CHAPTER

5

Double Bond Equivalent

DOUBLE BOND EQUIVALENTS (DBE) OR HYDROGEN DEFICIENCY INDEX OR DEGREES OF UNSATURATION

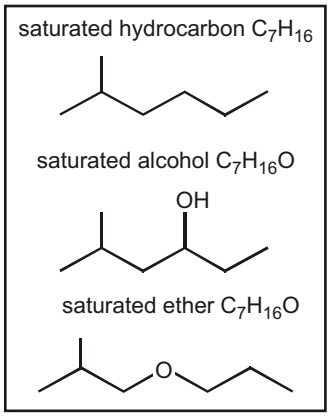
DBE help in the search for a structure

HOW TO CALCULATE DBE

Hello students! Have problems with calculating DBE ? No worries! Here is the tutorial which will help you step by step. Hopefully after reading this tutorial, you can calculate DBE faster and more accurately.

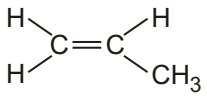
If DBE = 0

1. Ethylene, C_2H_6 is a saturated acyclic alkane and it does not have any bond or ring, so DBE = 0.



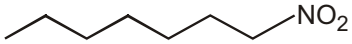
If DBE = 1

2. Propylene, C_3H_6 , contains a pi bond, so DBE = 1.



Propylene
DBE = 1

Cyclohexane
DBE = 1

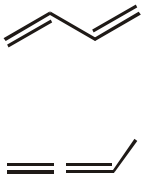


$C_7H_{15}NO_2$ = one DBE

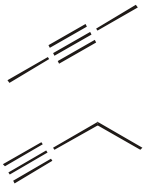
If DBE = 2

3. Propylene, C_4H_6 DBE = 2. There are several ways for a compound to possess two degrees of unsaturation : two double bonds, or two rings, or one double bond and one ring, or one triple bond. Let's explore all of these possibilities for C_4H_6 :

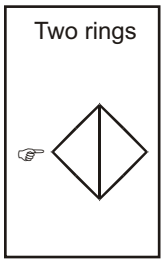
Two double bonds



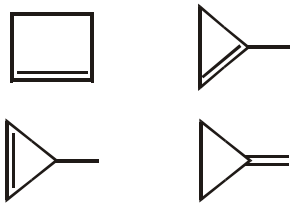
One triple bond



Two rings

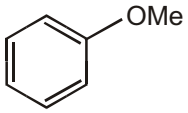


One ring and one double bond

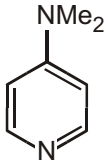


These are all of the possible constitutional isomers for C_6H_6. With this in mind, let's expand our skills set. Let's explore how to calculate the DBE when other elements are present in the molecular formula.

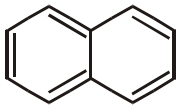
A benzene ring contains four DBE.



C_6H_8O = four DBE



$C_7H_{10}N_2$ = four DBE



only count two rings in this structure 5 pi bonds + 2 rings = > DBE = 5 + 2 = 7

HOW TO CALCULATE THE DBE IF WE DO NOT KNOW THE STRUCTURE OF THE CHEMICALS?

All the problems we have ever met talk about the organic chemicals which only contain carbon, oxygen, hydrogen, nitrogen, and halogens. Therefore, people summarized a DBE formula for our convenience.

$$\text{DBE} \quad C \quad \frac{H}{2} \quad \frac{N}{2} \quad 1$$

In this formula, C means the number of carbon. H means the number of hydrogen and X is number of halogen. N means the number of the nitrogen.

Let's apply the formula to the chemicals that we mentioned before.

Ethylene (C_2H_6) : DBE $\quad C \quad \frac{H}{2} \quad \frac{N}{2} \quad 1 \quad 2 \quad \frac{6}{2} \quad \frac{0}{2} \quad 1 \quad 0$

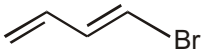
Propylene (C_3H_6) : DBE $\quad C \quad \frac{H}{2} \quad \frac{N}{2} \quad 1 \quad 3 \quad \frac{6}{2} \quad \frac{0}{2} \quad 1 \quad 1$

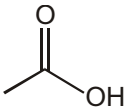
Cyclohexane (C_6H_{12}) : DBE $\quad C \quad \frac{H}{2} \quad \frac{N}{2} \quad 1 \quad 6 \quad \frac{12}{2} \quad \frac{0}{2} \quad 1 \quad 1$

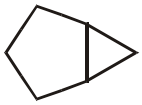
Solved Example

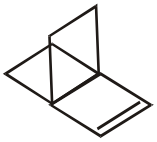
- Look at the chemical structure below and calculate the DBE.

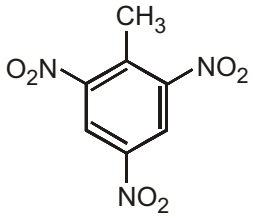
(1) 

(2) 

(3) 

(4) 

(5) 

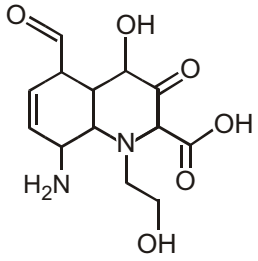
(6) 

Ans. (1) One pi bond. DBE = 1
(2) Two pi bond. DBE = 2
(3) One pi bond. DBE = 1
(4) Two rings. DBE = 2
(5) One pi bonds and three rings. DBE = 4
(6) Three pi bonds and one ring in the middle and three pi bonds on substituents. DBE = 7 exercise

EXERCISE

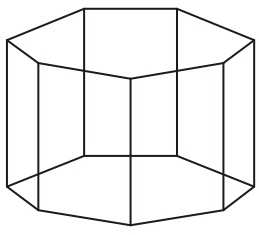
SINGLE CHOICE QUESTIONS

1. Find the sum of total number of different Functional groups and Double bond equivalent (DBE) value.



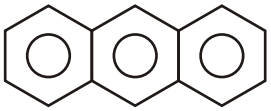
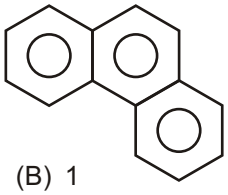
(A) 12 (B) 13 (C) 14 (D) 15

2. What is the Index of Hydrogen Deficiency (I.H.D) or Double Bond Equivalant (D.B.E.) for the following compound?



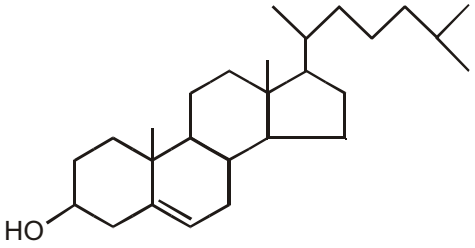
(A) 6 (B) 7 (C) 8 (D) 9

3. The difference in Double Bond Equivalent (DBE) value between

 and  is :

(A) 0 (B) 1 (C) 2 (D) 3

4. What is the correct molecular formula of following compound :



(Cholesterol)

(A) $C_{27}H_{46}O$ (B) $C_{25}H_{42}O$ (C) $C_{28}H_{46}O$ (D) $C_{23}H_{40}O$

5. Which of following compound. has D.B.E is 5 :

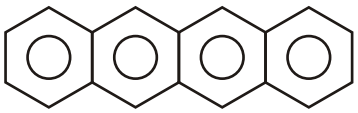
(A) 

(B) 

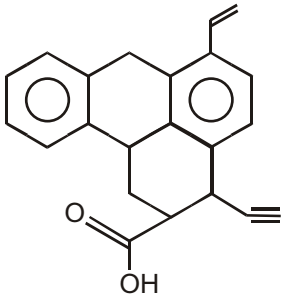
(C) 

(D) Both (B) & (C)

6. Number of p-bond present in given compound is



(A) 8 (B) 9 (C) 10 (D) 12

7. 

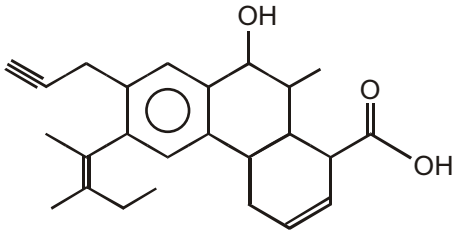
D.B. E of above compound is :

(A) 12 (B) 13 (C) 14 (D) 15

8. D.B.E of $(C_7H_5O_2)$ is :

(A) 3 (B) 5 (C) 5.5 (D) 4.5

9. How many degrees of unsaturation are there the following compound?



(A) 6 (B) 7 (C) 10 (D) 11

10. How many elements of unsaturation are implied by the molecular formula C_6H_{12}?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

11. How many elements of unsaturation are implied by the molecular formula C_5H_8O?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

12. How many elements of unsaturation are implied by the molecular formula $C_7H_{11}Cl$?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

13. How many elements of unsaturation are implied by the molecular formula $C_5H_5NO_2$?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

14. How many elements of unsaturation are implied by the molecular formula $C_8H_{11}N$?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

15. Consider molecules with the formula $C_{10}H_{16}$. Which of the following structural features are not possible within this set of molecules?

(A) 2 triple bonds (B) 1 ring and 1 triple bond
(C) 2 rings and 1 double bond (D) 2 double bonds and 1 ring
(E) 3 double bonds

16. A newly isolated natural product was found to have the molecular formula $C_{15}H_{28}O_2$. By hydrogenating a sample of the compound, it was determined to possess one -bond. How many rings are present in the compound?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

17. Which of the following molecular formulas corresponds to a monocyclic saturated compound?

(A) C_6H_6 (B) C_3H_7Br (C) C_3H_7N (D) C_3H_8O
(E) C_3H_8O

MULTIPLE CHOICE QUESTIONS

1. Which of the following statements applies to $C_{10}H_{14}O_2$ compound?

(A) It may have 2 double bonds and 2 rings. (B) It may have 3 double bond and Oxygen ring.
(C) It may have 1 triple bond and 2 rings. (D) It may have zero double bond and 3 rings

UNSOLVED EXAMPLE

1. How many hydrogens does each of the following compounds have?

(a) $C_8H_?O_2$, has two rings and one double bond
(b) $C_7H_?N$, has two double bonds
(c) $C_9H_?NO$, has one ring and three double bonds

2. Calculate the degree of unsaturation in each of the following formulas :

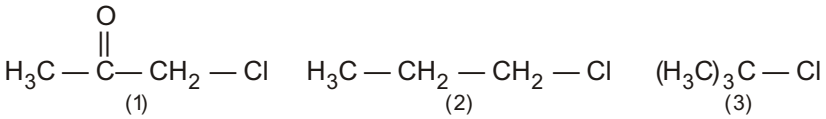
(a) Cholesterol, $C_{27}H_{46}O$ (b) DDT, $C_{14}H_9Cl_5$

(c) Prostaglandin E_1, $C_{20}H_{34}O_5$ (d) Caffeine, $C_8H_{10}N_4O_2$

(e) Cortisone, $C_{21}H_{28}O_5$ (f) Atropine, $C_{17}H_{23}NO_3$

SUBJECTIVE TYPE QUESTIONS

1. The order of S_N1 reactivity in aqueous acetic acid solution for the compounds :



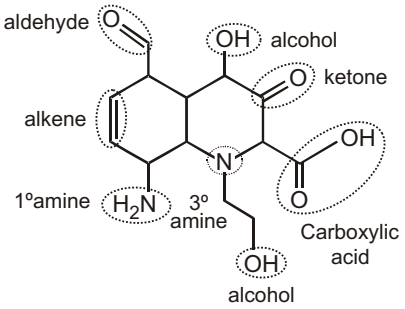
(a) 1 2 3 (b) 1 3 2 (c) 3 2 1 (d) 3 1 2

Answer

Single Choice Questions

1.	(B)	**2.**	(C)	**3.**	(A)	**4.**	(A)	**5.**	(D)	**6.**	(B)	**7.**	(C)	**8.**	(C)
9.	(D)	**10.**	(B)	**11.**	(C)	**12.**	(C)	**13.**	(E)	**14.**	(E)	**15.**	(A)	**16.**	(B)
17.	(C)														

1. D.B.E. value = 6



Different functional group = 7

2. The molecular formula of the compound shown is $C_{14}H_{14}$ D.B.E. value (14 1) 14 / 2 8

3. D.B.E. of both anthracene & phenanthrene is 10.

4. Calculate DBE value of given compound DBE value of given compound is 5

Multiple Choice Questions

1. (A,B, C)

$C_{10}H_{14}O_2$, DBE (C 1) $\frac{H \quad X \quad N}{2}$

DBE (4) means = 2 double bonds + 2 rings

= 1 triple bond + 2 rings

Unsolved Example

1.	(a) 12	(b) 13	(c) 13				
2.	(a) 5	(b) 8	(c) 4	(d) 6			
	(e) 8	(f) 7					

Subjective Type Questions

1. (c)

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