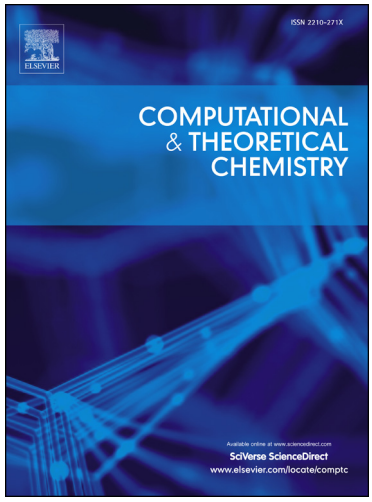

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The polarizability of organometallic bonds

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Abstract

The distributed atomic polarizabilities enable the investigation of the coordination of organic ligands to transition metals giving new insight of some organometallic complexes used in catalytic processes. This approach is useful to appreciate the enormous changes occurring upon complexation to a metal, which is mainly responsible for the augmented reactivity of these species. The method we have developed allows calculating the polarizability of an atom in a molecule upon a partitioning of the electron density, for example using the Quantum Theory of Atoms in Molecules. The polarizabilities result from numerical differentiation of the atomic dipole moments with respect to the electric field. From the polarizability tensors, other useful quantities derive, for example a mathematically precise definition of *bond polarizability*. In terms of chemical reactivity, the distributed polarizabilities are complementary to the traditional analysis of the electrostatic potential, which informs only on susceptibility towards *hard*, charge-controlled chemical reactions. On the contrary, atomic polarizabilities enable addressing the sites more keen on *soft*, orbital-controlled reactions.

Keywords: Electron Density; Polarizabilities; Organometallic Chemistry; Atoms in Molecules

Graphical abstract