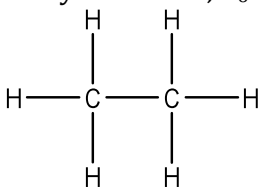
How to Calculate DBE

Hello friends! 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.

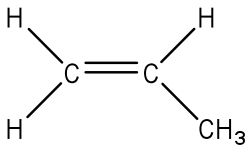
- What is DBE?

DBE=double bond equivalent. It is also called degree of unsaturation. From the structure of the chemicals, each pi bond or ring will generate one DBE.

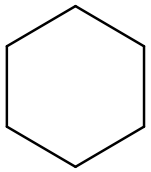
- For example:
  1. Ethylene, C_2H_6, is a saturated acyclic alkane and it does not have any pi bond or ring, so DBE=0.
  2. Propylene, C_3H_6, contains a pi bond, so DBE=1.
  3. Cyclohexane, C_6H_{12}, contains a ring, so DBE=1.



Ethylene
DBE=0



Propylene
DBE=1



Cyclohexane
DBE=1

The chemical formula and the chemical structure are highly related: each pi bond or ring will cause a pair of H less than the maximum number. Therefore, for hydrocarbon, each pair of H less than max H count, which is equal to the saturated acyclic alkane, is count for one DBE.

- Think question: How many DBE is in C_2H_5Cl?

- Why we need to know DBE?

Infrared spectroscopy is very useful tool to analyze the structure of an unknown chemical. Calculating DBE is an important step before analyzing the functional groups and it will offer us more clues to narrow down the options of function groups and make the work easier.

- How to calculate the DBE if we do not know the structure of the chemicals?

For Chem 14C, 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.

$$DBE = C - \frac{H}{2} + \frac{N}{2} + 1$$

In this formula, C means the number of carbon. H means the number of hydrogen and 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=C-(H/2) + (N/2) +1=2-(6/2) + (0/2) +1=0
Propylene (C_3H_6): DBE= C-(H/2) + (N/2) +1=3-(6/2) + (0/2) +1=1
Cyclohexane (C_6H_{12}): DBE= C-(H/2) + (N/2) +1=6-(12/2) + (0/2) +1=1

- Think question: How did people get this formula?

- Other important things you need to know about DBE:

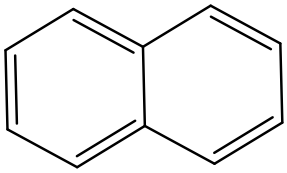
1. DBE is a nonnegative integer. If you got a negative or a fraction DBE, you will have to go back and check your math mistake!

2. Memorize the following facts and it will be more convenient when you apply DBE to figure out the chemical structure:

Double bond contains one DBE.
Triple bond contains two DBE.
A benzene ring contains four DBE.

3. Do NOT double count the rings in the chemical structure.

E.g.



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

Before we start the practice problem, let me explain the think questions first:

- Question 1: How many DBE is in C_2H_5Cl?

In this case, C_2H_5Cl is not hydrocarbon, so we cannot simply tell the DBE from how much H does it lack. However, halogens usually form one single bond to with other atoms, which is the same as hydrogen. We can imagine that the structure of C_2H_5Cl is similar to C_2H_6, in which case DBE=0.

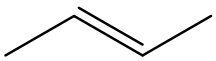
- Question 2: How do we get this formula?

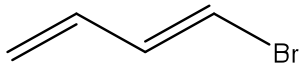
According to the Hydrogen/Halogen Rule, max number of hydrogens + halogens= 2C+N+2. We discussed that each pair of hydrogen and halogens less than max hydrogens and halogens count equals DBE.

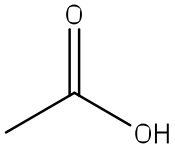
$$DBE = \frac{[\text{Max (Hydrogen + halogens)} - \text{ (Hydrogen + halogens)}]}{2} = \frac{2C + N + 2 - H}{2}$$

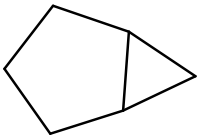
$$= C - \frac{H}{2} + \frac{N}{2} + 1$$

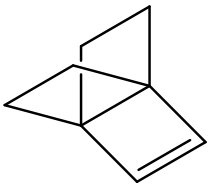
- Practice problem
  1. Look at the chemical structure below and calculate the DBE.

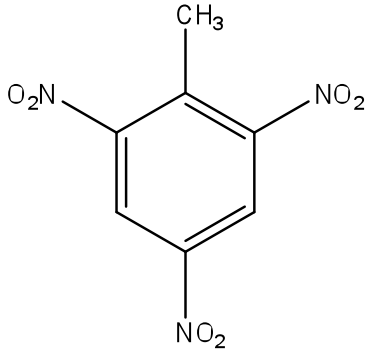
1) 

2) 

3) 

4) 

5) 

6) 

  2. Use the formula to calculate their DBE.

  1) C_8H_{10} 2) $C_6H_{12}O_6$ 3) $C_3H_4Cl_2$

  4) C_8H_7N 5) $C_{13}H_{10}$ 6) C_4H_9NO

- Answer key for the practice problems:
  1. 1) One pi bond. DBE=1

     2) Two pi bonds. 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

  2. 1) DBE= C-(H/2) + (N/2) +1= 8-(10/2) + (0/2) +1=4

     2) DBE= C-(H/2) + (N/2) +1= 6-(12/2) + (0/2) +1=1

     3) DBE= C-(H/2) + (N/2) +1= 3- (6/2) + (0/2) +1= 1

     4) DBE= C-(H/2) + (N/2) +1= 8- (7/2) + (1/2) +1= 6

     5) DBE= C-(H/2) + (N/2) +1= 13- (10/2) + (0/2) +1=9

     6) DBE= C-(H/2) + (N/2) +1= 4-(9/2) + (1/2) +1=1

Reference:

Hardinger, Steven. *Chemistry 14C: Structure of Organic Molecules : Course Thinkbook : Concept Focus Questions, OWLS Problems, Practice Problems*. Plymouth, MI: Hayden-McNeil, 2011. Print.

Hardinger, Steven. *Chemistry 14C: Organic Molecular Structures and Interactions : Lecture Supplements*. Plymouth, MI: Hayden-McNeil Pub., 2008. Print.