

Mechanisms of *Cis-Trans* Isomerization and C^α epimerization of (D-*allo*,L-isoIeucinato)copper(II)

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Our recent (unpublished) experimental observations revealed that the *cis*-to-*trans* transformation can happen relatively fast for (D-*allo*,L-isoIeucinato)copper(II) in methanolic solution at room temperature. On the other side, *trans*-to-*cis* isomerization, which might be accompanied by C^α epimerization to bis(L-isoIeucinato)copper(II), occurred in aqueous solution after several weeks.

To rationalize the transformations, we study the transition state structures for the *cis*-*trans* isomerization of bis(L-isoIeucinato)copper(II) and (D-*allo*,L-isoIeucinato)copper(II), and the C^α epimerization of the two complexes using the density functional B3LYP. For the former mechanism, we can calculate transition state structures with unbroken copper-donor bonds, and verify their nature as saddle points by frequency calculations. For the later, a keto-enol tautomerism is tried. This seems to include too high activation energy barriers, so solvent molecule participation should be expected.

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