Forming silicate and alumina dust in the wind of the O-rich AGB IK Tau

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We model the circumstellar envelope of the oxygen-rich Mira star IK Tau, characterized by a C/O ~ 0.75, and a pulsation period of ~ 470 days. Periodic shocks induced by pulsation with speeds of 10-32 km/s temporarily enable a non-equilibrium chemistry to take place between 1 and 10 R* above the photosphere. The impact of shocks on the circumstellar gas is modelled in two stages (ref. Cherchneff (2006, 2012)):

1. a thin 'chemical' dissociation layer corresponding to after the shock front, and
2. a hydrodynamic adiabatic cooling region.

We describe the formation of several molecules pertaining to O-rich environments using a chemical kinetic approach applied to the above shock conditions. The chemistry model also includes the formation pathways to small clusters of silicates (enstatite, $Mg_2Si_2O_6$, and forsterite, $Mg_4Si_2O_8$ dimers), and clusters of alumina (Al_8O_{12}), metal oxides and sulphides. We perform quantum mechanic calculation on the DFT level to gain insight on cluster structures, energetics, reaction mechanisms and finally possible formation routes.

The results for the gas phase agree well with the most recent observational data for IK Tau. Major 'parent' molecules form in the shocked gas under non-equilibrium conditions and include CO, H_2O, SiO, SiS, SO, SO_2 and CO_2. Silicate clusters form efficiently very close to the star at small pulsation phase whereas alumina clusters form at larger pulsation phases close to the star. Forsterite dimers are the most abundant clusters at 5 R*, followed by enstatite and alumina. The mass of dust estimated from our cluster abundances agree with the dust-to-gas mass ratio derived for IK Tau.

We also present preliminary results on the formation of molecules and dust clusters for a grid of models, varying in shock speed, metallicity, stellar evolution stage, and initial elemental abundances. Our best results for IK Tau are obtained for a one solar mass star of C/O = 0.75, shock speeds of 32 km/s and 25 km/s, and the photosphere with solar abundances. These results indicate that 'parent' molecules and dust grains form under non-equilibrium conditions in the inner wind of IK Tau.