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Maxim L. Kuznetsov and Armando J. L. Pombeiro*: Radical Formation in the [MeReO₃]-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 H₂O₂, alkyl derived from the alkane, and metal complex radicals) in the system [MeReO₃](MTO)/H₂O₂/H₂O–CH₃CN 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 H₂O₂. In one of them,¹ the authors observed, by EPR, the formation of a methyl radical by homolysis of the Re–CH₃ bond upon encapsulation of MTO into polystyrene in a heterogeneous system.

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