# *Degree of Unsaturation*

*How to determine the number of rings and multiple bonds in a compound from its molecular formula*

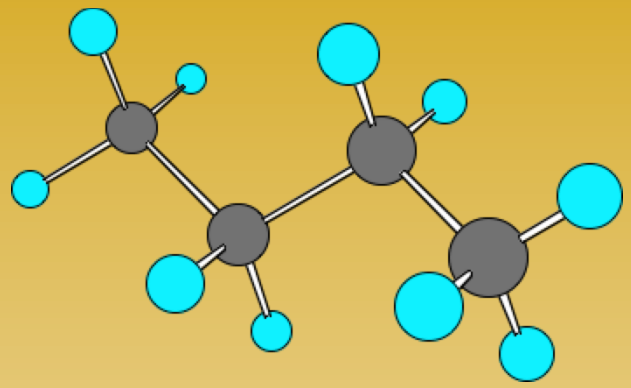
*No hydrocarbon can contain a greater number of hydrogens than fits the formula* $C_nH_{2n+2}$

*The number of hydrogens is always even.*

*All such compounds are acyclic*

*They may be straight (normal) chains as in n-butane ($C_4H_{10}$)*

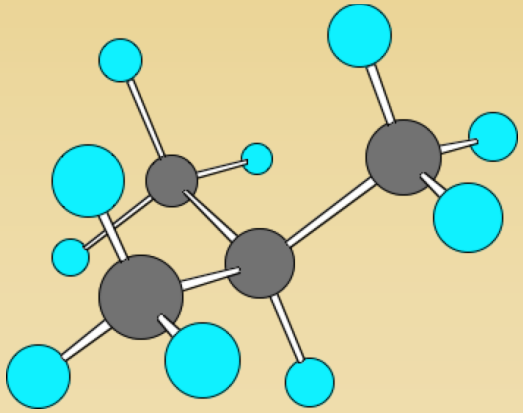
$CH_3CH_2CH_2CH_3$



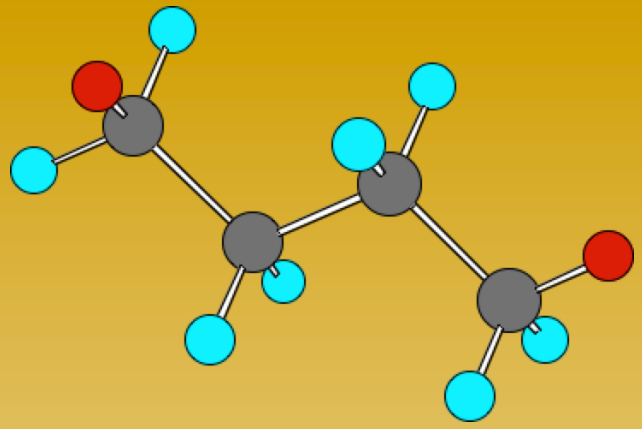
*or*

*they may be branched as in isobutane ($C_4H_{10}$)*

$CH_3CH(CH_3)CH_3$

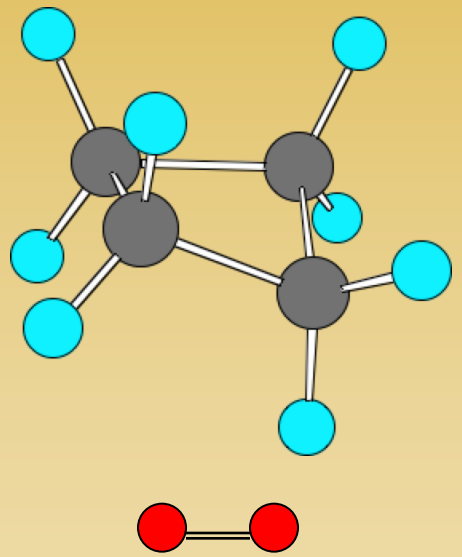


*If two hydrogen atoms on non-adjacent carbons of n-butane ($C_4H_{10}$) are removed*



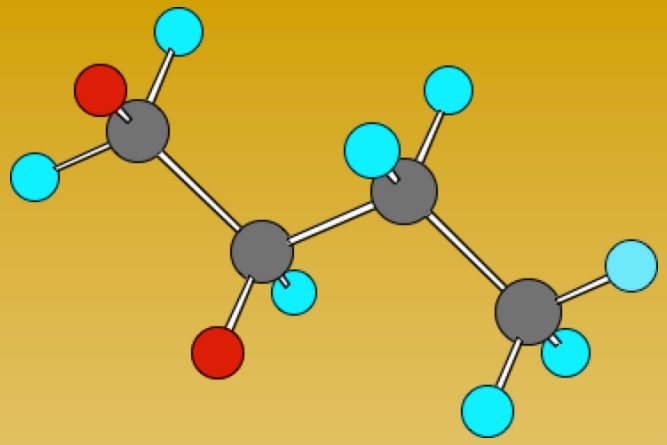
*then*

*a ring, cyclobutane ($C_4H_8$), is formed with the loss of $H_2$*



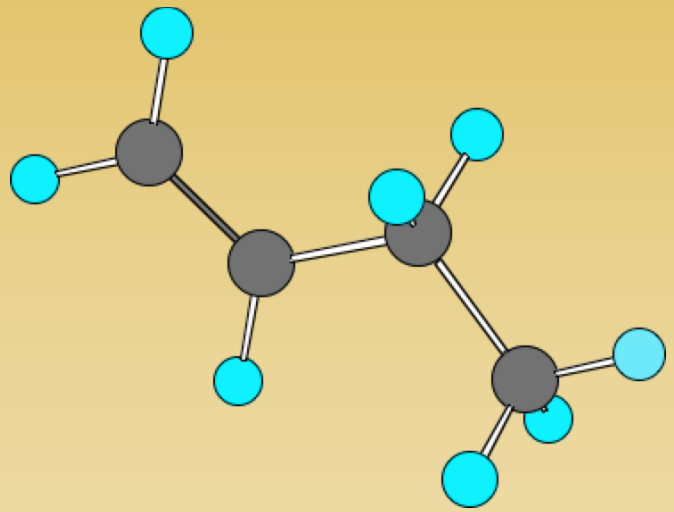
*This process is not necessarily a chemical reaction but rather a conceptual device.*

*If two hydrogen atoms on adjacent carbons of n-butane ($C_4H_{10}$) are removed*



*then*

*a double bond is formed with the loss of $H_2$.*

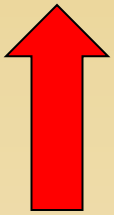


*In this case, the alkene, 1-butene ($C_4H_8$), is formed.*

*A compound with the molecular formula $C_4H_8$ is either an acyclic alkene (olefin) or cycloalkane.*

*How to determine the Degree of Unsaturation (DU) of this compound?*

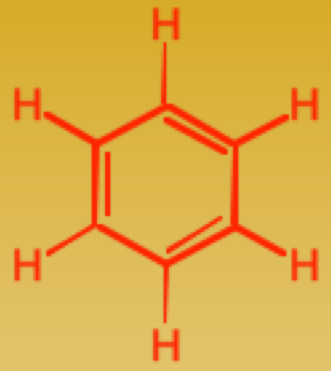
$C_4H_{10}$ - $C_4H_8$ = $H_2$ *divided by 2 = 1 DU*

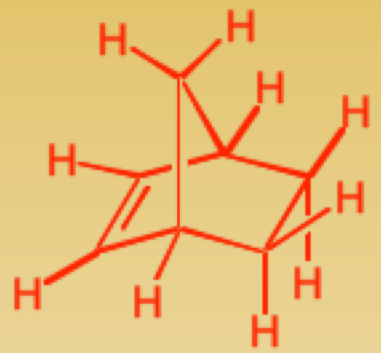


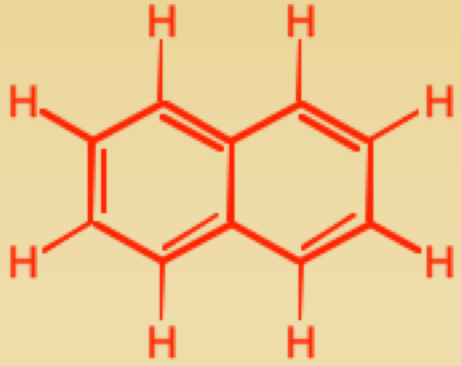
*most saturated $C_4$ compound*

*Try the following formulas:*

| | *DU* | *Example* |
|---|---|---|
| $C_6H_6$ | *4* | *benzene* |
| $C_7H_{10}$ | *3* | *norbornene* |
| $C_{10}H_8$ | *7* | *naphthalene* |







*How is the Degree of Unsaturation of a hydrocarbon containing halogen, or other monovalent atom, determined?*

*Every halogen in a hydrocarbon replaces a hydrogen.*

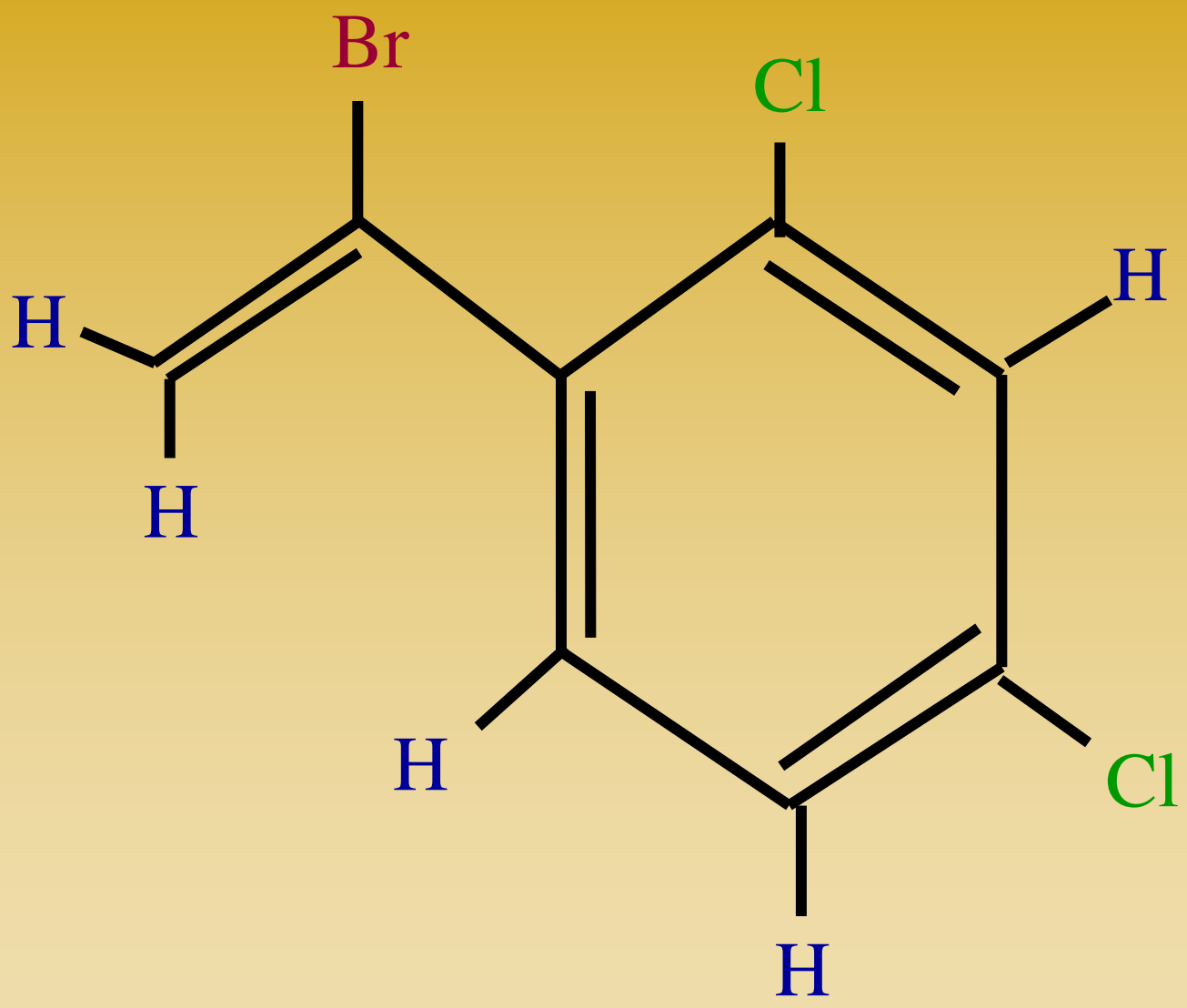
*Replace each halogen with hydrogen and then compare this hydrocarbon with the most saturated hydrocarbon.*

*The alkyl halide* $C_8H_5BrCl_2$ *becomes*

$$C_8H_8$$

$$C_8H_{18} - C_8H_8 = H_{10}/2 = 5\ DU$$

# *One example of an alkyl halide $C_8H_5BrCl_2$*




*1 DU - $C_6$*

*3 DU*

*1 DU - $C_8$*

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*5 DU*

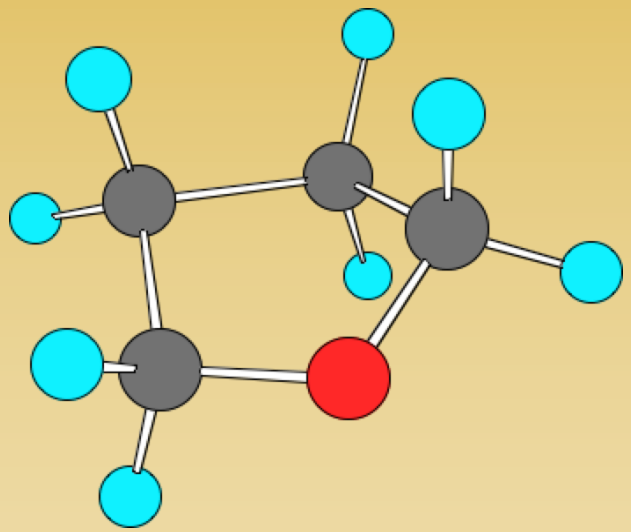
$C_8H_5BrCl_2$

*How is the Degree of Unsaturation of a hydrocarbon containing oxygen, or other divalent atom, determined?*

# *Ignore divalent atoms!*

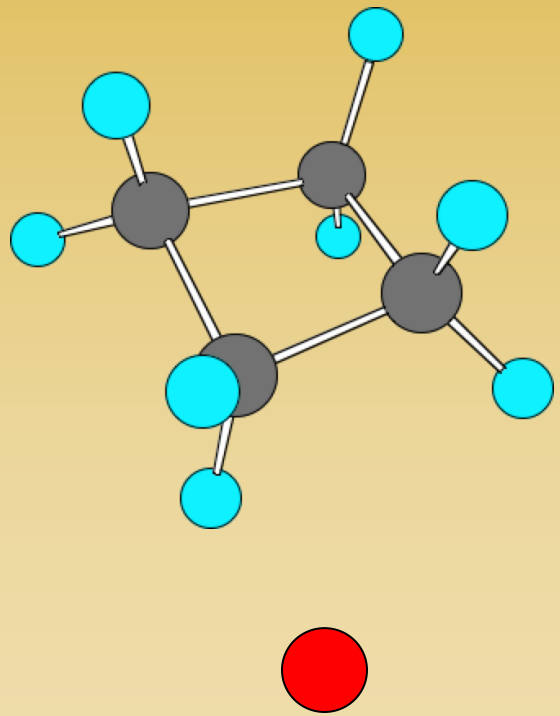
$C_4H_8O$

*1 DU*



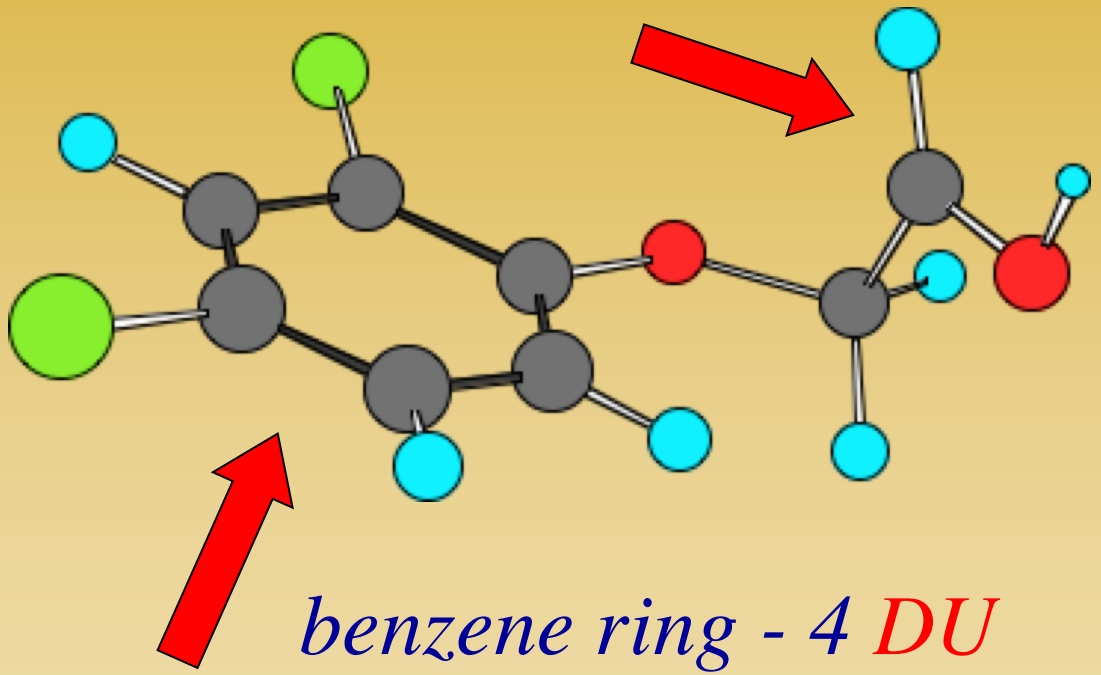
$C_4H_8$

*1 DU*



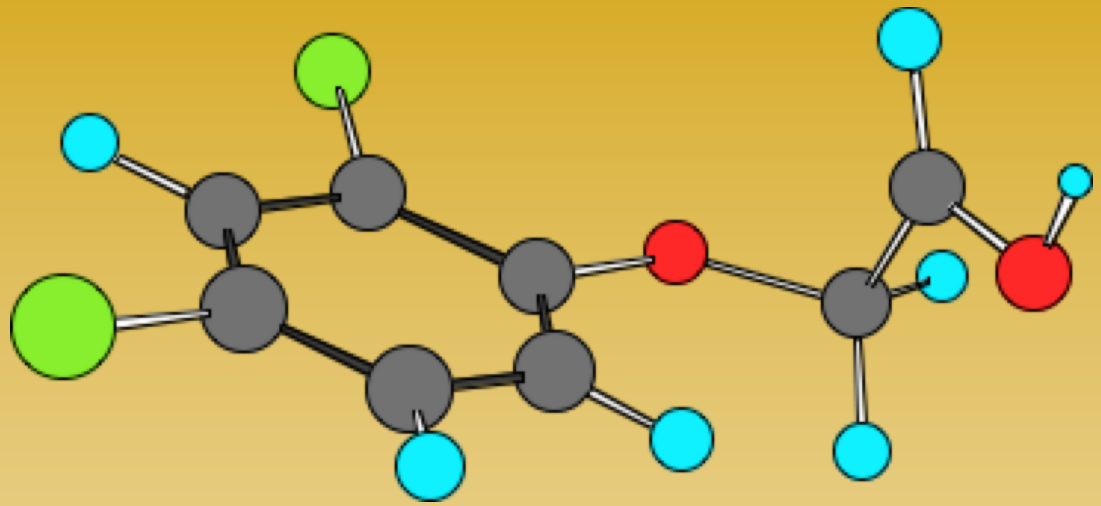
# *2,4-Dichlorophenoxyacetic acid*

*carbonyl - 1 DU*



*benzene ring - 4 DU*

# *2,4-Dichlorophenoxyacetic acid*



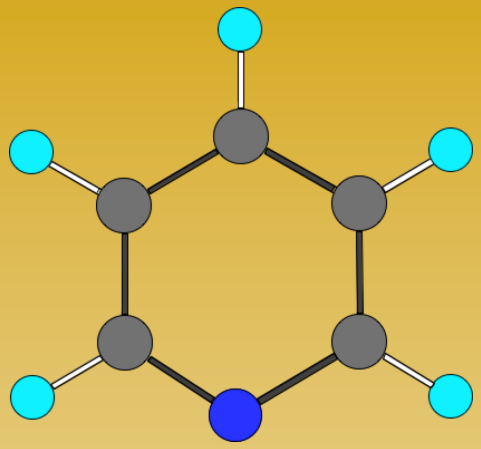
$C_8H_6Cl_2O_3$ → $C_8H_6Cl_2$ → $C_8H_8$

(drop $O_3$) (- $Cl_2$ + $H_2$)

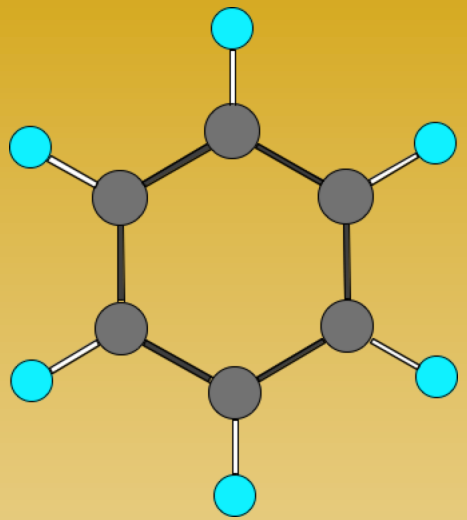
$C_8H_{18} - C_8H_8 = H_{10} / 2 = 5$ *DU*

*How is the Degree of Unsaturation of a hydrocarbon containing nitrogen, or other trivalent atom, determined?*

*Substitute CH for every N.*



(- N + CH)



*pyridine*

$C_5H_5N$

*benzene*

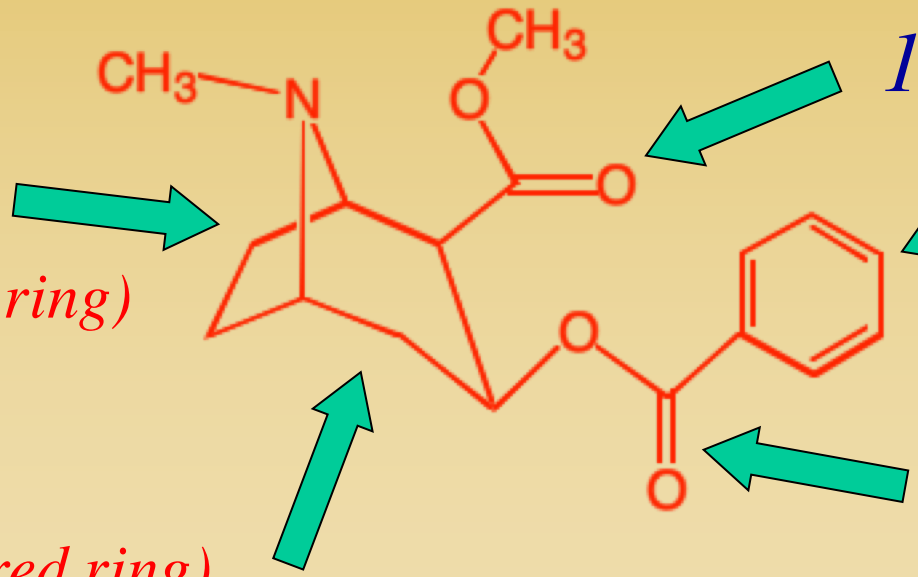
$C_6H_6$

$$C_6H_{14} - C_6H_6 = H_8 / 2 = 4\ DU$$

# Cocaine - $C_{17}H_{21}NO_4$

$C_{17}H_{21}NO_4$ → $C_{17}H_{21}N$ → $C_{18}H_{22}$

$C_{18}H_{38} - C_{18}H_{22} = H_{16} / 2 = 8$ DU




1 DU

1 DU
(5-membered ring)

4 DU

1 DU
(6-membered ring)

1 DU

# *Degree of Unsaturation*

*The End*

*F. E. Ziegler 2003*