Prediction of structure and energetics of CO_2-Ar_n clusters: a DFT study

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In this preliminary work, density functional theory (DFT) has been performed to predict possible stable structures of CO_2-Ar_n clusters for increasing number of Ar atoms. Previously, we have studied these systems by using a classical molecular-dynamics simulation and the pair wise-additive approximation to construct the potential energy function in classical mechanics (CM) [1]. Such complexes, CO_2 in Argon clusters, are still actively investigated at nano-scale [2]. However, there is still lack of quantum mechanical calculations (QM) in the literature. Some of the findings computed with DFT/B3LYP/6-311++g level theory [3] may be compared with previous results as one of our progressive studies.

Optimised geometries of CO_2-Ar_n (n=1-21) with CM aproaches were reported in our previous study [1] as given in Figure 1. The stability functions, second finite differences, of their total energies are given in Figure 2. Energy values are in Table.

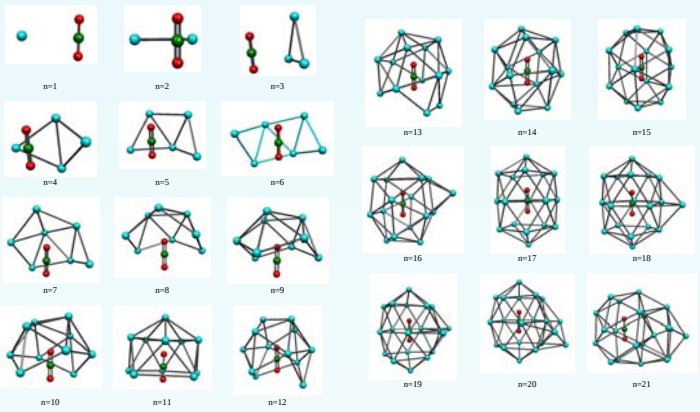

Figure 1 Optimized structures of the complexes CM [1]

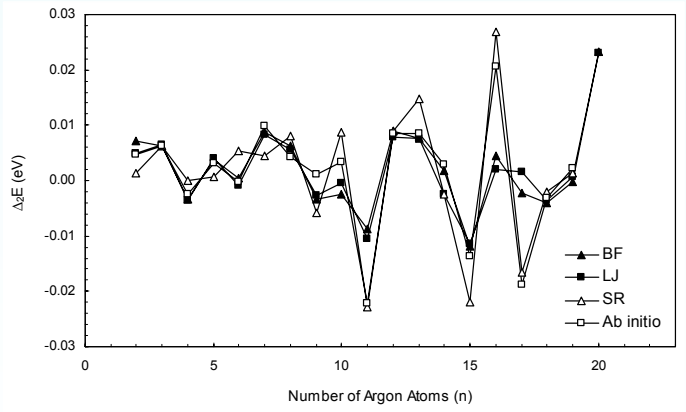

Figure 2 Stability functions

Table Energy comparison for some sizes

	This work			Literature		
N	BF	LJ	Aziz	SR	*ab initio*	3A[a]
1	-0.023	-0.023	-0.023	-0.025	-0.026	-0.024
2	-0.056	-0.055	-0.057	-0.063	-0.064	-0.061
3	-0.099	-0.093	-0.093	-0.101	-0.108	-0.098
4	-0.148	-0.137	-0.143	-0.146	-0.157	-0.136
5	-0.192	-0.178	-0.164	-0.191	-0.204	-0.179

DFT/B3LYP/6-311++g level theory are the progressive study of the present investigation. Similarly, the geometries are optimized. We attempt to determine a suitable functionals and basiss set for DFT. For Ar_2 interatomic distance is 2.69 Å and the frequiency is 178 cm^{-1}. The selected theory gives various imaginary frequiencies. For CO_2-Ar_2 there are nine frequiency modes and two of them are negative. Atomic charges are just negative on Oxygen atom and the others are positive. For n=5 there are 7 negative frequiencies in 18 modes. Its IR frequiencies are in Figure 3. Similarly the rest of the further structures are in consideration and the structure is given in Figure 4 as a sample for n=8. As shown the Ar atoms mainly prefer to sit around the CO_2 molecule.

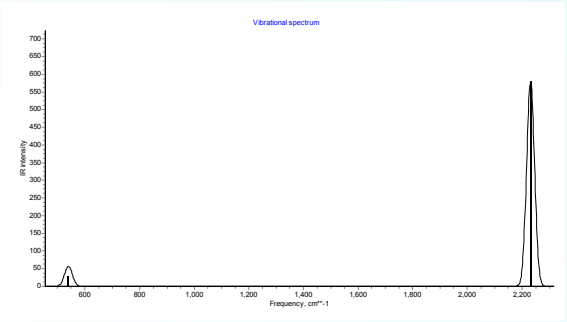

Figure 3 IR frequiencies for n=5.

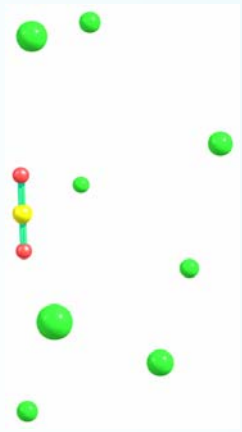

Figure 4 The QM structure for n=8.

As a result the suitable theory may be constructed to investigate the Ar surraunded CO_2 molecular complexes. By the way at least quantitative computations can lead any suitable data for further studies at nano-scale.

REFERENCES

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