Hyperfine parameters of pyridyl-containing iminoxy radicals generated from oximes by γ-irradiation and in zeolite lattice: EPR spectroscopy and density functional study.

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Streszczenie

Incorporation of pyridyl oximes into the channels of thermally activated pentasil zeolite ZSM-5 gives rise to iminoxy radicals. EPR spectrum of the species derived by dehydrogenation of di-2-pyridilketone oxime is fully anisotropic and characteristic for the iminoxy σ-type neutral radical. The EPR spectra of the radicals derived from 2-pyridinealdoxime and 4-pyridinealdoxime exhibit additional splitting due to the azomethine hydrogen. The ĝ and Â tensor parameters were determined on the basis of EPR spectra. In order to identify a geometric isomer (*E* or *Z*) of the iminoxyls obtained in the pores of the zeolite and within γ-irradiated samples of solid oximes, hyperfine interaction parameters of the generated radicals were compared with the parameters calculated using density functional theory (DFT); these calculations allow to characterize the iminoxy radical isomers formed in zeolite and oxime matrices.

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