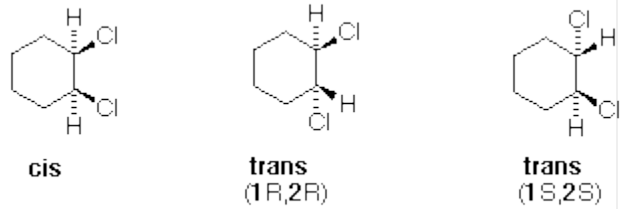
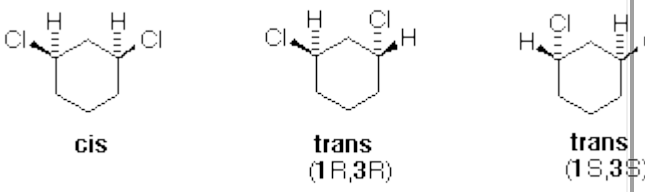
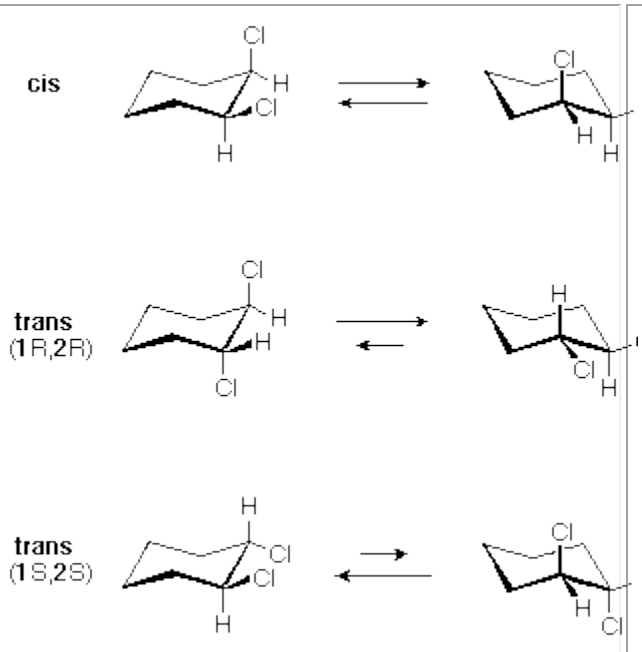
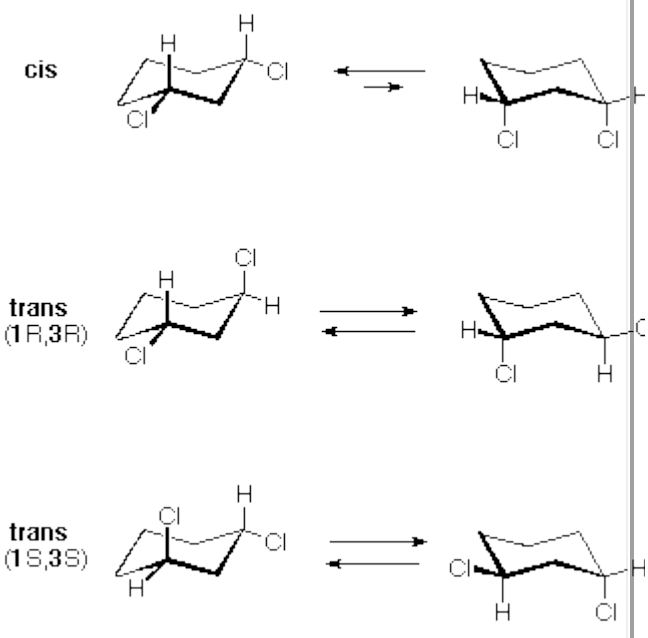
Stereoisomerism in Disubstituted Cyclohexanes

The distinction between configurational stereoisomers and the conformers they may assume is well-illustrated by the disubstituted cyclohexanes. The following discussion uses the various isomers of dichlorocyclohexane as examples. The 1,1-dichloro isomer is omitted because it is an unexceptional **constitutional isomer** of the others, and has no centers of chirality (asymmetric carbon atoms). The 1,2- and 1,3-dichlorocyclohexanes each have two centers of chirality, bearing the same set of substituents. The cis & trans-1,4-dichlorocyclohexanes do not have any chiral centers, since the two ring groups on the substituted carbons are identical.

There are three configurational isomers of 1,2-dichlorocyclohexane and three configurational isomers of 1,3-dichlorocyclohexane. These are shown in the following table.

The 1,2-Dichlorocyclohexanes	The 1,3-Dichlorocyclohexanes
	
	

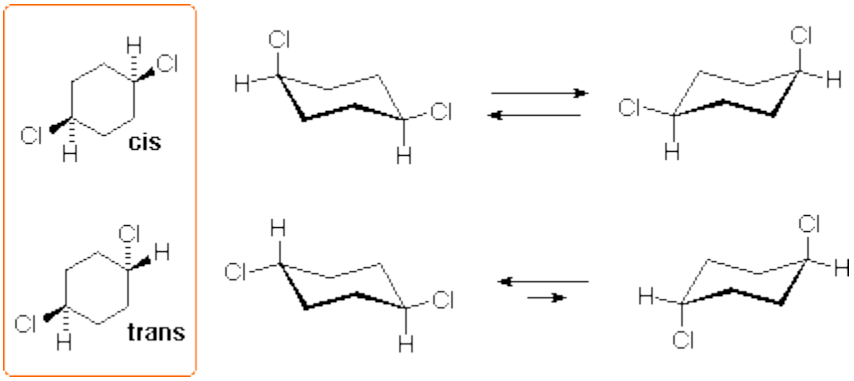
All the 1,2-dichloro isomers are **constitutional** isomers of the 1,3-dichloro isomers. In each category (1,2- & 1,3-), the (*R,R*)-trans isomer and the (*S,S*)-trans isomer are enantiomers. The cis isomer is a diastereomer of the trans isomers. Finally, all of these isomers may exist as a mixture of two (or more) conformational isomers, as shown in the table.

The chair conformer of the cis 1,2-dichloro isomer is chiral. It exists as a 50:50 mixture of enantiomeric conformations, which interconvert so rapidly they cannot be resolved (ie. separated). Since the cis isomer has two centers of chirality (asymmetric carbons) and is optically inactive, it is a meso-compound. The corresponding trans isomers also exist as rapidly interconverting chiral conformations. The diequatorial conformer predominates in each case, the (*R,R*) conformations being mirror images of the (*S,S*) conformations. All these conformations are diastereomeric with the cis conformations.

The diequatorial chair conformer of the cis 1,3-dichloro isomer is achiral. It is the major component of a fast equilibrium with the diaxial conformer, which is also achiral. This isomer is also a meso compound. The corresponding trans isomers also undergo a rapid conformational interconversion. For these isomers, however, this interconversion produces an identical conformer, so each enantiomer (*R,R*) and (*S,S*) has predominately a single chiral conformation. These enantiomeric conformations are diastereomeric with the cis conformations.

The 1,4-dichlorocyclohexanes may exist as cis or trans stereoisomers. Both are achiral, since the disubstituted six-membered ring has a plane of symmetry. These isomers are diastereomers of each other, and are constitutional isomers of the 1,2- and 1,3- isomers.

The 1,4-Dichlorocyclohexanes



All the chair conformers of these isomers are achiral, and the diequatorial conformer of the trans isomer is the predominate species at equilibrium.

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