Ab initio QUANTUM CHEMICAL INVESTIGATION ON THE GEOMETRICAL ISOMERS OF DINITROGENTETRAOXIDE

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ABSTRACT

Many people worked and given more details about Dinitrogentetraoxide (N_2O_4). But the geometry of N_2O_4 is still subjected to discussion.

There are many methods available, but the theoretical *Ab initio* Quantum chemical calculation is very suitable. It is very accurate with experimental values, but a time consuming method. Because it takes considerable amount of CPU time in computation.

In this study we used some experimental values, from these values the equilibrium geometry and its structural parameters were found by using computation. Total energies of the each isomer were also found.

These calculated values were correlated with experimental values and a possible geometry of the N_2O_4 was determined.

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