Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Degradation Mechanism of Sulfamethoxazole under Ozonation: A DFT Study

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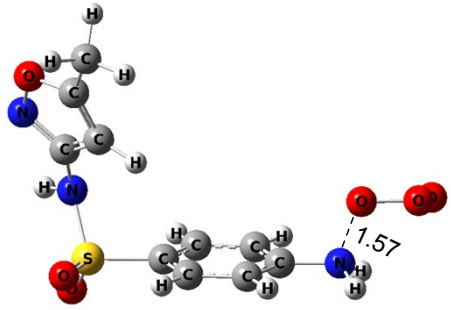
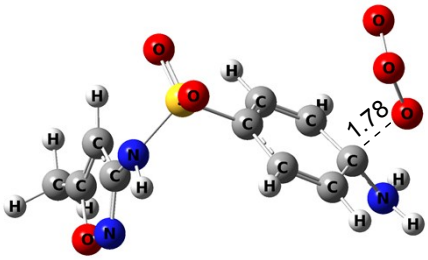


TS_{DA1}



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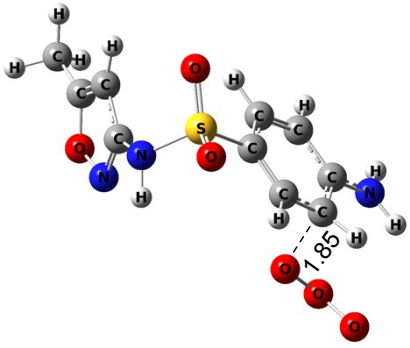

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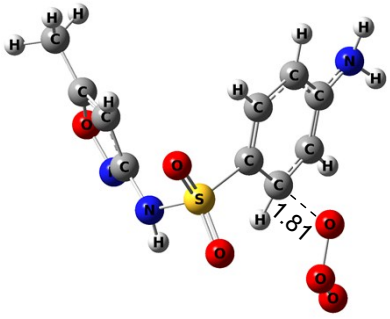
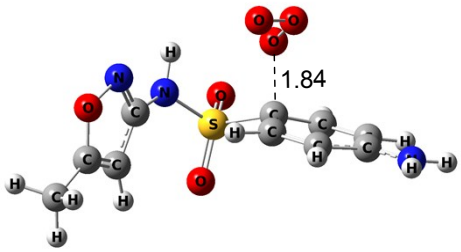


TS_{DA4}



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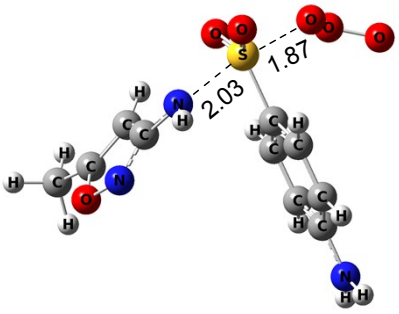
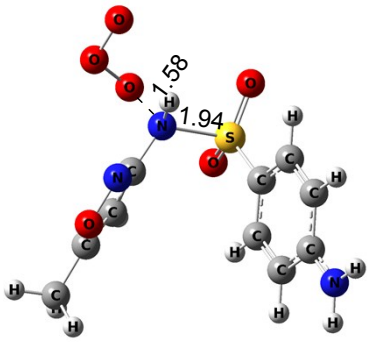


TS_{DA6}



TS_{DA7}

Figure S1. Optimized geometries of transition states (TSs, mentioned in Figure 2) for possible attack of O_3 at sites 1-7 in SMX (Interatomic distances are in Å)

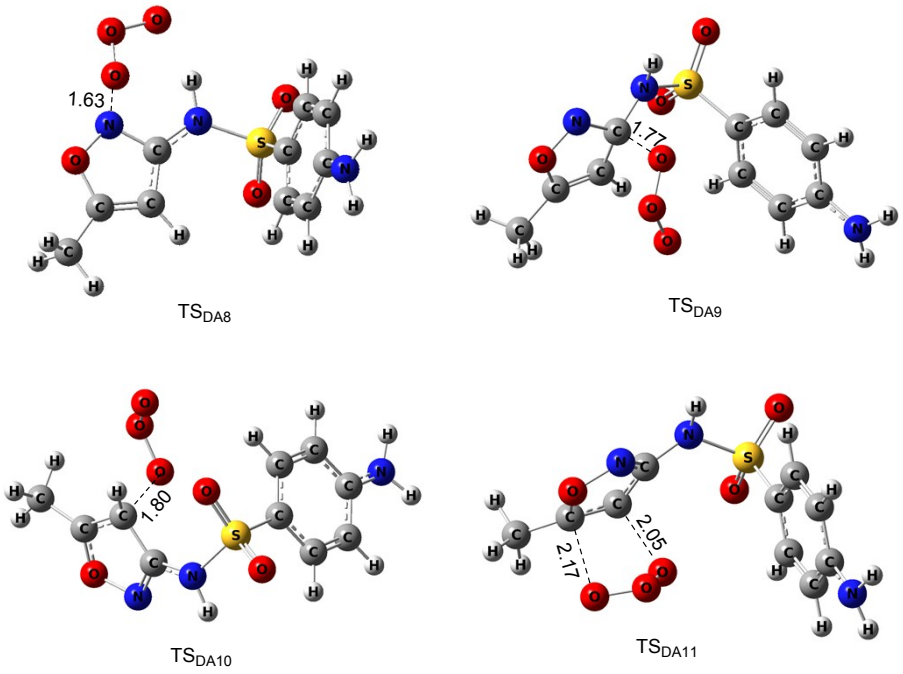


Figure S2. Optimized geometries of TSs (mentioned in Figure 3) for possible attack of O_3 at isoxazole moiety of SMX (Interatomic distances are in Å)

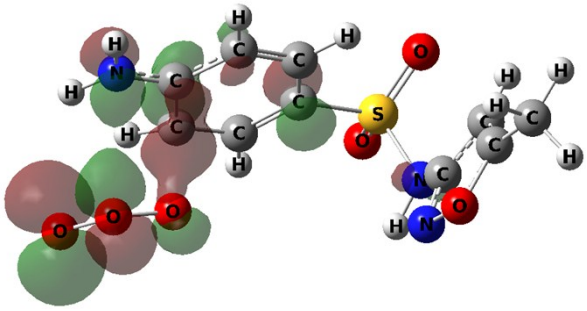


Figure S3. HOMO of TS_{DA3} (Isovalue of 0.04)

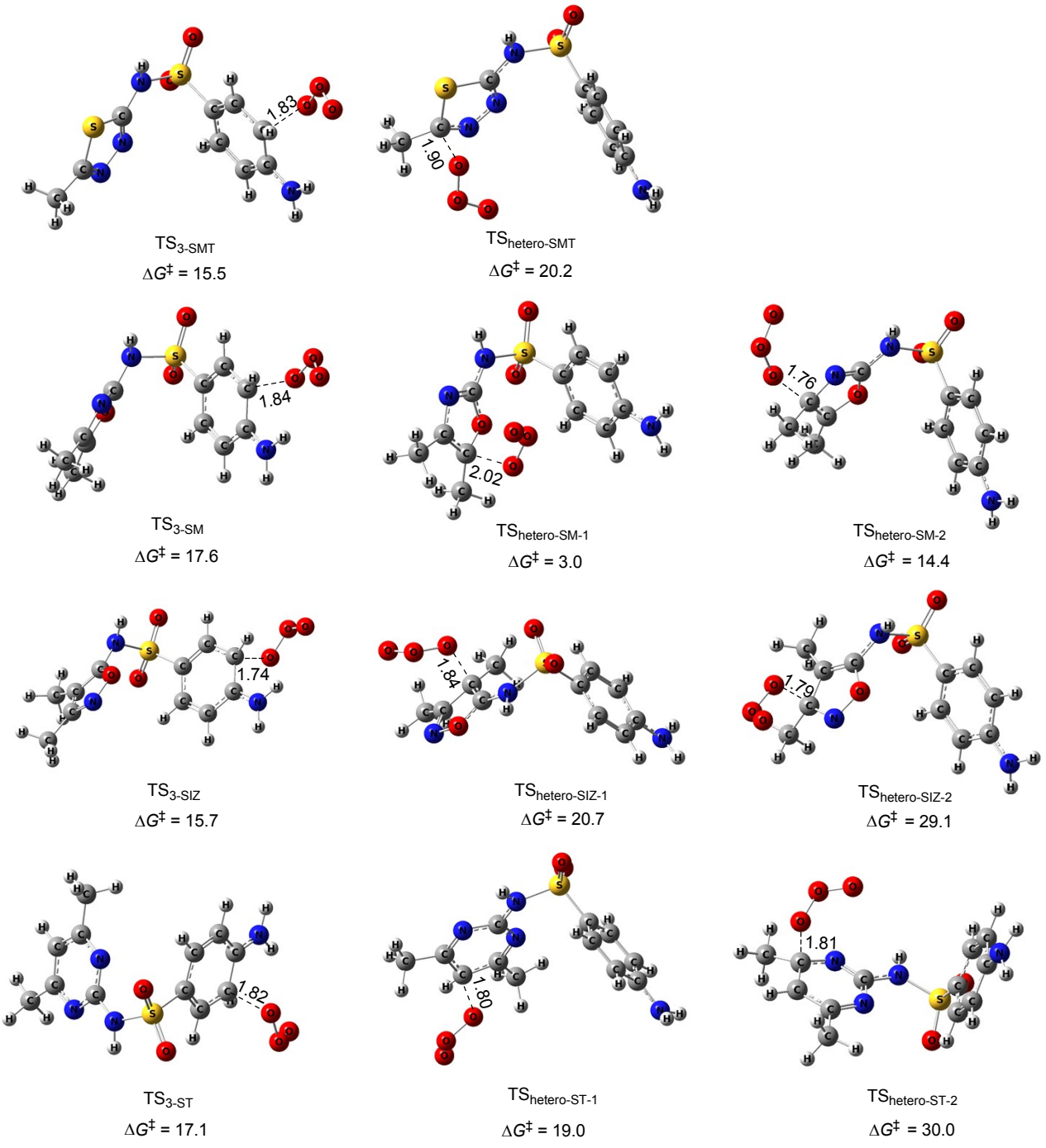


Figure S4. Optimized geometries of TSs (mentioned in Figure 5) for O_3 addition of other sulfonamides and corresponding energy barriers shown under the structure (The relative Gibbs free energies are given in kcal mol^{-1} and interatomic distances are in Å)

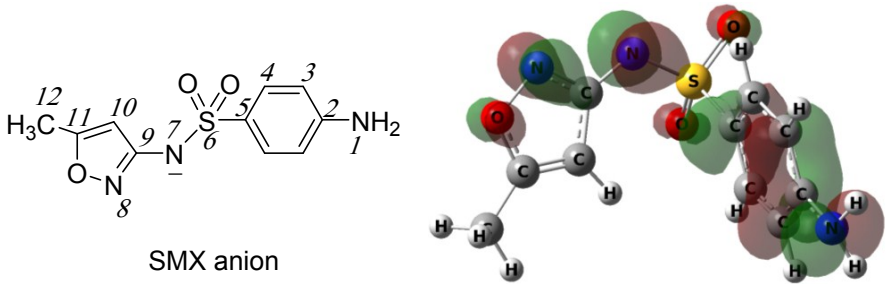


Figure S5. The atom labelling (attack sites) shown in the structure of SMX anion (left) and the HOMO of SMX anion (right) shown at the isovalue of 0.04

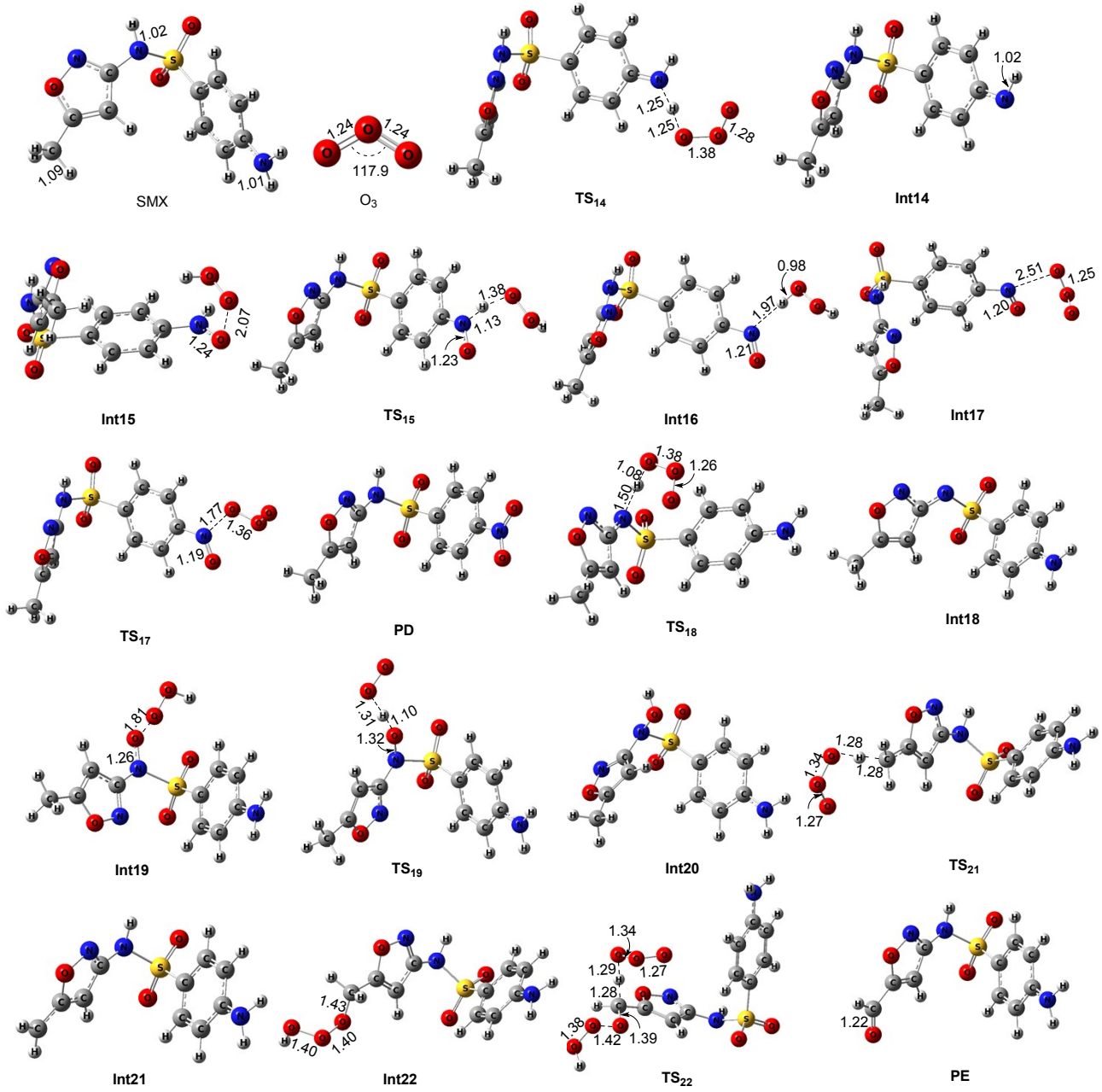


Figure S6. Optimized geometries of TSs and intermediates shown in Figure 7 (Interatomic distances are in Å)

Table S1. Activation energies (kcal mol^{-1}) for oxidation at different sites presented in Figures 2 and 3 and Table 1.

	DA mechanism	HAT mechanism
site 1	28.2	7.9
site 2	20.8	-[b]
site 3	14.4	31.0
site 4	24.7	33.3
site 5	18.8	-[b]
site 6	38.5	-[b]
site 7	39.1	13.9
site 8	27.9	-[b]
site 9	31.4	-[b]
site 10	21.9	50.8[c]
site 11	21.0	-[b]
site 12	-[a]	20.5

[a] All attempts to locate this TS were fruitless. [b] Not available. [c] This TS has several small imaginary frequencies corresponding to weak rotation of functional groups, which could have minor entropy contribution.