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Chemical constraints and microstructure in TMC-1 Core D

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Abstract. Microstructure has been detected in Core D of TMC-1. Unless it is confined or replenished by an as yet unexamined mechanism, this microstructure will dissipate on the sound-crossing timescale, which is less than 10^5 yr. We reconsider the large number of models that have been proposed to explain chemical variations in TMC-1 in an effort to determine whether chemical constraints require the microstructure to be confined or replenished for times much longer than the sound crossing timescale. We explore here a chemical model which, though consistent with the assumption of an age of 6 10^4 yr and a number density of H nuclei of 2 10^5 cm^{-3}, shows the richness in both molecular variety and abundances observed in Core D. In particular, the computed HC_3N fractional abundance relative to H_2 is 6 10^{-8}, in agreement with the latest observations of Ohishi & Kaifu (1998). Apparently, the chemistry of TMC-1 cannot be used to discard the possibility that TMC-1 Core D is young. This model has the following characteristics: the cosmic ray ionization rate is consistently larger than that usually assumed for dark regions; carbon atoms and hydrocarbons that strike grains are rapidly hydrogenated and promptly returned to the gas phase as methane; CO and N_2 striking grains are immediately returned to the gas phase unaltered; other chemical species containing at least one atom more massive than helium colliding with dust grains remain frozen on their surfaces; and the material other than hydrogen was initially in atomic form. For such a model to be viable, collapse of Core D must have been triggered by a stellar wind-driven shock of several km s^{-1}. This speed is low enough that magnetic moderation of the shock would have prevented the activation of a high temperature chemistry. The model results indicate that Core D would have fractional abundances of H_2O and O_2 at a core age of 6 10^4 yr consistent with the upper limits placed by very recent observations of Core D made with SWAS. The implications of this study are (1) that hydrogenation of atoms at the surfaces of dust grains may be a significant contributor to the chemistry of dark clouds; (2) that the special chemical nature of TMC-1 is due primarily to the exceptional youth of Core D.

Key words. ISM: clouds – ISM: TMC-1 – ISM: molecules

1. Introduction

The evolutionary age of an interstellar cloud, or of a clump within a cloud, is an important parameter in our understanding of the star formation process. Interstellar chemistry provides a powerful and widely-used method of age determination of interstellar clouds and clumps. The comparison of observational data of molecular abundances with results from the theoretical time-dependent models of interstellar chemistry gives information about the evolution of the gas in both static and dynamically changing environments. It would, however, be useful to have an independent measure of the age of interstellar material. In this paper, we question whether the microstructure observed in TMC-1 (Core D) may provide – through dynamical considerations – an independent upper limit to the age of material within that microstructure. If we could find no chemical model consistent with the age inferred from the dynamical arguments employed, we would have to conclude that the answer to our question will remain "no" at least until the dynamics have been explained with a more complicated hydrodynamic or hydromagnetic model.

TMC-1 is a ridge of dense cores that – partly because of its proximity – is one of the most frequently observed molecular sources in the sky. Its structure and chemical variations with position have been observed in a number of molecular lines (e.g. Hirahara et al. 1992; Ohishi et al. 1996; Harju et al. 2000), and it has been shown to be uniquely rich in chemical variety. The region in which the cyanopolyyne emissions peak is now often referred to as Core D (Hirahara et al. 1992).

Langer et al. (1995); Wolkovitch et al. (1997); and Peng et al. (1998) have resolved microstructure in Core D. Peng et al. (1998) have concluded that 19 of the 45 microclumps they found appear to be gravitationally unbound. The radii of the microclumps are typically about 3 10^{-2} pc. If unconfined, a microclump would disperse at roughly the

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internal sound speed of about 0.3 kms^{-1} on a timescale of around 1 10^5 yr. Though Peng et al. (1998) suggested that the Core D microclumps may be confined by a mechanism similar to that supposed by Bertoldi & McKee (1992) to confine translucent clumps detected in CO surveys of Giant Molecular Clouds (e.g. Williams et al. 1995), there is no compelling observational evidence requiring them to be older than 10^5 yr. In addition, no precise mechanism for continuously replenishing highly nonlinear microstructure that dissipates on the sound crossing time has been suggested. However, failure to find a chemical model compatible with Core D being younger than the sound crossing time in the microstructure would point to a confinement or replenishment mechanism being at work. In this paper, we consider the chemical models of TMC-1 in light of the possibility that Core D and the microclumps within it are younger than $\sim 10^5$ yr. For comparisons with chemical models, we shall adopt an age indicated by these arguments of 6 10^4 yr.

2. Previous chemical models

The variations with position in TMC-1 of chemical abundance, including in particular those of the cyanopolyynes, have been the subject of many theoretical studies.

In the 1980s TMC-1 was generally considered by chemical modellers to be a quiescent region in which dynamics play little role (e.g. Millar & Freeman 1984; Millar 1990). In fact, steady-state, purely gas phase chemical models cannot account for the high fractional abundances of cyanopolyynes and other complex carbon-bearing species measured towards TMC-1 (e.g. Millar 1990). However, relatively quiescent dark cores can generate high fractional abundances of such molecules if freeze-out of species more massive than helium on to dust grains occurs, but does so on a timescale larger than that required for the gas phase reactions to produce a gas phase chemical quasi-equilibrium (Ruffle et al. 1997). Hartquist et al. (1996, 1998) suggested that such a scenario might be appropriate to Core D. Clearly, models of Core D envisioned as a quiescent core are not consistent with an age less than the 10^5 yr indicated by the microclumps within it.

That dynamics might play a role in establishing high abundances of complex carbon-bearing species was the theme of papers by Chièze et al. (1991) and Williams & Hartquist (1991) who considered possible consequences of the microscopic mixing of material turbulently transported between different chemical states. While Williams & Hartquist (1991) took the view that such mixing would be confined to a boundary layer (cf. Rawlings & Hartquist 1997), Chièze et al. (1991) considered it to be a more extended phenomenon. However, in neither picture would Core D be a particularly young object, as the mixing would maintain a complex equilibrium chemistry.

Another model in which dynamics is invoked to explain the chemistry of Core D is that of Markwick et al. (2000). In this model Core D is again not a particularly young object. In their picture, Core D is an object which has existed for some time and in which wave activity has been recently triggered, with the consequence that explosive desorption of complex species formed on grain surfaces has occurred.

Time-dependent, purely gas phase models of dark cloud chemistry show that the abundances of complicated carbon-bearing species reach maxima and then decline as equilibrium is approached from atomic initial conditions (e.g. Millar 1990). Thus, Hirahara et al. (1992) suggested that Core D is a particularly young object, an idea explored further by Howe et al. (1996). Gwenlan et al. (2000) constructed time-dependent dense core chemistry models in which the material, except H_2, is initially in atomic form. They examined a wide range of assumptions in an attempt to find models compatible with the high HC_3N fractional abundance (relative to hydrogen nuclei number) of 6 10^{-8} measured towards Core D by Ohishi & Kaifu (1998). Several models were found by Gwenlan et al. (2000) to give fractional abundances of HC_3N in excess of 2 10^{-8}. These models are those in which atoms striking the grain surfaces are rapidly hydrogenated and returned to the gas phase as saturated species. Earlier work on the consequences of CH_4 injection into the gas phase for TMC-1 was reported by Brown & Charnley (1991). The only one of the Gwenlan et al. models in which such a high peak abundance of HC_3N is reached in less than 10^5 yr is one in which the cosmic ray induced ionization rate is an order of magnitude larger than 1.3 10^{-17} s^{-1}, often taken as typical for dense cores (e.g. Caselli et al. 1998). In this model, CO and N_2 are returned to the gas phase unchanged immediately on collision with grains. This assumption was made on the grounds that the interaction of CO and N_2 with the surface is known to be particularly weak (cf. Millar & Nejad 1985).

3. A chemical model of Core D

As reviewed in the previous section, few models of the chemistry of Core D in TMC-1 are based on the assumption that it is a dynamically young object. Indeed, only one detailed model that has been described in the recent literature (Model 9 in Gwenlan et al. 2000) gives an age of less than 10^5 yr and a HC_3N fractional abundance in harmony with that measured by Ohishi & Kaifu (1998). We therefore present more complete results for a model similar to that one, and refer to it as Model A.

The material is assumed to be dark (i.e. the ambient interstellar radiation field is excluded). We assume that atoms and molecules stick to grains efficiently and we set the parameter, S (the product of grain surface area per unit volume and the sticking probability, cf. Rawlings et al. 1992) equal to unity, which implies that a commonly adopted standard value of the grain surface area to hydrogen nuclei number has been used. (Note that Table 1 in Gwenlan et al. 2000 contains a typographical error as $S = 1$ also for Model 9). The adopted value of the cosmic ray induced ionization rate, ζ, is 1.3 10^{-16} s^{-1}. The adopted temperature is 10 K, the visual extinction is taken to be 10 mags, the number density of hydrogen nuclei is assumed constant at 4 10^4 cm^{-3} (a mean density for Core D), and the material is taken to be initially atomic except that all hydrogen is in H_2. It is also assumed that any CO and N_2 molecules striking the grains are returned promptly to the gas phase, while other molecules are retained on the grain surfaces. Atoms are assumed to be hydrogenated and returned to the gas promptly, i.e. oxygen is returned as H_2O and carbon as CH_4, etc. These hydrogenated molecules then contribute to the network of gas phase reactions. Elemental abundances by number relative to hydrogen nuclei were set equal to 7 10^{-2}, 1 10^{-4}, 8 10^{-5}, 2 10^{-4}, 2 10^{-8}, 3 10^{-9}, 2 10^{-7}, and 7 10^{-9} for helium, carbon, nitrogen, oxygen, sulphur, magnesium, sodium, and silicon respectively. The UMIST chemical database (Millar et al. 1997) was adopted for the network of gas-phase reactions, and the effects of a cosmic ray induced radiation field (Prasad & Tarafdar 1983) were included.

The most important differences between Model A and Model 9 of Gwenlan et al. (2000) are:
1) The electronic recombination reactions

$$CH_5^+ + e \rightarrow CH_4 + H \tag{1}$$

$$CH_5^+ + e \rightarrow CH_3 + H_2 \tag{2}$$

were removed and replaced with the following:

$$CH_5^+ + e \rightarrow CH_3 + H + H \tag{3}$$

$$CH_5^+ + e \rightarrow CH_2 + H_2 + H \tag{4}$$

(cf. Viti et al. 2000; Semaniak et al. 1998). The obvious gas phase route to CH_4 is, therefore, suppressed.
2) We adopt a more accurate treatment for the cosmic ray induced photodissociation of CO in that the Gwenlan et al. model did not include the temperature dependence of this reaction (see Millar et al. 1997). At 10 K, the Gwenlan et al. model contains an overestimate of the CO photodissociation induced by cosmic rays for $A_V >$ 4 mags.

Results for Model A are displayed in Fig. 1 (a and b) At a time of about 6 10^4 yr, the Model A fractional abundances of NH_3, HC_3N, CS and H_2CO are within a factor of around 2 of the corresponding fractional abundances measured by Ohishi & Kaifu (1998). SO is a factor of 5 underabundant, but this is not surprising considering the uncertainty of the sulphur depletion (e.g. Ruffle et al. 1999). Harju et al. (2000) determined the distribution of OH in TMC-1 and found that it is similar to that of HC_3N, peaking towards the cyanopolyyne maximum. They found a total column density of 2.6 10^{15} cm^{-2}. In Model A, the OH peak corresponds in time to the cyanopolyyne peak with its column density only slightly overabundant with respect to the observed value. The model fractional abundances of C_3H and CH_2CN (not shown) are too high, conceivably a result of poor knowledge of the rates of reactions affecting their production and removal. For the most part, however, the agreement between model and measured abundances is reasonable.

The chemical youth of Core D according to this model is consistent with its microstructure being transient. The high value of ζ is required to drive the gas-phase chemistry to generate such a large abundance of HC_3N at such an early time. A similarly high value of ζ in Core D has been advocated by Caselli et al. (1998), who concluded that Core D was the only one of the many dense cores they considered in which a high HC_3N abundance cannot simply be taken to be a sign of advanced depletion, as in the models described by Hartquist et al. (1996, 1998). Caselli (2000) has reviewed the evidence and physical grounds for variation in the cosmic ray ionization rate at different locations in the interstellar medium. Acceleration in a wind termination shock may increase the cosmic ray intensity in TMC-1, while variations of magnetic field orientation over the surface of the object may give variation within TMC-1 of the induced ionization rate if energies are low enough (Hartquist & Morfill 1994).

The H_2O and O_2 fractional abundances predicted by Model A greatly exceed those measured towards dense cores in regions of low-mass star formation with SWAS (Goldsmith et al. 2000; Snell et al. 2000). Published SWAS data for TMC-1 were obtained for the line-of-sight towards the region (Core B) where the NH_3 emission peaks. Core B is far from Core D, and has not been reported to possess microstructure. It was suggested by Hirahara et al. (1992) to be a much older object than Core D. Hence, published SWAS results do not directly constrain models of Core D.

4. SWAS observations of Core D

While an earlier version of this paper was being considered for publication, Melnick & Bergin (2001) noted the high abundances predicted by Model A, and kindly agreed to make observations of Core D using the SWAS facility. Their conclusions are that neither H_2O nor O_2 is detectable, and that upper limits for these species relative to H_2 are about 2 10^{-7} and 9 10^{-6}, respectively. The methods Melnick and Bergin have adopted to derive these abundances are summarized in Snell et al. (2000) for H_2O, and in Goldsmith et al. (2000) for O_2. For a description of the SWAS observatory see Melnick et al. (2000).

5. Revised chemical models

It is evident that while Model A is capable of producing a rich chemistry at very early times with molecular abundances comparable with those observed, it fails to meet the criteria set by SWAS for H_2O and O_2. Since the dynamical constraint is independent of any chemical arguments we have therefore examined some parameter variations of Model A to determine whether the rich hydrocarbon chemistry can be retained and the H_2O and O_2 abundances significantly reduced at the canonical age of 6 10^4 yr.

We have examined three types of modification to Model A. These are the adoption of higher density, modification of the gas/dust interaction, and reduction of the

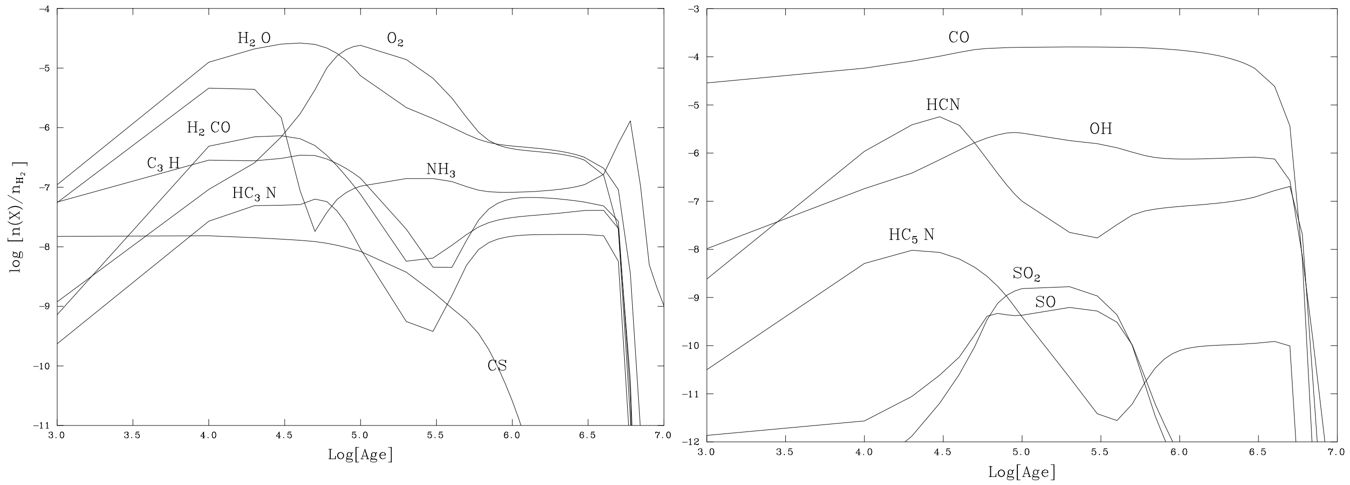

Fig. 1. Fractional abundances of selected species as function of time for Model A

total oxygen abundance. The modified surface chemistry is the same as that in Model A except that while atomic carbon and hydrocarbons striking the grains form methane which is immediately ejected into the gas phase, we now assume that all other species except H, H_2, He, CO and N_2, freeze out on to the dust and are retained there.

The result of an extensive search of this parameter space is that a new model, here called Model B, with an enhanced density of 2 10^5 cm^{-3} (consistent with microstructure densities inferred by Peng et al. 1998), and a chemistry modified as indicated above, produces high hydrocarbon abundances and satisfies the SWAS constraints for H_2O and O_2 at the canonical age of 6 10^4 yr. Figure 2 shows some results for Model B.

The adopted higher density shifts the peak abundances of H_2O and O_2 to a time earlier than the supposed dynamical age of the core, and the modified surface processes (about which there is no laboratory information at present) ensure a rich hydrocarbon chemistry. At the dynamical age of 6 10^4 yr, the Model B fractional abundances, relative to H_2, for H_2O and O_2 are 8 10^{-8} and 3 10^{-7}, which easily meet the SWAS constraints, while that of HC_3N is 6 10^{-8}, consistent with the abundance determinations from the observations of Core D by Ohishi & Kaifu (1998). The fractional abundance of other species, such as NH_3 and H_2CO, in Model B are also consistent with observations. Note that Model B, like Model A, has a near-solar total oxygen to total carbon ratio.

The use in the model of a density that is constant in time is appropriate only if Core D was imploded on a timescale shorter than 6 10^4 yr. Hartquist et al. (1996) drew attention to the sharp gradient in cyanopolyyne emission (cf. the map in Hirahara et al. 1992) throughout most of the TMC-1 ridge on the side furthest from the young star near the NH_3 emission peak. They suggested that this gradient may be associated with the termination shock of a stellar wind mass-loaded through the ablation of the cores in TMC-1. They noted that – in this case – the outer shock of the wind-blown bubble had already passed through the cores and that the drop in density along the ridge with increasing distance from the star inferred by Hirahara et al. (1992) is compatible with the cores having been imploded by the passage of a shock driven by the wind of the star. Microstructure in Core D may well have been due to the development of an instability (e.g. Wardle 1991) in the shock.

The issue arises of whether the passage of the shock might have affected the chemical initial conditions. At the distance of TMC-1 10 min of arc correspond to only about 0.4 pc, a distance which a shock propagating at only 4 $km\,s^{-1}$ would cross in 10^5 yr. The TMC-1 ridge is much narrower than this, so that perhaps the shock causing the compression need not have even been as fast as 4 $km\,s^{-1}$ to have done so on an acceptably short timescale. Given magnetic moderation of the shock (e.g. Draine et al. 1983), one as slow as 4 $km\,s^{-1}$ probably cannot induce a high temperature chemistry. Thus, there is no contradiction between shock implosion on a timescale shorter than 6 10^4 yr and the use of primarily atomic initial conditions in a chemical model of Core D.

6. Conclusions

The existence within Core D of TMC-1 of microstructure on a scale of 3 10^{-2} pc may indicate that the evolutionary age of this core should be less than about 10^5 years. This independent dynamical constraint would make very severe demands on existing chemical models which must account for the unusual richness in both abundance and variety of molecules found in Core D very early in its chemical evolution.

We propose a chemical model in which gas-phase reactions, driven quickly by an enhanced rate of cosmic ray ionization, are supplemented by a simple hydrogenation of carbon atoms and molecules at grain surfaces, while many other species freeze out. In addition, we also assume that CO and N_2 molecules do not stick to grain surfaces or are rapidly desorbed from them. With a hydrogen nuclei number density of 2 10^5 cm^{-3} such a model is capable of accounting for the unusually high HC_3N and other

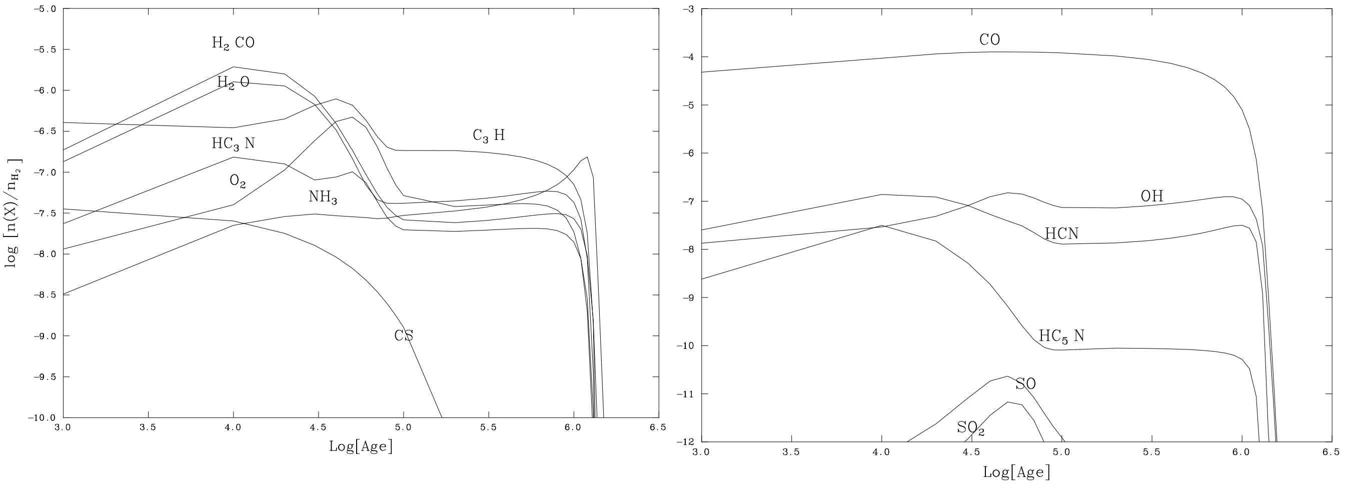

Fig. 2. Fractional abundances of selected species as function of time for Model B

abundances observed in Core D at the young evolutionary age of 6 10^4 years, while being in harmony with the SWAS upper limits for H_2O and O_2. Large scale CI mapping of Heiles Cloud 2 (Maezawa et al. 1999) shows regions with higher values of the ratio of $n(\mathrm{C^o})$ to $n(\mathrm{CO})$. We have pointed out above that the high value of the ionization rate can be localized to core D of TMC-1; thus higher values of the ratio need not indicate that the regions are much younger than core D of TMC-1.

The implications of this study are profound. If the assumption of extreme youth of Core D, as may be indicated by the presence of the microstructure, is valid, then the chemical model we propose provides powerful evidence in support of chemically active grains in dark clouds. This activity appears to be a simple hydrogenation of carbon, rather than any more complex chemistry, but with selective effects. Some atoms apparently freeze out. This indication adds greater urgency to the laboratory study of relevant gas/surface interactions. The extreme richness of the chemistry – in both variety and abundance of detected molecules – appears to be a consequence of both a fast gas-phase network and an efficient surface catalysis. Much of the gas-phase network is moderately well understood, but the surface catalysis should be studied in detail theoretically and experimentally. The consequences of such a contribution in diffuse clouds has already been investigated (Viti et al. 2000; O'neill et al., in preparation).

The special nature of TMC-1 – a long standing interstellar mystery – is here attributed to the extreme youth of Core D. In comparison, Core B (the location of NH_3 peak) is relatively old. A search to confirm the absence of microstructure in Core B should be undertaken. In Core D we may be observing by chance a very young object; most dark clouds are much older. The special chemical nature of Core D will decline in time (as Fig. 2 indicates) until it is no longer a chemically prominent object. Note that Fig. 2 suggests that the fractional abundance of HC_3N should decline to the range (1−3) 10^{-8} for a relatively long period of several million years. This is the range of HC_3N abundances commonly found in dark clouds. Finally, the implied age of less than 10^5 years for Core D implies rather special circumstances to set up the physical conditions in the object. The proposal made here is that this is a consequence of a low velocity shock passing through diffuse material that is largely atomic (apart from H_2).

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