Energetically non interacting system of molecules can display the Ring current effects manifesting in Chemical shifts. Such exclusive manifestations of Ring current effect must be resulting in comparable values for ring current shifts by QM calculations and Classical Dipole model indicating that in the limit of no energetically significant perturbations the QM chemical shift values are derivable by equations based on classical dipole model.

Sheet No.	Description of contents of the display sheet
1	**INTRODUCTION & INDEX to contents**
2	Independently optimized BENZENE and METHANE molecules drawn in structure editor & job submitted for QM Chemical shift calculation without any G.O. of combined system. Also depicting the system of BENZENE and HYDROGEN molecules
3	The Results of QM calculations as a function of distance (in the range 14 to 2 Angstrom) between the molecules are displayed (for a given relative orientation / paramagnetic shielding) in Sheets 3 & 4 for Benzene-Methane. The distance between molecules in this sheet range from 13.4 to 5.3 Angstroms. The benzene NMR consists of single line at the (nearly) same position in this range while the Methane PMR spectrum shows variations accounting for the difference in the 4 protons. Thus the benzene protons are not perturbed significantly over this range of distance while the methane protons show differences in Chemical shift. The interaction energy calculated by single point energy calculation is not significant (see inset graphical representation of energy difference vs. distance). Thus the differences in proton chemical shifts of methane must be due to the secondary fields arising by aromatic ring current contribution and not by perturbations that are energetically significant. http://nehuacin.tripod.com/1-crsi2015-1.jpg
4	The QM calculations as described in Sheet 3 continued (range of distance from 4.3 to 2.6). When the distance of separation is about 3 Angstroms the energy of interaction is significant and the benzene proton show differences in line position. Even at a distance of 3.8 Angstroms the interaction energy is of the order of 1 Kcals /mole and the perturbation on benzene protons is discernible. The methane proton differences are obvious and both the energetic perturbation and the ring current effect must be contributing to observe Chemical shifts in the range of distances. http://nehuacin.tripod.com/1-crsi2015-1.jpg
5	Similar distance dependence for comparable range when the Methane molecule is at a point along the symmetry axis of benzene molecule. The non interacting energy (sum of the separately calculated optimized energy for the two molecules) and the energy of the combined system subjected to single point energy calculation are given. In sheet-5 there is no significant difference in the Benzene PMR line. http://nehuacin.tripod.com/1-crsi2015-2.jpg
6	The trend as in sheet -5 for the distance range 4.3 to 2.6 Angstrom containing the single line benzene PMR and obvious variation in Methane PMR lines. Inference can be as per the logistics for the contents of sheets 3 &4. http://nehuacin.tripod.com/1-crsi2015-2.jpg
7	The contents of this sheet are for such distance between Benzene – Methane (and the Benzene-Hydrogen system) when the energetic perturbations are minimal and the aromatic ring current effect on the Methane PMR is evident. At this distance, the angular dependence (for the orientation of Methane molecule with respect to the benzene symmetry axis) is displayed in several perspectives for the possibility of finding situations when QM results for Chemical shift variations can be comparable to the values obtained by calculations on the basis of classical Magnetic Dipole Model. http://nehuacin.tripod.com/crsi15/
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12	Intermolecular distance dependence of Benzene- Methane and Benzene-Hydrogen systems by QM calculation and by Classical dipole model; Comparison seems to substantiate the inferences of the aromatic ring current effect, convincing that when only secondary field effect is significant QM and classical-model calculation are equivalent and the QM results must in such limit must tend to point out the validity of classical model. (Ref. Mc Connel’s derivation from Ramsey’s equation) http://nehuacin.tripod.com/1-crsi2015-8.jpg