

Stereochemical Relationships of H-sets

chemically equivalent H's - have the same chemical shift and coupling to other H's.

1. homotopic H's - those which are identical in all environments (usually related by a rotational symmetry operation, C_n)

2. enantiotopic H's - those which are identical in an achiral environment but different in a chiral environment (usually related by a mirror, s , or inversion, i , symmetry operations)

chemically inequivalent H's - have different chemical shifts and couple independently to other H's

3. diastereotopic H's - those which are chemically different by virtue of being in diastereomeric environments in the molecule (not symmetry related)

determination of stereochemical relations - consider the stereochemical relationship between molecules derived from changing one H set to D and the other H set to D. If the same molecule results, the H sets are homotopic; if enantiomers result, the H sets are enantiotopic; and if diastereomers result, the H sets are diastereotopic.

examples:

