Isomer Chemistry: Design Ligands to Adjust Thermodynamics and Kinetics for Rare-Earth Metal Extraction and Rhodium Catalyzed Hydroformylation

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There is a clear lack of a systematic method to develop ligands for scientific and industrial applications in drug delivery, nanomaterial engineering, disease treatment and solar energy. By leveraging steric and electrostatic properties of isomers, this work proposes a new and general approach to systematically design ligands with desirable stability and reactivity, altering the overall thermodynamics and kinetics of the reaction. We demonstrate its applicability and effectiveness by using butyl phosphine to modify metal complexes in two systems, one for rare-earth metal extraction and the other for rhodium catalyzed hydroformylation reaction of propene. They were examined both computationally and experimentally. We designed the two systems using computational chemistry approaches, then experimentally verified the theoretical results through rare-earth metal extraction experiments and hydroformylation inorganic synthesis. It was found that different butyl isomers do alter thermodynamic and kinetic properties; however, not always in a parallel manner. The data collected in this work and the following analysis lay the foundation for optimizing metal complex catalysts. This work develops a novel prospective for the design of new ligands to extract needed rare-earth metals from environments and to produce ideal catalysts for hydroformylation for the efficient production of plastics. It could be applied to other fields to systematically design new ligands as well.

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