QM Chemical Shift Calculations to infer on the Long-range Aromatic Ring Current-induced Field Contributions

S.Aravamudhan, Department of Chemistry, North Eastern Hill University,
Shillong 793022 Meghalaya, India.
saravamudhan@hotmail.com

The Quantum Mechanical NMR chemical shift calculations are usually carried out for the NMR parameter at intra molecular proton sites. The nature of the shielding includes the induced secondary fields arising due to electron circulation changes, and such fields arising from aromatic ring currents can be much larger and can probably be present at regions outside the specific molecular dimensions. The usual way these values are obtained is by the proton coordinates specified and most of the time the specified protons are present within the molecule.

For the sake of specifying a coordinate for extraneous (outside the molecule in the proximity) sites, it is possible to include a molecule (a sensor - well optimized independently for energetically stable geometry) at any specified distance from the Aromatic compound and *without subjecting this combination of molecules to any Geometry Optimization (for energetic structural stability),* the combination of molecules can be submitted for a chemical shift calculation.

The distance of the second molecule can be varied from the first aromatic compound, and the calculation made as a function of distance and also relative angular disposition. From the criterion of classical magnetic dipoles it should also be possible to estimate the induced field (chemical shift values) at the neighboring sensor molecule which may give rise to queries which can be discussed from the quantum mechanical formalisms point of view. Such a case study would be reported and consequences discussed.

Such considerations may have bearing on the interpretations of experimentally determined shielding tensor values by High Resolution PMR studies on Single Crystal Specimen of Aromatic Molecules and for the interpretation of ring current shifts observable in Biological Macromolecules, in particular the 3D structure determination by NMR.

Abstract Presentation: 17th CRSI National Symposium in Chemistry, February 06-08, 2015
crsi2015@ncl.res.in
Add to contacts
21-11-2014

To: saravamudhan@hotmail.com

Dear **Dr. ARAVAMUDHAN, Sankarampadi**,

Greetings from CSIR- National Chemical Laboratory, Pune.

Thank you for submitting an abstract for the **17th CRSI National Symposium in Chemistry**, which will be held during **February 06-08, 2015** at **CSIR-NCL, Pune**.

We have great pleasure in informing you that your contribution entitled QM Chemical Shift Calculations to infer on the Long-range Aromatic Ring Current-induced Field Contributions has been accepted for an **POSTER** presentation. You are requested to go through the details of the presentation guidelines given on the website.

Abstract Title: QM Chemical Shift Calculations to infer on the Long-range Aromatic Ring Current-induced Field Contributions
Presenting Author: Dr. ARAVAMUDHAN, Sankarampadi
Presentation Type: POSTER
Click to view the website.

If you need any further information, please contact us at **crsi2015@ncl.res.in** .

Regards,

Gopinath,Dr.C.S.,
Organizing Secretary/ Convener,
17th CRSI National Symposium in Chemistry,
February 06-08, 2015,
CSIR- National Chemical Laboratory,
Dr. Homi Bhabha Road,
Pune- 411008, India.