Computational Studies on Ion Pairing and Hydrogen Bonding

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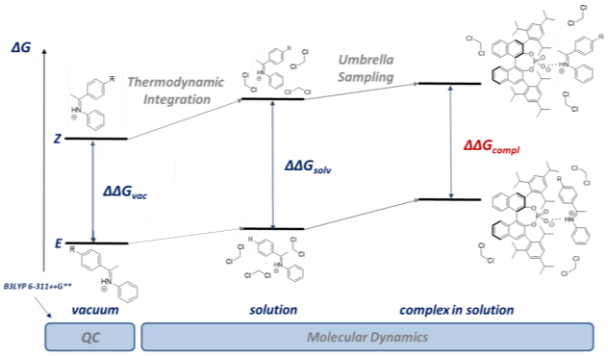

Quantum chemical calculations of the enantioselectivity in the transfer hydrogenation of imines in dichloromethane catalyzed by BINOL phosphoric acids showed poor performance.

Here we present a thermodynamic cycle that predicts the enantioselectivity using a combination of quantum chemistry and QUBEKit (Quantum mechanical Bespoke Kit) force field molecular dynamics simulations. [1] This combined QC/MD approach results in better agreement with experimental data for two selected imines. Details of the force field development are presented.

[1] J. T. Horton, A. Allen, L. S. Dodda, D. J. Cole, *J. Chem. Inf. Model.*, **2019**, *59*, 1366-1381.