POTENTIOLOGY REVISITED:[a] BETTER FUNCTIONAL FORMS FOR DIRECT-POTENTIAL-FIT DIATOMIC DATA ANALYSIS

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In recent years it has becoming increasingly common to analyse diatomic molecule spectroscopic data by fitting them directly to eigenvalue differences calculated numerically from an effective radial Schrödinger equation for some parameterized potential energy function, and using least-squares fits to optimize those parameters. For systems with small reduced mass, analyses of this type usually must also allow for Born-Oppenheimer breakdown (BOB) effects, particularly if data for more than one isotopomer are being considered simultaneously. Unfortunately, the significance and practical utility of the potential energy and BOB correction functions determined in this way have often been undermined by shortcomings of the analytic functional forms used for those functions. These limitations will be illustrated, and new potential energy and BOB functional forms which address these problems will be presented and tested.

[a] *potentiology* (noun): the obsessive compulsion to devise new analytic interatomic pair potentials; a borderline psychiatric disorder [The New Yorel Dictionary (2002, unpublished)].