

Rapid Calculation of the Number of π -bonds, σ -bonds, Single and Triple Bonds in Aliphatic Unsaturated Open Chain and Cycloalkynes

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Abstract Prediction of number of π -bonds, σ -bonds, single and triple bonds of aliphatic unsaturated open chain and cycloalkynes is a vitally important tool for students of chemistry at undergraduate and graduate level for solving different kinds of problems regarding different chemical reactions. In this manuscript, we try to present a simple and innovative method for easy calculation of number of π -bonds, σ -bonds, single and triple bonds with the help of completely 8 (eight) new formulae.

Keywords: open chain and cycloalkynes, π and σ -bond, triple and single bond, number of carbon, hydrogen atoms

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1. Introduction

The number and types of bonds in open chain and cycloalkynes having complex molecular formula is a Herculean task. Keeping this in view, a rapid method has been proposed for the calculation of number of π -bonds, σ -bonds, single and triple bonds with the help of following 08 (eight) completely new formulae for certain aliphatic unsaturated open chain and cycloalkynes.

Earlier eight new innovative methods including sixteen new formulae have been introduced on the easy prediction of 'Bond-Order of mono and diatomic homo and heteronuclear molecules or ions', 'Bond-order of oxide based acid radicals', 'Hybridization', 'IUPAC nomenclature of spiro and bicyclo compounds', 'spin multiplicity value calculation and prediction of magnetic properties of diatomic hetero nuclear molecules and ions, 'Aromaticity' and 'magnetic properties of homo and hetero nuclear diatomic molecules and ions [1-7].

The present study involves eight formulae by just manipulating the number of carbon and hydrogen atoms by using some factors.

We think it would go a long way to help the students of organic chemistry and applied chemistry also who would choose the subject as their carrier. Experiment *in vitro* on 100 students show that by using these new methods strike rate is 1Q/30secs.

On the basis of this, we can strongly recommend that by using these new formulae the students can calculate number of π -bonds, σ -bonds, single and triple bonds for aliphatic unsaturated open chain and cycloalkynes.

2. Result and Discussion

2.1. Open Chain Aliphatic Alkynes

2.1.1. Calculation of π -bonds (P)

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in a given unsaturated hydrocarbon containing triple bonds. The formula to calculate the number of π bonds for an aliphatic open chain alkyne, where there is one or more than one triple bonds is

$$P = [(2X - Y) / 2] + 1$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and P = number of π bonds.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore $P = [(2X - Y) / 2] + 1 = [(2 \times 16 - 30) / 2] + 1 = 1 + 1 = 2$ number of π bonds.

2.1.2. Calculation of σ -bonds (S)

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in a given unsaturated hydrocarbon containing triple bonds.

The formula to calculate the number of σ bonds for an aliphatic open chain alkyne, where there is one or more than one triple bonds is

$$S = [X + Y - 1]$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and S = number of σ bonds.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore, S = $[X+Y-1] = [16+30-1] = 45$ numbers of σ bonds.

2.1.3. Calculation of Single bonds (A)

The total number of single bond for an aliphatic open chain alkyne, where there is one or more than one triple bonds is $A = [\{ (2X+5Y)/2 \} - 3] / 2$

Where, A = number of single bonds, X = number of carbon atoms and Y = number of hydrogen atoms.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore, A = $[\{ (2X+5Y) / 2 \} - 3] / 2 = [\{ (2 \times 16 + 5 \times 30) / 2 \} - 3] / 2 = [91 - 3] / 2 = 44$ numbers of single bonds.

2.1.4. Calculation of Triple Bonds (T)

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in a given unsaturated hydrocarbon containing triple bonds. The formula to calculate the number of triple bonds for an aliphatic open chain alkyne, where there is one or more than one triple bonds is

$$T = [\{ (2X - Y) / 2 \} + 1] / 2$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and T = number of triple bonds.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore, T = $[\{ (2X - Y) / 2 \} + 1] / 2 = [\{ (2 \times 16 - 30) / 2 \} + 1] / 2 = 2 / 2 = 1$ triple bond.

Table 1.

Example for Open Chain Alkyne (C_xH_y)	π bonds $[\{ (2X - Y) / 2 \} + 1]$	σ bonds $[X + Y - 1]$	Single bonds $[\{ (2X + 5Y) / 2 \} - 3] / 2$	Triple bond/bonds $[\{ (2X - Y) / 2 \} + 1] / 2$
$C_{10}H_{18}$	2	27	26	1
$C_{11}H_{20}$	2	30	29	1
$C_{12}H_{22}$	2	33	32	1
$C_{13}H_{24}$	2	36	35	1
$C_{14}H_{26}$	2	39	38	1
$C_{15}H_{28}$	2	42	41	1
$C_{16}H_{30}$	2	45	44	1
C_6H_6	4	11	9	2
$C_{12}H_{14}$	6	25	22	3

2.2. Cycloalkynes

2.2.1. Calculation of π -bonds (P_c)

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in the given unsaturated cycloalkyne. The formula to calculate the number of π bonds for an aliphatic cycloalkyne is

$$P_c = [(2X - Y) / 2]$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and P_c = number of π bonds in the cycloalkyne system.

E.g.: In Cycloheptyne (C_7H_{10}), X = 7, Y = 10, therefore $P_c = (2 \times 7 - 10) / 2 = 2$ number of π bonds.

2.2.2. Calculation of σ -bonds (S_c)

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in the given unsaturated cycloalkyne. The formula to calculate the number of σ bonds for an aliphatic cycloalkyne is

$$S_c = [X + Y]$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and S_c = number of sigma bonds (σ -bonds) in cyclo alkyne system.

E.g.: In Cycloheptyne (C_7H_{10}), X = 7, Y = 10, therefore $S_c = (7 + 10) = 17$ number of σ bonds.

2.2.3. Calculation of Single bonds (A_c)

The total number of single bond for an aliphatic cyclo alkyne is

$$A_c = [\{ (2X + 5Y) / 2 \}] / 2$$

Where, A_c = number of single bonds in cycloalkyne, X = number of carbon atoms and Y = number of hydrogen atoms.

E.g.: In Cycloheptyne (C_7H_{10}), X = 7, Y = 10, therefore, $A_c = [\{ (2X + 5Y) / 2 \}] / 2 = [\{ (2 \times 7 + 5 \times 10) / 2 \}] / 2 = 32 / 2 = 16$ numbers of single bonds.

2.2.4. Calculation of Triple bonds (T)

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in a given unsaturated cyclo system containing triple bond. The formula to calculate the number of triple bond is

$$T_c = [\{ (2X - Y) / 2 \}] / 2$$

Where, X = number of carbon atoms; Y = number of hydrogen atoms and T_c = number of triple bond.

E.g.: In Cycloheptyne (C_7H_{10}), X = 7, Y = 10, therefore, $T_c = [\{ (2X - Y) / 2 \}] / 2 = [\{ (2 \times 7 - 10) / 2 \}] / 2 = 2 / 2 = 1$ triple bond.

3. Conclusions

In conclusion here we approach a new rapid innovative method on easier calculation of number of π -bonds, σ -bonds, single and triple bonds for aliphatic unsaturated open chain and cycloalkynes. This new method is very helpful to undergraduate and graduate level students of chemistry. By using these methods we can easily predict nature of bonds in alkyne system in a very simple and metabolic way.

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