Simulated and experimental NMR – a powerful tool to explore yet unknown structures

Thomas Heine

School of Engineering and Science, Jacobs University Bremen, 28759 Bremen, Germany, E-Mail: t.heine@jacobs-university.de

NMR is a powerful tool to characterise molecules and solids, as it allows the meaningful analysis of the chemical interactions of the investigated nuclei – in particular if the shielding tensor is available. Further, the combination of experimental and theoretical NMR techniques may allow the identification of small quantities of material, in quantities which are insufficient for an X-ray diffraction measurement. My presentation will be focused on the following subjects:

1. Density-Functional Theory and NMR – how theory differs from experiment
2. The induced magnetic field as tool of analysis for the stability of planar molecules
3. The importance of intermolecular contributions to $^1$H NMR chemical shieldings
4. Application to fluxional systems – $^{13}$C NMR in fullerene derivatives
5. Transition NMR on polyoxometalates

Related references: