Degree of Unsaturation

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

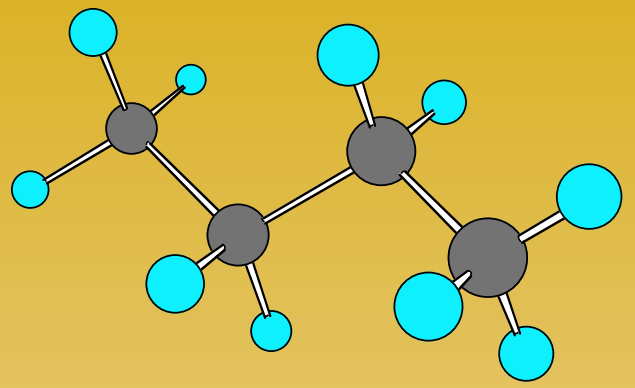
No hydrocarbon can contain a greater number of hydrogens than fits the formula C_nH_{2n+2}

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})

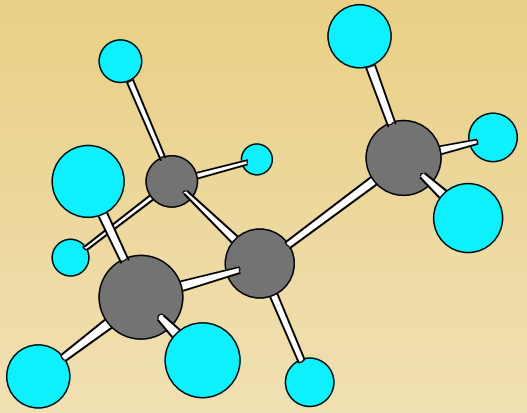
$CH_3CH_2CH_2CH_3$



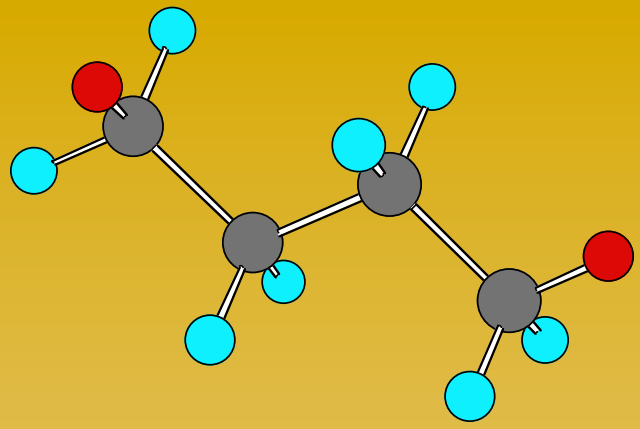
or

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

$CH_3CH(CH_3)CH_3$

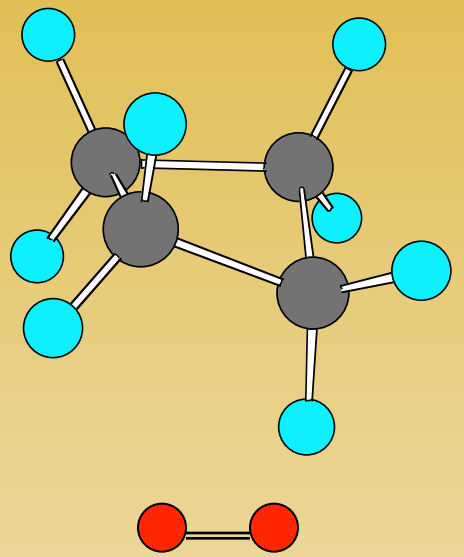


If two hydrogen atoms on non-adjacent carbons of n-butane (C_4H_{10}) are removed



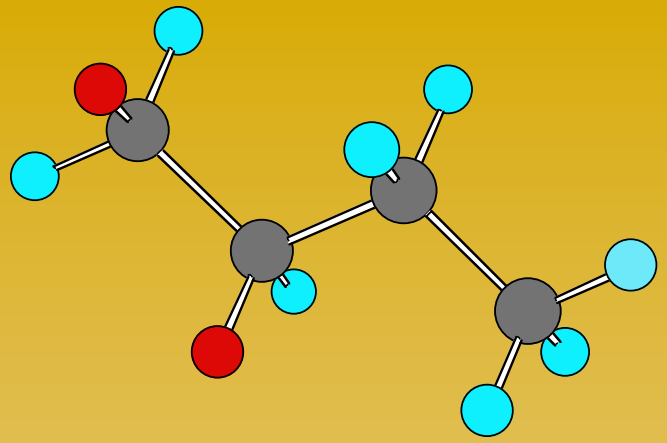
then

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



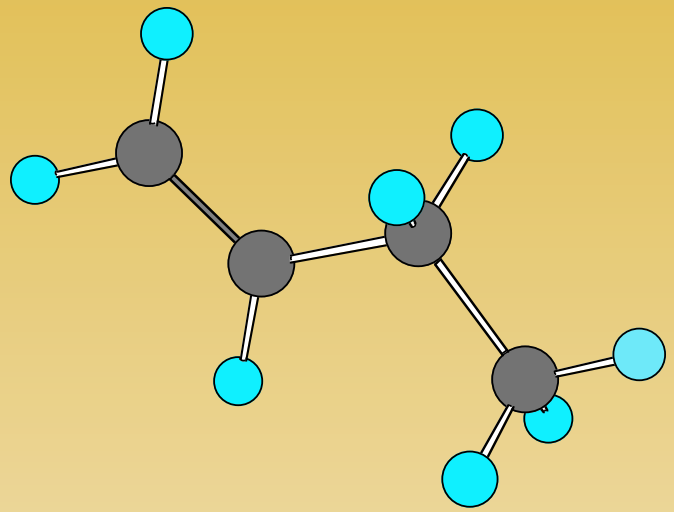
This process is not necessarily a chemical reaction but rather a conceptual device.

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.

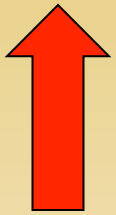


In this case, the alkene, 1-butene (C_4H_8), is formed.

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

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

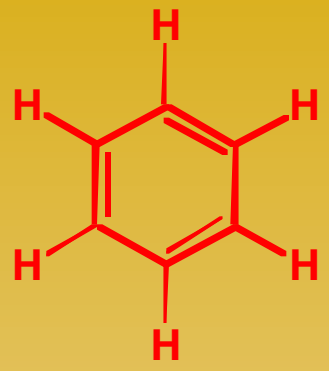
C_4H_{10} - C_4H_8 = H_2 divided by 2 = 1 DU

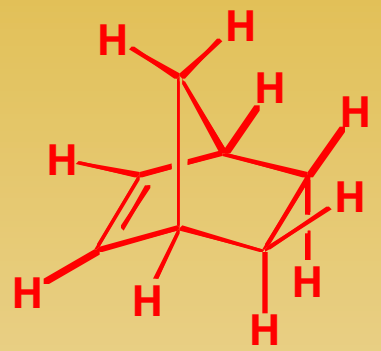


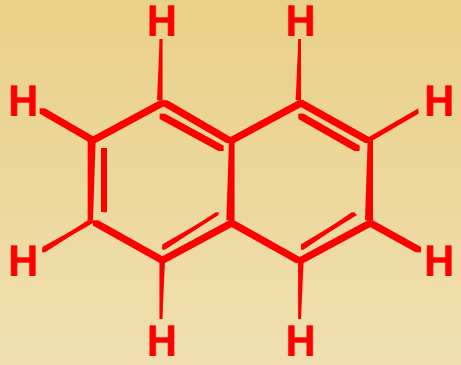
most saturated C_4 compound

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.

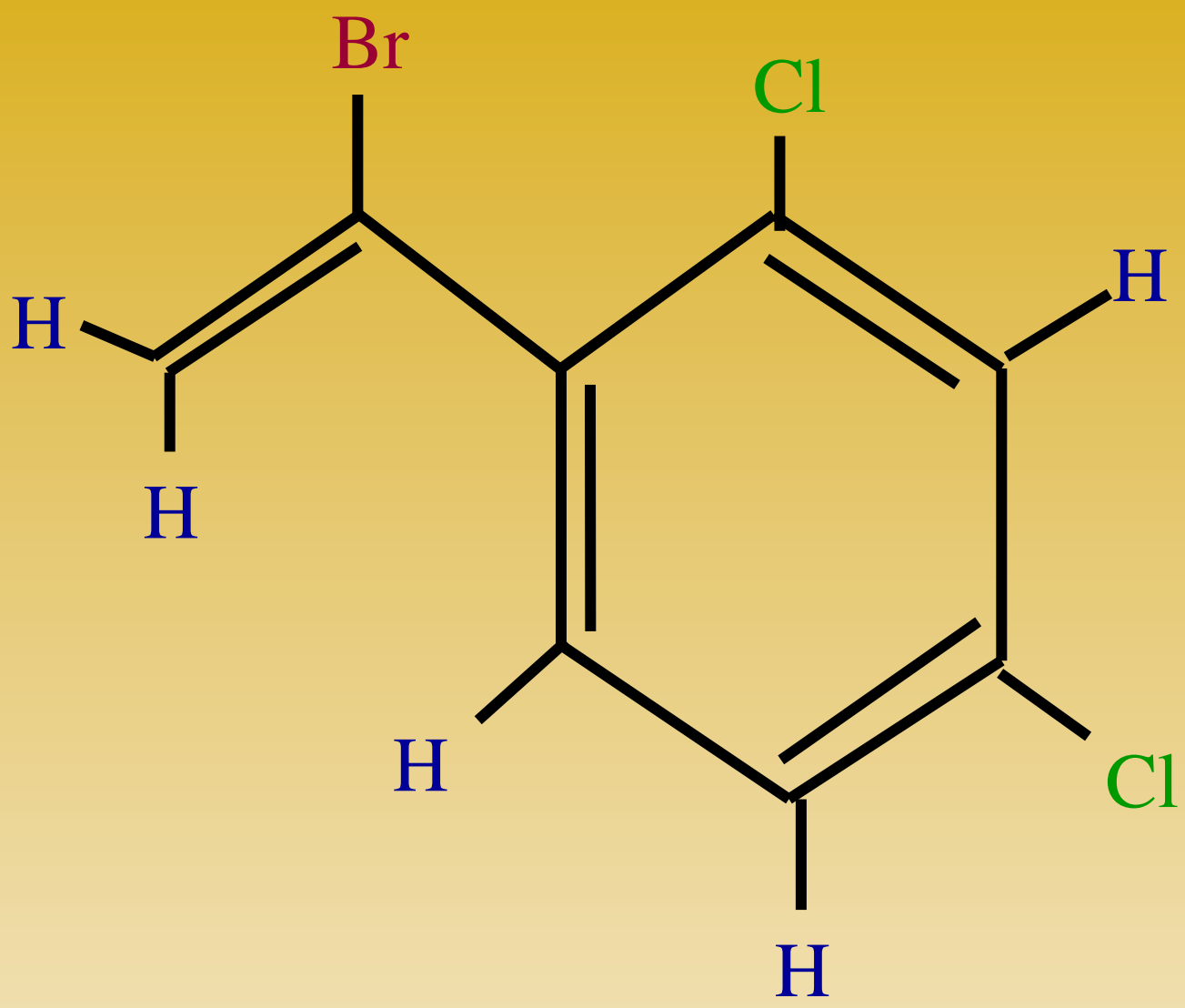
Replace each halogen with hydrogen and then compare this hydrocarbon with the most saturated hydrocarbon.

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

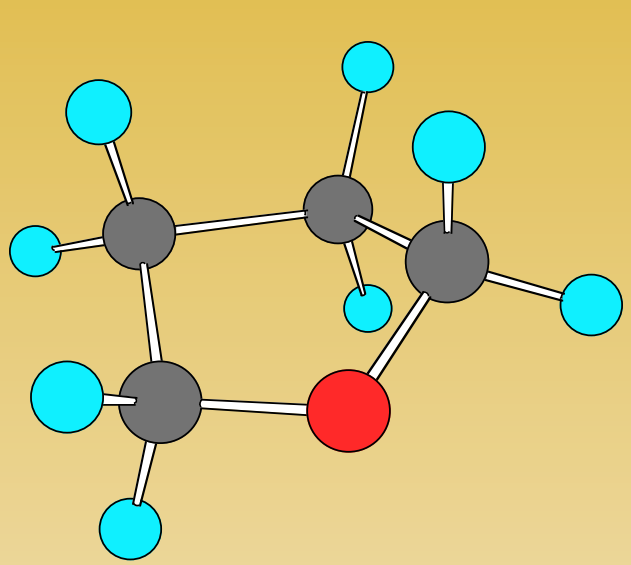
$C_8H_5BrCl_2$

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

Ignore divalent atoms!

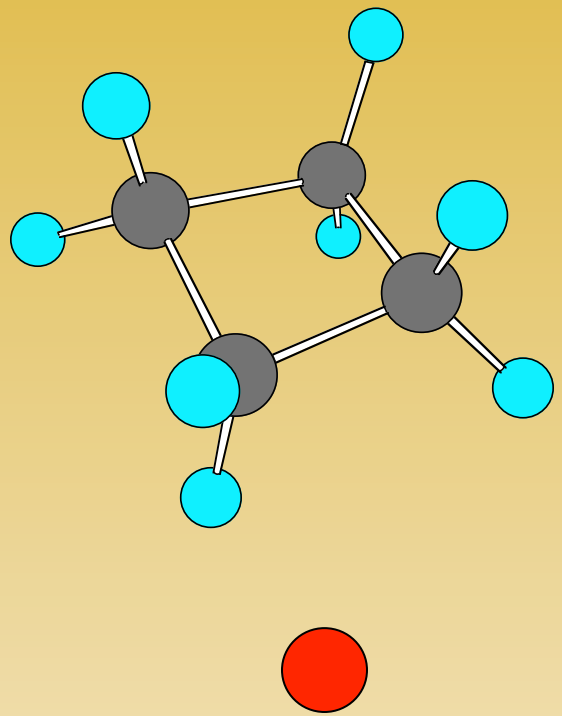
C_4H_8O

1 DU



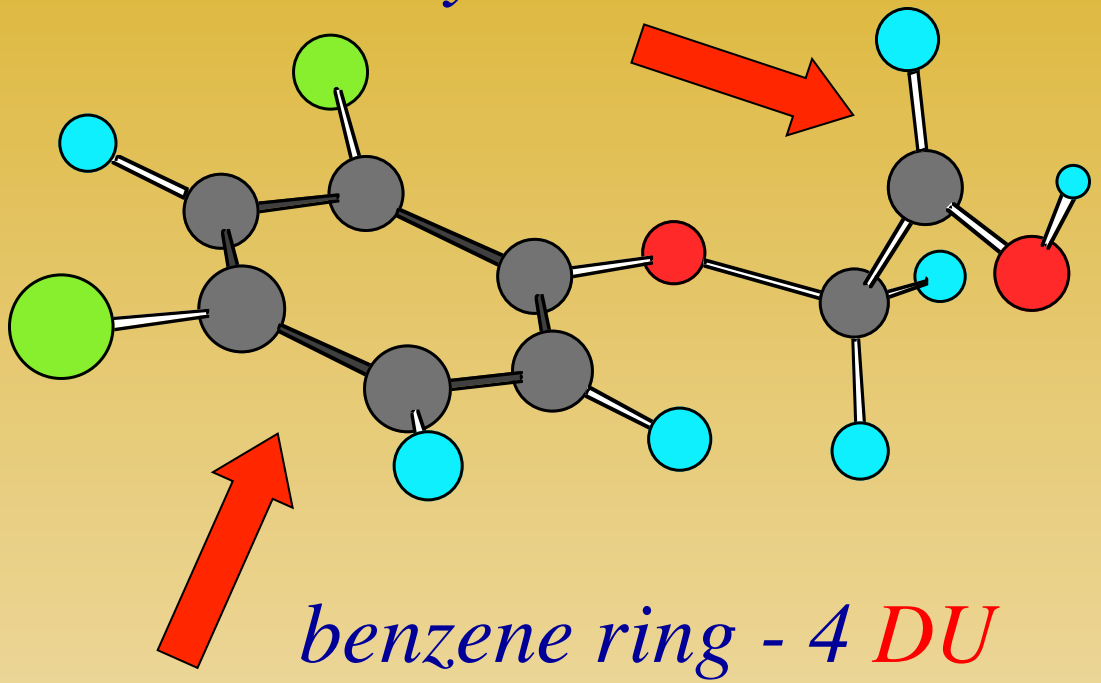
C_4H_8

1 DU



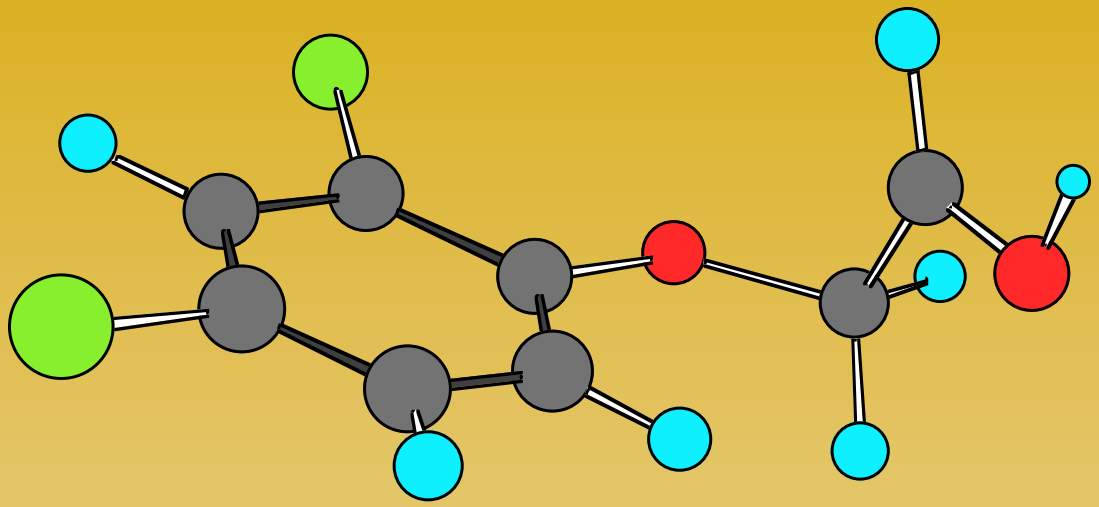
2,4-Dichlorophenoxyacetic acid

carbonyl - 1 DU



benzene ring - 4 DU

2,4-Dichlorophenoxyacetic acid



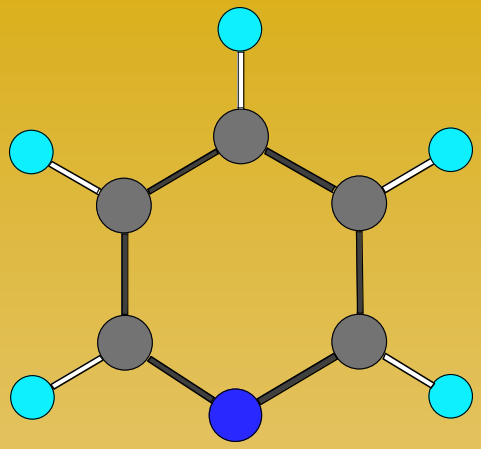
$C_8H_6Cl_2O_3$ → $C_8H_6Cl_2$ → C_8H_8

(drop O_3) (- Cl_2 + H_2)

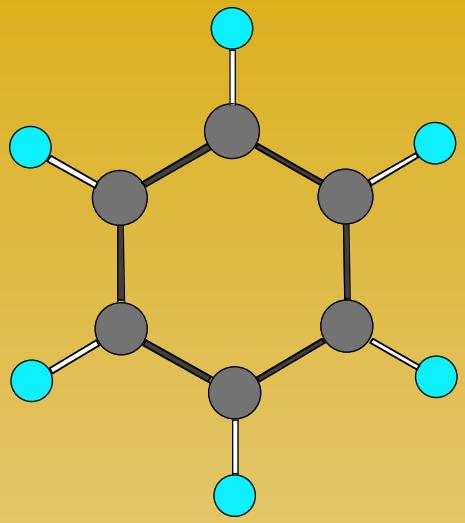
$C_8H_{18} - C_8H_8 = H_{10} / 2 = 5\ DU$

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

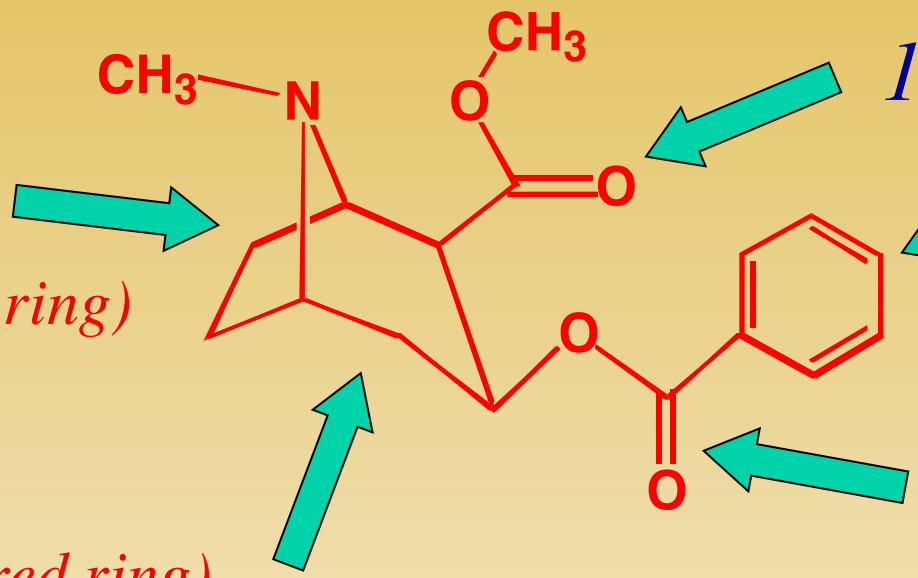
C_6H_6

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

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

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