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The Structure and Symmetry of Metal Tris Chelates

A Web Resource by Marion E. Cass (Carleton College) and Henry S. Rzepa (Imperial College London)

The goal in generating this website was to create and collect a set of visualizations to teach students about the structure and symmetry of chiral metal tris chelates (and a few metal tris chelates that are not chiral). Specifically, my goals are to help students: 1. Visualize and identify the C_n axes and rotations in this class of chiral molecules, 2. Assign the Λ or Δ absolute configuration, 3. Recognize λ and δ ligand conformations in given chelates, 4. Visualize the Bailar and Rây-Dutt non-dissociative motions that can racemize or racemize/isomerize these molecules and 5. Determine if these non-dissociative twisting motions racemize and/or isomerize (facial to meridional) tris chelate molecules. Two examples from the research literature and eight problems with several questions are included.

The website is designed to reinforce materials introduced in class. Interactive tools have been scripted to aid student learning. The visualizations and animations have been designed so that students can view the operations from any perspective however can always “Reset” to a preferred view or views. In addition, since these are web-based materials, they are available to students at their convenience. This work was originally published with my colleague Henry S. Rzepa of Imperial College, London, in the *Journal of Chemical Education* in 2008 (<http://pubs.acs.org/doi/pdfplus/10.1021/ed085p750>). I have updated the scripting from Jmol to JSmol (April 2014), updated links that have moved or changed, and have made some corrections in the content (resulting from some new experimental findings in the examples sections). I welcome any of you to write me with suggestions from the current literature to include in the examples section or examples to include in the exercise section.

The updated Web site, The Structure and Symmetry of Metal Tris Chelates can be found here: <http://www.people.carleton.edu/~mcass/TrisChelates/jsmol/Index.html>

Learning goals:

Working through these web-based materials:

1. Students should be able to locate the C_3 and possible C_2 axes in chiral metal tris chelates.
2. Students should be able to assign the Λ or Δ absolute configuration of a given complex.
3. Students should be able to assign a λ or δ ligand conformation in relevant molecules.
4. Students should be able to describe the Bailar Twist and Rây-Dutt mechanism.
5. Students should be able to determine if the Bailar Twist motion results in racemization and/or isomerization (facial to meridional isomerization) of a metal tris chelate molecule.
6. Students should be able to determine if the Rây-Dutt Twist motion results in racemization and/or isomerization (facial to meridional) of a metal tris chelate molecule.