PolyMLR: AN ANALYTIC MODEL FOR POLYATOMIC POTENTIALS WITH FEWER UNPHYSICAL PARAMETERS. APPLICATION TO CO_2.

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One has to calculate thousands or millions of *ab initio* points for potential energy surfaces even for molecules with only a few atoms. For diatomics, the MLR (Morse/long-range)[b,c] model has been very successful, making it possible to represent the entire curve accurately with just a few *ab initio* points, or a few spectral lines. With the MLR model it is also possible to extrapolate and interpolate in a way that allows successful predictions of energy level locations several thousand cm^{-1} away from the data region[d].

However no analogous model has existed yet for the intramolecular potentials of polyatomic molecules. A simple model is presented which accurately describes some small molecules with far fewer parameters than previous models, and can be extended to larger molecules too. The benefit of having a good model function is orders of magnitude greater for polyatomics than for diatomics since the amount of data needed for an accurate potential is reduced in each dimension. For example if the calculation of 100 *ab initio* points is reduced to 10 in a diatomic molecule, we may estimate that this factor of 10 reduction in cost becomes at least 10^{10} for a molecule whose potential depends on 10 radial coordinates.

As an example, an analytic potential for CO_2 is built, which requires fewer parameters than the previous state-of-the-art analytic potential, and obeys the theoretical long-range behavior more closely than all previous potentials, including inclusion of the Axelrod-Teller three-body interaction. The model is based on accurate diatomic potentials representing all atom-atom pairwise interactions, and for CO_2, a three-body correction representing the rest of the energy. This emphasizes the value of accurate molecular spectroscopy for simple diatomics, which is sometimes considered to be less interesting than research involving large molecules. Diatomic potentials are valuable as building blocks for large-molecule potentials.

An open-source computer program for building PolyMLR potentials for polyatomic molecules is introduced.

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