

INFLUENCE OF THE COUNTER ANION IN ORGANOMETALLIC CHEMISTRY FROM A THEORETICAL PERSPECTIVE.

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Many catalytic systems in organometallic chemistry are cationic species and, most of the time, the nature of the counter anion and its potential influence on the structure and/or reactivity of the catalyst are not considered with great caution. However NOE and PGSE NMR experiments have now developed to a point where it is possible not only to quantify the state of aggregation of charged species in solution (ion pairs, quadrupole), but also to specify the relative geometry of the anion and the cation in the ion pair (or quadrupole). When coupled with calculations (DFT or ONIOM), this allows a deeper understanding of the various interactions responsible for the aggregation, in particular when several geometries for the ion pairs are competitive. Moreover, in some cases, it has been shown that the nature of the counter anion dramatically influences the outcome of the reaction. DFT calculations have allowed to show that the nature of the product is dependent upon the role (spectator or actor) played by the counter anion in the transformation.