INTRODUCTION:

The following two WebPages consist of my poster contents for IBS2006 and IBS 2007 where in I have tried to illustrate the kind of averaging techniques useful for averaging the chemical shift values corresponding to the confirmation changes during a fluctuation of a given MEAN CONFIRMATION.

"http://aravamudhan-s.ucoz.com/inboxnehu_sa/IBS2006/ForIbs2006.html"

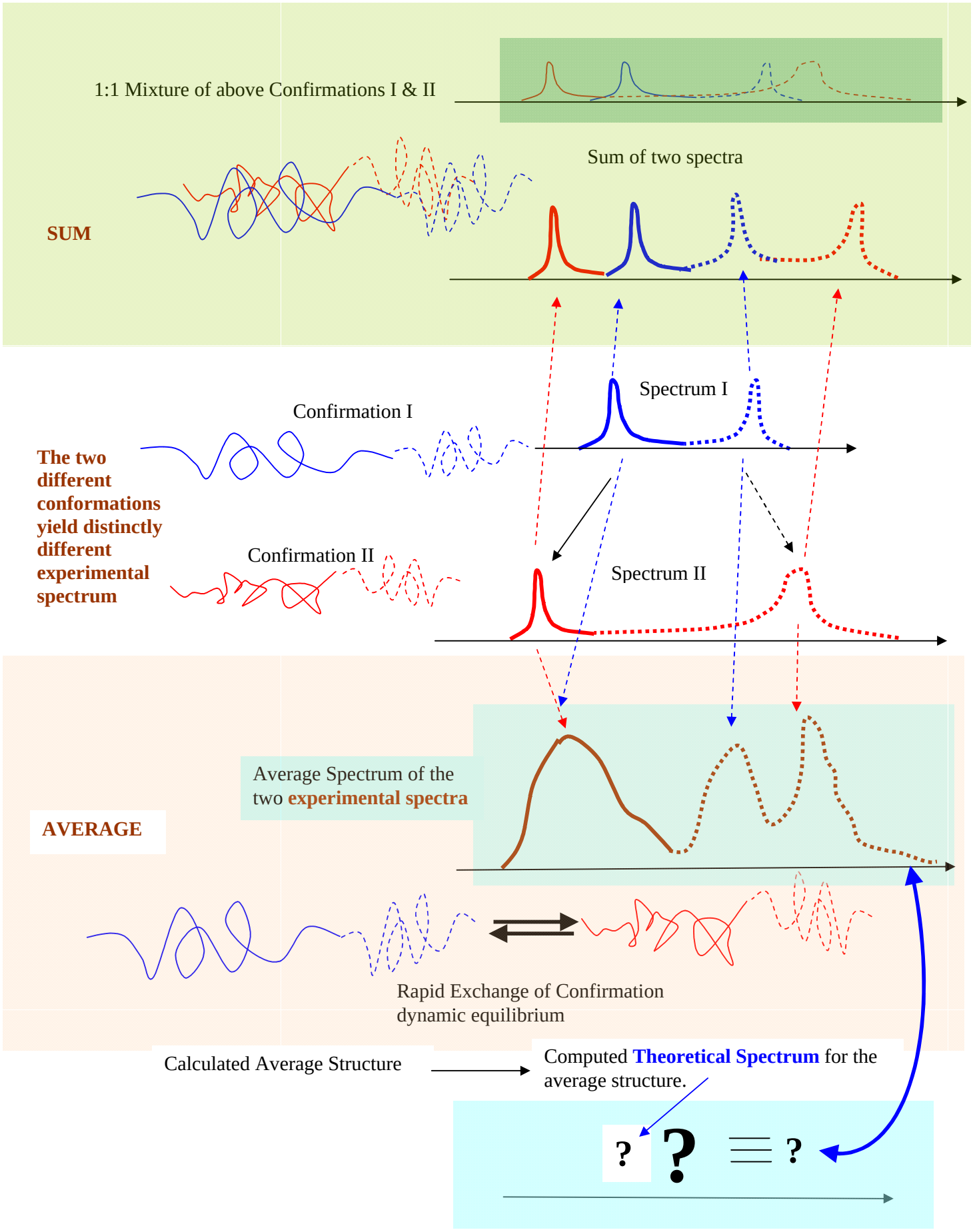
"http://aravamudhan-s.ucoz.com/Posters_nsc9_nmrs2007_ibs2007.html#IBS2007"

As per what is now known, the advantages of the NMR technique in comparison with Xray technique are that the solution structures can be determined by NMR. However, it is also necessary to consider the determination of the Macromolecular structure in Solution by NMR methods entails obtaining the several contributing structures for a given Biological macromolecule while the x-Ray method would be resulting in a single conformation as the structural investigation.

If a given solution structure obtained by NMR is a superposition of several structures, then each contributing structure must be recognized as a MEAN structure exhibiting fluctuations from the mean thus each of the contributing structure must be subjected to fluctuation characteristics while processing.

Thus when a molecule is having several confirmations in equilibrium, arriving at the effective structure accounting for the experimental NMR features would depend upon the appropriate characteristic times, and it may either require summing the experimental spectra or averaging the chemical shift values and then contructing a single spectrum corresponding to the experimental spectrum.

This situations is illustrated in the next SHEET.


1:1 Mixture of above Confirmations I & II
Sum of two spectra
SUM
Spectrum I
Confirmation I
The two different conformations yield distinctly different experimental spectrum
Confirmation II
Spectrum II
Average Spectrum of the two experimental spectra
AVERAGE
Rapid Exchange of Confirmation dynamic equilibrium
Calculated Average Structure
Computed Theoretical Spectrum for the average structure.
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