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Quantum Mechanical Calculation of Thermodynamic Properties and Infrared Spectra of Zirconium Complexes for Selective Oxidation Catalysis[1] CHAO DONG, THOMAS MANZ, New Mexico State University — Selective oxidation of organic substrates is an important process for producing chemical intermediates used in industry, lab chemicals, and pharmaceutical products. It is still challenging not to produce unwanted co-products. Recently published computations predict efficient molecular oxygen activation and selective oxidation of organic substrates using a newly designed zirconium organometallic complex that does not require any co-reductant (B. Yang and T. A. Manz, Theor. Chem. Acc., 2016, 135, 21:1-19 and RSC Adv., 2016, 6, 88189-88215). Here, quantum mechanical calculations are performed using Density Functional Theory to obtain the enthalpy and Gibbs free energy of this zirconium organometallic complex. These results provide insights for designing an experiment to synthesize this Zr complex and test its reactivity in lab. Infrared and hydrogen NMR spectra are calculated for various reaction intermediates to enable a comparison to experimentally measured spectra in order to elucidate the reaction mechanisms and side reactions.

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