

Organic Chemistry Take Home Assignment: Stereochemistry

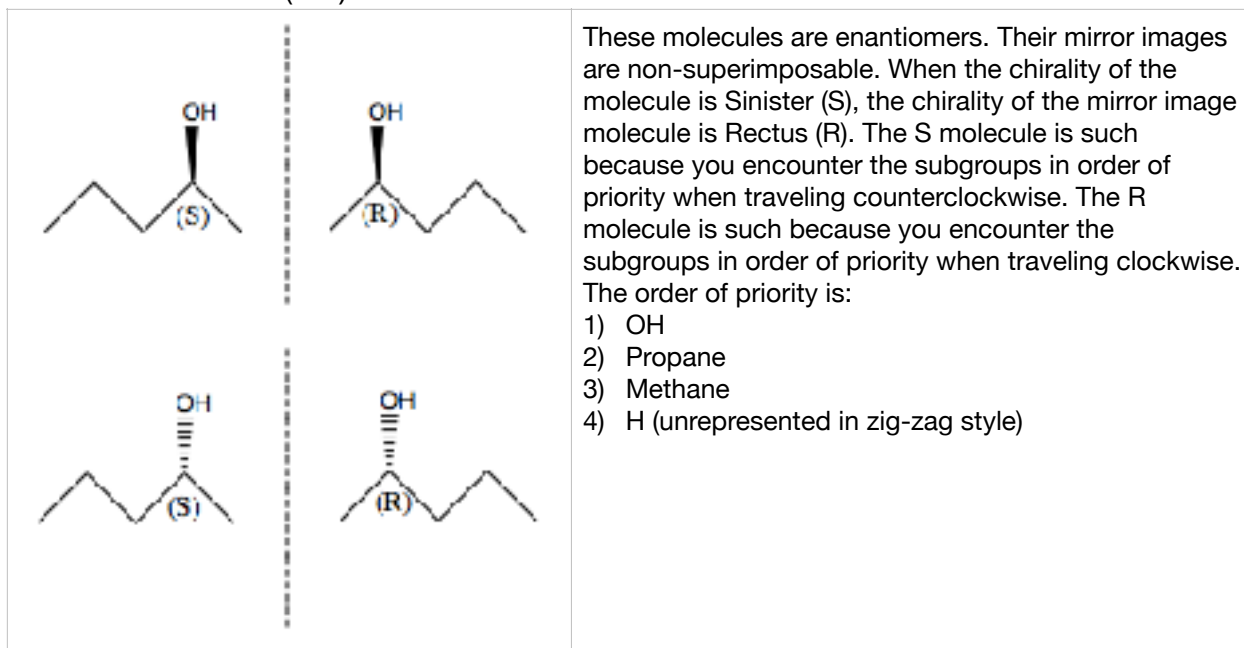
Kaitlyn Armstrong - 8544417

TA: Yousef Risha

Submitted on: February 9 2018

1. Enantiomers and Diastereomers:

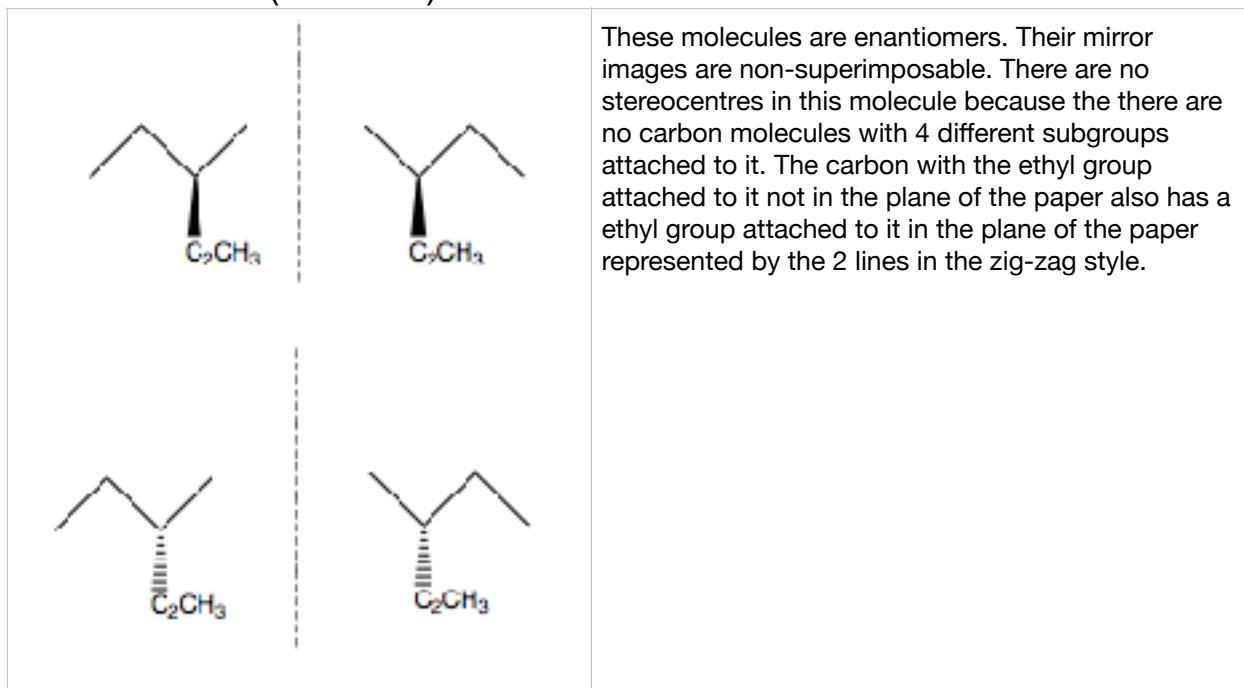
A. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$



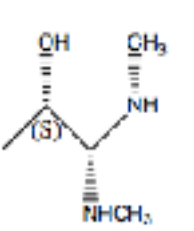
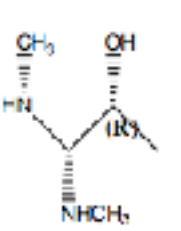
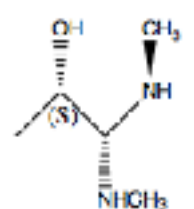
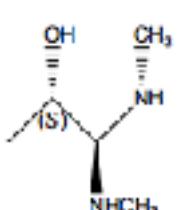
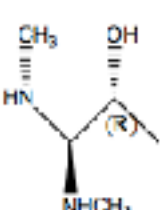
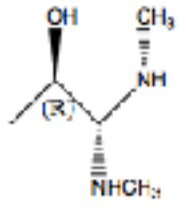
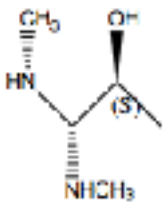
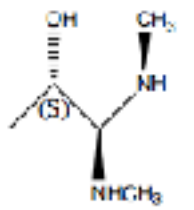
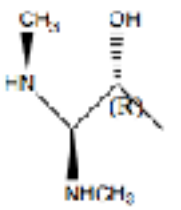
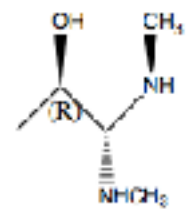
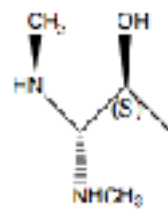
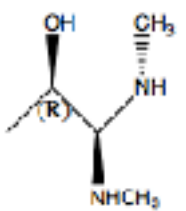
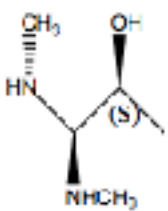
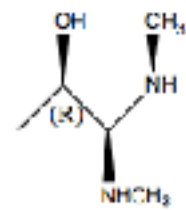
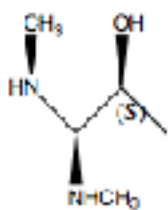
B. $\text{CH}_3\text{CClHCH}(\text{NH}_2)\text{CH}_3$

		<p>These molecules are enantiomers. Their mirror images are non-superimposable. For the first molecule both stereocentres have R chirality because the priority subgroups fall in a clockwise direction. The mirror image therefore has S chirality.</p> <p>The priority of the first centre is: 1) Cl 2) $\text{CH}(\text{NH}_2)\text{CH}_3$. 3) CH 4) H</p> <p>The priority of the second centre is: 1) NH_2. 2) CH_3CClH 3) CH_3. 4) H</p> <p>The priority does not change for all isomers.</p>
		<p>These molecules are enantiomers. Their mirror images are non-superimposable. For the first molecule the first stereo centre has S chirality and the second has R chirality. The mirror image switches the chiral centres causing them to be the opposite to it's pair.</p>
		<p>These molecules are also enantiomers. Their mirror images are non-superimposable. For the first molecule the first stereo centre has R chirality and the second has S chirality. The mirror image again switches the chiral centres causing them to be the opposite to it's pair.</p>
		<p>These molecules are also enantiomers. Their mirror images are non-superimposable. For the first molecule the first stereo centre has R chirality and the second has S chirality. The mirror image again switches the chiral centres causing them to be the opposite to it's pair.</p>

C. $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_3$



D. $\text{CH}_3\text{NHCH}(\text{NHCH}_3)\text{CHOHCH}_3$

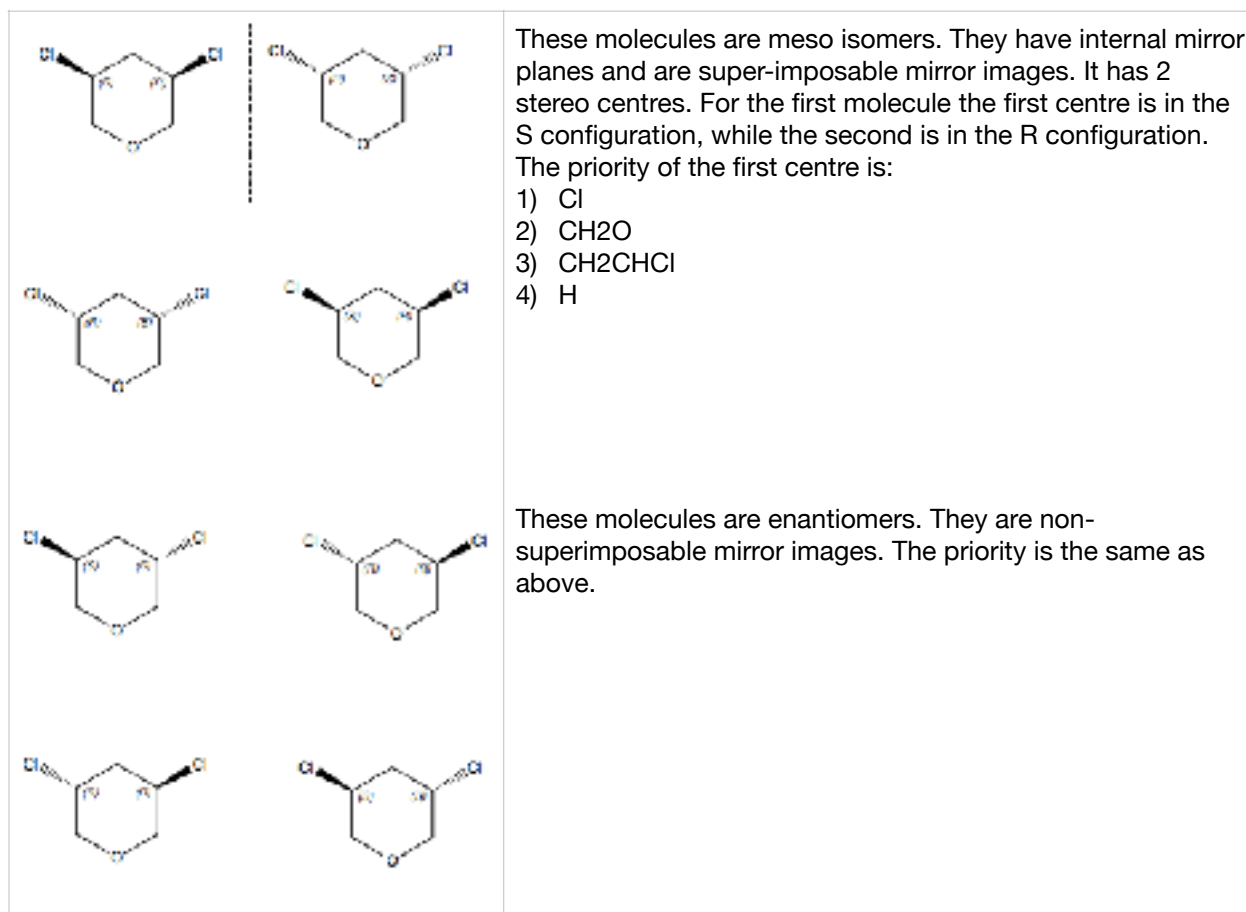


All of these molecules shown are enantiomers. The molecules cannot be imposed on their mirror images. Also, None are meso isomers because there is no internal plane of symmetry in any of the molecules. There is one stereo centre because it is the only carbon with 4 different subgroups attached.

The order of priority for the subgroups are:

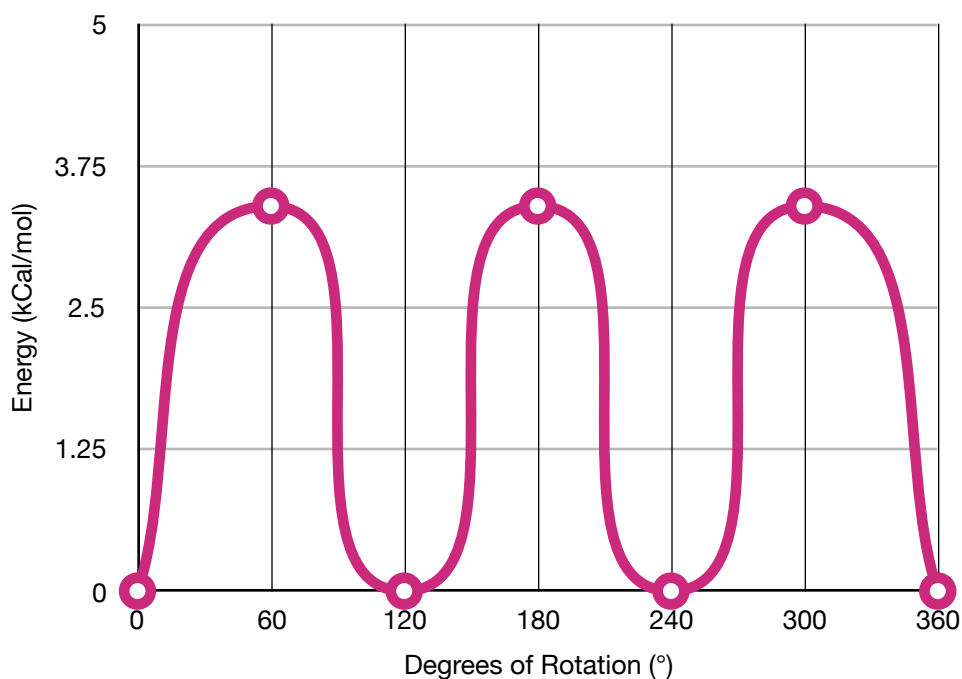
- 1) OH
- 2) CH₃NHCH(NHCH₃)
- 3) CH₃
- 4) H

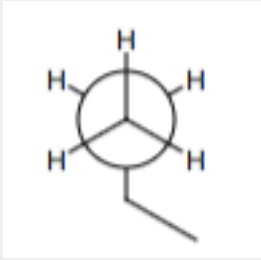
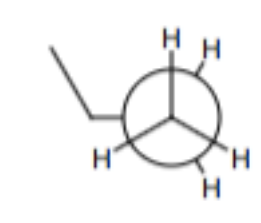
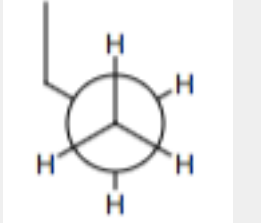
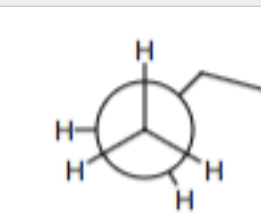
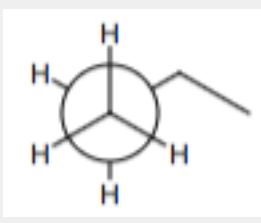
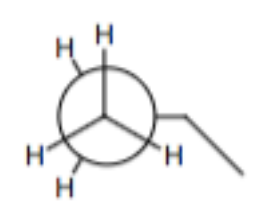
E. 3,5 dichloride - Oxocyclohexane

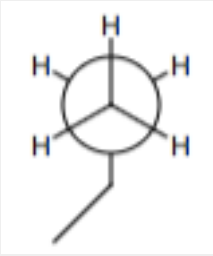


2. Newman Projections

Energy Diagram of n-Butane Newman Projections

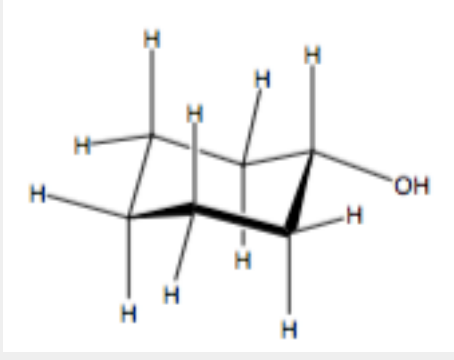
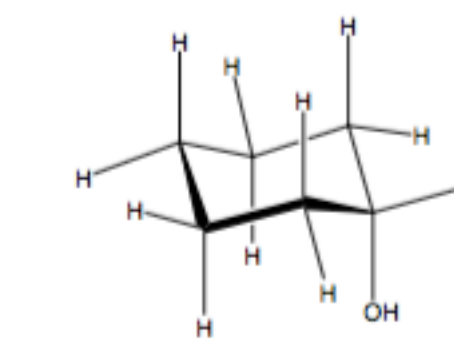


	Angle	Newman Projection
1	0°	 <p>A Newman projection of ethane looking down the C-C bond. The front carbon has three hydrogen atoms (H) at the 12, 2, and 4 o'clock positions. The back carbon has three hydrogen atoms (H) at the 10, 2, and 4 o'clock positions. An ethyl group is attached to the back carbon, pointing downwards.</p>
2	60°	 <p>A Newman projection of ethane looking down the C-C bond. The front carbon has three hydrogen atoms (H) at the 12, 2, and 4 o'clock positions. The back carbon has three hydrogen atoms (H) at the 10, 2, and 4 o'clock positions. An ethyl group is attached to the back carbon, pointing to the left.</p>
3	120°	 <p>A Newman projection of ethane looking down the C-C bond. The front carbon has three hydrogen atoms (H) at the 12, 2, and 4 o'clock positions. The back carbon has three hydrogen atoms (H) at the 10, 2, and 4 o'clock positions. An ethyl group is attached to the back carbon, pointing to the left.</p>
4	180°	 <p>A Newman projection of ethane looking down the C-C bond. The front carbon has three hydrogen atoms (H) at the 12, 2, and 4 o'clock positions. The back carbon has three hydrogen atoms (H) at the 10, 2, and 4 o'clock positions. An ethyl group is attached to the back carbon, pointing to the right.</p>
5	240°	 <p>A Newman projection of ethane looking down the C-C bond. The front carbon has three hydrogen atoms (H) at the 12, 2, and 4 o'clock positions. The back carbon has three hydrogen atoms (H) at the 10, 2, and 4 o'clock positions. An ethyl group is attached to the back carbon, pointing to the right.</p>
6	300°	 <p>A Newman projection of ethane looking down the C-C bond. The front carbon has three hydrogen atoms (H) at the 12, 2, and 4 o'clock positions. The back carbon has three hydrogen atoms (H) at the 10, 2, and 4 o'clock positions. An ethyl group is attached to the back carbon, pointing to the right.</p>

7	360°	
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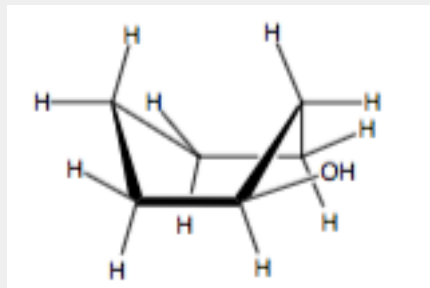
There are 6 possible Newman projections with 60° rotations between them. Newman projection 1 and 7 are identical, having done a full rotation. Out of these options, 4 conformations are equally stable, the ones at rotations 0°, 120°, 240°, and 360°. This is because there is the furthest possible distancing between the groups. The energy differences between these four conformers is zero because they are essentially the same compound.

3. Cyclohexanol

Line Drawings	
<p>This first conformation of cyclohexanol, the chair conformation, shows the most stable form. This is because the hydroxyl group, the largest group on the ring, is in an equatorial position. This positioning limits steric strain on the molecule.</p>	
<p>This second conformation shows the second "chair flip" or second chair conformation of cyclohexanol. When a chair flip occurs all axial positions become equatorial so now the hydroxyl group is in an axial position. This causes an unfavourable steric strain known as the 1,3-diaxial interaction.</p>	

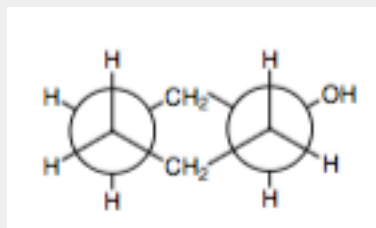
The third conformation is known as the boat conformation. This occurs mid flip between the two chair conformers. This conformer causes steric strain between the atoms, in this case Hydrogens, in the "flagpole positions" above the atom, although it is favourable that hydroxyl is equatorial.

Like the chair conformation, this boat conformation can be flipped which would produce a less stable conformer. In this conformer the hydroxyl group would be in the axial position which would cause the same strain issues as with the less stable chair conformer.

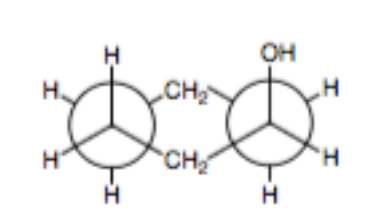


Newman Projections

Stable:
Chair conformer with the hydroxyl group in the equatorial position

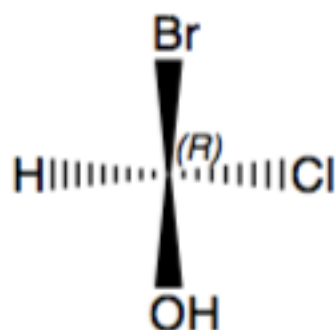
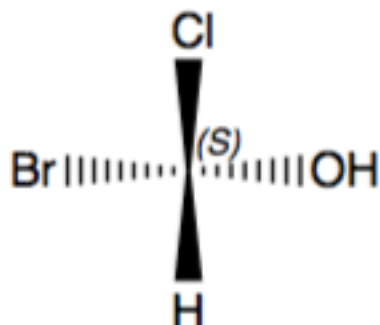


Less stable:
Chair conformer with the hydroxyl group in the axial position

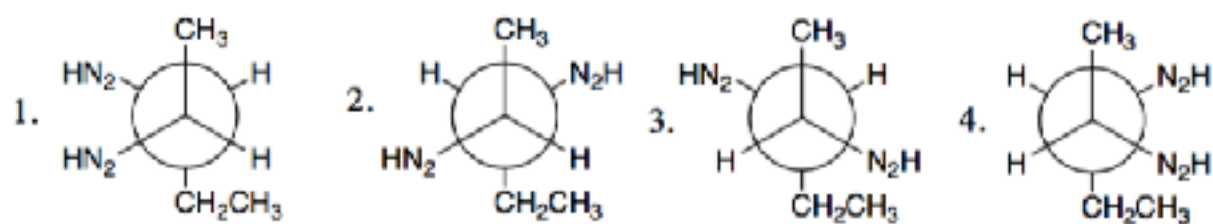
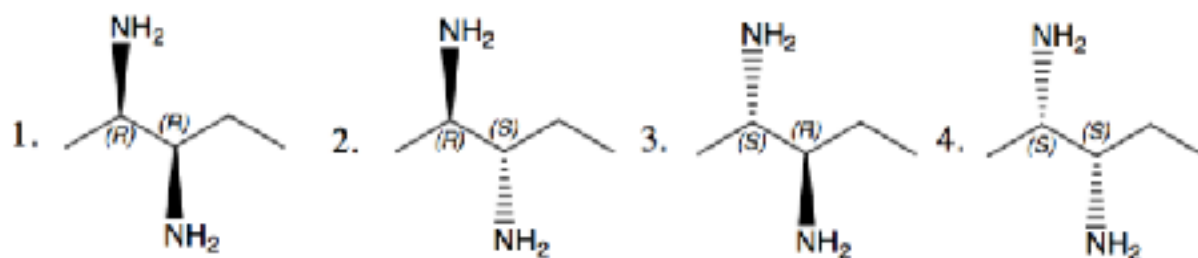


Questions:

1.



2.



3.

