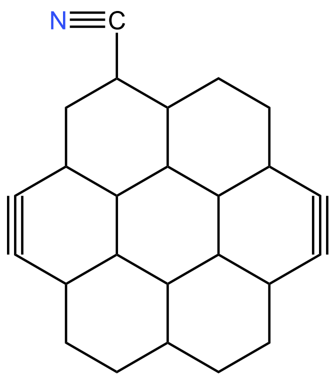


Figure 26. Second theoretical molecular structure with rings and triple bonds.

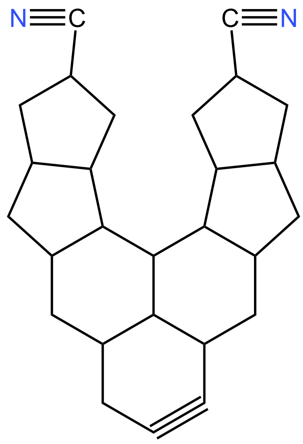


Figure 27. Third theoretical molecular structure with rings and triple bonds.

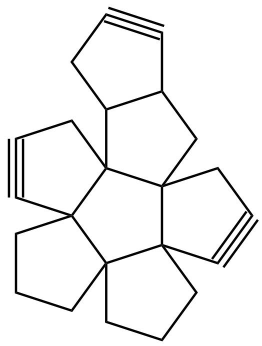
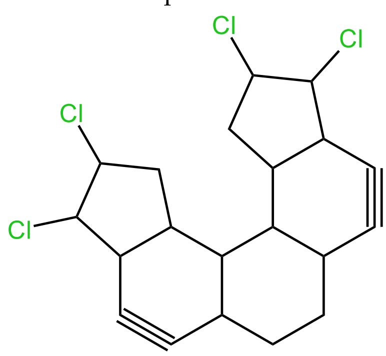


Figure 28. Fourth theoretical molecular structure with rings and triple bonds.

3.4.2. Second example



Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

Figure 29. First theoretical molecular structure with rings and triple bonds $\mathbf{C_{20}H_{20}Cl_4}$

$$n_\pi + n_r = DOU \text{ and } n_\pi + n_r = 1 + \frac{1}{2}\sum_i n_i(v_i - 2)$$

$$n_\pi + n_r = 1 + \frac{1}{2}n_C(4-2) + \frac{1}{2}n_{Cl}(1-2) + \frac{1}{2}n_H(1-2) => n_\pi + n_r = 9 \text{ and } n_\pi = 4 \ ; \ n_r = 5$$

$$p_\pi + p_r = TU \text{ and } p_\pi + p_r = 100\% \quad (5)$$

$$p_\pi = \frac{4 \cdot 100\%}{9} = 44.44444444\% \text{ and } p_r = \frac{5 \cdot 100\%}{9} = 55.55555556\%$$

Now we will substitute p_π and p_r in all the presented equations with percentages using the total unsaturation formula, where $p_\pi = 44.44444444\%$ of TU and $p_r = 55.55555556\%$ of TU.

$$p_\pi + p_r = TU \quad (5)$$

$$p_\pi + p_r = 100\% \ ; \ 44.44444444\% + 55.55555556\% = 100\%$$

$$n_\sigma = \frac{\sum_i n_i(v_i+2) + \left(\frac{55.55555556\%}{44.44444444\%} - 1\right)\sum_i n_i v_i - 2}{4 + 2\left(\frac{55.55555556\%}{44.44444444\%} - 1\right)}$$

$$n_\sigma = \frac{\sum_i n_i(v_i+2) + 0.25\sum_i n_i v_i - 2}{4 + 2 \cdot 0.25}$$

$$\mathbf{n_\sigma = \frac{\sum_i n_i(1.25v_i + 2) - 2}{4.5}} \quad (45)$$

$$n_s = \frac{\sum_i n_i(v_i+6) + 2\left(\frac{55.55555556\%}{44.44444444\%} - 1\right)\sum_i n_i v_i - 6}{8 + 4\left(\frac{55.55555556\%}{44.44444444\%} - 1\right)}$$

$$n_s = \frac{\sum_i n_i(v_i+6) + 0.5\sum_i n_i v_i - 6}{8 + 4 \cdot 0.25}$$

$$\mathbf{n_s = \frac{\sum_i n_i(1.5v_i + 6) - 6}{9}} \quad (46)$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2\left(\frac{55.55555556\%}{44.44444444\%} - 1\right)}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4 + 2 \cdot 0.25}$$

$$\mathbf{n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4.5}} \quad (47)$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + \left(\frac{55.55555556\%}{44.44444444\%} - 1\right)\left(\sum_i n_i(v_i - 2) + 2\right) + 2}{4 + 2\left(\frac{55.55555556\%}{44.44444444\%} - 1\right)}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_r = \frac{\sum_i n_i(v_i - 2) + 0.25\sum_i n_i(v_i - 2) + 0.5 + 2}{4 + 2 \cdot 0.25}$$

$$n_r = \frac{1.25\sum_i n_i(v_i - 2) + 2.5}{4.5} => \mathbf{n_r} = \frac{\sum_i \mathbf{n_i(v_i - 2) + 2}}{\mathbf{3.6}} \tag{48}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{8 + 4\left(\frac{55.55555556\%}{44.44444444\%} - 1\right)}$$

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{8 + 4 \cdot 0.25}$$

$$\mathbf{n_t} = \frac{\sum_i \mathbf{n_i(v_i - 2) + 2}}{\mathbf{9}} \tag{49}$$

After deducing the general equations for the calculation of the number of covalent bonds and rings for all the cyclic unsaturated organic molecules with triple bonds where $p_\pi = 44.44444444\%$ and $p_r = 55.55555556\%$, we will apply them on a molecular formula as an example: $C_{23}H_{36}P_2O_4$

$$n_\sigma = \frac{\sum_i n_i(1.25v_i + 2) - 2}{4.5} \tag{45}$$

$$n_\sigma = \frac{n_P(1.25 \cdot 5 + 2) + n_C(1.25 \cdot 4 + 2) + n_O(1.25 \cdot 2 + 2) + n_H(1.25 \cdot 1 + 2) - 2}{4.5}$$

$$n_\sigma = \frac{16.5 + 161 + 18 + 117 - 2}{4.5} \quad => \ \mathbf{n_\sigma = 69}$$

$$n_s = \frac{\sum_i n_i(1.5v_i + 6) - 6}{9} \tag{46}$$

$$n_s = \frac{n_P(1.5 \cdot 5 + 6) + n_C(1.5 \cdot 4 + 6) + n_O(1.5 \cdot 2 + 6) + n_H(1.5 \cdot 1 + 6) - 6}{9}$$

$$n_s = \frac{27 + 276 + 36 + 270 - 6}{9} \quad => \ \mathbf{n_s = 67}$$

$$n_\pi = \frac{\sum_i n_i(v_i - 2) + 2}{4.5} \tag{47}$$

$$n_\pi = \frac{n_P(5 - 2) + n_C(4 - 2) + n_O(2 - 2) + n_H(1 - 2) + 2}{4.5}$$

$$n_\pi = \frac{6 + 46 + 0 - 36 + 2}{4.5} \quad => \ \mathbf{n_\pi = 4}$$

$$n_r = \frac{\sum_i n_i(v_i - 2) + 2}{3.6} \tag{48}$$

$$n_r = \frac{n_P(5 - 2) + n_C(4 - 2) + n_O(2 - 2) + n_H(1 - 2) + 2}{3.6}$$

$$n_r = \frac{6 + 46 + 0 - 36 + 2}{3.6} \quad => \ \mathbf{n_r = 5}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

$$n_t = \frac{\sum_i n_i(v_i - 2) + 2}{9} \tag{49}$$

$$n_t = \frac{n_P(5-2) + n_C(4-2) + n_O(2-2) + n_H(1-2) + 2}{9}$$

$$n_t = \frac{6 + 46 + 0 - 36 + 2}{9} \quad => \ \mathbf{n_t = 2}$$

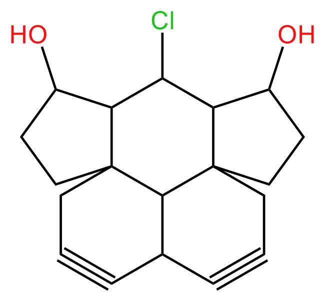
Other molecular formulas where their corresponding molecules can have $p_\pi = 44.44444444\%$ of TU and $p_r = 55.55555556\%$ of TU, will be presented in the following table:

Table 8. Calculation of covalent bonds and rings for unsaturated cyclic molecules with triple bonds

$$p_\pi = 44.44444444\% \quad and \quad p_r = 55.55555556\%$$

Examples of Unsaturated Cyclic Molecules with triple bonds	σ-bonds $\frac{-2}{4.5} + \frac{1}{4.5}(\sum_i n_i(1.25v_i + 2))$	Single bonds $\frac{-2}{3} + \frac{1}{9}(\sum_i n_i(1.5v_i + 6))$	π-bonds and triple bonds $\frac{2}{4.5} + \frac{1}{4.5}(\sum_i n_i(v_i - 2))$; $\frac{2}{9} + \frac{1}{9}(\sum_i n_i(v_i - 2))$	Ring/Rings $\frac{2}{3.6} + \frac{1}{3.6}(\sum_i n_i(v_i - 2))$
$C_{21}H_{28}N_2O_2$	57	55	4 n_π ; 2 n_t	5
$C_{35}H_{47}P_3N_2$	96	92	8 n_π ; 4 n_t	10
$C_{35}H_{49}S_2N_5$	100	96	8 n_π ; 4 n_t	10
$C_{50}H_{52}N_4$	120	114	12 n_π ; 6 n_t	15
$C_{54}H_{54}Cl_2$	124	118	12 n_π ; 6 n_t	15
$C_{62}H_{74}S_5O_{10}$	170	162	16 n_π ; 8 n_t	20
$C_{63}H_{71}P_5O_{10}$	168	160	16 n_π ; 8 n_t	20
$C_{78}H_{68}O_3$	173	163	20 n_π ; 10 n_t	25
$C_{71}H_{57}N_7Cl_4$	163	153	20 n_π ; 10 n_t	25

Some examples of molecular structures for cyclic unsaturated molecules with triple bonds where $p_r > p_\pi$ and $p_\pi = 44.44444444\%$; $p_r = 55.55555556\%$ from the total unsaturation are the following ones:



Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 4 March 2025 doi:10.20944/preprints202503.0108.v1

Figure 30. Second theoretical molecular structure with rings and triple bonds.

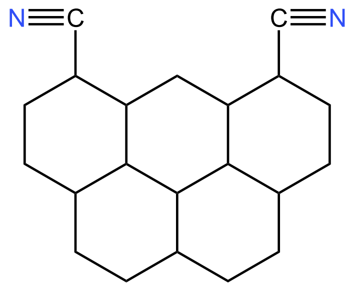


Figure 31. Third theoretical molecular structure with rings and triple bonds.

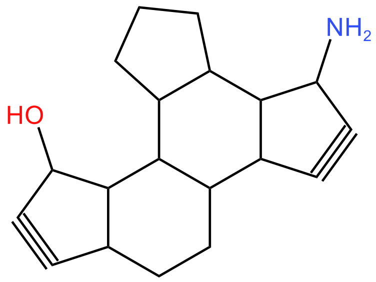


Figure 32. Fourth theoretical molecular structure with rings and triple bonds.

4. Conclusions

In this manuscript we have presented a new mathematical model for the calculation of covalent bonds and rings that can be used for any type of inequality established between p_π and p_r in cyclic unsaturated molecules with double or triple bonds, moreover, the model also works when p_π and p_r have the same values. Therefore, this research highlights a new methodology [26] that could serve as a starting point for multiple future studies based on ideas such as: similar equations for the calculation of covalent bonds in acyclic and cyclic unsaturated molecules with both double and triple bonds [27,28], integration of electric charges in order to account for anionic and cationic molecular species [29,30], taking into consideration delocalized π electrons [31,32] by modifying the numerical value of p_π from the total unsaturation and the possibility of inventing other equations for ionic and coordinate covalent bonds [33,34]. Another important aspect of this study is represented by the complexity that arises from the simmetry [35] and simplicity of the primary twelve novel equations which are made up by the number of atoms, their valences, and the percentages of pi(π) bonds and rings from TU in a molecule. These equations share a common structure in order to be easy to understand and simplified for any type of real or theoretical cyclic unsaturated compound [36]. Lastly, the mathematical model that was shown in this article could be used in computational chemistry to create tables and databases [37,38] that rely solely on the molecular formula of an organic compound and it's total unsaturation for the calculation of the number of covalent bonds and rings or to combine these equations with computer programs that already exist [39,40] in order to enhance the possibility of getting better results for certain theoretical approaches.

Author Contributions: The manuscript was conceptualized by Vlad Cristian Gavrilă, and investigation, review and editing processes were conducted by both authors. Both authors agreed to the final version of the manuscript.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Bonchev, D.; Rouvray, D.H. Chemical Graph Theory Introduction and Fundamentals. *CRC Press LLC* **2018**.
2. Gutman, I. Chemical Graph Theory—The Mathematical Connection. *Adv. Quantum. Chem.* **2006**, *51*, 125-138.
3. Leite, L.S.G.; Banerjee, S.; Wei, Y.; Elowitt, J.; Clark, A.E. Modern chemical graph theory. *WIREs. Comput. Mol. Sci.* **2024**, *14*.
4. Balaban, A.T. Applications of Graph Theory in Chemistry. *J. Chem. Inf. Comput. Sci.* **1985**, *25*, 334-343.
5. Zhao, L.; Schwarz, W.H.E.; Frenking, G. The Lewis electron-pair bonding model: the physical background, one century later. *Nat. Rev. Chem.* **2019**, *3*, 35–47.
6. Shaik, S.; Danovich, D.; Hiberty, P.C. Valence Bond Theory—Its Birth, Struggles with Molecular Orbital Theory, Its Present State and Future Prospects. *Molecules* **2021**, *26*, 1624.
7. Badertscher, M.; Bischofberger, K.; Munk, M.E.; Pretsch, E. A novel formalism to characterize the degree of unsaturation of organic molecules. *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 889-893.
8. Raheja, L.; Quick Calculation of Sigma and Pi bonds. *AIJRA* **2017**, *2*.
9. Gavrilă, V. C.; Nicolescu, T. O. A Theoretical Framework for the Calculation of the Number of Covalent Bonds in Unsaturated Organic Compounds. *Am. J. Phys. Chem.* **2024**, *13*, 72-82.
10. Das, A.; Adhikari, S.; Pal, D.; Paul, B.; Sanjeev, R.; Jagannadham, V. Rapid Calculation of the Number of π-bonds, σ-bonds, Single and Triple Bonds in Aliphatic Unsaturated Open Chain and Cycloalkynes. *World Journal of Chemical Education* **2014**, *2*, 1-3.
11. Gavrilă, V. C.; Nicolescu, T. O. New Equations for Rapid Calculation of π-bonds, σ-bonds, Single, Double and Triple Bonds in Open Chain Alcohols and Cycloamines. *Int. J. chem. math. phys*. **2024**, *8*, 9-15.
12. Xiaoyue, M. Development of Computational Chemistry and Application of Computational Methods. *Journal of Physics: Conference Series* **2022**, *2386*, 12005.
13. Alberts, M.; Laino, T.; Vaucher, A.C. Leveraging infrared spectroscopy for automated structure elucidation. *Commun. Chem.* **2024**, *7*.
14. Reguant, A.I.; Reis, H.; Medved, M.; Luis, J.M.; Zaleśny, R. A new computational tool for interpreting the infrared spectra of molecular complexes. *Phys. Chem. Chem. Phys***.** **2023**, *25*, 11658-11664.
15. Leniak, A.; Pietruś, W.; Kurczab, R. From NMR to AI: Designing a Novel Chemical Representation to Enhance Machine Learning Predictions of Physicochemical Properties. *J. Chem. Inf. Model.* **2024**, *64*, 3302-3321.
16. Hu, F.; Chen, M. S.; Rotskoff, G. M.; Kanan, M. W.; Markland, T. E. Accurate and Efficient Structure Elucidation from Routine One-Dimensional NMR Spectra Using Multitask Machine Learning. *ACS Cent. Sci.* **2024**, *10*, 2162-2170.
17. Scheubert, K.; Hufsky, F.; Böcker, S. Computational mass spectrometry for small molecules. *J. Cheminform.* **2013**, *5*.
18. Beck, A.G.; Muhoberac, M.; Randolph, C.E.; Beveridge, C.H.; Wijewardhane, P.R.; Kenttämaa, H.I.; Chopra, G. Recent Developments in Machine Learning for Mass Spectrometry**.** *ACS Meas. Sci. Au* **2024,** *4*, 233-246.
19. López, C.S.; Faza, O.N. Overview of the computational methods to assess aromaticity. *Aromaticity* **2021**, 41-71.
20. Ponting, D.J.; Deursen, R.V.; Ott M.A. Machine Learning Predicts Degree of Aromaticity from Structural Fingerprints**.** *J. Chem. Inf. Model.* **2020**, *60*, 4560–4568.
21. Kumar, M.D. A Study on Importance of Microsoft Excel Data Analysis Statistical Tools in Research Works. *Journal of Management & Educational Research Innovation* **2023**, *1*, 76-83.
22. Einax, J.W.; Crouch, S.R.; Holler, F.J. Applications of Microsoft® Excel in analytical chemistry, 2nd ed.. *Anal. Bioanal. Chem.* **2013**, *405*, 7559–7560.
23. Ferreira, C.T.T.; Silva, C.C. The Roles of Mathematics in the History of Science: The Mathematization Thesis. *Transversal: International Journal for the Historiography of Science* **2020**, *6*, 6-25.
24. Miller, D.D. Chapter 7 - The calculated uncertainty of scientific discovery: From Maths to Deep Maths. *Handbook of Statistics* **2023**, *49*, 203-226.
25. Liu, J.B. Novel Applications of Graph Theory in Chemistry and Drug Designing. *Combinatorial Chemistry & High Throughput Screening* **2022**, *25*, 439-440.
26. Lê, J. K.; Schmid, T. The Practice of Innovating Research Methods. *Organ. Res. Methods* **2022**, *25*, 308-336.
27. Wang, Z.X.; Livingstone, K.; Hümpel, C.; Daniliuc C.G.; Lichtenfeld, C.M.; Gilmour, R. Regioselective, catalytic 1,1-difluorination of enynes. *Nat. Chem.* **2023**, *15*, 1515–1522.

 doi:10.20944/preprints202503.0108.v1

28. Kitazawa, Y.; Kochi T.; Kakiuchi F. Hydroarylative cyclization of enynes with aromatic ketones catalyzed by a low-valent iron-phosphine complex. *Tetrahedron Letters* **2025**, *155*.
29. Sharma, B.; García, L.P.; Chaudhary, G.R.; Kaur, G. Innovative approaches to cationic and anionic (catanionic) amphiphiles self-assemblies: Synthesis, properties, and industrial applications. *Adv. Colloid Interface Sci.* **2025**, *337*.
30. Gao, H.; Jiang, J.; Huang, Y.; Wang, H.; Sun, J.; Jin, Z.; Wang, J.; Zhang, J. Synthesis of hydrogels for adsorption of anionic and cationic dyes in water: ionic liquid as a crosslinking agent. *SN Appl. Sci.* **2022**, *4*, 118.
31. Bradley, D.; Branley, C.P.; Peeks, M.D. A straightforward method to quantify the electron-delocalizing ability of π-conjugated molecules. *Phys. Chem. Chem. Phys.* **2022**, *24*, 11486-11490.
32. Box, V.G.S.; Yu, H.W. Pi-Electron Delocalization in Organic Molecules with C-N Bonds. *Journal of Chemical Education* **1997**, *74*, 1293.
33. Walton, J.R.; Rivera, L.A.R.; Lucchese, R.R.; Bevan, J.W. Is there any fundamental difference between ionic, covalent, and others types of bond? A canonical perspective on the question. *Phys. Chem. Chem. Phys*. **2017**, *19*.
34. Hei, X.; Liu, W.; Zhu, K.; Teat, S.J.; Jensen, S.; Li, M.; O'Carroll, D.M.; Wei, K.; Tan, K.; Cotlet, M.; Thonhauser, T.; Li, J. Blending Ionic and Coordinate Bonds in Hybrid Semiconductor Materials: A General Approach toward Robust and Solution-Processable Covalent/Coordinate Network Structures. *J. Am. Chem. Soc.* **2020**, *142*, 4242-4253.
35. Yanofsky, N.S.; Zelcer, M. The Role of Symmetry in Mathematics. *Found. Sci.* **2017**, *22*, 495–515.
36. Tantillo, D.J.; Applied Theoretical Organic Chemistry. *WORLD SCIENTIFIC (EUROPE)*, **2018**.
37. Mitchell, J. M.; Flight, R. M.; Moseley, H. N. B. Deriving Lipid Classification Based on Molecular Formulas. *Metabolites* **2020**, *10*, 122.
38. Feller, D. The role of databases in support of computational chemistry calculations. *J. Comput. Chem.* **1996**, *17*.
39. Hasan, M.R.; Alsaiari, A.A.; Fakhurji, B.Z.; Molla, M.H.R.; Asseri, A.H.; Sumon, M.A.A.; Park, M.N.; Ahammad, F.; Kim, B. Application of Mathematical Modeling and Computational Tools in the Modern Drug Design and Development Process. *Molecules* **2022**, *27*, 4169.
40. Sadybekov, A.V.; Katritch, V. Computational approaches streamlining drug discovery. *Nature* **2023**, *616*, 673 –685.