Magnetic Properties of Nitroxide Spin Probes: Reliable Account of Molecular Motions and Nonspecific Solvent Effects by Time-Dependent and Time-Independent Approaches

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Application of a new integrated computational approach for two widely used nitroxide spin probes allows to show unequivocally that proper account of stereoelectronic, environmental, and dynamical effects leads to magnetic properties in quantitative agreement with experimental results without the need of any empirical parameter. Together with their specific interest, our results point out, in our opinion, the importance of developing and validating computational approaches able to switch on and off different effects, including environmental and dynamical ones, in order to evaluate their specific role in determining the overall experimental outcome.

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https://www.acs.org/content/acs/en.html