ATOMIC DIAGNOSTICS OF X-RAY-IRRADIATED PROTOPLANETARY DISKS

R. MEIJERINK AND A. E. GLASSGOLD
Astronomy Department, University of California, Berkeley, CA 94720; rowin@astro.berkeley.edu, glassgol@astro.berkeley.edu

AND

J. R. NAJITA
National Optical Astronomy Observatory, Tucson, AZ 85719; najita@noao.edu

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ABSTRACT

We study atomic-line diagnostics of the inner regions of protoplanetary disks with our model of X-ray-irradiated disk atmospheres, which was previously used to predict observable levels of the Ne ii and Ne iii fine-structure transitions at 12.81 and 15.55 μm. We extend the X-ray ionization theory to sulfur and calculate the fraction of sulfur in S, S+, S2+, and sulfur molecules. For the D’Alessio generic T Tauri star disk, we find that the S i fine-structure line at 25.55 μm is below the detection level of the Spitzer Infrared Spectrometer (IRS), in large part due to X-ray ionization of atomic S at the top of the atmosphere and to its incorporation into molecules close to the midplane. We predict that observable fluxes of the S ii λ6718/λ6732 forbidden transitions are produced in the upper atmosphere at somewhat shallower depths and smaller radii than the neon fine-structure lines. This and other forbidden-line transitions, such as the O i λ6300/λ6363 and C i λ9826/λ9852 lines, serve as complementary diagnostics of X-ray-irradiated disk atmospheres. We have also analyzed the potential role of the low-excitation fine-structure lines of C i, C ii, and O i, which should be observable by SOFIA and Herschel.

Subject headings: accretion, accretion disks — infrared: stars — planetary systems: protoplanetary disks — stars: formation — stars: pre–main-sequence — X-rays: stars

Online material: color figures

1. INTRODUCTION

There is growing evidence for the existence of warm atmospheres in the inner disks of low- and intermediate-mass young stellar objects (YSOs). They first became apparent from observations of the CO overtone band head emission near 2.3 μm in Herbig Ae stars and T Tauri stars (e.g., Carr 1989; Najita et al. 2000). More recently, emission from the fundamental CO vibrational band near 4.6 μm has been observed in many T Tauri stars (Najita et al. 2003), as has the UV fluorescence of molecular hydrogen (e.g., Herczeg et al. 2002). These observations indicate that temperatures in the range 1000–2000 K occur over a considerable vertical column density of hydrogen, ~1021 cm–2 in the inner disk region. This and other spectroscopic evidence for warm gaseous disk atmospheres were reviewed by Najita et al. (2007), where extensive references are given to earlier work.

Calvet et al. (1991) pioneered the now widely accepted view that disk atmospheres are heated by stellar radiation. In previous publications (Glassgold et al. 2004, hereafter GNI04) we argued that stellar X-rays play an important role in heating the upper gas layers of circumstellar disks on the following basis. First, significant X-ray emission appears to be a universal aspect of low-mass YSOs; second, X-rays couple strongly to the gas; and third, hard X-rays with energies ≥1 keV can penetrate deeply into disk atmospheres.

One special aspect of X-ray irradiation is that temperatures as large as 4000–5000 K are achieved high in the atmosphere. We recently pointed out that this hot layer gives rise to significant flux levels of the fine-structure lines of neon at 12.81 and 15.55 μm (Glassgold et al. 2007, hereafter GNI07).

The Ne ii 12.81 μm line has now been detected in many YSOs by the Spitzer Infrared Spectrometer (IRS) in nearby star-forming regions (Pascucci et al. 2007; Lahuis et al. 2007; Espaillat et al. 2007) and by MICHELLE at Gemini North (Herczeg et al. 2007). The measured fluxes are in good agreement with the predictions in GNI07. These observations support the hypothesis that disk atmospheres are heated and ionized by photons energetic enough to ionize Ne (which has first and second ionization potentials of 21.56 and 41.0 eV), most likely X-rays. A key motivation in the work of GNI07 was the search for clear diagnostics of the effects of X-ray irradiation. The Ne lines seemed particularly appropriate because hard X-rays generate high ionization states of neon via the Auger effect and because neon chemistry is especially simple. U. Gorti & D. Hollenbach (2006, private communication) have suggested that EUV radiation may contribute to the neon fluxes, although the emission characteristics of YSOs in this wavelength band are poorly known compared to X-rays.

In this paper we extend the considerations of GNI07 and seek other fine-structure and forbidden transitions that have a potential to complement the neon lines. We have been guided in part by the intrinsic strength of a line, which we can take as the thermalized emissivity in a transition from an upper to a lower level $u \rightarrow l$,

$$j(u, l) = P(u) x_{n1} A(u, l) E(u, l).$$

(1)

Here $x_{n1}$ is the density of the emitting species, $P(u)$ is the population of the upper level, and $A(u, l)$ and $E(u, l)$ are the Einstein $A$ value and energy of the transition. The last two factors in equation (1) emphasize high-frequency transitions, but the other factors are crucial, since they require a theory for the ionization of the carrier species (the $x$-factor) and the excitation of the level [the factor $P(u)$], as they are sensitive to the physical conditions. We have chosen to focus here on the lines of oxygen, sulfur, and, to a lesser extent, carbon. Some spectral lines of particular interest...
are the 25.25 μm fine-structure transition of Si, which has been searched for, mostly without success, by Spitzer; the fine-structure lines of O i, which should be detectable with SOFIA and the PACS imaging spectrometer on Herschel; and various optical-infrared forbidden transitions accessible from the ground.

The atomic carriers of these lines appear in the many disk chemical models developed over the last 10–15 yr (reviewed by Bergin et al. 2007). They are closely related to the photon-dominated models (PDR) developed for the interstellar medium. In this case stellar and interstellar radiation generate warm atomic regions in the upper and lower layers of the disks until the UV radiation is absorbed and molecule formation becomes efficient. Jonkheid and Kamp and their collaborators (Jonkheid et al. 2004, 2006, 2007; Kamp et al. 2003) have gone farther and calculated the emissivity and line shape of the fine-structure lines of C i, C ii, and O i.

The 63 μm fine-structure line of O i was detected in YSOs with the KAO (e.g., Cohen et al. 1988; Ceccarelli et al. 1997) and ISO (e.g., Nisini et al. 1999; Spinoglio et al. 2000; Creech-Eakman et al. 2002; Liseau et al. 2006), but the interpretation of the results is hampered by the low spatial and spectral resolution of the observations, so that it is unclear what fraction of the emission arises from the disk. Disks have also been considered as a possible source of forbidden-line emission by Hartigan et al. (1995), Kwan (1997), and Störzer & Hollenbach (2000). The forbidden lines have been well studied in YSOs (see, e.g., the review by Ray et al. 2007), and some of the observed “low-velocity components” of the emission may originate from the disks in these systems (e.g., Kwan & Tademaru 1988, 1995). We return to the observations of the fine-structure and forbidden lines in § 5.

The calculations reported in this paper are exploratory in nature, as were those in GNI07. They examine the ability of X-rays, a well-characterized property of T Tauri stars, to produce atomic-line emission from T Tauri disks. The model employs the continuous disk density distribution developed by D’Alessio et al. (1999) for a generic T Tauri star, and features stellar X-ray heating and ionization in the context of a simplified thermal-chemical model, which is discussed in more detail in § 2. We do not attempt to fit the observations for any specific system, but instead try to derive conclusions that might be applicable to any protoplanetary disk.

The plan of the rest of this paper is as follows. In the next section we review and update the thermal-chemical model of GNI04. In § 3 we summarize the essentials of the basic ionization theory and extend it to include the X-ray ionization of sulfur. In § 4 we outline the excitation and flux calculations for the lines of interest, and then discuss the relevant observations in § 5. The last section summarizes the main results of this paper.

2. REVIEW OF THE MODEL

We use the thermal-chemical model of GNI04 with minor corrections and updates. The important processes in determining the thermal balance are X-ray heating, gas-grain heating and cooling, mechanical heating (e.g., from disk accretion or the wind-disk interaction), and line cooling (Lyα, recombination lines, O i fine-structure and forbidden lines, and CO rotational and rovibrational lines). The chemical network contains about 125 reactions and 25 species. Errors in the specification of these processes have been corrected, and the entire reaction base has been reevaluated and updated. None of the changes affect the conclusions of GNI04 and GNI07 in any major way. GNI04 provide a detailed description of the physical processes, and the chemical reaction base is available from the authors on request, or can be downloaded from the University of California, Berkeley, Web site.1

Following GNI04 and GNI07, we calculate the chemical and thermal structure of the gas in a protoplanetary disk for the smooth density distribution of the generic T Tauri disk model of D’Alessio et al. (1999) using an updated version of the code developed by GNI04. D’Alessio et al. (1999) did not distinguish between the thermal properties of the dust and the gas, and their density structure is in hydrostatic equilibrium. However, at high altitudes and low vertical column densities, the temperature of the gas is much higher than that of the dust (GNI04), and this implies that our model is no longer in hydrostatic equilibrium. Were we to treat the gas and dust as two separate fluids and require hydrostatic equilibrium, the results would differ somewhat from the exploratory calculations reported here and in GNI07. For example, we would expect the gaseous disk to be puffed up close to the star and to shield the outer part of the disk from stellar radiation. On the other hand, the flaring of the outer disk would also be increased, and thus it would be illuminated more directly by the central star (Dullemond et al. 2002; Gorti & Hollenbach 2004). A quantitative evaluation of such effects on the diagnostic line fluxes must await the development of a more complete model that treats both the gas and the dust self-consistently.

The D’Alessio model does not include X-rays. In our previous studies based on this density distribution, we adopted a “reference” X-ray luminosity of \( L_X = 2 \times 10^{30} \text{ erg s}^{-1} \) and a thermal spectrum with \( kT_X = 1 \text{ keV} \). It is well known that both the X-ray luminosity and spectrum of young stellar objects can change with time, and that they vary widely from source to source. The ionization rate is not very sensitive to the temperature of the spectrum, as shown in Figure 5 of Igea & Glassgold (1999). In the Chandra Orion Ultracold Project (COUP) study of the Orion Nebula Cluster (Getman et al. 2005), the X-ray luminosity function for the entire cluster spans five decades from log \( L_X = 27 \) to 32. Two of these decades of variation may be associated roughly with the dependence of \( L_X \) on stellar mass and one on a dependence on stellar age (Feigelson et al. 2005), leaving two or more unexplained decades. Thus, the X-ray luminosity of a pre-main-sequence object with specific mass and age may vary over 2 orders of magnitude. This is consistent with the findings of Wolk et al. (2005) for a subset of 28 solar-mass stars in the Orion Nebula Cluster with masses in the range \( M_* = 0.9–1.2 M_\odot \), which have a median X-ray luminosity of log \( L_X = 30.25 \text{ erg s}^{-1} \). The spread of 2 orders of magnitudes can only be partly explained by variability, including flares. Similar results have been found in the XMM-Newton study of the Taurus-Aurigae cluster (Güdel et al. 2007; Telleschi et al. 2007), where the X-ray luminosity ranges over three decades (log \( L_X = 28–31 \)).

Our previous choice \( L_X = 2 \times 10^{30} \text{ erg s}^{-1} \) was consistent with the observations of young T Tauri stars with masses \( M_* \approx 1 M_\odot \) and with the X-ray luminosity of well-studied sources such as TW Hya (Kastner et al. 2002; Stelzer & Schmitt 2004). The median X-ray luminosity measured by XEST for classical T Tauri stars (with disks) in the Taurus-Aurigae cluster is \( L_X = 5 \times 10^{27} \text{ erg s}^{-1} \), 4 times smaller than our reference value. In recognition of this difference, as well as the observed 1–2 dex spread in measured luminosity, we consider a range of X-ray luminosities between \( L_X = 2 \times 10^{29} \) and \( 2 \times 10^{31} \text{ erg s}^{-1} \). X-ray luminosities in this range are likely to yield fluxes for the lines of interest that can be detected with current facilities.

In order to improve the numerical accuracy of the flux calculations in § 4, the calculations reported here cover an extended

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1 See http://astro.berkeley.edu/~rowin/MGN_rates.pdf.
range of radii from 0.25 to 100 AU, in contrast to GNI07, who considered the range 1–40 AU. In making this extension, we do not consider any structural and physical modifications that might occur at very small and very large radii. For example, spectral energy distributions measured with the Spitzer IRS indicate the occurrence of inner holes and rims at distances of the order of several AU (Dullemond et al. 2007). Since we use the D’Alessio model calculations, which varies continuously from 0.028 to >500 AU, the present calculations do not take into account structures such as holes, gaps, and rims.

The elemental abundances used here and in the flux calculations to follow are \( \chi_{\text{H}} = 0.1 \), \( \chi_{\text{C}} = 2.8 \times 10^{-4} \), \( \chi_{\text{O}} = 6.0 \times 10^{-4} \), \( \chi_{\text{S}} = 7.0 \times 10^{-6} \), \( \chi_{\text{Ne}} = 1.0 \times 10^{-4} \), and \( \chi_{\text{Na}} = 1.0 \times 10^{-6} \). The abundance of sulfur that we have adopted is in the range suggested by the recent modeling of sulfur molecules observed in the Horsehead Nebula (Goicoechea et al. 2006). It is much closer to the solar photospheric/meteoritic value (Asplund et al. 2005) than the heavily depleted values used in modeling dark clouds (e.g., Millar & Herbst 1990). UV absorption-line studies of the diffuse interstellar medium provide no evidence for depletion of sulfur, as they do for more refractory elements (Savage & Sembach 1996). Figure 1 shows the thermal structure of the reference disk model. The stellar and disk parameters that define the D’Alessio et al. (1999) model are given in the caption. For high altitudes (\( N_{\text{H}} < 10^{21} \text{ cm}^{-2} \)) and moderate radii (\( R < 25 \) AU), temperatures as high as 4000–5000 K are reached. Going deeper into the atmosphere, \( T \) undergoes a sharp drop toward midplane temperatures in the range from 30 to 200 K, depending on radius. Near the midplane, where the density is high (\( n = 10^{6}–10^{10} \text{ cm}^{-3} \)), the gas and the dust are thermally coupled. For these radii (<25 AU), the temperature starts high at the top of the atmosphere and then increases further with increasing vertical column density or decreasing altitude (see also Fig. 2 of GNI04). This is a consequence of the balance between X-ray heating and Ly{\( \alpha \)} cooling that controls the temperature at the very top of the atmosphere. The heating and the cooling are both proportional to the first power of the volume density. The small increase in temperature arises from its logarithmic dependence on optical depth, which of course increases with increasing vertical column density. Beyond 25 AU, the \( \text{O} \) i fine-structure lines are the dominant coolants at the disk surface.

3. IONIZATION THEORY

The GNI07 thermal-chemical program includes the elements H, He, C, and O, plus a generic heavy atom represented by Na. X-ray ionization of H, He, H{\( \beta \)}, and C are included explicitly, and that of O implicitly. Generally speaking, X-ray ionization of a cosmic gas occurs by the absorption by the K and L shell electrons of heavy atoms and ions. The resultant photo and Auger electrons then generate many more secondary electrons by the collisional ionization of H and He. The ionization state of a heavy atom A or ion in a mainly atomic gas is determined by several processes: direct X-ray ionization (rate \( \zeta_{\text{dir}} \)), secondary electron ionization (rate \( \zeta_{\text{sec}} \)), electronic recombination, and charge transfer to H and He. The latter process may be fast (rate coefficient \( \sim 10^{-9} \text{ cm}^{3} \text{ s}^{-1} \)) or slow. In the case of neon (GNI07), charge transfer is relatively slow and fosters high abundances of neon ions. The ionization rates for atom A, \( \zeta_{\text{dir}}(A) \) and \( \zeta_{\text{sec}}(A) \), are always per atom, whereas the total ionization rate \( \zeta \) is per H nucleus.

On the basis of its elemental X-ray absorption cross section, we estimate that the oxygen ionization rates are \( \zeta_{\text{dir}}(\text{O}) = 17 \zeta \) and \( \zeta_{\text{sec}}(\text{O}) = 2.4 \zeta \), where \( \zeta \) is the X-ray ionization rate of the cosmic mix of disk gas. However, near-resonant charge exchange of \( \text{H}^{+} \) and O is fast, and dominates the ionization of oxygen. Thus, direct X-ray ionization of oxygen can be ignored, as in GNI04. In the case of carbon, we estimated \( \zeta_{\text{dir}}(\text{C}) = 6 \zeta \) and \( \zeta_{\text{sec}}(\text{C}) = 4 \zeta \), but now charge exchange of \( \text{H}^{+} \) and \( \text{He}^{+} \) with C is very slow, and therefore X-ray ionization of carbon is important and is included explicitly in the thermal-chemical program.

Figure 2 shows the electron fraction calculated for our model; it exceeds 0.01 at the top of the atmosphere down to a depth of \( N_{\text{H}} \sim 10^{19} \text{ cm}^{-2} \). The electron fraction decreases more smoothly with vertical column than the temperature. Near the midplane, its value is larger than that given by GNI07 because ionization due to the radioactive decay of \( ^{26}\text{Al} \) has been included at a rate \( \zeta_{26} = 4 \times 10^{-19} \text{ s}^{-1} \) (Stepinski 1992; Glassgold 1995; Finocchiaro & Gail 1997). This assumes that the entire disk is optically thick with respect to the 1.809 MeV decay γ-rays, and that the \( ^{26}\text{Al}/^{27}\text{Al} \) ratio has the canonical value found in meteoritic calcium-aluminum inclusions (\( 5 \times 10^{-5} \)). It also ignores the effects of the 1 Myr mean life of \( ^{26}\text{Al} \) and the possibility that the initial distribution of \( ^{26}\text{Al} \) is spatially inhomogeneous. In light of these simplifying assumptions, it is likely that the rate is even smaller than the one we have adopted, but the exact value is not crucial for the main subject of
Abundances of the order $10^{19}$ cm$^{-3}$ are found at high altitudes ($N_{\text{H}} < 10^{14}$ cm$^{-3}$). It is remarkable that X-ray ionization produces significant abundances of Ne$^+$ and Ne$^{2+}$ out to radii as large as 30 AU.

The closed shell character of neon means that the complexities of molecule formation and destruction do not enter, and only three species, Ne, Ne$^+$, and Ne$^{2+}$, have to be considered in estimating their line fluxes. This is not the case for the calculation of the S and S$^+$ fine-structure and forbidden lines. In order to calculate the abundances of S and S$^+$, we have to consider the transition into sulfur molecules, such as SO, SO$_2$, and CS, which occurs at large vertical column densities. Figure 4 gives a schematic overview of sulfur ionization including a simplified warm chemistry, following Leen & Graff (1988).

Sulfur ions in the disk are mainly produced by X-ray ionization. Sulfur has L and K edges near 0.2 and 2.5 keV and, since we consider X-ray spectra that are not particularly hard ($T_\chi \gtrsim 1$ keV), photons with energies between the L and K edges are the ones most strongly absorbed by sulfur. Because charge exchange with H is fast for highly ionized sulfur ions, X-ray ionization of sulfur accompanied by the Auger process leads primarily to S$^{2+}$ and S$^{3+}$. Calculations by Butler & Dalgarno (1980) and Christensen & Watson (1981) suggest that S$^{2+}$ charge exchange with atomic hydrogen is also fast, while that of S$^{3+}$ is slow. Therefore, we only include ions up to S$^{2+}$, as we did in the case of neon (GNI07).

However, in addition to electronic recombination and charge exchange of sulfur ions with atomic hydrogen, we also include the S$^+$ + H$^+$ charge-exchange reaction, which can ionize S at a significant rate below 10,000 K according to the theoretical calculations of Zhao et al. (2005). Furthermore, the reaction S$^{2+}$ + H$_2$, which has been measured to be fast (Chen et al. 2003), can significantly reduce the abundance of S$^{3+}$.

As for carbon and oxygen, we can estimate the direct X-ray ionization rate of sulfur from its X-ray absorption cross section. Its energy dependence is very similar to that of the mean X-ray absorption cross section averaged over interstellar or solar abundances. Thus, the direct ionization rate of sulfur, resulting from the $(L$ to $K)$ 0.2–2.4 keV band, is basically given by the ratio of the two absorption cross sections at these energies. For example, at 1 keV the ratio is $\approx 500$. This then is the approximate ratio of the primary or direct X-ray ionization of sulfur (per sulfur nucleus) to that of the mean interstellar atom (per hydrogen nucleus, since abundances are conventionally normed to hydrogen). However, most of the ionization of the gas as a whole comes from secondary-electron ionization of hydrogen (atomic and molecular) and helium. Since there are roughly 25 such electrons produced per primary ionization, the ratio of the direct sulfur ionization rate per sulfur nucleus to the total X-ray ionization per H nucleus is 500/25 = 20:

$$\zeta(S)_{\text{dir}} \approx 20\zeta.$$  \hspace{1cm} (2)

The secondary electrons generated by X-ray ionization of all of the cosmic elements collisionally excite and ionize S at a rate that is roughly given by the ratio of the electronic ionization cross section of sulfur to that of hydrogen (Maloney et al. 1996). This leads to the approximate value

$$\zeta(S)_{\text{sec}} \approx 5\zeta.$$  \hspace{1cm} (3)

The direct ionization rate is mainly responsible for producing higher S ions, which we lump together into S$^{2+}$ because of fast charge transfer. The secondary ionization rate primarily produces an additional electron, e.g., it generates S$^+$ from S. Some of the sulfur ion rate coefficients are listed in Table 1. Those for radiative recombination are well calculated. As in the case of neon, however, the rate coefficients for electron transfer from atomic...
The dominant species at large columns. Column densities larger than 0 star. We find that sulfur is completely locked up in molecules for above the disk midplane at a radial distance of 20 AU from the constriction of the sulfur molecules, SO, SO₂, CS, and OCS, by species near the midplane, we include the formation and de-

hydrogen are not well established. They represent an important uncertainty in the results of this paper.

To address the question of whether S remains the dominant species near the midplane, we include the formation and destruction of the sulfur molecules, SO, SO₂, CS, and OCS, by using the warm neutral sulfur chemistry of Leen & Graff (1988). We also include X-ray ionization and destruction of these molecules, assuming that X-ray cross sections for molecules are additive over the constituent atoms, and using the atomic rates discussed above. We also make the simplifying assumptions that a direct absorption of an X-ray by a sulfur molecule always leads to a molecular ion. The sulfur molecular ions are rapidly produced, whereas S assumes that role at intermediate altitudes. Beyond R > 25 AU, X-ray ionization of sulfur is not strong enough to maintain S⁺ as the dominant species. At low altitudes, we find a clear cut-off in the atomic S abundance, with almost all of the sulfur in molecules.

4. EXCITATION AND FLUX CALCULATIONS

The flux calculations for the atomic ions considered in this paper are relatively straightforward because one needs to deal with a few levels of relatively low excitation, even for the forbidden lines. For neon, we continue to focus on the ground fine-structure transitions of Ne⁺ and Ne²⁺. For O, S, and C, we treat the five lowest levels in the ground electronic configuration: a fine-structure triplet that generates the famous 158 μm line. Simplications often occur. For example, the fine-structure transitions of C i and C ii have low critical densities and, because of the high disk densities, are near-thermalized. Similarly, the forbidden lines are usually optically thin and the effects of line trapping are small. In the following sections, we discuss specific issues that arise in the calculation of the emissivities of the lines of interest. We use the line frequencies and A values in the NIST database. Electronic excitation rates are now reasonably well established, but those for excitation by H, H₂, He, and H⁺ are often unknown, except perhaps for O i, C i, and C ii. References for our choice of rate coefficients are given in Table 2. In those cases where trapping plays a role, e.g., for the O i and S i fine-structure lines, our results apply to a face-on disk.

4.1. Neon

We calculate the optically thin Ne ii and Ne m lines’ fine-structure lines at 12.81 and 15.55 μm in the manner of GNI07 with the following change. While retaining the two-level population formula for the ground-level doublet of Ne ii, we solve exactly for the populations of the ground-level triplet of Ne m. This more complete excitation calculation leads to an increase in the population of the upper J = 0 level and, to a lesser extent, the J = 1 level, and increases the line intensities.

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**TABLE 1**

| Reactants | Products | Symbol | Rate Coefficient | Reference |
|-----------|----------|--------|------------------|-----------|
| S⁺ + e    | S + hν   | o₁     | $4.65 \times 10^{-13} T_2^{-0.63}$ | Aldrovandi & Pequignot (1973); Gould (1978) |
| S⁺⁺ + e   | S⁺ + hν  | o₂     | $3.37 \times 10^{-12} T_2^{-0.50}$ | Nahar & Pradhan (1995) |
| S⁺⁺ + e   | S⁺ + hν  | o₃     | $5.23 \times 10^{-12} T_2^{-0.50}$ | Nahar & Pradhan (1995) |
| H⁺ + S    | S⁺ + H   | k₁     | $5 \times 10^{-12}$ | Zhao et al. (2005) |
| S⁺ + H    | H⁺ + S   | k₂     | Negligible      | Zhao et al. (2005) |
| S⁺⁺ + H   | H⁺ + S²⁺ | k₃     | $10^{-14}$ | Butler & Dalgarno (1980); Christensen & Watson (1981) |
| S⁺ + H⁺   | H⁺ + S²⁺ | k₄     | $3 \times 10^{-9}$ | Butler & Dalgarno (1980); Christensen & Watson (1981) |
| S⁺ + H₂   | S etc.   | BK     | $2 \times 10^{-9}$ | Chen et al. (2003) |
| S⁺ + H₂   | S etc.   | (1 − B)K | $2 \times 10^{-9}$ | Chen et al. (2003) |
| S + X-ray | S⁺ + e   | $\zeta(S)$ | $5 \times \zeta$ | This work |
| S + X-ray | S⁺ + 2e  | $\zeta(S)$ | $20 \times \zeta$ | This work |
| S⁺ + X-ray| S⁺ + e   | $\zeta(S)$ | $25 \times \zeta$ | This work |

* Approximate value valid from 500 to 5000 K.

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**Fig. 5.—** Fractional sulfur abundances vs. vertical column density measured from the top of the disk at a radial distance of 20 AU from the star. SO₂ becomes the dominant species at large columns.
Figure 7 shows the distribution of the Ne ii 12.81 µm emissivity throughout the disk for the reference X-ray luminosity. Most of the emission is produced at high temperature (≈4000 K) and high electron abundance, corresponding to radial distances \( R < 25 \) AU and vertical column densities \( N_H < 10^{21} \) cm\(^{-2}\). The largest emissivity does not always occur at the highest altitude above the midplane. This is due to an increase of the Ne\(^{+}\) density and its specific emissivity with increasing depth. The upper \( J = 1/2 \) level is subthermally populated and its population is proportional to electronic collisions. However, we have been reminded that, as the electron fraction decreases with height, collisions with atomic hydrogen begin to play a role (D. J. Hollenbach 2006, private communication). Using the results of Bahcall & Wolf (1968), Hollenbach & McKee (1989) estimated the rate coefficient for collisional deexcitation of the 12.81 µm transition in collisions with atomic hydrogen to be \( 1.3 \times 10^{-9} \) cm\(^3\) s\(^{-1}\). Although the theory of Bahcall & Wolf may give the right order of magnitude (as it does for the excitation of the O\( ^i \) fine-structure transitions), it is incorrect in principle since it implies that the excitation cross section is proportional to the scattering cross section. According to Bahcall & Wolf, the rate coefficient in a collision with a neutral atom varies with temperature as \( T^{1/6} \) (cf. the van der Waals potential) and as a constant in a collision with an ion (cf. the Langevin potential). However, collisional excitation of a fine-structure transition requires an exchange of a spin between the incident H atom and the target electrons, and thus depends on differences between potentials, differences which decrease more rapidly than \( 1/T^6 \) and \( 1/T^4 \) for neutral and ionic collisions, respectively.

The full quantum-mechanical calculations for O\( ^i \) and C\( ^i \) (Launay & Roueff 1977a; Abrahamsson et al. 2007) and for C\( ^{ii} \) (Launay & Roueff 1977b; Barinovs et al. 2005) bear out the fact that the Bahcall & Wolf theory predicts the wrong temperature dependence for the collisional excitation rate coefficients by atomic hydrogen. We have compared the recent calculations of Barinovs et al. (2005) for H + C\( ^{ii} \) with the Bahcall & Wolf theory, and find that the latter overestimates the rate coefficient by factors of 7.5–5 in the temperature range from 500 to 4000 K. If something like this reduction factor also applies to H + Ne\(^{+}\), then the order of magnitude of its rate coefficient for collisional deexcitation of the Ne\(^{+}\) fine-structure doublet is \( \approx 2 \times 10^{-10} \) cm\(^3\) s\(^{-1}\). We have calculated the 12.81 µm emissivity (including line trapping) with this value for the H deexcitation rate, and find that it increases the flux by about a factor of 2. This increase arises mainly at large radial distances, where the deviations from a thermal population are the greatest. We conclude that our calculations based on electronic excitation alone underestimate the Ne\(^{+}\) 12.81 µm flux, but possibly not by a large factor. Actual calculations of the atomic hydrogen excitation rate would be most welcome.

### 4.2. Oxygen

Figure 8 gives the five levels that we consider in calculating fine-structure and forbidden-line emission from atomic oxygen and sulfur. According to Table 2, collisional excitation rates for the fine-structure levels of O\( ^i \) are available for collision partners

| Ion | References |
|-----|------------|
| Ne \( ^{ii} \) fine structure | Griffin et al. (2001) (e) |
| Ne \( ^{iii} \) fine structure | Butler & Zeippen (1994) (e) |
| O\( ^i \) fine structure | Launay & Roueff (1977a); Abrahamsson et al. (2007) (H); Jaquet et al. (1992) (H\(_2\)); Monteiro & Flower (1987) (He); Chambaud et al. (1980) (p); Pequignot (1990) (e) |
| O\( ^i \) forbidden | Krems et al. (2006) (H); Zatsarinny & Tayal (2003) (e) |
| S\( ^i \) fine structure | Tayal (2004) (e) |
| S\( ^{ii} \) forbidden | Tayal (1997) (e) |
| C\( ^i \) fine structure | Launay & Roueff (1977a); Abrahamsson et al. (2007) (H); Monteiro & Flower (1987) (He, H\(_2\)) |
| C\( ^{ii} \) forbidden | Pequignot & Aldrovandi (1976); Zatsarinny et al. (2005) (e) |
| C\( ^{iii} \) fine structure | Barinovs et al. (2005) (H); Launay & Roueff (1977b) (H\(_2\)); Wilson & Bell (2002) (e) |

Note.—The collision partners are specified inside the parentheses.
Atomic hydrogen tends to dominate and, even without line trapping, the critical densities are modest, typically $n_{cr}(H) < 10^6 \text{ cm}^{-3}$. At large radii ($>25$ AU), densities of this order are not reached until vertical column densities $N_H / C_2 > 10^{20} \text{ cm}^{-2}$. The full emissivity calculation is particularly relevant at large radii.

Figure 9 shows the spatial distribution of the emissivity of the $^{1}D_2 \rightarrow ^{1}P_J$ transitions of O $\lambda 6300/\lambda 6363$ and the $^{1}S_0 \rightarrow ^{1}D_2$ transitions of S. Significant emission occurs beyond columns of $N_H = 10^{22} \text{ cm}^{-2}$ as a consequence of the fact that the excitation energy is relatively low ($\approx 230$ K) and contributes $\approx 10\%$ of the total line flux.

The $^{1}D_2 \rightarrow ^{1}P_J$ transitions are optically thin and subthermally excited. In addition to the electronic rate coefficients (Zatsarinny & Tayal 2003), the collisional deexcitation rate of the $^{1}D_2$ level by atomic hydrogen has been calculated by Krems et al. (2006). It varies little between 500 and 6000 K, where it has a mean value of $8 \times 10^{-11} \text{ cm}^{3} \text{s}^{-1}$ for the $^{1}S_0$ level, so electronic collisions dominate over those with atomic hydrogen for $x_e > 2.5 \times 10^{-4}$. If we consider only electronic collisions, then an upper limit to the critical density for the $^{1}D_2 \rightarrow ^{1}P_J$ transitions is $n_e \approx 10^6 \text{ cm}^{-3}$, while that for the $^{1}S_0 \rightarrow ^{1}D_2$ transition is $n_e \approx 10^7 \text{ cm}^{-3}$. In the absence of calculations for the $^{1}S_0$ level, we have adopted the value $10^{12} \text{ cm}^{-2}$ for the $^{1}P_J$ level, so electronic collisions dominate over those with atomic hydrogen for $x_e > 2.5 \times 10^{-4}$. If we consider only electronic collisions, then an upper limit to the critical density for the $^{1}D_2 \rightarrow ^{1}P_J$ transitions is $n_e \approx 10^6 \text{ cm}^{-3}$, while that for the $^{1}S_0 \rightarrow ^{1}D_2$ transition is $n_e \approx 10^7 \text{ cm}^{-3}$. In the absence of calculations for the $^{1}S_0$ level, we have adopted the value $10^{12} \text{ cm}^{-2}$ for the $^{1}P_J$ level.
the critical density. The emissivity for both lines is then given by equation (1). The $^{1}S_{0}$ uppermost level is so far from being thermalized that we can calculate the flux of the 5577 Å line by using the extreme low-density collisional-excitation limit, in which every excitation leads to the production of a photon.

Figure 11 shows that the O i forbidden lines trace the upper atmosphere of the disk, where the atomic oxygen abundance is constant. The O i 6300 Å lines are generated within 25 AU, a somewhat smaller range than the neon fine-structure lines, while the 5577 Å line (not shown) originates from radii inside 15 AU. The calculations of forbidden-line fluxes necessarily ignore an effect of the UV photodissociation of OH, which leads to its destruction at large radii. Figure 11, however, already demonstrates that OH photodissociation by the stellar irradiation is not important at large radii due to OH photodissociation by the stellar or interstellar/intracluster FUV radiation field.

4.3. Sulfur

We focus on the mid-IR fine-structure lines of S i and the 6718 Å/6732 Å forbidden transitions of S ii; the fine-structure lines of S iii are likely to be too weak to be observable at the present time. In accord with Figure 8, the calculation of the S i fine-structure emission is similar to that just described for O i. The big difference is that little if anything is known about the excitation of these lines by collision partners other than electrons. Thus, the present flux estimates are lower limits. The calculations take line trapping into account and solve the three-level fine-structure population problem exactly, including the the weak $J = 0 \rightarrow 2$ quadrupolar transition.

Figure 12 shows the spatial distribution of the S i 25.25 μm fine-structure line emissivity for the reference model. The appearance of the 56.33 μm emissivity (not shown) is similar, but it is concentrated toward smaller radii and higher altitudes. As in the case of O i, the variation of the fine-structure emission with depth at fixed radius is nonmonotonic, and again there are several factors that contribute to this behavior. First, there are the chemical changes already mentioned, where sulfur changes from S$^{+}$ to S at high altitudes and from S to sulfur molecules at low altitudes. Thus, the emission peaks at intermediate altitudes, at a vertical column of $N_{H} \sim 10^{21} \text{ cm}^{-2}$ at $R = 0.25$ AU and near $N_{H} \sim 10^{19} \text{ cm}^{-2}$ at $R = 25$ AU. Second, the increase of volumetric density with depth also promotes fine-structure emission, whereas the overall temperature decrease has the opposite effect.

Figure 13 shows the variation of the specific emissivity with vertical column at fixed radius. For radii in the range 1–25 AU, the emissivity per S atom of the $J = 1 \rightarrow 0$ level changes from subthermal to thermal as the density increases with increasing depth. At somewhat larger column densities, the specific emissivity decreases due to decreases in both temperature and electron density.

The transition of atomic sulfur into molecules such as SO and SO$_2$ has little effect on the absolute level of the S i fine-structure emission. This is due to the fact that electronic excitation has already become ineffective for $N_{H} < 10^{23} \text{ cm}^{-2}$ before molecule formation occurs. In order to gauge the importance of H atom collisions, we carried out a calculation where we assumed that the S i fine-structure deexcitation rates are about the same as for O i; specifically, $k(H) = (5.0 \times 10^{-13}) T^{1/2}$ for all transitions. The S i 25.25 and 56.33 μm emission is then increased by factors of 10 or more over that for electron collisions only. This serves to indicate the importance of extending the calculation of H excitation rates to heavy atoms and ions such as Ne ii and S i.

We estimate the emission of the S ii forbidden lines in the optically thin approximation. We concentrate on the $^2D_{5/2,3/2} \rightarrow ^4S_{3/2}$ transitions with wavelengths near 6700 Å. Using the electron collisions strengths from Tayal (1997) we find electron critical densities $n_{cr} \sim 10^{7} \rightarrow 10^{9} \text{ cm}^{-3} \text{ s}^{-1}$, and conclude that the lines are almost thermalized. We also considered the possible role of
the H$^+$ + S $\rightarrow$ S$^+$ + H charge exchange, which mainly branches to the upper $^2P_j$ level of S$^+$, and then decays with the emission of photons with wavelengths near 4070 Å, 6700 Å, and 1 μm. We find that this process does not increase the 6718 and 6732 Å line emissivities, probably because the rate coefficient for charge exchange is small ($\sim$5 × 10$^{-12}$ cm$^3$ s$^{-1}$) and because the high density tends to a thermalize the level population. In Figure 14 we show the emissivity of S $\equiv$ 6718 line (the 6733 Å line is very similar). These lines trace the warm upper layers of the disk. Significant emission arises only from regions with temperatures in the range 2000–5000 K.

4.4. Carbon

The energy levels of the ground configuration of C i are similar to those of O i and S i shown in Figure 8, except that the scale of the energy level separations is reduced and the ordering of the total angular momentum quantum number $J$ in the ground-state triplet is inverted. The upper fine-structure levels have energies $E_2/k = 62.5$ K and $E_1/k = 23.62$ K and give rise to far-infrared lines with wavelengths $\lambda(1-0) = 609.135$ μm and $\lambda(2-1) = 370.144$ μm. In addition to these lines, we calculate the emissivity of the forbidden lines at 9827 and 9853 Å that emanate from the first $^1D_2$ level of C i above ground. For C ii, we only consider the fine-structure doublet, with excitation energy and wavelength $\Delta E(3/2-1/2)/k = 91.2$ K and $\lambda(3/2-1/2) = 157.7$ μm, and ignore the 2300 Å lines that arise from the next $^4P$ level.

The $A$ values of the C i and C ii fine-structure transitions are very small ($\sim$10$^{-7}$ s$^{-1}$ for C i and 2.3 × 10$^{-6}$ s$^{-1}$ for C ii), which implies that the critical densities for all of these transitions are low ($<10^4$ cm$^{-3}$, based on the collisional rate coefficients referenced in Table 2). Thus, we can estimate the emissivities assuming that the fine-structure levels are in thermal equilibrium (but we do include line trapping). The integrated fluxes for a nominal distance of 140 pc are given in Table 3. The flux of the C $\equiv$ 158 μm line is very small, but the 369 μm line of C i appears to be in the observable range, as may even be the case for the 609 μm line.

We estimate the C i 29827 and 29853 forbidden-line emission in the optically thin approximation. Using Table 2, the critical density of the $^1D_2$ level at 4000 K is $1.96 \times 10^4$ cm$^{-3}$ s$^{-1}$, and the level is close to being thermalized. The density-dependent correction for subthermal excitation is made in the same way as for O i, as described in § 4.2. The spatial distribution of the C i 29827 emission is shown in Figure 15. The emission is peaked at small vertical column densities, much like the O i 6300 emission in Figure 11. The integrated line flux given in Table 3 is somewhat smaller than the flux of the O i 6300 line, but still in the potentially observable range. Of course, all of these statements about the detectability of neutral carbon lines stand to be corrected (and reduced) when interstellar/intracluster UV radiation is included in the ionization theory.

5. DISCUSSION

In this section we discuss the most important results of this paper in the context of both existing and prospective observations. We treat high- and low-excitation lines separately, since they trace different parts of the disk. We first summarize in Table 3 the line fluxes for five values of the stellar X-ray luminosity that range from $L_X = 2 \times 10^{29}$ to $2 \times 10^{31}$ erg s$^{-1}$. To ensure accurate

| Table 3 |
|-------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Lx (erg s$^{-1}$) | 2.0 × 10$^{29}$ | 6.0 × 10$^{29}$ | 2.0 × 10$^{30}$ | 6.0 × 10$^{30}$ | 2.0 × 10$^{31}$ |
| Line (1) | (2) | (3) | (4) | (5) | (6) |
| Ne $\equiv$ 12.82 μm | $4.1 \times 10^{-16}$ | $1.5 \times 10^{-15}$ | $6.4 \times 10^{-15}$ | $2.3 \times 10^{-14}$ | $9.6 \times 10^{-14}$ |
| Ne $\equiv$ 15.55 μm | $3.0 \times 10^{-17}$ | $1.4 \times 10^{-16}$ | $7.4 \times 10^{-16}$ | $3.3 \times 10^{-15}$ | $1.7 \times 10^{-14}$ |
| O i 63 μm | $1.9 \times 10^{-14}$ | $3.1 \times 10^{-14}$ | $6.6 \times 10^{-14}$ | $1.6 \times 10^{-13}$ | $4.3 \times 10^{-13}$ |
| O i 146 μm | $9.6 \times 10^{-16}$ | $1.2 \times 10^{-15}$ | $1.8 \times 10^{-15}$ | $3.8 \times 10^{-15}$ | $1.1 \times 10^{-14}$ |
| O i 6300 Å | $1.1 \times 10^{-15}$ | $3.6 \times 10^{-15}$ | $1.3 \times 10^{-14}$ | $4.5 \times 10^{-14}$ | $1.7 \times 10^{-13}$ |
| O i 6557 Å | $2.7 \times 10^{-17}$ | $1.4 \times 10^{-16}$ | $7.3 \times 10^{-16}$ | $2.8 \times 10^{-15}$ | $1.1 \times 10^{-14}$ |
| S i 25.25 μm | $7.0 \times 10^{-17}$ | $1.3 \times 10^{-16}$ | $3.4 \times 10^{-16}$ | $9.5 \times 10^{-16}$ | $3.1 \times 10^{-15}$ |
| S i 56.23 μm | $6.4 \times 10^{-18}$ | $9.0 \times 10^{-18}$ | $1.7 \times 10^{-17}$ | $4.0 \times 10^{-17}$ | $1.2 \times 10^{-16}$ |
| Si $\equiv$ 6718 Å | $4.1 \times 10^{-17}$ | $1.7 \times 10^{-16}$ | $8.3 \times 10^{-16}$ | $3.5 \times 10^{-15}$ | $1.6 \times 10^{-14}$ |
| Si $\equiv$ 6733 Å | $9.2 \times 10^{-18}$ | $3.9 \times 10^{-17}$ | $2.0 \times 10^{-16}$ | $8.6 \times 10^{-16}$ | $4.2 \times 10^{-15}$ |
| C i 158 μm | $1.2 \times 10^{-18}$ | $3.2 \times 10^{-18}$ | $9.8 \times 10^{-18}$ | $2.8 \times 10^{-17}$ | $9.0 \times 10^{-17}$ |
| C i 369 μm | $9.8 \times 10^{-16}$ | $1.2 \times 10^{-15}$ | $1.6 \times 10^{-15}$ | $2.0 \times 10^{-15}$ | $2.6 \times 10^{-15}$ |
| C i 609 μm | $3.2 \times 10^{-16}$ | $3.8 \times 10^{-16}$ | $4.5 \times 10^{-16}$ | $5.4 \times 10^{-16}$ | $6.4 \times 10^{-16}$ |
| C i $\equiv$ 9827 Å | $3.5 \times 10^{-16}$ | $1.4 \times 10^{-15}$ | $6.3 \times 10^{-15}$ | $2.5 \times 10^{-14}$ | $1.1 \times 10^{-13}$ |

Notes.—A nominal distance of 140 pc has been assumed. Luminosities can be obtained by multiplying by 4π(140 pc)$^2$ = 2.35 × 10$^{25}$ cm$^2$. Col. (4) refers to the reference model.

The O i 6363 and C i 29853 fluxes can be obtained by multiplying the fluxes of O i 6300 by 0.244 and C i 29827 by 0.248, respectively.
results for values of $L_X$ larger than standard, we have calculated the disk properties and emissivities out to 100 AU. The calculations pertain to the case in which X-ray heating of the disk atmosphere dominates mechanical heating ($\alpha_k = 0.01$ in the notation of GNI04). As discussed in §2, the underlying density model is the generic T Tauri disk model of D’Alessio et al. (1999); the parameters for the model are given in the caption of Figure 1. The “reference” model that we have used throughout has an X-ray luminosity of $L_X = 2 \times 10^{30}$ erg s$^{-1}$; the fluxes for this case are given in column (4) of Table 3.

The values shown in the other columns illustrate how sensitive the modeling results are to the choice of X-ray luminosity. Table 3 encompasses a range of 100 in X-ray luminosity, which is roughly the spread seen by the COUP and XEST projects for T Tauri stars in the Orion Nebula and Taurus-Aurigae clusters of the same mass and age. Were we to choose the median $L_X$ for Taurus-Aurigae (Telleschi et al. 2007) for the reference model, the second column of fluxes would be appropriate. According to the discussion in the previous sections, all of the flux estimates are uncertain to varying degrees due to uncertainties in the rate coefficients and other limitations of the model. In particular, the fluxes for the neon and sulfur fine-structure lines are lower limits because of the omission of collisional excitation by H atoms.

The sensitivity of the integrated line fluxes to the X-ray luminosity can vary from one line to another, since they may originate in different parts of the disk with different physical properties. We illustrate this in Figure 16, which shows how some of the line fluxes vary with $L_X$, normalized to the standard model. The C i 369 $\mu$m line luminosity depends very weakly on $L_X$, since most of the emission is produced at intermediate column densities ($N_{H_2} \sim 10^{22}$ cm$^{-2}$) where the X-ray flux is strongly attenuated. The O i 63 $\mu$m luminosity shows a somewhat steeper dependence, because it is produced both at high altitudes, where the X-ray flux is large, and close to the midplane, where the X-ray flux is small (and the gas and dust temperatures are almost the same). The optically thin O i 5577 emission displays the strongest dependence on $L_X$ because, with its relatively high excitation temperature, it is only produced in the warmest part of the disk fully exposed to stellar X-rays. The other forbidden lines and the S i fine-structure lines (not shown) behave very much like the Ne ii fine-structure line. The almost linear relation between Ne ii line flux and $L_X$ arises from the dependence of the emissivity on $n_e^2$ (cf. eq. [4-1] of GNI07). In its present form, Figure 16 is not meant to suggest a general empirical correlation of line fluxes with X-ray luminosity, simply because the stellar and disk properties of the reference model have been held fixed in the calculations for this figure.

5.1. High-Excitation Lines

5.1.1. Neon Fine-Structure Lines

The neon fine-structure line fluxes (Table 3) are close to but more accurate than those of GNI07. The Ne ii flux is 40% larger, since the calculations extend to smaller radii ($R = 0.25$ AU). The Ne ii 12.81 $\mu$m line emission arises from the top of the atmosphere, where the temperature and electron density are high. We find significant contributions to the integrated emission out to $R = 25$ AU. The emissivity per unit radius is determined by the column density in the upper level (cf. eq. [3-7] of GNI07). This quantity is plotted in Figure 17 (top) against the radius $R$. In contrast to Figure 4 of GNI07, there is no dip near 5 AU, thanks to more accurate and closer spaced calculations. When we assume Keplerian rotation to convert from column density to a velocity distribution function $P(v)$ (cf. eq. [3-8] of GNI07), the peak in $P(v)$ occurs at $v = 0.25 \pi (1$ AU), which corresponds to a peak in the emissivity per unit area at 16 AU. Figure 17 (bottom) shows that $P(v)$ has a long tail extending to high velocity. The ratio of the Ne ii 15.55 $\mu$m to the Ne ii 12.81 $\mu$m flux is of order 0.1. GNI07 considered the detection of the Ne ii line to be a near-definitive diagnostic of X-ray ionization of neon. However, using a disk model dominated by stellar EUV radiation, D. Hollenbach & U. Gorti (2007, private communication) find a range of possible Ne ii/Ne ii ratios (0.1–6) depending on the nature of the EUV spectrum. Thus, it is not immediately clear whether the Ne ii/Ne ii fine-structure line ratio can serve as a discriminant between EUV and X-ray irradiation.

The Ne ii 12.81 $\mu$m line has now been detected in T Tauri disks in about 20 cases from the ground and from space (by IRS on Spitzer; Pascucci et al. 2007; Lahuis et al. 2007; Espaillat et al. 2007; and MICHELLE on Gemini North: Herczeg et al. 2007). The detected flux levels are of order $10^{-14}$ erg cm$^{-2}$ s$^{-1}$; they are within a factor of a few agreement with our model calculations. The weaker 15.55 $\mu$m of Ne iii line has been tentatively detected in only one case (Sz 102; Lahuis et al. 2007). Based on the $3 \sigma$ detection of the Ne ii line, the Ne ii/Ne ii ratio is $\approx 0.06$, which might be compared with a ratio $\approx 0.1$ derived from Table 3. Perhaps what is most interesting about this T Tauri star is that it has the second brightest Ne ii line detected in the Lahuis et al. survey.
Its flux is an order of magnitude larger than the value for our reference model, after correction for the distance of 200 pc. Detailed modeling of the disk around this star would be of considerable interest. For the case of the nearby TW Hya, Herczeg et al. (2007) measure the luminosity for the Ne II 12.81 μm line to be 4.8 × 10⁻⁶ \( L_\odot \), which is 20% larger than the result for our reference model in Table 3.

From a small number of detections of the Ne II 12.81 μm line the Spitzer Legacy program Formation and Evolution of Planetary Systems (FEPS), Pascucci et al. (2007) have suggested that a linear correlation may exist between the Ne II and X-ray luminosities. Together with their detection of the Ne II line in CS Cha and that for TW Hya, based on data obtained by Uchida et al. (2004), Espaillat et al. (2007) argue against such a correlation. The range of \( L_X \) in these papers is small, 1.5 for Pascucci et al. (2007) and 2.25 for Espaillat et al. (2007), the same order of magnitude as the observed variability in the X-ray luminosity. Aside from the intrinsic difficulty of deducing a meaningful correlation on the basis of a small dynamical range in YSO X-ray luminosity, it is important to keep in mind that the line fluxes depend on many other stellar and disk properties, e.g., the stellar temperature, mass, and age, the disk mass, the accretion rate, and the amount of dust grain growth and settling. The theoretical calculations shown in Figure 16 may not be relevant in this context because they assume that the disk structure is fixed while \( L_X \) is varied. To pursue the question of the existence of a correlation with \( L_X \), T Tauri stars with similar properties, both stellar and disk, should be considered. A more practical approach might be to focus in depth on a few specific cases with well-observed properties and to use observed X-ray spectra.

Using the MICHELLE spectrometer at Gemini North, Herczeg et al. (2007) have obtained a spectrally resolved Ne II line profile for TW Hya, which has a nearly face-on disk. The line is centered at the stellar radial velocity, consistent with a disk origin, but the line is broad, with FWHM of ~22 km s⁻¹. The rotational broadening in our models (Fig. 5 of GNI07 and Fig. 17 of this paper), when corrected for inclination, cannot explain the observed line width, even though the present calculations extend to radii as small as 0.25 AU. Although our calculations agree with the measured Ne II luminosity, the rotational broadening in the model is small because it arises from relatively large radii, as shown in Figure 17. As discussed by Herczeg et al. (2007), two interesting explanations of the line width seen in TW Hya that deserve consideration are transonic turbulence and photoevaporative outflows from the disk (Hollenbach et al. 2000; Font et al. 2004). These possibilities raise interesting challenges for future research. If the hole is produced by photoevaporation, then the wind itself will generate line emission. Furthermore, the inner rim of the hole will be irradiated more or less directly by the star, as in the model of Chiang & Murray-Clay (2007), again producing characteristic line emission.

5.1.2. Sulfur Fine-Structure Lines

We consider the S i fine-structure lines to be “high-excitation” because the associated excitation energies, 476 and 825 K, are larger than the temperatures characteristic of the outer disk, as are the fine-structure levels of the neon ions. As discussed in § 3, the X-ray ionization theory for neon and sulfur, where charge exchange plays an important role, is also similar. Reference to Table 3 shows that the integrated S i fine-structure emission for our reference model is ~20 smaller than for the Ne II line. Figure 12 shows that the strongest emission of the S i 25.25 μm line comes from a relatively thin layer between \( N_H = 10^{19} \) and \( 10^{21} \) cm⁻² for \( R < 10 \) AU. This situation and the attendant weakness of the 25.25 μm line occur because sulfur is in the form of S⁺ at higher altitudes and electronic excitation becomes weak at lower altitudes (cf. Figs. 5 and 6).

The S i 25.25 μm line was not detected by the Spitzer c2d and FEPS teams. Pascucci et al. (2007) put upper limits on the residual gas in the disks around their survey of older T Tauri stars with ages between 5 and 100 Myr using the model calculations of Gorti & Hollenbach (2004). From Table 3, which is based on pure electronic excitation, the S i fine-structure lines from younger T Tauri disks would be similarly difficult to detect. However, if the atomic H collision rates for S i are similar to those for O i, the predicted fluxes would approach the observable range. It is important to recall several other caveats that pertain to our calculations: the uncertainties in sulfur chemistry, the total abundance of gaseous sulfur in disks, and the poorly known charge-exchange rate coefficients.

5.1.3. Forbidden Lines

Table 3 gives the fluxes for our reference model of a sample of forbidden lines, as calculated in § 4: O i \( \lambda 6300/\lambda 6363 \), O i \( \lambda 5577 \),
S II λ6718/6731, and C I λ9827/9853. We have identified them as potential diagnostics of the warm and highly ionized gas produced by X-ray irradiation in the upper atmosphere of the inner disk. These lines are generated within the same radial distance range as the Ne II 12.81 and 15.55 μm lines, but at somewhat higher elevations. In principle, they can provide complementary checks on our picture of X-ray irradiation. As discussed in § 4, the accuracy of the calculations varies somewhat from line to line, depending on the reliability of the atomic data and on the completeness of the model itself. For example, we have ignored the role of stellar or interstellar/intracluster FUV radiation, which could enhance the ionization of carbon at high altitudes and thereby reduce the amount of neutral carbon and the strength of the C II forbidden lines. Similarly, the S II λ6718 line strength is affected by the sulfur atoms being converted into molecules. With this proviso, we can see from Table 3 that many of the forbidden lines generated in the upper disk atmosphere are observable in nearby star-forming regions such as Taurus-Aurigae, in the sense that the predicted fluxes are \( \lesssim 10^{-15} \text{erg cm}^{-2} \text{s}^{-1} \), notably O I \( \lambda6300/6363 \), C I \( \lambda9827/9853 \), and perhaps S I \( \lambda6718/6733 \).

Many of these lines have been measured in T Tauri stars. The most dramatic manifestation of the forbidden lines is their tracing of high-velocity outflows or jets from YSOs (e.g., Ray et al. 2007). But these flows have a low-velocity as well as a high-velocity component (Kwan & Tademaru 1988, 1995; Hirth et al. 1997). Kwan (1997) suggested that the low-velocity component (LVC) originates in the inner regions of T Tauri disks (\( R < 2 \text{AU} \)).

Other possible sources for the origin of the LVC are a MHD disk wind (e.g., Paditz et al. 2007) or a photoevaporative outflow (e.g., Hollenbach et al. 2000; Font et al. 2004).

Hartigan et al. (1995) have obtained extensive data on forbidden emission from T Tauri stars. The LVC is ubiquitous, with a typical line luminosity of \( \sim 10^{-4} \text{L}_\odot \), an order of magnitude smaller than the luminosity of our reference model, \( 8 \times 10^{-6} \text{L}_\odot \). They also find O I \( \lambda5577 \) to O I \( \lambda6300 \) line ratios in the range \( \sim 0.2-0.5 \); our model predicts \( \sim 0.1 \). These numbers may signify the difficulty of applying our X-ray-irradiated disk model to observations such as the optical forbidden lines that are sensitive to the other dynamic entities that are operative in accreting young stars, e.g., the various flows that arise near the inner edge of the disk. Hartigan et al. define the LVC to include velocities as high as 60 km s\(^{-1}\), thereby increasing the possibility of including emission from such flows. A cleaner comparison case for our model might be provided by an X-ray-bright star with a relatively low accretion rate, where the emission from outflows would be reduced.

Because TW Hya has a low mass-loss rate and a small accretion rate, it would be a good case for detailed modeling. Herzeg et al. (2007) detected the O I \( \lambda6300/6363 \) lines in TW Hya at moderately high spectral resolution. The luminosity of the 6300 Å line, \( 7.0 \times 10^{-6} \text{L}_\odot \), is close to the result given in Table 3, \( 8.0 \times 10^{-6} \text{L}_\odot \), recalling the good agreement for the luminosity of the Ne II 12.81 μm line. The 6300 Å line is centered on the stellar velocity, and it has a significantly narrower width than the Ne II line, but one that is still too large to be explained by pure rotational broadening. Again, interesting possible explanations to consider in future modeling are a turbulent atmosphere and photoevaporation.

5.2. Low-Excitation Lines

We next consider the low-excitation lines that arise from the fine-structure levels of O I (excitation energies 228 and 327 K), C I (excitation energies 23.6 and 62.5 K), and Ne II (excitation energy 91.2 K); they give rise to far-infrared emission at 63 and 145 μm (O I), 609 and 370 μm (C I), and 158 μm (Ne II). Table 3 shows that the O I fine-structure lines are potential diagnostics of both the moderately warm, ionized gas produced by X-rays, and the cooler gas at large perpendicular column densities. As shown in Figure 9, O I 63 μm line emission extends down toward the midplane region, especially at small radial distances, due to the incomplete conversion of atomic oxygen into molecules and the relatively low excitation temperature of the \( J = 1-2 \) transition.

The 63 μm line has been observed around T Tauri stars with the KAO (e.g., Cohen et al. 1988; Ceccarelli et al. 1997) and ISO (e.g., Spinoglio et al. 2000; Creech-Eakman et al. 2002; Liseau et al. 2006). These observations were made with large beams (tens of arcseconds) and with moderate spatial resolution (50–300 km s\(^{-1}\)). A typical flux for a T Tauri star in Taurus-Aurigae is quite large, \( \sim 10^{-12} \) to \( 10^{-11} \text{erg cm}^{-2} \text{s}^{-1} \), and may include emission from other circumstellar material and not just disks. On the other hand, the flux calculations in Table 3 probably underestimate the flux, even though they integrate out to 100 AU, especially for the carbon lines. Jonkheid et al. (2004) have applied a code developed for (UV) photon-dominated regions to the surface layers of a flaring disk, and find that the fluxes of the O I, C I, and C II fine-structure lines are all of comparable brightness, and that much weaker than the CO(\( J = 1-0 \)) line. Photoionization of neutral carbon by external FUV radiation can enhance the abundance of C\(^+\) and increase the flux of the C II 158 μm line. Our model would have to be extended to include UV irradiation in order to get a fuller understanding of these low-excitation diagnostic lines.

Our estimate of the O I 63 μm line flux provides a good estimate of the emission of this line from the inner disk. Since its detection requires airborne or space observations, the identification with inner disk emission requires resolved line profiles and the assumption of Keplerian disk rotation. Such measurements could be made with heterodyne detectors aboard SOFIA or with Herschel (PACS).

6. SUMMARY

We have used a simplified thermal-chemical and structural model to explore the diagnostics of the atomic gas in protoplanetary disks irradiated by stellar X-rays. Our focus has been on moderate disk radii out to roughly 25 AU, where stellar X-rays play an important role in ionizing and heating the upper layers of the disk. We find several diagnostics for this region, all of which arise from relatively high excitation levels \( \sim 1000 \text{K} \): Ne II and Ne III fine-structure lines and O I, S II, and C I forbidden lines. Some low-excitation fine-structure lines are also of interest in the context of X-ray irradiation, especially the O I fine-structure lines, which generate strong disk emission over a substantial range of vertical column density, extending close to the midplane of the disk.

The atomic lines probe different depths of the disk at moderate radii. The forbidden transitions are generated at the top of the atmosphere, where the temperature and ionization levels are the highest. The mid-infrared fine-structure lines probe greater depths, where the temperature and ionization level have decreased. Neon is the cleanest case, since it does not easily form molecules, and its fine-structure lines originate from intermediate as well as the top layers of the disk. On the other hand, the S I fine-structure lines are produced mainly in intermediate layers, since atomic sulfur has a low abundance in the top layers due to X-ray ionization, and also near the midplane, due to molecule formation. By contrast, the O I fine-structure lines are formed at almost all depths, including close to the midplane, where the density is high and the upper...
levels of the transitions are more commensurate with the temperatures there.

The X-ray-generated atomic lines discussed here are produced over a range of radii, extending from the inner radius of the disk out to 20–30 AU. To resolve these regions in nearby star-forming clusters at a nominal distance of 140 pc requires a spatial resolution of ~0.1″–0.2″, as well as resolved line profiles. For example, the Ne ii 12.81 μm line should be detectable with TEMES or comparable spectrometers on large ground-based telescopes. A promising step in this direction is its detection with MICHELLE on Gemini North (Herczeg et al. 2007). The far-infrared lines of C i, C ii, and O i will be detectable with instruments on board SOFIA and Herschel.

In presenting these results for a simplified T Tauri disk model irradiated by stellar X-rays, we have tried to mention and discuss its limitations. To summarize, there are, first of all, many uncertainties in the underlying atomic physics, such as missing rate coefficients for charge exchange with atomic hydrogen and for collisional excitation by abundant particles other than electrons. These uncertainties, of course, hold for all thermal-chemical/excitation models. Another limitation is the reliance on one type of disk, represented by the smooth density distribution of the generic T Tauri model of D’Alessio et al. (1999). Removing this restriction is one of our immediate goals. It will enable us to discuss disks of different ages and disks with nonmonotonic density distributions such as holes, gaps, and rims. The improvements that are needed to treat situations such as disks with holes require a higher level model than used here. More generally, a three-dimensional treatment is needed, and this dictates a greatly improved treatment of the radiation transfer, especially for the cooling lines and the external UV irradiation.

Focusing on X-rays to the exclusion of UV irradiation is another limitation that needs to be dealt with in future modeling. It is very likely that the well-documented X-rays produced by essentially all YSOs are the dominant external radiation source for radii less than 25 AU. At larger radii, however, ambient UV, from the general interstellar medium or from the host star cluster members, can affect disk properties. At smaller radii, UV radiation originating close to the star may also play a role, although it is more easily attenuated than moderately hard keV X-rays. We have ignored stellar UV radiation, which is poorly determined, in favor of the well-measured X-rays.

Granted that the X-rays likely play the dominant role within 25 AU or so, the relatively high excitation transitions that they generate may be produced by some of the other dynamical components of the star formation system that lie near and even inside the inner edge of the disk. The most obvious examples are the forbidden optical transitions produced by jets and accretion streams that are the signatures of actively accreting YSOs. In this situation, the high-excitation line strengths that we calculate for disks may only represent lower limits to those measured in spatially unresolved observations. A similar conclusion pertains to the low-excitation lines, where significant emission can arise from large disk radii where external UV can dominate. Of course, the contributions of the various parts of the star formation complex can in principle be disentangled by observations with the appropriate spatial and spectral resolution, together with more complex models. The present results demonstrate the importance of X-ray irradiation in the ongoing process of elucidating the nature of the gas in protoplanetary disks.

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APPENDIX A: ABSOLUTE FUNDAMENTAL LINES
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