

## UniSysCat Colloquium

Prof. Dr. Odile Eisenstein

ICGM - Institut Charles Gerhardt Montpellier

Start Time: Wednesday, October 16, 2019 05:45 pm

End Time: Wednesday, October 16, 2019 07:15 pm

Room BEL 301

Technische Universität Berlin, Villa Bell, Marchstraße 6, 10587 Berlin

### The $^{13}\text{C}$ solid state NMR signature of metal-bonded carbon: An information for bonding and reactivity

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Metal-bonded carbon atoms in metal-alkyl, metal-carbene/alkylidene and metal-carbyne/alkylidyne species show significantly more deshielded isotropic chemical shifts than their organic counterparts (alkanes, alkenes and alkynes). While isotropic chemical shift is universally used to characterize a chemical compound in solution, it is an average value of the three principal components of the chemical shift tensor ( $d_{11} > d_{22} > d_{33}$ ). The tensor components, which are accessible by solid-state NMR spectroscopy, can provide detailed information about the electronic structure (frontier molecular orbitals) of the observed nuclei. This information can be accessed in detail by quantum chemical calculations, most notably by an analysis of the paramagnetic term of the NMR shielding tensor. Analysis of this term shows that deshielding in specific directions can be directly related to the nature of the metal-carbon bond and in many cases to the presence of metal-carbon p character. Since reactivity is also determined by the nature of the bonding framework, NMR can be reporter of reactivity patter.

The consequence of these finding in several organometallic systems and reactions will be presented

Prof. Dr. Martin Kaupp (TU Berlin)

Organizer

