Some Condensation Calculations Using Chemical Equilibria

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A number of extensive chemical equilibrium calculations have recently been performed for temperatures below 2000 K, with mixtures containing over 200 gaseous species and the allowance for the formation of over 60 condensates. These calculations were based on the minimization of the Gibb's free energy.

For calculations performed with a solar mixture (C/O=0.55, but excluding the inert gases) at a total pressure of 500 dyn cm^{-2}, we found the most important condensed species to appear are $MgSiO_3$ and Mg_2SiO_4, with SiO_2 not appearing, which is in good agreement with Lattimer et al. (1978) and Tarafdar (1987). As expected, those gaseous species like SiO that contain at least one element that is also present in a condensed species, decrease sharply in abundance when the corresponding condensate appears. However, many flourine, chlorine and sulfur bearing species such as CS, increase in abundance relative to the case when condensation is neglected. This can be explained by these elements being released from other molecules containing an element that does condense out, such as SiS releasing sulfur when silicon condenses as silicates.

Calculations performed for a number of different C/O ratios show that for the carbon rich cases the condensation of graphite and SiC decrease the gas phase C/O ratio, and in the oxygen rich cases oxides and silicates increase the gas phase C/O ratio; in both cases this ratio moves closer to unity. Of particular interest are the weakly oxygen rich mixtures with C/O ratios greater than about 0.83, as sufficient oxygen is removed from the gas phase by oxides and silicates that graphite can condense out, and species like HCN and C_2H_2 which would otherwise have negligible abundances, can increase by several orders of magnitude.

Lattimer, J.M., Schramm, D.N., and Grossman, L. (1978), Ap.J. 219, 230.

Tarafdar, S.P. (1987), in Astrochemistry, M.S. Vardya and S.P. Tarafdar, Eds., IAU Symposium No. 120, 559.

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