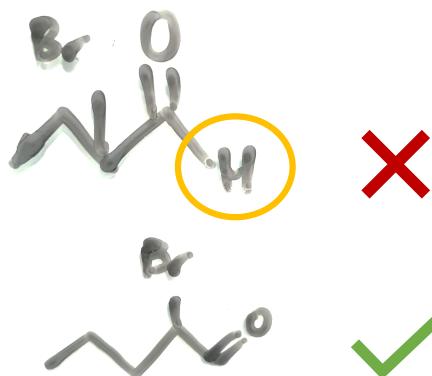


Introduction to Organic Chemistry

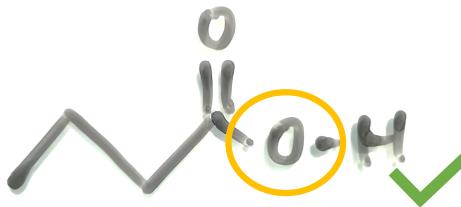
- Types of formula:
 1. Empirical formula
 2. Molecular formula
 3. Structural formula
 - a. Full structural formula/ displayed formula
Show trigonal planar and bent arrangement (if any)
 - b. Condensed formula
Use conventional grouping like COOH/ CO₂H
 - c. Stereochemical formula
Use dash wedge convention
 - d. Skeletal formula

2-bromopentanal



A H directly bonded to a C atom should not be drawn in skeletal formula.

CH₃CH₂CH₂CO₂H



CH₃CH₃OH



- For full structural formula, should try to show trigonal planar/ linear arrangement as much as possible. (Otherwise, it is hard to illustrate stereoisomers like cis-trans isomers clearly)
- Have a system for identifying isomers to prevent repeats:
 1. Start with straight chain
 2. Explore branching
 3. Explore positional isomers
 4. Explore functional group isomers
 5. Explore stereoisomers (cis-trans and enantiomers)

- Classification of hydrocarbons
 1. Saturation
Single bonds → Saturated
Double bonds → Unsaturated
 2. Aliphatic compounds
No aromatic ring
 3. Aromatic compounds
With delocalised π electron systems like benzene ring where continuous overlap of unhybridized p orbitals results in delocalisation of electrons above and below the ring, stabilising the ring
 4. Homologous series
 - a. Have general formula
 - b. Differ by CH_2 from one member to the next
 - c. Same FG → similar chemical properties
 - d. Gradual change in physical properties as Mr increases
- IUPAC

Root naming system:
Meth, Eth, Prop, But,
Pent, Hex, Hept, Oct,
Non, Dec

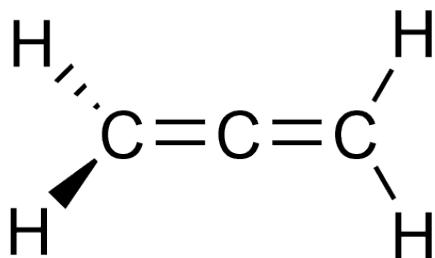
PREFIX-ROOT-SUFFIX

Prefix: Arrange in alphabetical order (di/ tri does not affect ordering), Smaller numbering of C atoms preferred

Root: If alicyclic, cyclo- added in front of root.

Suffix: Principal FG- marks 1st C atom. If no ambiguity no need give position locant.

- NOT all H atoms on prop-1,2-diene are on the same plane!!



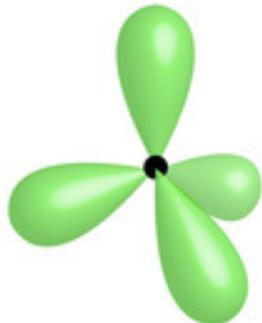
Explanation:

Since C2 has a hybridisation of sp, it has 2 un-hybridised p orbitals that are perpendicular to each other as well as the sp hybrid orbitals. The sideways overlap of the p orbitals formed between C1 and C2 is therefore perpendicular to that between C2 and C3.

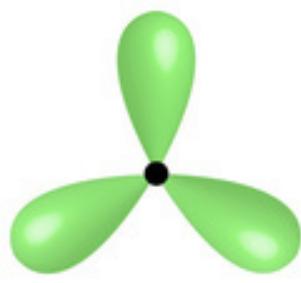
You may be tricked if the question gives you the structure w/o dash wedge convention and you fail to consider orbitals in your analysis!!

- Hybridisation¹

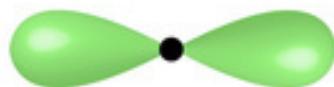
Hybridisation refers to the mixing of atomic orbitals in various combinations to give a set of hybrid orbitals of equivalent energy.



sp^3 hybrid orbitals
tetrahedral



sp^2 hybrid orbitals
trigonal planar



sp hybrid orbitals
linear

Should have the **asymmetrical dumbbell shape!** (Not well illustrated here)

Explanation:
Increased % s character, closer the hybrid orbitals to the nucleus, and smaller in size, bond stronger

Formation of hybrid orbitals require energy.

Hence, it is only natural that hybrid orbitals go towards formation of (stronger) sigma bonds instead of pi bonds.

Are you able to identify the hybridisation state of other central atoms besides C?

→ Consider the **bond angle**
180- sp, 120- sp², 109.5- sp³

(Don't use other things to compare; specific to carbon central atom only)

- Overlap head on → sigma bond
- Overlap sideways → pi bond
- Hybrid orbitals of the same type are equivalent and degenerate
- No of hybrid orbitals used in hybridisation = No of orbitals formed
- Electrons assigned to hybridisation by Pauli Exclusion Principle, Hund's Rule

¹ a concept that ties atomic structure with chemical bonding

Number of electron pair around central atom	Hybrid state of central atom	Number of valence orbital of central atom involved		Character		Number of hybrid orbitals	Number of bonds		Arrangement of hybrid orbital (IMPT)	Examples
		s	p	s	p		Sigma	Pi		
2	sp	1	1	50.0%	50.0%	2	2	2	linear	ethyne
3	sp ²	1	2	33.3%	66.7%	3	3	1	trigonal planar	ethene, benzene
4	sp ³	1	3	25.0%	75.0%	4	4	0	tetrahedral	methane, ethane

Isomers are compounds with the same molecular formula, but different arrangement of atoms in 3-dimensional space.

Constitutional/ Structural Isomers are compounds with the same molecular formula, but different structural formula.

Stereoisomers have the same molecular and structural formula but differ in the spatial arrangement of their atoms.

Chain isomers are isomers with the same functional group, but different carbon chains.

Positional isomers are isomers with the same carbon chain but differ in the position of FG.

FG isomers are isomers which differ in their FGs.

Different physical properties
Different chemical properties (for FG isomers)

Cis-trans isomers are a pair of molecules that exhibit cis-trans isomerism.

Condition

- (1) **Restricted rotation about a C=C bond** (as will break π bond for e.g.)
- (2) **Two different groups/ atoms attached to each C =C bond**

Cis-isomers are isomers with identical groups on the same side of double bond.

Trans-isomers are isomers with identical groups on the opposite sides of double bond.

Different physical properties
May have same chemical properties

Enantiomers are stereoisomers with non-superimposable mirror images. (Have chiral carbon; opposite- achiral)

Condition

- (1) **At least 1 chiral carbon (C*)** with 4 different groups arranged tetrahedrally around it
- (2) **No internal plane of symmetry**

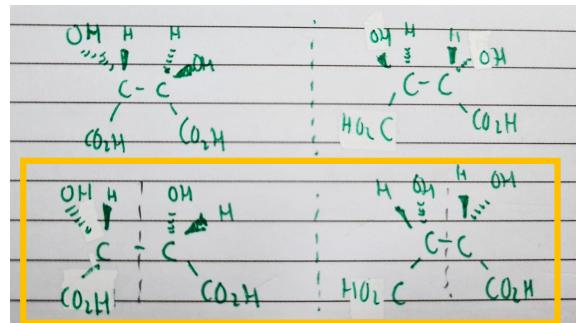
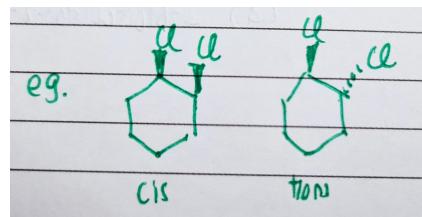
Identical physical properties (except for effect on plane polarized light) → optically active and a pair of " can rotate plane polarized light by equal but opposite angles

Identical chemical properties (except when interacting with other chiral molecules)

- Stereoisomerism
 - When question wants you to show stereoisomerism, and 3D arrangement around chiral carbon for enantiomers not shown → 0m. For cis-trans isomerism, usually 2D arrangement will suffice unless compound has a ring structure.
 - If there are 2 chiral carbons, for ease of drawing, ensure **2 chiral carbons are on the same plane**.
 - When you switch the positions of 2 groups (around the chiral centre) in enantiomers, a new compound is formed.
 - Hence, **number of possible enantiomers = $2^{\text{number of chiral carbons in the compound}}$** .
 - If there is an **internal plane of symmetry** (when there are 2 chiral carbons), there will be superimposable mirror images (as mirror image is the same as itself).

This is also the reason why there may only be 3 enantiomers (Tut Q9: 2,3-dihydroxybutanedioic acid).

Explanation: Molecule A and B each possess two chiral carbons and no internal plane of symmetry. Hence, they are mirror images of each other that are non-superimposable (i.e. enantiomers of each other). They are chiral molecules and are optically active. Although molecule C contains 2 chiral centres it contains an internal plane of symmetry. The mirror images are superimposable. Hence it is achiral and optically inactive.



Same stereoisomer due to internal plane of symmetry

- More information on FGs

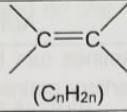
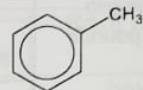
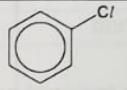
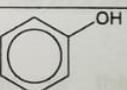
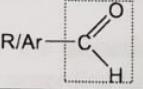
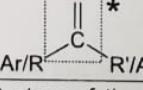
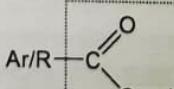
Table 3.2 Common functional groups arranged in increasing priority down the table

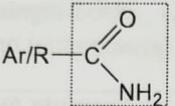
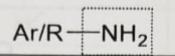
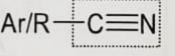
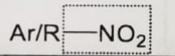
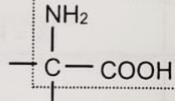
Formula	Name of functional group	Suffix	Prefix
	alkane	-ane	alkyl-, e.g. methyl- (-CH ₃), ethyl- (-CH ₂ CH ₃)
	alkene	-ene	-
	arene	-benzene	phenyl-
$-\text{C}\equiv\text{C}-$	alkyne	-yne	-
Ar/R-X (X = F, Cl, Br, I)	aryl/ alkyl halide	-	fluoro- (-F) chloro- (-Cl) bromo- (-Br) iodo (-I)
Ar/R-NO ₂	nitro-	-	nitro-
Ar/R-NH ₂	primary amine	-amine	amino-
Ar/R-O-H	primary, secondary or tertiary alcohol	-ol	hydroxy-
	ketone	-one	oxo-
	aldehyde	-al	oxo-
Ar/R-C≡N	nitrile	-nitrile	cyano-
	amide	-amide	-
	acyl chloride (X = Cl) acyl bromide (X = Br)	-oyl halide	-
	ester	-oate	-
	carboxylic acid	-oic acid	-

Table 2.1 Homologous series in the A-level syllabus

R/ R' represents alkyl groups of general formula C_nH_{2n+1} ; Ar/ Ar' represents an aryl group which is drawn as 

functional group form
simple aromatic ring
compounds where
one hydrogen atom
is removed from
ring

	Homologous Series	Formula (with functional group highlighted)	Example
Hydrocarbons	Alkane	C_nH_{2n+2}	CH_4 methane
	Alkene		$CH_2=CH_2$ ethene
	Arene	Ar-R	 methylbenzene
Halogen derivatives	Alkyl halide	R-X (X = F, Cl, Br, I)	CH_3Cl / chloromethane
	Aryl halide	Ar-X	 chlorobenzene
Hydroxy compounds	Alcohol	R-OH	CH_3OH methanol
		Alcohols can be further classified into primary, secondary or tertiary alcohols. This will be covered under the topic "Hydroxy Compounds".	
Carbonyl compounds	Phenol	Ar-OH	 phenol
	Aldehyde		CH_3CHO ethanal
	Ketone		CH_3COCH_3 propanone
<p>* The C atom of the C=O group (carbonyl group) must be bonded to 2 C atoms on both sides (i.e. cannot be bonded to a H).</p>			
Carboxylic acids and derivatives	Carboxylic acid		CH_3COOH ethanoic acid

	Homologous Series	Formula (with functional group highlighted)	Example
Organic nitrogen compounds	Amide		CH_3CONH_2 ethanamide
		Amides can be further classified into primary, secondary or tertiary amides. This will be covered under "Organic Nitrogen Compounds".	
	Amine		CH_3NH_2 methylamine
		Amines can be further classified into primary, secondary or tertiary amines. This will be covered under "Organic Nitrogen Compounds".	
	Nitrile		CH_3CN ethanenitrile
	Nitro compound		CH_3NO_2 nitromethane
	Amino acid		$\text{CH}_2(\text{NH}_2)\text{COOH}$ 2-aminoethanoic acid (also known as glycine)
		Contains both the amine and the carboxylic acid functional groups.	

- Phenyl (C_6H_5)
- Phenol ($\text{C}_6\text{H}_5\text{OH}$)
- Benzene (C_6H_6)
- Benzoate ($\text{C}_6\text{H}_5\text{COO}^-$)
- Types of reactions
Addition, Substitution, Elimination, Condensation, Hydrolysis, Oxidation, Reduction
- Definitions
 - Nucleophile is the electron pair donor and has a lone pair of electrons to be donated. (-ve charge/ neutral with partial -ve charge)
 - Electrophile is the electron pair acceptor and is electron deficient. (+ve charge/ neutral with partial +ve charge)
 - Homolytic fission: The covalent bond is broken such that each of the bonding atoms takes one of the bonding electrons, giving rise to free radicals.
 - Heterolytic fission: The covalent bond is broken such that one of the bonding atoms takes both bonding electron (and becomes an anion) while the remaining part of the molecule becomes a cation.
 - Free radicals are species with unpaired electrons.
 - Compounds/ mixtures of compounds that can rotate plane polarised light are termed optically active.
 - A mixture containing equal amounts of both enantiomers is called a racemic mixture or a racemate.