Chemical models of interstellar gas–grain processes – III. Molecular depletion in NGC 2024

S. B. Charnley

1Astronomy Department, University of California, Campbell Hall, Berkeley, CA 94720, USA
2Space Science Division, NASA Ames Research Center, MS 245-3, Moffett Field, CA 94035, USA

ABSTRACT

The chemistry arising from the exchange of molecules between dust and gas in ultradense \( n_H \geq 10^7 \, \text{cm}^{-3} \) cool cores is described. Under certain assumptions concerning molecule–grain binding energies and dust temperature, slight warming of cold dust grains can induce selective desorption of mantle volatiles. It is theoretically possible for ultradense cores to become depleted in CO but to remain abundant in \( \text{N}_2 \) and so be relatively rich in nitrogen-bearing molecules. This effect may explain the apparent depletion of CO and the presence of ammonia in several cores within the NGC 2024 cloud. The theory implies that heavy metal atoms should be almost entirely absent from the gas phase of high-density cores, and that a mantle of CO, \( \text{O}_2 \), \( \text{N}_2 \) and other weakly bound molecules should cover water ice mantles, forming a ‘volatile crust’. Molecular observations are suggested which will allow a test of this model.

Key words: molecular processes – ISM: clouds – ISM: individual: NGC 2024 – ISM: molecules.

1 INTRODUCTION

In dense molecular clouds, atoms and molecules collide and stick to the surfaces of cold dust grains to form molecular ice mantles (see for example Millar & Williams 1993). In the limit of zero desorption from grain surfaces, the entire heavy element component of the gas phase should condense out within a characteristic time of about \( 3 \times 10^9 / n_H \, \text{yr} \) (Iglesias 1977), where \( n_H \) is the hydrogen nucleon density. The presence of gas-phase molecules attests to a non-zero desorption rate for at least some of the surface species (Brown & Charnley 1990, 1991, hereafter Papers I and II).

Simple theories predict that, prior to warming by nearby protostars, there may exist, transiently, ultradense \( (n_H > 10^8 \, \text{cm}^{-3}) \) regions with gas and dust temperatures, \( T \) and \( T_g \), of about 20 K or less, in which all heavy gas-phase material has been incorporated into grain mantles (Brown, Charnley & Millar 1988). In such objects, where the gas–grain collision time-scale is extremely short, the problem of the precise nature of the cycling of molecules between gas and dust becomes manifest.

Seven ultradense dust emission cores (FIR1–7) have been identified in NGC 2024 \( (n_H \sim 10^8 \, \text{cm}^{-3}; T \sim 18 - 40 \, K; T_g \sim 19 \, K) \) which appear to show depletions of gas-phase \( \text{C}^{18}\text{O} \), CO and CS (Mezger et al. 1988, 1992; Mauersberger et al. 1992; Wilson, Mehringer & Dickel 1995). It has been argued that these cores are cool protostellar condensations and are regions where accretion on to grains is dominating the gas-phase evolution. Although this interpretation has been the subject of debate (Schulz et al. 1991; Chandler & Carlstrom 1996), these cores are promising candidates in which to develop an understanding of gas–grain processes at extremely high densities. Associated, and in some cases coincident, with the FIR sources are several clumps detected in ammonia (NGC 2024: NH\(3\)1–7) with fractional abundances relative to \( \text{H}_2 \) in the range of \( 10^{-10} \) to a few \( 10^{-9} \) (Gaume, Johnston & Wilson 1992; Mauersberger et al. 1992), factors of 100–1000 less than dark cloud ammonia abundances. If the NGC 2024: FIR/NH\(3\) cores are indeed regions of ongoing accretion, it is puzzling that a molecule with a large binding energy for physisorption such as \( \text{NH}_3 \) is present at all in gas in which material of much higher volatility (i.e. CO) is being removed. As \( \text{N}_2 \) is most probably the major reservoir of nitrogen in dense molecular clouds (Womack, Ziturys & Wyckoff 1992a), the solution to this problem could be connected to the volatility of \( \text{N}_2 \).

In this paper the molecular chemistry of ultradense cores is explored with particular reference to the observed cores in NGC 2024. Three of these cores (FIR 4, 5 and 6) are in a more evolved state of protostellar evolution, as evidenced by the presence of outflows and 2-\( \mu \)m emission (Moore & Chandler 1989; Richer 1990; Richer, Hills & Padman 1992; Moore & Yamashita 1995). The theory developed here is based on the observational interpretation, due to Mezger and co-workers, that the NGC 2024 FIR cores are isothermal protostellar condensations. In Section 2 the basic model is described. Results are given in Section 3 and conclusions summarised in Section 4.
2 STEADY-STATE THEORY

It is assumed that ultradense cores form by isothermal (~10 K) gravitational contraction to their present state. At some point, late in this evolution, conventional interstellar chemistry ends and all the heavy gas-phase material has condensed out on to the dust to form icy mantles (Brown et al. 1988). Model calculations (e.g. Paper I) show that these mantles will include CO, N2 and O2, abundantly produced by gas-phase reactions in clouds older than a few million yr, as well as CH4, H2O and NH3, formed by grain-surface hydrogenation of C, O and N atoms. Subsequent heating, by a protostar adjacent to, or within, the core, leads to modest warming of the grains to Tgr~30~30 K. Based on the physics/chemistry binding energies of the pure substance (Nakagawa 1980; Tielens & Allamandola 1987), only H2, CO, N2 and O2 could evaporate in the NGC 2024 cores (Tgr~19 K) and provide the material from which other molecules may form (see Section 2.2 below for discussion of this point).

As all the C, O and N available for gas-phase reactions are contained in only three molecules, this means that it is not necessary to compute the detailed chemistry of core formation; this fact, with the assumption of dynamical and chemical steady states, greatly simplifies the analysis of the core chemistry. By neglecting chemical destruction of CO and N2, their abundances can be calculated from the position of the accretion-desorption equilibrium. In fact the gas-phase chemistry is only in a quasi-steady state: neglect of this evolution, conventional interstellar chemistry ends and hydrogenation of C, O and N atoms. Subsequent heating, by a protostar adjacent to, or within, the core, leads to modest warming of the grains to Tgr~30~30 K. Based on the physics/chemistry binding energies of the pure substance (Nakagawa 1980; Tielens & Allamandola 1987), only H2, CO, N2 and O2 could evaporate in the NGC 2024 cores (Tgr~19 K) and provide the material from which other molecules may form (see Section 2.2 below for discussion of this point).

As all the C, O and N available for gas-phase reactions are contained in only three molecules, this means that it is not necessary to compute the detailed chemistry of core formation; this fact, with the assumption of dynamical and chemical steady states, greatly simplifies the analysis of the core chemistry. By neglecting chemical destruction of CO and N2, their abundances can be calculated from the position of the accretion-desorption equilibrium. In fact the gas-phase chemistry is only in a quasi-steady state: neglect of gas-phase production of CO, N2 and O2 means that these molecules would eventually be destroyed by ion-molecule reactions or by cosmic-ray-induced photons, and the core chemistry would ‘wind down’ as the product atoms and ions accrete on to the grains. However, the time-scale to attain a chemical quasi-steady state in the NGC 2024: FIR cores (~10^7 yr) is much shorter than estimates of both their dynamical ages (~10^6 yr: Chandler & Carlstrom 1996) and the chemical destruction time-scales of CO and N2 (~10^8 yr).

2.1 Gas–grain interaction

The model considers sticking, charging and neutralizing collisions by gas-phase species to produce three populations of spherical grains, G^0, G^- and G^+. The steady-state treatment is similar to that of Umebayashi & Nakano (1990) who considered sticking and charging of grains by ions and electrons, as well as between the three grain populations, but neglected accretion of neutral molecules. In steady-state models one must have some molecular desorption present, and in this paper it is by thermal evaporation of CO, N2 and O2; all other heavy neutrals have zero desorption rates.

2.1.1 Accretion

The collision rate of a gas-phase ion X^+ with the dust grains can be written as

\[ \lambda(X^+) = \frac{1.45 \times 10^7}{M_X} \left( \frac{T}{M_X} \right)^{0.5} n_H^2 n_g, \]

where n_g is the number density of spherical grains of radius a, k is the Boltzmann constant, T is the gas temperature, M_X is the molecular weight of X, and Ze is its charge. Unit sticking efficiency on neutral grains is assumed. In writing equation (1), there are the facts that n(G^-)~n_g for the density range of interest has been used (Umebayashi & Nakano 1990). For neutral molecules the exact expression is obtained by setting Z=0 in equation (1). It is assumed that H2 molecules and He atoms do not stick to the grains. For collisions of electrons and atomic ions with grains of opposite charge, it is assumed that grains are neutralized and that the atoms are ejected back into the gas phase.

2.1.2 Desorption of mantle volatiles

A neutral molecule X evaporates at a rate

\[ \xi(X) = n(H_2) \exp \left[ -\frac{E_b(X)}{kT_{gr}} \right], \]

where n(H2) is the vibrational frequency of X in a surface binding site and E_b(X) is its binding energy for physisorption (e.g. Watson & Salpeter 1972; Leger, Jura & Omont 1985; Sandford & Allamandola 1993). For each of CO, N2 and O2 a representative value of \( n(H_2) = 2 \times 10^{12} \text{s}^{-1} \) is taken (Sandford & Allamandola 1993).

The gas-phase abundances of CO, N2 and O2 are set primarily by E_b(X), Tgr and \( \lambda(X) \). For example, denoting the total number density of N2 molecules available in a core as ntot(N2) (i.e. gas plus solid), then the steady-state gas-phase number density is

\[ n(N_2) = \frac{n_{tot}(N_2)}{1 + \lambda(N_2) \xi(N_2)} \]

Equation (3) and similar expressions for CO and O2 implicitly assume that their destruction by gas-phase processes is negligible over the time-scales of interest (see above). To obtain the number densities of CO, O2 and N2 we compare \( \xi(X) \) from equation (2), for various assumptions concerning the relevant binding energies for physisorption.

2.1.3 Gas-phase number densities

The dense gas is ionized by cosmic rays at a rate \( \xi(X) \) to produce the H^+, H_2^+ and He^+ that drive the ion–molecule chemistry. When hydrogen atoms are produced from H2 destruction and lost in re-formation of H2 on dust grains, one finds that n(H)~1 cm^{-3} (e.g. Duley & Williams 1984).

Useful analytic formulae can be obtained for the steady-state number densities of the species most important for the ammonia chemistry. For a species, i, with a total production rate per unit volume of \( P_i \) and a total destruction rate per unit volume of \( D_i \), the steady-state value of \( n(i) \) is just \( P_i/L_\xi(i) \) (cf. Lepp, Dalgarno & Sternberg 1987). These formulae are listed below; the grain collision terms are included even when gas-phase processes dominate the destruction. All reaction rate coefficients are taken from Millar et al. (1991) except where stated. The number of helium ions per cm^3 is

\[ n(He^+) = \frac{0.5 \xi_0 n(He)}{1.6(n(CO) + n(N_2)) + \alpha n(H_2) + \lambda_0 n(He^+)} \]

where \( \xi_0 = 10^9 \xi, \lambda_0(He^+) = 10^9 \lambda(He^+) \) and \( \alpha = 3.7 \times 10^{-5} \exp(-35/7) \).

The number density of hydrogen ions is

\[ n(H^+) = \frac{0.017 \xi_0 n(H_2)}{1.2(n(O_2) + 3.5 \times 10^{-3} T_3^{-0.75} n_e + \lambda_0 n(H^+))} \]

where \( n_e \) is the electron density. The number density of H_2^+ ions is

\[ n(H_2^+) = \frac{\xi_0 n(H_2)}{1.7(n(CO) + 1.8n(N_2) + 220 T_3^{-0.5} n_e + \lambda_0 n(H_2^+))} \]

where \( T_3 = (T/300) K \) and the dissociative recombination rate coefficient is \( 2.2 \times 10^{-7} \text{cm}^3 \text{s}^{-1} \).

© 1997 RAS, MNRAS 291, 455–460

© Royal Astronomical Society • Provided by the NASA Astrophysics Data System
The number density of protonated N2 is
\[ n(\text{HCO}^+) = \frac{1.7n(H^+) + 0.88n(N_2H^+)}{110T_3^{-2}n_e + \lambda_9(HCO^+)}n(\text{CO}). \]  
(7)
The number density of protonated N2 is
\[ n(N_2H^+) = \frac{1.8n(H^+)n(N_2)}{0.88n(\text{CO}) + 170T_3^{-2}n_e + \lambda_9(N_2H^+).} \]  
(8)
Ammonia formation is initiated by the reaction
\[ N^+ + H_2 \rightarrow NH^+ + H, \]  
(9)
where the N\(^+\) ion is formed in the reaction of He\(^+\) with N\(_2\). Reaction (9) is the first step in the rapid NH\(_3\) \( \rightarrow \) H\(_2\) chain leading to NH\(_3\) and ultimately to NH\(_3\). Theoretical and experimental studies show that the rate coefficient of reaction (9), \( k_0 \), can be appreciable in cold gas despite an activation energy barrier: the N\(^+\) ion produced from N\(_2\) by He\(^+\) is kinetically excited (Adams, Smith \& Millar 1984) and can overcome the barrier. For the kinetic temperature of the coolest NGC 2024 cores (~18 – 23 K) the non-thermal value of \( k_0 \) at 20 K calculated by Yee, Lepp \& Dalgarno (1987; see also Herbst, Defrees \& McLean 1987) is probably appropriate under these conditions: \( k_0 = 6 \times 10^{-11} \text{cm}^3 \text{s}^{-1} \). The steady-state ammonia concentration can be written as
\[ n(\text{NH}_3) = \frac{0.48n(\text{He}^+)n(N_2)}{R + \lambda_9(\text{NH}_3)}, \]  
(10)
where
\[ R = 2.2n(\text{HCO}^+) + 2.3n(N_2H^+) + 5.2n(H^+) \]  
\[ + 2.2n(\text{He}^+) + 2.7n(H^+). \]  
(11)
The derivation of equation (10) makes use of the relation
\[ n(N^+) = \frac{0.96n(\text{He}^+)n(N_2)}{k'n(H_2) + 0.45n(\text{CO}) + 0.61n(O_2) + \lambda_9(N^+)} \]  
(12)
where \( k' \) is \( 10^9k_0 \).

2.2 Grain-surface desorption

2.2.1 Molecular binding energies
A fundamental assumption concerns the appropriate values of \( E_b \): low \( E_b \) values are essential if the ammonia observations of NGC 2024: NH\(_3\)-1–7 are to be explained by thermal evaporation of N\(_2\) from 19 K dust. Hereafter, the convention is followed of expressing \( E_b \) values in kelvin. Interstellar ice mantles are known to consist mostly of H\(_2\)O molecules, and the estimated binding energy of, for example, CO on H\(_2\)O is measured to be about 1740 K (Sandford \& Allamandola 1993). Hence, in the range \( T_g = 15 – 30 \text{ K} \), CO would be entirely depleted from the gas. No experimental information is available for either N\(_2\) or O\(_2\) binding on H\(_2\)O ice. For each of N\(_2\), O\(_2\) and CO, binding energies of 890, 1120 and 1030 K have been adopted (Léger et al. 1985), corresponding to the \( E_b \) values of the pure substances (i.e. N\(_2\) on N\(_2\), CO on CO etc.).

2.2.2 Mantle structure
The adoption of the ‘pure’ \( E_b \) values is tantamount to postulating the existence of a volatile ‘crust’ of CO, O\(_2\) and N\(_2\) molecules surrounding a mantle comprising mostly H\(_2\)O and other refractory species (although some of these molecules could also be incorporated into this mantle). The interchange of atoms and molecules between this ‘crust’ and the gas phase is then the key process that regulates the chemistry of cool ultradense cores. Accretion and mantle formation may naturally produce a dirty ice where the inner layers will be mainly saturated molecules and the outer layers simple diatomic species. Early in the core evolution \( (T > 10 \text{ K}; n_H \sim 10^{-10} \text{ cm}^{-3}) \), when H atoms are more abundant than the total abundance of C, O and N atoms, the heavy atoms will accrete and be hydrogenated to CH\(_2\), H\(_2\)O and NH\(_3\) (e.g. d’Hendecourt, Allamandola \& Greenberg 1985; Paper I). A few million y r into the core evolution the gas phase is primarily CO, N\(_2\) and O\(_2\); these molecules eventually condense out to form a layer on the mostly H\(_2\)O ice. The physisorption binding energy of gas-phase molecules on surfaces involves the induced dipole moment between the surface molecules and the gas-phase species; hence, one might expect that the appropriate \( E_b \) values should be closer to those of surfaces covered predominantly by non-polar or weakly polar molecules, i.e. CO on CO rather than CO on H\(_2\)O.

2.2.3 Atoms and metals
Modest dust warming evaporates CO, O\(_2\) and N\(_2\) into the gas where chemical reactions release C, O and N atoms which then collide and stick to the dust grains. For simplicity, it is assumed that accreted heavy atoms (and radicals) are not thermally desorbed but take part in surface hydrogenation reactions. Atoms of C, N and O have lower \( E_b \) values for physisorption than the volatile diatomics; however, at the relevant values of \( T_g (=20 – 30 \text{ K}) \), the surface migration timescale of each is much shorter than both the associated evaporation timescale and the migration time for hydrogen atoms (Tielens \& Allamandola 1987). Therefore, heavy atoms will either scan the surface to find sites where they can be strongly chemisorbed (Watson \& Salpeter 1972) or, since hydrogen atoms are more abundant than heavy atoms in the accreting gas, encounter an H atom, ultimately forming saturated molecules which remain in the mantle. It is clear that during the core formation phase, longer than an accretion time, any Fe, Na, Mg or Si atoms should have become entirely depleted from the gas: the estimated \( E_b \) values for metal atoms are so high (Jura \& Morris 1985) that, once accreted, they cannot be returned to the gas by thermal evaporation at \( \sim 20 \text{ K} \) (see Turner 1991). These cores therefore contain zero-metallicity gas.

2.3 Model
Equations (4)–(8) and (10), together with the relevant equations for \( n(\text{CO}), n(N_2), n(O_2), n(\text{G}^0), n(\text{G}^+), n(\text{G}^2+) \) and a charge conservation equation to calculate the gas-phase electron density, were solved numerically. The cosmic ray ionization rate \( \dot{\zeta} \) was taken to be \( 1.3 \times 10^{-17} \text{ s}^{-1} \); \( n_{\text{gr}} = 10^{-12}n_H, T = T_g, a = 0.1 \mu \text{m} \); the electron sticking efficiency on \( \text{G}^0, \text{S}^0 \), was taken equal to 0.6 (Nishi, Usheyashi \& Nakano 1991). The total He number density was taken to be \( 7 \times 10^{-2}n_H \). To be consistent with dark cloud observations of gas-phase CO, the total number density of CO molecules available to the gas and solid phases, \( n_{\text{tot}}(\text{CO}) \), was taken equal to \( 5 \times 10^{-5}n_H \). Using the abundance of N\(_2H^+\) measured in TMC-1 by Womack, Ziurys \& Wyckoff (1992b) and equation (8) yields an undepleted N\(_2\) gas-phase abundance of \( n_{\text{tot}}(N_2) = 2 \times 10^{-5}n_H \). Finally, \( n_{\text{tot}}(O_2) = 1 \times 10^{-5}n_H \), consistent with observational upper limits (Goldsmith \& Young 1989).
3 RESULTS AND DISCUSSION

3.1 Steady-state model

Fig. 1 shows fractional abundances as a function of density for dense cores where the chemistry is sustained by thermal desorption from grains at 19 K. At increasingly higher densities, for fixed \( T_g \), accretion eventually dominates over evaporation and the heavy molecular species become more severely depleted. Except for \( \text{N}_2 \text{H}^+ \), the runs of ion, electron and grain abundances with \( n_H \) are similar to those of Umebayashi & Nakano (1990). Note that \( \text{H}^+ \) is more abundant than \( \text{H}_2^+ \) since \( \text{O}_2 \) is depleted from the gas. Also shown in Fig. 1 are the derived \( \text{NH}_3 \) abundances for each of the ammonia cores (Mauersberger et al. 1992) plotted at the density of each associated FIR core (solid circles) derived from their dust masses (Mezger et al. 1992). From Fig. 1 it is clear that cycling of \( \text{CO} \) and \( \text{N}_2 \) molecules between gas and 19-K dust grains can resolve the problem of co-existing \( \text{CO} \) depletions and finite \( \text{NH}_3 \) abundances only in the the cores with the lowest \( \text{NH}_3 \) abundances, NGC 2024: \( \text{NH}_3 \)4 and 5.

Mauersberger et al. (1992) have emphasized that the ammonia emission probably originates from lower density gas on the surfaces of the FIR cores. Lower densities for all the FIR cores are also suggested by virial analysis estimates (Wilson et al. 1995). Fig. 1 also shows the \( \text{NH}_3 \) abundances of NGC 2024: \( \text{NH}_3 \)1–3 and NGC 2024: \( \text{NH}_3 \)6 and 7 assuming that the corresponding densities are 10 times lower (open circles). For four of the cores, except NGC 2024: \( \text{NH}_3 \)7, the agreement is much better. Taking the model results at face value implies that there is a strong variation in density between the \( \text{NH}_3 \)-emitting regions. The fact that \( n_H \sim 10^6 \text{ cm}^{-3} \) is suggested for NGC 2024: \( \text{NH}_3 \)4 and 5 is consistent with these regions being more evolved than the others (Chandler & Carlstrom 1996). In this interpretation the others have \( n_H \sim 10^5 \text{ cm}^{-3} \), except NGC 2024: \( \text{NH}_3 \)7 which has \( n_H \sim 10^6 \text{ cm}^{-3} \).

The selective retention of \( \text{CO} \) in grain mantles yields an \( \text{N}_2 \text{H}^+ \) abundance of \( \sim 10^{-10} \) in NGC 2024: \( \text{NH}_3 \)4 and 5, very close to the value of \( \sim 2 \times 10^{-10} \) determined for FIR 5 by van Dishoeck et al. (1992). Such high abundances are symptomatic of regions where \( \text{CO} \) and \( \text{N}_2 \) molecules are unequally partitioned between gas and grain surfaces. Fig. 1 shows that, since \( \text{CO} \) destroys it, \( \text{N}_2 \text{H}^+ \) should be detectable towards the NGC 2024: \( \text{NH}_3 \) sources with an almost uniform abundance.

3.2 Time-dependent model

The ammonia chemistry and the spread in NGC 2024 \( \text{NH}_3 \) abundances could be a time-dependent effect. Fig. 2 shows the results of a time-dependent calculation at a fixed density of \( 2 \times 10^7 \text{ cm}^{-3} \), with the model parameters described above. With all the the available \( \text{CO} \), \( \text{O}_2 \) and \( \text{N}_2 \) contained in the ices, the grain temperature was raised to 19 K and the chemical evolution induced by the volatile outgassing followed. The model used was that of Charnley, Tielens & Millar (1992) and considers 1554 reactions amongst 152 species. An alternative scenario for the gas-grain chemistry of these cores is that the grains were heated to \( \sim 30 \text{ K} \) followed by cooling to 19 K; here all the surface \( \text{CO} \), \( \text{O}_2 \) and \( \text{N}_2 \) will have been desorbed and the approach to steady state involves their recondensation. Fig. 3 shows the corresponding chemical evolution at a fixed density of \( 2 \times 10^6 \text{ cm}^{-3} \).

From Figs 2 and 3 it is clear that time-dependent effects cannot explain the \( \text{NH}_3 \) observations. Figs 2 and 3 also show, as solid circles at \( 10^5 \text{ yr} \), the steady-state abundances computed in Section 3.1, confirming the accuracy of the analytical formulae and the steady-state assumption.

3.3 Other explanations

Chandler & Carlstrom (1996) have proposed that discrepancies in the estimated mass of FIR 5 derived from CS and dust observations can be brought into agreement, by invoking molecule depletions, or anomalous grain properties, or much higher dust temperatures \( (T_g \sim 100 \text{ K}) \). Such high dust temperatures would rule out the depletion scenario for FIR/\( \text{NH}_3 \)5; however, it then becomes difficult to account for the observed \( \text{N}_2 \text{H}^+ \) abundance and the fact that \( \text{NH}_3 \) is less abundant in this region. Assuming that the mantles in each core are composed of 10 per cent \( \text{NH}_3 \) then, in the Chandler & Carlstrom interpretation, FIR 5 should have much more gas-phase \( \text{NH}_3 \) than the other cores, not less, as is observed. When dust grains...
Figure 2. Chemical evolution for a model with \( n_H = 2 \times 10^7 \) cm\(^{-3}\) in which all available CO, N\(_2\) and O\(_2\) were initially present in the mantles and the dust temperature was raised instantaneously to 19 K at \( t = 0 \). Solid circles at \( 10^4 \) yr denote the corresponding abundances from the steady-state model.

Figure 3. Chemical evolution for a model with \( n_H = 2 \times 10^8 \) cm\(^{-3}\) in which all the available CO, N\(_2\) and O\(_2\) were initially present in the gas and the dust temperature was instantaneously lowered to 19 K at \( t = 0 \). Solid circles at \( 10^4 \) yr denote the corresponding abundances from the steady-state model; the electron and ammonia abundances are equal.

Perhaps the best observational test of whether thermal or non-thermal evaporation is responsible for the presence of ammonia at such high densities is to measure the relevant \( \text{NH}_2\text{D}/\text{NH}_3 \) abundance ratio for each core. The theory described in this paper requires that \( \text{NH}_3 \) be synthesized directly in the gas. There have been no calculations of interstellar deuteration at the relevant temperatures and densities; however, existing calculations show that the \( \text{NH}_2\text{D}/\text{NH}_3 \) ratio could be expected to be less than that attained in 10-K gas (Millar, Bennett & Herbst 1989) or on grain surfaces (Brown & Millar 1989). In particular, as NGC 2024: \( \text{NH}_3 \)4 and 5 have gas temperatures in excess of 40 K (Mauersberger et al. 1992), the theory would predict much less, if any, deuteration in \( \text{NH}_3 \).

Alternatively, if \( \text{NH}_3 \) is non-thermally desorbed from the dust then it must have formed either in cold gas or on grain surfaces; both theory and observations show that the observed \( \text{NH}_2\text{D}/\text{NH}_3 \) ratios should then lie in the range more typical of hot cores: 0.003–0.06 (Sutton et al. 1995; Turner 1990).

4 CONCLUSIONS

A theory for the gas–grain chemistry in the seven dense FIR cores of NGC 2024 has been developed. The cores are in a chemical steady state and, adopting pure physisorption binding energies for the volatiles (cf. Léger et al. 1985), \( n_H < 10^{10} \) cm\(^{-3}\), and the grain
temperature of 19 K determined by Mezger and co-workers, the theory can explain the co-existence of CO depletions and the presence of NH$_3$ as being due to the difference in volatility of CO and N$_2$: the latter molecule can remain abundant (but undetectable) in the gas where reactions with He$^+$ initiate NH$_3$ formation. Alternatively, if the physisorption binding energies of N$_2$ and CO are taken to be those for binding to water ice (~1740 K for CO), then both molecules are strongly depleted and the theory fails. However, if the lower values are applicable, the presence of a thick "volatile crust" enclosing the water ice and containing mostly molecules with low or zero dipole moments is indicated. There should be no refractory metal atoms or compounds in dense gas as their binding energies are too large. There is observational support for low metallicity in dense gas (Turner 1991), and for the presence of hierarchical structure in interstellar ices (Whittet 1996).

Assuming that the NH$_3$ is present in gas with density equal to that of the associated FIR core (Mezger et al. 1992), the model best explains the lowest NH$_3$ abundances, in FIR/NH$_3^4$ and 5, and suggests that the observed NH$_3$ emission from the others should originate in gas that is about 10 times less dense, consistent with previous suggestions (Mauersberger et al. 1992; Wilson et al. 1995). Calculations with a time-dependent model show that the observed ammonia distribution amongst the seven cores is not an evolutionarily fixed effect, as well as demonstrating the validity of the steady-state assumption.

More molecular observations of these cores are required to determine their chemical state. N$_2$H$^+$ observations offer a test of the depletion scenario: the theory predicts an almost uniform abundance across the cores. Cores with "normal" CO abundances will contain much lower N$_2$H$^+$ abundances. Searches for well-known "hot core" molecules, particularly NH$_2$D, may allow a test of this theory against other possible explanations involving higher dust temperatures and non-thermal desorption mechanisms.

ACKNOWLEDGMENTS

This work was supported by NASA's Origins of Solar Systems Program (RTOP No. 452-99-96-01).

REFERENCES


This paper has been typeset from a TEXILATEX file prepared by the author.