THE IONIZATION FRACTION OF BARNARD 68: IMPLICATIONS FOR STAR AND PLANET FORMATION

Sébastien Maret and Edwin A. Bergin

Department of Astronomy, University of Michigan, 500 Church Street, Ann Arbor, MI 48109-1042

Received 2007 January 18; accepted 2007 April 24

ABSTRACT

We present a detailed study of the ionization fraction of the Barnard 68 prestellar core, using millimeter H$^{13}$CO$^+$ and DCO$^+$ lines observations. These observations are compared to the predictions of a radiative transfer model coupled to a chemical network that includes depletion on grains and gas-phase deuterium fractionation. Together with previous observations and modeling of CO and isotopologues, our H$^{13}$CO$^+$ and DCO$^+$ observations and modeling allow us to place constraints on the metal abundance and the cosmic ionization rate. The H$^{13}$CO$^+$ emission is well reproduced for metal abundances lower than $3 \times 10^{-9}$ and a standard cosmic-ray ionization rate. However, the observations are also consistent with a complete depletion of metals, i.e., with cosmic rays as the only source of ionization at visual extinctions greater than a few $A_V$. The DCO$^+$ emission is found to be dependent of the ortho-to-para H$_2$ ratio and indicates a ratio of $\sim 10^{-2}$. The derived ionization fraction is about $5 \times 10^{-9}$ with respect to H nuclei, which is about an order of magnitude lower than that observed in the L1544 core. The corresponding ambipolar diffusion timescale is found to be an order of magnitude larger than the free fall timescale at the center of the core. The inferred metal abundance suggests that magnetically inactive regions (dead zones) are present in protostellar disks.

Subject headings: astrochemistry — ISM: abundances — ISM: individual (Barnard 68) — ISM: molecules — stars: formation

Online material: color figures

1. INTRODUCTION

The ionization fraction (or the electron abundance) plays an important role in the chemistry and the dynamics of prestellar cores. Because of the low temperature, the chemistry is dominated by ion-neutral reactions (Herbst & Klemperer 1973), and electronic recombination is one of the major destruction pathways for molecular ions. Furthermore, the ionization fraction sets the coupling of the gas with the magnetic field (Shu et al. 1987).

Several attempts have been made to estimate the electron fraction in dense clouds and prestellar cores (Guélin et al. 1982; Wootten et al. 1982; de Boissinger et al. 1996; Williams et al. 1998; Caselli et al. 1998). These studies rely on measurements of the degree of deuterium fractionation (through the DCO$^+$ over HCO$^+$ abundance ratio, for example), which has been found to be roughly inversely proportional to the electron abundance (Langer 1985). However, this simple approach has caveats (Caselli 2002), as it does not consider line-of-sight variations of the electron fraction. Large density gradients exist in prestellar cores, and therefore, one may anticipate similar variations in the electron abundance. In addition, the freeze-out of molecules onto the grain surfaces (e.g., Tafalla et al. 2002; Bergin et al. 2002) influence the degree of deuterium fractionation independently of the electron fraction (Caselli et al. 1998). Finally, these studies usually consider simple chemical networks that may neglect important ingredients for the electron fraction.

In this paper, we study the ionization fraction in the Barnard 68 core, using H$^{13}$CO$^+$ and DCO$^+$ line observations. These observations are interpreted with a chemical network including gas-grain interactions that is coupled to a radiative transfer model. This technique allows us to infer the electron abundance along the line of sight and to place constraints on the abundance of metals, the cosmic-ray ionization rate, and the ionization state of material that is provided by infall to the forming protoplanetary disk.

The paper is organized as follows. In § 2 we present the observations. The model used to interpret these observations is detailed in § 3. Results are presented in § 4. Implications of our findings are discussed in § 5, and § 6 concludes this paper.

2. OBSERVATIONS

The H$^{13}$CO$^+(1–0)$ ($\nu = 86.754288$ GHz) and the DCO$^+(2–1)$ ($\nu = 144.077319$ GHz) transitions were observed toward B68 ($\alpha = 17^h22^m38^s.2^e$ and $\delta = -23^\circ49'34.0''$; J2000.0) in 2002 April and September using the IRAM 30 m telescope. The core was mapped with a spatial sampling of 12$''$. The half-power beam size of the telescope is $29''$ at 87 GHz and $17''$ at 144 GHz. System temperatures were typically $\sim 110–150$ K at 3 mm and $\sim 160–350$ K at 2 mm. Pointing was regularly checked using planets and was found to be better than $\sim 2''$. The data were calibrated in antenna temperature ($T_A^*$) units using the chopper wheel method and were converted to the main beam temperature scale ($T_{mb}$) using the telescope efficiencies from the IRAM Web site. All observations were carried out in frequency switching mode. The H$^{13}$CO$^+(1–0)$ data were also presented in Maret et al. (2006).

Figure 1 shows a comparison between the integrated line-intensity maps of DCO$^+(2–1)$ and H$^{13}$CO$^+(1–0)$ with the visual extinction map obtained by Alves et al. (2001). The C$^{18}$O(1–0) map from Bergin et al. (2002) is also shown. In this figure we see that the peak of H$^{13}$CO$^+(1–0)$ line emission does not correspond to the maximum visual extinction in the core. The C$^{18}$O(1–0) line emission shows a similar behavior; it peaks in a shell-like structure with a radius of $\sim 50''$ around the maximum visual extinction. The DCO$^+(2–1)$ line emission, on the other hand, seems to correlate well with the visual extinction. These differences are likely a consequence of chemical effects. Because of the freezeout on grain mantles, the abundance of CO and its isotopologues decrease by about 2 orders of magnitude toward the center of the core (Bergin et al. 2002). Since H$^{13}$CO$^+$ is mainly formed from the reaction of $^{13}$CO with H$^+$, its abundance is also expected to decrease toward the core center. DCO$^+$ should also be affected by the depletion of...
CO. However, the deuterium fractionation increases as CO is removed from the gas phase. Thus, the disappearance of CO might be compensated by the increased deuterium fractionation. In what follows we interpret the emission of these species using a chemical model coupled with a Monte Carlo radiative transfer model, in order to precisely derive their abundance profiles.

3. ANALYSIS

We have used a technique that combines the predictions of a chemical network with a Monte Carlo radiative transfer (Bergin et al. 2002, 2006; Maret et al. 2006). The outline of this technique is the following. Chemical abundances are computed as a function of the visual extinction in the core. Using these abundance profiles, the line emission is computed with a Monte Carlo radiative transfer code. The resulting map is convolved to the resolution of the telescope and is compared to the observations. Free parameters of the chemical model (e.g., cosmic ionization rate, metal abundances) are adjusted until a good agreement is obtained between the model and the observations. Thus, this technique allows for a direct comparison between the predictions of the chemical network and the observations.

We have used the chemical network of Bergin et al. (1995). This network contains about 150 species (including isotopologues; see below) and focuses on the formation of simple molecules and ions (e.g., CO and HCO\(^{+}\)). The network includes the effect of depletion on grains, and the desorption by thermal evaporation, UV photons, and cosmic rays (Hasegawa & Herbst 1993; Bringa & Johnson 2004). It also includes the effect of fractionalization of \(^{13}\)C and \(^{18}\)O, using the formalism described by Langer & Penzias (1993). We have extended this network to include the effect of deuterium fractionation, following the approach used by Millar et al. (1989).

Because of the importance of multiply deuterated species in the deuterium fractionation process, these species were also included in the network, following Roberts et al. (2004). It also includes neutralization reactions of ions on negatively charged grains. The predictions of our network were checked against the UMIST network (Millar et al. 1997) for consistency.

We adopt the density profile determined by Alves et al. (2001) from observations of near-infrared extinction from background stars. This profile is assumed to be constant as a function of time. The dust temperature profile was computed using the analytical formulae from Zucconi et al. (2001). For the gas temperature we have adopted the profile determined by Bergin et al. (2006) from observations and modeling of CO and its isotopologues. The gas temperature is relatively low (7–8 K), and increases slightly (10–11 K) at the center of the core as indicated by ammonia lines observations (Lai et al. 2003). This increase in the temperature is a result of grain coagulation at the center of the core, which produces a thermal decoupling between the gas and the cooler dust.

The cloud is supposed to have the initial composition summarized in Table 1. In our model, we assume that the density profile of the core does not evolve with time. Therefore, we also assume that the chemistry has already evolved to a point where hydrogen is fully molecular, and all the carbon is locked into CO. Our treatment of the initial atomic oxygen pool deserves special mention. Bergin & Snell (2002) examined this question in the context of the nondetection of water vapor emission in B68 by the Submillimeter Wave Astronomy Satellite (SWAS). They found that if atomic oxygen were present in the gas phase in the dense core center, then the well-studied reaction chain that forms H\(_2\)O (via H\(_2\)O\(^{+}\)) would have yielded detectable water vapor emission. The simplest way to stop this reaction chain is to remove the fuel for the gas-phase chemistry, atomic oxygen. This happens when oxygen is trapped on grain surfaces in the form of water ice (e.g., Bergin et al. 2000). Thus, we have assumed initial conditions in which all nonrefractory oxygen is in the form of water ice and CO gas with no atomic oxygen left. In this fashion our initial abundances assume the core formed out of gas that reached out to \(A_V \sim 2\), where H\(_2\) and CO have formed and water ice mantles are observed. On the other hand, nitrogen is assumed to be mostly in atomic form (Maret et al. 2006).

A grain size of 0.1 \(\mu\)m is assumed. The cosmic-ray ionization rate and the abundance of low ionization potential metals (<13.6 eV) are free parameters of our study (see §2.1 and 4.2). In our models we combine all metals (e.g., Fe\(^{+}\), Mg\(^{+}\)) into one species, labeled as M\(^{+}\) with the Fe\(^{+}\) recombinations rate of \(\alpha(\text{M}^{+}) = 3.7 \times 10^{-12}(T/300 \text{ K})^{-0.65} \text{ cm}^3 \text{ s}^{-1}\). Because of the low ionization

### Table 1

| Species         | Abundance$^a$ |
|-----------------|---------------|
| H\(_2\)         | 0.5           |
| He              | 0.14          |
| H\(_2\)O\(_{ex}\) | 2.2 \times 10^{-4} |
| H\(^{13}\)O\(_{ex}\) | 4.4 \times 10^{-7} |
| CO              | 8.5 \times 10^{-5} |
| \(^{13}\)CO    | 9.5 \times 10^{-7} |
| C\(^{18}\)O    | 1.7 \times 10^{-7} |
| N                | 1.50 \times 10^{-3} |
| N\(_2\)        | 2.5 \times 10^{-8} |
| HD              | 1.6 \times 10^{-8} |
| Grains          | 10^{-12}       |

$^a$ Relative to H nuclei.

---

**Fig. 1.**—Comparison between integrated intensity maps (contours) of C\(^{18}\)O(1–0) (left; from Bergin et al. 2002), H\(^{13}\)CO\(^{+}\)(1–0) (center), and DCO\(^{+}\)(2–1) (right) superposed on the map of visual extinction obtained by Alves et al. (2001). C\(^{18}\)O(1–0) contours start at 0.2 K km s\(^{-1}\) and step by 0.2 K km s\(^{-1}\). H\(^{13}\)CO\(^{+}\)(1–0) contours start at 0.15 K km s\(^{-1}\) and step by 0.15 K km s\(^{-1}\). DCO\(^{+}\)(1–0) contours start at 0.1 K km s\(^{-1}\) and step by 0.1 K km s\(^{-1}\). The A\(_r\) images range from 0 to 27 mag.
potentials these metals are assumed to be fully ionized at the start of the calculation. The network also includes the neutralization of ions of negatively charged grains with one electron per grain.

The core is assumed to be bathed in a UV field of 0.2 (in Habing units; Habing 1968), as determined by Bergin et al. (2006). The chemical abundances are computed as a function of time by solving the rate equations using the DVODE algorithm (Brown et al. 1989). This is done until a time of 10\(^5\) yr is reached. This corresponds to the “best-fit” model of Bergin et al. (2006). However, as discussed by Bergin et al., this time is a lower limit of the real age of the cloud, since the CO is assumed to be preexisting at \(t = 0\) in these models.

Modeling the line emission requires the knowledge of velocity profile in the core. As a first approach, we have neglected systematic motions (see Lada et al. 2003; Redman et al. 2006), and we have used the turbulent velocity profile determined by Bergin et al. (2006) from \(^1\)C\(^1\)O and \(^1\)C\(^2\)O lines. The turbulent velocity is \(\sim 0.3\) km s\(^{-1}\) at the edge of the cloud, and decreases significantly (\(\sim 0.15\) km s\(^{-1}\)) toward the center of the core.

4. RESULTS

4.1. Metals Depletion

Metal ions (e.g., Fe\(^{++}\) and Mg\(^{++}\)) play an important role in setting the electron abundance in prestellar cores, because they are destroyed relatively slowly by radiative recombination. For example, the recombination rate of H\(^+\) is 4 orders of magnitude higher than the rate for Fe\(^{++}\).

Guélin et al. (1982) measured the electron abundance in a sample of dense molecular clouds using HCO\(^++\) and DCO\(^++\) line observations and obtained values of between \(10^{-8}\) and \(10^{-7}\). The authors concluded that the metal abundance is lower than \(10^{-7}\) in these clouds. Caselli et al. (1998) determined the electron abundance in a sample of 24 low-mass isolated cores (some with embedded stars and others starless, similar in properties to B68) from CO, HCO\(^++\), and DCO\(^++\) observations and obtained values in the range \(10^{-8}\) to \(10^{-6}\). Caselli et al. argued that the differences between cores are due to changes in metal abundance and a variable cosmic ionization rate (\(\zeta\)). The best fit between their chemical model predictions and the observations indicates metal abundances in the range \(2 \times 10^{-9}\) to \(3 \times 10^{-7}\). Williams et al. (1998) determined the electron abundance in a similar sample of low-mass cores using a slightly different approach and obtained metal abundances of between \(5 \times 10^{-9}\) and \(4 \times 10^{-8}\) (assuming a constant \(\zeta\)). All these studies indicate low metal abundances with respect to their solar values. Indeed, observations of far-ultraviolet (FUV) Fe \(II\) absorption lines, and other metal lines, toward diffuse clouds find depletion factors of over 2 orders of magnitude with respect to solar values (Savage & Bohlin 1979; Jenkins et al. 1986; Snow et al. 2002).

Our H\(^{13}\)CO\(^++\) observations can be used to set limits on the metal ion abundance in B68. H\(^{13}\)CO\(^++\) is sensitive to the electron abundance inside the core, because it is mainly destroyed by electronic recombination. It is also sensitive to the H\(^+\) and \(^1\)CO abundances, since it is formed from the reaction between these two species. H\(^+\) itself is mainly formed from H\(^+\) ionization by cosmic rays. The remaining parameter in determining the chemical abundance profile is the time dependence of the chemistry. In this case our analysis is simplified, because Bergin et al. (2006) used multiple transitions of \(^1\)C\(^1\)O and \(^1\)C\(^2\)O and a similar modeling technique to derive the \(^1\)CO abundance and constrain the “chemical age” of Barnard 68 to \(t = 10^5\) yr. Thus, the only free parameters for our modeling of the H\(^{13}\)CO\(^++\) emission are the cosmic ionization rate \(\zeta\) and the metal ion abundance. These two parameters are difficult to constrain simultaneously. In Maret et al. (2006) we found that the H\(^{13}\)CO\(^++\) line emission in B68 is well reproduced by our chemical network if one assumes a metal abundance of \(3 \times 10^{-5}\) with respect to H nuclei and a standard cosmic ionization rate (\(\zeta = 3 \times 10^{-17}\) s\(^{-1}\); see § 4.2). In the following, we explore the parameter space in more detail to place constraints on the metal abundance in the core.

In Figure 2 we show the predicted intensity of the H\(^{13}\)CO\(^++\) line for different metal ion abundances and cosmic ionization rates. In these models, metals are assumed to be initially fully ionized. In Figure 2 we see that for \(\zeta = 3 \times 10^{-17}\) s\(^{-1}\), our model predicts the same intensities for \(x(M^+) = 0\) and \(x(M^+) = 3 \times 10^{-10}\). The predicted emission is in fairly good agreement with the observations. On the other hand, for a higher metal abundance \(x(M^+) = 3 \times 10^{-9}\) the model predicts an intensity slightly lower than that observed, but is in better agreement with the observations at the center of the core. A metal abundance of \(3 \times 10^{-8}\) is clearly ruled out by the model and observation comparison. We conclude that \(x(M^+) \leq 3 \times 10^{-9}\). This value is at the low end of that obtained by Caselli et al. (1998) and Williams et al. (1998). Compared to the abundance of metals in the solar photosphere \((x(M) \sim 8.5 \times 10^{-5}\); Anders & Grevesse 1989\)), this represents a depletion factor of more than 4 orders of magnitude. Indeed, our observations are also consistent with a complete depletion of metals in the core, i.e., with cosmic rays as the only source of ionization at \(A_{\perp}\) greater than a few magnitudes (see Fig. 2). It should be noted, however, that the result depends on the value of \(\zeta\) adopted. For example, our observations are fully consistent with a cosmic ionization rate of \(3 \times 10^{-16}\) s\(^{-1}\) and \(x(M^+) = 3 \times 10^{-8}\). The effects of varying \(\zeta\) are discussed in § 4.2.

4.2. Cosmic-Ray Ionization Rate

Cosmic rays play a crucial role in the chemistry of prestellar cores, because they set the abundance of the pivotal H\(^+\) ion and are the only source of ionization at \(A_{\perp}\) greater than a few magnitudes. Despite its importance, the cosmic-ray ionization rate is difficult to constrain (see Le Petit et al. 2004; van der Tak et al. 2006; Dalgarno 2006 for recent reviews). Early estimates in diffuse clouds from HD and OD observations indicate \(\zeta = 7 \times 10^{-17}\) s\(^{-1}\) (van Dishoeck & Black 1986), a value in agreement with the lower limit of \(3 \times 10^{-17}\) s\(^{-1}\) measured by the Voyager and Pioneer satellites (Webber 1998). H\(^3\)O\(^+\) observations toward the \(\zeta\) Persei cloud suggest a significantly higher rate (\(\zeta = 1.2 \times 10^{-15}\) s\(^{-1}\); McCall et al. 2003). However, Le Petit et al. (2004) argued that a value of \(\zeta = 2.5 \times 10^{-16}\) s\(^{-1}\) is more consistent with both H\(^3\)O\(^+\) and HD observations. In denser regions, HCO\(^+\) observations indicate a lower ionization rate than in diffuse clouds; van der Tak & van Dishoeck (2000) obtained \(\zeta = (2.6 \pm 1.8) \times 10^{-17}\) s\(^{-1}\) from HCO\(^+\) line observations toward massive protostars. In prestellar cores, Caselli et al. (1998) inferred a value of between \(10^{-19}\) and \(10^{-16}\) s\(^{-1}\). The difference in the cosmic-ray ionization rate between diffuse and dense clouds could be due to the scattering of cosmic rays (Padoan & Scalo 2005). In addition, large variations are inferred as a function of the Galactic center distance (Oka et al. 2005; van der Tak et al. 2006).

Cosmic rays are also heating agents of the gas. Bergin et al. (2006) examined the value of \(\zeta\) in B68 by comparing the predictions of a chemical and thermal model to observations of CO and its isotopologues. Bergin et al. found that their model provides reasonable fits to the data for \(\zeta = 1 - 6 \times 10^{-17}\) s\(^{-1}\). Their best-fit model has \(\zeta = (1.5-3) \times 10^{-17}\) s\(^{-1}\). Here we examine the constraints placed by our H\(^{13}\)CO\(^++\) observations. In Figure 2 we see
that our model produces a good fit to the data for \( \zeta = 3 \times 10^{-17} \) s\(^{-1} \), except for \( x(M^+) = 3 \times 10^{-8} \), where the model predictions underestimate the observation by a factor 2. Models with \( \zeta = 3 \times 10^{-18} \) s\(^{-1} \) consistently underestimate the observations. Conversely, models with \( \zeta = 3 \times 10^{-16} \) s\(^{-1} \) overestimate the model, except for the one with \( x(M^+) \leq 3 \times 10^{-8} \). This is in agreement with Bergin et al. (2006), who found that their observations are not reproduced by models with \( \zeta = 6 \times 10^{-16} \) s\(^{-1} \).

To summarize our conclusions regarding the metal abundances and the cosmic ionization rate, models with \( x(M^+) \leq 3 \times 10^{-9} \) in B68. This implies that the abundance of ionized metals is reduced in the center of B68. Charge transfer from molecular ions (e.g., \( \text{H}_2^+ \), \( \text{HCO}^+ \)) to metals can be important, and a reduction in the abundance of ionized metals also requires the lowering of the neutral metal abundance. In the case of Fe, a potential reservoir is FeS (Keller et al. 2002), or organometallic molecules (Serra et al. 1992). Another possibility is that Fe is incorporated into grain cores.

4.3. Ortho-to-Para \( \text{H}_2 \) Ratio

The ortho-to-para \( \text{H}_2 \) ratio influences the degree of ion and molecule deuteration in prestellar cores (Pineau des Forêts et al. 1991; Flower et al. 2006a). In the gas phase, deuteration fractionation is mainly due to the reaction (see Roberts et al. 2004 and references therein)

\[
\text{H}_2^+ + \text{HD} = \text{H}_2\text{D}^+ + \text{H}_2. \tag{1}
\]

The reverse reaction has an activation barrier of \( \sim 232 \) K, and therefore, the reaction becomes essentially irreversible at low...
temperature. Gerlich et al. (2002) measured the forward and reverse rates of the above reaction at 10 K and found them to be very different than commonly adopted values. The forward reaction rate was found to be about 5 times higher than previous estimates (Sidhu et al. 1992), while the reverse reaction rate was found to be 5 orders of magnitude larger than previously used (e.g., Caselli et al. 1998). In addition, Gerlich et al. (2002) determined via a laboratory measurement that the reverse reaction rate is very sensitive to the ratio of ortho-to-para molecular hydrogen, because o-H$_2$ in its ground rotational level ($J = 1$) has a higher energy ($\Delta E \approx 170.5$ K) when compared to the ground state of p-H$_2$ ($J = 0$). Consequently, o-H$_2$ can more easily cross the energy barrier than p-H$_2$, and the rate of the reverse reaction increases with the ortho-to-para H$_2$ ratio.

Our DCO$^+$ observations can be used to estimate the H$_2$D$^+$ abundance and, thus, the efficiency of the deuterium fractionation process. DCO$^+$ is mainly formed by the reaction

$$\text{H}_2\text{D}^+ + \text{CO} \rightarrow \text{DCO}^+ + \text{H}_2$$

(2)

and is mainly destroyed by electronic recombination. Thus, the DCO$^+$ emission depends on both the CO and H$_2$D$^+$ abundances, the electron fraction (induced by cosmic rays and by preexisting metal ions), the ortho-to-para H$_2$ ratio, and on time. Here we benefit from our previous analysis of CO, which constrained the CO abundance and “chemical age,” and our analysis of H$^{13}$CO$^+$, which limited the metal ion abundance and cosmic-ray ionization rate. Thus, the primary free parameter is the ortho-to-para H$_2$ ratio (o/p) when we adopt our best-fit parameters of $\chi(M^+) = 3 \times 10^{-9}$ and $\zeta = 3 \times 10^{-17}$ s$^{-1}$.

In Figure 3 we compare the observed DCO$^+(1-0)$ line emission as a function of $A_V$, with the predictions of our model for different o/p. Note that in these models, no o/p conversion is considered; the o/p is assumed to be constant. The best agreement between the observations and the model is obtained for an o/p of $\sim 1.5 \times 10^{-2}$, well above the Boltzmann equilibrium value at 10 K ($3.5 \times 10^{-7}$). Figure 3 also shows the derived DCO$^+$ abundance inside the core. The abundance peaks at an $A_V$ of $\sim 5$ and decreases slightly toward the core center as a consequence of CO depletion (see § 5.1).

It is interesting to compare the o/p H$_2$ we obtain with the predictions of other models. Walmsley et al. (2004) modeled the o/p in prestellar cores, assuming a complete depletion of heavy elements. In their model, an initial o/p of $3.5 \times 10^{-7}$ is assumed. For a density of $10^6$ cm$^{-3}$, steady state is reached in $10^5$ yr, a time comparable to the age of B68 inferred from CO depletion observation and modeling (Bergin et al. 2006). At steady state, the o/p obtained is $6 \times 10^{-5}$, i.e., about 2 orders of magnitude lower than the value determined in this work. However, as noted by Flower et al. (2006b), the o/p conversion reactions are very slow, and it is not clear if the steady state equilibrium is reached in molecular clouds prior to the formation of dense cores. Using an initial o/p of 3 (a value appropriate for H$_2$ formation on grains), Flower et al. (2006a) obtain a steady state ratio of $3 \times 10^{-5}$. This value, although still about a factor 5 lower, is in better agreement with our estimate. We note that for o/p = $3 \times 10^{-3}$, our model predicts a DCO$^+(1-0)$ emission about 2 times higher than the observations (see Fig. 3).

5. DISCUSSION

5.1. Electron Abundance and Main Charge Carriers

In Figure 4 we show the derived electron and main ion abundances inside the core. The electron abundance is $\sim 5 \times 10^{-9}$ with respect to H nuclei throughout most of the core. At low $A_V$, the
electron abundance increases as a result of photodissociation of CO. In this region, the most abundant ion is C\(^+\). At higher \(A_T\), the most abundant ion is H\(_3^+\), which carries about \(\sim\)20% of the electric charge. The remainder of the charge is shared between more complex ions. Deuterated ions do not contribute significantly to the ionization fraction. In the innermost region of the core, where the deuteration increases as a result of CO depletion, the main deuterated ion, D\(_3^+\), is about 10 times less abundant than H\(_3^+\). H\(_2\)D\(^+\) and D\(_2\)H\(^+\) have similar abundances (\(2 \times 10^{-11}\) with respect to H). This is in agreement with recent observations (Vastel et al. 2004).

Recently, Hogerheijde et al. (2006) reported a probable detection of the \(\nu_2\)-H\(_2\)D\(^+\) fundamental line toward B68, which can be compared to our model predictions. The measured flux is, however, quite uncertain, given the relatively low signal-to-noise ratio of this observation (2.7 \(\sigma\) and 5.2 \(\sigma\) on the peak and integrated intensity, respectively). Assuming a thermal excitation (10 K) and optically thin conditions, Hogerheijde et al. derive an H\(_2\)D\(^+\) column density of \(1.5 \times 10^{12}\) cm\(^{-2}\). Assuming an H\(_2\) column density of \(3.6 \times 10^{22}\) cm\(^{-2}\) (Alves et al. 2001), this corresponds to an H\(_2\)D\(^+\) abundance of \(2.1 \times 10^{-11}\) with respect to H nuclei, averaged in the Atacama Pathfinder Experiment (APEX) beam (17\(\arcsec\)). This is in excellent agreement with our model, which predicts an H\(_2\)D\(^+\) abundance of \(2 \times 10^{-11}\), roughly constant across the envelope. Of course, if the excitation is nonthermal, the detection implies a higher abundance. Assuming a 5 K excitation temperature, Hogerheijde et al. derive a beam-averaged abundance of \(1.5 \times 10^{-10}\) with respect to H nuclei. This is about an order of magnitude higher than our model predictions. Since no collisional rates exist in the literature for H\(_2\)D\(^+\), it is unclear whether or not the excitation of this line is thermal. Hogerheijde et al. estimate a critical density of \(2 \times 10^6\) cm\(^{-3}\), which exceeds the density at the center of B68 (3 \(\times 10^5\) cm\(^{-3}\)) by about an order of magnitude. However, the collisional rate, and therefore, the critical density, is uncertain by an order of magnitude (van der Tak et al. 2005; Hogerheijde et al. 2006). Our model predictions regarding the deuteration chemistry could be also tested via observations of the D\(_2\)H\(^+\) 1\(_{0,0}\) \(\rightarrow\) 1\(_{0,1}\) (\(\nu = 691.66044\) GHz). Assuming an excitation temperature of 10 K, we predict a line intensity of 10 mK. Unfortunately, this is too weak to be detected with current ground-based telescopes.

We would like to compare the electron abundance profile we obtained with that derived by Caselli et al. (2002) in L1544. In the Caselli et al. best-fit model, the electron abundance at the center of L1544 is \(5 \times 10^{-10}\) (with respect to H), while we obtain an electron abundance an order of magnitude higher at the center of B68. These differences are probably a consequence of different central densities; the L1544 central density is about an order of magnitude higher than that of B68, and the electron fraction is expected to scale as \(n(H_2)^{-1/2}\) (McKee 1989). Another important difference is the dominant ion; Caselli et al. (2002) predicts that the most abundant ion is H\(_2\)O\(^+\), while in our modeling the main charge carrier is H\(_3^+\). These differences are due to different assumptions on the atomic oxygen abundance. Caselli et al. (2002) assumes that oxygen is initially mostly atomic. As a consequence, the H\(_2\)O\(^+\) abundance is relatively large, because atomic oxygen reacts with H\(_3^+\) to form H\(_2\)O\(^+\) (after successive protonations by H\(_2\) followed by recombination). In our modeling, oxygen is assumed to be initially locked in water ices and gas-phase CO (see Table 1), and the atomic oxygen gas-phase abundance is relatively low.

Finally, we would like to comment on the effect of grain size evolution on the electron fraction in the core. Walmsley et al. (2004) computed the electron abundance and main charge carrier in a prestellar core for different grain sizes. For a grain size of 0.02 \(\mu\)m, the main charge carrier in their model is H\(_3^+\), while for larger grains (0.1 \(\mu\)m), the most abundant ion becomes H\(^+\). In their models, H\(^+\) recombines primarily on grains, while H\(_3^+\) recombines with free electrons. Since the recombination timescale on grains depends on the grain size, the H\(^+\) over H\(_3^+\) abundance ratio, and in turn the electron abundance, depends on the grain size as well. However, these models assume a complete depletion of heavy elements, which is not the case for B68. In B68 we do find evidence for strong molecular, but not complete, heavy-element freezeout, at the core center. The reaction with H\(^+\) with molecules containing these elements (e.g., NH\(_3\), OH) can transfer the charge to molecular ions with faster recombination timescales. This would probably reduce the dependence of the electron abundance on the grain size.

5.2. Core Stability

The electron abundance in the core is also important for its dynamical evolution, since it affects the efficiency of ambipolar diffusion. In a weakly ionized subcritical core, the ions are supported against collapse by the magnetic field, but neutrals can slowly drift with respect to the ions (see Shu et al. 1987 for a review). The timescale for this phenomenon is given by Walmsley et al. (2004),

\[
\tau_{ad} = \frac{2}{\pi G m_n^2} \sum_i \frac{n_i}{n_H} \frac{m_{ion}}{m_n} \left\langle \sigma v \right\rangle_{in},
\]

where \(G\) is the gravitational constant, \(m_n\) and \(m_i\) are the masses of the neutrals and the ions, respectively, \(n_i\) and \(n_H\) are the number densities, \(\left\langle \sigma v \right\rangle_{in}\) is the rate coefficient for the momentum transfer, and the summation goes over all ions. At low temperature, the rate coefficient for momentum transfer is (Flower 2000)

\[
\left\langle \sigma v \right\rangle_{in} = 2\pi e \left( \frac{1}{\alpha} + \frac{m_i}{m_n} m_n \right)^{1/2},
\]

where \(\alpha\) is the polarizability of H\(_2\). Assuming that H\(_3^+\) is the dominant ion, we obtain

\[
\tau_{ad} \sim 2 \times 10^{14} \chi(e) \text{ yr},
\]

where \(\chi(e)\) is the electron abundance, with respect to H. Thus, at the center of the core, the ambipolar diffusion timescale is 10\(^6\) yr. It is interesting to compare this to the free-fall timescale, which is given by

\[
\tau_{ff} = \left( \frac{3\pi}{32 G \rho} \right)^{1/2},
\]

where \(\rho = n_{H_2} m_{H_2}\) is the mass density. When expressed as a function of \(n_{H_2}\), this gives

\[
\tau_{ff} = 3.6 \times 10^7 n_{H_2}^{-1/2} \text{ yr}.
\]

At the center of B68 we obtain \(\tau_{ff} = 7 \times 10^4\) yr, which is about an order of magnitude faster than the ambipolar diffusion timescale. Thus, if present, the magnetic field may provide an important source of support.

The strength of the magnetic field that is needed to support the cloud can be obtained from the critical mass (Mouschovias & Spitzer 1976)

\[
M \sim \frac{0.13}{G^{1/2} \phi_B},
\]

where \(G\) is the gravitational constant, and \(\phi_B\) is the magnetic field strength.
where $\phi = \pi R^2 B$ is the magnetic flux, $R$ is the core radius, and $B$ is the magnetic field strength. The strength of the magnetic field that is needed to support the cloud is therefore

$$B \sim \frac{G^{1/2} M}{0.13 \pi R^2},$$

where $M$ is the mass of the core. Using $R = 12,500$ AU and $M = 2.1 M_\odot$ (Alves et al. 2001), we obtain a critical magnetic field of 76 $\mu$G for B68. No magnetic field measurements for B68 exist in the literature, but we can compare this value to the one measured in other cores from dust submillimeter polarization. Ward-Thompson et al. (2000) and Crutcher et al. (2004) measured plane-of-the-sky magnetic field strengths of 80 $\mu$G in L183, 140 $\mu$G in L1544, and 160 $\mu$G in L43. Kirk et al. (2006) measured lower fields of 10 and 30 $\mu$G in the L1498 and L1517B cores. Therefore, if the magnetic field strength in B68 is at the lower end of the values measured in other cores, then it might be supercritical (i.e., the magnetic field is too weak to balance gravity). If it is higher, then the core is probably subcritical. One may argue B68 has nearly round shape (albeit with an asymmetrical extension to the southeast), which potentially is indicative of a weak magnetic field.

5.3. Implications of the Metals Depletion for Accretion in Protostellar Disks

One important conclusion of this study is the large metal depletion inferred for B68. Here we examine the implication of this finding for the mechanism of angular momentum transport in protostellar disks. The most favored theory for angular momentum transport in disks predicts that accretion occurs via magnetorotational instability (MRI; Balbus & Hawley 1991), which produces magneto-hydrodynamic (MHD) turbulence. Since this is a magnetic process, the ion-neutral coupling is therefore important. Typically, the ionization fraction should be greater than $10^{-12}$ for disks to be able to sustain MHD turbulence (see Ilgner & Nelson 2006 and references therein). Gammie (1996) suggested a model wherein the accretion is layered. The electron abundance is high at the surface of the disk because of the ionization of the gas by UV, X-rays, and cosmic rays, but it decreases toward the midplane. Thus, disks may have magnetically active zones at high altitude, where the electron fraction is sufficient to maintain MHD turbulence, and “dead zones” closer the midplane of the disk, where the electron fraction is lower, and accretion cannot occur.

Our results have some import on this process, because the chemical structure of the prestellar stage sets the initial chemical conditions of the gas that feeds the forming protoplanetary disk. Because of their influence on the ionization fraction, metal ions can have dramatic effects on the size of the dead zone, assuming that they are provided by infall to the disk (Fromang et al. 2002; Ilgner & Nelson 2006). The latter authors computed the ionization fraction in a protostellar disk and found that for $x(M^+) \leq 3 \times 10^{-10}$, the dead zone extends between 0.5 and 2 AU, while it disappears completely for $x(M^+) \geq 10^{-8}$. In B68, we obtain a metal abundance of $x(M^+) \leq 3 \times 10^{-9}$, which is below the threshold for a complete disappearance of the dead zone. Thus, if B68 is representative of the initial conditions for the formation of protostellar disks, and cosmic rays do not penetrate deeply to the midplane, dead zones should exist in those disks.

6. CONCLUSIONS

We have presented a detailed analysis of the electron abundance in the B68 prestellar core using H$^{13}$CO$^+$(1−0) and DCO$^+$(2−1) line observations. These observations were compared to the predictions of a time-dependent chemical model coupled with a Monte Carlo radiative transfer code. This technique allows for a direct comparison between chemical model predictions and observed line intensities as a function of radius (or the visual extinction) of the core. Our main conclusions are:

1. The metal abundance is difficult to constrain independently from the cosmic ionization rate. However, accounting for thermal balance considerations and to reproduce H$^{13}$CO$^+$(1−0) emission, we estimate that $x(M^+) \leq 3 \times 10^{-9}$ and $\zeta = (1-6) \times 10^{-17}$ s$^{-1}$.

2. The DCO$^+$(2−1) line emission is sensitive to the ortho-to-para ratio. The emission is well reproduced by our model for an ortho-to-para ratio of 1.5 $\times 10^{-2}$, well below the equilibrium value, and in reasonable agreement with previous work.

3. The inferred electron abundance is $5 \times 10^{-9}$ (with respect to H), and is roughly constant in the core at $A_F > 5$. It increases at lower $A_F$ because of the photodissociation of CO and photionization of C. In the dense part of the core, the dominant ion is H$_3^+$, HD$^+$, and D$_2$H$^+$. They have similar abundances and are about 2 orders of magnitude less abundant than H$_3^+$. In the center of the core, our model predicts D$^+_2$ to be the most abundant deuterated ion.

4. The inferred electron abundance implies an ambipolar diffusion timescale of 10$^6$ yr at the center of the core, which is about an order of magnitude higher than the free-fall time (10$^3$ yr).

5. The metal abundance we obtain is below the threshold for a protostellar disk to be fully active. Consequently, if the chemical composition of B68 is representative of the initial conditions for the formation of a disk and cosmic rays do not penetrate to the disk midplane, then dead zones should exist in protostellar disks.

Both authors are grateful to C. Lada for a fruitful collaboration that led to this work and to T. Huard and E. Aguti for obtaining a portion of these data. We are also grateful to the referee and to the editor J. Black for useful and constructive comments. S. M. wishes to thank H. Roberts for helping us in testing the predictions of our model for the ortho-to-para ratio, L. Hartmann and F. Heitch for discussions about the ortho-to-para ratio, L. Hartmann and F. Heitch for discussions about the dynamics of B68, and S. Fromang for discussions about MRI in protostellar disks. This work is supported by the National Science Foundation under grant 0335207.

Facilities: IRAM.30m, CSO, APEX

REFERENCES

Alves, J. F., Lada, C. J., & Lada, E. A. 2001, Nature, 409, 159
Anders, E., & Grevesse, N. 1989, Geochim. Cosmochim. Acta, 53, 197
Balbus, S. A., & Hawley, J. F. 1991, ApJ, 376, 214
Bergin, E. A., Alves, J., Huard, T., & Lada, C. J. 2002, ApJ, 570, L101
Bergin, E. A., Langer, W. D., & Goldsmith, P. F. 1995, ApJ, 441, 222
Bergin, E. A., Maret, S., van der Tak, F. F. S., Alves, J., Carcmondy, S. M., & Lada, C. J. 2006, ApJ, 645, 369
Brown, P. N., Byrne, G. D., & Hindmarsh, A. C. 1989, SIAM J. Sci. Stat. Comput., 10, 1038
Caselli, P. 2002, Planet. Space Sci., 50, 1133
Caselli, P., Walsmley, C. M., Terzieva, R., & Herbst, E. 1998, ApJ, 499, 234
Bergin, E. A., & Snell, R. L. 2002, ApJ, 581, L105
Bergin, E. A., et al. 2000, ApJ, 539, L129
Briga, E. M., & Johnson, R. E. 2004, ApJ, 603, 159
Brown, P. N., Byrne, G. D., & Hindmarsh, A. C. 1989, SIAM J. Sci. Stat. Comput., 10, 1038
Caselli, P. 2002, Planet. Space Sci., 50, 1133
Caselli, P., Walmsley, C. M., Zucconi, A., Tafalla, M., Dore, L., & Myers, P. C. 2002, ApJ, 565, 344
Crutcher, R. M., Nutter, D. J., Ward-Thompson, D., & Kirk, J. M. 2004, ApJ, 600, 279
Dalgarno, A. 2006, Proc. Natl. Acad. Sci., 103, 12269
de Boisanger, C., Helmich, F. P., & van Dishoeck, E. F. 1996, A&A, 310, 315
Flower, D. R. 2000, MNRAS, 313, L19
Flower, D. R., Pineau Des Forêts, G., & Walmsley, C. M. 2006a, A&A, 449, 621
———. 2006b, A&A, 456, 215
Fromang, S., Terquem, C., & Balbus, S. A. 2002, MNRAS, 329, 18
Gammie, C. F. 1996, ApJ, 457, 355
Gerlich, D., Herbst, E., & Roueff, E. 2002, Planet. Space Sci., 50, 1275
Guêlin, M., Langer, W. D., & Wilson, R. W. 1982, A&A, 107, 107
Habing, H. J. 1968, Bull. Astron. Inst. Netherlands, 19, 421
Hasegawa, T. I., & Herbst, E. 1993, MNRAS, 261, 83
Herbst, E., & Klemperer, W. 1973, ApJ, 185, 505
Hogerheijde, M. R., et al. 2006, A&A, 454, L59
Ilgner, M., & Nelson, R. P. 2006, A&A, 445, 223
Jenkins, E. B., Savage, B. D., & Spitzer, L., Jr. 1986, ApJ, 301, 355
Keller, L. P., et al. 2002, Nature, 417, 148
Kirk, J. M., Ward-Thompson, D., & Crutcher, R. M. 2006, MNRAS, 369, 1445
Lada, C. J., Bergin, E. A., Alves, J. F., & Huard, T. L. 2003, ApJ, 586, 286
Lai, S.-P., Velusamy, T., Langer, W. D., & Kuiper, T. B. H. 2003, AJ, 126, 311
Langer, W. D. 1985, in Protostars and Planets II, ed. D. C. Black & M. S. Matthews (Tucson: Univ. Arizona Press), 650
Langer, W. D., & Penzias, A. A. 1993, ApJ, 408, 539
Le Petit, F., Roueff, E., & Herbst, E. 2004, A&A, 417, 993
Maret, S., Bergin, E. A., & Lada, C. J. 2006, Nature, 442, 425
McCall, B. J., et al. 2003, Nature, 422, 500
McKee, C. F. 1989, ApJ, 345, 782
Millar, T. J., Bennett, A., & Herbst, E. 1989, ApJ, 340, 906
Millar, T. J., Farquhar, P. R. A., & Willacy, K. 1997, A&AS, 121, 139
Mouschovias, T. C., & Spitzer, Jr., L. 1976, ApJ, 210, 326
Oka, T., Geballe, T. R., Goto, M., Usuda, T., & McCall, B. J. 2005, ApJ, 632, 882
Padoan, P., & Scalo, J. 2005, ApJ, 624, L97
Pineau des Forêts, G., Flower, D. R., & McCarroll, R. 1991, MNRAS, 248, 173
Redman, M. P., Keto, E., & Rawlings, J. M. C. 2006, MNRAS, 370, L1
Roberts, H., Herbst, E., & Millar, T. J. 2004, A&A, 424, 905
Savage, B. D., & Bohlin, R. C. 1979, ApJ, 229, 136
Serra, G., Chaudret, B., Saillard, Y., Le Beuze, A., Rabaa, H., Ristorcelli, I., & Klotz, A. 1992, A&A, 260, 489
Shu, F. H., Adams, F. C., & Lizano, S. 1987, ARA&A, 25, 23
Sidhu, K. S., Miller, S., & Tennyson, J. 1992, A&A, 255, 453
Snow, T. P., Rachford, B. L., & Figsoski, L. 2002, ApJ, 573, 662
Tafalla, M., Myers, P. C., Caselli, P., Walmsley, C. M., & Comito, C. 2002, ApJ, 569, 815
van der Tak, F. S. F., Belloche, A., Schilke, P., Güsten, R., Philipp, S., Comito, C., Bergman, P., & Nyman, L.-Å. 2006, A&A, 454, L99
van der Tak, F. S. F., Caselli, P., & Ceccarelli, C. 2005, A&A, 439, 195
van der Tak, F. S. F., & van Dishoeck, E. F. 2000, A&A, 358, L79
van Dishoeck, E. F., & Black, J. H. 1986, ApJS, 62, 10
Vastel, C., Phillips, T. G., & Yoshida, H. 2004, ApJ, 606, L127
Walmsley, C. M., Flower, D. R., & Pineau des Forêts, G. 2004, A&A, 418, 1035
Ward-Thompson, D., Kirk, J. M., Crutcher, R. M., Greaves, J. S., Holland, W. S., & André, P. 2000, ApJ, 537, L135
Webber, W. R. 1998, ApJ, 506, 329
Williams, J. P., Bergin, E. A., Caselli, P., Myers, P. C., & Plume, R. 1998, ApJ, 503, 689
Wootten, A., Loren, R. B., & Snell, R. L. 1982, ApJ, 255, 160
Zucconi, A., Walmsley, C. M., & Galli, D. 2001, A&A, 376, 650