We thank the Referee for the constructive comments on our manuscript. Below are our point-to-point replies to the different questions raised by the Referee. For clarity, the Referee's comments are reproduced in blue color text and modified/inserted text in the revised manuscript are in red color text.

Authors are Narcisse Tchinda Tsona and Lin Du

Recommendation: This paper is publishable subject to minor revisions noted. Further review is not needed.

Comments: The authors have theoretically studied the role of the superoxides such as O2- in SO2 oxidation. The simulations were performed using a combination of DFT and CC levels of theory (CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ). Calculations were performed in the gas phase with and without one water molecule. Two possible mechanisms for the titled reaction were suggested and considered.
It is well known, that sulfur oxidation products play an important role in the atmosphere: formation of secondary aerosols, clouds and acid rains. Therefore, this theoretical work is an important contribution to a better understanding of the total mechanism of atmospheric sulfuric acid formation. I recommend publication this paper in the Atmospheric Chemistry and Physics Discussions after minor revisions.

Referee's comment:
Page 1, line 18. Misspelling the word "modelling". It does not need double LL.

Authors' reply
This has been corrected.

Referee's comment:
Page 3, line 9. Does not need a dot in the middle of sentences "with O3. in"

Authors' reply
This has been corrected.

Referee's comment:
Page 6, line 10. Delete the empty space between "4. 5"

Authors' reply
This has been corrected.

Referee's comment:
Page 12, line 16. Need to add a negative charge to the formula O2SOO.

Authors' reply

This has been corrected.

Authors' reply

The sentence at Page 3, Line 25-27 was re-written as:

"As the substrate in this study is a radical anion, all stationary points in the energy surface were optimized using density functional theory (DFT) based on the UM06-2X density functional (Zhao and Truhlar, 2008) and the aug-cc-pVTZ basis set (Dunning Jr et al., 2001), setting the charge to -1 and the spin multiplicity to 2."

Authors' reply

The IRC analysis was performed as indicated at Page 3, Line 4, they indeed connected the transition states to the pre-reactive complexes and the products.

Authors' reply

The reaction was performed in the gas-phase, exclusively. In the gas-phase, it was shown that only one water molecule can attach to O2SOO- and we also verified from our calculations that the addition of a second water vapor molecule to RC2 is not favorable under atmospheric conditions. It is, however, possible that O2SOO- would bind several water molecules in the liquid phase and the reaction properties would then be greatly affected.

The energy of TSW2 being lower than the energy of RCW2 is likely the effect of correlation since without CCSD(T) correction, TSW2 lies above RCW2. This difference in energy can also be explained by the difference in the electronic configurations of the two outer oxygen atoms of the O_3 moiety in the two transition states.

This information has been updated in the revised manuscript at Page 9, Lines 16-18 as:

"Another reason for this substantial drop in energy barrier is the difference in the electronic configurations of the two outer oxygen atoms of the O_3 moiety in the two transition states that form O_2 with different multiplicities in the products."

Authors' reply

The units used in Eq. (4) are CGS units, whereas SI units are used in Eq. (5).

Constants and variables	CGS units	SI units
T	K	K
k_B	1.38×10^{-16} erg K^{-1}	1.38×10^{-23} J K^{-1}
h	6.63×10^{-27} erg s	6.63×10^{-34} J s
q	4.80×10^{-10} statC	1.60×10^{-19} C
ε_0	$1/(4\pi)$	8.85×10^{-12} F m^{-1}
μ	g	kg
α	cm^3	F m^2
α_D	StatC cm	C.m

The following related sentences were added in the manuscript.
Page 6, Lines 13-15:
"The constants and variables in Eq. (4) and Eq. (5) are given in centimetre-gram-second (CGS) system of units and International System (SI) units, respectively. Details on these units are given in the Supplement."