MODELS OF CHEMISTRY, THERMAL BALANCE, AND INFRARED SPECTRA FROM INTERMEDIATE-AGED DISKS AROUND G AND K STARS

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ABSTRACT

We model gas and dust emission from regions 0.3–20 AU from a central low-mass star in intermediate-aged (~10^7 yr) disks whose dust is fairly optically thin to stellar radiation. The models treat thermal balance and chemistry self-consistently and calculate the vertical density and temperature structure of the gas in a disk. The gas and dust temperatures are calculated separately. The models cover gas masses 10^{-3} to 1 M_J and dust masses 10^{-7} to 10^{-4} M_J and treat solar-type (G and K) stars. We focus on mid-infrared and far-infrared emission lines from various gas species such as the rotational lines of H_2, OH, H_2O, and CO molecules and the fine-structure lines of carbon, oxygen, sulfur, iron, and silicon atoms and ions. These lines and the dust continuum are observable by the Spitzer Space Telescope and future missions including SOFIA and the Herschel Space Observatory. We find that the [S[i] 25.23 μm line is the strongest emission line for a wide range of disk and stellar parameters, followed by emission from [Si ii] 34.8 μm, [Fe ii] 26 μm, and [O i] 63 μm. [Fe i] 24 μm and rotational lines of OH and H_2O are strong when gas masses are high (≥0.1 M_J). Emission from the rotational lines of H_2 is more difficult to detect unless disk gas masses are substantial (≥0.1 M_J). For emission from H_2 lines to be observable and yet for the dust to be optically thin in stellar light, the ratio of gas to small submillimeter-sized dust particle mass in the disk needs to be ≥1000, or at least an order of magnitude higher than that in the interstellar medium. This may be possible at intermediate stages in disk evolution, such as in the gas-gathering stage of the core accretion scenario for giant planet formation, in which most of the dust has coagulated into larger objects (>1 mm) but the gas has not yet fully dispersed. Whereas the absolute fluxes observed in some lines such as [Fe i] 24 μm and H_2S(0) 28 μm primarily measure the gas mass in the disks, various line ratios diagnose the inner radius of the gas and the radial temperature and surface density distribution of the gas. Many lines become optically thick and/or suffer chemical or thermal effects such that the line luminosities do not increase appreciably with increasing gas mass. We predict that it may be difficult for the Spitzer Space Telescope to detect ≤1 M_J of gas in optically thin (in dust) disks at distances ≥150 pc. The models presented here will be useful in future infrared studies of the timescale for the dispersion of gas in a planet-forming disk and tests of core accretion models of giant planet formation.

Subject headings: circumstellar matter — infrared: general — planetary systems: protoplanetary disks — stars: formation

1. INTRODUCTION

Circumstellar disks evolve from gas-rich structures with 1% of the total mass in dust to disks that are observed to be completely devoid of gas and dominated by emission from dust particles. During this process of evolution, the disk, which is initially very optically thick in dust with radial midplane optical depths in the visual τ_V ≥ 10^3, becomes optically thin with τ_V ≥ 1 in a few million years (Haisch et al. 2001). At this intermediate stage of disk evolution planetary formation is probably underway with dust particles colliding and growing to form larger objects (which greatly reduces τ_V) and with some residual gas. Disks with ages ≥10^7 yr are observed to have almost no gas (Zuckerman et al. 1995; Duvert et al. 2000). Smaller dust particles in these disks either have dispersed or have coagulated to larger sizes, and these disks are very optically thin in dust, with τ_V ≤ 10^{-2}. These very optically thin disks are called “debris disks,” as the dust in these disks is generally not primordial but is continually generated debris from colliding rocky bodies and planetesimals.

The evolution of the dust component of disks has been extensively studied (e.g., Weidenschilling 1977; Weidenschilling et al. 1997) in models in which the dust grains in disks grow in size via collisional agglomeration. As dust grains grow and planetesimals eventually form, the disk becomes optically thin to stellar radiation and the fractional dust luminosity, f_D = L_IR/L_Bol, the ratio of the disk infrared luminosity to the stellar bolometric luminosity, is observed to decrease with the age of the disk as t^{-1.76} (Habing et al. 1999; Spangler et al. 2001; Zuckerman 2001). This decrease in dust luminosity occurs as micron-sized or smaller particles are lost through the effects of radiation pressure, Poynting-Robertson drag, and collisions (e.g., Backman & Paresce 1993), and the population of larger bodies that are the ultimate source of the dust dwindles.

Gas evolution in disks is less well understood. CO observational studies seem to indicate that gas beyond about 30 AU disappears rather abruptly at disk ages ≥10^7 yr (e.g., Zuckerman et al. 1995; Duvert et al. 2000). Theoretical studies also indicate short gas dispersal timescales (Hollenbach et al. 2000; Clark et al. 2001). However, there is some controversy regarding the
presence or absence of gas in disks of ages \( \sim 10^7 \) yr. Seemingly contradicting the CO observations, there may have been detection of \( \sim 0.1-1 \) \( M_J \) of molecular hydrogen gas in three younger (ages \( \geq 10^7 \) yr) debris disks by Thi et al. (2001) using the Infrared Space Observatory (ISO). These ISO results are controversial (see Lecavelier des Etangs et al. 2001; Richter et al. 2002; Sheret et al. 2003; Brandeker et al. 2004). If the ISO observations are confirmed, then perhaps CO is not a reliable tracer of gas mass in such systems and may be subject to chemical effects such as freezing onto cold dust grain surfaces in the outer disks and optical depth effects in the inner disk. On theoretical grounds, although gas in the outer regions \( (r \geq 10-100 \) AU) may be subject to photoevaporation due to stellar radiation, gas inside these radii does not photoevaporate because it is more tightly bound gravitationally to the star. Viscous accretion onto the central star and viscous spreading to the outer photoevaporating disk likely dominates the gas dispersal of the inner \( (r \leq 10-100 \) AU) disk (Johnstone et al. 1998; Hollenbach et al. 2000; Clarke et al. 2001). However, the timescale for viscous dispersal at \( r \sim 10-100 \) AU is uncertain.

A determination of gas dispersal timescales in disks is important for understanding the formation of planetary systems. Two competing theories exist for the formation of gas giants. Gaseous Jovian-type planets are believed to form in disks via accretion of gas onto rocky cores of a few earth masses (e.g., Lissauer 1993; Pollack et al. 1996; Kornet et al. 2002) or by gravitational instability in disks leading to the formation of clumps, which subsequently contract to form giant planets (e.g., Boss 2003). The presence or absence of gas in intermediate-aged or transitional disks \( (\tau_T \sim 1, \text{ages} \sim 10^7 \) yr) can potentially discriminate between these two theories. In the gravitational instability scenario, gas giants form quickly and the gas may dissipate rapidly. Longer gas disk lifetimes \( (\sim 10^8 \) yr) facilitate the formation of gas giant planets through conventional core accretion models, allowing sufficient time for the building of a rock/ice core of a few earth masses and subsequent accretion of gas. At the accretion stage, there would be little dust (or equivalently, particles small enough to significantly radiate at infrared/submillimeter wavelengths and be observed) in the giant gas regions of disks, and substantial amounts \( (\geq M_J, \text{or a Jupiter mass}) \) of gas. Core accretion theory suggests that systems may reside in this state for a significant length of time (a few Myr; e.g., Pollack et al. 1996). At this stage, the ratio of gas mass to dust mass (where dust is defined as particles with sizes \( \lesssim 1 \) mm) would initially increase from the interstellar value of 100 before the final gas dispersal reduces the ratio to values \( \leq 100 \) characteristic of the older debris disks. The detection of gas infrared emission during this epoch of gas accretion onto rock/ice cores would help support the core accretion scenario. Conversely, if very little gas \( (\sim 1 \) \( M_J \)) is present at the moment when the dust disk first becomes optically thin (signaling the buildup of several earth mass cores), then the core accretion model is likely invalid.

In the terrestrial planet region of the disk, the residual gas content of the disk at the epoch when embryos or protoplanets assemble to form terrestrial planets helps determine the ultimate mass and eccentricity of the planet and therefore the eventual habitability of the planet (Agnor & Ward 2002; Kominami & Ida 2002, 2004). In particular, a finite range of gas masses produces earth-mass planets on circular orbits. If the gas mass inside 3 AU at ages of \( 10^6-10^7 \) yr is much greater than \( 10^{-2} \) \( M_J \), the tidal interaction of the planets with the gas is sufficient to circularize the orbits of lunar-mass protoplanets, making it difficult for collisions between them to build earth-mass planets. On the other hand, if the gas inside 3 AU is much less than \( 10^{-2} \) \( M_J \), earth-mass planets can be produced but in orbits considerably more eccentric than that of the Earth.

At later debris disk stages, \( t \sim 10^7 \) yr, the presence of even small amounts of gas \( (\sim 10^{-2} \) \( M_J \)) can affect dust dynamics because of the drag forces they induce, and therefore, this gas may affect the disk structure significantly. This effect weakens the interpretations of gaps and ring signatures observed in dusty disks as being due to the presence of planets, as the presence of gas could give rise to the same structures (Klahr & Lin 2001; Takeuchi & Artymowicz 2001; Takeuchi & Lin 2002).

In the work presented here, we model gas emission from a disk that has optically thin or marginally optically thick \( (\tau_T \lesssim 5) \) dust\(^1\) and so is perhaps at a stage at which considerable rock/ice planetesimal and planet formation has already taken place, but may still retain appreciable amounts \( (\sim 10^{-2} \) to \( \lesssim 1 \) \( M_J \)) of gas left over from the rock/ice planet-building phase. We predict expected emission from such a range of gas masses in optically thin dust disks as a function of the gas mass, dust mass, and stellar properties. The results will aid future observational programs that plan to look for gas emission in disks in order to understand the evolution of gas in disks, the timescales for gas dispersal, and the process of giant planet formation. New observational facilities such as the Spitzer Space Telescope, SOFIA, and the Herschel Space Observatory are sensitive enough to detect infrared and submillimeter emission from small amounts of gas using tracers other than CO. These IR tracers may be better suited than CO for detecting gas in the 1–20 AU planet-forming region around solar-type stars. The possibility of detection of gas emission from the planet-forming regions around intermediate-aged and evolved debris disks by future IR observational studies is one of the main motivations of the present paper.

There has been extensive work on disk modeling of both young optically thick disks and older optically thin disks. However, most of this work either has concentrated on solving the disk structure by setting the gas and dust temperatures to be equal (e.g., D’Alessio et al. 1998, 1999; Dullemont et al. 2002; Dullemont et al. 2002; Lauchame et al. 2003) or has assumed a gas density and temperature distribution and solved for the chemistry (Willacy et al. 1998; Aikawa et al. 1999, 2002; Markwick et al. 2002; Iglner et al. 2004). We solve for both the gas and dust temperatures and the chemistry simultaneously in our models and use the gas temperature to calculate the vertical density profile. A similar theoretical study has been made by Kamp & van Zadelhoff (2001), who attempted to explain the observed \( H_2 \) emission from disks around two A stars, Vega and \( \beta \) Pictoris as seen by ISO, and the lack of CO emission from these disks. These authors calculate the gas temperature by balancing the different heating and cooling mechanisms but do not solve for the vertical structure of the disk. Our work adds the computation of vertical structure and is complementary to their model, since we focus on the inner regions of the disk, within about 20 AU from the star where the gas and dust are both warm \((\sim 100 \) K), whereas Kamp & van Zadelhoff (2001) considered disk regions from \( \sim 40 \) to 200 AU. The inner regions are more interesting from the planet formation point of view.

\(^1\) Henceforth, we call our models “optically thin” even though, as discussed in § 2.1, they apply for \( \tau_T \lesssim 5 \), where \( \tau_T \) is the radial optical depth through the midplane.
view, as many planets are expected to form close to the central star, within a few tens of AU if our solar system is typical. Furthermore, gas in regions far beyond this radius may be subject to photoevaporation from the central star and may be lost from the system early in its evolution. Our models are also complementary to the work of Glassgold et al. (1997) and A. Glassgold, J. Najita, & J. Igea (2004, in preparation), who model the very innermost regions \( r < 1\) AU of young optically thick disks with emphasis on the problem of heating the surface layers and the near-infrared spectra.

The paper is organized as follows. In the next section, we briefly describe some of the physical processes we consider. In § 3, we describe our model in detail. We present the results of a fiducial case (§ 4) and then in § 5 present results where we vary most of the parameters to see how disk emission is affected by their values. This is followed by a discussion of our results and conclusions (§ 6).

2. PHYSICAL PROCESSES IN DISKS

Our disk models include chemistry and thermal balance in a self-consistent manner and calculate the density and temperature structure of the disk in both the radial and vertical directions. The vertical structure of the disk is calculated by balancing the hydrostatic thermal pressure gradient with the vertical component of gravity from the central star. The inner \( r_i \) and outer \( r_o \) boundaries of the disk and the distribution of the gas and dust surface density \( \Sigma(r) \) within these boundaries are input parameters. Our focus is on the IR emission detectable by the *Spitzer Space Telescope*, SOFIA, or *Herschel*, and we therefore constrain our models to radial distances \( 0.3–20 \) AU from the central star, where gas temperatures range from \( \sim 1000 \) to \( 100 \) K, respectively. The dust grains in this region are sufficiently warm to prevent ice formation on their surfaces, and therefore significant depletion of relatively volatile species such as gas-phase O, C, or S does not occur. We assume no significant opacity inside the inner edge at \( r_i \), so that there is an “inner hole.”

Although we focus on intermediate-aged and older debris disks, which are relatively optically thick in dust opacity, the gas opacity can in fact be quite large at the line center of strong transitions and even for some far-UV (FUV) continuum bands, which lead to photodissociation and photoionization of abundant gas species. It is instructive to calculate a fiducial radial (hydrogen) gas column density \( N_H \) in the equatorial plane. Assuming a gas surface density distribution \( \Sigma(r) \propto r^{-3/2} \), a vertical scale height of \( H = 0.1r \), a gas mass of \( \sim 0.1 M_\odot \), and an outer radius \( r_o = 20 \) AU for a vertically isothermal disk, we find

\[
N_H \approx 2.6 \times 10^{25} \left( \frac{1 \text{ AU}}{r_i} \right)^{3/2} \left( \frac{M_{\text{gas}}}{0.1 M_\odot} \right) \text{ cm}^{-2}.
\]

Since cross sections in the UV and X-ray for trace species can approach \( 10^{-17} \text{ cm}^{-2} \) (or \( 10^{-21} \) per H nucleus), we see that even small masses of gas can become optically thick in relevant bands. We also note that most of the opacity for radially declining surface densities is produced at \( r_i \). If stellar photons make it through the shielding at \( r_i \), they will generally penetrate the rest of the disk.

We emphasize that our disk model is hydrostatic and our thermal and chemical solutions are steady state. Therefore, we implicitly assume that the timescales to reach chemical/thermal steady state are short compared to dynamic timescales, i.e., the timescale for radial or vertical migration of gas. Because of the high densities and subsequent rapid cooling timescales, the assumption of thermal balance is well justified. Chemical timescales, however, can be quite long in cool \( (T \lesssim 300 \) K) gas shielded from photodissociation. In such gas, cosmic-ray ionization sets the equilibrium timescales to \( \sim 10^6 \) yr, which is comparable to radial drift timescales. However, this work represents an important first step in predicting the chemical and thermal structure of the warm \( T \sim 100–1000 \) K, \( r \sim 1–20 \) AU regions of evolved disks and predicting their spectrum. We briefly describe below the chemical and physical processes considered in our models and refer the reader to the Appendices for greater detail.

2.1. Dust Physics

Coagulation processes in intermediate-aged disks may lead to a distribution of solid particles that range in size from \( 1 \mu m \) to \( 10^4 \) km (planets). We define “dust” to consist of all particles \( \lesssim a_{\text{max}} = 1 \) mm in radius. We assume that the size distribution of particles between \( a_{\text{min}} \) and \( a_{\text{max}} \) follows a power law \( n(a) \propto a^{-s} \), where \( 3 < s < 4 \) such that most of the surface area is in the smallest particles and most of the mass is in the largest particles. Observational studies of disks estimate the “dust” mass from emission at wavelengths \( \gtrsim 0.4–2 \) mm. If the size distribution has the above power-law form, these observational studies are only sensitive to the mass of dust in particles with sizes \( \lesssim 1 \) mm.

Implicit in these assumptions is that most of the mass of solids will be “hidden” in large particles, rocks, boulders, and planetesimals, which emit insignificant amounts of infrared and millimeter wavelength radiation. Thus, at intermediate disk ages \( \sim 10^7 \) yr, when dust has coagulated up to planetary sizes but significant quantities of gas may not yet have been dispersed, the gas-to-“dust” (meaning \( a \lesssim 1 \) mm) mass ratio may increase above the value \( \sim 100 \) characteristic of interstellar conditions. For example, if 90% of the mass of the primordial dust in a disk grows by runaway accretion to cores/embryos of sizes \( 10^2–10^4 \) km and the remaining 10% of the mass is in solids with a distribution characterized by \( a_{\text{min}} = 1 \mu m, a_{\text{max}} = 100 \) km, and \( s = 3.5 \), the gas-to-“dust” mass ratio increases to \( 10^8 \) without any gas or solid dispersion. Later, as the gas disperses, the gas-to-dust mass ratio may fall below the interstellar value.

In order to express the large range of gas to (small) dust mass ratios and the absolute values of the gas or dust mass that may exist as intermediate-aged or older disks evolve, we consider a range of gas masses \( M_{\text{gas}} \sim 10^{-3} \) to \( 1 M_\odot \) and a range of dust masses \( M_{\text{dust}} \sim 10^{-7} \) to \( 10^{-4} M_\odot \) (or \( f_D \sim 10^{-4} \) to \( 10^{-1} \)). \( M_{\text{gas}} \) and \( M_{\text{dust}} \) are treated as independent variables, so that we cover gas-to-dust mass ratios of \( 10^{-7}–10 \). We emphasize that these masses lie at \( r \lesssim 20 \) AU. We do not consider gas masses smaller than \( 10^{-3} M_\odot \) because we find such small masses to be undetectable by the *Spitzer Space Telescope*, SOFIA, or *Herschel*. We do not consider dust masses higher than \( 10^{-4} M_\odot \) because we find that the dust becomes significantly optically thick in the equatorial plane, and our model is valid only for small to moderate dust optical depths.

Our models consider gas and dust separately but as a coupled system, and they are capable of treating the dust grain density distribution independently of the gas density distribution as a function of radius \( r \) and vertical height \( z \). In addition, the grain size distribution can be arbitrarily varied with \( r \) and \( z \). However, for simplicity and to limit the number of models to be presented, we make the following assumptions.
1. We assume that the dust mass density distribution $\rho_\text{d}(r, z)$ is proportional to the gas mass density distribution $\rho(r, z)$. That is, for a given disk we assume that the same gas-to-dust mass ratio applies everywhere in the disk. This assumption means that we ignore settling by grains to the midplane. Turbulence may stir the gas and dust sufficiently to justify this assumption (e.g., Balbus & Hawley 1991). However, our main motivation is simplicity in the models; presumably by using an average (vertical) mass ratio of gas to dust, we will obtain a first-order solution for the more complicated case of vertical differentiation.

2. We assume that the grain size distribution does not vary with $r$ or $z$. We consider our minimum grain size to be much larger than that in the interstellar medium. In intermediate-aged disks, the population of very small grains dwindles as coagulation processes lead to grain growth (e.g., Beckwith & Sargent 1996; Throop et al. 2001; Natta et al. 2004). In more evolved debris disks, small grains are continually replenished by the grinding down of larger objects by collisions, but radiation pressure forces act on submicron-sized dust grains to rapidly remove them from the disk (Backman & Paresce 1993) on short timescales. Observations nevertheless seem to indicate the presence of small submicron-sized particles (Li & Greenberg 1998) in a debris disk. We adopt a minimum grain size of $a_{\text{min}} = 1 \, \mu$m for our standard case but also consider other cases in which we vary $a_{\text{min}}$. In this paper, we only consider $n(a) \propto a^{-3.5}$, i.e., $s = 3.5$.

For a given mass in grains, the surface area $\propto a_{\text{min}}^{-1/2}$. Gas-grain collisional heating can be important in disks, and because of their large surface area, small grains dominate the heating of the gas. Therefore, lowering $a_{\text{min}}$ raises the gas-grain coupling and usually raises the gas temperature in the disk. Lowering $a_{\text{min}}$ tends to raise the gas temperature for two other reasons. Smaller grains have higher efficiencies of heating the gas through the grain photoelectric heating mechanism (see Watson 1972; Weingartner & Draine 2001), which may dominate the heating once $a_{\text{min}} \leq 10^{-5} \, \mu$m. More importantly for this paper, smaller grains are hotter than larger grains because of the heating by stellar radiation and the inefficient radiative cooling of small grains. Grain absorption and emission efficiencies are dependent primarily on their physical size relative to the wavelength of emission or absorption, and their composition. For our models, we choose silicate (amorphous olivine) grains, and the absorption coefficients are calculated from a Mie code (S. Wolf 2003, private communication) based on optical constants from the Jena database (Henning et al. 1999). We divide the grain size distribution into 32 logarithmically spaced bins in size $a$, and each size grain has a different temperature at a fixed point in space.

We conclude this subsection with a discussion of the dust optical depths in the model disks. Using the absorption coefficients discussed above, we calculate the optical depth $\tau_\nu$ in the $V$ band (0.5 $\mu$m) of dust grains radially outward in the equatorial plane of the disk. For most of our models, $\tau_\nu \leq 1$. We do, however, run a few cases where the optical depth in the midplane $\tau_\nu \sim 5$. These disks are still optically “thin” in comparison to the younger, primordial dust disks where $\tau_\nu \sim 10^2$–10$^4$. In our calculation of dust temperatures we ignore the heating of dust grains due to the infrared radiation field emitted by the surrounding dust, but we include extinction of starlight by dust grains along the line of sight to a particular point in the disk. Even at optical depths $\tau_\nu = 5$, the dust grains are still primarily heated by attenuated starlight rather than by the reradiated IR continuum field, so that our error in calculating the dust temperature is still small ($\leq 10\%$), and our models are still valid. Typically, debris disks ($t > 10^7$ yr) have $\tau_\nu \leq 10^{-2}$. However, intermediate-aged disks ($t \sim 10^6$ yr) may have $10^{-2} < \tau_\nu < 5$.

### 2.2. Gas Chemistry

The chemical composition of the gas disk is critical to the structure and evolution of the disk. Although H$_2$ cooling is often important in the radial range we consider, trace species such as S, O, CO, and H$_2$O are often significant or even dominant coolants, and for an accurate determination of the strength of emission lines, the abundances of atoms and molecules need to be calculated. Our treatment of disk chemistry is an adaptation of the photodissociation region (PDR) models of Tielens & Hollenbach (1985, hereafter TH85) and subsequent work (Kaufman et al. 1999). Elemental gas-phase abundances are taken from Savage & Sembach (1996) (Table 5, Appendix A). We use interstellar depletions of these elements, allowing for refractory dust but no ices in the $r \leq 20$ AU disk region, where the dust is sufficiently warm to prevent ice formation. We have added sulfur chemistry and reactions of CH$_3$ and CH$_4$, and there are a total of 73 species with atoms and ions of H, He, C, O, S, Fe, Mg, and Si and molecules and molecular ions of H, C, O, S, and Si (Table 6, Appendix A). To the PDR network of ion-neutral, neutral-neutral, and photodissociation reactions, we have added X-ray photoreactions and some high-temperature reactions of importance under typical disk conditions. We have 537 reactions in all, with reaction rates in most cases taken from the UMIST Astrochemistry database (Le Teuff et al. 2000). A list of the added reactions, as well as the rates when they differ from the UMIST data, can be found in Table 7 (Appendix A).

The formation mechanism of H$_2$ in disks may differ from the processes at work in the interstellar medium. In the ISM, H$_2$ forms mainly on the surfaces of cold dust grains, with $T_{\text{dust}} \leq 25$ K, typically. Dust in disks at 0.3–20 AU typically has temperatures $T_{\text{dust}} \approx 100$ K. It is not clear whether H atoms would stick to such warm dust grains for sufficient time to allow formation of H$_2$ molecules (Hollenbach & Salpeter 1971; Cazaux & Tielens 2002). We have conservatively omitted grain formation of H$_2$. We find that other processes such as three-body reactions in dense regions and formation through H$^-$ can completely convert atomic hydrogen to molecular hydrogen in self-shielded regions. We have also run cases including grain formation of H$_2$ and find that the resultant infrared spectrum is not significantly altered.

Because the dust is optically thin, stellar and interstellar UV radiation is mainly attenuated in the disk by different gas species in various bands and lines. Large gas columns in the inner disk shield the outer regions from UV photodissociation caused by the central star. Similarly, the gas columns in the upper layers shield the midplane from the interstellar radiation field (ISRF). The self-shielding of H$_2$ and CO, which involves absorption of specific resonance lines rather than continuum radiation, is treated analytically as in TH85. Attenuation of continuum FUV radiation by atoms and molecules is determined by splitting the FUV stellar radiation field into energy intervals, and the photon flux in each interval is calculated from the stellar (and ISRF) spectrum. The eight intervals from 0.74 to 13.6 eV include 0.74–2.6, 2.6–3.5, 3.5–4.3, 4.3–5.12, 5.12–7.5, 7.5–10.36, 10.36–11.26, and 11.26–13.6 eV, where the lower and upper bounds in each case were chosen to correspond to dominant photoabsorption thresholds.
of species in each energy bin. The attenuated photon flux in each bin at a given position in the disk is dependent on the column densities of all the absorbing species toward the line of sight to the source. Photodissociation and photoionization reaction rates are thus accurately computed by taking into account the attenuation of photons in the energy range where absorption cross sections peak.

We also consider the effects of X-ray radiation from the star on the disk. X-ray luminosities of $\sim 10^{-4} L_{\text{bol}}$ have been observed in stars as old as $10^7 - 10^8$ yr and therefore include not only intermediate-aged disks but also a number of observed “debris disks.” X-rays affect the chemical structure of the disk through ionizations and heat the gas via collisions with secondary electrons generated by the X-ray–produced primary electron. X-ray heating and chemistry may dominate in the inner regions of the disk and the surface layers where attenuation by gas is low. Stellar X-ray spectra from weak-line T Tauri stars (wTTSs) peak at about 1–2 keV (e.g., Feigelson & Montmerle 1999), and the flux drops rapidly as the X-ray photon energy increases. Soft X-rays, with energies $\lesssim 1$ keV, do not penetrate significantly through a massive disk, their typical attenuation columns being about $10^{21} - 10^{22}$ cm$^{-2}$ of gas. The penetration columns are larger by about 2 orders of magnitude for harder (3–10 keV) X-rays, but the stellar flux and photoabsorption cross sections decrease sharply to make their influence on disk chemistry relatively unimportant in the shielded regions of the disk. On the other hand, in disks with low masses or lower column densities toward the line of sight to the star (disks with large inner radii, for example), X-rays incident on the disk heat, ionize, and dissociate significant numbers of atoms and molecules in the gas, and our chemical code treats this chemistry in detail. For simplicity, we do not consider double or higher ionizations, as in Maloney et al. (1996). The total X-ray photoabsorption cross section of the gas is taken from Wilms et al. (2000), adapted to our gas-phase abundances (see Appendix B). We use the photoionization cross sections as originally published by Werner et al. (1993) and later updated by Werner & Yakovlev (1995). The primary ionization rates for each species are calculated for each species by integrating the product of the attenuated photon flux and the absorption cross section over the X-ray energy range (Maloney et al. 1996). We also include secondary ionization rates and X-ray–induced FUV radiation and the resulting photochemistry (Maloney et al. 1996). The details of our treatment of X-ray chemistry and heating are given in Appendix B.

2.3. Heating and Cooling Processes

One of the major innovations of this paper in terms of disk modeling is the separate calculation of gas and dust temperatures. Most previous models (with the exception of Kamp & van Zadelhoff 2001) assume that the gas temperature equals the dust temperature. While this is certainly true in the midplanes or central regions of very optically thick disks, it is not as true for debris disks, intermediate-aged disks, or the upper regions of younger, optically thick disks. Here the relatively weak thermal coupling between gas and dust, as well as the different processes that heat and cool the gas and dust, can lead to significant temperature differences. This point was also made by Chiang & Goldreich (1997), who note that the gas temperature in the superheated layers of passive, optically thick dust disks can be significantly lower than the dust temperature because of molecular cooling.

Gas in disks can be heated through many different mechanisms, and we consider the physical and chemical processes that are likely to dominate in these environments. The heating of dust grains by the stellar radiation field and subsequent collisions with gas molecules transfers kinetic energy to the gas, thereby heating it. Gas-dust collisions are the dominant heating mechanism for the gas through most of the disk, except in regions where the gas is heated to temperatures higher than the dust by other processes, and here collisions with dust cool the gas. In regions where the columns through the disk are small enough to allow the penetration of FUV radiation, and H$_2$ is photodissociated to form atomic hydrogen, the heat associated with the formation of H$_2$ raises the temperature of the gas. X-rays from the central star directly heat the gas and dominate the gas heating at the surface and in the inner disk. In addition to these mechanisms, we also include heating due to collisional deexcitation of vibrationally excited H$_2$ molecules, grain photoelectric heating, drift heating due to dust, exothermic chemical processes, photoionization of neutral carbon, and cosmic rays. All the heating mechanisms considered are described in some detail in Appendix C.

The gas in the disk is mainly cooled through radiative transitions of the different species and, where the gas is warmer than the dust, through gas-grain collisions. We include cooling due to the fine structure and metastable lines of C i, C ii, O i, O ii, Fe i, Fe ii, S i, S ii, Si i, and Si ii and the rotational lines of H$_2$, H$_2$O, OH, CO, CH, HCO$^+$ and by Ly$\alpha$. We also include cooling due to the collisional ionization of atomic species and vibrational cooling due to H$_2$. Vibrational cooling due to CO was found to be unimportant for the disk parameters considered in this paper. For all the molecular rotational levels, except for H$_2$ and CO, we use the analytical formulae of Hollenbach & McKee (1979, hereafter HM79). We derive new fits to their formulae for H$_2$O (ortho and para states) and OH (see Appendix D) using collisional rate data for 167 and 45 levels, respectively. It was computationally expensive to include a detailed multilevel calculation for these molecules in the code, and we estimate the strengths of individual H$_2$O and OH lines using the derived density and temperature structure and solve for the level populations after a disk solution for the temperature, density, and chemical abundance structure (i.e., the $r, z$ dependence) has been obtained with the new analytical approximations for the total cooling by OH and H$_2$O molecules. We note that cooling transitions are often optically thick, and we use the escape probability formalism described in HM79.

We solve for the rotational cooling due to H$_2$ in detail because one of our primary aims is to calculate the strength of the H$_2$ emission lines from the disk. We include the first 20 levels of molecular hydrogen in our calculation of the cooling and derive the population of each individually excited level. We have also added vibrational cooling of H$_2$ as in HM79 and cooling due to collisional dissociation of H$_2$ molecules. We do a similar calculation of the first 20 rotational levels of CO and solve for the level populations to compute the total CO cooling.

3. DISK MODEL

In this section, we describe our disk model, discuss some of our assumptions, and give the details of our numerical scheme for obtaining a disk solution. Because our main aim is to characterize observed emission from disks and infer disk properties from the comparison of observed spectra with our
models, we have varied most of our input parameters across a wide range. However, we define a “standard case” in which we assign typical values to each parameter. The results from the standard model are described in § 4.

3.1. Surface Density Distribution

We assume a power-law distribution of surface density of both gas and dust with radius, \( \Sigma(r) \propto r^{-\alpha} \), where \( r \) is the distance from the star. The nominal value for \( \alpha \) is often taken to be 3/2 in the literature (Lynden-Bell & Pringle 1974; Chiang & Goldreich 1997). For our standard case, we assume a flatter surface density distribution defined by \( \alpha = 1 \), motivated by observations of disks (Dutrey et al. 1996; Li & Greenberg 1999). The main effect of changing the slope of the surface density distribution is to alter the relative distribution of mass in the inner and outer disk. This changes both the slope of the dust continuum emission at longer wavelengths and the relative strengths of the gas emission lines that preferentially originate either in the warmer inner disk or the colder outer disk region. We study the effects of a change in the surface density distribution by varying \( \alpha \). As long as \( \alpha < 2 \), most of the disk mass is in the outer regions; and for \( \alpha > 0 \) (and assuming a vertical scale height \( H \) that increases with \( r \)), most of the radial opacity occurs in the inner regions.

3.2. Radial Extent

Our model disk is defined to have both an inner and outer edge. It is not, however, certain whether an inner (gas) hole would exist in evolved disks, even if the dust is heavily depleted in the inner regions. Theoretical models of dust disks often assume an inner truncation radius determined by the dust sublimation temperature, interior to which there is no dust (e.g., Bell et al. 1997; Chiang & Goldreich 1997; D’Alessio et al. 1998; Duellmond et al. 2002). Spectral energy distribution modeling of observed dust disk emission also argues for the presence of inner (dust) holes in many disk systems (e.g., Natta et al. 2001; Duellmond et al. 2001). In evolved disks, where planetary formation is likely to have taken place, an inner gas cavity may be generated by massive planets that prevent outer gas from accreting onto the star, whereas viscous accretion of gas interior to the massive planets may rapidly drain gas there.

The inner disk radius \( r_i \) is an important parameter of our models because it determines the penetration of stellar radiation into the disk and contains the hottest gas and dust. Emission from this region, therefore, is a dominant contributor to the higher frequency continuum from the dust and the higher excitation lines of the gas. Small values of \( r_i \) imply higher densities and column densities at the inner edge, and radiation can penetrate only a short distance into the disk before being attenuated. If disks with the same gas mass have larger \( r_i \), there is less rapid attenuation of stellar photons. Consequently, photodissociation and photoionization by X-rays and FUV radiation extends farther into the disk and affects more of the gas mass. Observations of intermediate-aged and debris disks indicate disk inner radii ranging from a few tenths of an AU to tens of AU (e.g., Liu et al. 2004; Calvet et al. 2002; Li & Greenberg 1998). For our standard case, we assume an inner radius of \( r_i = 1 \) AU. However, we include several cases in which we vary the inner radius to see how this parameter affects disk thermal structure and chemistry and the resultant spectrum.

We also define an outer disk radius \( r_o \). Our fiducial disk is truncated at \( r_o = 20 \) AU. Unlike \( r_i \), the exact choice of \( r_o \) does not affect our results significantly because any gas beyond \( r_o \) will be too cold to significantly contribute to the IR lines that we focus on in this study. The choice of 20 AU is motivated by the following four reasons. (1) Disks may lose much of the outer gas through the process of photoevaporation early in their evolution (Hollenbach et al. 1994; Adams et al. 2004). (2) Our interest lies in the planet-forming regions of the disk, and from our understanding of the formation of the solar system and of the evolution of disks, planet formation appears to take place within a few tens of AU from a star. (3) A. Glassgold, J. Najita, & J. Igea (2004, in preparation) present models of inner (<1 AU) disks, whereas Kamp & van Zadelhoff (2001) present models of outer (>30 AU) disks. We therefore present this complementary study, which is especially relevant to the Spitzer Space Telescope, SOFIA, and Herschel, since the gas and dust temperatures span a range (~50–500 K) that produces copious IR emission in the 4–200 \( \mu \)m wavelength range. Mid-infrared emission from gas species at temperatures less than ~100 K is likely to be insignificant, so the neglect of any gas beyond \( r_o \) does not affect our emission-line calculations. (4) Gas molecules, such as \( \text{H}_2\text{O} \), may freeze on grain surfaces when the dust grain temperature drops below ~80–100 K. We therefore truncate the disk at a radius where ice mantle formation is likely to become important on grains, i.e., when dust grain temperatures fall below ~100 K. To summarize points 3 and 4, the outer edge need not correspond to a real cutoff in surface density. We are interested in the IR emission from warm gas in the \( r \leq 20 \) AU region. Material beyond this outer radius will be either too cold or frozen on grain surfaces to radiate appreciably as IR line emission from gaseous species.

3.3. Stellar Spectrum

The stellar spectrum is chosen to be a modified Kurucz model, and we consider stars of two spectral types, a G star at 6000 K and a cooler K star with a temperature of 4000 K. The central star at these disk ages is expected to have a significantly higher FUV luminosity than its main-sequence counterpart, and we account for this increased luminosity in our stellar models. An accurate determination of the FUV flux is especially important in solving for the disk chemistry, as the FUV initiates numerous photodissociation and photoionization reactions. We follow a prescription by Kamp & Sammar (2004) for our age-dependent FUV fluxes, where the FUV flux scales inversely with the age of the star (Ayres 1997). We assume an age of 10^7 yr for the G star in our models. IUE and rocket experiment data are added to a Kurucz photosphere model to thus obtain a semiempirical age-dependent spectrum for a G2 spectral type star. We use chromospheric models by M. Cohen (2003, private communication) for the star \( \epsilon \) Eri as our input stellar model for the K star. Figure 1 shows the spectra we use; the solid line indicates the G star, and the dashed line, the K star.

For the stellar X-ray spectrum, we use a broken power-law fit to ROSAT observations (Feigelson & Montmerle 1999) for a wTTS, where the luminosity per keV peaks at about 2 keV. The luminosity per keV is thus given by \( L(E) \propto E^{-1.75} \), \( E \geq 2 \) keV, and \( L(E) \propto E \) for \( E < 2 \) keV. This X-ray spectrum is normalized to the stellar X-ray luminosity between 0.5 and 10 keV. For our fiducial case, the X-ray luminosity is assumed to be 10^-4 times the bolometric luminosity of the star.

3.4. Numerical Model

The disk density and temperature structure is calculated iteratively from the midplane to the surface starting at \( r = r_i \)
and then working radially outward in the disk. We start with an estimate of the gas density at the point \((r = r_1, z = 0)\) and compute the dust and gas temperatures.

The dust temperature is calculated from thermal balance between the absorption of stellar radiation by the dust and subsequent reemission in the infrared. Heating of a grain due to absorption of infrared radiation coming from surrounding dust particles is ignored in our optically thin dust disk models. The dust temperature (at a given size \(a\)) needs to be iterated only because the dust vertical distribution is determined by the gas vertical distribution, and the dust temperature is a function of \(z\) because of the varying distance to the star.

The gas temperature is determined by thermal balance between the heating and cooling processes described earlier, and this then determines the gas pressure. The condition of vertical hydrostatic pressure equilibrium,

\[
\frac{dP}{dz} = -\frac{GM_\star m_\text{H} n_\text{H}(r,z)}{(r^2 + z^2)^{3/2}},
\]

(2)
determines the pressure as a function of disk height, where \(P = k_B[n(\text{H}) + n(\text{H}_2) + n(\text{He})]T_{\text{gas}}\), \(\mu\) is the mean molecular weight, \(n_\text{H}\) is the mass of a hydrogen atom, \(n_\text{H}\) is the hydrogen nucleus number density, and \(n(\text{H}), n(\text{H}_2), n(\text{He})\) are the number densities of atomic and molecular hydrogen and helium, respectively. At each height \(z\) from the midplane, the density and temperature combination that gives the pressure from equation (2) is found. The vertical grid is adaptive in nature and determined by the condition of pressure gradient balancing gravity. The vertical increments in height are chosen to correspond to equal factors of decrease in thermal pressure (a factor of 0.8 in most cases), and for regions where the temperature slowly varies with \(z\), this also corresponds to a logarithmically decreasing column density in each cell. This ensures that the escape probabilities for the cooling transitions increase slowly and smoothly as we get farther from the midplane and enables accurate determination of the gas temperature. We ensure that the density contrast from surface to midplane is at least 4 orders of magnitude, and the number of cells and their spacing are calculated to meet all these criteria. After the entire vertical grid has been solved, the gas density is integrated over \(z\) and compared with the required gas surface density, \(\Sigma(r)\). The midplane density is rescaled, and the vertical temperature and density structure is thus iterated until the surface density converges to the required value.

Once we have the solution at \(r_1\), we move outward to solve at the next radial grid point. The radial grid is logarithmically divided in \(r\), except for the inner disk, which is more finely subdivided. The column density toward the star is dominated by the dense inner regions, and this is where the gas absorbs most of the stellar FUV and X-rays. This attenuation needs to be calculated accurately, and we have divided the inner disk into cells of slowly increasing column density going outward in \(r\), with the first radial cell (at midplane) having a hydrogen gas column density \(10^{20}\) cm\(^{-2}\), which corresponds to a small attenuation of the X-ray and UV fluxes.

### 4. STANDARD DISK MODEL RESULTS

In this section, we describe in some detail the results of our fiducial disk model (“the standard case”), the input parameters for which are listed in Table 1. The standard model has a gas mass \(M_{\text{gas}} = 10^{-2} M_\odot\) and dust mass \(10^{-5} M_\odot\). In the next section we present a full parameter study varying both the gas mass and the dust mass, the main parameters of this work. The other parameters we treat as “minor” parameters, and in the next section we vary each of these parameters in turn, holding all other parameters at the fiducial values, and study the effect on disk structure and emission. These minor parameters include the disk inner radius, the minimum grain size, the stellar X-ray flux, and the surface density distribution.

Our fiducial gas-to-dust mass ratio of \(10^2\) is higher than the interstellar value, but, as we have discussed, this is possible at an intermediate stage at which dust has coagulated but gas has not yet dispersed. We have chosen this value for our fiducial case primarily because, as is shown below, this ratio allows detection of gas emission lines over the continuum for the smallest gas masses with the dust midplane optical depth still being \(\lesssim 1\).

Our standard model disk solution results in a flared disk with an inner puffed region where the gas is subject to the

### TABLE 1

** Input Parameters for Standard Disk Model **

| Parameter                  | Value |
|----------------------------|-------|
| Gas mass                   | \(10^{-2} M_\odot\) |
| Inner radius \(r_i\)       | 1 AU  |
| Outer radius \(r_o\)       | 20 AU |
| Surface density power-law index \(\alpha\) | 1.0 |
| Stellar age (for FUV flux) | 10\(^7\) yr |
| Stellar X-ray luminosity   | \(4.0 \times 10^{29}\) ergs s\(^{-1}\) |
| Stellar temperature \(T_s\) | 5780 K |
| Dust mass                  | \(10^{-5} M_\odot\) |
| Minimum grain size \(a_{\text{min}}\) | 1.0 \(\mu\)m |
| Maximum grain size \(a_{\text{max}}\) | 1.0 mm |
| Grain size distribution index \(s\) | 3.5 |
| Grain composition          | Amorphous olivine |
| Stellar bolometric luminosity | \(4.0 \times 10^{13}\) ergs s\(^{-1}\) |
unattenuated, strong stellar radiation field and heated to high temperatures. Dullemond et al. (2002) find a similar effect in younger, optically thick (in dust) disks. Figure 2 shows the disk surface where the density is $10^{-4}$ times the density in the midplane and contours where the vertical column densities to the surface are $10^{21}$ and $10^{22}$ cm$^{-2}$. Stellar UV and X-ray fluxes are absorbed at these column densities and hence in these regions. The hot inner edge or rim has a somewhat lower density than gas just beyond the edge because it is hotter and more extended vertically. This region shields much of the rest of the disk from UV and X-ray photodissociation and photodestruction by starlight. The density increases slightly with radius progressing from this inner edge as the temperature falls steeply, and the disk scale height decreases. Recall that for a vertically isothermal disk the scale height $H$ of the disk is given by $H \propto \frac{r^2}{T(r)}$ (e.g., Adams et al. 1988; Shakura & Sunyaev 1973). Therefore, for a radial temperature gradient steeper than $1/r$, the scale height decreases with radius. X-rays are a strong heating agent in the unshielded innermost regions of the disk but get attenuated rapidly because of the high midplane radial column density $N(r)$ (see eq. [1]). The penetration column for 2 keV X-ray photons, where the X-ray spectrum peaks, is $\sim 1/\sigma(E) \sim 5 \times 10^{22}$ cm$^{-2}$, which implies a penetration depth of $\sim 0.003$ AU. Heating due to X-rays becomes unimportant in the midplane for $r > 10^3$ AU, however, can penetrate farther at the surface of the disk, where the attenuation columns of gas toward the line of sight to the star are low. X-rays are the dominant heating mechanism at the surface. Gas-grain collisions are the strongest gas-heating source through most of the equatorial regions of the disk even though the dust surface area per H nucleus is much smaller than the interstellar value (about $10^{-3}$ times that in the ISM for the standard case). Note that in the innermost regions, the gas-grain collisions become a cooling mechanism, rather than a heating mechanism, as the gas becomes hotter than the dust grains because of X-ray and H$_2$ formation heating. Heating due to cosmic rays, grain photoelectric heating, and drift heating are negligible in this disk model.

4.1. Heating, Cooling, and Temperature Structure

Figures 3, 4, 5, and 6 show the heating, cooling, and the radial temperature and density structure in the disk at the midplane and the vertical temperature and density structure in the disk at two typical radii, 2 and 10 AU. Figure 3 shows the main heating terms for our standard case in the midplane of the disk as a function of disk radius. Heating due to formation of H$_2$ is high where hydrogen is predominantly atomic but quickly decreases as self-shielding turns the gas molecular, at hydrogen nuclei column densities of $\sim 10^{21}$--$10^{22}$ cm$^{-2}$. X-rays are a strong heating agent in the unshielded innermost regions of the disk but get attenuated rapidly because of the high midplane radial column density $N(r) \sim 10^{24}$ cm$^{-2}$ (see eq. [1]). The penetration column for 2 keV X-ray photons, where the X-ray spectrum peaks, is $\sim 1/\sigma(E) \sim 5 \times 10^{22}$ cm$^{-2}$, which implies a penetration depth of $\sim 0.003$ AU. Heating due to X-rays becomes unimportant in the midplane for $r > 10^3$ AU. X-rays, however, can penetrate farther at the surface of the disk, where the attenuation columns of gas toward the line of sight to the star are low. X-rays are the dominant heating mechanism at the surface. Gas-grain collisions are the strongest gas-heating source through most of the equatorial
Zadelhoff (2001) find drift heating to be the dominant heating agent in their models of gas disks around A stars, but we find that our more careful calculation of drift velocities yields values that are typically too low ($\sim 10^3$ cm s$^{-1}$ or less) for viscous heating to be important in our $\sim 20$ AU disks. Nevertheless, we include this mechanism, as it may become important in other regions of parameter space. The dominant coolants in the midplane of the disk (Fig. 4) are OH, H$_2$O, Si $\equiv$, Si $\equiv$, H$_2$, and Fe $\equiv$ in the inner regions and O $\equiv$, CO, and OH in the outer disk. Above the midplane S $\equiv$ and O $\equiv$ are strong coolants. At radii larger than $\sim 7$ AU, the IR continuum field from the warmer dust excites the upper level of the [S $\equiv$] line, and subsequent collisional deexcitation leads to a gas heating rather than cooling by this line, as seen by the sharp cutoff in the S $\equiv$ cooling in Figure 4.

The gas temperature in the midplane of the disk (Fig. 5) decreases with radius approximately as $T_{\text{gas}} \propto r^{-0.8}$. The plot also shows the dust temperatures of the smallest and largest grains. These temperatures are higher than that of the gas over most of the disk interior, and therefore gas-grain collisions heat the gas here. In the outer regions of the disk midplane, the gas temperature falls well below the dust temperature, as the decreasing density leads to a decrease in collisional coupling between grains and dust, which lowers the heating rate of the gas. Figure 5 also shows the number density of gas in the midplane, which falls approximately as $1/r^2$.

Figure 6 shows the variation of gas temperature with height at two different disk radii, 2 and 10 AU, and the gas number density with height at 2 AU, with the dominant heating sources and coolants marked at various heights. In the equatorial region where gas-grain collisions dominate the heating, the density (Fig. 6, dashed line) can be seen to decrease rapidly with $z$ [recall that for isothermal disks, $n \propto \exp(-z^2/H^2)$, where $H$ is the scale height], leading to a reduced gas-grain coupling and heating and causing a drop in temperature with height. Several scale heights above the midplane, the attenuating column to the star drops to sufficiently low values that X-ray heating begins to dominate and the gas temperature rapidly rises. The main coolant at the surface is [O $\equiv$] 63 $\mu$m, which is optically thick at these column densities. The column to the surface decreases with height, and the line becomes more optically thin and more efficient at cooling. This leads to a drop in temperature again in the upper disk atmosphere. Figure 6 also shows the temperature profile at a larger disk radius (10 AU), where gas temperatures are much lower. The main heating sources remain gas-grain collisions at the midplane and X-rays at the disk surface, but the main coolants in these regions are CO and O $\equiv$, as the temperatures are too low ($< 100$ K) to significantly excite the transitions of H$_2$, S $\equiv$, Si $\equiv$, or Fe $\equiv$, and the densities and OH and H$_2$O abundances are too low for OH and H$_2$O to dominate the cooling.

4.2. Chemistry

Figure 7 shows the abundances of various species as a function of height above the disk at a radius of 2 AU. We discuss below the essential species in the hydrogen, OH/H$_2$O, C$^+$/C/CO, Si$^+$/Si, Fe$^+$/Fe, and S$^+$/S chemistry.

In the innermost disk, for $r \leq 1.1$ AU, hydrogen is predominantly atomic. H$_2$ is formed via reactions of H with H$^-$ and three-body reactions but is rapidly destroyed by reactions with O to form OH and by photodissociation. In regions high above the midplane, where there is less attenuation of stellar UV photodissociation of H$_2$ dominates. Beyond 1.1 AU, self-shielding prevents UV photodissociation of H$_2$. The destruction reaction with O has a high activation barrier at $\Delta E/k = 3200$ K, and this reaction rate rapidly falls as the temperature decreases radially outward. Consequently, hydrogen turns fully molecular in the dense midplane at $r \sim 2$ AU. At the surface of the disk at $r = 2$ AU, lower attenuation columns lead to photodissociation of H$_2$, and hydrogen is atomic as is shown in Figure 7.

Carbon turns molecular in the midplane even at the inner edge of the disk where hydrogen is still atomic and is in the
form of CO throughout the disk midplane. In the upper regions of the disk, CO is photodissociated into atomic carbon, which gets ionized even higher up in the disk to form C+ (Fig. 7). CO is formed via the reaction of C with OH in the inner disk where the temperatures are high and OH is more abundant. O reacts with CH to form CO in the outer disk. The main destruction routes of CO are photodissociation by the stellar UV field at the inner edge of the disk and in regions above the midplane everywhere in the disk. In the shielded interior of most of the disk, all the available carbon forms CO, as the only destruction mechanism for CO molecules is collisions with the very few He + ions that are formed by cosmic rays.

The gas-phase elemental oxygen abundance is a factor of 2.3 higher than the carbon abundance (Table 5, Appendix A), and all the oxygen not locked up in CO is in the form of O i throughout the disk. The stellar photons are not energetic enough to ionize oxygen, and trace amounts of the atomic oxygen form O2, OH, and H2O. In the inner disk, where the temperature is high (T > 300 K), O reacts with H2 to form OH, which then reacts again with H2 to form water. OH also reacts with O to form O2 throughout the disk, which is destroyed by photodissociation. H2O and OH are the dominant coolants at the high densities and temperatures in the innermost disk. Water is photodissociated through the disk more readily than OH, as it has a lower photodissociation threshold (~4.3 eV). In disks that are more massive, larger attenuation columns shield H2O from photodissociation, and because of its high abundance, it dominates the cooling, as will be discussed later. As the temperature drops farther into the disk, the production of OH and H2O drops because the reactions of O and OH with H2 have high activation barriers. The resulting decrease in the abundance of OH lowers its strength as a coolant farther into the disk. The destruction of OH is mainly via photodissociation, which rapidly decreases with disk radius as the optical depth in the relevant FUV band increases, and this keeps the abundance of OH from dropping sharply. The main reaction for the production of OH and H2O in the cooler outer regions is recombination of H3O+, which is initiated by cosmic-ray ionization of H2.

Sulfur is predominantly atomic throughout most of the disk, except very near the midplane, where it is partly molecular, and at the disk surface, where it is ionized to form S ii. In more massive disks, which shield sulfur molecules from photodissociation, we find that most of the sulfur is SO2 at regions near the midplane. Silicon and iron are ionized through most of the disk and are neutral only in denser disks.
where there is sufficient shielding from photoionization. Limited silicon chemistry is included in our models, and we find that silicon is ionized through most of the disk. For more massive disks with \( M_{\text{gas}} > 0.1 M_\odot \), silicon is atomic in dense regions, such as near the midplane, but does not turn molecular even for our most massive disks.

\( \text{S} \) i, Si ii, Fe ii, and H\(_2\) S(0) all have their first excitation level \( \sim 500 \) K above ground and are excited under similar conditions. The gas needs to be warm, \( \gtrsim 100 \) K for emission from these lines, to be strong. Note that sulfur is a much stronger coolant than \( \text{H}_2 \), although both species have similar excitation energies. At disk gas densities, these coolants are in LTE, so their cooling is proportional to their abundance times their spontaneous transition probability. Although the abundance of sulfur is 4.5 orders of magnitude lower than that of \( \text{H}_2 \), its spontaneous transition probability is \( 4.7 \times 10^7 \) that of \( \text{H}_2 \) S(0). Thus, at high densities, and assuming the lines are optically thin, \( \text{S} \) i 25.23 \( \mu \)m should dominate \( \text{H}_2 \) 28 \( \mu \)m by a factor \( \sim 1000 \). In fact, the \( \text{S} \) i 25 \( \mu \)m transition is optically thick, so the \( \text{S} \) i 25 \( \mu \)m line is typically \( \sim 10 \) times the \( \text{H}_2 \) line strengths. Cooling from \( \text{S} \) i decreases as the gas temperature decreases, and in the outer disk the most important coolants are CO and O i at the midplane and O i at the surface where CO is photodissociated.

### 4.3. Disk Emission and Spectrum

Figure 8 shows a model spectrum for this standard disk at a distance of 30 pc, with the dominant lines in the 5–40 \( \mu \)m band, superposed on the dust continuum. (The resolution of Spitzer IRS in the high-resolution mode (\( R = 600 \)) has been assumed for computing the emission spectra.) The lines shown in the emission spectrum are strong enough for nearby sources (\( \lesssim 100 \) pc) to be potentially observable by the Spitzer Space Telescope or future infrared telescopes, such as SOFIA or Herschel. The IRS instrument on the Spitzer Space Telescope has a 3 \( \sigma \) flux detection limit of \( \sim 10^{-18} \) W m\(^{-2}\), with an integration time of \( \sim 500 \) s.

The \( \text{S} \) i 25.23 \( \mu \)m line stands out as a strong coolant in our disk spectrum and as an important diagnostic of the presence of gas at \( \sim 1 \) AU in disks. The possible detection of gas disks in sulfur is one of our main results, as in many cases this line dominates the spectrum and is stronger than the \( \text{H}_2 \) lines. The [O i] 63 \( \mu \)m and [S i] 56.0 \( \mu \)m lines may also be strong enough for detection by SOFIA. Other detectable lines in this figure are the \( \text{H}_2 \) S(1) and S(2) lines, the [Fe ii] 26.0 \( \mu \)m line, the [Si ii] 34.8 \( \mu \)m line, and water lines at 33 \( \mu \)m (ortho-H\(_2\)O, \( 6_0^1 \rightarrow 5_0^0 \)) and 36 \( \mu \)m (ortho-H\(_2\)O, \( 6_2^2 \rightarrow 5_1^1 \)).

Figure 9 shows a similar spectrum for a disk with an inner radius of 10 AU, which is seen to have no strong OH or H\(_2\)O lines but has detectable \( \text{H}_2 \) S(1), \( \text{H}_2 \) S(2), [S i] 25.23 \( \mu \)m, [Fe ii] 26 \( \mu \)m, and [Si ii] 34.8 \( \mu \)m lines. The effect on the gas of changing the inner disk radius is discussed in more detail in § 5.2.

Table 2 lists the observable mid-infrared and far-infrared lines with their wavelengths and the telescope instruments that can observe them.

Gas emission lines are potentially important diagnostic tools of physical and chemical conditions of gas in disks and could be useful in detecting even very small amounts of gas. However, most of these lines are optically thick, with the exception of \( \text{H}_2 \) S(0), and would correspondingly diminish in strength with the inclination of the disk, being the strongest for a face-on orientation. Molecular hydrogen remains optically thin in the S(0) 28 \( \mu \)m line, and the line strength is not affected by the orientation angle of the disk. Moreover, it is less dependent on the chemical network and the cosmic abundances assumed and directly traces the gas in the disk. However, the \( \text{H}_2 \) S(0) line is weaker than other gas emission lines and hence is more difficult to detect. For pure sensitivity
TABLE 2  
**Infrared Emission Lines, Their Wavelengths, and Observing Instruments**

| Species | $\lambda$ (\textmu m) | Transition | Telescope Instruments |
|---------|------------------|----------|-----------------|
| H$_2$ S(2) | 12.3 | ... | Spitzer IRS, SOFIA EXES |
| H$_2$ S(1) | 17.0 | ... | Spitzer IRS, SOFIA EXES |
| H$_2$ S(0) | 28.2 | ... | Spitzer IRS, SOFIA EXES |
| OH......... | 15–200 | ... | Spitzer IRS, SOFIA EXES, GREAT, SAFIRE, Herschel SPIRE |
| H$_2$O..... | 15–200 | ... | Spitzer IRS, SOFIA EXES, GREAT, SAFIRE, Herschel SPIRE |
| Fe i......... | 24.0 | $^2$$D_{5/2}$–$^2$$D_{3/2}$ | Spitzer IRS, SOFIA EXES |
| Si i......... | 25.2 | $^3$$P_{1/2}$–$^3$$P_{3/2}$ | Spitzer IRS, SOFIA EXES |
| Fe ii........ | 26.0 | $^6$$D_{9/2}$–$^6$$D_{7/2}$ | Spitzer IRS, SOFIA EXES |
| Si ii........ | 34.8 | $^2$$P_{3/2}$–$^2$$P_{1/2}$ | Spitzer IRS |
| Fe i......... | 34.2 | $^3$$D_{3/2}$–$^3$$D_{1/2}$ | Spitzer IRS |
| Fe ii........ | 35.4 | $^6$$D_{7/2}$–$^6$$D_{5/2}$ | Spitzer IRS |
| Si i......... | 56.6 | $^3$$P_{0}$–$^3$$P_{1}$ | SOFIA FIFI-LS |
| O i......... | 63.1 | $^3$$P_{1}$–$^3$$P_{2}$ | SOFIA FIFI-LS, GREAT, Herschel PACS |
| Fe ii........ | 145.6 | $^3$$P_{3}$–$^3$$P_{1}$ | SOFIA SAFIRE, GREAT, Herschel SPIRE |
| C ii......... | 157.7 | $^2$$P_{3/2}$–$^2$$P_{1/2}$ | SOFIA SAFIRE, GREAT, Herschel SPIRE |
| C i......... | 369.0 | $^3$$P_{2}$–$^3$$P_{1}$ | SOFIA CASIMIR, SAFIRE, Herschel HIFI |
| H i......... | 609.2 | $^3$$P_{1}$–$^3$$P_{0}$ | SOFIA SAFIRE, Herschel HIFI |

The $S(1)$ and $S(2)$ lines of H$_2$ arise from gas with temperatures $\gtrsim 150$–$200$ K, whereas S(0) emission has a significant contribution from slightly cooler gas ($T \gtrsim 100$ K). At very low gas masses ($10^{-3}$ $M_J$), the midplane column density through the disk is $\sim 10^{23}$ cm$^{-2}$ and hence low enough to allow penetration by stellar UV and X-ray photons through much of the inner disk and to photodissociate H$_2$. The low amount of warm H$_2$ gas results in very low line strengths of all three H$_2$ lines, as can be seen in Figure 10. As the disk gas mass is increased to $10^{-2}$ $M_J$, the column density increases, allowing shielding of H$_2$, increasing its abundance in the inner, warm regions of the disk. The gas in the inner disk, where the emission from the S(1) and S(2) lines peaks, is heated by collisions with dust, H$_2$ formation heating, and by X-rays. The increased amounts of warm H$_2$ gas ($\gtrsim 100$ K) result in a sharp increase in the line strengths. As the gas mass is further increased to 0.1 $M_J$, the gas temperature at a fixed radial column density initially decreases because the H$_2$O cooling rises faster than the X-ray heating with density. Thus, there is less mass and surface area of warm gas. As the gas mass increases to 0.2 $M_J$, the gas heating by dust-gas collisions is negligible. At very low gas masses, the observed H$_2$ S(0) emission directly correlates with the mass of warm gas in the disk, regardless of the dust or total gas masses, and the warm gas ($T \gtrsim 100$ K) mass in a disk at 30 pc needs to be above $\sim 10^{-3}$ $M_J$ for detection by the Spitzer Space Telescope. At higher gas masses, $\sim 1 M_J$, dust collisions are the main heating mechanism that heat H$_2$ gas. In these relatively massive disks, H$_2$ line emission does not increase proportionately with mass, as the lines start to become optically thick at disk gas masses $\gtrsim 0.05 M_J$ for S(1) and S(2) and $\gtrsim 0.2 M_J$ for S(0). Figure 10 shows that for line luminosities $\sim 5 \times 10^{-8}$ $L_{\odot}$, the luminosity generally scales with a low power ($<1$) of gas mass. This means that for disks at distances $d \gg 30$ pc, considerably more gas mass is required for detection than if $L \propto M_{gas}$ is assumed. This important point is discussed more in $\S$ 6.

An increase in total dust mass of the disk produces increased emission because of an increase in heating of the gas.

to the presence of small amounts of gas at $r \sim 1$–2 AU, the [S i] 25.23 $\mu$m line is predicted to be the best probe.

5. PARAMETER SURVEY AND EMISSION-LINE DETECTABILITY

5.1. Variation of Spectra with $M_{gas}$ and $M_{dust}$

We have conducted a parameter survey to explore the probability of gas emission line detection above the dust continuum emission for a range of gas masses and dust masses and for a range of stellar and disk parameters (Table 3). We limit the range of parameters to those that might give us detectable infrared line fluxes and those whose dust optical depths $\tau_r \lesssim 5$. Figure 10 shows the change in IR line luminosities due to variations in gas and dust masses. For a disk at a distance of 30 pc, the flux detection limit of the IRS (high resolution) instrument on Spitzer for a 3 $\sigma$ 500 s detection corresponds to a line luminosity of $\sim 3 \times 10^{-8}$ $L_{\odot}$ (or $10^{-18}$ W m$^{-2}$). For comparison, SOFIA at these wavelengths ($10^{-28}$ $\mu$m) has a minimum detectable 3 $\sigma$ line flux of $10^{-17}$ W m$^{-2}$ ($3 \times 10^{-7}$ $L_{\odot}$), and Herschel, $\sim 7 \times 10^{-18}$ W m$^{-2}$ ($2 \times 10^{-7}$ $L_{\odot}$) at its shortest observing wavelengths (60–200 $\mu$m). Instruments on both telescopes have resolving powers $\sim 10^{3}$–$10^{4}$.

Figure 11 presents these results in an alternate way, which readily shows the parameter space where lines are detectable.

TABLE 3  
**Parameter Range for Disk Model**

| Parameter | Range |
|----------|-------|
| Gas mass | $10^{-3}$ to 1 $M_J$ |
| Inner radius $r_i$ | 0.3–10 AU |
| Outer radius $r_o$ | 20 AU |
| Surface density power-law index $\alpha$ | 0.5–2.0 |
| Stellar X-ray luminosity | $10^{-2}$ to $10^{-5}$ $L_{\odot}$ |
| Dust mass | $10^{-7}$ to $10^{-4}$ $M_J$ |
| Minimum grain size $a_{min}$ | 0.1–10.0 $\mu$m |
| Maximum grain size $a_{max}$ | 1.0 mm |
| Grain size distribution index $s$ | 3.5 |
| Stellar temperature $T_*$ | 4500 and 5780 K |
via gas-dust collisions. Dust collisions are an important heating mechanism in the bulk of the H$_2$-emitting regions. As the dust mass is decreased, the decreased coupling between gas and dust lowers the gas-heating rate and the gas temperature and therefore the emission. On the other hand, dust produces IR continuum emission, which can obscure the detection of infrared lines (typically, systematics introduce baseline variations that make it impossible to detect lines at the less than around a few percent continuum level). There is thus an optimal gas-to-dust mass ratio $\sim 10^3$ to $10^5$ and gas mass $\geq 10^{-2}M_J$ (for disks at 30 pc) where H$_2$ emission can be detected. Given $\geq 10^{-2}M_J$ of total gas mass, a gas-to-dust mass ratio $\leq 100$ produces a line-to-continuum ratio of $\leq 5\%$ for the highest Spitzer Space Telescope resolving power ($R = 600$), rendering the line difficult to detect above the strong continuum. On the other hand, if the dust abundance is lowered to the point where the gas-to-dust ratio is $\geq 10^5$, then the grain-gas collisional heating is so drastically reduced that the gas is cold, and the H$_2$ lines are too weak to detect in the absence of other gas-heating mechanisms.

The S i, Fe ii, and Si ii emission line strengths are complicated by chemistry in the disk. For disks of low gas mass ($10^{-3}$ to $10^{-2}M_J$), the main sulfur species in the denser regions near the midplane of the disk is atomic sulfur, and sulfur is photoionized near the surface. Iron and silicon are completely ionized throughout such disks. In this low gas mass limit, the emission increases as the gas mass increases and as the dust mass increases. A higher dust mass in general implies more heating through gas-grain collisions and hence warmer gas. As the gas mass increases to 0.1 $M_J$ or higher, the main sulfur-bearing species near the midplane is SO$_2$, as sulfur turns molecular at these high densities and opacities. Here most of the atomic sulfur is in a layer above the midplane where there is enough penetration of stellar radiation to photodissociate SO$_2$ but not sufficient to ionize sulfur. Similarly, chemistry also affects the Fe ii and Si ii lines, as there are substantial amounts of neutral iron and silicon in the denser regions (i.e., near the inner midplane) of the more massive disks. The S i line is optically thick for all the gas masses considered here, and at higher gas masses, the line luminosity is approximately independent of mass. There is a slight increase in the line strength at $10^{-2}M_J$, as X-rays also contribute to the gas heating making the gas warmer, and a sharp decrease at lower gas masses, as sulfur gets ionized because of lower column densities.
For the minimum detectable gas mass for different dust masses in the disk for each dusty) disks. Emission from the \([C_20]r\) lines get optically thick for gas masses of mass: the lines get optically thick for gas masses \(\text{in} \), making them strong coolants. OH is a strong coolant when the gas temperature is high (around a few hundred kelvins), and OH line emission mostly arises from the dense, hot inner disk where H\(_2\)O photodissociates to OH more readily. Cooling by H\(_2\)O dominates in the dense equatorial regions of these massive disks at all radii, but the emission is spread in various lines in the mid-IR, only some of which lie in the Spitzer Space Telescope band from 10 to 37 \(\mu\)m. The abundance of lines also implies that the cooling luminosity is distributed over many lines, which reduces the strength of each individual line. Table 4 lists the strongest infrared line luminosities of the ortho- and para-H\(_2\)O species and OH for a disk with a gas mass of \(0.1 M_J\) and dust mass of \(10^{-5} M_J\), with all other parameters having their fiducial values.

5.2. Variation of Spectra with Other Parameters

The position of the inner radial cutoff, \(r_i\), is an important parameter that can alter the observed strength of emission lines. We have run cases with four different values of this inner radius equal to 0.3, 1.0, 3.0, and 10 AU from the central star, keeping all other parameters identical to our standard disk model (see Fig. 12). Disks with smaller inner holes have a small mass of hotter, denser gas that lies closer to the central star and might be expected to have increased line luminosities as compared to disks with large inner holes. However, larger inner holes increase the gas mass heated and chemically altered by X-rays and UV, so the situation is in fact more complicated. The fluxes for all the lines (except \([Fe \ i]\) are seen to drop when the inner radius is decreased from 1 to 0.3 AU. The higher disk densities in the inner disk cause sulfur to turn molecular and reduce the ionization of iron and silicon. With lower abundances of S, Fe, and Si and a smaller surface area of warm gas, their line luminosities correspondingly decrease. The line luminosity from the \([Fe \ i]\) line, however, increases because of a higher abundance of neutral iron. The strength of the H\(_2\) lines is also seen to decrease slightly, and this is due to lower masses of \(\geq 100\) K H\(_2\) gas for the \(r_i = 0.3\) AU disk because of effective self-shielding from UV and X-rays. When the disk inner radius is increased from 3 to 10 AU, emission from all the lines except \([Si \ i]\) and H\(_2\) S(0) increases again. A disk with such a large inner radius has a significantly low radial column density \(\sim 4 \times 10^{23} \text{cm}^{-2}\) through the midplane) so that X-rays more effectively penetrate the disk and now dominate gas-grain collisions as the main heating mechanism. The enhanced emission in most of the lines is due to a higher gas temperature due to X-ray heating through most of the disk. Emission from the \([Si \ i]\) lines is seen to decrease, however, and this is because of a higher ionization rate of sulfur, which lowers the atomic sulfur abundance and lowers the effective area of warm \([Si \ i]\) gas relative to a disk with a smaller inner disk radius.

Variations in the surface density power-law profile (Fig. 13) have effects on the line intensities similar to those of changing \(r_i\). The amount of warm gas in the inner regions is sensitive to the power-law index \(\alpha\), and for a steeper power law there is more mass in the inner region as compared to a shallower surface-density profile. We have considered three different power-law indices, \(\alpha = 0.5, 1, 1.5\). For the largest value of \(\alpha\), there is a decrease in the strength of the \([Si \ i]\) 34.8 \(\mu\)m and \([Fe \ i]\) 26 \(\mu\)m lines, as the increased densities in the inner regions increase the shielding of these species from photoionization, and their abundances decrease. Correspondingly, the \([Fe \ i]\) 24 \(\mu\)m line increases sharply for large \(\alpha\).
The X-ray luminosity of the star was taken to be $10^{-4}$ times the bolometric luminosity in the standard case, as is typical for a wTTS or more evolved stars (Feigelson et al. 2003). However, this value may be higher or lower depending on the age of the star and other factors, and we have run cases where we assume an X-ray luminosity of $10^{-5}$ to $10^{-3}$ times the bolometric luminosity. The X-ray spectrum is assumed to remain the same, peaking at around 2 keV and ranging from 0.5 to 10 keV. The X-ray luminosity has surprisingly little effect on the Spitzer Space Telescope lines as can be seen from

| Species | $\lambda$ (µm) | Line Luminosity ($L_{\odot}$) |
|---------|----------------|-------------------------------|
| OH      | 30.54          | $9.8 \times 10^{-8}$          |
|         | 30.63          | $1.0 \times 10^{-7}$          |
|         | 33.80          | $1.4 \times 10^{-7}$          |
|         | 33.93          | $1.4 \times 10^{-7}$          |
|         | 37.01          | $1.8 \times 10^{-7}$          |
|         | 37.08          | $1.8 \times 10^{-7}$          |
|         | 38.84          | $7.7 \times 10^{-7}$          |
|         | 38.88          | $6.5 \times 10^{-7}$          |
| o-H$_2$O| 21.15          | $2.6 \times 10^{-7}$          |
| p-H$_2$O| 21.17          | $2.6 \times 10^{-7}$          |
| o-H$_2$O| 21.18          | $3.0 \times 10^{-7}$          |
| p-H$_2$O| 21.18          | $3.0 \times 10^{-7}$          |
| o-H$_2$O| 21.85          | $3.1 \times 10^{-7}$          |
| p-H$_2$O| 21.89          | $2.7 \times 10^{-7}$          |
| o-H$_2$O| 23.19          | $3.0 \times 10^{-7}$          |
| p-H$_2$O| 23.90          | $3.2 \times 10^{-7}$          |
| o-H$_2$O| 25.17          | $2.9 \times 10^{-7}$          |
| p-H$_2$O| 25.22          | $3.1 \times 10^{-7}$          |
| o-H$_2$O| 25.94          | $4.0 \times 10^{-7}$          |
| p-H$_2$O| 25.98          | $3.1 \times 10^{-7}$          |
| o-H$_2$O| 27.03          | $3.1 \times 10^{-7}$          |
| p-H$_2$O| 27.99          | $3.1 \times 10^{-7}$          |
| o-H$_2$O| 28.59          | $2.7 \times 10^{-7}$          |
| p-H$_2$O| 28.59          | $2.7 \times 10^{-7}$          |
| o-H$_2$O| 28.91          | $2.7 \times 10^{-7}$          |
| p-H$_2$O| 29.36          | $2.7 \times 10^{-7}$          |
| o-H$_2$O| 29.84          | $3.0 \times 10^{-7}$          |
| p-H$_2$O| 29.88          | $2.9 \times 10^{-7}$          |
| o-H$_2$O| 30.47          | $2.6 \times 10^{-7}$          |
| p-H$_2$O| 30.53          | $2.7 \times 10^{-7}$          |
| o-H$_2$O| 30.53          | $2.8 \times 10^{-7}$          |
| p-H$_2$O| 30.87          | $2.5 \times 10^{-7}$          |
| o-H$_2$O| 30.90          | $3.4 \times 10^{-7}$          |
| p-H$_2$O| 31.74          | $2.5 \times 10^{-7}$          |
| o-H$_2$O| 33.00          | $2.9 \times 10^{-7}$          |
| p-H$_2$O| 33.01          | $3.0 \times 10^{-7}$          |
| o-H$_2$O| 34.40          | $2.0 \times 10^{-7}$          |
| p-H$_2$O| 34.55          | $2.7 \times 10^{-7}$          |
| o-H$_2$O| 35.43          | $2.7 \times 10^{-7}$          |
| p-H$_2$O| 35.47          | $3.2 \times 10^{-7}$          |
| o-H$_2$O| 35.67          | $2.2 \times 10^{-7}$          |
| p-H$_2$O| 35.90          | $2.9 \times 10^{-7}$          |
| o-H$_2$O| 36.21          | $2.7 \times 10^{-7}$          |
| p-H$_2$O| 66.44          | $2.6 \times 10^{-7}$          |
| o-H$_2$O| 75.38          | $3.6 \times 10^{-7}$          |
| p-H$_2$O| 100.98         | $8.1 \times 10^{-7}$          |
| o-H$_2$O| 108.07         | $3.3 \times 10^{-7}$          |
| p-H$_2$O| 138.53         | $5.9 \times 10^{-7}$          |
| o-H$_2$O| 179.53         | $2.2 \times 10^{-7}$          |

Figure 14. The line luminosities seem largely insensitive to the amount of X-ray flux, and this can be understood by referring to the temperature structure (Figs. 5 and 6) for the standard case. The X-rays only penetrate and heat a very small fraction of the mass of the disk, and in these regions, most of the heating is carried away as infrared emission from dust and by the [O i] 63 µm line. The strength of this line correlates with the X-ray flux, as it comes mostly from the upper surface regions of the inner disk where the gas is warm and heated by X-rays (see Fig. 6).

Figure 13. Changes in the line luminosities due to variations in the slope of the power-law index $\alpha$ of the surface density distribution.
The infrared line emission from gas is quite sensitive to the stellar flux, with stronger emission from gas disks around more luminous stars. We have run our disk models for two different stellar types, a G2 star and a K4 star. In both cases, all disk parameters were the same, and the X-ray luminosity in both cases was $10^{34}$ ergs s$^{-1}$. With lower X-rays and UV flux and with the dust grains around the less luminous K star being colder, the gas temperature is much lower in the disk around the K4 star. Consequently, the line emission strengths are correspondingly lower (Fig. 15). The [S\textsc{i}] 25.23 \mu m, [Si \textsc{ii}] 34.8 \mu m, [Fe \textsc{ii}] 26 \mu m, and [O \textsc{i}] 63 \mu m lines may still be strong enough for detection by the \textit{Spitzer Space Telescope} and SOFIA for disks at $d \leq 30$ pc, especially if the X-ray luminosities are higher than average.

Lowering the minimum grain size in the dust distribution increases line emission, as can be seen from Figure 16. In our standard case, the minimum grain size $a_{\text{min}}$ was chosen to be 1 \mu m, and we have run cases where the minimum grain size was 0.1 and 10 \mu m. Smaller dust grains are less efficient at reradiating stellar radiation and get hotter as the grain size decreases. In addition, for a fixed dust mass and $s = 3.5$, the grain surface area is proportional to $a_{\text{min}}^{-1/2}$, and therefore decreasing $a_{\text{min}}$ increases the surface area. Both of these effects raise the gas temperature, since the gas heating is largely by gas-grain collisions and this heating rate is proportional to $T_{\text{dust}} - T_{\text{gas}}$ and the dust surface area. The resultant higher gas temperatures raise the total infrared line emission from the disk.

In all our models, we did not allow the formation of H$_2$ on dust grains. It is not clear whether hydrogen atoms stick on warm dust grains long enough to allow the formation of H$_2$ (Cazaux & Tielens 2002), and we have run the standard model in which we allow the grain formation of H$_2$. We find that there are no significant differences in the resultant spectrum of the disk in the two cases. Even when grain formation of H$_2$ is set to zero, H$_2$ is formed efficiently by reactions with H$^-$ and by three-body reactions.

6. DISCUSSION, SUMMARY, AND CONCLUSIONS

We have modeled the \~0.3–20 AU regions of “intermediate-aged” and “debris” disks with a range of dust masses $10^{-7}$ to $10^{-4}$ $M_J$ (or $f_d = L_{IR}/L_{bol} = 10^{-4}$ to $10^{-1}$) and gas masses $10^{-3}$ to 1 $M_J$. We define dust as grains with size $a \leq 1$ mm, and, assuming a size distribution $n_{\text{dust}}(a) \propto a^{-3.5}$, we find that these disks are reasonably optically thin to starlight for $M_{\text{dust}} < 10^{-4} M_J$. Therefore, we have covered all of parameter space relevant to intermediate-aged and debris disks with sufficient gas and dust to be detected in IR emission lines in...
the next decade by observatories such as the *Spitzer Space Telescope*, SOFIA, and *Herschel*.

Although the dust is optically thin to stellar photons, the gas is optically thick at UV and X-ray wavelengths. Therefore, we find that the dominant gas-heating mechanism for the bulk of the gas, which is shielded from heating by UV or X-rays by gas in the inner regions or at the surface, is gas-dust collisions. In these regions the dust is heated by stellar photons and colder gas is heated by collisions with warmer dust grains. However, at the surface of the disk and at the inner edge of the disk (assuming a hole or a gap between disk and star), the UV and X-rays heat the gas, and the gas temperature can exceed the temperature of even the smallest grains. We find that the gas temperature in the 0.3–20 AU regions of debris disks ranges from \(\sim 1000\) to \(\sim 50\) K.

The chemistry in the innermost regions and at the surface of the disk is dominated by photodissociation and photodissociation caused by UV and X-rays. However, in the cooler, shielded regions the chemistry is dominated, like interstellar cloud chemistry, by ion-neutral reactions with ionization by cosmic rays, UV, and X-rays. We assume that at \(r < 20\) AU, the grains are too warm (\(T_{\text{dust}} \gtrsim 100\) K) to support icy mantles or to allow surface catalysis of \(H_2\). However, \(H_2\) is still efficiently formed by the reaction of \(H\) with \(H^-\) and by three-body reactions. In warmer regions (\(T_{\text{gas}} \gtrsim 300\) K) neutral-neutral reactions with activation barriers become important, with the general result of enhanced production of \(OH\) and \(H_2O\). In addition, the reaction of \(O\) with \(H_2\) to form \(OH\) can dominate the destruction of the \(H_2\) molecule. Photodissociation of molecules by UV photons plays a large role in molecular destruction and creation of ions such as \(Fe^+\) and \(Si^+\). We find that sulfur is \(S^+\) at the disk surface, \(S\) at intermediate gas opacities, and \(SO_2\) in regions well shielded by overlying gas opacity. Because \(H_2\) and \(CO\) so readily self-shield and are shielded by atomic \(C\), we find that for cases with sufficient gas mass to be detected (\(M_{\text{gas}} \gtrsim 10^{-2}\) \(M_J\)), the bulk of hydrogens is \(H_2\) and the bulk of carbon is \(CO\) in the disks. Unlike in the case of interstellar clouds, the carbon becomes \(CO\) before the hydrogen becomes \(H_2\) as one moves to greater depths from the disk surface, a result caused by the lack of production of \(H_2\) on grain surfaces in the warm disk regions.

Surprisingly, we find that the strongest mid-IR line is [S i] 25.23 \(\mu\)m. This results from the high value of the product of its abundance times its spontaneous decay rate (or \(A\) value). We find that [S i] is a strong coolant in the inner disk for all our disk models with various input parameters. We have included detailed sulfur chemistry to determine the abundance of atomic sulfur in the disk, and emission is strong enough for detection even when substantial amounts of gas have turned molecular (mainly \(SO_2\)). The total mass of gas in disks is a little more difficult to obtain from measurements of the [S i] 25.23 \(\mu\)m line alone, as the amount of neutral atomic sulfur is affected by the chemistry of the disk. In addition, the [S i] line tends to be optically thick and therefore not sensitive to the total gas mass.

Other strong mid-IR lines include [Si ii] 34.8 \(\mu\)m, [Fe i] 26 \(\mu\)m, [Fe i] 24 \(\mu\)m, and OH and \(H_2O\) rotational transitions. We assume depleted gas-phase silicon and iron abundances (see Table 5, Appendix A) similar to ice-free regions of the ISM. However, we have no iron chemistry in our models other than ionization and recombination. We do include more chemistry for silicon and consider some molecular species of Si, such as \(SiO\) and \(SiH_2\). However, the abundances of the silicon molecules are calculated to be very low, primarily because of photodissociation. In disks with low gas masses (\(M_{\text{gas}} \lesssim 10^{-2}\) \(M_J\)), Si and Fe are ionized through most of the disk, and the line intensities we compute are probably reasonably accurate even though we do not treat the chemistry of these species in detail. In disks with higher gas masses, Si and Fe are shielded from photodissociation and the [Fe i] 24 \(\mu\)m line becomes strong. The \(OH\) and \(H_2O\) lines become detectable at relatively high gas masses, \(M_{\text{gas}} \gtrsim 10^{-2}\) \(M_J\).

Pure rotational \(H_2\) lines such as S(0) 28 \(\mu\)m and S(1) 17 \(\mu\)m are roughly an order of magnitude weaker than the [S i] 25.23 \(\mu\)m line. The highest spectral resolving power of the *Spitzer Space Telescope* is \(R \approx 600\), and this modest resolution makes it difficult to detect weak mid-IR (10–37 \(\mu\)m) lines in the presence of strong (dust) mid-IR continuum. Detection of the relatively weak \(H_2\) lines above the dust continuum requires a relatively large ratio (\(\gtrsim 1000\)) of gas mass to dust mass. Such large ratios are possible at a transition epoch (\(\sim 10^7\) yr) when much of the dust mass has coagulated into particles of sizes \(a \approx 1\) mm, but the gas has not yet appreciably dispersed.

Most of the *Spitzer Space Telescope* high spectral resolution emission arises from gas at \(r \lesssim 5\) AU in our models, whereas longer wavelength (lower excitation) emission such as from low to mid-J \(CO\) lines and O i 63 \(\mu\)m has significant contribution from gas at \(r \gtrsim 5\) AU. The O i line arises from the entire disk and is a good probe of the conditions throughout the disk. While the mid-IR lines observable by the *Spitzer Space Telescope* are insensitive to the strength of the X-ray flux, the intensity of the [O i] 63 \(\mu\)m line does increase with the X-ray luminosity. SOFIA is capable of observing this transition and may be able to detect smaller amounts of gas in disks around stars that are strong X-ray sources. Our models indicate that CO emission is strong enough to be detectable, and it is a strong coolant in the outer cold regions of the disk. CO line luminosities are \(\sim 10^{-9}\) \(L_\odot\) in the 2 \(\rightarrow\) 1 line and \(\sim 10^{-7}\) \(L_\odot\) in the higher 15 \(\rightarrow\) 14 transition for our fiducial disk. Higher J transitions of CO in the far-infrared and the submillimeter wavelength regions can be easily detected by *Herschel* and can reveal the extent of the gas disk.

Line ratios are also diagnostic of the gas characteristics. The [Fe i] 24 \(\mu\)m line is only strong when there is high shielding (or high columns and densities) in the inner disk regions. This requires either high gas masses, steep surface density distributions, small inner holes, or a combination of these. The Fe i/S i ratio is especially suited to probing these parameters. Significant amounts of [O i] 63 \(\mu\)m and CO (\(J = 15 \rightarrow 14\)) 187 \(\mu\)m radiation emanate from regions \(r \gtrsim 5\) AU, in contrast to the S i or \(H_2\) 17 \(\mu\)m lines. Therefore, the ratios [O i] 63 \(\mu\)m/S i, [O i] 63 \(\mu\)m/\(H_2\) 17 \(\mu\)m, and CO 187 \(\mu\)m/\(H_2\) 17 \(\mu\)m are sensitive to the relative masses of gas at \(r \lesssim 5\) AU compared with that at \(r \gtrsim 5\) AU. In other words, these ratios are sensitive to the steepness of the surface density distribution.

The overall strength of the mid-IR lines primarily depends on the mass of warm (\(T \gtrsim 100\) K) gas, which typically lies within 5 AU of the central star. Disks with more total gas mass, with smaller inner holes, or with steeper surface density distributions produce stronger mid-IR emission. Because gas-dust collisions mainly heat the bulk of the gas, the line emission also increases either with greater dust mass or, holding dust mass fixed, with smaller minimum grain size \(a_{\min}\). In the latter case, the smaller size grains are warmer and have greater surface area than their larger counterparts and therefore heat the gas more vigorously.

As little as \(10^{-3}\) \(M_J\) of warm gas at \(r \lesssim 5\) AU can be detected by the *Spitzer Space Telescope* in the [S i] 25 \(\mu\)m line for
sources at \( \sim 30 \) pc from the Sun. However, to better diagnose the physical characteristics of the gas requires the detection of several lines, and this requires roughly an order of magnitude greater gas mass (\( \sim 10^{-2} M_J \)) at this distance. We emphasize that the line luminosities in the strongest lines ([Si i], [Si ii], [Fe ii], and [O i]) increase very slowly or even decrease with increasing gas mass (see Fig. 10). This is because the gas temperature in these disks is largely controlled by the dust temperature, which is independent of gas mass, and the gas emission lines at high gas mass become optically thick, so their luminosities saturate. Our results show that at the distance of Taurus (140 pc), even 1 \( M_J \) of gas in intermediate-aged optically thin dust disks could be difficult to detect. However, typical disks in Taurus are more likely to be younger and therefore abundant in small grains (\( a_{\text{min}} \sim 50 \) Å). A younger central star is also more luminous in FUV. This will lead to an increase in both collisional gas-grain heating (due to the larger surface area of small grains) and grain photoelectric heating, which will make the gas warmer and increase gas line emission significantly.

Assuming that we know the distance to the source, the X-ray and FUV luminosities of the central star, and the dust mass and dust distribution from the IR and submillimeter/millimeter continuum observations, we can readily constrain the gas properties by comparing the observed fluxes in various emission lines with our models. Ultimately, if the lines are spectrally resolved by high-resolution instruments on SOFIA or Herschel, the line profiles will also help constrain the gas dynamics and spatial distribution.

To conclude, we find exciting prospects for the detection by the Spitzer Space Telescope, SOFIA, or Herschel of infrared line emission from the gas in 0.3–20 AU regions of intermediate-aged disks at distances \( \leq 150 \) pc. The core accretion model of giant planet formation strongly suggests an epoch (\( t < 10^6 \)–\( 10^7 \) yr) when the dust in the 1–20 AU region is relatively optically thin, because of the growth of several earthmass cores, but when \( \geq 1 \) \( M_J \) of gas persists for an extended period. Therefore, the observations of line emission coupled with the models presented here will provide a measure of the evolution of gas in disks as they transition from planet-forming disks to the older, gas-free, debris disks and a test of the core-accretion scenario for gas giant planet formation. The presence of even small amounts of gas at times \( t \sim 10^7 \)–\( 10^8 \) yr has important effects on planet formation in the 0.3–20 AU region.

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**APPENDIX A**

**CHEMISTRY**

We adopt gas-phase abundances from Savage & Sembach (1996) toward the line of sight through a diffuse cloud to the star \( \zeta \) Oph. The abundances are listed in Table 5. Table 6 lists the atomic, ionic, and molecular species included in our chemical code. Reaction rates are mostly from the UMIST'99 database, except for some reactions that are listed in Table 7. Apart from those listed here, X-ray photoionization rates are calculated as described in Appendix D, and reactions involving polycyclic aromatic hydrocarbons and vibrationally excited \( \text{H}_2 \) are from TH85. The UV photoionization rates of atoms and molecules are calculated using their photoabsorption cross sections multiplied by the stellar flux and integrated over frequency.

**TABLE 5**

**Elemental Gas-Phase Abundances**

(from Savage & Sembach 1996)

| Element | Abundance |
|---------|-----------|
| He      | 0.1       |
| C       | \( 1.4 \times 10^{-4} \) |
| O       | \( 3.2 \times 10^{-4} \) |
| Si      | \( 1.7 \times 10^{-6} \) |
| Mg      | \( 1.1 \times 10^{-6} \) |
| Fe      | \( 1.7 \times 10^{-7} \) |
| S       | \( 2.8 \times 10^{-5} \) |

**TABLE 6**

**Chemical Species Included in the Models**

| \( \text{H} \) | \( \text{He}^+ \) | \( \text{C}^+ \) | \( \text{O}^+ \) | \( \text{H}_2 \) | \( \text{O}_2 \) | \( \text{OH} \) | \( \text{CO} \) | \( \text{H}_2\text{O}^+ \) | \( \text{HCO}^+ \) | \( \text{H}_3\text{O}^+ \) |
|-------------|----------------|-------------|-------------|-------------|-------------|-------------|-------------|----------------|----------------|----------------|
| \( \text{H}_2^+ \) | \( \text{He}^+ \) | \( \text{C}^+ \) | \( \text{O}^+ \) | \( \text{H}_2 \) | \( \text{O}_2 \) | \( \text{OH} \) | \( \text{CO} \) | \( \text{H}_2\text{O}^+ \) | \( \text{HCO}^+ \) | \( \text{H}_3\text{O}^+ \) |
| \( \text{Si} \) | \( \text{Si}^+ \) | \( \text{SiH}^+ \) | \( \text{SiH} \) | \( \text{SiO} \) | \( \text{Fe} \) | \( \text{Fe}^+ \) | \( \text{S} \) | \( \text{S}^+ \) | | |
| \( \text{SiO}^+ \) | \( \text{HOSi} \) | \( \text{H}^+ \) | \( \text{CH}_4 \) | \( \text{CH}_2 \text{CH}_2 \) | \( \text{HS}^+ \) | \( \text{H}_2\text{S} \) | \( \text{H}_2\text{S} \) |
| \( \text{HS} \) | \( \text{H}_2\text{S} \) | \( \text{CS} \) | \( \text{CS}^+ \) | \( \text{HCS}^+ \) | \( \text{HCS} \) | \( \text{OCS} \) | \( \text{OCS}^+ \) | \( \text{HOC} \) |
| \( \text{SO} \) | \( \text{SO}^+ \) | \( \text{HSO}^+ \) | \( \text{SO}_2 \) | \( \text{SO}_2 \text{H}_2\text{O}^+ \) | \( \text{H}_2\text{CS} \) | \( \text{H}_2\text{CS}^+ \) | \( \text{H}_2\text{CS}^+ \) |
is the total column density of the gas toward the source, \( n \) the absorption cross section. We obtain \( F \) given by

\[
L_{\text{b}} = \frac{4 \pi d^2}{4 \pi D^2} \left( \frac{1}{n_{\text{H}} f_b} \right) \int_{0.5}^{10} F(E) \sigma(E) n_{\text{H}} f_b dE \text{ ergs cm}^{-3} \text{ s}^{-1},
\]

where \( \sigma(E) \) is the total gas X-ray photoabsorption cross section per H nucleus, \( \tau_X \) is the X-ray optical depth given by \( \sigma(E) n_{\text{H}} \), \( n_{\text{H}} \) is the total column density of the gas toward the source, \( n_{\text{H}} \) is the number density, and \( f_b \) is the fraction of absorbed energy that goes into heating the gas. We also include secondary heating of X-rays due to photoionization from the \( n = 2 \) state of atomic hydrogen and follow exactly the treatment of Shang et al. (2002).

B2. X-RAY PHOTOABSORPTION CROSS SECTION \( \sigma(E) \)

We use the model of Wilms et al. (2000) for the X-ray photoabsorption cross section per H nucleus. They obtain the total photoionization cross section of the ISM by summing the cross sections of the gas, molecules, and grains. They use cosmic abundances for the various elements and add the contribution from grains. Our grains are large, and typical X-ray penetration depths are \( \sim 0.1 \mu m \), and therefore X-rays do not penetrate even our smallest dust grains. We use only the gas-phase abundances in our calculation of the cross section, and we adopt abundances from Savage & Sembach (1996) through a diffuse cloud toward the star \( \zeta \) Oph.

We correct Figure 1 of Wilms et al. (2000) to correspond to our depleted abundances and then fit a power law to find the absorption cross section. We obtain

\[
\sigma(E) = 1.2 \times 10^{-22} \left( \frac{E}{1 \text{ keV}} \right)^{-2.594}.
\]

Compare with the fit to the Wilms et al. (2000) cross section

\[
\sigma(E) = 2.27 \times 10^{-22} \left( \frac{E}{1 \text{ keV}} \right)^{-2.485}.
\]

B3. X-RAY PHOTOIONIZATION RATES OF ATOMS AND MOLECULES

The absorption cross section of a species \( i \) for ionization is approximated to be of the functional form

\[
\sigma_i(E) = \sigma_0 \left( \frac{E}{1 \text{ keV}} \right)^{\alpha}.
\]
We use the partial photoionization cross sections of Verner & Yakovlev (1995) and the fitting formulae they provide (Table 1 of their paper). These formulae for the cross sections in the range 0.5–10 keV are then fitted again with a power law of the above form for each neutral atomic species. In some cases, the cross section is fitted with a broken power law within this range. Table 8 lists the values of \( \sigma_0 \) in barns, \( \alpha \), and the energy ranges in keV where the fits are valid. The primary rate of photoionization is given by the integral of the photon number flux and the cross section

\[
\zeta_i = 6.25 \times 10^8 \int_{0.5}^{10} \sigma_i(E) \frac{F(E)}{E} e^{-\tau_X(E)} dE \text{ s}^{-1},
\]

where \( F(E) \) is in units of ergs s\(^{-1}\) keV\(^{-1}\) and the energy \( E \) is in keV. The attenuation factor \( \tau_X \) has the same definition as before and is equal to the product of the total photoabsorption cross section and the column density toward the source.

Secondary ionizations are important for hydrogen and helium. The fraction of primary electron energy going into secondary ionization is (Shull & van Steenberg 1985)

\[
\Phi_{\text{H}} = 0.391 \left( 1 - \frac{13.6}{E} \right) \approx 0.35,
\]

\[
\Phi_{\text{He}} = 0.0554 \left( 1 - \frac{24.6}{E} \right) \approx 0.05,
\]

where \( E \) is now in eV. The number of secondary photoionizations produced by a primary electron of energy \( E \) is equal to \( E \Phi_{\text{H}}/13.6 \) and \( E \Phi_{\text{He}}/24.6 \) for hydrogen and helium. The number of secondary ionizations by a photon of energy \( E \) is therefore 25.7\((E/1 \text{ keV})\) for hydrogen and 2.0\((E/1 \text{ keV})\) for helium. The total photoionization rates for hydrogen and helium are therefore

\[
\zeta_{\text{H},i} = 6.25 \times 10^8 \int_{0.5}^{10} \sigma_i(E) \frac{F(E)}{E} e^{-\tau_X(E)} (1 + 25.7E) dE \text{ s}^{-1},
\]

\[
\zeta_{\text{He},i} = 6.25 \times 10^8 \int_{0.5}^{10} \sigma_i(E) \frac{F(E)}{E} e^{-\tau_X(E)} (1 + 2.0E) dE \text{ s}^{-1},
\]

where \( E \) is in units of keV. We ignore secondary ionizations of all other species. Photoionization rates of molecules are assumed to be the sum of the rates of their constituent atoms, e.g., \( \zeta_{\text{OH}} = \zeta_O + \zeta_H \), etc. These integrals are numerically evaluated for each species with the expressions for the cross sections and the X-ray flux as a function of column \( N_{\text{H}} \) toward the star.

**APPENDIX C**

**GAS-HEATING MECHANISMS**

**C1. GAS-GRAIN COLLISIONS**

Dust grains in the optically thin disk are heated by the stellar radiation field, and collisional gas-grain energy transfer is often the dominant heating mechanism for the gas. The dust grain temperature is size dependent; smaller grains are less efficient at reradiating stellar light and are thus warmer than larger grains. Collisions of gas molecules with dust grains can either heat or cool...
the gas, depending on the gas and dust grain temperatures. Our treatment is similar to that of HM79 but adapted for an arbitrary grain size distribution. The net heating (or cooling) due to collisions is given by

$$\Gamma_1 = \alpha_T n_{H1} v_{\text{gas}} \sum_{a_{\text{min}}}^{a_{\text{max}}} \pi a^2 n_{\text{dust}}(a) [2k_B T_{\text{dust}}(a) - 2k_B T_{\text{gas}}] \text{ ergs cm}^{-3} \text{ s}^{-1},$$

where $\alpha_T = 0.3$ is the thermal accommodation coefficient (Burke & Hollenbach 1983); $n_{H1}$, the gas hydrogen nucleus number density; $v_{\text{gas}}$, the thermal velocity of the gas; $a$, the dust grain radius, which ranges from $a_{\text{min}}$ to $a_{\text{max}}$; $n_{\text{dust}}(a)$, the number density of particles of size $a$; and $T_{\text{dust}}(a)$ and $T_{\text{gas}}$, the temperatures of a dust grain of size $a$ and the gas, respectively.

C2. FUV PUMPING OF H$_2$ AND COLLISIONAL DEEXCITATION

H$_2$ molecules absorb FUV photons from the star and from the ISRF and are excited to a higher vibrational state. Subsequent deexcitation by collisions with H atoms and ground-state H$_2$ molecules deposits the excess energy as heat into the gas. H$_2$ molecules can also be directly photodissociated from the vibrationally excited state, which again leads to heating. (See TH85 for a detailed discussion.) The heating due to FUV pumping and collisional deexcitation is given by

$$\Gamma_2 = 3.18 \times 10^{-12} n(H_2) \left[ 10^{-12} T^{0.5} \exp \left( \frac{-1000}{T} \right) n(H) \right] + 1.4 \times 10^{-12} T^{0.5} \exp \left( \frac{-18}{T+1200} \right) n(H_2) \right]$$

$$+ G_{11.26} \left\{ 1.36 \times 10^{-23} [n(H_2) \beta_1(\tau) n(H_2)] / \beta_2(\tau) \right\}$$

$$+ 5.8 \times 10^{-24} n(H_2) \right\} \text{ ergs cm}^{-3} \text{ s}^{-1},$$

where $n(H_2)$ and $n(H_2^*)$ are the number densities of H$_2$ and vibrationally excited H$_2$, respectively, $\beta_1(\tau)$ and $\beta_2(\tau)$ are the corresponding self-shielding factors, and $G_{11.26}$ is the local photon energy flux in the range 11.26–13.6 eV (from the star and the ISRF, attenuated by dust and other gas species), normalized to the Habing flux in the same band ($2.26 \times 10^{-4}$ ergs cm$^{-2}$ s$^{-1}$). We use self-shielding factors for CO from van Dishoeck & Black (1988) and for H$_2$ from Draine & Bertoldi (1996).

C3. X-RAY HEATING

X-rays incident on gas photoionize atoms and molecules, and the primary electrons thereby generated are energetic enough to cause multiple secondary ionizations. The heating term arises from the thermalization of some of the energy of these secondary electrons and is proportional to the ionization rate due to X-rays. The heating due to X-rays is given by

$$\Gamma_3 = \int_{E_{\text{min}}}^{E_{\text{max}}} F(E) e^{-N_{H1} \sigma(E)} \sigma(E) n_{H1} f_h dE \text{ ergs cm}^{-3} \text{ s}^{-1},$$

where $F(E)$ is the X-ray photon flux, $N_{H1}$ is the hydrogen nucleus column density of gas toward the source, $\sigma(E)$ is the X-ray absorption cross section of the gas per hydrogen nucleus (see Appendix B), and $f_h$ is the fraction of energy that is converted to heat, equal to 0.1 for atomic gas and 0.4 for molecular gas. (See Maloney et al. 1996 for details.) We also include indirect heating by X-rays due to atomic hydrogen ionization, the recombinig H$^+$ resulting in a substantial $n = 2$ population of H because of the trapping of Ly$\alpha$ photons, followed by photoionization or collisional deexcitation of $n = 2$ hydrogen atoms (see Shang et al. 2002). We ignore X-ray scattering from the surface layer into the disk, as we estimate the contribution from this process to be negligible.

C4. GRAIN PHOTOELECTRIC HEATING

Energetic electrons emitted from dust grains due to the absorption of stellar FUV photons can collide with and heat the gas (Bakes & Tielens 1994). The efficiency of this process is dependent on the size of the dust grain and decreases with increasing grain size. As we consider large dust grains in our disk models, this process is not as efficient as in the ISM where small submicron-sized dust grains are abundant. The grain photoelectric heating term has been revised to include the effects of a cooler radiation field (stars of lower spectral type) and increased grain sizes. We use corrected grain photoelectric efficiencies from Weingartner & Draine (2001) and J. C. Weingartner (2002, private communication) for our calculations of grain photoelectric heating in disks.

$$\Gamma_4 = G_0 \sum_{a_{\text{min}}}^{a_{\text{max}}} n_{\text{dust}}(a) \pi a^2 \epsilon(T_{\text{FUV}}, a) \text{ ergs cm}^{-3} \text{ s}^{-1},$$

where $\epsilon$ is the photoelectric heating efficiency and is a function of the grain size $a$, the equivalent blackbody temperature of the stellar FUV flux $T_{\text{FUV}}$, and $G_0$ and $e_r$ (which determine the grain charge). The FUV flux spectrum from the star (Fig. 1) has a characteristic temperature $T_{\text{FUV}} \sim 10,000$ K. $G_0$ is the local stellar flux between 6.0 and 13.6 eV, normalized to the Habing flux. A similar term for the ISRF is also included, where $T_{\text{FUV}}$ is replaced by the temperature of the ISRF, 30,000 K, although this contribution is generally negligible.
C5. DRIFT HEATING

Dust grains and gas molecules are subject to different forces in the disks, with radiation pressure acting only on dust and gas being constrained by thermal pressure gradients. They could have different disk velocities and orbits, and this causes a viscous heating term that could be important in dense disks (Kamp & van Zadelhoff 2001; Takeuchi & Artymowicz 2001). We add drift heating to our disk models, although we do not solve for the disk orbital dynamics of the dust or gas. The heating due to drift is given by

\[
\Gamma_5 = 0.5 \mu_H n_H \sum_{a_{\text{min}}}^{a_{\text{max}}} n_{\text{dust}}(a) \pi a^2 v_{\text{drift}}(a) \text{ ergs cm}^{-3} \text{ s}^{-1},
\]

where \(v_{\text{drift}}(a)\) is the drift velocity between gas and a dust particle of size \(a\). We use the equations of Takeuchi & Artymowicz (2001) for the calculation of the drift velocity.

C6. HEATING DUE TO FORMATION OF H\(_2\)

We include heating due to the formation of H\(_2\) in our model. The formation of H\(_2\) either on grain surfaces or by reactions of H atoms with H\(^-\) leads to heating of the gas. The grain formation mechanism provides \(\sim 0.2\) eV of kinetic energy going into the newly formed H\(_2\) molecule and \(\sim 4.2\) eV of energy initially deposited as rovibrational internal energy of the molecule (Hollenbach et al. 1971). The reaction with H\(^-\) is an exothermic reaction that liberates \(\sim 3.53\) eV of energy, and we assume that most of this energy is initially in rovibrational internal energy of the molecule. Generally, in disks, the gas densities are much greater than the critical density \(n_c\) to deexcite the vibrationally excited H\(_2\) molecule. Therefore, the rovibrational energy is quickly converted into heat.

Grain formation of H\(_2\) is not included in our standard runs, and this heating mechanism is only included for the case in which we allow formation of H\(_2\) on grains. Heating due to formation of H\(_2\) by H\(^-\) is given by

\[
\Gamma_6 = 7.34 \times 10^{-21} n_H^2 x(H^-) x(H) \left( \frac{1}{1 + n_c/n_H} \right) \text{ ergs cm}^{-3} \text{ s}^{-1},
\]

where

\[
\frac{n_c}{n_H} = \frac{10^6 T^{-1/2}}{1.6x(H) \exp \left[-(400/T)^2\right] + 1.4x(H_2) \exp \left[-12,000/(T + 1200)\right]} \text{ cm}^{-3}
\]

and \(x(H), x(H^-),\) and \(x(H_2)\) are the abundances of H, H\(^-\), and H\(_2\), respectively (HM79). Heating due to formation of H\(_2\) on dust grains is given by

\[
\Gamma_7 = 4.8 \times 10^{-29} n_H^2 f_{\text{dust}} x(H) \left( 0.2 + \frac{4.2}{1 + n_c/n_H} \right) \text{ ergs cm}^{-3} \text{ s}^{-1},
\]

and \(f_{\text{dust}}\) is a factor that accounts for the change in dust surface area per H nucleus caused by changes in the size distribution and the gas-to-dust mass ratio as compared to interstellar values.

C7. COSMIC-RAY HEATING AND OTHER HEATING MECHANISMS

Apart from the processes discussed above, we consider cosmic-ray heating (\(\Gamma_8\)), photoionization of neutral carbon (\(\Gamma_9\); see TH85), and heating by the excitation of the [O i] 63 \(\mu\)m upper level by the IR continuum radiation field followed by the collisional deexcitation of this level (\(\Gamma_9\); see Appendix D).

\[
\Gamma_8 = 1.5 \times 10^{-11} \zeta n_H [x(H) + 2x(H_2)] \text{ ergs cm}^{-3} \text{ s}^{-1},
\]

where \(\zeta\) is the primary cosmic-ray ionization rate.

\[
\Gamma_9 = 4.16 \times 10^{-29} n_H x(C) G_{11.26} \exp \left(-3A_e - \frac{\tau_{11.26}}{\beta_c}\right) \text{ ergs cm}^{-3} \text{ s}^{-1},
\]

where \(x(C)\) is the abundance of neutral carbon, \(\tau_{11.26}\) is the optical depth due to gas absorption toward the star in the FUV band that photoionizes carbon, and \(\beta_c\) is a self-shielding factor (van Dishoeck & Black 1988). To this term we also add similar terms for the contribution from the ISRF, and use optical depths and self-shielding factors due to gas columns vertically up and down from the spatial position in the disk.
Gas cooling processes

Gas cooling occurs by gas-grain collisions when the gas is warmer than the dust (eq. [C1]) and by collisional excitation followed by line radiation of gaseous atoms, ions, and molecules. We essentially follow the treatment of TH85, in which the cooling due to a transition from level \( i \) to level \( j \) is given by

\[
\Lambda_{ij} = n_i \lambda_{ij} \left( \frac{1}{S_{ij}} \right) \frac{P_{ij}}{S_{ij}},
\]

where \( n_i \) is the population density of the species in level \( i \), \( \lambda_{ij} \) is the spontaneous transition probability, \( h \nu_j \) is the energy of the emitted photon, \( \tau_j \) is the optical depth in the line, and \( \beta_{esc}(\tau_j) \) is the associated escape probability; \( P_{ij} \) is the background radiation term, which consists of the sum of the cosmic microwave background radiation and the infrared emission from the dust grains of different temperatures at the wavelength of the transition. The source function \( S(\nu_j) \) is determined by solving for the level populations assuming statistical equilibrium. We generally assume that radiation can escape from any point in the disk either vertically up or down or radially out the inner radius. We calculate the column densities in each level of the cooling species in all three directions. From the column densities we determine the optical depth in the line and the escape probability of a photon, which then gives the cooling rate in a given line. If the gas temperature is lower than that of dust, and the background radiation stronger than the source function, the transition can heat the gas as the term \( 1 - \frac{P(\nu_j)}{S(\nu_j)} \) becomes negative. In this case, a background photon is absorbed by a particular species and subsequent collisional deexcitation transfers the excitation energy to gas heating.

We treat CO and H₂O cooling in a detailed multilevel calculation but treat OH and H₂O somewhat differently. Analytical approximations to multilevel line-cooling calculations of OH and H₂O are derived for use in the gas disk code. The full level population calculation was prohibitively expensive to include in the code, and instead, we derived analytic fits for the total cooling similar to HM79. For H₂O, we used collisional rate data for approximately 170 levels for both the ortho and para species and new approximations to multilevel line-cooling calculations of OH and H₂O are derived for use in the gas disk code. The full level population calculation was prohibitively expensive to include in the code, and instead, we derived analytic fits for the total cooling similar to HM79 that best fit the data, \( \sigma = 2.0 \times 10^{-15} \text{ cm}^{-2} \), \( E_0/K = 23.0 \text{ K} \), and \( A_0 = 6.0 \times 10^{-3} \text{ s}^{-1} \). The collisional rate data for OH for the first 45 levels are used to obtain the values, \( \sigma = 8.0 \times 10^{-16} \text{ cm}^{-2} \), \( E_0/K = 5.4 \text{ K} \), and \( A_0 = 7.6 \times 10^{-4} \text{ s}^{-1} \).
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