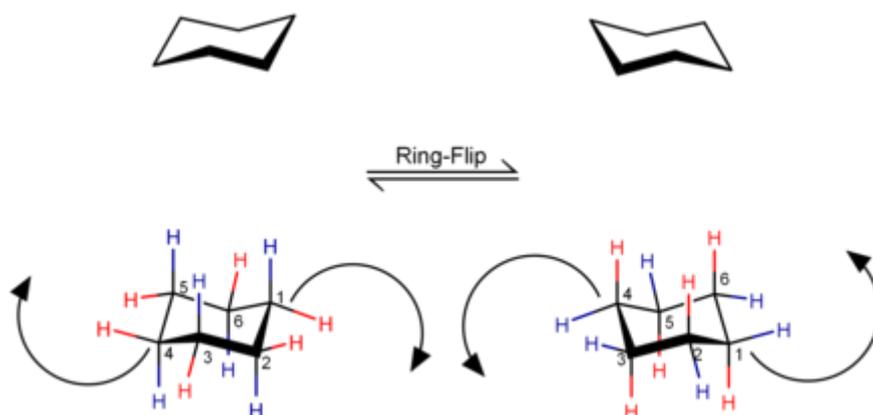


# Ring flip

In organic chemistry, a **ring flip** (also known as a **ring inversion** or **ring reversal**) is the interconversion of cyclic conformers that have equivalent ring shapes (e.g., from a chair conformer to another chair conformer) that results in the exchange of nonequivalent substituent positions.<sup>[1]</sup> The overall process generally takes place over several steps, involving coupled rotations about several of the molecule's single bonds, in conjunction with minor deformations of bond angles.

Most commonly, the term is used to refer to the interconversion of the two chair conformers of cyclohexane derivatives, which is specifically referred to as a **chair flip**, although other cycloalkanes and inorganic rings undergo similar processes.



Two chair conformations of cyclohexane. The entirety of axial positions become equatorial, and vice versa, upon ring flip.

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## Cyclohexane

Cyclohexane is a prototype for low-energy degenerate ring flipping. The 'chair' is the strongly preferred conformation. Two <sup>1</sup>H NMR signals should be observed in principle, corresponding to axial and equatorial protons. However, due to the cyclohexane chair flip, only one signal is seen for a solution of cyclohexane at room temperature, as the axial and equatorial proton rapidly interconvert relative to the NMR time scale. The coalescence temperature at 60 MHz is ca.  $-60\text{ }^{\circ}\text{C}$ .<sup>[2]</sup>

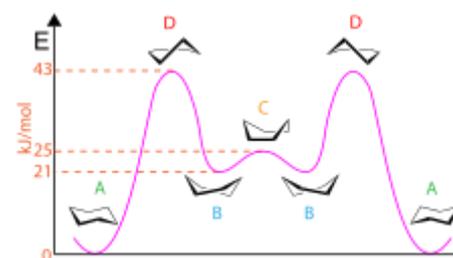
The molecular motions involved in a chair flip are detailed in the figure on the right: The half-chair conformation (**D**, 10.8 kcal/mol,  $C_2$  symmetry) is the energy maximum when proceeding from the chair conformer (**A**, 0 kcal/mol reference,  $D_{3d}$  symmetry) to the higher energy twist-boat conformer (**B**, 5.5 kcal/mol,  $D_2$  symmetry). The boat conformation (**C**, 6.9 kcal/mol,  $C_{2v}$  symmetry) is a local energy maximum for the interconversion of the two mirror image twist-boat conformers, the second of which is converted to the other chair confirmation through another half-chair. At the end of the process, all axial positions have become equatorial and vice versa. The overall barrier of 10.8 kcal/mol corresponds to a rate constant of about  $10^5\text{ s}^{-1}$  at room temperature.

Note that the twist-boat ( $D_2$ ) conformer and the half-chair ( $C_2$ ) transition state are in chiral point groups and are therefore chiral molecules. In the figure, the two depictions of **B** and two depictions of **D** are pairs of enantiomers.

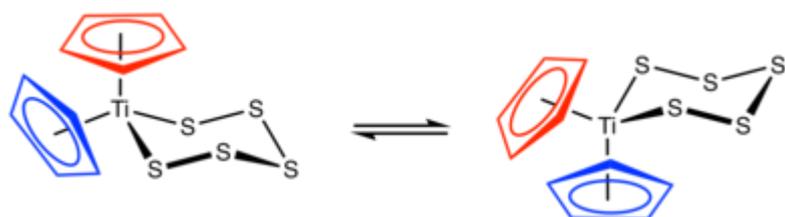
As a consequence of the chair flip, the axially-substituted and equatorially-substituted conformers of a molecule like chlorocyclohexane cannot be isolated at room temperature. However, in some cases, the isolation of individual conformers of substituted cyclohexane derivatives has been achieved at low temperatures ( $-150\text{ }^\circ\text{C}$ ).<sup>[3]</sup>

## Other cases

Most compounds with nonplanar rings engage in degenerate ring flipping. One well-studied example is titanocene pentasulfide, where the inversion barrier is high relative to cyclohexane's. Hexamethylcyclotrisiloxane on the other hand is subject to a very low barrier.



The conformational changes that occur in a cyclohexane ring flip take place over several stages. Structure **D** (10.8 kcal/mol) is the highest energy transition state of the process.



The  $^1\text{H}$  NMR spectrum of titanocene pentasulfide features two signals at room temperature, a consequence of its relative rigidity.

## See also

- Cyclohexane conformation
- Conformational isomerism

## References

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