
Correct representation of stereochemical configurations for publications and computer treatment

Most molecular entities are inherently three-dimensional, but they are commonly depicted on two-dimensional media such as paper or computer displays. Historically, the varying conventions for depiction of configuration have caused confusion among chemists and can lead to misinterpretation by computer programs while property predictions and structure search.

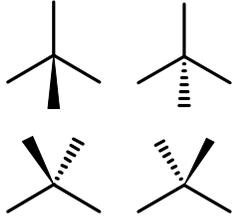
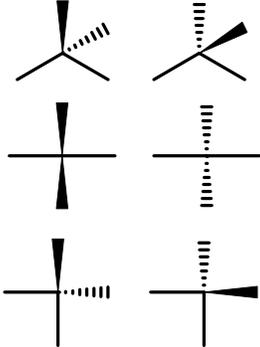
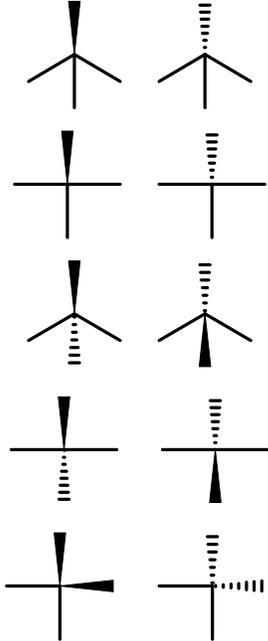
The recent publication by International Union of Pure and Applied Chemistry (IUPAC) "*Graphical representation of stereochemical configuration*" provides a self-consistent series of recommendations for the unambiguous depiction of molecules in two dimensions using standards that are, for the most part, understandable by both human and computer programs.

Main principles of these recommendations are:

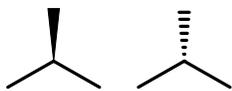
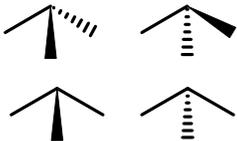
- Diagrams that have a wide audience should be **drawn as simply as possible**.
- **Use** as most as possible **preferred drawing styles** and avoid ambiguous styles.
- **Avoid** the use of **perspective diagrams** and **class-specific drawing styles** (Fischer projections, Haworth projections, *etc.*) when structures are to be interpreted by computers.
- **Use solid wedges** to indicate bonds that project above the plane of the paper **and hashed wedges** to indicate bonds that project below the plane of the paper.
- The bonds must be oriented with the narrow end pointed at the stereogenic center.
- Avoid connecting stereogenic centers with a stereobond.

The following table illustrates the main styles used to represent stereochemical configurations and their classification based on potential ambiguity.

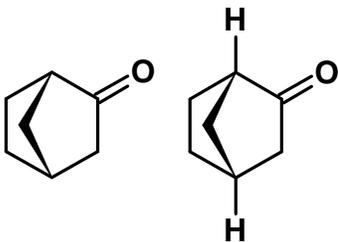
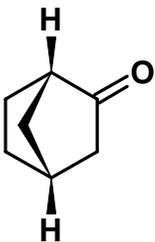
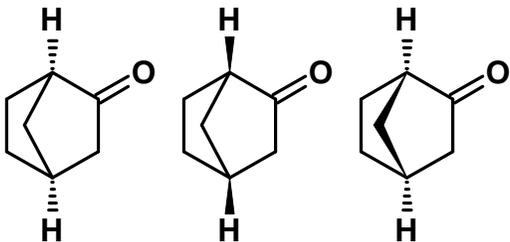
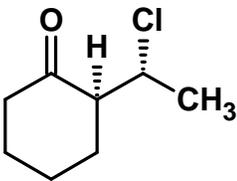
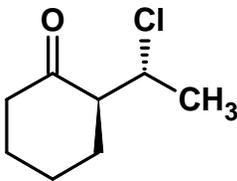
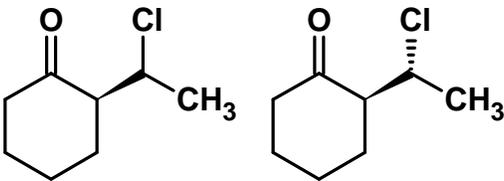
Tetrahedral configurations depicted with four explicit bonds

Preferred	Acceptable	Not Acceptable or Wrong
		

Tetrahedral configurations depicted with three explicit bonds

Preferred	Acceptable	Not Acceptable or Wrong
		

These principles can be illustrated with the following representations of two distinct chemical structures:

Preferred	Acceptable	Not Acceptable or Wrong
		
		

More detailed description of recommended drawing styles that takes into account the specific types of chemical structures can be found in the official publication:

- [Graphical representation of stereochemical configuration \(IUPAC Recommendations 2006\)](#). *Pure Appl. Chem.* **78**, 1897 (2006).