Integration of Graph Theory and Quantum Chemistry

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The objective of this talk is to present an integrated approach to graph theory and quantum chemistry. Indeed this cross-fertilization is quite natural in that concepts in both areas are intertwined. We will present several examples of this unification which lead to not only significant new insight into both areas but also important results which can be derived elegantly by this cross-fertilization. Several computational schemes for computation and characterization of structures and their properties will be presented. Several applications to structures and their properties and to spectroscopy will be considered including Inverse-Euclidian geometry for NMR spectroscopic applications. Applications to structure-activity, NMR spectroscopy, quantum chemistry, fullerenes, etc., will be considered.