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The role of Eucalyptol in new particle formation

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Aerosols are ubiquitous in the Earth's lower atmosphere. Sulfuric acid and water probably have an important role in the formation of new atmospheric particles. However, in many cases the observed rates of particle formation greatly exceed those expected on the basis of binary sulfuric acid-water nucleation. Several alternative processes have been proposed, one of the less known is the ternary nucleation involving organic compounds.

Recent field measurements carried out in Australia (1) shows some nucleation events related with the organic compounds liberated to the atmosphere by eucalypt forest, one of the dominant compounds found during measurement campaign was the Eucalyptol (1,8-cineole), with the empirical formula $C_{10}H_{18}O$.

In order to evaluate the potential role of this compound in new particle formation, we have performed quantum chemical calculation on clusters containing up to four sulfuric acids and one eucalyptol. We have calculated the formation free energy in the conditions found in filed measurements, and we have compared it to the formation energy of pure sulfuric acid clusters and ammonia containing clusters.

We have found that the presence of eucalyptol lowers the nucleation barrier for sulfuric acid clusters, this lowering effect comparable to the effect of ammonia. The results support the role of eucalyptol in nucleation events observed in field measurements.

(1) M. Kulmala, T. Suni, et al: A new feedback mechanism linking forests, aerosols, and climate, Atmos. Chem. Phys. Discuss., 3, 6093-6107, 2003