Quasi-Symmetry of Potential Energy Surfaces as Symmetry-Breaking of Energy Component Surfaces

Paul G. Mezey

Canada Research Chair in Scientific Modeling and Simulation
Department of Chemistry and
Department of Physics and Physical Oceanography
Memorial University of Newfoundland
283 Prince Philip Drive
St. John's, NL, Canada A1B 3X7
tel.: 709 737 8768, fax: 709 737 3702, email: paul.mezey@gmail.com
and
External Faculty
Institute For Advanced Study, Collegium Budapest,
H-1014 Budapest, Szentharomsag u. 2
Hungary

Potential energy hypersurfaces can be represented as sums of energy component hypersurfaces, where the components often show characteristic behavior suitable to analyze various chemical processes, including conformational changes and chemical reactions. The changes along component hypersurfaces often show dominant effects not obvious from the complete potential energy hypersurface. Various interrelations between the components are often manifested in approximate symmetries. These quasi-symmetries that are in fact manifested as the deviations from perfect symmetry, can be analysed in terms of symmetry deficiency measures, also used in molecular shape analysis. Some of the consequences of these interrelations between energy components are discussed, with special emphasis on the identity and transformations of molecular species.

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