

# Modeling $^{13}\text{C}$ and $^{15}\text{N}$ Chemical Shifts in Crystalline Systems<sup>#</sup>

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<sup>#</sup> This project is partially funded by the NSF International and Chemistry Divisions under grant INT-0071032 and by grants to MBF from University of Buenos Aires (UBACYT-TX063), Agencia nacional de Promoción de Ciencia y Tecnología and CONICET (Argentina).



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# What are Chemical Shifts ?

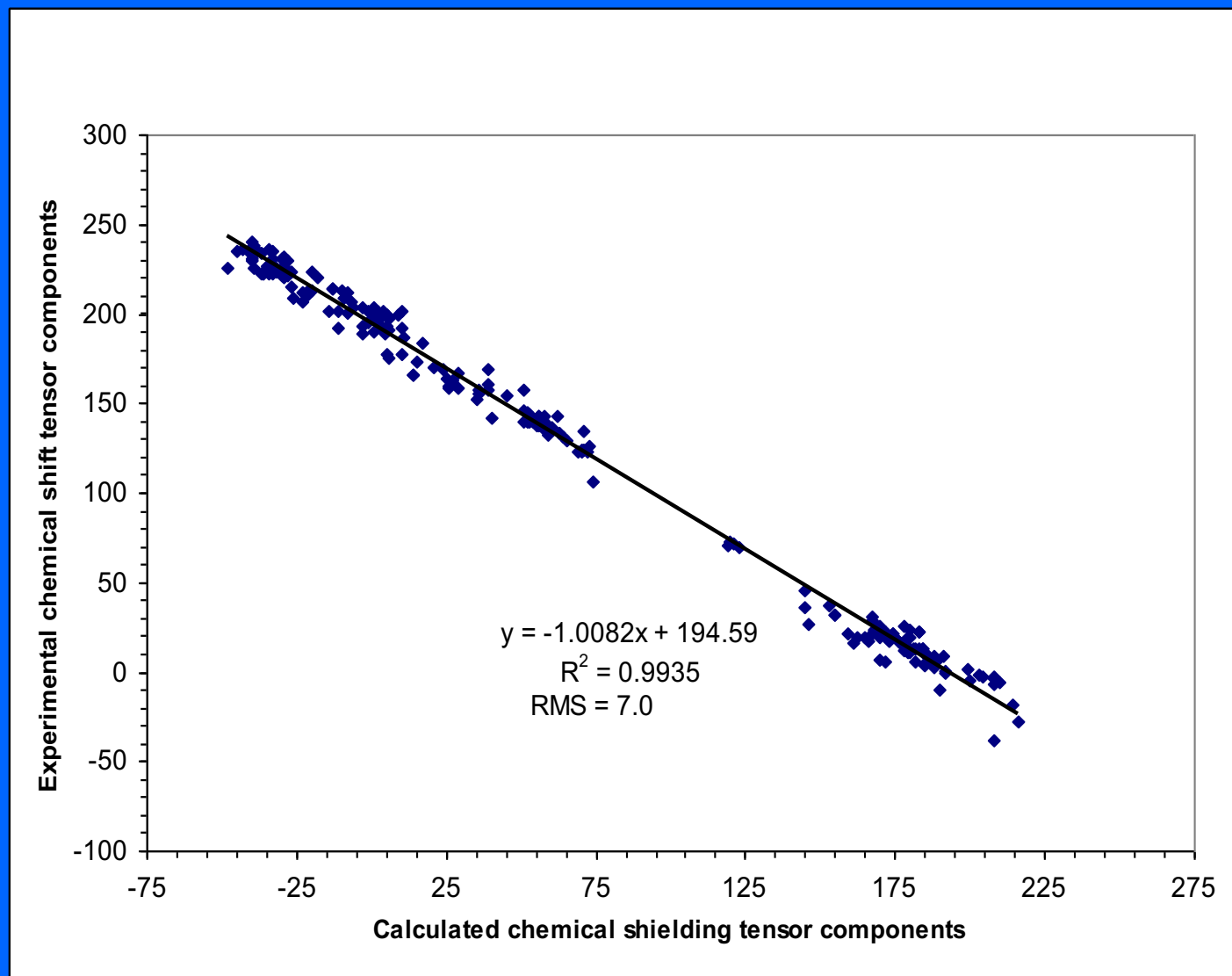
- Are the “shift” of the NMR signal due to the molecular and crystalline environment.
- Tensorial quantity, i.e. the shifts depends on the orientation of the molecule in the magnetic field.



# Why Chemical Shift Calculations are Important ?

- Chemical shifts are highly dependent of Molecular and Crystalline Structure.
- Chemical Shifts Calculations provide the link between “structure” and “measurements”





# Remaining problems

- Intermolecular effects are important
- Calculations are very dependent of the molecular geometry
- Heavy nuclei (relativistic effects)



# N-15 BENZAMIDE SHIFT TENSOR

Effects of Hydrogen Bonding

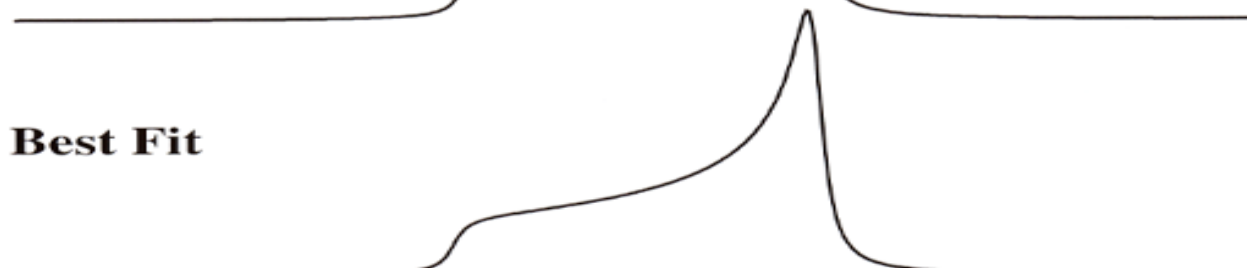
**Theory**  
**No H-Bonding**



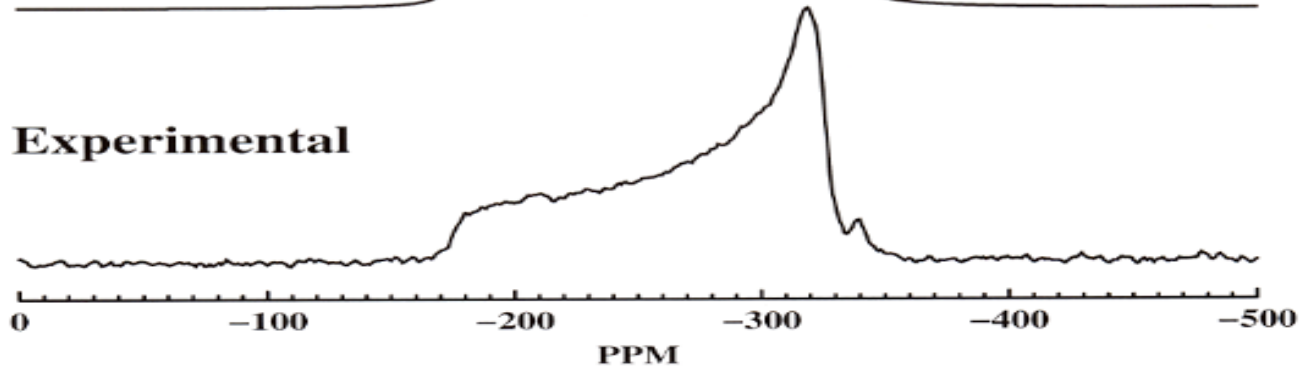
**Theory**  
**H-Bonding**



**Best Fit**



**Experimental**



# Objectives of the Collaboration

- Leverage expertise and resources available in Utah and Buenos Aires
- Develop robust techniques to include intermolecular effects in the calculations
- Apply these techniques to solve structural problems in biologically active compounds from marine invertebrates from the South Atlantic (Dr. Jorge Palermo, Organic Chemistry, FCEyN, Universidad de Buenos Aires)



# Critical Network Needs

- Connectivity from FCEyN to CHPC
  - Remote access to systems (windows)
  - File transfers
  - Distributed processing





# Desirable Network Needs

- 12 type of services from FCEyN to CHPC
  - Teleconferencing,
  - Distributed white boards and
  - Remote instrument operation

