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Residual Dipolar Couplings in NMR Spectroscopy Using Lanthanide Tags

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Abstract : Nuclear Magnetic Resonance (NMR) spectroscopy is an indispensable technique used in structure determination of small and macromolecules to study their physical properties, elucidation of characteristic interactions, dynamics and thermodynamic processes. Quantum mechanics defines the theoretical description of NMR spectroscopy and treatment of the dynamics of nuclear spin systems. The phenomenon of residual dipolar coupling (RDCs) has become a routine tool for accurate structure determination by providing global orientation information of magnetic dipole-dipole interaction vectors within a common reference frame. This offers accessibility of distance-independent angular information and insights to local relaxation. The measurement of RDCs requires an anisotropic orientation medium for the molecules to partially align along the magnetic field. This can be achieved by introduction of liquid crystals or attaching a paramagnetic center. Although anisotropic paramagnetic tags continue to mark achievements in the biomolecular NMR of large proteins, its application in small organic molecules remains unspread. Here, we propose a strategy for the synthesis of a lanthanide tag and the measurement of RDCs in organic molecules using paramagnetic lanthanide complexes.

Keywords : lanthanide tags, NMR spectroscopy, residual dipolar coupling, quantum mechanics of spin dynamics
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