Relation between molecular electronic structure and nuclear spin-induced circular dichroism
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Relation between molecular electronic structure and nuclear spin-induced circular dichroism

The recently theoretically described nuclear spin-induced circular dichroism (NSCD) is a promising method for the optical detection of nuclear magnetization. NSCD involves both optical excitations of the molecule and hyperfine interactions and, thus, it offers a means to realize a spectroscopy with spatially localized, high-resolution information. To survey the factors relating the molecular and electronic structure to the NSCD signal, we theoretically investigate NSCD of twenty structures of the four most common nucleic acid bases (adenine, guanine, thymine, cytosine). The NSCD signal correlates with the spatial distribution of the excited states and couplings between them, reflecting changes in molecular structure and conformation. This constitutes a marked difference to the nuclear magnetic resonance (NMR) chemical shift, which only reflects the local molecular structure in the ground electronic state. The calculated NSCD spectra are rationalized by means of changes in the electronic density and by a sum-over-states approach, which allows to identify the contributions of the individual excited states. Two separate contributions to NSCD are identified and their physical origins and relative magnitudes are discussed. The results underline NSCD spectroscopy as a plausible tool with a power for the identification of not only different molecules, but their specific structures as well.

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