Chapter-11

INNOVATIVE METHODS FOR THE CALCULATION OF CHEMICAL BONDS IN ALKYNES

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In the previous chapter 10, some speedy innovative formulae have been proposed for calculating the number of chemical bonds (π-bonds, σ-bonds, single and double bonds) in aliphatic unsaturated open-chain and cyclic olefinic hydrocarbons without drawing their exact structures. But in this chapter 11, some brisk innovative formulae have also been proposed for the calculation of the number of chemical bonds (π-bonds, σ-bonds, single and triple bonds) in aliphatic unsaturated open-chain alkynes and cycloalkynes without drawing their accurate structures. It also helps students to solve multiple choice type questions (MCQs) on the calculation of chemical bonds in alkynes at different competitive examinations in a time economic ground without drawing their correct structures. The molecular formula, which defines a very large number of hydrocarbon units (H & C) in alkynes, in this particular case, it is a formidable task for students and educators to calculate the number of chemical bonds without drawing their precise structures. Keeping it in view, some hasty innovative methods have been introduced for the calculation of the number of chemical bonds such as π-bonds, σ-bonds, single and double bonds by merely counting number of carbon and hydrogen atoms with the help of 08 (eight) innovative formulae for aliphatic unsaturated open-chain and cycloalkynes[1,2,3].

METHODOLOGY

A. Innovative methods for calculation of chemical bonds in open chain aliphatic alkynes

(i) Calculation of π-bonds (P):

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1. A. Das *et.al.* , "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* 2 (Dec 2013**):** 1-3, doi:10.12691/wjce-2-1-1, http://pubs.sciepub.com/wjce/2/1/1/#.
2. A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education", *International Journal of Physics & Chemistry Education* 10 (June 2018): 27-40, doi: 10.12973/ijpce/81589, http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html.
3. A. Das, "Innovative Mnemonics Make Chemical Education Time Economic – A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept2018):154-174, doi:10.12691/wjce-6-4-2, http://pubs.sciepub.com/wjce/6/4/2/index.html.

The number of π bonds for an aliphatic open chain alkyne is **P= [(2X-Y)/2] + 1**; where X = number of carbon atoms; Y = number of hydrogen atoms and P = number of π bonds.

(ii) Calculation of σ-bonds (S):

The number of σ bonds for an aliphatic open chain alkyne is **S = [X + Y - 1]**; where X = number of carbon atoms; Y = number of hydrogen atoms and S = number of sigma bonds (σ-bonds).

(iii) Calculation of Single bonds (A):

The total number of single bond for an aliphatic open chain alkyne, where there are 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.

(iv)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 are one or more than one triple bond is **T= [{(2X-Y)/2} + 1]/2**; where, X = number of carbon atoms; Y = number of hydrogen atoms and T = number of triple bonds.

B. Innovative methods for calculation of chemical bonds in cycloalkynes

(i) 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.

(ii) Calculation of σ-bonds (S_c):

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 cycloalkyne system.

(iii) Calculation of Single bonds (A_c):

The total number of single bond for an aliphatic cycloalkyne 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.

(iv) Calculation of Triple bonds (T):

The number of triple bonds is **T_c= [{(2X-Y)/2}]/2**; where X = number of carbon atoms; Y = number of hydrogen atoms and T_c = number of the triple bond.

RESULTS AND DISCUSSION

Chemical bonds (π-bonds, σ-bonds, single and triple bonds) in the open chain and cycloalkynes having complex molecular formulae like $C_{15}H_{28}$, $C_{16}H_{30}$ can be calculated without drawing their literal structures by using different formulae, involving the number of carbon and hydrogen atoms only.

A. Innovative methods for calculation of chemical bonds in open chain aliphatic alkynes

Ex.a. For $C_{10}H_{18}$, number of carbon atoms, X = 10 and number of hydrogen atoms, Y = 18, therefore, number of π bonds, P = [(2X-Y)/2+1] = 2; σ bonds, S = [X+Y-1] = 27; single bonds, A = [{(2X+5Y)/2}-3]/2 = 26 and triple bond, T = [(2X-Y)/2 + 1] / 2 = 1.

Ex.b. For $C_{11}H_{20}$, number of carbon atoms, X = 11 and number of hydrogen atoms, Y = 20, therefore, number of π bonds, P = [(2X-Y)/2+1] = 2; σ bonds, S = [X+Y-1] = 30; single bonds, A = [{(2X+5Y)/2}-3]/2 = 29 and triple bond, T = [(2X-Y)/2 + 1] / 2 = 1. Adequate examples for the calculation of chemical bonds (π bonds, σ bonds, single and triple bonds) in open chain alkynes without drawing their exact structures have been illustrated in **Table 11.10**.

B. Innovative methods for calculation of chemical bonds in cycloalkynes

Ex.c. In cycloheptyne (C_7H_{10}), X =7, Y = 10, therefore, number of π bonds (P_c) = [(2X-Y)/2] = (2x7-10) / 2 = 2; number of σ bonds (S_c) = [X + Y] = (7+10) = 17; numbers of single bonds (A_c) = [{(2X+5Y)/2}]/2 = [{(2x7+5x10)/2}]/2 = 32/2 = 16 and number of triple bonds (T_c) = [{(2X-Y)/2}]/2 = [{(2 x 7 – 10)/2}] / 2 = 2/2 = 1.

APPLICATION OF INNOVATIVE METHODS ON ALKENES AND ALKYNES IN DESIGNING CBL ACTIVITY

Mnemonics on the calculation of chemical bonds in alkene and alkyne system, described in chapters 10 & 11, are very suitable for designing computer-based learning (CBL) activities and for developing computer programs to produce chemistry educational software tool like 'Hydrocarbons Parser'[4]. This tool will validate the formulas of hydrocarbons by storing these in an array and mapping its elements to a PHP regular expression pattern. This tool is used to count chemical bonds, degrees of unsaturation (DoU), discriminate between functional isomers, and predict physical properties. All this is done without consulting molecular orbital theory or a chemical database.

This tool will encourage educators, scholars, and chemistry students in solving a chemistry problem on the calculation of chemical bonds in the alkene and alkyne system. Data miners, computational chemists, chemical engineers, chemists can also use this tool.

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4. A.Das *et.al.*,'Hydrocarbons Parser', *minerazzi.com* (Aug 2015), http://www.minerazzi.com/tools/hydrocarbons/parser.php.

It may be expected that these time economic organic innovative mnemonics for calculation of chemical bonds in open chain and cycloalkynes without drawing their precise structures would go a long way to help the students of chemistry from Undergraduate to Post-Graduate level. Experiments, *in vitro*, on 100 students, showed that by using these formulae students can save up to 3-5 minutes' time in the examination hall. On the basis of this, I can strongly recommend using these time economic innovative mnemonics in the field of organic chemical education.

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