Structure Determination of Twinned and Disordered Cyclopentadienyl Complexes

Ulrich Baisch, Oliver Oeckler, Sandro Pagano, Wolfgang Schnick *Department of Chemistry and Biochemistry, University of Munich (LMU), Munich, Germany.* E-mail: ulrich.baisch@cup.uni-muenchen.de

Cp_3 lanthanides (Cp = cyclopentadienyl) represent one of the best investigated agents in modern organolanthanide chemistry [1]. However, only eight of the 14 possible solvent free lanthanide Cp_3 complexes have been yet characterized successfully by X-ray diffraction methods [2]. Many problems in the synthesis of suitable crystals and refinement of the crystal data have been reported [3].

We observed the intrinsic twinning and/or disorder in the crystal structure of the Cp complexes of cerium and holmium. Single-crystal X-ray and powder diffraction measurements at different temperatures have been elaborated in order to explain this phenomenon from a crystallographic and chemical point of view.

$HoCp_3$ and $CeCp_3$ crystallize in different crystal shapes, depending on the temperature at which they were crystallized. Pseudomerohedral and reticular pseudomerohedrical twinning as well as disorder were detected in monoclinic primitive crystal systems. The sharing of one C atom between the molecular units of the complex produces polymeric zigzag chains along the cell axis.

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