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The role of ammonia in sulfuric acid ion induced nucleation

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Abstract. We have developed a new multi-step strategy for quantum chemical calculations on atmospherically relevant cluster structures that makes calculation for large clusters affordable with a good accuracy-to-computational effort ratio. We have applied this strategy to evaluate the relevance of ternary ion induced nucleation; we have also performed calculations for neutral ternary nucleation for comparison. The results for neutral ternary nucleation agree with previous results, and confirm the important role of ammonia in enhancing the growth of sulfuric acid clusters. On the other hand, we have found that ammonia does not enhance the growth of ionic sulfuric acid clusters. The results also confirm that ion-induced nucleation is a barrierless process at high altitudes, but at ground level there exists a barrier due to the presence of a local minimum on the free energy surface.

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