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BIO: Dr. Cláudio F. Tormena is Associate Professor of the Institute of Chemistry at University of Campinas – Campinas - São Paulo - Brazil. He received his PhD (in chemistry) from University of Campinas in 2000, under supervision of Professor Roberto Rittner. Part of his doctoral was developed at the University of Liverpool from 1998 to 1999 under supervision of Professor R. J. Abraham. He was a postdoctoral fellow at the University of Campinas from 2000 to 2003. From 2009 to 2010 during a sabbatical period, Dr. Tormena stayed in the School of Chemistry at the University of Manchester working with Prof. Gareth A. Morris. He has published more than 150 peer-review papers and more than 100 communications in national and international meetings. His research interests are focused on the experimental and theoretical NMR parameters, conformational analysis and Matrix-Assisted DOSY for mixtures analyses and pulse sequence development.

He is a member of Advisory board of Magnetic Resonance in Chemistry and member of São Paulo Academy of Science.

NMR: Beyond Structural Assignment

ABSTRACT: NMR parameters, such as chemical shift and coupling constants, are mainly used for molecular structure assignments. The remarkable potential of nuclear spin-spin coupling constants and chemical shifts as probes for the study of molecular electronic structures is remarkably enhanced if the experimental values are adequately complemented with theoretical analysis. However, obtaining accurate calculations of coupling constants and chemical shifts proved to be a non-trivial task for quantum chemistry. In this talk, the effects of electron-donating (NH₂) and electron-withdrawing (NO₂) groups on ¹³C NMR chemical shifts in substituted benzenes are investigated by molecular orbital analyses, since the π orbitals system do not explain^{i,ii,iii} the substituent effects in the ¹H and ¹³C NMR spectra as conventionally suggested in textbooks. Similarly, the ¹J_{CH} coupling constant in substituted benzaldehydes^{iv} is not governed by π orbitals system. Some unexpected experimental behaviour, such as, higher values for ⁵J_{FH} than for ³J_{FH} in heteroaromatic rings^v and higher ¹³C chemical shifts values for anion in comparison with carbocation will be discussed.^{vi} We intent to highlight during this talk the application of ³J_{CH} coupling for configurational and conformational assignment on trisubstituted double bond derivatives.^{vii}

References:

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