Information on reactivity from NMR? An approach combining solid state NMR and quantum calculations.

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NMR is without any doubt one of the most versatile methods for characterisation of chemical species. It is used widely in all domains of chemistry and biology. Among various recent improvements, it has gained considerable sensitivity due to the implementation of the dynamic nuclear polarization (DNP) and can be used to inform on details of structures. In the presented lecture, it will be shown that the chemical origin of the 3-dimensional property of the chemical shift (chemical shift tensor) can be easily understood and can inform on reactivity. For this purpose, one combines experimental determination of the chemical shift tensors by solid state NMR with quantum calculations of the same quantities. These calculations reveal that regions of shielding and deshielding around an atom can be very predicted from the localisation and energy pattern of the frontier orbitals at the active atoms. In particular, low-lying orbitals are indicative of regions of deshielding in specific directions, hence the link with reactivity. Thus, combining the information derived from solid state NMR with simple molecular orbitals analysis it is possible to understand specific reactions associated with transition metal complexes. Several examples will be presented.[1-4]

References
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