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Catalytic Conversion of Ethanol to Butanol: Synthesis and Application of Naphthaquinone and Anthraquinone Coordinated Iridium Compounds

Abstract:

The catalytic upgrading of ethanol to higher-order alcohols such as butanol is a critical step toward the development of sustainable liquid fuels and energy-dense bio-based chemicals. In this study, we report the synthesis and characterization of a new class of iridium complexes coordinated with redox-active naphthaquinone and anthraquinone ligands. These complexes were synthesized via ligand substitution reactions starting from $[Ir(COD)Cl]_2$ (COD = 1,5-cyclooctadiene), and structurally confirmed by NMR, IR, and single-crystal X-ray diffraction.

Catalytic evaluations reveal that these quinonoid-ligated iridium compounds exhibit enhanced activity in the Guerbet-type coupling of ethanol to butanol under mild conditions. The redox non-innocence of the quinone ligands appears to facilitate key dehydrogenation and C–C bond-forming steps through ligand-assisted electron transfer. Compared to classical phosphine- or nitrogen-based systems, these organometallic quinone complexes demonstrate improved selectivity, turnover number (TON), and thermal stability. This work highlights the potential of utilizing redox-active ligands in transition metal catalysis to promote complex multi-step transformations and lays the groundwork for designing advanced catalytic systems for renewable fuel production.

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Biography:

Dr. A. K. Fazlur Rahman earned his M.A. in Chemistry from Brandeis University and his Ph.D. in Organometallic Chemistry from the Australian National University in Canberra. He pursued postdoctoral research at the University of Tasmania (Australia), Ames Laboratory (Iowa State University, USA), and the University of Oklahoma (USA). Dr. Rahman is a distinguished recipient of the Southwest Regional Award of the American Chemical Society (2009) and the Oklahoma Chemist Award (2015).

Over the course of his career, he has held visiting faculty positions at several prestigious institutions, including Texas A&M University, University of Rochester, California Institute of Technology (Caltech), University of California at Berkeley, Free University of Berlin, Friedrich Schiller University (Jena), Rutgers University, and Columbia University in New York City. Currently, Dr. Rahman holds an endowed professorship and serves as the Sarkeys Energy Foundation Chair in Chemistry at the Oklahoma School of Science and Mathematics. In addition, he serves as an Affiliate Professor of Chemistry and Chemical Engineering at the University of Oklahoma, where he has taught Organic Chemistry as an adjunct professor for many years.