

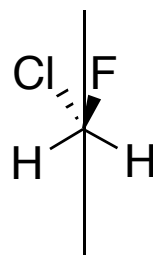
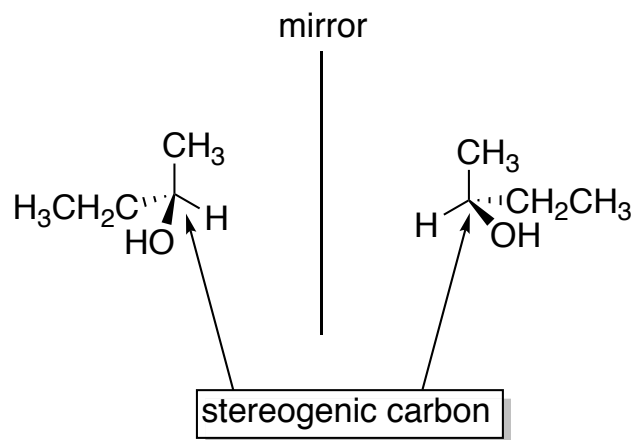
# Absolute Stereochemistry: Cahn-Ingold- Prelog Rules

Instructor: Olivia Chesniak

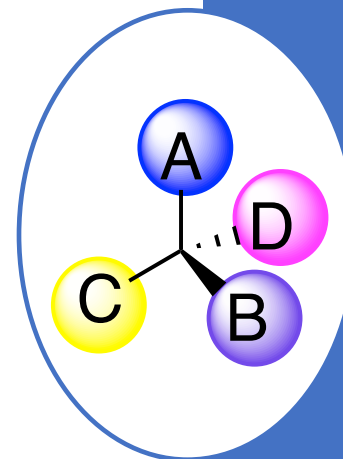
April 9, 2018

# Recap: Chiral Molecules

- 4 different groups attached to stereogenic carbon
- Non-superimposable mirror image
- No internal plane of symmetry



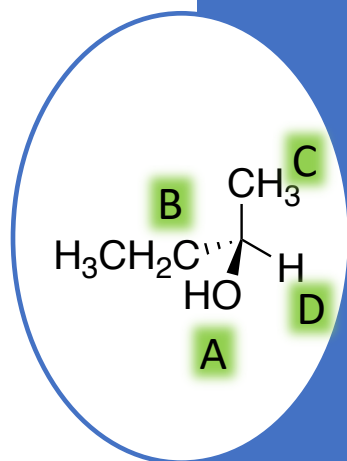
internal plane of symmetry



# R-S Convention: Describing the Absolute Configuration of a Molecule

- Cahn-Ingold-Prelog Rules

- Assign priority to each substituent attached to the stereogenic carbon:
  - A (highest) > B > C > D (lowest)
  - Highest atomic number = highest priority
  - Lowest atomic number = lowest priority
- In case of a tie, move to the next atom and compare
- If an atom is doubly or triply bonded, count it 2x, 3x



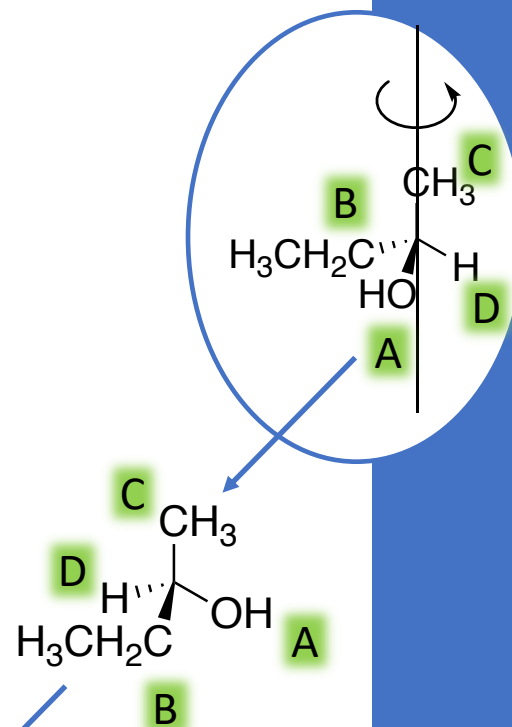
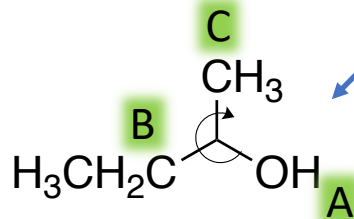
IUPAC Periodic Table of the Elements

1 H Hydrogen 1.00794	2 He Helium 4.002602	Key Symbol Element name Atomic number																18 Ar Argon 39.948
3 Li Lithium 6.941	4 Be Beryllium 9.012182	5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.006434	8 O Oxygen 15.999	9 F Fluorine 18.9984032	10 Ne Neon 20.1797	11 Na Sodium 22.98976928	12 Mg Magnesium 24.304	13 Al Aluminum 26.9815386	14 Si Silicon 28.08558	15 P Phosphorus 30.973762	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.948			
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.9216	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798	
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium 98	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.36	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.29	
55 Cs Cesium 132.90545196	56 Ba Barium 137.327	57-71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.9804	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222	
87 Fr Francium 223	88 Ra Radium 226	89-103 Actinoids	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 263	107 Bh Bohrium 264	108 Hs Hassium 265	109 Mt Meitnerium 266	110 Ds Darmstadtium 267	111 Rg Roentgenium 268	112 Cn Copernicium 269	113 Nh Nihonium 270	114 Fl Flerovium 271	115 Mc Moscovium 272	116 Lv Livermorium 273	117 Ts Tennessine 274	118 Og Oganesson 276	

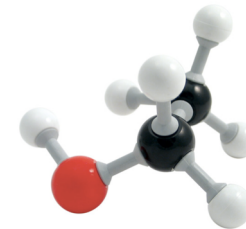
# R-S Convention: Describing the Absolute Configuration of a Molecule

4. Arrange the molecule such that the lowest priority group is pointing away from you
- Trace a path from  $a \rightarrow b \rightarrow c$  (highest to lowest priority)
  - If the path is clockwise, the molecule has the configuration R (Latin *rectus*, right)
  - If the path is counterclockwise, the molecule has the configuration S (Latin *sinister*, left)

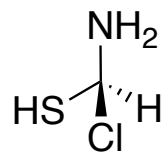
(*R*)-butan-2-ol



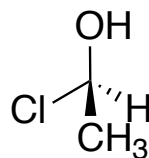
# Molecular Models Activity



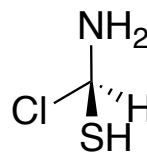
**Group 1**



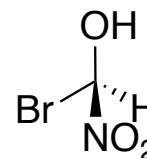
**Group 2**



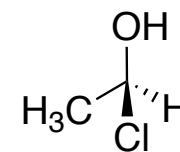
**Group 3**



**Group 4**



**Group 5**

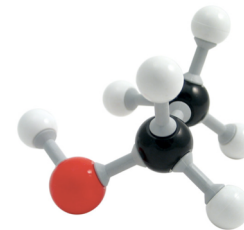


1. Assign priority
2. Put lowest group to the back
3. Trace path from a → b → c
  - Clockwise?
    - R
  - Counterclockwise?
    - S

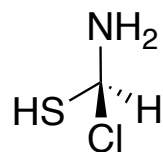
Color	Atom	Atomic No.
White	Hydrogen	1
Black	Carbon	6
Blue	Nitrogen	7
Red	Oxygen	8
Yellow	Sulphur	16
Green	Chlorine	17
Gray	Bromine	35

## Question Time!

# Molecular Models Activity

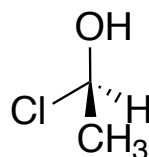


Group 1



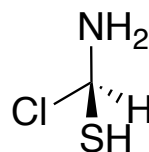
R

Group 2



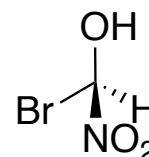
R

Group 3



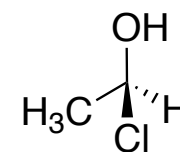
S

Group 4



R

Group 5



S

1. Assign priority
2. Put lowest group to the back
3. Trace path from a → b → c
  - Clockwise?
    - R
  - Counterclockwise?
    - S

Color	Atom	Atomic No.
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