Efficient Computational Methods for Transition Metal Complexes: Computational Characterization of a Hydrogen-Bonded Bidentate Catalyst

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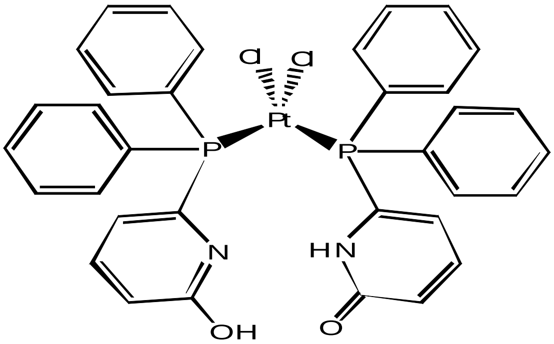
Rapid calculation of the structures and energies of transition metal complexes is desirable for understanding and optimizing catalysts. Here we present results from a molecular mechanics (MM) based strategy for this purpose. The VALBOND force field [1] developed by Landis *et al.* has been implemented into CHARMM and extended into VALBOND-TRANS by adding terms that account for the trans influence of ligands on bond lengths and relative energies.[2] This approach can also be combined with other force field methods developed in our group, for example molecular mechanics with proton transfer (MMPT). [3]



Pt[Cl_2(6-DPPon)$_2$] is among a series of homogeneous catalysts proposed, characterized and tested by Breit *et al.* [4], which constitute the self-assembly of monodentate ligands through hydrogen bonding and provide high activity and regioselectivity in hydroformylation. Here we show that MM force field are suitable for a detailed atomistic characterization of structures and energetics of such complexes. The results demonstrate that force field-based methods are quantitative compared to experimental and other computational methods while they are several orders of magnitudes faster. Nanosecond molecular dynamics (MD) simulations of this Platinum catalyst were carried out in both gas phase and explicit solvation. Infrared, UV/Vis and NMR spectra were computed from MD trajectories and compared with experimental measurement, and the hydrogen bonding situation in the complex is studied. Combining force field methods with *ab initio* calculations and experimental data, modes of action of cis-Pt[Cl_2(6-DPPon)$_2$] can be characterized in atomistic detail. [5, 6]

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[6] J. Huang, U. Gellrich, W. Seiche, B. Breit, M. Meuwly, *in prepration.*