Supporting Information

Accurate calculation of optically induced birefringences in chiral systems using efficient polarized basis sets

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FIG. 1: CCSD basis set convergence of the medium constants in asymmetric methane. \( \lambda = 632.8 \) nm, \( P = 1 \) atm, and \( T = 273.15 \) K. The wavelength is the same for the pump and the probe beams. Units are \( m^2 V^{-2} \). Symbol aVXZ denotes the aug-cc-pVXZ (X= D, T, Q, 5) series of bases, and daVXZ the d-aug-cc-pVXZ (X= D, T, Q, 5) one.
FIG. 2: DFT/B3LYP basis set convergence of the medium constants in asymmetric methane. $\lambda = 632.8\,\text{nm}$, $P = 1\,\text{atm}$, and $T = 273.15\,\text{K}$. The wavelength is the same for the pump and the probe beams. Units are $m^2 V^{-2}$. Symbol $aVXZ$ denotes the aug-cc-pVXZ ($X = D, T, Q, 5$) series of bases, $daVXZ$ the d-aug-cc-pVXZ ($X = D, T, Q, 5$) one, and "reference" the CCSD/d-aug-cc-pVQZ results.