This manuscript investigated the gas-phase formation mechanism of nitric sulfuric acid (NSA) from the SO_3+ HNO_3 reaction, as well as its subsequent enhancement in sulfuric acid–ammonia nucleation. The results found that NSA is a novel nucleation precursor. The topic is relevant to atmospheric chemistry and the manuscript is generally readable. In my opinion, the present work may be suitable for publication in ACP. However, I note the absence of any discussion regarding field observations of NSA. I also have several comments and suggestions, which follow.

1) Please provide the description of the calculation method for the reactions of SO_3 with HNO_3.
2) In global minimum search step, how did you deal with the calculation results that failed during optimization or that ended up with imaginary frequencies?
3) Where did the authors take the SA-A data from? Or were the clusters recalculated in the present work?
4) Please clarify whether the NSA has determined the most stable structure.
5) Since NA have been detected in the atmosphere of various polluted cities, it would be interesting to see the nucleation rate and cluster growth pathway at ambient conditions more typical to polluted urban environments, that is, higher coagulation sink value, e.g., 2×10^{-2} s^{-1}.
6) In the ACDC simulation, why are the low level energies calculated at M06-2X method used in the input file, rather than high level energies calculated at DLPNO-CCSD(T) method?
7) Figure3. In some cases, the structure obtained from the optimization method may differ from the result of the dual-level calculation; the authors need to explain why the most stable structures obtained at the DLPNO-CCSD(T)/aug-cc-pVTZ//M06-2X/6-311++G(2df,2pd) level were not presented.
8) Line 246, 271-277, missing references.
9) Line 297-298, How is the NSA/SA ratio determined?
10) Figure 1, the figure is unclear and what is the reference state? I think it is sufficient to provide ΔE and there is no need to provide the ICR.
11) Move Figure 2 to SI
12) Figure 4, it is difficult to understand. What do the circles of different sizes represent? It is recommended to provide specific values.
13) Figure 6a, Provide values of flux out.