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Assessing nucleation in cloud formation modelling for Brown Dwarf and Exoplanet atmospheres

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Context. Substellar objects such as Brown Dwarfs and hot Jupiter exoplanets are cool enough that clouds can form in their atmospheres (Helling & Casewell 2014; A&ARv 22)). Unlike Earth, where cloud condensation nuclei are provided by the upward motion of sand or ash, in Brown Dwarf and hot Jupiters these condensation seeds form from the gas phase. This process proceeds in a stepwise chemical reaction of single monomer addition of a single nucleation species, referred to as homogeneous nucleation. The rate at which these seeds form is determined by the local thermodynamic conditions and the chemical composition of the local gas phase. Once the seed particles have formed, multiple materials are thermally stable and grow almost simultaneously by chemical surface reactions. This results in the growth of the condensation seeds to macroscopic particles of μm size. At the same time, the gas phase becomes depleted. Once temperatures become too high for thermal stability of the cloud particle, it evaporates until its constituents return to the gas phase. Convection from deeper atmospheric layers provides element replenishment to upper, cooler layers allowing the cloud formation process to reach a stationary state (Woitke & Helling 2003; A&A 399).

Aims. The most efficient nucleation is a 'winner takes all' process as the losing molecules will condense on the surface of the faster nucleating seed particle. We apply new molecular $(TiO_2)_N$-cluster and SiO vapour data to our cloud formation model in order to re-asses the question of the primary nucleation species.

Methods. We apply density functional theory (B3LYP, 6-311G(d)) using the computational chemistry package GAUSSIAN 09 to derive updated thermodynamical data for $(TiO_2)_N$-clusters as input for our TiO_2 seed formation model. We test both TiO_2 and SiO as primary nucleates assuming a homogeneous nucleation process and by solving a system of dust moment equations and element conservation for a pre-scribed Brown Dwarf/hot Jupiter DRIFT-PHOENIX atmospheric model temperature-pressure structure.

Results. We present updated Gibbs free energies for the new $(TiO_2)_N$-clusters. We discuss the effect of this new data on the resulting cloud structure and cloud properties like particle number density, grain sizes and grain composition. We find SiO to be the more efficient nucleation species. However, subsequent SiO condensation onto seed particle mantles result in element depletion, reducing the number density of gaseous SiO and reducing the efficiency of nucleation. Therefore, TiO_2 remains therefore the primary nucleation species (Lee et al. 2014; arXiv:1410.6610).