Chapter-10

INNOVATIVE METHODS FOR THE CALCULATION OF
CHEMICAL BONDS IN ALKENES

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This chapter 10 is totally different from the other chapters. In this chapter, some hasty innovative formulae have been proposed for the calculation of 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. This chapter helps students to solve multiple choice type questions (MCQs) on the calculation of chemical bonds in alkenes at different competitive examinations in a time economic ground.

The molecular formula, which defines an exceptionally large number of hydrocarbon units (H & C) in alkenes, in this particular case, it is a herculean task for students and educators to calculate the number of chemical bonds without drawing their precise structures. Earlier Badertscher *et.al.* studied a novel formalism to characterize the degree of unsaturation of organic molecules[1]. But no such work has not been taken till now, to calculate the number of chemical bonds in the open chain olefinic system having complex molecular formulae like $C_{176}H_{250}$, $C_{2000}H_{2000}$. Keeping it in view, some rapid innovative mnemonics have been introduced for the calculation of the number of chemical bonds such as π-bonds, σ-bonds, single and double bonds by simply counting number of carbon and hydrogen atoms with the help of 06 (six) innovative formulae for certain aliphatic unsaturated open-chain and cyclic olefinic hydrocarbons[2,3].

METHODOLOGY

A. Innovative methods for calculation of chemical bonds in open chain olefinic hydrocarbons

(i) Calculation of π-bonds and double bonds (P):

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1. M. Badertscher *et.al.,* "A Novel Formalism To Characterize the Degree of Unsaturation of Organic Molecules", *J.Chem.Inf.   Comput.   Sci.*   41(May   2001)**:**   889-893,   doi: 10.1021/ci000135o, https://pubs.acs.org/doi/abs/10.1021%2Fci000135o.

2. A. Das *et.al.*, "Rapid calculation of the number of π-bonds, σ-bonds, single and double bonds in the aliphatic unsaturated open-chain and cyclic olefinic hydrocarbons", *Education in Chemical Science and Technology* 2 (Aug 2014):41-46.

3. 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.

The number of π bonds or double bonds for a olefin is $P = [(2X-Y)/2] + 1$; where, X = number of carbon atoms; Y = number of hydrogen atoms and P = number of π bonds/double bonds.

(ii) Calculation of σ-bonds (S):

The number of σ bonds for a straight chain olefin 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 a straight chain olefin is $A = [(3Y/2)-2]$; where A = number of single bonds and Y is the number of hydrogen atoms.

B. Innovative methods for calculation of chemical bonds in cyclic aliphatic olefinic hydrocarbons

(i) Calculation of π-bonds and double bonds (P_c):

The number of π bonds or double bonds for an aliphatic cyclic olefin is $P_c = [(2X-Y)/2]$; Where X = number of carbon atoms; Y = number of hydrogen atoms and P_c = number of π bonds or double bonds in the cyclic olefinic system.

(ii) Calculation of σ-bonds (S_c):

The number of σ bonds for an aliphatic cyclic olefin 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 the cyclic olefinic system.

(iii) Calculation of Single bonds (A_c):

The total number of single bonds in aliphatic cyclic olefin can be calculated by using the formula $A_c = [3Y/2]$; where A_c = number of single bonds and y is the number of hydrogen atoms in aliphatic cyclic olefin.

RESULTS AND DISCUSSION

Chemical bonds (π-bonds, σ-bonds, single and double bonds) in the open chain and cyclic olefinic hydrocarbons having complex molecular formulae like $C_{176}H_{250}$, $C_{2000}H_{2000}$ 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 olefinic hydrocarbons

Ex.a. For C_2H_4 ($H_2C=CH_2$), number of carbon atoms, X = 2 and number of hydrogen atoms, Y = 4, therefore, number of π bond, P = [(2X-Y)/2+1] = 1; σ bonds, S = [X+Y-1] = 5; single bonds, A = [(3Y/2)-2] = 4 and double bond = [(2X-Y)/2 + 1] = 1.

Ex.b. For C_3H_6 ($H_2C=CH-CH_3$), number of carbon atoms, X = 3 and number of hydrogen atoms, Y = 6, therefore, number of π bond, P = [(2X-Y)/2+1] = 1; σ bonds, S = [X+Y-1] = 8; single bonds, A = [(3Y/2)-2] = 7 and double bond = [(2X-Y)/2 + 1] = 1.

Adequate examples for the calculation of chemical bonds (π bonds, σ bonds, single and double bonds) in open chain olefinic hydrocarbons without drawing their structures have been illustrated in Table 10.8.

Table 10.8 Calculation of bonds in open chain olefinic hydrocarbons

Example (C_xH_y)	Straight-chain Structure	π bond/ bonds [(2X-Y)/2+1]	σ bonds [X+Y-1]	Single bonds [(3Y/2)-2]	Double bond/bonds [(2X-Y)/2 + 1]
C_2H_4	$H_2C=CH_2$	1	5	4	1
C_3H_6	$H_2C=CH-CH_3$	1	8	7	1
C_3H_4	$H_2C=C=CH_2$	2	6	4	2
C_4H_8	i)$H_2C=CH-CH_2-CH_3$ ii)$H_3C-HC=CH-CH_3$	1	11	10	1
C_4H_6	i)$H_2C=C=CH-CH_3$ ii)$H_2C=CH-CH=CH_2$	2	9	7	2
C_4H_4	$H_2C=C=C=CH_2$	3	7	4	3
$C_{176}H_{250}$	-	52	425	373	52
$C_{2000}H_{2000}$	-	1001	3999	2998	1001
$C_{99}H_4$	-	98	102	4	98

B. Innovative methods for calculation of chemical bonds in cyclic olefinic hydrocarbons

Ex.c. For cyclopropene (C_3H_4), number of carbon atoms, $X = 3$ and number of hydrogen atoms, $Y = 4$, therefore, number of π bond, $(P_c) = [(2X-Y)/2] = 1$; σ bonds, $(S_c) = [X+Y] = 7$; single bonds, $(A_c) = [(3Y/2)] = 6$ and double bond $= [(2X-Y)/2] = 1$.

Adequate examples for the calculation of chemical bonds (π bonds, σ bonds, single and double bonds) in cyclic olefinic hydrocarbons without drawing their structures have been illustrated in Table 10.9.

Table 10.9 Calculation of bonds in Cycloalkene system

Example (C_xH_y)	Cycloalkene	π bond / bonds (P_c) = [(2X-Y)/2]	σ bonds (S_c) [X+Y]	Single bonds (A_c) [(3Y/2)]	Double bond/bonds [(2X-Y)/2]
C_3H_4	Cyclopropene	1	7	6	1
C_4H_4	Cyclobutadiene	2	8	6	2
C_5H_6	Cyclopentadiene	2	11	9	2
C_6H_8	Cyclohexadiene	2	14	12	2
C_7H_8	Cycloheptatriene	3	15	12	3
C_8H_8	Cyclooctatetraene	4	16	12	4

Conclusion

It may be expected that these time economic organic innovative mnemonics for calculation of chemical bonds in open chain and cyclic olefinic hydrocarbons without drawing their literal structures would go a long way to help to 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. Based on this, I can strongly recommend using these time economic innovative mnemonics in the field of organic chemical education.

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