POTENTIOLOGY[a] IN SPECTROSCOPY: IT MATTERS

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Spectroscopists have long attempted to summarize what they know about small molecules in terms of a knowledge of potential energy curves or surfaces. For most of the past century, this involved deducing polynomial-expansion force-field coefficients from energy level expressions fitted to experimental data, or for diatomic molecules, by generating tables of many-digit RKR turning points from such expressions. In recent years, however, it has become increasingly common either to use high-level *ab initio* calculations to compute the desired potentials, or to determine parametrized global analytic potential functions from direct fits to spectroscopic data. In the former case, this invoked a need for robust, flexible, compact, and 'portable' analytic potentials for summarizing the information contained in the (sometimes *very* large numbers of) *ab initio* points, and making them 'user friendly'. In the latter case, the same properties are required for potentials used in the least-squares fitting procedure. In both cases, there is also a cardinal need for potential function forms that extrapolate sensibly, beyond the range of the experimental data or *ab initio* points. This talk will describe some recent developments in this area, and make a case for what is arguably the 'best' general-purpose analytic potential function form now available. Applications to both diatomic molecules and simple polyatomic molecules will be discussed.

[a] *potentiology* (noun): study focusing on the development of new interatomic pair potential forms; sometimes pursued in an obsessive compulsive manner [The New Yorel Dictionary (2002, unpublished)].