Investigating Water-Oxidation Using a Ru(III) Carboxamide Water Coordinated Complex

Authors : Yosra M. Badiei, Evelyn Ortiz, Marisa Portenti, David Szalda

Abstract : Water-oxidation half-reaction is a critical reaction that can be driven by a sustainable energy source (e.g., solar or wind) and be coupled with a chemical fuel making reaction which stores the released electrons and protons from water (e.g., H_2 or methanol). The use of molecular water-oxidation catalysts (WOC) allow the rationale design of redox active metal centers and provides a better understanding of their structure-activity-relationship. Herein, the structure of a Ru(III) complex bearing a doubly deprotonated N,N'-bis(aryl)pyridine-2,6-dicarboxamide ligand which contains a water molecule in its primary coordination sphere was elucidated by single-crystal X-ray diffraction. Further spectroscopic experimental data and pH-dependent electrochemical studies reveal its water-oxidation reactivity. Emphasis on mechanistic details for O₂ formation of this complex will be addressed.

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Keywords : water-oxidation, catalysis, ruthenium, artificial photosynthesis

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