

Generation of accurate potential energy surfaces of molecular systems of astrophysical and atmospheric interest

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We use different *ab initio* methods to compute multi-dimensional potential energy surfaces (PESs) of molecular systems of atmospheric and astrophysical interest. These PESs are incorporated later to solve the nuclear motion problem to deduce the spectroscopy of these species. After benchmarks that include the use of standard coupled cluster, complete active space self consistent field, internally contracted multi reference configuration interaction and the newly developed CCSD(T)-F12 methods, we show that the CCSD(T)-F12/aug-cc-pVTZ approach represents a compromise for good description of the PES and computation cost. This technique leads to results as accurate as those obtained using CCSD(T)/aug-cc-pV5Z whereas the CPU time and the disk used are reduced by ~30 [1,2]. This is valid for monoconfigurational electronic states. For multi configurational systems and electronically excited states, we should use the costly configuration interaction methods (MCSCF, MRCI). Several examples will be treated including the rigid molecules, charge transfer systems and weakly bound van der Waals molecular systems.