# Macro-Molecules in Model Atmospheres

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We present calculations of partial pressures of macro-molecules in stellar photospheric MARCS (Jørgensen et al. 1992, *A&A*, 261, 263) models of carbon stars. The molecular equilibrium data included were taken from Cherchneff & Barker (1992, *ApJ*, 394, 703). Our aim is to study the molecular route to the formation of carbonaceous grains. In our hydrostatic models the largest molecule that appears in a significant amount is $C_6H_2$. Open-shell species (radicals) have comparable abundances but all of them are found to be too rare to support grain formation, or to affect the photospheric structure by levitation.

A hydrodynamic model atmosphere (kindly provided to us by A. Fleischer) has higher pressure in the outer atmosphere, and much larger density, than our corresponding hydrostatic model. Although the dynamical model extends to much lower gas pressures, the $T - P_{\rm gas}$ structures of the dynamical and hydrostatic models are quite similar in the region of overlap. The same molecular species are therefore formed in about the same amount in the overlap-region of the two models. Chemical equilibrium calculations for $(T, P_{\rm gas})$ values corresponding to a hydrodynamic (wind) model show large concentrations of PAHs (polycyclic aromatic hydrocarbons) in the layers with $T \leq 850\,{\rm K}$ (i.e., cooler than the photospheric models). Larger PAH molecules such as $C_{22}H_{14}$-benzo[c]crysene dominate over smaller PAHs and other hydrocarbon molecules. An exploration of the $T - P_{\rm gas}$ plane, $T\epsilon\,[750\,{\rm K}, 1300\,{\rm K}]$ and $\log P_{\rm gas}\,\epsilon\,[-5{,}3]$ (dyn/cm$^2$), shows that macro-molecules bind a large fraction of the available C not bound in CO and can bind even more C than CO for $C/O \geq 5.0$. The time scale of a realistic wind model is, however, much shorter than the time required for PAH formation. Hence, the hydrostatic as well as the hydrodynamic models have problems with forming carbon grains via the PAH route.

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