NMR CHEMICAL SHIFTS BEYOND NUMBERS: UNDERSTANDING ELECTRONIC STRUCTURE AND COORDINATION ENVIRONMENTS

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Chemical shift has been successfully used since the beginning of NMR to identify the signature of molecules (and materials) making NMR an invaluable tool of characterizations. Because of its power to elucidate molecular structure, NMR interpretation is taught at early stage, often in laboratory courses, even before one understand the fundamentals of spectroscopy and their selection rules. All chemistry students remember solving organic and inorganic puzzles based on 1D and 2D NMR spectra during our undergraduate (and graduate…) times,[1] while physics students remember the Block equation

This lecture will concentrate on developing a detailed understanding of the origin of NMR chemical shift, and how it can be used to reconstruct the electronic structure of molecules and materials. This lecture will also aim to show that the angular momentum operator has an "ideal" symmetry, that makes NMR a privilege spectroscopic descriptor of structure and reactivity.[2]

1) Spectral identification of organic compounds, Eds. Silverstein, Webster and Kiemle, Wiley&Sons, **2005**.

2) a) Metal Olefin Complexes: Revisiting the Dewar-Chatt-Duncanson Model and Deriving Reactivity Patterns from Carbon-13 NMR Chemical Shift. C. P. Gordon, R. A. Andersen, C. Copéret *Helvetica Chim Acta* **2019**, *102*, e1900151. b) Carbon-13 NMR Chemical Shift: A Descriptor for Electronic Structure and Reactivity of Organometallic Compounds C.P. Gordon, C. Raynaud, R.A. Andersen, C. Copéret, O. Eisenstein, *Acc. Chem. Res.* **2019**, *52*, 2278-2289. c) Nuclear Magnetic Resonance: A Spectroscopic Probe to Understand the Electronic Structure and Reactivity of Molecules and Materials. C. P. Gordon, L. Lätsch, C. Copéret *J. Phys. Chem. Lett.* **2021**, *12*, 2072-2085.