INTERACTIONS BETWEEN RELATIVISTIC QUANTUM CHEMISTS AND NMR EXPERIMENTALISTS: SOME RESULTS

W.A. DE JONG, Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Mail Stop K1-83, P.O. Box 999, Richland, WA 99352.

The electric field gradients of uranyl, at the uranium nucleus and oxygen nuclei, in carbonate complexes have been calculated. The calculated results are used to estimate the T_1 spin-lattice relaxation times and first-order nuclear spin transition energies in uranium and oxygen nuclei. These parameters are then used as a guideline for possible NMR experiments on uranyl compounds. Future plans for calculations of NMR properties and further interaction between theory and experiment will be discussed.