Oxidation of 2-Propanol by Peroxo Titanium Complexes: A Combined Experimental and Theoretical Study

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Received: July 24, 2010; Revised Manuscript Received: September 23, 2010

The oxidation of 2-propanol by titanium peroxo complexes is investigated in a combined synthetic, spectroscopic, and computational study. We find in quantum chemical calculations for the thermal reaction in protic solvents that the temporary protonation of the peroxo group activates the latter as electrophile. This transient species is amenable to a concerted transfer of two electrons and a proton from the secondary C atom of 2-propanol. Simultaneously, the carbonyl group is formed and the alcoholic proton is transferred to the solvent. In line with the results of the calculations, we find experimentally that the activity of the titanium peroxo complexes as oxidant depends on the pH value of the reaction medium.