Work Plan of Ayda Badri

Spectroscopy of molecules trapped in CO matrix X-$(CO)_n$
Application: the CO_2-CO van der Waals complex

Recently, explicitly correlated quantum chemistry methods [1] have been widely used for generation of highly accurate intermolecular potential surfaces of van der Waals complexes. The carbon dioxide molecule, CO_2, plays important role in many atmospheric, environmental and industrial applications. The complexes that involve CO_2, including homodimer CO_2-CO_2 as well as CO_2 with the interacting partner with such as CS_2, N_2, *etc*, have been the subject of many theoretical [2-5] and experimental studies [5-7].

As the first step of theoretical study, the explicitly correlated coupled cluster method with single, double, and perturbative triple excitations, CCSD(T)-F12 level of theory in conjunction with an augmented correlation consistent Valence Triple Zeta (aug-cc-pVTZ) basis set has been applied to calculate a large set of the single point energies in 4D intermolecular coordinate space.

As the next steps, within the short-term scientific mission (STSM), the following analysis will be performed:

1. The fit of the analytical 4D-PES to the calculated single energies points.
2. Estimation of the accuracy of the calculated CCSD(T)-F12 PES by comparison to the conventional CCSD(T) at the CBS limit for a few cuts including the stationary points.
3. Comparison of the generated PES to the previously reported by Uteva *et al.* [8].
4. Analysis of the PES in order to extract the relevant structural and dynamical information of the complex. Calculation of the structures and harmonic frequencies for the determined minimum configurations.
5. Calculation of the bound states of CO_2-CO.
6. Preparing the report on the studies needed to write the manuscript appropriate for publishing in scientific journal.

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