Supporting Infomation

Computational theoretical study of reaction path of the unimolecular decomposition of malonic acid in the gas phase using the NEB method

by

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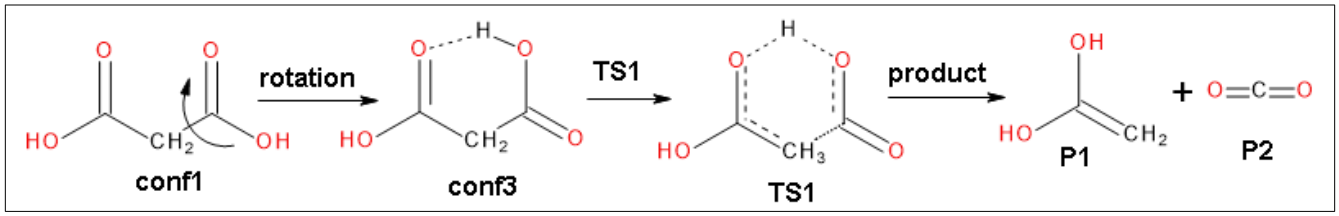
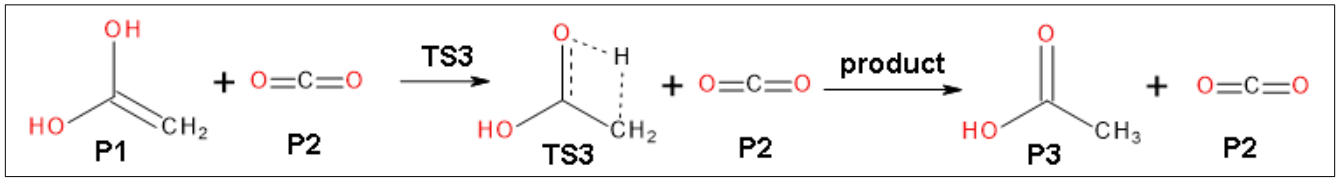
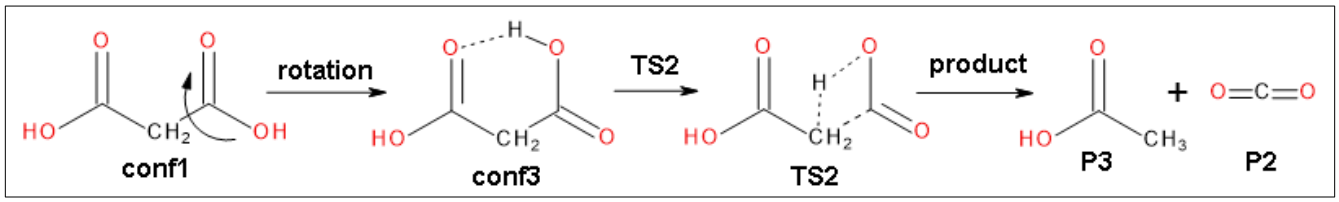
Scheme of Reactions



Scheme 1. Reaction step for the formation of Enol and CO_2.



Scheme 2. Reaction step for the conversion of enol to acetic acid.



Scheme 3. Reaction mechanism in a unique step for the decomposition of malonic acid.

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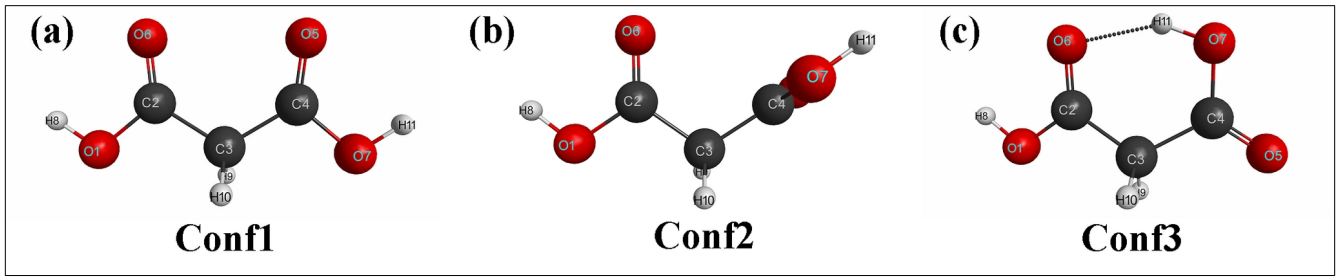


Figure 1. Conformations of the malonic acid.

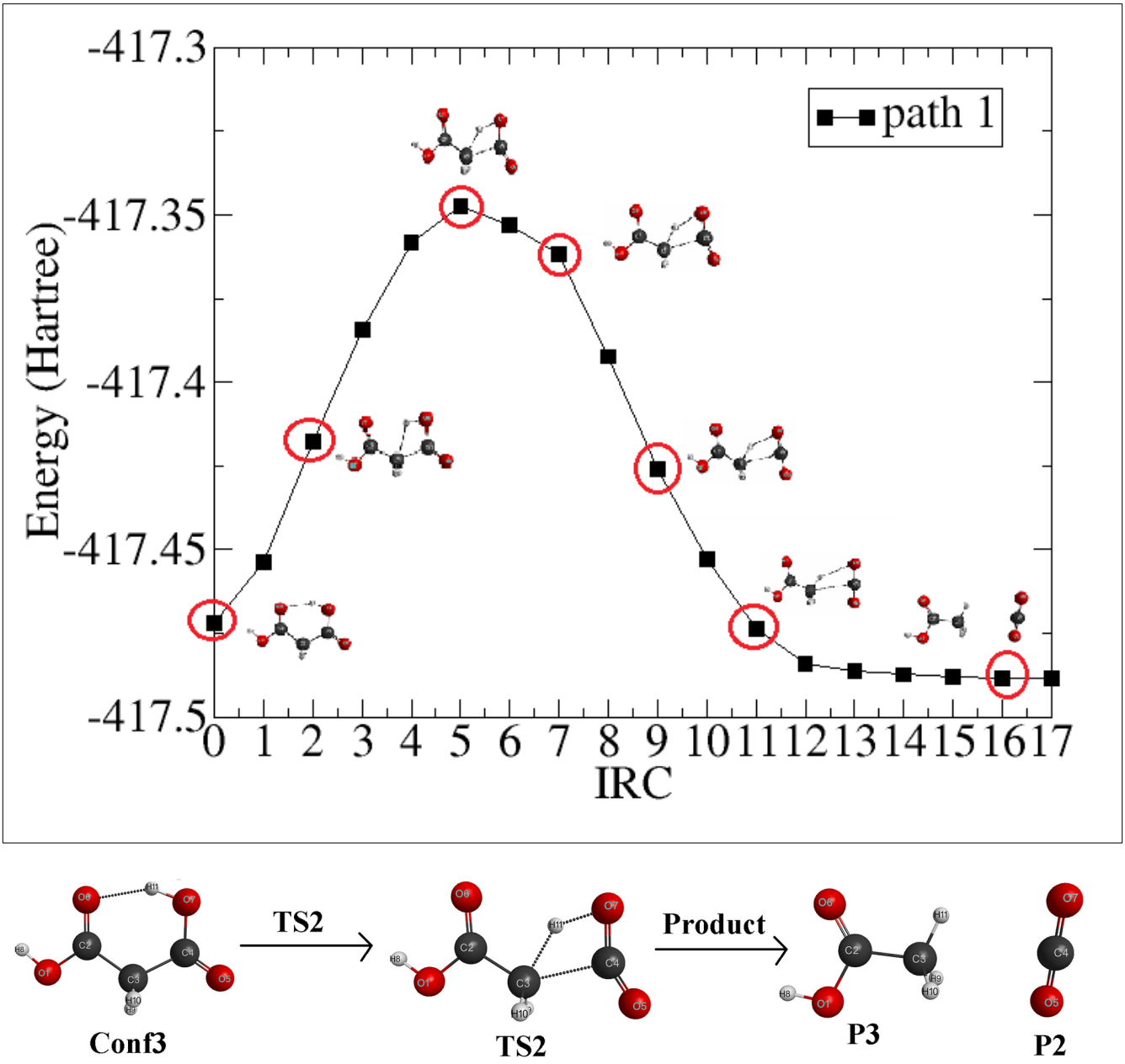


Figure 2. Energy profile obtained from the NEB method implementation for the reaction step path 1 that correspond to the transition state TS2.

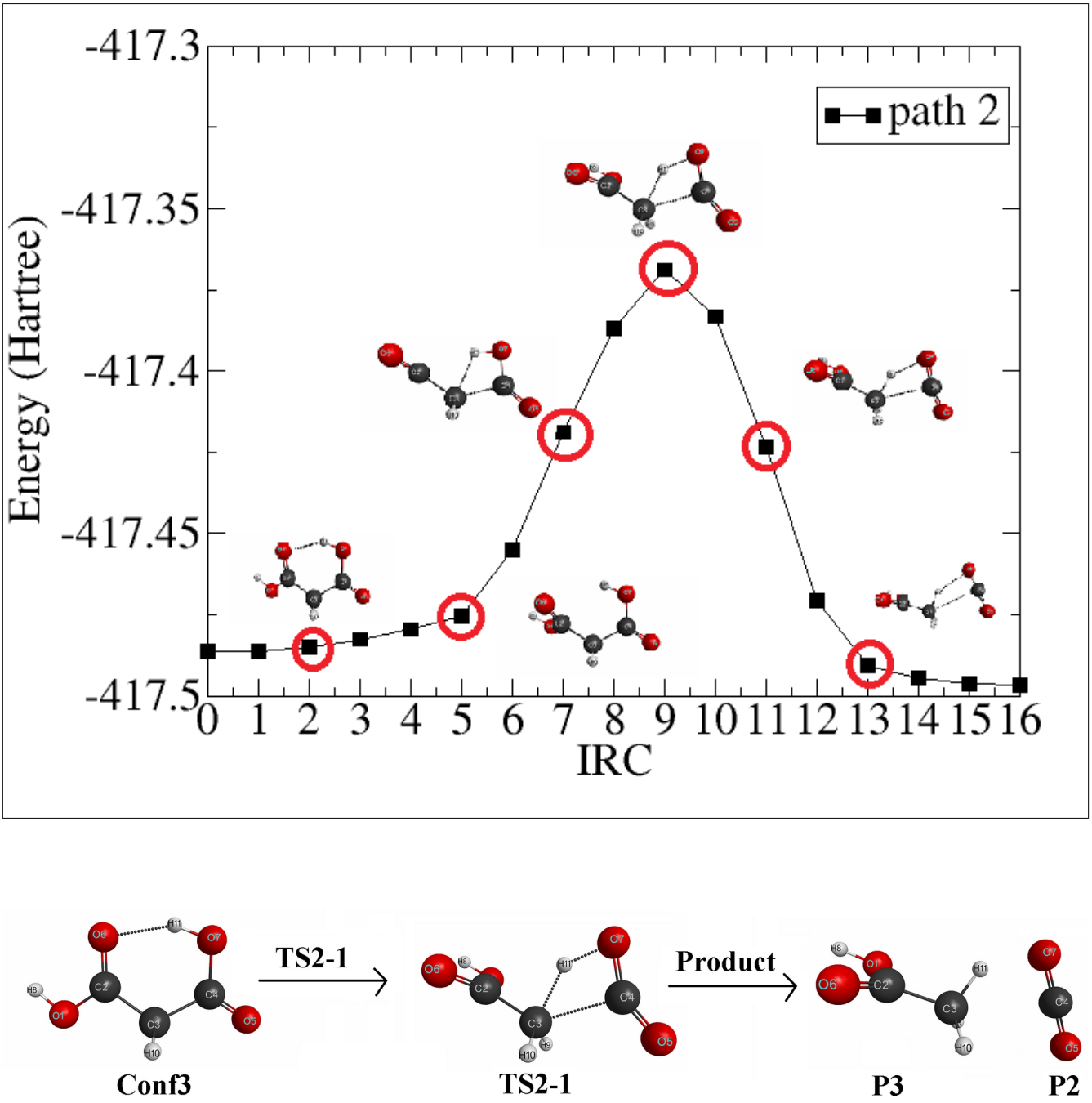
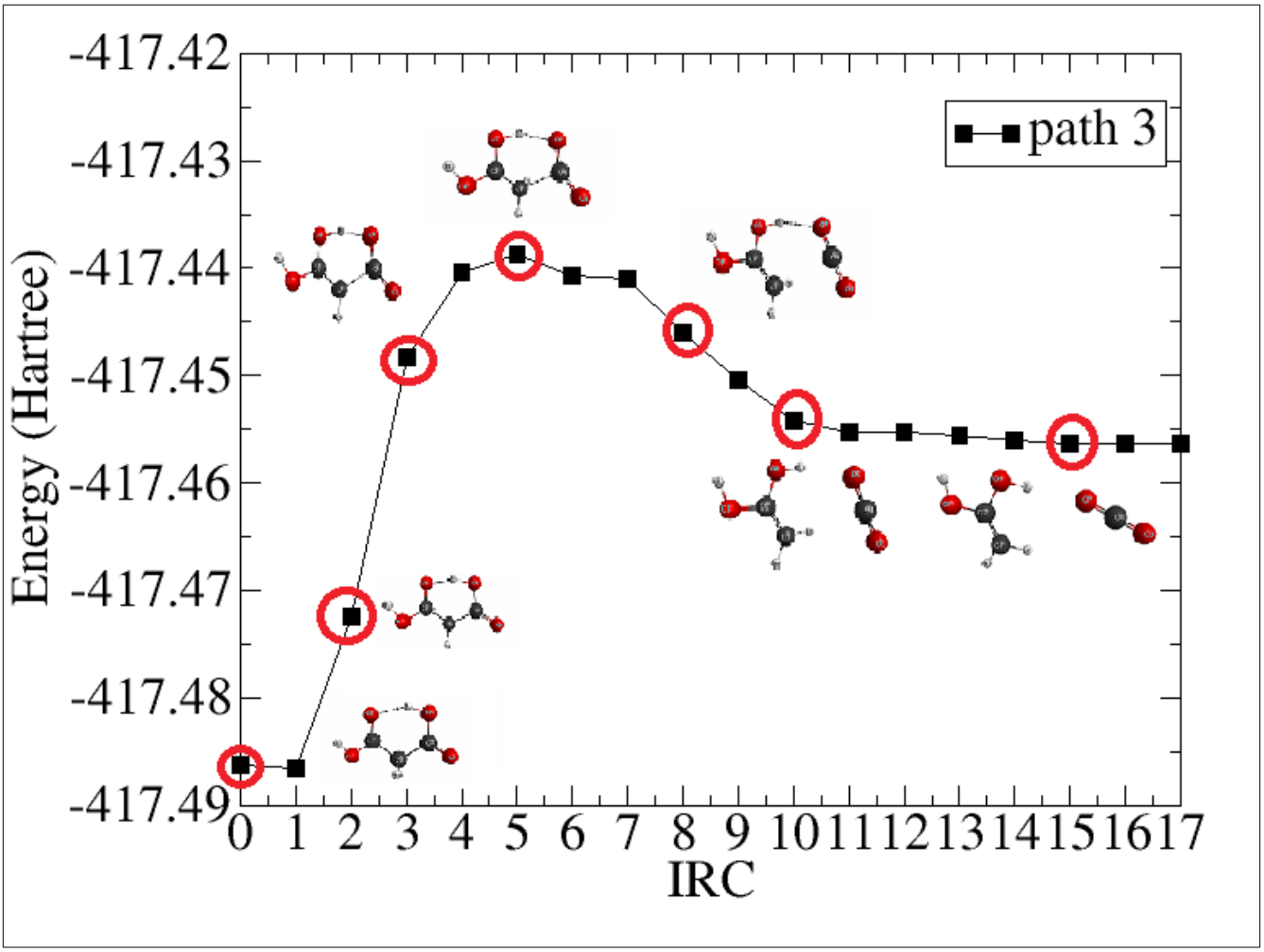


Figure 3. Energy profile obtained from the NEB method implementation for the reaction step path 2 that correspond to the transition state TS2-1.



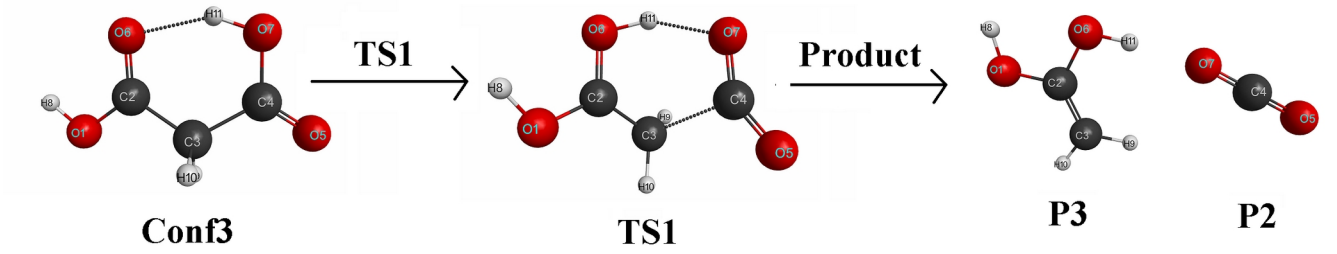


Figure 4. Energy profile obtained from the NEB method implementation for the reaction step path 3 that correspond to the transition state TS1.

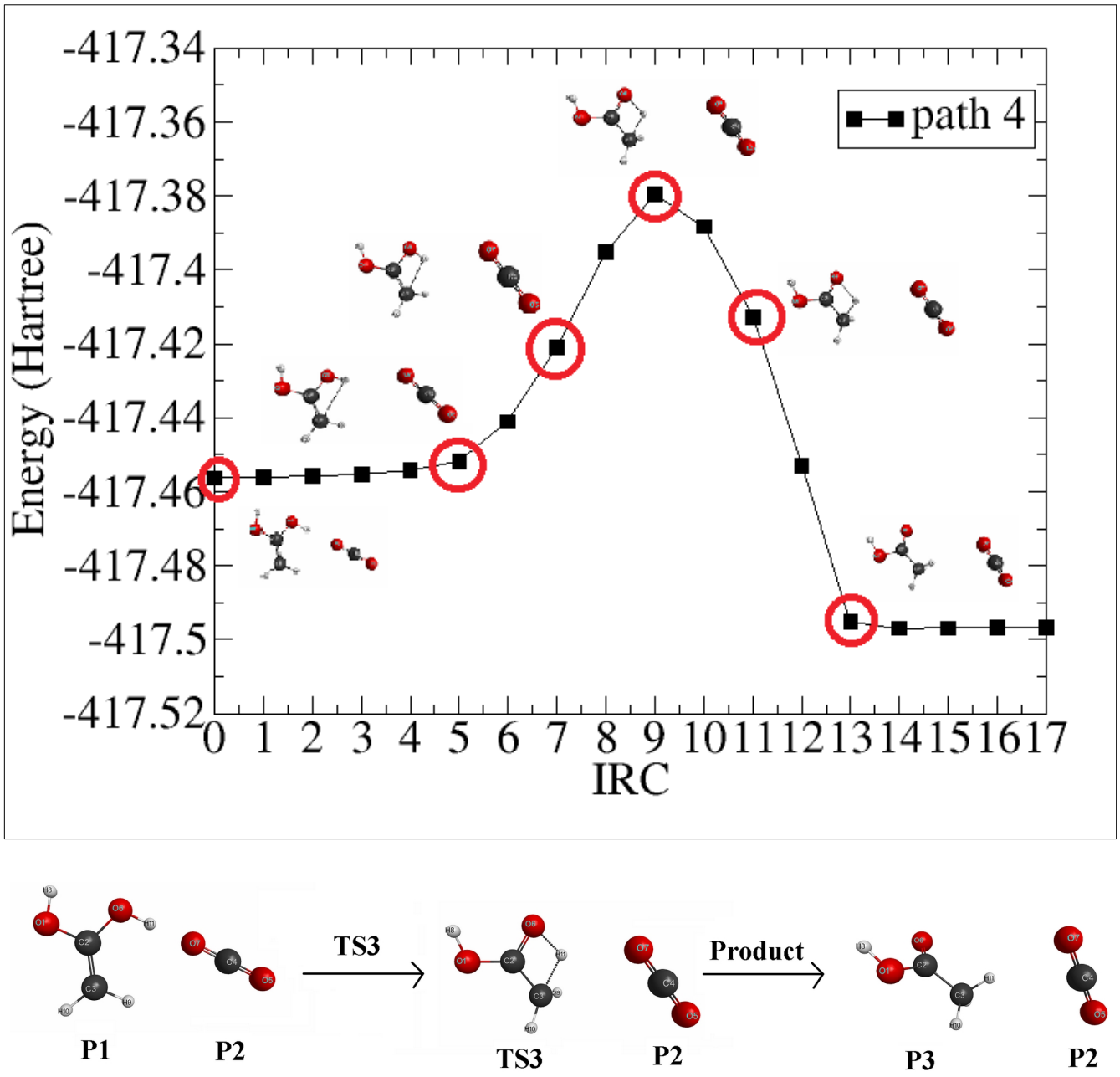


Figure 5. Energy profile obtained from the NEB method implementation for the reaction step path 4 that correspond to the transition state TS3.