

A total conformational analysis of diastereomeric esters and calculation of their conformational shielding models
Tamp, Sven; Danilas, Kady; Kreen, Malle; Vares, Lauri; Kiirend, Ene; Vija, Sirje; Pehk, Tõnis; Parve, Omar; Metsala, Andrus
Journal of molecular structure : THEOCHEM 2008 / 1/3, p. 84-91 : ill
https://www.researchgate.net/publication/244272489_A_total_conformational_analysis_of_diastereomeric_esters_and_calculation_of_their_conformational_shielding_models

An assessment of alternative low level calculation methods for the initial selection of conformers of diastereomeric esters
Metsala, Andrus; Tamp, Sven; Danilas, Kady; Lille, Ülo; Villo, Ly; Vija, Sirje; Pehk, Tõnis; Parve, Omar Journal of theoretical chemistry 2014 / p. 1-10 : ill

Conformity analysis with structured query language

Liv, Innar; Kuusik, Rein, inform.; Võhandu, Leo 6th WSEAS International Conference on Artificial Intelligence, Knowledge Engineering and Data Bases : Corfu Island, Greece, February 16-19, 2007 2007 / p. 187-189
https://www.academia.edu/3807457/Conformity_analysis_with_structured_query_language

Improved efficiency of focal point conformational analysis with truncated correlation consistent basis sets

Kahn, Kalju; Kahn, Iiris Journal of computational chemistry 2008 / 6, p. 900-911 <https://onlinelibrary.wiley.com/doi/abs/10.1002/jcc.20848>

Quantum chemical evaluation of the yield of hydroxybenzophenones in the Fries rearrangement of hydroxyphenyl benzoates

Metsala, Andrus; Usin, Eve; Vallikivi, Imre; Villo, Ly; Pehk, Tõnis; Parve, Omar Journal of molecular structure : THEOCHEM 2004 / p. 215-221 : ill <https://www.sciencedirect.com/science/article/pii/S016612800400750X>

Reaction path scans : Aza-Michael reactions of isatin imines

Metsala, Andrus; Žari, Sergei; Kanger, Tõnis Computational and theoretical chemistry 2017 / p. 30-40 : ill
<https://doi.org/10.1016/j.comptc.2017.07.014> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

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](#)

Supramolecular chirogenesis in a sterically hindered porphyrin: a critical theoretical analysis

Osadchuk, Irina; Luts, Hanna-Eliisa; Norvaiša, Karolis; Borovkov, Victor; Senge, Mathias O. Chemistry : a European journal 2023 / art. e202302275 <https://doi.org/10.1002/chem.202302275> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)