Department of Mathematical Sciences Colloquium

MARION LAWRENCE ELLZEY, JR.

Department of Chemistry, UTEP

Molecular Structure, Molecular Symmetry and Groups

Our research has been in the application of the theory of group representations to quantum mechanical studies on molecules. We have published papers on symmetry adaptation of bases of the Hilbert space to relevant groups and on the application of irreducible tensorial operators to the parameterization of the matrix representation of the Schrödinger equation. Computational techniques for applying group theory to large molecules have been developed, including symmetry-generation and symmetry-averaging. Of particular interest has been the symmetry of the icosahedral point group, the symmetry of the C_{60} buckminsterfullerene molecule and an approximate symmetry for a number of enzymes and viruses. We have also developed an axis-angle formulation of the irreducible rotation matrices $D^{(l)}$ which is computationally more efficient than the traditional Euler angle formulation $D(\alpha, \beta, \gamma)^{(l)}$.

Friday, November 2, 2007 at 3 pm in Bell Hall 143
The University of Texas at El Paso

Refreshments will be served in front of the colloquium room, 15 minutes before the start of the colloquium.

For further information, please contact Dr. Pavel Solin, Bell Hall 220. Phone: (915) 747-6770, email: `solin@utep.edu`.