

Supplementary Material

Computational study of photodegradation process and conversion products of the antidepressant citalopram in water

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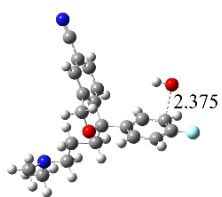
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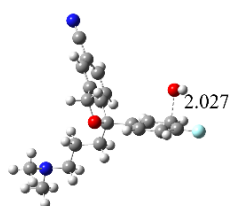
9 Pages

8 Figures

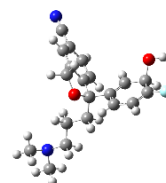
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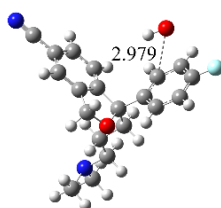
C1_R



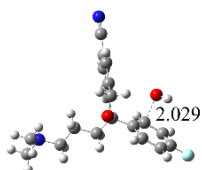
C1_TS



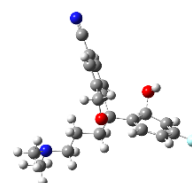
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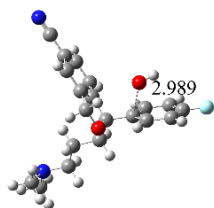
C2_R



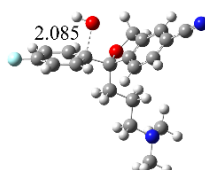
C2_TS



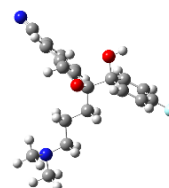
C2_P



C3_R



C3_TS



C3_P



N



H



C



O



F

Figure S1. Optimized geometries of reactant (R), transition state (TS), and product (P) at C1-C3 sites for the indirect photodegradation pathways of CIT with $\cdot\text{OH}$.

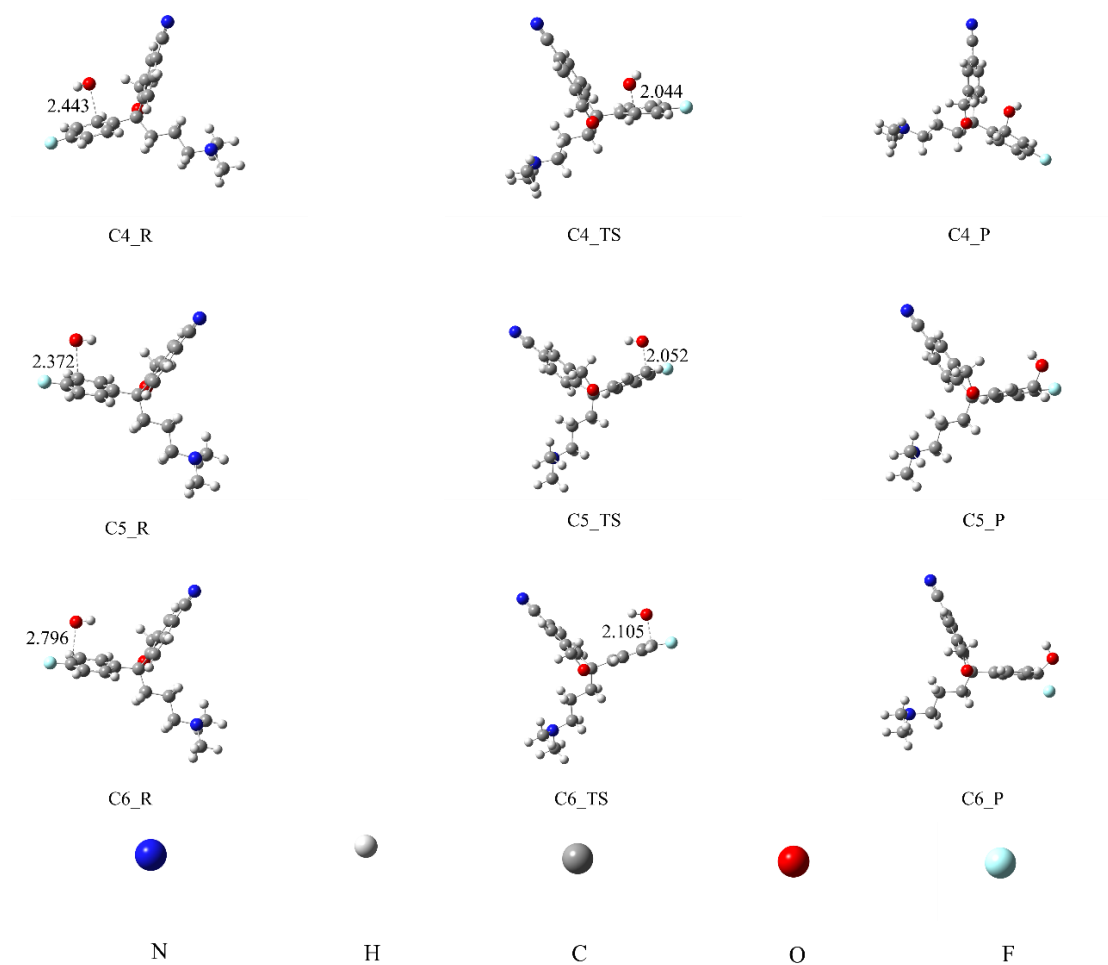


Figure S2. Optimized geometries of reactant (R), transition state (TS), and product (P) at C4-C6 sites for the indirect photodegradation pathways of CIT with $\cdot\text{OH}$.

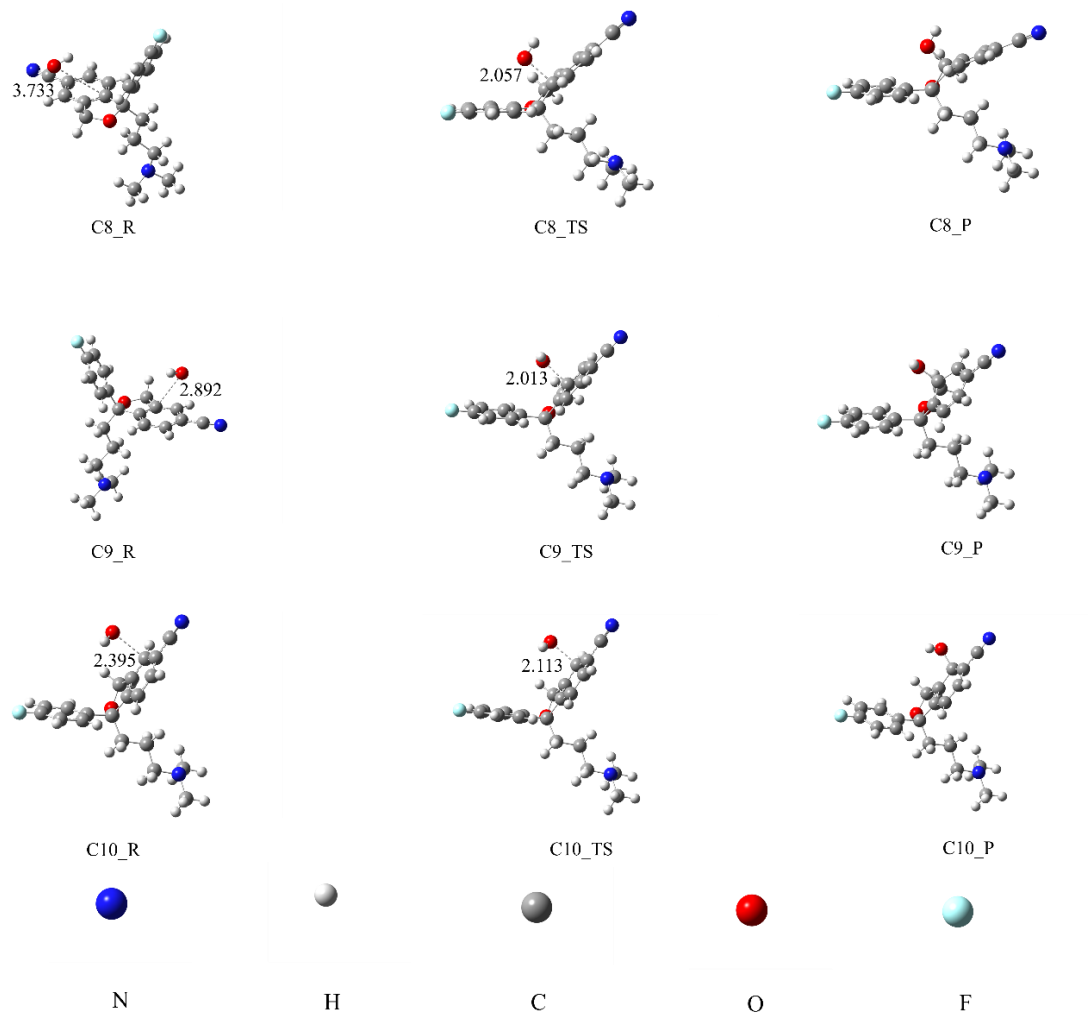


Figure S3. Optimized geometries of reactant (R), transition state (TS), and product (P) at C8-C10 sites for the indirect photodegradation pathways of CIT with $\cdot\text{OH}$.

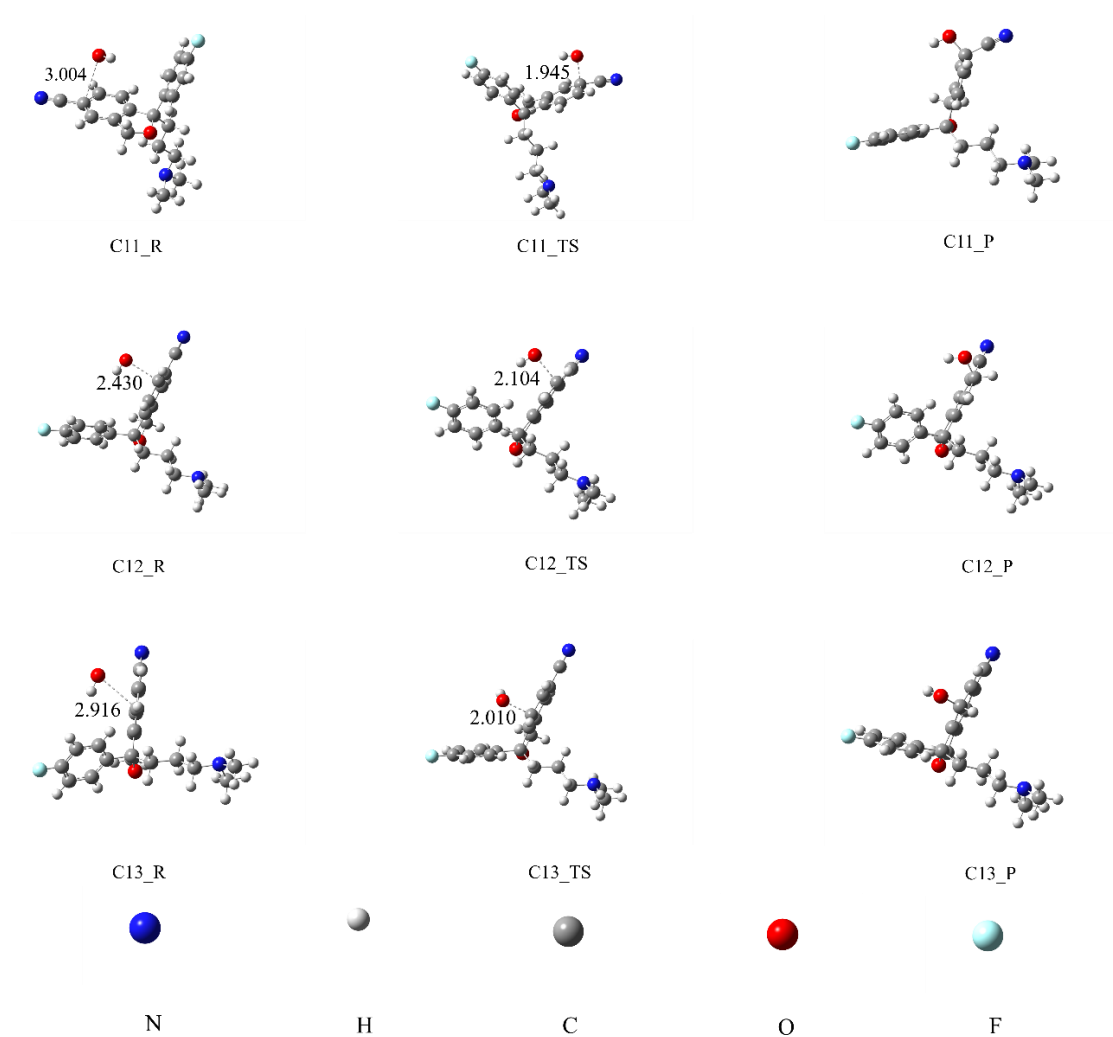


Figure S4. Optimized geometries of reactant (R), transition state (TS), and product (P) at C11-C13 sites for the indirect photodegradation pathways of CIT with $\cdot\text{OH}$.

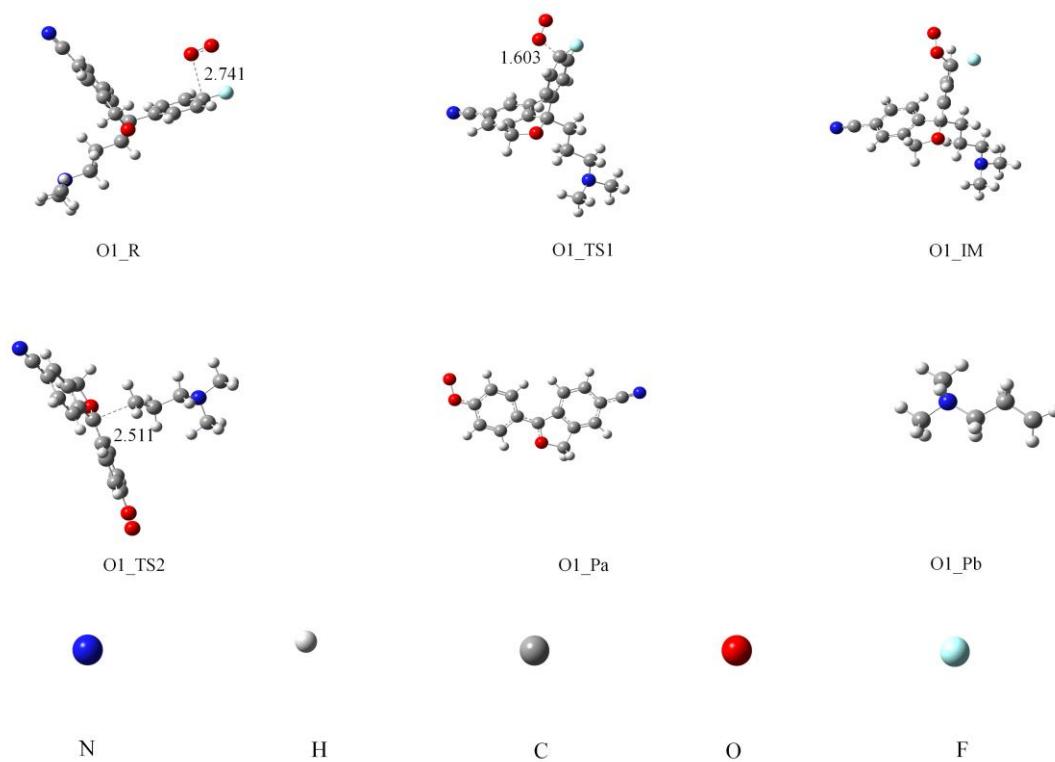


Figure S5. Optimized geometries of reactant (R), transition state (TS), intermediate (IM), and product (P) in Path O1 for the indirect photodegradation pathways of CIT with $^1\text{O}_2$.

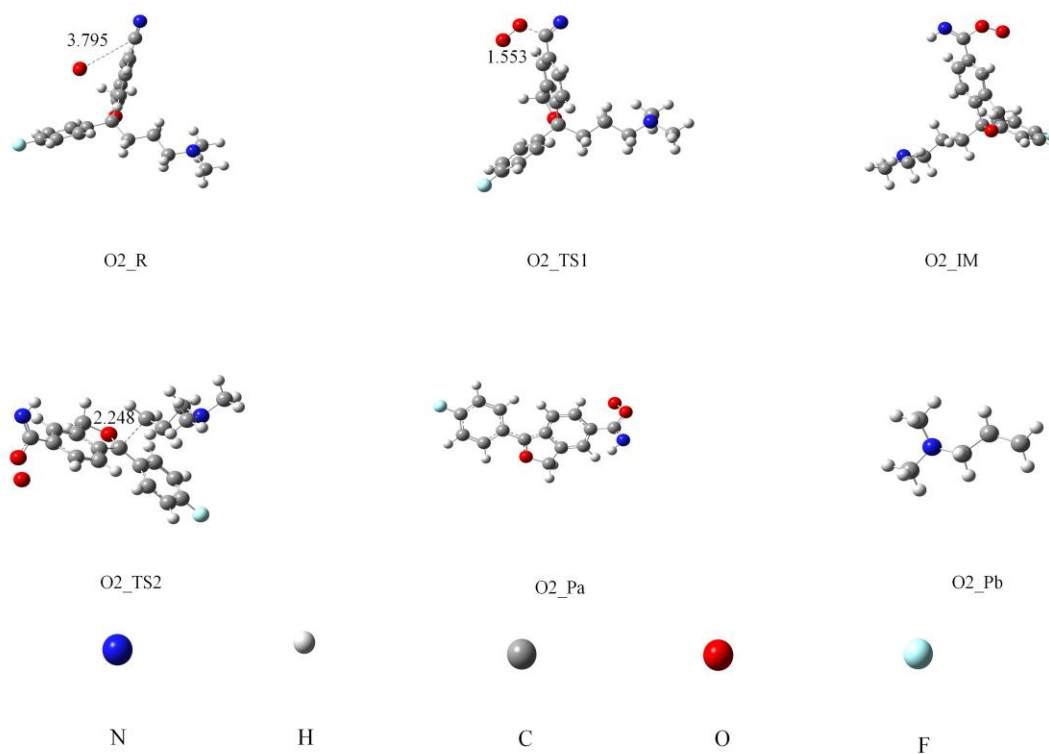


Figure S6. Optimized geometries of reactant (R), transition state (TS), intermediate (IM), and product (P) in Path O2 for the indirect photodegradation pathways of CIT with $^1\text{O}_2$.

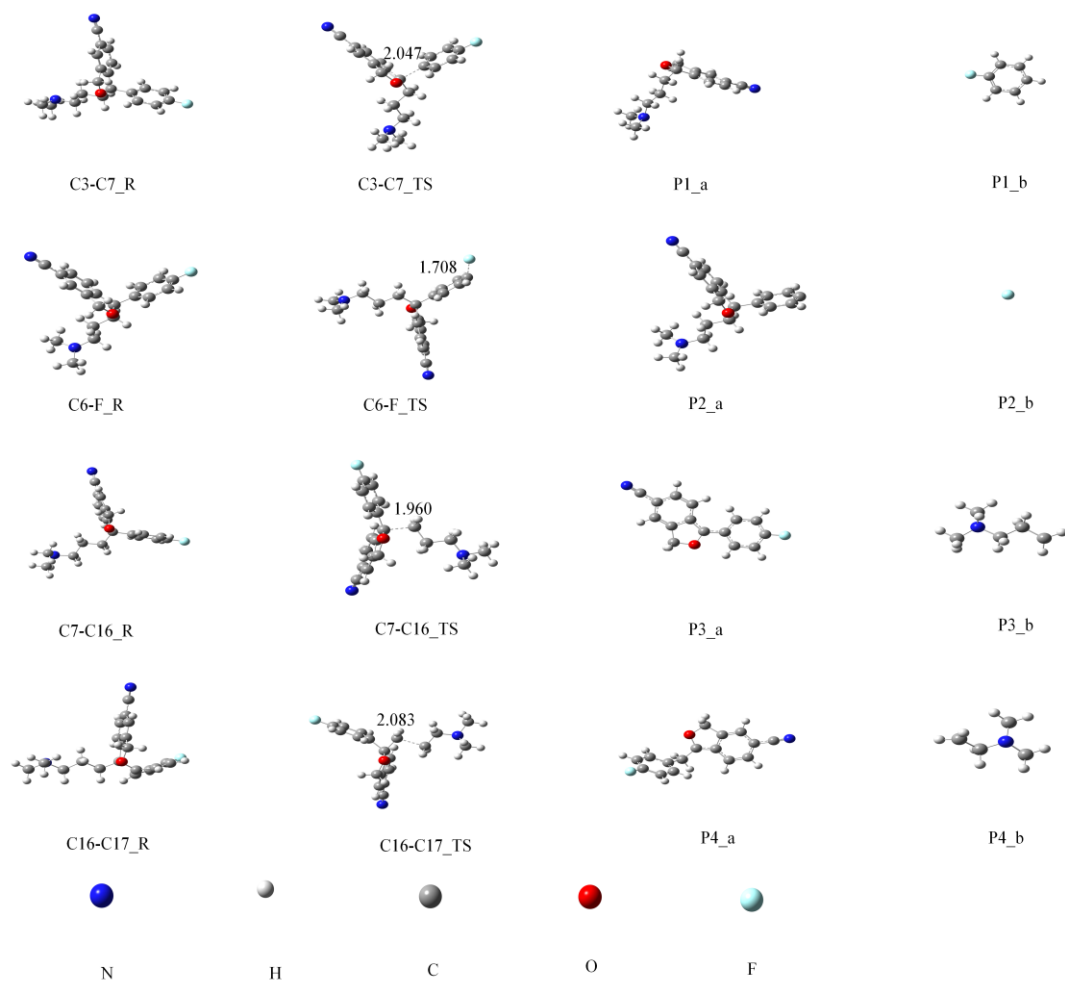


Figure S7. Optimized geometries of reactant (R), transition state (TS), product (P) in C3-C7/C6-F/C7-C16/C16-C17 for the direct photodegradation pathways of CIT.

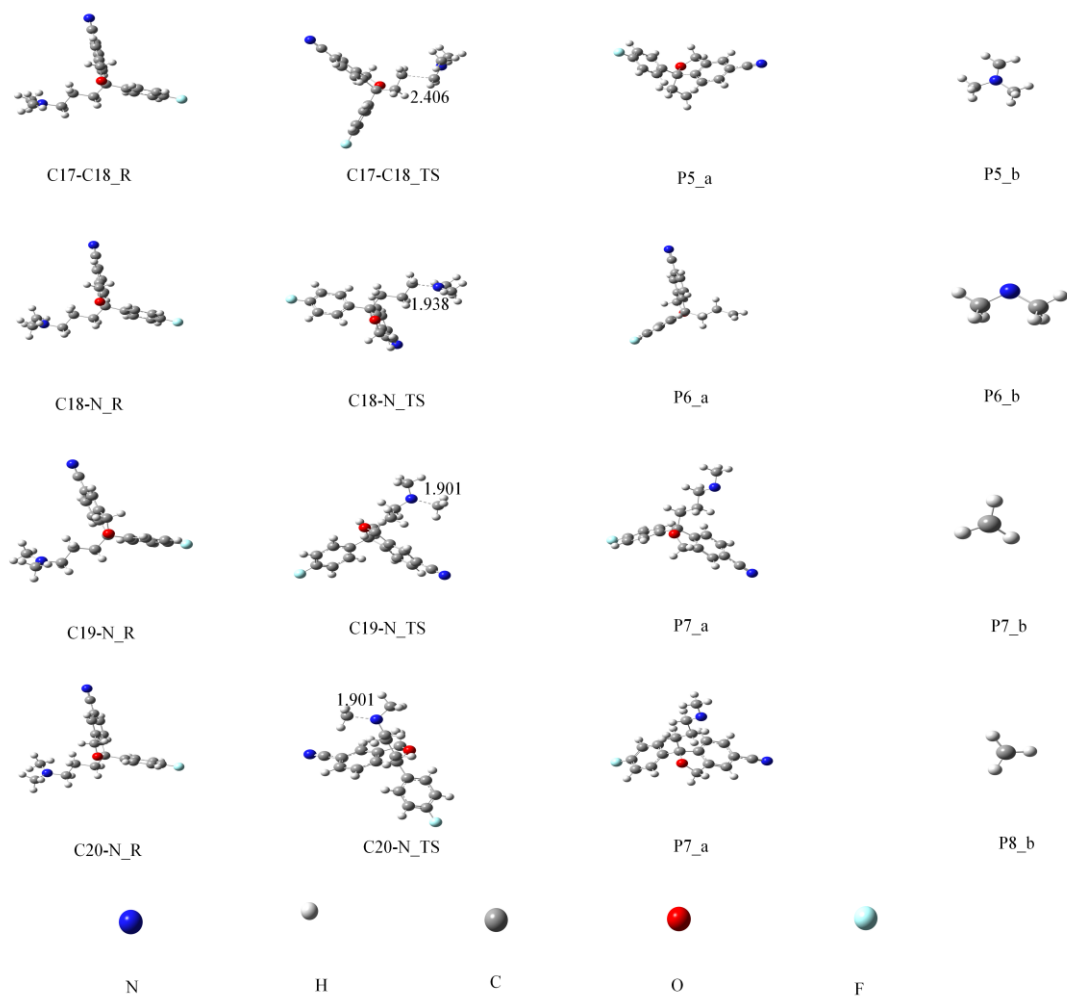


Figure S8. Optimized geometries of reactant (R), transition state (TS), product (P) in C17-C18/C18-N/C19-N/C20-N for the direct photodegradation pathways of CIT.