

Deuterium Isotope Effects in ^{13}C NMR Spectra of Mono- and Binuclear Aromatic Compounds

Vilko Smrečki,^{a,*} Predrag Novak,^b Dražen Vikić-Topić,^a and Zlatko Meić^{b,†}

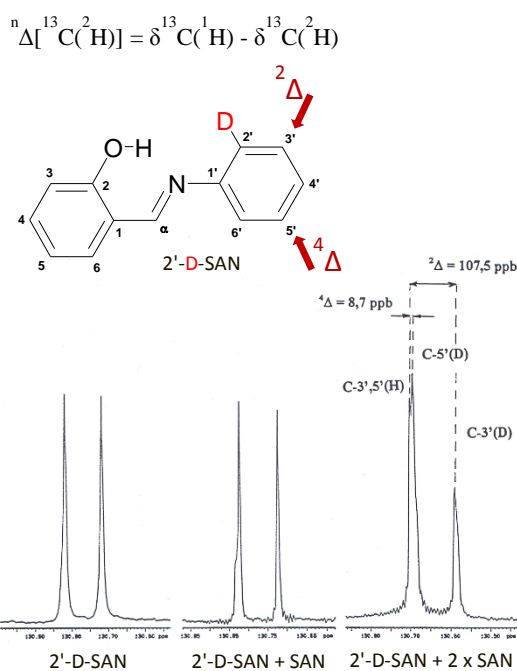
^a NMR Centre, Ruđer Bošković Institute, Bijenička cesta 54, HR-10000 Zagreb, Croatia

^b Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, HR-10000 Zagreb, Croatia

* smrecki@irb.hr

† dedicated to the Memory of the late Professor Zlatko Meić

Isotopic substitution produces changes in the reactivity of a molecule and causes a redistribution of molecular internal vibrational and rotational energy. In NMR, it causes changes in chemical shifts (nuclear shielding), coupling constants and relaxation times.



The most studied by far are deuterium effects on nuclear shielding owing to the large fractional change in mass on isotopic substitution and relative ease of their determination from high resolution NMR spectra.

The focus of this talk will be put to unsaturated systems containing one or two bridged phenyl groups where isotopic perturbation can be transmitted many bonds away from the isotope substitution site. The sign alternation and specific magnitudes of such long-range isotope effects will be discussed in terms of subtle charge shifts throughout the molecule as a

consequence of bond shortening upon isotopic substitution. Moreover, the linear correlation between long-range isotope effects and molecular torsional angle can serve as a conformational probe [1] for studied type of molecules.

- [1] P. Novak, D. Vikić-Topić, V. Smrečki, and Z. Meić, Isotope Effects in NMR Spectra as a Structural Tool for Organic Molecules, in: Atta-ur-Rahman (Ed.), *New Advances in Analytical Chemistry*, Harwood Academic Publishers, Amsterdam, **2000**, 135-168.