SHEET-04

Visualizing a Cycloaddition by the Abinitio SCF Methods; a Case Study of Finding Rationale of a Fictitious "Spin bookkeeping" Structure to Simulate NMR spectra.

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As described in the introductory material in document of this author (1), the rationalization of "average structures" which results in experimental NMR spectra -with the theoretically possible "averagable structures", has been not straightforward in particular with biological macromolecules. The organic molecular polymers are included among the category of macromolecules whose structures have been characterized by NMR spectroscopy by Heatley and Bovey (2). Among these, the specific instance of Polystyrene stands out as a typical case where the backbone proton NMR spectrum of isotactic polystyrene lends itself for an exact simulation but only by invoking a cyclic (dimeric-) structure presenting 6 spin system, that structure which is stated not to be taken too literally.

Such a fictitious structure makes possibile the inclusion of certain spin-spin coupling constants for simulation which, otherwise, is not simple enough to infer. Obviously these Spin-Spin interactions occur by mechanisms transmitted through bonds, and it is surprising that a structure which is "fictitious", can be revealing such through-bond routes by which the exact simulation of the observed NMR spectra. Hence, it was considered worth the while, trying to find out the possibility of the stability criterion for a dimeric Styrene with the possible QM methods by Geometry Optimization and verify with the calculation of the chemical shifts for such a dimer. A thorough literature survey of the possibility for the occurrence of such dimeric structure of styrene molecule was not be undertaken lest those conditions may build up a bias, for an "Only Theoretical Model" by Abinitio Calculations.

There have been reports earlier on Biological molecules extensively using merely the SCF method with STO 3G basis sets, calculating mainly using the Specifically varied fixed geometries, inferring on the environments in biological systems; and, no detailed potential energy surfaces were profiled. Only limited structures and resulting plots were seemed to enable quite a lot to infer. Hence, a similar approach using the Abinitio SCF method with the STO 3G basis set at the working online-demo version of the http://www.webmo.net certain convincing trends arrived at. The progress of such Optimization calculations could be conveniently downloaded and archived at anyone's personal internet domain as displayable material, which can be downloaded at any convenient terminal for a review. This case study and its convenience would be reported (3) along with the simulated Spectra and Optimized Geometries.

(1)http://www.ugc-inno-nehu.com/WMBS/0_Introduction/WMBS_Context_myIBSpresentations.pdf
(2) F.Heatleyand F.A.Bovey, Macromolecules, Vol.1, page 301 (1968). Reference #7 on page 129, Section IV, in the Book "High Resolution NMR of Macromolecules" by Frank A. Bovey, Academic Press, NY,London (1972).
(3) Webpage under construction: http://www.ugc-inno-nehu.com/crsi_nsc14.html