

**Chirogenesis in Zinc porphyrins : theoretical evaluation of electronic transitions, controlling structural factors and axial ligation**

**Osadchuk, Irina; Aav, Riina; Borovkov, Victor**; Clot, Eric ChemPhysChem 2021 / p. 1817–1833 : ill

<https://doi.org/10.1002/cphc.202100345> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

**Controlling chirogenic effects in porphyrin based supramolecular systems: theoretical analysis versus experimental observations**

**Osadchuk, Irina; Luts, Hanna-Eliisa; Zahharova, Aleksandra; Tamm, Toomas; Borovkov, Victor** ChemPhysChem 2024 / art.

e202400104 <https://doi.org/10.1002/cphc.202400104>

**Shortfall of B3LYP in reproducing NMR JCH couplings in some isomeric epoxy structures with strong stereoelectronic effects : a benchmark study on DFT functionals**

**Adamson, Jasper**; Nazarski, Ryszard B.; Jarvet, Jüri; Pehk, Tõnis; **Aav, Riina** ChemPhysChem 2018 / p. 631-642 : ill

<https://doi.org/10.1002/cphc.201701125> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)