

All the QM Calculations were carried out at <http://www.webmo.net> as 1 min jobs
 "Gaussian" / HF - SCF - STO3G

For Classical Dipole model Calculations the descriptions at http://www.ugc-inno-nehu.com/repository/FP/2006_IBS2006_FP_p1to16.pdf
 contain Procedure and Parameters for Susceptibility Anisotropy of Benzene ring

<http://nehuacin.tripod.com/1-crsi2015-8.jpg>

Quantum Mechanical Abinitio Calculation of Chemical Shift for Optimized Hydrogen Molecule Placed at varying distances in the range 5 Angstrom to 12 Angstrom Units from Benzene ring. At such a distances the two independently optimized molecules 1. Benzene 2. Hydrogen Molecule do not seem to indicate any specific interaction, only the secondary field is significant even at such distance. See the relative dispositions in Fig below

At hydrogen 15 (25 Angstroms away from center), no significant change with distance and the shielding is the same as it would be for an isolated hydrogen molecule in the absence of benzene.

LEFT Column: QM results
 13 & 14 Protons of Hydrogen Molecule along the C6 Symmetry axis
 16 & 17 perpendicular to symmetry axis in molecular plane

Since it is merely a secondary field without any specific orbital interactions (for energy considerations), these QM results must be the same as the Classical dipole model where the Magnetic dipole is placed at the ring center of optimized benzene.

Results of the Two methods seem to compare well to be able to use the results of calssical model confidently with the QM results as a transferable quantity

RIGHT Column: Classical Dipole model

This classical equation was used for calculating secondary field at one point corresponding to the distance on the x-axis. Hence only one point is plotted for each of diamagnetic and diamagnetic locations

