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Shielding by Ring Current Effect Contributions Isotropic Shielding Values by the Traditional Equations and from the Full Tensor Calculations

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The efforts to find the advantages- which might be added when full shielding tensor calculations are obtained, while trying to interpret the Biomolecular Structures on the basis of the ring current effects- have been leading to the necessity to obtain the isotropic values of the shielding by calculating the trace of the Full Shielding Tensor calculated from an equation based on the magnetic dipole model1. The contents of the Webpage http://geocities.com/inboxnehu_sa/NSCMB2004.html would indicate that a preliminary effort could lead to the conclusion that the comparison of values of isotropic shielding by this approach and the values listed earlier based on the traditional equations for the isotropic shielding parameter has been encouraging. A more detailed effort to use the magnetic dipole model and calculate the Shielding Tensor as a function of the distances around the aromatic ring would be reported in this contributions with the highlights on the additional advantages of such effort.

Reference:

http://saravamudhan.tripod.com/
http://geocities.com/amudhan20012000/Confview_link.html