

Shaping complicated *ab initio* potential energy surfaces from the bottom of the well to the dissociation limit: application to the ozone PES

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An accurate determination of the potential energy surfaces (PES) is a prerequisite for high-resolution spectra predictions as well as for calculations involving kinetics of molecular formation, dissociation and recombination. In this work we compare spline PES approximations and various analytical PES representations available in the literature by applying this to the ozone molecule as a benchmark example. The ozone molecule has quite complicated electronic structure, consequently various issues for an accurate description of the shape of the ozone potential on the entire range of nuclear configurations are still unsolved and are considered as a challenge for the *ab initio* theory [1,2,3]. In order to extend the validity of the PES at higher energy range we propose a new analytical PES representation in order to describe a complicated shape of the surface along the transition state (TS) to the dissociation [4]. To build the ozone PES along the minimum energy path the electronic structure calculations have been extended [3,4] to a larger grid of nuclear configurations. Graphical software useful for the study of the shape of the PES was developed in particular to describe the eventual "reef" structure and van der Waals wells and also for matching *ab initio* points computed with different basis sets and methods.

Vibration energies up to dissociation will be presented as well as comparisons of predictions with available experimental data [5-7]. The impact of the reef structure on the high energy ozone vibration states will be discussed elsewhere [8].

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