EXTRAPOLATION PROPERTIES OF MORSE-LENARD JONES POTENTIAL

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The accuracy of the potential energy curves for diatomic molecules determined from experimental data is confirmed empirically with numerous examples in the literature. Usually PECs are determined from a limited set of experimental data and this in turns limits the range of internuclear distances where the shape of the potential is unambiguously fixed. While the uncertainty for interpolation could be assessed, the extrapolation is usually questionable and needs careful analyses. The Morse/Long-Range potential (Mol. Phys. 105, 663 (2007)) has been reported to have a built in long-range asymptotic behavior and therefore it is plausible to expect that one can expect good extrapolation properties and even possibility to determine important molecular parameters like D_e or/and C_6 from limited set of experimental data. In this contribution we undertake a systematic study which confirms these expectations in the case of Ca_2 ground state.

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