Structures and reaction rates of the gaseous oxidation of SO₂ by an $O_3^{-}(H_2O)_{0-5}$ cluster – a density functional theory investigation

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General Comments

The manuscript reports and discusses computational results that are relevant to understanding the atmospheric chemistry of SO₂. I am less concerned than the other reviewer about the reliability of the quantum chemistry method, although I agree that CCST(T) calculations should be performed on some of the reactions. The manuscript merits final publication in *Atmospheric Chemistry and Physics* after a few issues are addressed. My only concerns are with the organization and use of scientific terminology.

Specific Comments

p. 29653, line 28 (for example): The authors' use of "tight" and "loose" to describe transition states is non-standard. A tight transition state is one that corresponds to a first-order saddle point on both the potential energy and free energy surfaces, while a loose transition state (often involving a simple bond homolysis) corresponds to a first-order saddle point only on the free energy surface.

p. 29654, line 6: It is actually a well-established fact that in $S_N 2$ reactions, solvation preferentially stabilizes reactants more than transition states because charge is much more delocalized at transition states. See, for example, the work of J. I. Brauman (*J. Am. Chem. Soc.* **1977**, *99*, 4219).

p. 29656, lines 15-16: Please clarify this sentence.

Section 3.4 and Figure 9: This discussion of equilibrium should be clarified as well. One change that would help is moving the last sentence of Section 3.5 into Section 3.4.

Technical Corrections

p. 29656, line 6: "electronegativities" should be "electron affinities"

p. 29660, line 11: Please define "hTST"

p. 29665, line 19: The reference to Atkins' physical chemistry textbook is incorrect.