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Title:	Characterization of the ^{19}F chemical shielding tensor using cross-correlated spin relaxation measurements and quantum chemical calculations
Authors:	Dorai, K. (/jspui/browse?type=author&value=Dorai%2C+K.)
Keywords:	Ab initio method Basis sets Chemical shielding tensors Chemical shift anisotropy Flourinated
Issue Date:	2010
Publisher:	Elsevier B.V.
Citation:	Chemical Physics Letters, 489 (4-6), pp. 248-253.
Abstract:	The ^{19}F chemical shift anisotropy (CSA) tensor is an indispensable structure estimation tool in the NMR investigations of flourinated biomolecules. This work focuses on the characterization of the ^{19}F CSA tensor in small molecules, through the combined use of quantum chemical methods and liquid-state NMR cross-correlated spin relaxation experiments. The effect of different basis sets and quantum computational methods on the magnitude and orientation of the ^{19}F CSA tensor are discussed. The results from ab initio methods and the liquid-state relaxation experiments match well and are comparable to values of the CSA tensor obtained from previous solid-state studies and from theoretical investigations of similar molecules.
Description:	Only IISERM authors are available in the record.
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