

NUCLEAR SPIN-INDUCED CIRCULAR DICHROISM AND ITS RELATION TO THE MOLECULAR ELECTRONIC STRUCTURE

Petr Štěpánek, Jiří Mareš, Vasily A. Ovchinnikov, Dage Sundholm, Sonia Coriani, Juha Vaara

NMR Research Group, Faculty of Science, University of Oulu, PO Box 3000, 90014 Oulu, Finland

Nuclear spin-induced circular dichroism (NSCD) is a recently theoretically predicted spectroscopic method bordering optical and nuclear magnetic resonance spectroscopy[1]. The phenomenon manifests as a difference in absorption of left- and right- circularly polarized components of light, caused by polarization of nuclear spins along the light beam.

In order to help guide the near future experimental work, we present here a computational study of NSCD spectra of several nucleobase molecules calculated from first principles using density functional theory (DFT). Different nucleobases as well as different conformers thereof are discussed. It is shown that changes in the overall shape of the NSCD spectra are connected to the changes in the electronic density upon excitation, where similar differences in the excited state densities lead to similar NSCD spectra. Interactions with specific nuclei and their influence on the NSCD spectra is also illustrated.

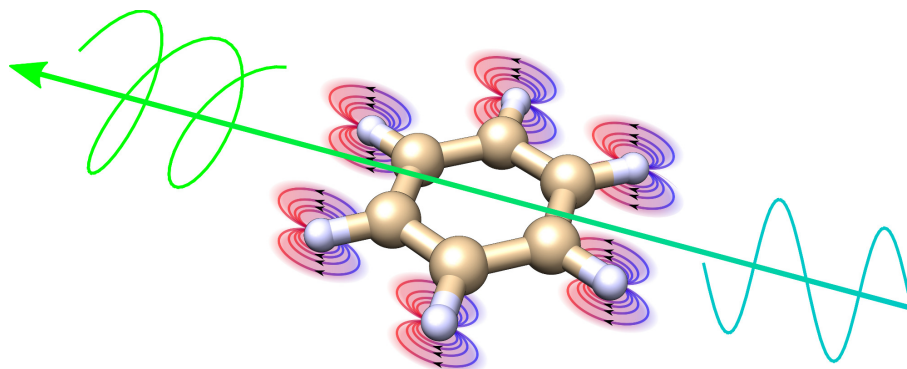


Figure 1: Illustration of the origin of ^1H nuclear spin circular-dichroism in benzene. The linearly polarized light beam becomes elliptically polarized upon interaction with nuclear spins aligned along the direction of the beam propagation.

[1] J. Vaara, A. Rizzo, J. Kauczor, P. Norman, S. Coriani, *The Journal of Chemical Physics* **140**, 134103 (2014).