

Unraveling CD spectra of G-quadruplexes

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Studying structures of G-quadruplexes (four-stranded nucleic acids comprised of guanine stacks) is a challenging issue. Such structures are usually very versatile so that classic methods like X-ray or NMR sometimes fail to determine even strands direction[1]. Circular dichroism (CD) spectroscopy is rapid and simple method which is commonly used to describe topological features of quadruplexes[2]. Nevertheless the origin of quadruplex CD spectra still remains unclear. Some efforts have recently been done to address this issue but there are many things yet to be clarified[3].

In this work we use recent state-of-the-art quantum chemistry techniques to provide detailed description of G-quadruplex CD. Our calculations reproduce the most prominent features of experimental spectra at 260 and 290 nm. The strong connection between quartet stacking mode, geometry and a shape of corresponding CD curve is shown. Results of quantum chemical calculations are compared with the classical dipole-dipole interpretation of CD spectra.

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