Relationships Between Conformations of Disubstituted Cyclohexanes

Summary of Relationships (both substituent groups the same)

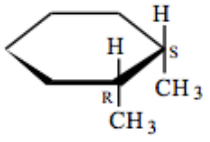
Compound	Conformational Equilibrium*	Relationship Between Conformations	Chirality of Conformers‡
cis-1,2	a e ⇌ e a	enantiomeric	Each is chiral, but not resolvable due to rapid ring flipping.
trans-1,2	a a ⇌ e e	diastereomeric	Both conformers are chiral and therefore resolvable.
cis-1,3	a a ⇌ e e	diastereomeric	Both conformers are achiral.
trans-1,3	e a ⇌ a e	identical	It is chiral and thus resolvable.
cis-1,4	a e ⇌ e a	identical	It is achiral.
trans-1,4	a a ⇌ e e	diastereomeric	Both conformers are achiral.

* "a" stands for axial and "e" stands for equatorial. In those instances where the interconverting conformations are diastereomeric, the more stable of the two has been indicated by relative lengths of the reversible arrows.

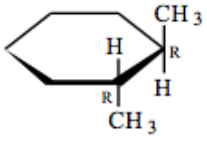
‡ Resolvable refers to a conformer which exists as a pair of enantiomers which are isolable from each other.

Example Discussion: 1,2-dimethylcyclohexanes

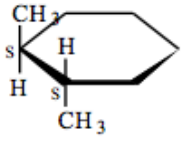
The chirality and optical activity of substituted cyclohexanes can be predicted from planar ring drawings. This is true even though the ring is not actually planar but rather has chair conformations. For example, consider the 1,2-dimethylcyclohexanes.



A



B

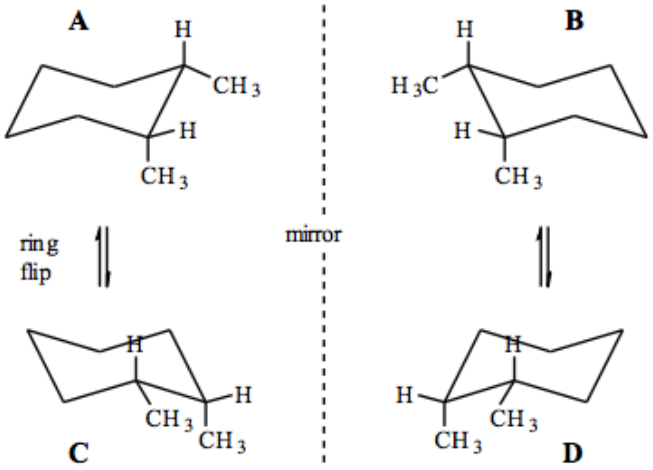


C

no plane of symmetry: B, C	has plane of symmetry: A	enantiomers: B & C
chiral: B, C	achiral: A	diastereomers: A & B, A & C
optically active: B, C	optically inactive: A	meso: A

From the above planar representations, it can be seen that there are three different isolable stereoisomers corresponding to 1,2-dimethylcyclohexane. Looking at the correct conformations allows one to understand why planar drawings give accurate predictions. Build models and convince yourself that the following information is true.

Cis-1,2 Diastereomer



chiral conformers: A, B, C, D

identical conformers: A=D, B=C

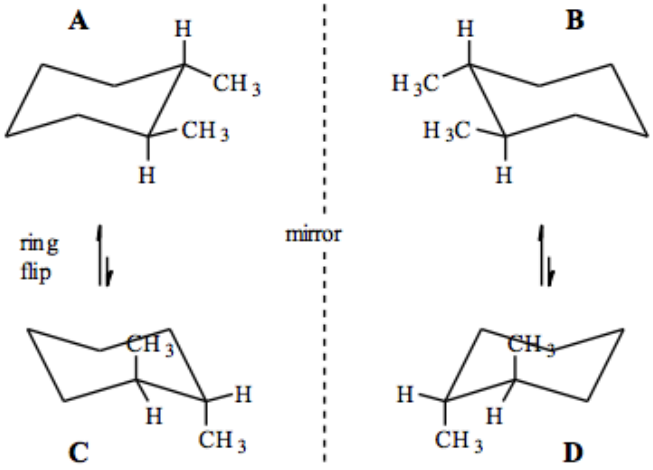
enantiomeric conformers:

A&B, C&D, A&C, B&D

diastereomeric conformers: none

The *cis* diastereomer consists of <u>one</u> pair of enantiomeric conformers (since A=D and B=C). They are not isolable or resolvable since rapid ring flipping interconverts them. Thus, the cis isomer is optically inactive and exists as a nonresolvable racemic mixture. There is only one distinct isolable substance from *cis*-1,2-dimethylcyclohexane.

Trans-1,2 Diastereomer



chiral conformers: A, B, C, D

identical conformers: none

enantiomeric conformers:

A&B, C&D

diastereomeric conformers:

A&C, A&D, B&C, B&D

The *trans* diastereomer consists of <u>two</u> pairs of enantiomeric conformers or alternatively, <u>four</u> pairs of diastereomeric conformers. Two diastereomeric pairs of conformers cannot be separated into two isomers since they are interconverted by rapid ring flipping. Each enantiomeric pair is isolable and resolvable since they are not interconverted by ring flipping. All conformations of each stereoisomer are chiral and therefore, each stereoisomer is chiral. As a result of all this, *trans*-1,2-dimethylcyclohexane exists as two optically active, isolable and resolvable substances. They have equal, but opposite specific rotations and thus, consist of a pair of enantiomers.