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Uncovering the formation mechanism of atmospheric nanoparticles[1]

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Atmospheric aerosol affect human health, visibility and radiation budget of the Earth. The current estimate is that 20-80% of aerosols particles are formed in the atmosphere by condensable gases. Experimental and theoretical data indicates that the formation of new particles in the atmosphere in most cases very likely involves sulphuric acid assisted with some base molecules. The role of ions in atmospheric particle formation is has been widely discussed during recent years. The diameter of the forming clusters is 1-2nm, falling between the smallest size where brute force quantum mechanical treatment is possible, and macroscopic size where bulk thermodynamics in applicable. Recent experiments at the CLOUD chamber in CERN have provided molecular-level information on the charged fraction of the nucleating clusters, but the theoretical framework needed to convert this into information on neutral clusters is still lacking. We have used a cost-effective multi-step computational chemistry method involving automated configurational sampling, density functional theory geometry optimizations and coupled-cluster energy calculations, to study the stability of charged and neutral sulfuric acid clusters containing ammonia and dimethylamine. Combined with a cluster dynamics model ACDC, we are able to replicate the formation rates observed in the CLOUD chamber, as well as match observed formation rates in Hyytiälä Smear II station in Finland.

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