DESORPTION MECHANISM OF GASES FROM INTERSTELLAR GRAINS AND PAH MOLECULES

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SUMMARY : Many gases, including CO, should be condensed at the temperature of interstellar grains in the absence of efficient desorption mechanisms. We consider such mechanisms and find that impulsive heating by X rays and *heavy cosmic rays* (iron group) are the most efficient ones.

For CO rich mantles, we conclude that species as CO, N_2, O_2 and probably H_2CO, NH_3, H_2O should be desorbed in most cases including dense and obscure regions. For mantles composed mainly of refractory ices (H_2CO, NH_3, H_2O) we expect very little desorption.

The case of PAH molecules that may offer a larger surface for condensation than grains is also discussed.

1. NEED FOR EFFICIENT DESORPTION MECHANISMS

Léger (1983) among others has considered the process of the condensation of CO onto grains as an example of the process of the depletion of gas phase material. His basic conclusions are (i) that when CO collides with a grain it sticks, and (ii) the time scale for such collisions is short compared to the lifetime of a typical cloud. As a result of (i) and (ii), inside a dark cloud where the grain temperature is low, if there is no desorption mechanism, grains must accumulate relatively quickly essentially all the CO (Fig. 1).

Observationally, it is clear that all the CO is not in grains. In particular, it is necessary to find an appropriate desorption mechanism.

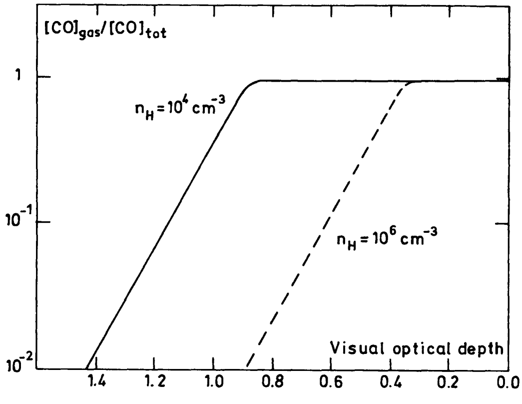

Figure 1 : Expected depletion of CO in a cold molecular cloud versus the radial visual optical depth if the only desorption mechanism is steady thermal desorption.

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2. IMPULSIVE HEATING BY X-RAYS AND COSMIC RAYS

Several mechanisms may act to desorb grain mantles. Turbulent collisions between grains can be important provided that the relative velocity of the grains is sufficiently high (d'Hendecourt et al., 1982). Turbulent convection to the outer parts of a cloud and subsequent photodesorption (Boland and de Jong, 1982) may be active. The rate for these processes are presently more uncertain than the desorption produced by X-rays and cosmic rays, and, in any case, the different desorption mechanisms are cumulative and not exclusive.

Léger, Jura and Omont (1985) concentrated on impulsive heating of grains by X-rays and cosmic rays, and used recent measurements of the fluxes of these particles that were not previously available. The temperature increase of the grains following impulsive heating is estimated using new laboratory specific heat measurements in both the classical thermal evaporation picture and the chemical explosion model of Greenberg and d'Hendecourt. Both whole grain heating and local hot spot desorption are considered. The effects of the relatively rare *heavy cosmic rays are found to dominate*, except for the smallest grains, because the energy deposition in matter depends as the square of the charge of the impinging particle.

The rate of desorption of CO by classical evaporation due to cosmic rays is displayed on Fig. 2 and that of chemical explosion on Fig. 3. The total expected depletions are in Table 1 and 2.

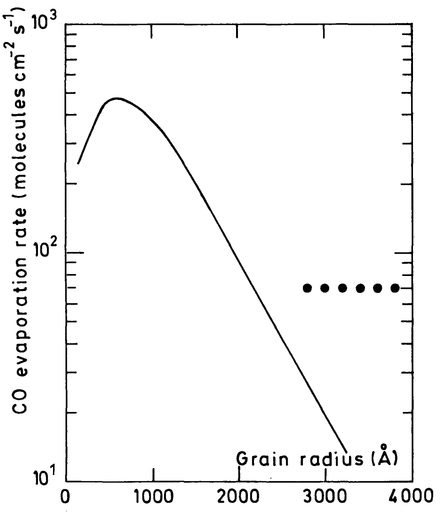

Figure 2 : Rate of CO molecules classical evaporation from silicate grains due to Cosmic Rays. The rate induced by the spot heating (•••) of energetic particle is remarkably independent of grain size and dominates for the largest grains.

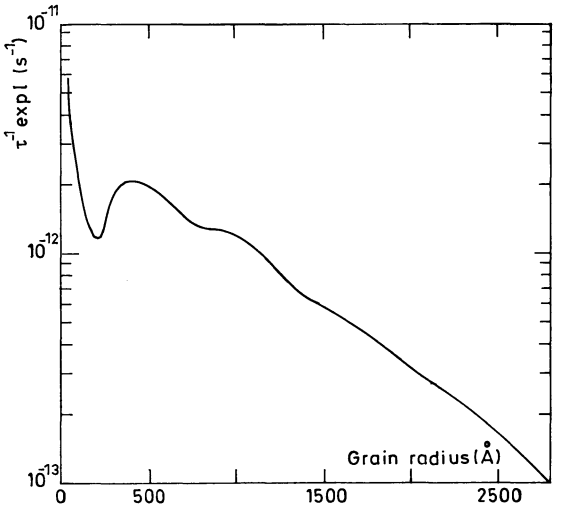

Figure 3 : Rate of chemical explosion per silicate grain (model by Greenberg and d'Hendecourt) triggered by Cosmic Rays.

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n_H	$a_+ = 0.25\,\mu m$		$a_+ = 1.2\,\mu m$	
	$\tilde{\beta} = f_{gas}$	$1-\tilde{\beta} = f_{cond}$	$\tilde{\beta} = f_{gas}$	$1-\tilde{\beta} = f_{cond}$
(cm^{-3})	(%)		(%)	
10^3	99	1	30	70
10^4	20	80	3	97
10^5	2	98	0.3	–
10^6	0.2	–	0.03	–

Table 1 : Expected depletion of CO for classical evaporation only. The grain size distribution is assumed bo be $n(a) \propto a^{-3.5}$ with upper cutoff either $a_+ = 0.25\ \mu m$ or $a_+ = 1.2\ \mu m$.

n_H	$\tilde{\beta} = f_{gas}$	$1-\tilde{\beta} = f_{cond}$
(cm^{-3})	(%)	
10^3	99.5	0.5
10^4	95	5
10^5	70	30
10^6	20	80

Table 2 : Expected depletions of CO for chemical explosions acting alone. $\tilde{\beta}$ is the gaseous fraction of CO while the ultraviolet flux in the medium is supposed to be efficient to provide the reacting radicals. The grain size distribution is assumed to be that derived by Mathis et al. (1977) from observations of the diffuse medium: $n(a) \propto a^{-3.5}$ with an upper cutoff $a_+ = 0.25\ \mu m$.

3. RESULTING DESORPTION

For CO rich mantles, the chemical explosions and the thermal desorption driven by the whole grain heating are quite efficient for grains with sizes $< 0.25\ \mu m$ in moderately obscure regions ($A_V < 5$ mag. measured from the interior to the cloud surface) with densities $< 10^4\ cm^{-3}$.

The spot heating evaporation operates even on very large grains and it is still active in obscure regions. While it cannot prevent a substantial depletion onto big grains, the e-folding time for the condensation onto these grains, $10^7(10^4/n)$ yr, is so long that steady state conditions may not be achieved in many clouds. Therefore, we find that *we can understand the small depletions (< 30%) of species such as CO observed in regions with $A_v < 5$ mag and $n(H) < 10^4\ cm^{-3}$.*

More refractory ices (H_2CO, NH_3, H_2O in very dense and obscure regions are expected to be efficiently desorbed from CO rich mantles if there are internal ultraviolet sources inside the clouds at the level of 10^{-4} times the diffuse interstellar flux (Prasad and Tarafdar, 1983 ; Norman and Silk, 1980). Even in the absence of UV at that level, if segregation between refractory and volatile species does not occur during the very fast ($< 10^{-10}$) spot heating process, some desorption of refractory ices from CO-rich mantles still proceeds. This could be a clue to understanding *the observations of these molecules (such as NH_3)* in the gas phase of dense clouds.

For mantles composed mainly of refractory ices (H_2O, NH_3, H_2CO) we expect very little desorption.

4. ROLE OF POLYCYCLIC AROMATIC HYDROCARBONS (PAHs) MOLECULES

There is now strong evidence of a new important component of the interstellar medium : clusters of size intermediate between the relatively

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small molecules observed mainly by radioastronomy and the conventional small grains, namely large PAH molecules (Léger and Puget, 1984). Their role in the interstellar chemistry has to be considered as they offer a geometrical cross section larger than grains. The first case to consider is the formation of H_2 (Omont, 1985). Large thermal fluctuations should allow desorption.

REFERENCES

- Boland, W., de Jong, T. : 1982, Astrophys. J. **261**, 110.
- d'Hendecourt, L.B., Allamandola, L.J., Baas, F., Greenberg, J.M. : 1982, Astron. Astrophys. **109**, L12.
- Léger, A. : 1983, Astron. Astrophys. **123**, 271.
- Léger, A., Puget, J.L. : 1984, Astr. & Astrophys. **137**, L5.
- Léger, A., Jura, M., Omont, A. : 1985, Astr. & Astrophys. **144**, 147.
- Norman, C., Silk, J. :1980, Astrophys. J. **238**, 158.
- Omont, A. : 1985, to be published in Astr. & Astrophys.
- Prasad, S.S., Tarafdar, S.P. : 1983, Astrophys. J. **267**, 603.

DISCUSSION

GREENBERG: In some recent (unpublished) experiments it has been shown that explosions can occur at temperatures lower than 27K if the heating is impulsive. We will be investigating this phenomenon in the future.

WILLIAMS: What is the concentration of radicals you have assumed to exist in your discussion of grain mantle explosions, and do you think that this value varies from point to point in the cloud?
LERGER: In fact, what we really need is the minimum ratio of UV flux versus molecular flux that permit the explosion. We have used the experimentally measured value ($\emptyset_{uv}/\emptyset_{mol} \geqq 0.1$).

BOLAND: A prediction of the circulation model of molecular clouds (cf. Boland and de Jong, 1984, Astron. Astrophys. 134, 87) is a relation between the circulation velocity and the abundances of HC_nN molecules in the sense that the highest HC_nN concentrations had to be found in clouds with the largest circulation velocities (= line widths).
(i) I suggest that the efficiency of evaporation of grain mantles decreases with the energy of the cosmic ray particles. What are the assumptions on the cosmic ray energies in your calculations? (ii) If evaporation of grain mantles by cosmic rays is efficient you should expect a correlation between cosmic ray fluxes and depletions. Can such a correlation be found in the existing observational data?
LEGER: (i) Conservatively we considered only H cosmic rays with E > 100 MeV and Fe cosmic rays with the same magnetic rigidity

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($E > 20$ MeV/nucl). (ii) It is correct that higher the cosmic ray flux higher is the expected depletion at least if you do not consider chemical explosions.

PIRRONELLO: Why the strong transient increase of temperature in the cylindrical region around the track of the impinging ion does not trigger, at least locally, a chemical explosion in the mantle?
LETER: Curiously enough, we found that the propagation of the chemical reaction is slower than the diffusion of heat ($t \sim 10^{-11}$ s). So conservatively we did not consider this triggering of chemical explosions.

CHADHA: You have shown the formation of a polycyclic hydrocarbon in your studies. How did you characterise this molecule and what would be the mechanism of its formation?
LEGER: The formation mechanism of PAHs is an open question. We suggest that graphite grain collisions can lead to graphite plane fragments which are PAHs when hydrogenated. Additional building up and erosion could be achieved by C, C^+ and O atoms respectively.