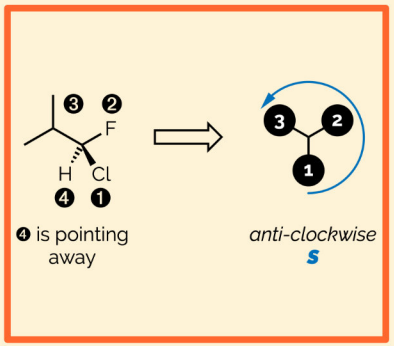
HIGHLIGHTS

- Determining the priority of substituents
- *R*/*S* - determining the descriptor for tetrahedral sp^3 stereocentres
- *E*/*Z* - determining the descriptor for trigonal planar sp^2 stereocentres
- An example



Structural isomers have different chemical names because they are different molecules. Stereoisomers will have the same constitution and have the same chemical name. Yet stereoisomers are different molecules as the spatial arrangement of atoms around a stereocentre differs. The full name of a compound must reflect these differences, and so a ***stereochemical descriptor***, defining the configuration, is added. This handout is a short introduction to determining the descriptor. As always, this is a simplification, with the complete rules being far more extensive.

CHEMISTRY CLASSICS

AN INTRODUCTION TO STEREOCHEMISTRY

STEREOCHEMICAL DESCRIPTORS

Introduction to Stereochemical Descriptors

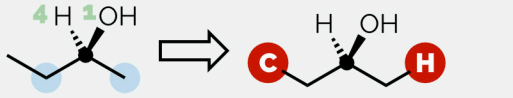
1. Assign Priorities

The substituents of a stereocentre are ranked in ***order of priority*** by the Cahn-Ingold-Prelog (CIP) rules.*

Highest priority = **1** and lowest = **4**.

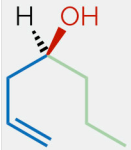
(i) ***Atomic Number*** - Rank the atoms attached directly to the stereocentre by highest atomic number.

(ii) ***Inspect same atoms along chain*** - If 1st atoms attached are the same move to the 2nd atoms, then 3rd etc until a difference is observed.



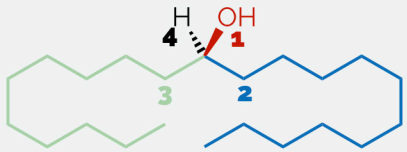
1st atom the same **C** | 2nd atom **C**,H,H *higher priority (2)* | *vs* | 2nd atom H,H,H *priority 3*

(iii) ***Multiple bonds count as the same number of single bonds*** - in carbonyl C=O, carbon attached to 2 x oxygen.



Group	H	OH	CH_2CHCH_2	C_3H_7
1st atom	H	O	C	C
2nd atom			C, H, H	C, H, H
3rd atom			C,**C**,H	C,H,H
priority	**4**	**1**	**2**	**3**

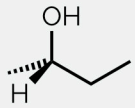
(iv) ***Keep moving along chain*** - there must be difference or not a stereocentre.



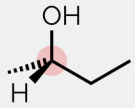
*These are a simplification or starting point, there are many more rules describing every possible kind of difference.

2. *R* or *S* Descriptor

How to determine the stereochemical descriptor for:



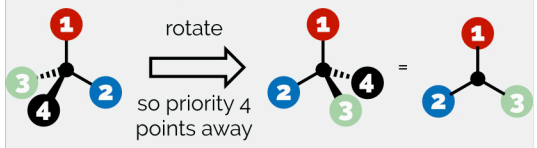
(i) ***Identify stereocentre*** - which atom(s) need a descriptor.



(ii) ***Assign priorities*** - use the CIP rules to rank the substituents of the stereocentre.

Group	H	OH	CH_2CH_3	CH_3
1st atom	H	O	C	C
2nd atom			C, H, H	H, H, H
priority	**4**	**1**	**2**	**3**

(iii) ***Orientate molecule so the lowest priority points away*** - priority 4 should face into the page.

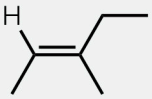


(iv) ***Draw arrow connecting 1→2→3***

anti-clockwise descriptor = ***S*** | *clockwise* descriptor = ***R***

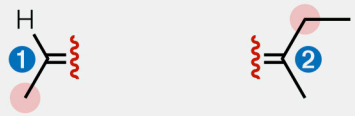
3. *E* or *Z* Descriptor

How to determine the stereochemical descriptor for an alkene:



(i) ***Divide in half*** - look at each carbon separately.

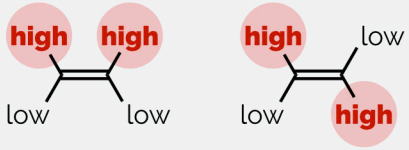
(ii) ***Assign priorities*** - determine highest priority substituent on each half.



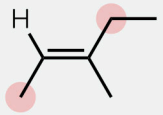
Group	H	CH_3
1st atom	H	C
priority	low	**high**

Group	Et	CH_3
1st atom	C	C
2nd atom	**C,H,H**	H,H,H
priority	**high**	low

(iii) ***Assign descriptor*** - if highest priorities are on the ***same*** side, descriptor = ***Z***. If they are on ***opposite*** sides of the alkene the descriptor = ***E***.



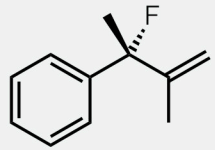
descriptor = ***Z*** | descriptor = ***E***



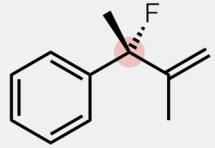
(***E***)-3-methylpent-2-ene

4. Example

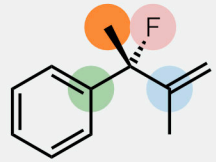
Determine the descriptor for:



(i) ***Identify stereocentre*** - sp^3 carbon with four different groups.

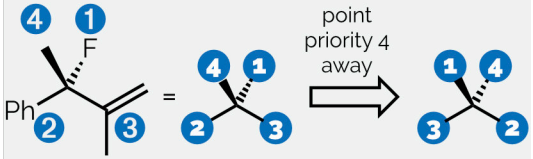


(ii) ***Assign priorities*** - follow chain until a difference.



Group	F	$CH(CH_3)CH_2$	C_6H_5	CH_3
1st atom	F	C	C	C
2nd atom		C,C,C	C,C,C	C,H,H
3rd atom		C,H,H	C,**C**,H	
priority	**1**	**3**	**2**	**4**

(iii) ***Orientate molecule so priority 4 points away*** - points into page



(iv) ***Draw arrow connecting 1→2→3*** - assign descriptor

clockwise = ***R***