Automatic Generation of Intermolecular Potential Energy Surfaces

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Abstract

A method is developed for automatic generation of intermolecular two-body, rigid-monomer potential energy surfaces. The potentials are based on symmetry-adapted perturbation theory (SAPT), or any other sufficiently accurate electronic structure method. The long-range component of the potential is obtained from a rigorous asymptotic expansion with *ab initio* computed coefficients which seamlessly connects to SAPT interaction energies at large separations. An accompanying software package has been developed and tested successfully on eight systems ranging in size from the Cl^-–H_2O dimer to the cyclotrimethylene trinitramine dimer containing 42 atoms total. The potentials have a typical fit errors of about 0.2 kcal/mol in the negative energy region. All aspects of potential development were designed to work reliably on a broad range of systems with no human intervention. The method is described in a recently published paper [M. P. Metz, K. Piszczatowski, and K. Szalewicz, Automatic generation of intermolecular potential energy surfaces, J. Chem. Theory Comput., 2016]. Additionally, a new method of selecting dimer configurations for fitting the potential is discussed, in which statistical information about the functional form of the fit is leveraged to reduce the number of dimer configurations required.