Title:	Using the 19F NMR chemical shift anisotropy tensor to differentiate between the zigzag and chiral forms of fluorinated single-walled carbon nanotubes
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Abstract:	The structural characterization of different kinds of zigzag and chiral single-walled carbon nanotubes (SWNTs) has been investigated theoretically using 19F NMR spectroscopy. The chemical shift anisotropy (CSA) tensor is computed at different levels of theory for the 19F nuclei in different forms of functionalized fluorinated carbon nanotubes (CNT). A set of fluorine CSA parameters comprising the span, skew, and isotropic chemical shift is computed for each form of the fluoronanotubes and multidimensional CSA parameter correlation maps are constructed. We show that these correlations are able to clearly distinguish between the chiral and zigzag forms of fluorinated carbon nanotubes (F-SWNTs). Implications for solid-state and liquid-state NMR experiments are discussed.
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