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HOMOCHIRAL CRYSTALS FOR SELECTIVE SYNTHESIS

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Abstract

Six new coordination compounds were prepared from monodentate sulfide ligands and copper(I) halides and their crystal structures were determined by single-crystal X-ray diffraction. The aim was to prepare coordination polymers that crystallize as conglomerates in order to use them in total spontaneous resolution. The anionic and neutral ligands were varied in order to examine how they would affect the crystallization. All six complexes formed racemic crystals, and five of them were polymeric.

Bidentate sulfide ligands were used to increase the possibility of obtaining a coordination polymer. Five new complexes were prepared and structurally characterized by single crystal X-ray diffraction. Three of the complexes formed coordination polymers but none of them crystallized as a conglomerate.

Tetrahedral metal complexes have been resolved by total spontaneous resolution for the first time. A cationic silver(I) complex with a bidentate sulfide ligand was prepared and it crystallized as a conglomerate. Enantioenriched crystal batches were obtained with enantiomeric excesses up to 90 %.

Three chiral Ru(II) complexes with bidentate sulfide ligands were prepared and all three crystallized as conglomerates. They were used in absolute asymmetric synthesis and oxidized enantioselectively. The oxidations resulted in a selectivity of > 98% without the use of a chiral catalyst. One of the Ru(II) complexes isomerizes when exposed to light. Four new phases, containing one or both isomers, co-crystallized from the same solution.

Keywords: Absolute asymmetric synthesis, total spontaneous resolution, optical activity, coordination compounds, coordination polymers, photoisomerization, enantioselective sulfide oxidation, single crystal X-ray crystallography, co-crystallization of diastereomers

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