Circumstellar Dust Shells Around Oxygen-Rich Long-Period Variable Stars

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We present a consistent model for circumstellar dust shells (CDS) around O-rich long-period variable stars (LPVs). Since almost all carbon is locked up in the chemically inert CO molecule in an O-rich environment, the grains only can be formed from molecules containing the remaining oxygen and the less abundant elements Mg, Si, S, Fe, Al, Ti. This leads to a heterogeneous element composition of the emerging dust component. Assuming chemical equilibrium in the gas phase, we describe the formation of the seed particles by means of a modified classical nucleation theory. The most promising seed nuclei appear to be TiO2 clusters, which grow by addition of those molecular species which have a stable solid phase under the local thermodynamic conditions prevailing in the CDS. For calculating the nucleation rates, the Gibbs free energies of Tix Oy clusters are used, resulting from quantum mechanical Density Functional Theory calculations of their structures. We present the results of a consistent dust shell model characterised by L. = $2*10^4~L_{\odot},~T_{*}$ = 2000K, M_{*} = 1 $M_{\odot},~\triangle u_{p}$ = 5 kms $^{-1},~P$ = 300d, and solar element composition. This model produces a mass loss rate of $\dot{M} \sim 5*10^{-5} {\rm M}_{\odot}$ /yr and an outflow velocity of $v_{\infty} \sim 15 \text{ kms}^{-1}$. The radii of most of the dust grains range between 0.01 and 0.1 μ m. The chemical composition and temporal evolution of the resulting dust grains and their influence on the generation of massive outflows from oxygen-rich LPVs will be discussed.