FORMATION OF SMALL IRON CLUSTERS IN CIRCUMSTELLAR ENVELOPES

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Abstract.

We have investigated the role of small iron clusters as possible seeds for the formation of dust particles in circumstellar envelopes. Using cluster data available in the literature we constructed a simple cluster model in order to calculate the partition function and the Gibbs energy of formation for Fe_N clusters ($N \leq 19$). Based on these data we have calculated the equilibrium densities of such clusters under different physical conditions.

The results are discussed with respect to the problem of the primary dust condensate in M–type stars.

1. Introduction

During the late stages of their evolution, low and intermediate mass stars undergo a phase of heavy mass loss forming a circumstellar dust shell. Details of the microscopic processes, which are responsible for the formation of dust are yet unrevealed. A major problem is the lack of fundamental data of molecules and clusters involved in the nucleation process. In this paper we focus on the basic thermodynamic properties of small iron clusters needed for the calculation of their nucleation rate.

2. Method

We calculated the thermodynamic properties, i.e. the entropie $S^{\ominus}$, the enthalpie of formation $\Delta_f H^{\ominus}$, and the Gibbs free energy of formation $\Delta_f G^{\ominus}$, of small iron cluster Fe_N ($N \leq 19$) directly from the molecular data. For a detailed discussion of the thermodynamic concepts and assumptions we refer to a forthcoming paper (John *et al.*, 1997).

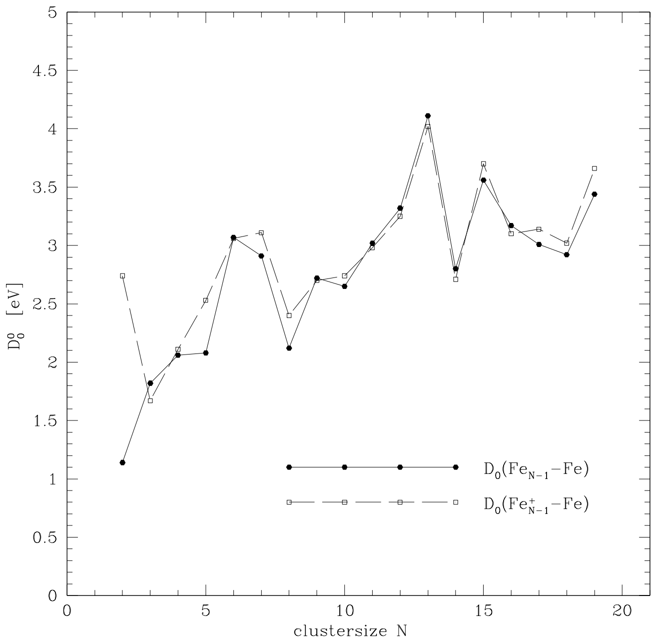

Figure 1. Dissociation energy D_0^0 of neutral (•) and ionized (□) iron clusters, measured by Lian *et al.* (1992). Maxima at N = 6, 7, 13, 15 and 19 belong to clusters that show enhanced stability.

Of particular importance for the aim of this work is the dissociation energy D_0^0 of the iron clusters, for which we used the experimental data of Lian *et al.* (1992), plotted in figure 1. It is important to note that the dissociation energy shows a strong dependence on the cluster size N. Especially the smaller clusters ($N = 2, 3$) are not very stable.

The other relevant data (i.e. vibrational frequencies, principle moments of inertia and deep lying electronic states) where deduced from data available in the literature (e. g. Moskovits and DiLella ,1980, Shim and Gingerich, 1982). Details of the method will be published in the above mentioned paper.

3. Results

Based on the derived thermodynamic properties of small iron clusters we calculated the equilibrium abundances of these clusters relative to the monomer ($f(N)/f(1)$) using the law of mass action. For the monomer, which is the Fe–atom, we assumed a density of $f(1) = 4 \cdot 10^5\,\mathrm{cm}^{-3}$, a typical value in the inner regions of a circumstellar envelope. The resulting cluster size distribution function is plotted in figure 2 for four different temperatures ($T = 600, 500, 450$ and 400 K). For the temperatures $T = 600\,\mathrm{K}$

and for $T = 500\,\mathrm{K}$ the critical cluster, defined as the least abundant species, is the Fe_5–molecule. As it can be seen from figure 2, effective nucleation can not take place at this temperatures due to the very low density of the critical cluster. One can infer from this figure that effective nucleation starts at temperatures between 500 and 450 K.

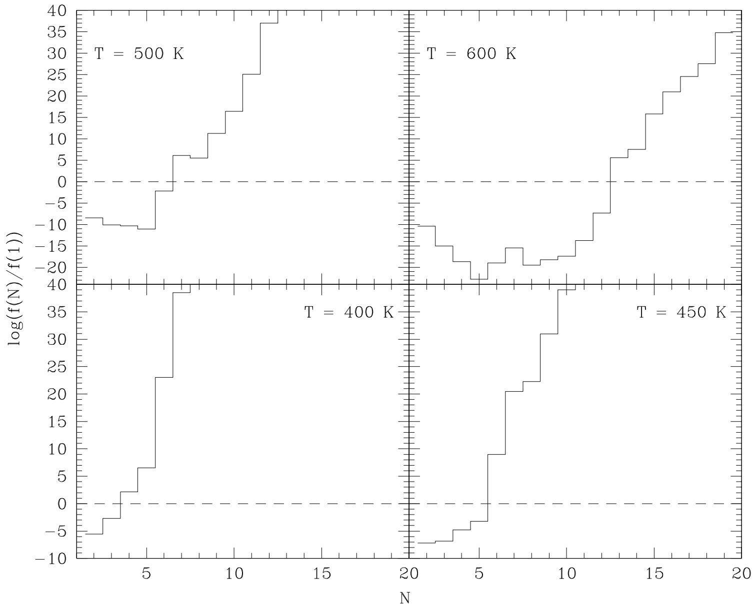

Figure 2. Equilibrium densities of small iron clusters normalized to a monomer density of $n_{mo} = 4 \cdot 10^5\,\mathrm{cm}^{-3}$.

Finally we calculated the equilibrium densities of small iron clusters in the stationary outflow of a M-type star, using a simple spherical symmetric wind model for the density ($n_{<H>} \propto r^{-2}$) and temperature structure (given by radiation dilution).

As can be seen from the resulting plot in figure 3, the cluster densities reach a maximum value at about $10R_*$, which corresponds to a temperature of approximately $540\,\mathrm{K}$. Due to the high abundance of the $Fe(OH)_2$ molecule (see lower panel in figure 3) the particle densities of clusters larger than the Fe_7–cluster are very low.

4. Conclusion

In view of these results it seems unlikely, that iron clusters could serve as the first seeds for the dust formation process in late M-type stars, because the onset of effective nucleation occurs at temperatures well below 600 K, which is much lower, than the typical values, inferred from observations of the inner edge of circumstellar dust shells (see e.g. van der Veen *et al.*, 1995).

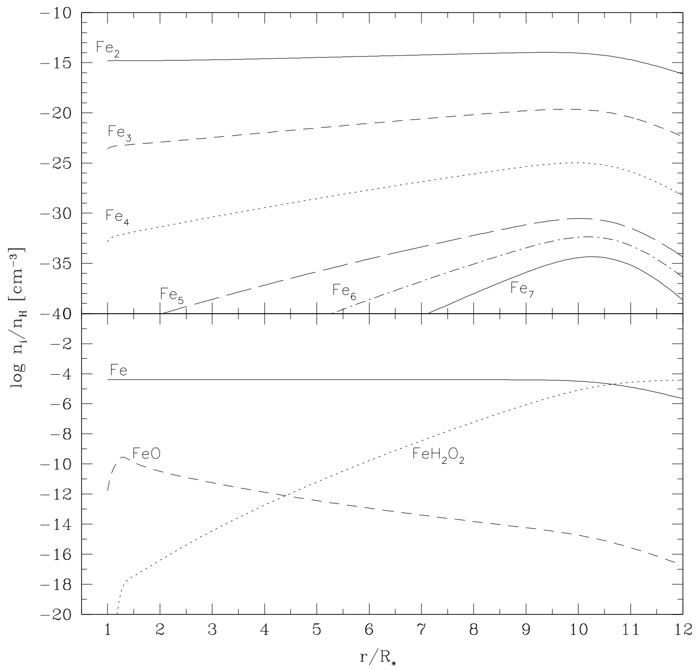

Figure 3. Equilibrium densities of small iron clusters ($N \leq 10$, upper panel) and some competitive molecules (lower panel) in the stationary outflow of a M-type giant star with a constant outflow velocity of 1 km/s, a luminosity of $10^4\,L_\odot$, an effective temperature of 2500 K, a mass loss rate of $10^{-6}\,M_\odot/$ yr and solar elemental abundances.

In some peculiar environments, which show for example an enrichment of iron, this picture may change and iron may nucleate effectively. In order to finally decide this question, a consistent description of the nucleation process of iron is needed. Some of the necessary data are now available. Up to then, the problem of the real primary condensation sequence in M-type stars still remains unsolved.

References

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