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Mixed metal oxides as primary dust condensates

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Metal oxides are promising candidates as a primary dust condensate in the atmospheres of oxygen-rich evolved stars. Typically, Al2O3 and TiO2 are considered as they represent the most prominent case studies. However, also mixed metal oxides, containing more than one metal, represent realistic alternatives to Al2O3 and TiO2 as a first solid in the rich gas mixture of
stellar atmospheres. Their related nano-sized metal oxide clusters, often referred to as seed particles, trigger the onset of stellar dust formation and the mass return into the interstellar medium.
However, the nature and the formation of these clusters are not well understood.
Nano-sized clusters are fundamentally different from crystalline bulk material.
As a result of their finite size and quantum interactions clusters exhibit a wide range of different structures and potential energies. The most favourable structures with the lowest potential energies are typically not spherical and can generally not be extrapolated from the bulk.
We aim to shed light on the initial steps of cosmic dust formation (i.e. nucleation) in oxygen-rich environments by a quantum-chemical bottom-up approach. Therefore, we study different metal oxide clusters containing Mg, Al, Si, Ti, and Ca, including various combinations and stoichiometries.
Starting with an elemental gas-phase composition including radioactive isotopes, we construct a detailed chemical-kinetic network describing the formation and destruction of molecules and dust-forming clusters up to the size of 16 atoms.
The reaction rates are derived from their potential energy surfaces using global optimisation techniques and transition state theory. Owing to the increasing computational complexity the subsequent coagulation of clusters with more than 16 atoms is calculated using accurate thermo-chemical data.
The resulting extensive network is applied to two model stars, representing a semi-regular variable and a Mira-type AGB star, and to different circumstellar gas trajectories including a non-pulsating outflow and a pulsating model.
We provide energies, bond characteristics, electrostatic properties and vibrational spectra of the clusters as a function of their size, oxygen content, and temperature.
Our preliminary model results predict temperature- and density dependent abundances of molecules and clusters, dust compositions and sizes, IR spectra, and chemical timescales that are compared to recent observations as well as to grain properties of meteoritic stardust.

Session

Dust and presolar grains

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