NEW EXPANSIONS OF POTENTIAL ENERGY FOR DIATOMIC MOLECULES

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We introduced new expansions of the internuclear potential energy for diatomic molecules in the form of a power series combining Dunham, Simons-Parr-Finlan and Ogilvie expansions[a], a continued fraction[b], and a combination of a power series and Padé approximants[c]. These functions satisfy all criteria applicable to real potential curves of molecules in a stable electronic state; they asymptotically approach a finite value in the dissociation limit, exhibit a minimum energy at the equilibrium internuclear separation, and approach a positive value greater than a dissociation energy as the separation decreases. The proposed expansions are applied in quantitative analysis of the infrared, microwave and Raman spectra of the selected diatomic molecules. Published wavenumbers of assigned transitions are reproduced with fewer parameters for potential energy than reported elsewhere.

[a] M. Molski, J. Mol. Spectrosc. 193, 244 (1999).
[b] M. Molski, Phys. Rev. A 60, 3300 (1999).
[c] M. Molski and J. Konarski, unpublished results.