Supporting Information

An Experimental and Theoretical Study of the Kinetics of the Reaction between 3-Hydroxy-3-Methyl-2-Butanone and OH radicals

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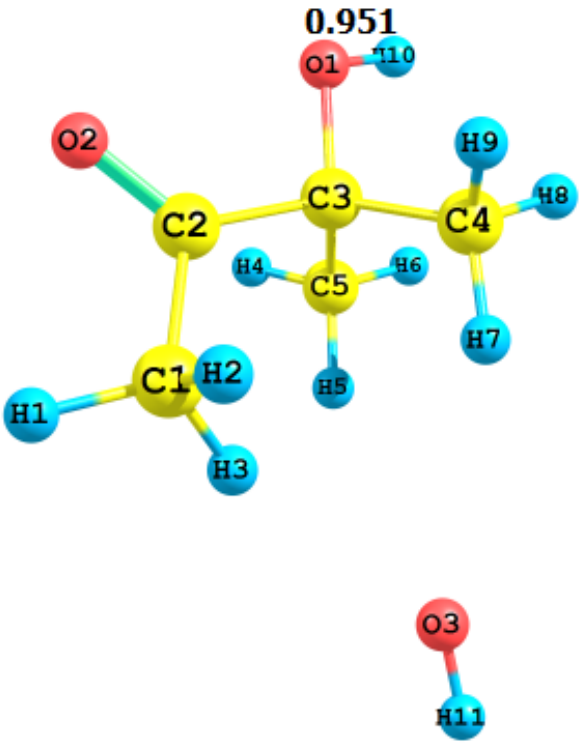
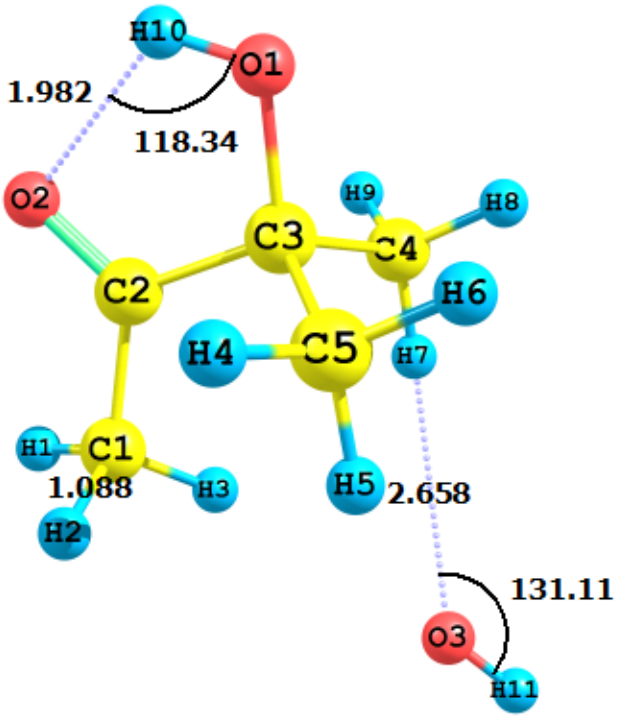
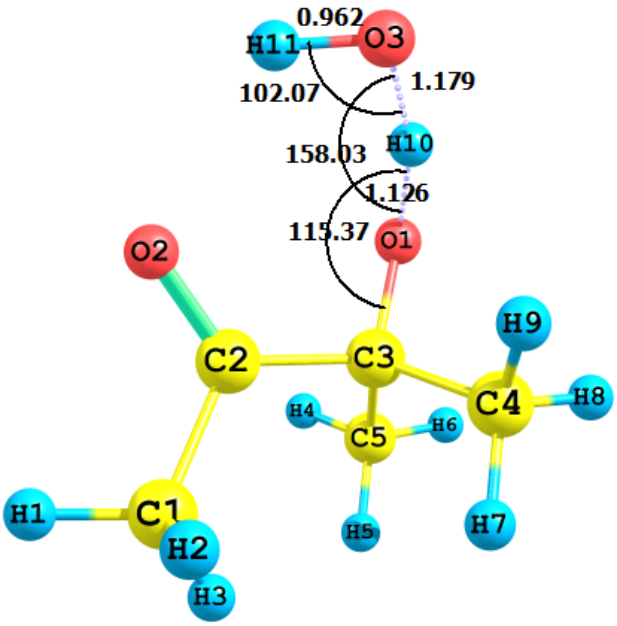


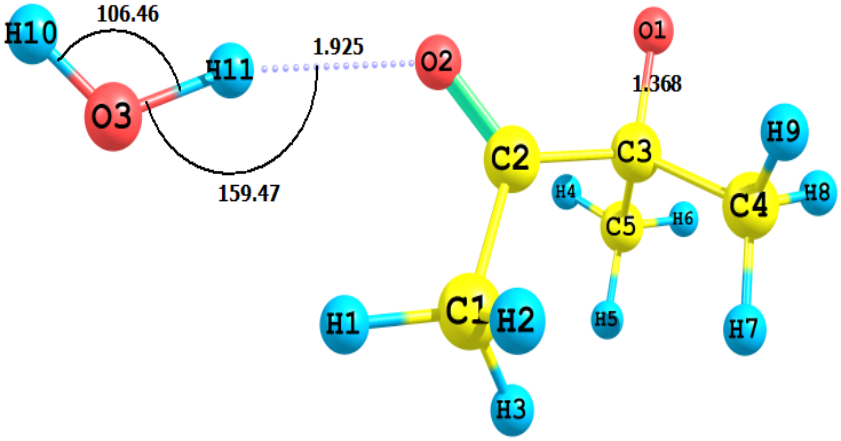
Reactant (R)



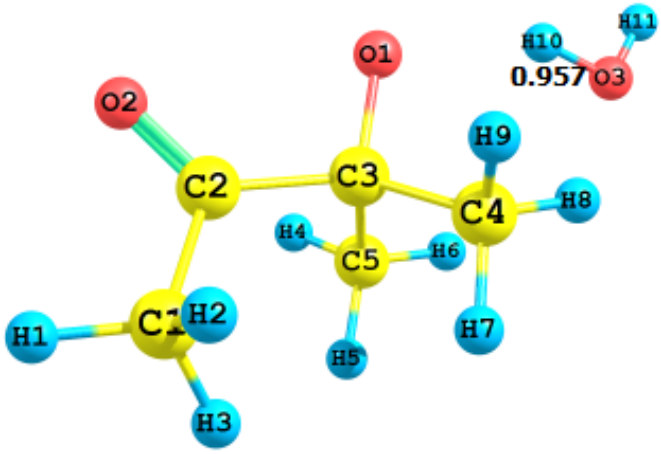
Reactant complex (RC)



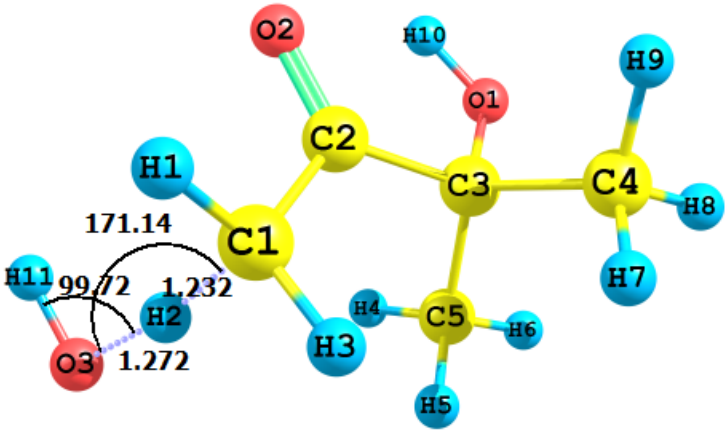
Transition State (TS1)



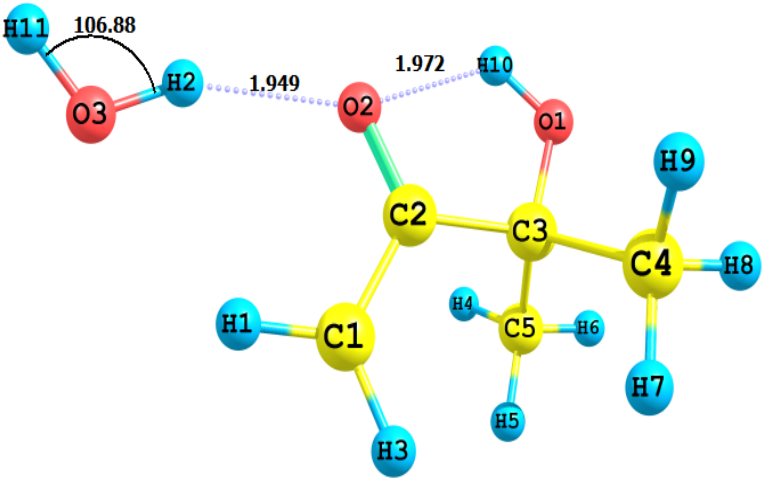
Product complex (PC1)



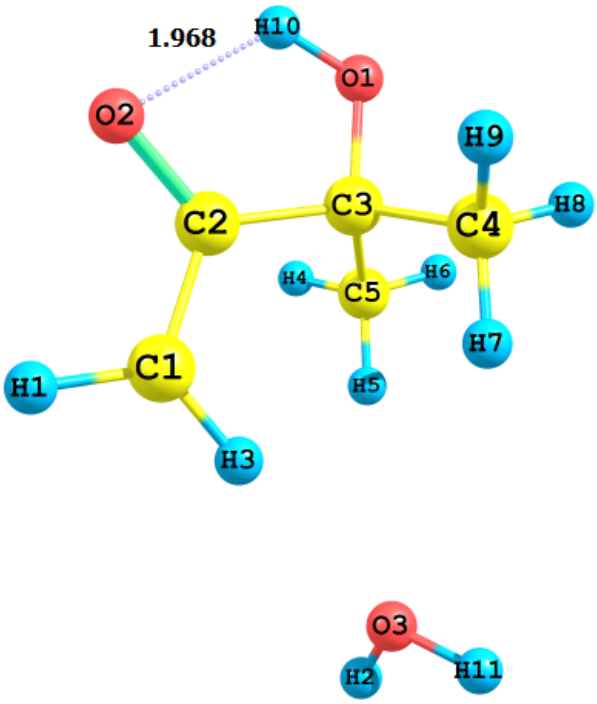
Product (P1)



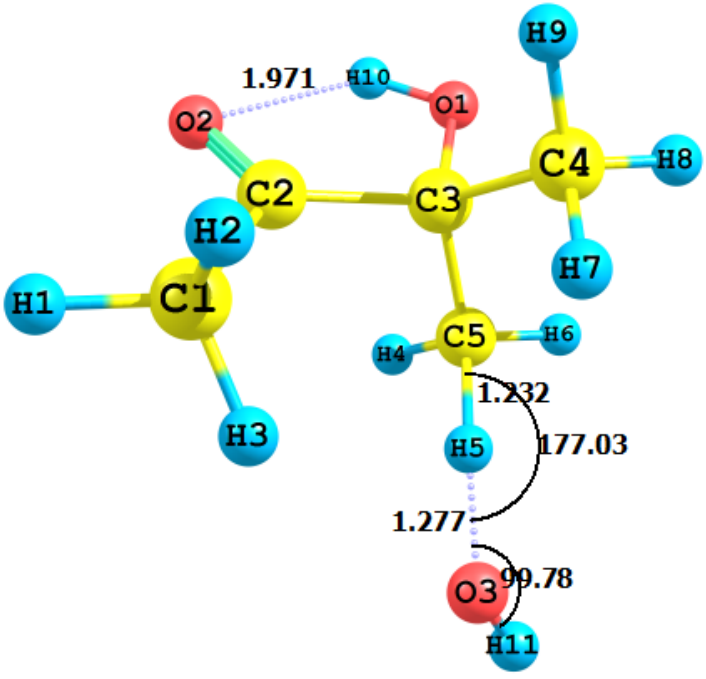
Transition State (TS2)



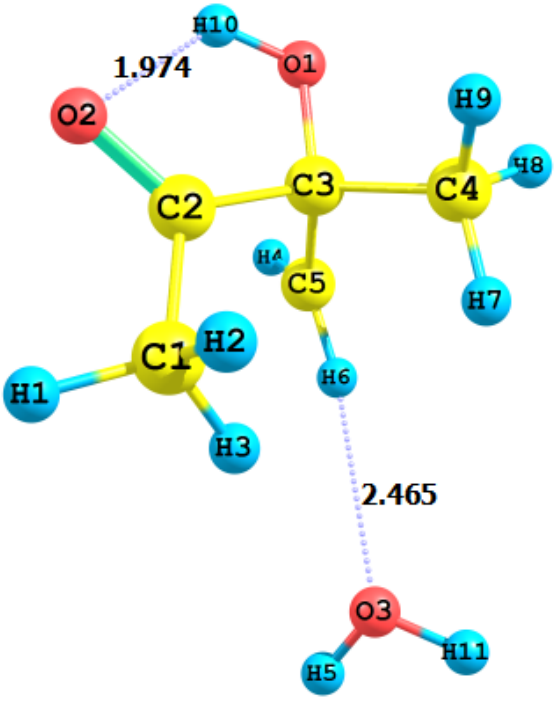
Product Complex (PC2)



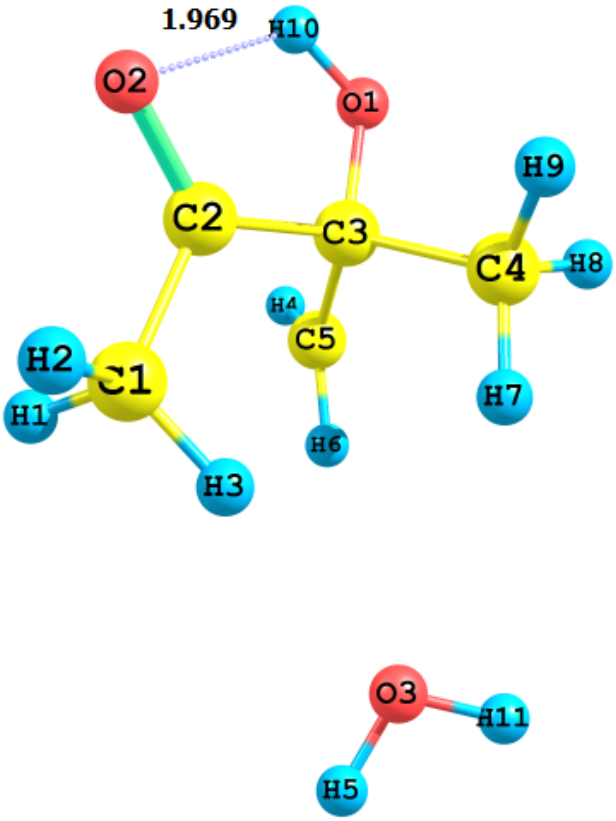
Product (P2)



Transition state (TS3)



Product complex (PC3)



Product (P3)

Fig.S1 Optimized reactive species of all reactants, reactant complex, transition states, products, product complexes at BH & HLYP level of theory with 6-311+G(d,p) basis set. Bond distances are in angstrom, bond angles are in degrees.