

# Fe-PDC as catalyst for the oxidation of organic contaminants: theoretical and experimental studies

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Reactions involving hydrogen peroxide decomposition catalyzed by new materials to generate radical \*OH, have received special attention due to the advantages in relation to the classic homogeneous process involving iron soluble salts. Understanding chemical oxidation mechanisms is one of the most relevant issues, in order to plan rational chemical treatments of organics in wastewaters and, in a broader view, a fundamental step on designing novel efficient and cost-effective technological processes for environmental remediation, in progressively widescale applications.

The goal of this work is to investigate the utilization of the complex Fe-PDC as a homogeneous catalyst for the degradation of organic dyes in the light of the theoretical and experimental techniques. For the preparation of Fe-PDC was used a solution of 60mM PDC (dipicolinic acid) that was added to a solution of 30mM Fe(NO<sub>3</sub>)<sub>3</sub>, the reaction mixture was subjected to 48 h of magnetic stirring. The synthesized material was characterized by XRD, XPS and FTIR measurements and the reaction mechanism was studied by ESI-MS analyses. Furthermore, in order to shed some more light on the formation of hydroxyl radicals and of the overall reaction mechanism, some thermodynamic calculations were performed. The theoretical calculations were performed with the Gaussian 98 program. All intermediate precursors involved and transition states were calculated using the DFT method at B3LYP basis function 6-31G (d, p). The results of this study show that the Fe-PDC is a good catalyst for oxidation of organic dyes *via* a Fenton-like mechanism. All theoretical data are in good agreement with the experimental results for the dyes degradation.

**Keywords:** Fe-PDC, theoretical calculations, Fenton, homogeneous catalysis.

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