PROBING PRE-PROTOSTELLAR CORES WITH FORMALDEHYDE

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ABSTRACT

We present maps of the 6 cm and 1.3 mm transitions of H₂CO toward three cold, dense pre-protostellar cores (PPCs): L1498, L1512, and L1544. The 6 cm transition is a unique probe of high-density gas at low temperature. However, our models unequivocally indicate that H₂CO is depleted in the interiors of PPCs, and depletion significantly affects how H₂CO probes the earliest stages of star formation. Multistage, self-consistent models, including gas-dust energetics, of both H₂CO transitions are presented, and the implications of the results are discussed.

Subject headings: astrochemistry — ISM: clouds — ISM: individual (L1498, L1512, L1544) — ISM: molecules — radio lines: ISM — stars: formation

1. INTRODUCTION

Molecular cloud cores that have yet to form a star provide the best opportunity to determine the initial conditions for star formation. However, the earliest evolution of a cloud core is very poorly constrained, and its evolutionary track is unclear. Recently, a number of compact objects without IRAS sources but with considerable submillimeter continuum emission have been identified (Ward-Thompson et al. 1994). Since these have no obvious source of internal luminosity but are characterized by high column density, they are plausible candidates for the stages just before formation of a central object. These objects are classified as pre-protostellar cores, or PPCs.

Several of these objects have been mapped in submillimeter continuum emission (Shirley et al. 2000), and the dust emission has been modeled using self-consistent calculations of the dust temperature (Evans et al. 2001). The calculations show that the dust deep inside the PPCs is very cold \( T_d \sim 8 \) K and that this low \( T_d \) affects the interpretation of the submillimeter emission. In particular, the PPCs may be more centrally condensed, with higher central densities, than previously thought. Study of these objects will be very valuable for our understanding of the formation of solar-type stars. The density distribution as a function of radius in such starless cores is a strong discriminator between theoretical models. The density structure is also of critical importance for assessing whether the cloud is in equilibrium or whether it may be beginning to collapse, and the density structure of PPCs strongly affects the nature of the collapse and star formation that follows (André et al. 2000).

Most density tracers employed by astronomers involve the use of a pair of rotational transitions of a linear molecule (e.g., isotopologues of CO, CS, HC₃N). Since the different transitions have different spontaneous decay rates, they require different collision rates to bring their populations into thermal equilibrium. At a specific density, their relative populations reflect the collision rate and thus allow determination of the hydrogen density. This method can work well, but there is an important caveat: the different rotational levels generally lie at significantly different energies above the ground state, given approximately by the rigid-rotor formula \( E(J) = hB_0 J(J + 1) \). For \( ^{13}\)CO, \( J = 1 \) is at 5.3 K, \( J = 2 \) is at 15.8 K, \( J = 3 \) is at 31.6 K, etc. When we are dealing with a very cold cloud \( (T \leq 10 \) K) or a cloud whose temperature structure is unknown, a significant uncertainty is introduced. The collisional excitation rates, as well as the LTE level populations, for a linear molecule having a large rotation constant, including \( ^{13}\)CO, depend sensitively on the kinetic temperature of the gas. The lack of detailed temperature information means that the density one determines becomes confused with the temperature. It is extremely difficult to disentangle the two, especially in the case of cold dark clouds that may have warm edges heated by the interstellar radiation field (ISRF). For PPCs, the heated edge can dominate the excitation effects and only with quite detailed models can we become confident that we have properly separated the temperature and the density structure.

Clearly a better probe of density for studying cold, dark clouds would be valuable. The lowest transition of orthoformaldehyde \( (H_2CO) \) at 6 cm is one possible candidate. The 6 cm line is seen in absorption against the cosmic background radiation (CBR) in molecular clouds. The discovery of absorption against the CBR by the lowest transition of \( H_2CO \) (Zuckerman et al. 1969) was quite surprising because it is impossible for any two-level system to have an excitation temperature below that of the CBR. The 6 cm transition occurs between the levels of the lowest \( K \)-doublet of \( H_2CO \) (the \( J_{Ku} = 1_{11} \) and \( 1_{10} \) levels). Townes & Cheung (1969) proposed a collisional pumping scheme to lower the excitation temperature; this scheme depends on collisions to higher rotational levels followed by radiative decay to the \( J = 1 \) levels. The propensity of collisions to favor the lower levels in each excited \( K \)-doublet transition leads to an overpopulation of the lower level of the \( J = 1 \) \( K \)-doublet. This pumping scheme operates over a range of densities up to about \( 10^4 \) \( \text{cm}^{-3} \), at which point collisions become dominant and drive the excitation temperature toward
2. OBSERVATIONS

Three PPCs, L1498 (04h10m51.s5, 25°09'58", J2000.0), L1512 (05h04m08.s2, 32°43'20"), and L1544 (05h04m17.s1, 25°10'48"), were observed in 2001 December and 2002 September using the 305 m telescope of the Arecibo Observatory.1 All of the sources were observed at 6 cm, the \( J_{K_{\alpha},K_{\beta}} = l_{11} - l_{10} \) transition of orthoformaldehyde. The observed frequency was 4829.6594 MHz, the weighted mean of the frequencies of the main hyperfine component (\( F = 2 - 2 \)) and the nearby \( F = 0 - 1 \) component as given in Tucker et al. (1971). The Arecibo telescope has a beam size of 60" at this frequency. We observed at least 15 positions for each of three PPCs in the 6 cm line, creating maps with spectra spaced at 60" intervals. The mapping strategy ensured mapping off the edge of the core as seen in the dust. The long direction of each map is perpendicular to the long axis of the dust core. For L1544 and L1498, the long axis runs northwest-southeast; therefore, the map runs northeast-southwest.

The first challenge was to develop an appropriate data-taking strategy. The standard Arecibo position-switching routine, with off position designed to have the telescope observe the same “track” across the sky, is problematic, as these sources are large, and the reference position could “contaminate” the data. Switching to a fixed reference position was an option but would have had negative implications for data reduction. Fortunately, taking total power “ON SOURCE” spectra revealed that the receiver and autocorrelator (with digital bandpass filters) gave a baseline that was limited only by the fluctuations expected from the radiometer equation. This method also gains a factor of 2 in sensitivity compared to position switching and should be of general value for observation of narrow spectral lines. As discussed in §3, this technique worked well for integration times as long as 200 minutes, resulting in rms fluctuations below 10 mK in a 1.5 kHz channel width.

Standard Arecibo calibration sources were observed at the beginning and end of each shift. In 2001 December, the average beam efficiency, \( \langle \eta_B \rangle \), including the main beam and the first sidelobe, from these observations was 0.61 ± 0.05. In 2002 September, \( \langle \eta_B \rangle = 0.59 ± 0.04 \). This beam efficiency, \( \eta_B \), accounts for radiation (ohmic) losses, rearward and forward scattering, and spillover. Assuming that the coupling efficiency is unity because of the extended nature of the dark clouds, we calculate the radiation (source) temperature, \( T_R \), using the equation

\[
T_R = T_A / \eta_B,
\]

where \( T_A \) is the measured antenna temperature. \( T_R \) is outside the atmosphere. Table 1 lists the observed and derived 6 cm line properties, including \( T_R \).

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1 The Arecibo Observatory is part of the National Astronomy and Ionosphere Center, which is operated by Cornell University under a cooperative agreement with the National Science Foundation.
In addition to the 6 cm observations, each PPC was observed with the 10.4 m Caltech Submillimeter Observatory\(^2\) (CSO) at 225.697787 GHz (1.3 mm), the frequency of the \(J_{K_{\text{C}}}=3_1^2-2_1^1\) transition of \(\text{H}_2\text{CO}\). The CSO has a beam size of 32'' at 1.3 mm. The central position of L1544 was observed in 1996. In 2002 January and 2003 September/October, the central position of L1512 was observed in 1996 October. In 2002 January and 2003 September/October, the central positions of L1498 and L1512 were observed, and point maps of all three PPCs were made. The four offset positions were along and perpendicular to the long axis of the core, all at 60'' from the central position.

\(^2\) The CSO is operated by the California Institute of Technology under funding from the National Science Foundation, contract AST 90-15755.

Observations of Mars and Jupiter as calibration sources gave an average main-beam efficiency at 230 GHz of \(\eta_{\text{MB}} = 0.57 \pm 0.11\) in 1996 October, \(\eta_{\text{MB}} = 0.53 \pm 0.04\) in 2002 January, and \(\eta_{\text{MB}} = 0.77 \pm 0.06\) in 2003 September/October. Because the CSO employs a chopper wheel for calibration, the measured quantity is \(T_A^*\), the antenna temperature corrected for atmospheric attenuation, radiation losses, and rearward spill-over and scatter. Therefore, \(\eta_{\text{MB}}\) is \(\eta_{\text{MB}}\) divided by \(\eta_{\text{MB}}\), the ohmic and backward scattering efficiency. The radiation temperature in this case, again assuming that the coupling efficiency is unity, is given by

\[ T_R = T_A^* / \eta_{\text{MB}}. \]
All data were reduced using the Continuum Line Analysis Single-dish Software (CLASS). CLASS was used to remove baselines, average weighted spectra, and calibrate the data. The spectra were weighted by $\sigma^{-2}$, where $\sigma$ is the rms noise. Spectra from different nights were averaged. The 6 cm data were then Hanning smoothed. The line-center velocities ($v_{\text{LSR}}$), line widths ($\Delta v$), and optical depths (τ) for the 6 cm data were determined by fitting a manifold of Gaussian profiles, one for each hyperfine component. Only one Gaussian component was necessary for the 1.3 mm data because the hyperfine structure is negligible as a result of the extremely close spacing of the components.

3. RESULTS

Strong H$_2$CO 6 cm absorption was observed toward every source. The absorption spectra obtained at the central positions are shown in Figure 2. The radiation temperature and rms noise at each observed position are listed in Table 1, and 15-point maps of each PPC are shown in Figures 3–5. We achieved an average rms of 0.014 K at the center positions. At the other positions, the average rms was 0.022 K. The 6 cm line strength stayed nearly constant across all of the PPCs, not weakening until 120$''$ from the central position.

We have achieved exceptionally good resolution of the hyperfine components of the 6 cm inversion doublet. The $F = 1$–0 hyperfine component ($\Delta \nu = -18.5$ kHz; Tucker et al. 1971) was easily resolved in all of the PPCs. In L1498 and L1512, the $F = 1$–2 and 2–1 hyperfine components ($\Delta \nu = +6.5$ and +4.1 kHz, respectively) were also clearly distinguishable from the strong blend of the $F = 2$–2 and 0–1 components, which are closest to the observed central frequency of 4829.6594 MHz. In L1544, all of the components...
were blended except the $F = 1-0$ component creating an asymmetrical line profile.

The observed 6 cm line widths are extremely narrow ($\sim 0.4$ km s$^{-1}$), indicating low turbulent velocity dispersion. Table 1 lists the line width ($\Delta v$) and the turbulent velocity dispersion ($\sigma_{\text{turb}}$) for each source. To calculate the latter, we assumed $T_K = 10$ K. At the central positions, the H$_2$CO line widths are comparable to those observed by Caselli et al. (2002a) in the N$_2$H$^+$ $J = 1-0$ line. However, they are about a factor of 2 smaller than those observed in the NH$_3$ $(J, K) = (1, 1)$ inversion line by Benson & Myers (1989).

Table 1 also lists the excitation temperature for each position observed at 6 cm in the PPC maps. The excitation temperature was calculated using the optical depth and $T_K$ (Heiles 1973).
We assumed that there was only one velocity component and that the continuum temperature is 2.725 K (Mather et al. 1999). We find an average excitation temperature of 1.5 K. This is consistent with the results of Heiles (1973), who found a mean excitation temperature of 1.6 K for nine positions in dark dust clouds using a CBR temperature of 2.8 K. Vanden Bout et al. (1983) found a slightly higher mean excitation temperature of 1.9 K for seven dark clouds.

A significant velocity gradient is seen across L1498. Overall, the velocity increases with distance away from the center position (Fig. 6). This gradient is not consistent with either rotation or infall but is suggestive of a cometary or prolate-shaped object seen face-on. A velocity gradient has been measured in C$^{18}$O (Lemme et al. 1995) and NH$_3$ (Goodman et al. 1993). However, the gradient runs southeast-northwest, along the main axis of the dust emission, which is very different from the H$_2$CO gradient. The apparent velocity gradient could be the result of two distinct velocity components, one associated with L1498 at 7.8 km s$^{-1}$ and a second unrelated component at a higher velocity. Kuiper et al. (1996) observed a second component toward L1498 in C$^{18}$O and CS at 8.1 km s$^{-1}$. Tafalla et al. (2002) suggested that the second velocity component might be the result of gas unrelated to the dark cloud and equivalent to the “red” component in CS toward L1498 described by Lemme et al. (1995). The 6 cm H$_2$CO observations also show some evidence of a second velocity component in a small wing near 8.3 km s$^{-1}$ (see also § 4.1). Wang (1994) observed the 6 cm H$_2$CO line toward L1498 with a smaller beam at the VLA. Wang did not observe a velocity gradient, providing further evidence that the velocity gradient we observed is due to an unrelated second component.

The 1.3 mm observations toward the center of each PPC are shown in Figure 2. The 1.3 mm five-point maps are shown in Figures 3–5 along with the 6 cm absorption maps. The average rms for the 1.3 mm observations was 0.057 K. The 1.3 mm line was not detected at one offset position in each map. The 2 $\sigma$ upper limits for $T_R$ are listed in Table 2 for positions with no detection along with $T_R$ and rms at the other positions for each PPC. The upper limits given are small in comparison with the detected values, especially in L1512 and L1544. Therefore, the nondetections may indicate a real decrease of H$_2$CO emission in that direction (southeast in L1498, north in L1512, and southwest in L1544). Table 2 also lists $v_{LSR}$, $\Delta v$, and $\sigma_{turb}$ for each position with a detection. The $\sigma_{turb}$ agree with those found for the 6 cm lines within a channel width ($\pm 0.06$ km s$^{-1}$ for the 1.3 mm data).

The H$_2$CO 6 cm maps indicate that the H$_2$CO absorption is considerably more extended than the dust continuum (Evans et al. 2001; Shirley et al. 2000). Vanden Bout et al. (1983) found that the 6 cm absorption extended over a region more than 10$''$ in size toward L1544. However, the 1.3 mm emission, which only extends to 60$''$, appears to drop off more quickly than the 6 cm H$_2$CO absorption in L1512 and L1544. Figure 7 shows normalized radial profiles of the H$_2$CO $T_R$ for both 6 cm and 1.3 mm and the 850 $\mu$m emission along the short axis of the dark clouds. The broad extent of the 6 cm absorption and the

![Fig. 6.—Top: Velocity gradient in the 6 cm line in L1498 in (right ascension, declination)-space. The size of the symbol increases with velocity. The central (and smallest) velocity is 7.85 km s$^{-1}$, and the largest velocity is 8.34 km s$^{-1}$. All velocities are listed in Table 1. Bottom: Velocity difference vs. the positional offset. This plot shows that the velocity, as well as the dispersion of velocities, increases with distance from the center.](image)

**TABLE 2**

| Source | Offset (arcmin) | $v_{LSR}$ (km s$^{-1}$) | $\Delta v$ (km s$^{-1}$) | $\sigma_{turb}$ (km s$^{-1}$) | $T_R$ (K) | rms (K) | $\eta_{MB}$ |
|--------|----------------|-------------------------|--------------------------|-----------------------------|-----------|--------|-----------|
| L1498  | (0, 0)         | 7.82                    | 0.23                     | 0.08                        | 0.23      | 0.043  | 0.53      |
|        | (0.7, 0.7)     | 7.85                    | 0.12                     | ...                         | 0.21      | 0.056  | 0.77      |
|        | (−0.7, 0.7)    | 7.82                    | 0.35                     | 0.14                        | 0.14      | 0.043  | 0.77      |
|        | (−0.7, −0.7)   | ...                     | ...                      | ...                         | $<0.16^a$ | 0.081  | 0.77      |
| L1512  | (0, 0)         | 7.01                    | 0.35                     | 0.14                        | 0.34      | 0.079  | 0.53      |
|        | (0, 1)         | ...                     | ...                      | ...                         | $<0.10^a$ | 0.051  | 0.77      |
|        | (0, −1)        | 7.17                    | 0.27                     | 0.10                        | 0.34      | 0.070  | 0.77      |
|        | (1, 0)         | 7.09                    | 0.31                     | 0.12                        | 0.17      | 0.029  | 0.77      |
|        | (−1, 0)        | 7.12                    | 0.13                     | 0.02                        | 0.18      | 0.034  | 0.77      |
| L1544  | (0, 0)         | 7.14                    | 0.41                     | 0.17                        | 0.47      | 0.063  | 0.57      |
|        | (0.7, 0.7)     | 7.06                    | 0.48                     | 0.20                        | 0.23      | 0.051  | 0.77      |
|        | (−0.7, 0.7)    | 7.27                    | 0.43                     | 0.17                        | 0.22      | 0.056  | 0.77      |
|        | (−0.7, −0.7)   | 7.12                    | 0.44                     | 0.18                        | 0.45      | 0.088  | 0.77      |

* The 2 $\sigma$ upper limit.
smaller region of 1.3 mm H$_2$CO emission indicate that the two transitions are probing different parts of the PPCs. The 1.3 mm emission is likely tracing denser gas than the 6 cm absorption. This conclusion is discussed further in the context of our models in § 4.4.

4. MODELS

The H$_2$CO line profiles of each PPC were modeled in the final stage of a three-step process. First, dust continuum data for the PPCs were modeled to determine the density and dust temperature profiles of each core. Second, the gas temperature structure was determined from the dust temperature with an energetics code. Finally, the density and gas temperature profiles were used to model the H$_2$CO lines using a Monte Carlo method code (Choi et al. 1995). The details of each stage are described below.

The observed sources have dust continuum maps at 450 and 850 µm (Shirley et al. 2000). The dust continuum radial intensity profile for L1498 was modeled by Y. Shirley et al. (2004, in preparation), and L1512 and L1544 were modeled by Evans et al. (2001) yielding a density and dust temperature profile for each source. The temperature structure was modeled with a one-dimensional radiative transfer code (Egan et al. 1988). The density structure was assumed to be that of a Bonnor-Ebert sphere (Evans et al. 2001). The cloud was assumed to have no internal energy source and to be heated only by the ISRF. A simulated observation of the cloud yielded a spectral energy distribution (SED) and a radial intensity profile. The model SED and radial profile were compared to the observations. The physical parameters of the model cloud were iteratively adjusted until a good fit was found to the observations. The best-fit model was judged by the reduced $\chi^2$ of the model fit to the 450 and 850 µm radial profiles and the SED.

We remodeled L1512 and L1544 with a slightly different method than that used by Evans et al. (2001) but in accordance with Y. Shirley et al. (2004, in preparation). Our models differed from the Evans et al. (2001) models in how the ISRF was treated. Evans et al. (2001) found that an ISRF reduced from the Black-Draine ISRF, which they adopted as a standard, improved the fit to the dust emission for L1512 and L1544. The ISRF (except for the CBR component) was multiplied by a factor of 0.3 in the model for L1512 and by a factor of 0.6 in the model for L1544. In the models presented here, the ISRF was instead attenuated to correspond to a certain visual extinction ($A_V$). The attenuated ISRF is reduced much more at ultraviolet and visible wavelengths but much less in the infrared than the ISRF reduced by a single multiplicative factor. Figure 8 plots both the reduced and attenuated ISRF for comparison.

The $A_V$ values resulting from the dust models correspond well to the known environments of the PPCs. The best-fit dust model of L1498 required 2 mag of visual extinction surrounding the core (Y. Shirley et al. 2004, in preparation). Cambrésy’s (1999) extinction map of Taurus shows L1498 to be fairly isolated and surrounded by ambient gas with $A_V = 1\pm 2$ mag. L1512 is on the edge of Taurus where $A_V$ is about 0.5 mag (Falgarone et al. 1998). For this PPC, attenuating the ISRF did not improve the fit to the dust, but since it was not a significantly worse fit, the $A_V = 0.5$ attenuated dust model was used for consistency. We found that attenuating the ISRF in the models for L1544 fitted the dust emission radial profiles better than simply reducing the ISRF. L1544 is the most heavily embedded core; our radiative transfer model indicates $A_V = 3$. This value is consistent with the extinction determined from star counts at a 5' radius ($A_V = 2\pm 3$; Minn 1991; Snell 1981).

Once the dust temperature profile had been determined from the dust emission, an energetics code (after Doty & Neufeld 1997) was used to calculate the temperature of the gas from the temperature of the dust. The calculation accounted for radiative cooling of the gas, transfer of energy from collisions between the gas and dust grains, heating by cosmic rays, and...
photoelectric heating. The Appendix provides complete details of the energetics calculations.

The strength of the heating on the outside of the cloud in the energetics code is primarily controlled by the factor $G_0$, which is the strength of the UV field relative to the standard ISRF at the outer PPC boundary. A value of $G_0$ less than unity results from the attenuation of the ISRF by the material surrounding the PPC, and a smaller $G_0$ indicates greater attenuation. In order to constrain the estimate of $G_0$ for each cloud, we modeled the CO $J = 1\rightarrow 0$ line and compared the models to observations for each PPC. This CO transition is completely thermalized. By comparing the strength of the modeled and observed CO lines, we are able to determine if the model temperature is too hot or cold on the outside of the cloud and, therefore, if $G_0$ is too high or low. We used the CO observations of Kuiper et al. (1996), Falgarone et al. (1998), and Tafalla et al. (1998) for L1498, L1512, and L1544, respectively. We did not attempt to fit the CO line profile in detail because our models have many parameters other than $G_0$. The CO models all had the same abundance and physical parameters. Different $G_0$ values were tested to find the one that produced a $T_0$ that was consistent with the observations.

We compared $G_0$ found using CO observations as a constraint to $G_0$ calculated from the $A_F$ value used to attenuate the ISRF in the dust model [see the equation for $G(r)$ in the Appendix] for each source. The CO-derived $G_0$ values were 0.06, 0.03, and 0.08 for L1498, L1512, and L1544, respectively. The $G_0$ values calculated from the dust model $A_F$ were 0.03, 0.005, and 0.41, respectively. The $G_0$ values derived from CO are larger than those calculated from the $A_F$ values for L1498 and L1544, indicating less extinction toward the PPCs. For L1512, the $G_0$ derived from CO is much smaller than the value calculated from the dust model $A_F$ but is consistent with the $G_0$ values derived from CO for the other sources. Complete photon-dominated region (PDR) analysis is needed in order to fully examine this inconsistency. The CO-derived $G_0$ values are used in the energetics code for this work because the CO is much more sensitive to $G_0$ than the dust models are to $A_F$. Further, the equation used to calculate $G_0$ for a given $A_F$ is for plane-parallel slabs and is not appropriate for spheres as discussed in the Appendix.

We used the best-fit density profile from the dust model and the gas temperature profile from the energetics calculations as input into a Monte Carlo (MC) method radiative transfer code (Choi et al. 1995) to model the H$_2$CO 6 cm and 1.3 mm lines. Figure 9 shows the density and temperature profiles resulting from the dust and energetics models for each PPC. The results from the MC code were convolved to the resolution of the observations for comparison with the data. The MC model has two free parameters, the outer radius of the cloud ($R_{\text{out}}$) and the microturbulent velocity dispersion ($\sigma_v$). The same outer radius was used for the dust and MC models (0.15 pc) for consistency; $\sigma_v$ was iterated on to find the best-fitting value for each PPC. Theoretical collision rates for H$_2$CO only exist down to 10 K, and the temperatures in dark starless cores drop below that. Therefore, for the purpose of these models, the H$_2$CO collision rates were linearly extrapolated down to 3 and 5 K from the known rates at 10 and 15 K (Green 1991). The convergence criterion in the MC code was set at 5%.

The components of the hyperfine structure of the 6 cm line were modeled independently with the exception of the $F = 2\rightarrow 2$ and $0\rightarrow 1$ components. These two components lie within 0.1 km s$^{-1}$ of one another, less than the turbulent velocity dispersion in the observed lines. Therefore, the relative intensities of these lines were added together for the purpose of our models. The frequency of the combined component was given as the relative intensity-weighted mean of the individual frequencies. The five modeled components were added for the complete modeled 6 cm line profile. We compared this method of modeling five components to modeling the full six hyperfine components and found that using all six components deepened the absorption by only about 10%.

Our models indicate that H$_2$CO is significantly depleted in these PPCs as predicted by various chemical models (Lee et al. 2004; Y. Aikawa 2003, private communication). Figure 10 shows the simulated 6 cm line profile for a dark cloud with a central density of $10^6$ cm$^{-3}$ and an undepleted H$_2$CO fractional abundance of $10^{-8}$. The model is plotted with the observed line profile of L1544 to show the large discrepancy between the expected undepleted line profile and what was actually observed. The undepleted model predicts 6 cm emission toward the center of the PPC, a qualitative discrepancy with the observation. Depletion significantly affects how the 6 cm H$_2$CO transition probes cold, dense gas. If H$_2$CO is depleted in the center of a PPC, then the 6 cm line will not be able to see the densest part of the core.

Depletion was introduced into the models with an abundance profile characterized by less H$_2$CO at small radii than at larger radii. Several different functional forms of the abundance profile were compared in the modeling process, including a power law, exponential, and step function (see Table 6 in Lee et al. 2003). The abundance at the outer edge of the cloud was set by $X_0$, the undepleted abundance. The shapes of the step function and exponential were characterized by a radial scale of depletion ($r_d$). The depth of the step function was set by $(f_0)$, the factor by which the abundance in the central portion of the PPC was decreased.

These simple functional forms of the abundance profile were also compared with the profile generated by chemical
network models (Lee et al. 2004), where the reactions between gas and grains, such as depletion and desorption of species, and gas-phase chemistry have been considered. Lee et al. (2004) used a series of Bonnor-Ebert spheres of various central densities ($n_c$) to calculate the evolution of chemistry in the PPC stage. They assumed that a Bonnor-Ebert sphere evolves from lower central density to higher central density, and the timescale of the evolution decreases as the central density increases. The total timescale for the PPC stage was assumed to be a million years. The abundance profile resulting from the chemical models was multiplied by a scale factor ranging from 0.3 to 2.0 in the models to best fit the data since the actual timescale is unknown. Figure 11 shows examples of the various abundance profiles. The values specifying the exact shape of the abundance profiles ($X_0, r_D, f_D, n_c$, etc.) were iterated on until a best fit for each type of profile was found for each source. The results of the models with different abundance profiles are compared in §§ 4.1–4.4 and Table 3.

Each model was compared to the observed 6 cm line at the center of each PPC and at offsets of 60° and 120° from the center. The model was also compared to the 1.3 mm line at the center and 60° offset. Figures 12–14 plot the data and the best-fitting model for each source. The offset spectra are the weighted average of the spectra in all directions at either 60° or 120° from the center of the cloud. For the 6 cm line, the 60° offset spectrum is the average of eight spectra, and the 120° spectrum is the average of six spectra for each source. For the 1.3 mm line, the 60° offset spectrum is the average of four spectra.

The best model was selected by comparing values of the absolute deviation that characterize the model fit to the data at both wavelengths and all offsets. The absolute deviation is defined as the sum of $|\text{model}(i) - \text{observed}(i)|$ over all data points $i$ (Press et al. 1992). The absolute deviation was chosen instead of the more common reduced $\chi^2$ value in order to eliminate artificial weighting of the noisier 1.3 mm data. For nearly all the models, the 1.3 mm reduced $\chi^2$ was low compared to that for the 6 cm lines even when the model clearly fitted the 6 cm data better than the 1.3 mm data. The high noise levels in the 1.3 mm data dramatically decreased the reduced $\chi^2$ values and, as a result, created a bias toward the 1.3 mm fits. The absolute deviation does not consider noise so it is free of this bias.

We have calculated the absolute deviation in two different ways. First, we calculated the absolute deviation between the integrated intensity of the model and the observations. A second absolute deviation compares the line profile shape of the model and data. Each of these values is calculated for 6 cm and 1.3 mm lines independently. The absolute deviation is also calculated independently for each observed offset. The average absolute deviation over all offsets for each wavelength is reported in Table 3.

We chose the model with the lowest integrated intensity and profile absolute deviation values at 6 cm for the best-fit model because the 6 cm data have high signal-to-noise ratio and provide good constraints for the models. All of the models presented in Table 3 are the best-fitting models for particular abundance profiles. There was often a discrepancy between the models with the lowest absolute deviation for the 6 cm data and the 1.3 mm data. We found that no reasonable models for the 6 cm data fitted the 1.3 mm data well. This discrepancy is discussed in further detail in § 4.4. The models are discussed by source in §§ 4.1–4.3.

### 4.1. L1498

L1498 is the most diffuse of the three PPCs discussed here. As a result, the best-fitting dust model has the lowest central density, $10^4$ cm$^{-3}$, of all the sources (Fig. 9). L1498 was modeled with an outer radius of 0.15 pc. This is smaller than the outer radius of the best-fitting dust radiative transfer model.
but is consistent with the outer radii used by Lee et al. (2004) for the chemical models and for L1512 and L1544 in this work. All the L1498 models use \( /C_14^v t = 0.1k \) ms.

The G0 derived from the CO observations of L1498 is 0.06. Table 3 gives a full listing of model parameters and absolute deviations for models of L1498 with differing abundance profiles.

The best-fitting model for L1498 (Fig. 12) uses a chemical model abundance profile (Fig. 11). The chemical model abundance profile was multiplied by a factor of 0.8 in order to best fit the data. The chemical model used had the same \( A_v \) as the dust model for L1498, \( A_v = 2 \), but a much higher central density of \( 10^7 \) cm\(^{-3} \). The higher central density in the chemical model results in more central depletion of \( H_2CO \) in the abundance profile. Further, the chemical model abundance profile used to fit the L1498 data is dramatically different from the other abundance profiles at large radii (Fig. 11). The chemical model abundance profile has a high maximum abundance \( /C_24^9 \) and decreases rapidly at large radii for \( A_v = 2 \).

The absorption predicted by the model at the center position resulted in a model that fitted the strength of the 6 cm H\(_2CO\) absorption well at 60\(^0\) and 120\(^0\).

The absorption predicted by the model at the center position

\( \text{Fig. 12: } \text{Dotted lines: } \text{H}_2\text{CO data. Solid lines: Best-fit MC model for L1498. The top panels show the 6 cm line at the offsets indicated in the figure, and the bottom panels are the 1.3 mm line. The model has a chemical model abundance distribution. Model parameters are given in Table 3.} \)

### Table 3: Model Parameters

| Source   | Abundance Profile | \( X_0 \)   | \( r_D \) (pc) | Other                  | Absolute Deviation (6 cm) | Absolute Deviation (1.3 mm) |
|----------|-------------------|-------------|---------------|------------------------|---------------------------|-----------------------------|
|          |                    |             |               |                        | Integrated\(^a\) Profile\(^b\) | Integrated\(^a\) Profile\(^b\) |
| L1498    | Step              | \( 4 \times 10^{-9} \) | 0.02          | \( f_D = 10 \)         | 0.17                       | 1.28                        | 0.053                       | 0.29                       |
|          | Power             | \( 7 \times 10^{-9} \) | ...           | \( p = 1' \)           | 0.25                       | 1.43                        | 0.055                       | 0.30                       |
|          | Exponential       | \( 5 \times 10^{-9} \) | ...           |                        | 0.17                       | 1.28                        | 0.055                       | 0.30                       |
|          | Chemical\(^e\)    | \( 0.8' \)   | ...           | \( A_v = 2, n_c = 10^7 \) \( \text{cm}^{-3} \) | 0.19                       | 1.24                        | 0.037                       | 0.25                       |
|          | Chemical\(^e\)    | \( 2.6' \)   | ...           | \( A_v = 2, n_c = 10^9 \) \( \text{cm}^{-3} \) \( G_0 = 0.6 \) | 0.26                       | 1.27                        | 0.058                       | 0.30                       |
| L1512    | Step\(^e\)        | \( 1 \times 10^{-8} \) | 0.05          | \( f_D = 20 \)         | 0.037                      | 0.96                        | 0.10                       | 0.71                       |
|          | Power             | \( 1.5 \times 10^{-8} \) | ...           | \( p = 1' \)           | 0.081                      | 1.04                        | 0.078                       | 0.65                       |
|          | Exponential       | \( 1.5 \times 10^{-8} \) | 0.05          | ...                    | 0.079                      | 1.24                        | 0.050                       | 0.60                       |
|          | Chemical\(^e\)    | \( 0.3' \)   | ...           | \( A_v = 3, n_c = 10^6 \) \( \text{cm}^{-3} \) | 0.13                       | 0.92                        | 0.078                       | 0.67                       |
| L1544    | Step\(^e\)        | \( 1.5 \times 10^{-8} \) | 0.04          | \( f_D = 10 \)         | 0.13                       | 1.07                        | 0.15                       | 0.97                       |
|          | Power             | \( 2.5 \times 10^{-8} \) | ...           | \( p = 1' \)           | 0.09                       | 0.91                        | 0.21                       | 1.12                       |
|          | Power + velocity\(^d\) | \( 2.5 \times 10^{-8} \) | ...           | \( p = 1' \), Plummer velocity | 0.084                     | 0.91                        | 0.23                       | 1.17                       |
|          | Exponential       | \( 2 \times 10^{-8} \) | 0.03          | ...                    | 0.11                       | 0.99                        | 0.20                       | 1.13                       |
|          | Chemical\(^e\)    | \( 0.5' \)   | ...           | \( A_v = 3, n_c = 10^6 \) \( \text{cm}^{-3} \) | 0.11                       | 0.89                        | 0.20                       | 1.10                       |

\(^a\) Average absolute deviation of the integrated intensity of the model vs. the observed lines over all offsets.

\(^b\) Average absolute deviation of the modeled profile shape vs. the observed profiles over all offsets.

\(^c\) Power-law exponent.

\(^d\) Best-fit model described in text and shown in Figs. 12–14.

\(^e\) Since the chemical models are not characterized by \( X_0 \), this value indicates the scale factor for the chemical model abundance profile.

\(^f\) These values for \( A_v \) and \( n_c \) describe the input for the chemical model and are independent of dust radiative transfer model values.

(0.17 pc; Y. Shirley et al. 2004, in preparation) but is consistent with the outer radii used by Lee et al. (2004) for the chemical models and for L1512 and L1544 in this work. All the L1498 models use \( \delta v_r = 0.1 \) km s\(^{-1} \). The \( G_0 \) derived from the CO observations of L1498 is 0.06. Table 3 gives a full listing of model parameters and absolute deviations for models of L1498 with differing abundance profiles.

The best-fitting model for L1498 (Fig. 12) uses a chemical model abundance profile (Fig. 11). The chemical model abundance profile was multiplied by a factor of 0.8 in order to best fit the data. The chemical model used had the same \( A_v \) as the dust model for L1498, \( A_v = 2 \), but a much higher central density of \( 10^7 \) cm\(^{-3} \). The higher central density in the chemical model results in more central depletion of \( H_2CO \) in the abundance profile. Further, the chemical model abundance profile used to fit the L1498 data is dramatically different from the other abundance profiles at large radii (Fig. 11). The chemical model abundance profile has a high maximum abundance (~9 \( \times 10^{-9} \)) and decreases rapidly at large radii for \( A_v = 2 \). This abundance profile resulted in a model that fitted the strength of the 6 cm \( H_2CO \) absorption well at 60\(^0\) and 120\(^0\).

The absorption predicted by the model at the center position...
appears too weak. The weak central line could indicate that there is not enough depletion at the center of the model, and the main hyperfine component is being driven toward emission. Alternatively, there could be less absorption in the main component because it is too optically thick in the model and is not probing as far into the cloud as the other components. Abundance profiles that have more central depletion but no outer decrease fitted the central 6 cm line better but were too deep at the offset positions.

An alternative model for L1498 was found by allowing $G_0$ to be a free parameter rather than constraining it with CO observations. An abundance profile, adopted from the chemical model with $A_F = 2$ at the time step at which $n_c = 10^4$ cm$^{-3}$ that is consistent with the model of the dust emission by Y. Shirley et al. (2004, in preparation), can fit the observed 6 cm H$_2$CO profiles if a $G_0$ $10$ times higher than what was found from the CO $J = 1$–0 line is used. The absolute deviations for this model are listed in Table 3 and Figures 9 and 13. As Figure 13 shows, the step function model predicts less 6 cm absorption in the main hyperfine component ($F = 2$–2) than observed at the center of L1512. The other abundance profiles modeled predict even less absorption than the step function model. The step function abundance profile differs significantly from the power law, exponential, and chemical model profiles in that H$_2$CO is depleted out to a larger radius. The other profiles fall off gradually, but the step function has a steep drop in abundance at 0.05 pc. Although the best-fit model is not a perfect match to the data, the model constrains the H$_2$CO abundance profile by ruling out profiles that are depleted too slowly toward the center of the core. The parameters characterizing the best-fit step function ($r_D, f_D, X_0$) are good within a factor of 2 to fit the data.

Again, the best-fit model produces 1.3 mm line profiles that are too weak compared to the data (see § 4.4). Additionally, there is a velocity shift between the model and 1.3 mm data at the 60'' offset position. The central velocity of the data appears higher than that of the model. The map of L1512 in Figure 4 shows that there is no obvious velocity gradient in the 6 cm data as is the case in L1498.

As with L1498, the models do not fit the wing to the right of the main 6 cm hyperfine component as shown in Figure 13, and we believe that this again is the result of a second velocity component. Falgarone et al. (1998) observed multiple velocity components in several transitions of CO toward L1512. They observed a second velocity component in the line profile of C$^{18}$O at a similar velocity (7.3–8.1 km s$^{-1}$) to the wing in the H$_2$CO line.

### 4.2. L1512

L1512 is best fitted with a model of a moderate central density ($n_c = 10^5$ cm$^{-3}$) and a step function abundance profile. All the L1512 models had an outer radius of 0.15 pc, a $b v_{\text{c}}$ of 0.1 km s$^{-1}$, and $G_0 = 0.03$. Model parameters and results are given in Table 3 and Figures 9 and 13. As Figure 13 shows, the step function model predicts less 6 cm absorption in the main hyperfine component ($F = 2$–2) than observed at the center of L1512. The other abundance profiles modeled predict even less absorption than the step function model. The step function abundance profile differs significantly from the power law, exponential, and chemical model profiles in that H$_2$CO is depleted out to a larger radius. The other profiles fall off gradually, but the step function has a steep drop in abundance at 0.05 pc. Although the best-fit model is not a perfect match to the data, the model constrains the H$_2$CO abundance profile by ruling out profiles that are depleted too slowly toward the center of the core. The parameters characterizing the best-fit step function ($r_D, f_D, X_0$) are good within a factor of 2 to fit the data.

### 4.3. L1544

L1544 is the most centrally condensed of the three PPCs. The models require a high central density ($n_c = 10^6$ cm$^{-3}$, Fig. 9) and a larger $G_0$ of 0.08 compared to the other PPCs. All the L1544 models have an outer radius of 0.15 pc and $b v_{\text{c}}$ of 0.19 km s$^{-1}$. There was no clear best-fitting model for L1544. The absolute deviation values were very similar for models with four different abundance profiles. The model parameters and absolute deviations are shown in Table 3. Even though the exact shape of the abundance profile for L1544 cannot be
determined by these models, the general shape of the abundance profile is constrained. All of the best-fitting abundance profiles have a similar shape at large radii, are depleted toward the center on a radial scale \( r_D \) of 0.03–0.04 pc, and have an outer edge undepleted \( H_2CO \) fractional abundance \( X_0 \) of about \( 2 \times 10^{-8} \) (Fig. 11). Changes in \( r_D \) and \( X_0 \) of 25% produce significantly different model results and absolute deviations, showing that the reported values characterize the general shape of the \( H_2CO \) abundance profile. Figure 14 shows the model fit to the data for a power-law abundance profile. The power-law models have slightly lower absolute deviations for the 6 cm data than the models with different abundance profiles.

In the L1544 models, the model 1.3 mm line at the center position shows self-absorption (Fig. 14). Self-absorption is not seen in our observations, although the spectra are noisy. We have tried to reconcile our models and the data in two ways. First, the density at large radii representing the ambient density have tried to reconcile our models and the data in two ways. Secondly, we increased the collision rates for the transitions that populate the upper level of the 1.3 mm transition by a factor of 3. This change did increase the model 1.3 mm emission by a factor of 1.75 on average. However, the transitions to the upper level of the 1.3 mm transition are also significant in the pumping mechanism that allows for 6 cm absorption against the CBR. The increase in collision rates increased the efficiency of cooling of the 6 cm absorption, and the absorption in the models deepened by more than a factor of 2. Therefore, a model with increased collision rates did not fit the 6 cm and 1.3 mm observed line profiles simultaneously.

Since changing the abundance profiles and collision rates did not solve the discrepancy between the 6 cm and 1.3 mm line models, we suggest that a density profile other than the Bonnor-Ebert sphere may be needed to simulate the observed 6 cm and 1.3 mm data. The two transitions are most sensitive to only slightly different densities in emission, but the 6 cm absorption can come from a region of significantly lower density (Fig. 1). The strong 6 cm absorption could mask weak 6 cm emission coming from the denser regions. Therefore, we are, in effect, seeing two different parts of the cloud with the two transitions, and a more complex density profile may be able to match both lines. The Bonnor-Ebert density profile has been found to fit submillimeter dust continuum data well in PPCs (Evans et al. 2001). Deviations from spherical symmetry in the PPCs not accounted for in the models may be contributing to the discrepancy in the 6 cm and 1.3 mm models. However, a three-dimensional radiative transfer model of the dust continuum emission from L1544 fits a power-law density profile to the data.

4.4. Discussion

An unambiguous aspect of our models is that all require depletion of formaldehyde in the center of the core. Depletion of carbon-bearing molecules such as CO and CS in the center of PPCs, including L1498, L1512, and L1544, is well known (e.g., Tafalla et al. 2002, 2004; Lee et al. 2003). Tafalla et al. (2004) modeled high angular resolution \( C^{15}O \) and CS observations toward L1498 with a similar method to the one in this work, except that they assumed a constant dust temperature and used a larger outer radius (0.25 pc). They found that the high-resolution data required a faster decrease in abundance than their previous models of lower resolution data had suggested (Tafalla et al. 2002). Their result is consistent with the findings presented here that, although the exact shape of the abundance profile cannot be uniquely determined, all the models suggest a significant drop in abundance toward the center of PPCs. Tafalla et al. (2004) fitted the CO and CS data with a step function abundance profile that drops to zero at a given radius. They found depletion radii about a factor of 2 larger for CO and CS than the depletion radius used in the step function abundance profile model of \( H_2CO \) in L1498 (Table 3). Lee et al. (2003) also found \( C^{18}O \) to be depleted out to larger radii \( (r_D = 0.075 \) and 0.045 pc) and by a larger factor \( (J_D = 25) \) in L1512 and L1544 than is required for \( H_2CO \) in the models presented here.

The depletion of \( H_2CO \) in PPCs may be related to the chemical processes of deuteration and the reaction between gas and grains. \( H_2CO \) is likely depleted in PPCs as a result of accretion onto cold dust grains (Carey et al. 1998). Maret et al. (2004) observed a jump in the abundance of gas-phase \( H_2CO \) where grain mantles evaporate \( (T_D = 100 \) K) in Class 0 protostellar envelopes, supporting the idea of depletion onto grains. In addition, at high density and very low temperature, \( D_2CO \) forms efficiently (Tielsens 1983) because of its lower zero energy level compared to that of \( H_2CO \). \( D_2CO \) is considered to form through both gas chemistry and surface chemistry (Ceccarelli et al. 2002). In dark cores without protostellar objects, abundant deuterated molecules in the gas phase are mainly driven by gas chemistry because the dust temperature is not high enough for deuterated molecules on grain surfaces to be desorbed. Gas-phase deuteration may be more efficient where CO and \( NH_3 \) are depleted, as in PPCs (Roberts & Millar 2000; Bacmann et al. 2003). \( D_2CO \), which is formed and accumulated on grain surfaces during the PPC stage, evaporates when a newly formed luminous source heats dust grains (Loinard et al. 2002).

In addition to depletion, another aspect of the model results warrants further discussion. No single model was able to fit the 6 cm and 1.3 mm data simultaneously. We have considered different explanations for this discrepancy. First, we have tried four different abundance profiles: step function, power law, exponential, and chemical model. Table 3 lists the model parameters for each type of abundance profile and the corresponding absolute deviations. The table shows that there is not one clear best-fitting model abundance profile for all of the sources. The power-law, exponential, and chemical model abundance profiles are all very similar (Fig. 11) and often result in comparable line profiles. None of the abundance profiles solve the problem of fitting the data at both wavelengths. For those models providing a good match to the 6 cm observations, the models consistently underpredict the 1.3 mm line strength in L1498 and L1512 and show 1.3 mm self-absorption in L1544.

Second, we increased the collision rates for the transitions that populate the upper level of the 1.3 mm transition by a factor of 3. This change did increase the model 1.3 mm emission by a factor of 1.75 on average. However, the transitions to the upper level of the 1.3 mm transition are also significant in the pumping mechanism that allows for 6 cm absorption against the CBR. The increase in collision rates increased the efficiency of cooling of the 6 cm absorption, and the absorption in the models deepened by more than a factor of 2. Therefore, a model with increased collision rates did not fit the 6 cm and 1.3 mm observed line profiles simultaneously.
and cannot rule out a Bonner-Ebert density profile similar to that of the best-fit one-dimensional model (S. Doty et al. 2004, in preparation). The strength of the 1.3 mm lines at both 0° and 60° suggests that there is more dense material farther out in the cloud than the Bonner-Ebert or power-law density profiles allow. One solution may be to include small regions of enhanced density in the models. High-density clumps would not be resolved in the dust continuum and may not be large enough to affect the strength of the 6 cm line but could provide enough dense material in the outer parts of the cloud to produce the observed 1.3 mm H$_2$CO lines. Additionally, the temperature and density dependencies are not as well decoupled in the observed 1.3 mm H$_2$CO lines. Higher temperature may also create the excess 1.3 mm emission. Thus, the density in the models. High-density clumps would not be resolved in the dust continuum and may not be large enough to affect the strength of the 6 cm line but could provide enough dense material in the outer parts of the cloud to produce the observed 1.3 mm H$_2$CO lines. Additionally, the temperature and density dependencies are not as well decoupled in the observed 1.3 mm H$_2$CO lines. Higher temperature may also create the excess 1.3 mm emission.

5. SUMMARY

We have presented maps of three PPCs in two transitions (6 cm and 1.3 mm) of formaldehyde showing strong absorption in the 6 cm transition toward all the sources. The absorption extended well beyond the edge of the observed dust emission. The 1.3 mm emission was observed out to 60° in all the PPCs. A velocity gradient, increasing away from the center of the core, was observed in L1498. The apparent gradient may be caused by unrelated gas in the region of L1498.

We have modeled both H$_2$CO transitions, including the offset positions, with a multistage method including dust radiative transfer, gas energetics, and gas radiative transfer. The attenuation of the ISRF, reflected in the parameter $G_0$ in the energetics code, was constrained by CO observations. However, since $G_0$ can have a significant effect on the model results, full PDR analysis is needed to better constrain this parameter and future PPC models.

The models described in this work indicate that H$_2$CO is depleted in the center of these PPCs as predicted by chemical network models. Undepleted models cannot reproduce the strong 6 cm absorption but predict 6 cm emission toward the center of the cold, dense PPCs. Therefore, the 6 cm H$_2$CO transition is not able to probe the densest parts of PPCs. Although all the models require depletion of H$_2$CO, the shape of the abundance profile in the best-fitting models varies from source to source. L1498 is fitted best with a chemical model abundance profile that is depleted both toward the center and at large radii. L1512 requires a large amount of depletion out to a relatively large radius, so it is fitted with a step function abundance profile. L1544 is fitted best with a power-law abundance profile that depletes smoothly toward the center. The models place strong constraints on the physical parameters of the core at large radii and unequivocally indicate depletion of H$_2$CO toward the center of PPCs.

The models also show that multiple velocity components may be present in the 6 cm H$_2$CO observations of L1498 and L1512. The 1.3 mm and 6 cm data cannot be well matched with a single model. Models that are reasonable fits to the 6 cm data are unable to reproduce the strength of the 1.3 mm emission. The 1.3 mm emission may be probing denser gas than the 6 cm absorption. A more complex density or temperature distribution may be needed to fit both sets of data.

APPENDIX

ENERGETICS

The gas temperature at each depth in the model is determined by balancing the local heating and cooling rates (Fig. 15). The approach used is patterned after that of Doty & Neufeld (1997), but with updates that we describe here.

Before discussing the detailed heating and cooling rates, we note that all references to $n$(H$_2$) correspond to H$_2$ number density. However, many of the adopted rates require the baryon number density, $n$(H) $\sim$ 2$n$(H$_2$) + 4$n$(He) (assuming that there is only neutral and molecular gas and low abundances of heavier elements). For a molecular gas with 25% helium by mass, $n$(He) = 0.166$n$(H$_2$) and $n$(H) = 2.66$n$(H$_2$). All expressions below have accounted for this fact.

The gas close to the surface is primarily heated by photoelectric heating. We follow the prescription of Bakes & Tielens (1994), namely,

$$\Gamma_{pe} = 10^{-24}\epsilon G(r)n(H) \text{ ergs cm}^{-3} s^{-1},$$

where the efficiency, $\epsilon$, is given by

$$\epsilon = \frac{4.87 \times 10^{-2}}{1 + 4 \times 10^{-3} [G(r)T_K^{0.5}/n_e]^{-0.75}} + \frac{3.65 \times 10^{-2} (T_K/10^4)^{0.7}}{1 + 2 \times 10^{-4} [G(r)T_K^{0.5}/n_e]}.$$  

(A2)

In this expression, $T_K$ is the temperature, $n_e$ is the electron number density, and $G(r) = J(r; E > 6 \text{ eV})/J(\text{ISRF}; E > 6 \text{ eV})$ is the ratio of the mean intensity of the local radiation field within the cloud to the mean intensity of the ISRF for energies above 6 eV, the energies above which photons can cause significant photoelectric heating (e.g., Juvela et al. 2003). The electron number density is taken from chemical models similar to those of Doty et al. (2002), which include UV processing and attenuation. In the clouds we study, the product $G(r)T_K^{0.5}/n_e$ is small enough that the total heating rate scales with $G(r)$ and is nearly independent of the exact value of the electron number density.
The depth-dependent radiation field is determined by a self-consistent solution to the radiative transfer problem using the code of Egan et al. (1988). In this case, we assume spherical symmetry, include scattering, and adopt the dust properties for coagulated grains with icy mantles described by Ossenkopf & Henning (1994; col. [5] of Table 1). These assumptions are identical to those adopted for the dust radiative transfer models, providing a consistent approach. While the radiation field is a complicated function of depth, it is interesting to note that it is generally much stronger than would be calculated by taking a simple attenuation law used for plane-parallel slabs such as \( G(r) = G_0 \exp(-a \tau_r) \), where \( \tau_r \) is the extinction at \( V \) and \( a \) is commonly taken to be in the range from 1.8 (e.g., A. G. G. M. Tielens 2003, private communication) to 2.5 (Hollenbach et al. 1971). In a spherical geometry, any point in space has a lower optical depth to the outside for nonnormal rays than for the equivalent ray in a slab geometry. As a result, the radiation field along nonnormal rays can penetrate farther into spherical sources, leading to a higher radiation field (e.g., Flannery et al. 1980). In the models described in the text, the value of \( G_0 \) is varied until agreement with the CO \( J = 1-0 \) line is reproduced. Physically, this has the effect of accounting for variations in the incident radiation field due to local sources and/or attenuation by the surrounding low-density cloud.

Grain photoelectric heating usually dominates in the exterior of the cloud. However, as a result of attenuation of the photon flux by the dust, cosmic-ray heating will often dominate in the interior (\( \tau_r > 1 \)), as can be seen in Figure 15. We assume a cosmic-ray ionization rate of \( 3 \times 10^{-17} \text{s}^{-1} \) (van der Tak & van Dishoeck 2000) and also take the energy input per ionization to be \( \Delta Q = 20 \text{ eV} \) (Goldsmith 2001). This yields a cosmic-ray heating rate per unit volume of

\[
\Gamma_{\text{gas,cy}} = 10^{-27} n(H_2) \left( \frac{\zeta}{3 \times 10^{-17} \text{s}^{-1}} \right) \left( \frac{\Delta Q}{20 \text{ eV}} \right) \text{ergs cm}^{-3} \text{ s}^{-1}.
\]

(A3)

For the gas cooling, we follow Doty & Neufeld (1997) in their adoption of the tabulated cooling functions of Neufeld et al. (1995) and Neufeld & Kaufman (1993) for CO, O, H_2, H_2O, and other diatomic and polyatomic molecules. As discussed in the text, molecular depletion is a key aspect of these clouds. However, we have not decreased the abundances of coolants because the abundances are strongly affected only at relatively high densities, where \( T_K \) is already closely coupled to \( T_d \). Depletion has only a small effect on gas temperature (Goldsmith 2001). Similar to Doty & Neufeld (1997), we find that the cooling in the exterior is dominated by CO. Likewise, the decrease in temperature on the outside of the models is due to the increased ability of radiation to escape, allowing the gas to cool. We tested the case in which the gas temperature is constant at the outer radii rather than decreasing and found that the drop-off in \( T_K \) at large radii causes a ~5% decrease in \( T_R \).

Collisions between gas and dust can either heat or cool the gas; the dust will cool the gas if the gas kinetic temperature, \( T_k \), is greater than the dust temperature, \( T_d \), and vice versa. Our formulation treats the interaction as a cooling term formally. There is of course a balancing heating or cooling of the dust in the process, but the effect on \( T_d \) is small compared to radiative processes, even deep in well-shielded clouds (Evans et al. 2001; Goldsmith 2001), and we ignore it here. We adopt the general prescription of Hollenbach & McKee (1989), assuming collisions between gas and dust where the dust has a power-law size distribution \( n(a) \propto a^{-3.5} \) (Mathis et al. 1977), with a minimum grain size \( a_{\text{min}} = 100 \text{ Å} \), a maximum grain size \( a_{\text{max}} = 0.25 \mu m \), a mass density \( \rho = 2 \text{ g cm}^{-3} \), and a dust-to-gas mass ratio of \( R_{d/g} = 4.86 \times 10^{-3} \). These assumptions lead to an average dust cross section per baryon of \( \Sigma_d = 6.09 \times 10^{-22} \text{ cm}^{-2} \). We adopt the temperature-dependent accommodation coefficient \( \alpha = 0.37[1 - 0.8 \exp(-75/T_K)] \)
This expression is similar in form to others in the literature. However, the coefficient is approximately the geometrical mean of the lower value of Goldsmith (2001) and the higher value of Hollenbach & McKee (1989). It is, however, within a factor of 5 of these two other values. This is reassuring as our expression does not represent an extremum on either end of the range of expected gas-dust cooling rates and agrees to within the intrinsic uncertainties in assumed microphysical properties (e.g., dust composition, size distribution, dust-gas mass ratio, sticking probabilities, gas composition). In practice, gas-dust cooling has the effect, as noted by other authors (e.g., Doty & Neufeld 1997; Goldsmith 2001), of strongly coupling the gas and dust temperatures at densities $n > 10^5$ cm$^{-3}$.

These heating and cooling rates are then solved for the temperature point by point within the cloud. The problem is treated as a root-finding problem in the gas temperature and solved using Brent’s method (Press et al. 1992) to a fractional accuracy of $10^{-8}$.

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(Burke & Hollenbach 1983). This expression comes from averaging over speeds for an astrophysical mixture of gases; thus, it must be used in conjunction with a mean speed for a hydrogen atom, $\langle v(m_H) \rangle$. With these conventions, our adopted expression for the gas-dust energy transfer rate is

$$\Lambda_{gd} = 9.0 \times 10^{-14} n(H)^2 (T_K)^{0.5} \left[1 - 0.8 \exp\left(-\frac{75}{T_K}\right)\right] (T_K - T_d) \left(\frac{\Sigma_d}{6.09 \times 10^{-22}}\right) \text{ erg cm}^{-3} \text{ s}^{-1}. \quad (A4)$$