

Double Bond Equivalents (D.B.E)

To calculate the number of double bonds or rings with a given formula, where one DBE is a double bond or a ring structure (it is not possible to determine whether it is a double bond or a ring – other evidence is necessary). Two DBEs are two double bonds or a triple bond or a double bond and a ring structure etc. Four DBEs is possible an aromatic ring structure e.g. benzene

Take No of C atoms = n ; Take No of H atoms = m

Calculate $a = 2n+2$; $x = a-m$

DBE = $x/2$

e.g. benzene C_6H_6 , ($n = 6, m = 6$); Therefore $a = 14$; $x = 8$; DBE = 4

Therefore benzene has 4 DBE. 3 double bonds and 1 ring.

e.g. cyclohexane C_6H_{12} , ($n = 6, m = 12$); Therefore $a = 14$; $x = 2$; DBE = 1

Therefore cyclohexane has 1 DBE. Therefore cyclohexane 1 ring.

e.g. hexane C_6H_{14} , ($n = 6, m = 14$); Therefore $a = 14$; $x = 0$; DBE = 0

Therefore hexane has 0 DBE. Therefore hexane no rings or double bonds.

e.g. naphthalene $C_{10}H_8$, ($n = 10, m = 8$); Therefore $a = 22$; $x = 14$; DBE = 7

Therefore naphthalene has 7 DBE. Therefore naphthalene 2 rings and 5 double bonds.

For heterosystems containing nitrogen

Take No of C atoms = n

Take No of H atoms = m

Take No of N atoms = p

Calculate $a = 2n+2$

$x = a-(m-p)$

DBE = $x/2$

e.g. pyrrole C_4H_5N , ($n = 4, m = 5, p=1$); Therefore $a = 10$; $x = 6$; DBE = 3

Therefore pyrrole has 3 DBE. 2 double bonds and 1 ring.

e.g. pyridine C_5H_5N , ($n = 5, m = 5, p=1$); Therefore $a = 12$; $x = 4$; DBE = 4

Therefore pyridine has 4 DBE. 3 double bonds and 1 ring.

For heterosystems containing halogens, X

Take No of C atoms = n

Take No of H atoms = m

Take No of X atoms = q

Calculate $a = 2n+2$

$x = a-(m+q)$

DBE = $x/2$

e.g. chlorobenzene C_6H_5Cl , ($n = 6, m = 5, q=1$); Therefore $a = 14$; $x = 6$; DBE = 4

Therefore chlorobenzene has 4 DBE. 3 double bonds and 1 ring.

For oxygen or sulphur compounds - ignore the O or S.

Therefore $C_{19}H_{21}NO$, ($n = 19, m = 21, p=1$); Therefore $a = 40$; $x = 20$; DBE = 10

Therefore $C_{19}H_{21}NO$ has 10 DBE.