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Maxim L. Kuznetsov and Armando J. L. Pombeiro*: Radical Formation in the [$MeReO_3$]-Catalyzed Aqueous Peroxidative Oxidation of Alkanes: A Theoretical Mechanistic Study

Pages 307−318. In this paper, we presented DFT calculations of plausible mechanisms of the formation of radicals (hydroperoxyl and hydroxyl derived from H_2O_2, alkyl derived from the alkane, and metal complex radicals) in the system [$MeReO_3$](MTO)/H_2O_2/H_2O−CH_3CN used for the catalytic oxidations of alkanes. Discussing the state of the art in this field, we overlooked a few papers by Crucianelli et al.,[1−4] which describe experimental studies of alkane oxidations catalyzed by MTO and polymer-supported MTO in the presence of H_2O_2. In one of them,[1] the authors observed, by EPR, the formation of a methyl radical by homolysis of the Re−CH_3 bond upon encapsulation of MTO into polystyrene in a heterogeneous system.

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