

Molecular geometry and hyperfine interactions in iminoxy radicals with C=O or CH₂ group - DFT and EPR studies in liquid and rigid media.

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Two series of iminoxy radicals, $R_1C(O)C(NO)R_2$ and $R_1CH_2C(NO)R_2$, were studied using DFT calculations and EPR spectroscopy. The role of stereochemistry in long-range spin density distribution was discussed in terms of the configurational and conformational effects. To identify the geometric isomers (*E* or *Z*) of the iminoxyls obtained in solution as well as in the matrices of zeolite and γ -irradiated oximes, the hyperfine parameters derived from the EPR spectra were compared with those predicted by DFT. The spectra indicate that $C_6H_5COC(NO)H$ and $CH_3COC(NO)H$ undergo isomerization in the solid oxime. The contribution of a particular isomer, dependent on temperature, corresponds to the calculated relative energies of the isomers.

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