Development of a "first principles" carbon dioxide potential and its application to clusters up to $(CO_2)_{13}$

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A "first principles" potential energy function with flexible monomers is developed for carbon dioxide (CO_2) gas phase systems. This function is constructed through a fit to the electronic energies of CO_2 monomers and dimers at the CCSD(T)-F12b/aug-cc-pVTZ level of theory and basis set. In total, over 300,000 configurations of CO_2 were used to train the potential function, which was then used to determine the minimum energy structures of CO_2 clusters ranging in size from 3 – 13 molecules. A separate potential function was fit to MP2 reference energies and was directly compared to clusters optimized at the MP2/aug-cc-pVDZ level of theory.