MolecModels3D™

Cat.No. 1021000

Organic Stereochemistry (Student) Set

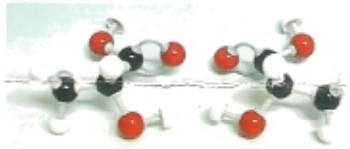
Contents

Qty	Element	colour	holes / type	Dia mm
30	Hydrogen **H**	white	1molydome®	17
14	Carbon **C**	black	4 tetrahedral.	23
6	Carbon **C**	black	5 tribipyramid	23
6	Oxygen **O**	red	2 angular	23
4	Nitrogen **N**	blue	4 tetra.	23
8	Chlorine **Cl**	green	1 hole.	17
2	Bromine **Br**	orange	1 hole	17
2	Iodine **I**	purple	1 hole	17
2	Metal	grey	6 holes	23
	Orbitals			
6	p-orbital	Pink	2D flat	
6	p-orbital	purple	2D flat	
	Bonds			
40	Link -medium	grey	single bonds	19 / 31 *
12	Link –long flexible	grey	double/triple	32 / 43 *
50	Link -short	white	all	2 / 10 *
1	Tool			* total

Isomerism – Molecules with the same molecular formula but different structures.

Stereoisomers – Molecules that differ because of the different locations the atoms adopt in space.

Optical isomerism
e.g. Lactic acid



Enantiomers – Mirror images of each other

Positional isomerism
e.g. Butene C_4H_8

The position of the non-carbon group, atom or multiple bond varies, giving rise to more than one option.

Skeletal isomerism
e.g Butane C_4H_{10}

Note the carbon skeleton back bone differences

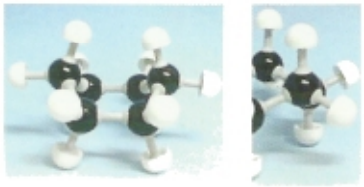
Functional groups e.g. C_2H_6O These give rise to 2 different functional groups.
In this example an alcohol (ethanol) and an ether are shown.

Geometric isomerism
Where rotation along a bond is not possible, such as in a double bond when a ***cis***- or ***trans*** isomer is possible.

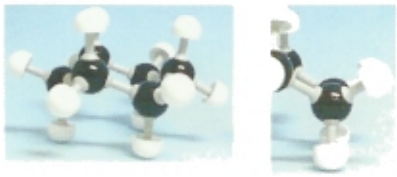
***Cis* & *trans* versions of 1,2-Cyclopentanediol**
Puckered versions.

Conformational isomerism
Free rotation about the carbon-carbon single bond.
e.g. ethane

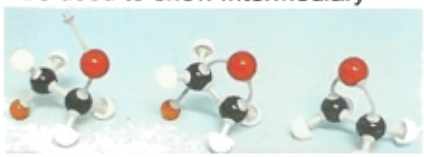
Conformations of Cyclohexane
Boat (perfectly staggered)
Note the "crowding of the 2 flagpole hydrogens".



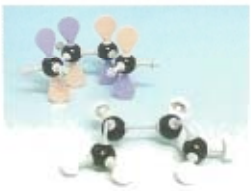
Now "flip" the model into the Chair conformation.
Chair (eclipsed)



5-hole carbon atoms can be used to show intermediary stages during the hydrolysis of an epoxide, leading to 1,2-diols and is stereospecific.



Molecular orbital explanation of thermal cyclization of butadienes.
Ground state (homo)



Conrotation of the excited state

Benzene C_6H_6
Molecular orbital model of benzene made using the 5 hole carbons and pink and purple p-obital lobes.

Disassembly of Compact Models
Please read the following instructions for the recommended use of the Link Remover tool.