POINTWISE AND ANALYTICAL POTENTIALS FOR DIATOMIC MOLECULES. AN ATTEMPT FOR CRITICAL COMPARISON

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In the year of 2000, three publications appeared which demonstrated efficient and highly accurate description of the energy levels for electronic states in diatomic molecules by means of potential energy curves. Two of them suggested an analytical presentation of the potentials (Samuelis et al. Phys. Rev. A 63, 012710 (2000) and Seto et al. J. Chem. Phys. 113, 3067 (2000)), whereas Pashov et al. (Comp. Phys. Commun. 128, 622 (2000)) suggested a model-free point wise presentation. Since then all three methods were further developed and successfully used in a variety of problems. In this presentation a comparison between these three presentations is made, with the accent put on their applicability, convergence of the fitting process and the estimation of the uncertainties of the potential parameters.