# TRANSITION-METAL CONFORMERS IN IMPLICIT AND EXPLICIT SOLVENT

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The development of highly efficient catalysts depends on a comprehensive understanding of their properties. The emergence of flexible catalytic systems poses a number of new challenges in this context. To unlock the reaction mechanisms of such catalysts, a systematic and automatic exploration of the potential energy surface is essential to identify relevant conformations.
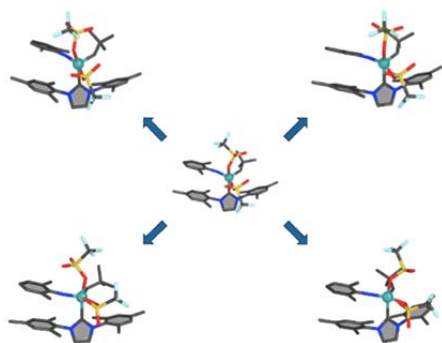
In this study, we focus on Mo-imido alkylidene-N-heterocyclic carbene catalysts for olefin metathesis, utilizing them as an illustrative example to develop and showcase our workflow for systematic conformational analysis. Our workflow commences with an initial sampling phase, encompassing both implicit and explicit solvent scenarios, for the purpose of conformer generation. In the implicit solvent, we employ the CREST tool, [1] while in an explicit solvent environment, we resort to classical molecular dynamics (cMD) simulations implemented in our PyConSolv tool. [2] This dual approach is designed to compare the performance of conformer generation between the two methodologies.

As the methods generate a vast amount of conformations, reduction of the structural ensemble is crucial. To this end, we evaluate different clustering algorithms, such as kmeans, dbscan and hierarchical, as well as alignments for their performance and sensitivity. Our searches identified conformers that were lower in energy than those found by chemical intuition and our results highlights the profound impact of alignment and clustering methods on structural representation.

[1] Pracht, Philipp and Bohle, Fabian and Grimme, Stefan "Automated exploration of the low-energy chemical space with fast quantum chemical methods", Phys. Chem. Chem. Phys., 22 (2020), 7169-7192. DOI: 10.1039/C9CP06869D.

[2] R. A. Talmazan and M. Podewitz.* "PyConSolv: A Python Package for Conformer Generation of (Metal-Containing) Systems in Explicit Solvent". Journal of Chemical Information and Modeling. DOI: 10.1021/acs.jcim.3c00798.