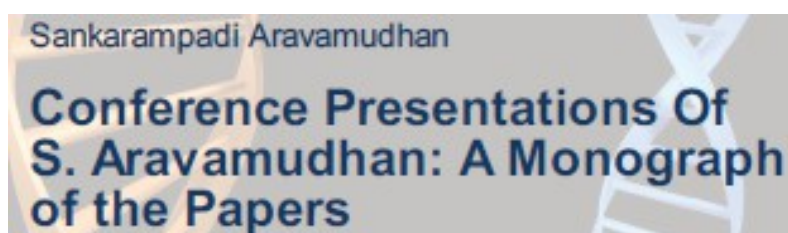


Excerpt from:

<http://www.ugc-inno-nehu.com/book-projs/03-1-book-sp-proj-2.pdf>
<http://www.ugc-inno-nehu.com/scope.html#books>

05-2013-ICETC2013

Importance of Small-molecule Computational Chemistry; Related to Macromolecular Computations



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have an authenticity that the path during these efficient mathematical procedures consists of chemically realizable intermediate structures. *“Indeed, it is tempting to take Variation Principle quite literally and then imagine that the variations are actually taking place. In that case at each moment or at each point, the system, whatever it is, is sampling all sorts of possible behavior, with the actual behavior then being selected on the basis that it will make the least change in something, that is, it will make some quantity stationary”*(13).

The above considerations would be dealt with as much as possible with the examples of computational results and the chemical intuitions. It is intended to highlight how these considerations

Follow up materials; occasion of FAMA-2018

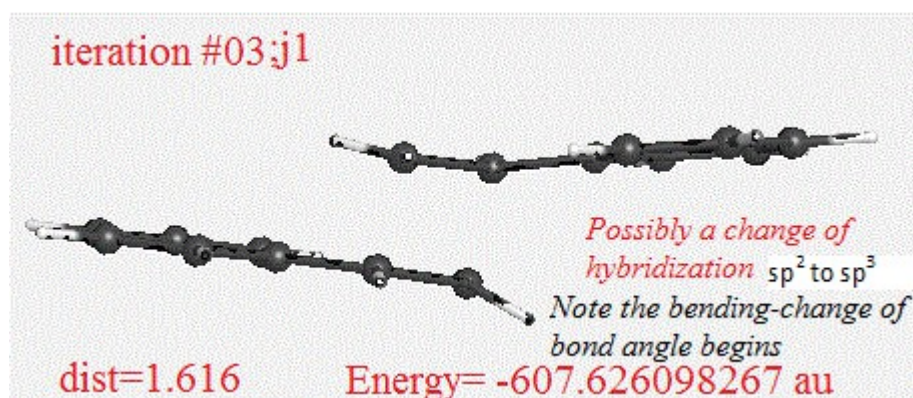
GIF Movie embedded show at <http://www.ugc-inno-nehu.com/events.html#bhc>

<http://saravamudhan.tripod.com/Animationwizard-60frames-20minutes.gif>

Contents of the third frame displayed in the above gif movie link

The contents of this animated GIF image set, is the results of QM calculation at the website <http://www.webmo.net> ; each job is a one minute job from which the structure images are obtained at the structure-editor at the website. SCF-minimal 3G basis set calculations are from the remote server by submission of guess structures at the portal displayed in desktop/laptop PC unit.

Below is the content of the 21st Frame displayed in the above gif movie link



The structures as above as one of the iterative sequence result indicates how to relate the energy criterion Produces a change in small variation in structure that appeals to chemists grasp of bond formation in terms of directed valence. Such inferences compiled should in turn the interpretations in terms of energy minimization towards the reaction conditions for a product from reactants.

<http://ugc-inno-nehu.com/IACS2015-ppt/IACS-2015.ppt>

<http://www.ugc-inno-nehu.com/IACS2015-jmiUni.jpg>

SCHEME FOR THE CONTENTS OF NEXT 9 SLIDES : Slide #2 to #9

