Doctoral Thesis

The impact of high-energy radiation on the chemistry of star-forming regions

Author(s):
Stäuber, Pascal

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The Impact of High-Energy Radiation on the Chemistry of Star-Forming Regions

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presented by
PASCAL STÄUBER
Dipl. Phys.

born October 4, 1971
citizen of Amriswil (TG)

accepted on the recommendation of
Prof. Dr. Arnold O. Benz, examiner
Prof. Dr. Ewine F. van Dishoeck and Prof. Dr. Jan O. Stenflo,
co-examiner

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Abstract

Young stars are deeply embedded in their natal molecular cloud. The youngest objects are surrounded by large amounts of dust and gas that completely absorb all radiation from the protostar at wavelengths shorter than optical. As a consequence, these objects can only be studied at infrared and (sub)millimeter wavelengths – the reign of dust and molecules. To trace the central high-energy radiation from UV to X-rays in those sources, their molecular environment has to be studied. The excitation and abundance of a molecule is sensitive to the condition of the gas (and dust), such as temperature, density and ionization rate. A careful study of the chemistry can thus provide information about the internal – invisible – processes of the protostellar object.

The introduction of this thesis provides a short review on star-formation of both low and high-mass objects, feedback processes from the innermost region on the molecular surroundings and a summary of some important chemical reactions. It contains also a description of how observations can be interpreted: from molecular excitation and radiative transfer to chemical models.

In Chapter 2\textsuperscript{1}, the influence of a central far ultraviolet (FUV) source on the chemistry in the surrounding spherically symmetric envelope is studied for the isolated massive star-forming region AFGL 2591. A code was developed based on a previously published chemical model that solves for the time and depth-dependent molecular abundances. It is found that enhanced FUV fluxes lead to abundant radicals and ions in the inner few hundred AU of the envelope. Comparison between observations and models is improved with moderate FUV fluxes at the inner edge of the envelope.

In Chapter 3\textsuperscript{2}, the chemical reaction network is extended to allow the

\textsuperscript{1} based on Stäuber et al. (2004a)
\textsuperscript{2} based on Stäuber et al. (2005)
impact of X-rays from the central source on the protostellar envelope. Specific reactions – such as the secondary ionization through primary photoelectrons – are discussed. The chemistry in the envelope of AFGL 2591 is studied for different X-ray fluxes. In contrast to FUV, X-rays can enhance certain species in the envelope out to distances of a few thousand AU from the central source. The X-ray models improve the fits to observations in comparison to the FUV models.

Water is an important coolant in molecular gas and – after $\text{H}_2$ and CO – one of the most abundant species in star-forming regions. It will be extensively studied with the upcoming Herschel Space Observatory. Chapter 4\textsuperscript{3} therefore presents a detailed study of the water abundance in star-forming environments under the influence of X-rays and FUV fields. It is found that X-rays destroy water on (relatively) short timescales in regions with gas temperatures of $\lesssim 300\, \text{K}$. At higher temperatures, water can persist with high abundances even for high X-ray fluxes. Central FUV fields were found to have negligible influence, unless the photons can escape through cavities and irradiate regions at larger distances from the source.

In Chapter 5\textsuperscript{4}, observations of molecular lines in two high-mass objects and nine low-mass sources are presented. The observations were carried out using the James Clerk Maxwell Telescope on Mauna Kea, Hawaii. The observed ions and radicals are found to trace X-ray and FUV fluxes from the central source. The observations towards the high-mass objects were best interpreted by a FUV field irradiating the outflow walls, suggesting that the high-mass objects have low opacity outflows that allow the FUV photons to escape the central region. X-rays are predicted to be more effective than FUV fields in the low-mass objects.

Chapter 6 presents results of chemical models and a radiative transfer analysis of hydrides which will be observed with Herschel in the near future. Hydride abundances are studied for different gas temperatures, hydrogen densities, and X-ray and FUV fluxes. Tracers for the FUV field as well as for X-rays are discussed. It is found that carbon hydrides are excellent tracers for enhanced FUV fluxes. Nitrogen hydrides, on the other hand, are good tracers for X-rays.

The thesis concludes with a summary and an outlook on future work.

\textsuperscript{3}based on Stäuber et al. (2006a)
\textsuperscript{4}based on Stäuber et al. (2006b)
Zusammenfassung


\[\text{aus Stäuber et al. (2004a)}\]
Zusammenfassung
dert AU führen. Modelle mit einem moderaten FUV Fluss im inneren Bereich der Hülle erzeugen, im Vergleich zu früheren Beobachtungen von Moleküllinien, bessere Resultate als jene ohne FUV Strahlung.


⁶aus Stäuber et al. (2005)
⁷aus Stäuber et al. (2006a)
⁸aus Stäuber et al. (2006b)
Röntgenstrahlung eine wichtigere Rolle als die FUV Strahlung.


Eine (englische) Zusammenfassung und ein Ausblick auf zukünftige Arbeiten befinden sich am Ende dieser Arbeit.
Chapter 1

Introduction

I can believe in anything, provided that it is quite incredible

Oscar Wilde

1.1 The formation of stars

The birth sites of stars are dense clouds of molecules and dust. Stars like our Sun (so called low-mass stars with $M \lesssim 1 \, M_\odot$) are believed to be formed by gravitational "inside-out" collapse from dense cores (e.g., Shu et al. 1987). The widely accepted picture of evolutionary stages in low-mass star formation is based on observations of the spectral energy distribution (SED), which has led to a classification scheme of four classes (e.g., Lada 1987; André et al. 1993). The Class 0 and Class I objects are in the main accretion phase with SEDs peaking in the submillimeter to far-infrared. The central object builds up its mass from a surrounding infalling envelope and accretion disk. The main accretion phase is always accompanied by powerful outflows and jets, where a small fraction of the accreted material is ejected into the molecular surrounding. The phase lasts between $10^4$–$10^5$ yrs. The protostellar envelope is gradually dispersed by the radiation pressure and outflows leading to Class II objects which have massive (0.01–0.1 $M_\odot$) protoplanetary disks of gas and dust. Their SEDs show emission in the visible and infrared spectrum typical for a star-disk system. After $\approx 10^6$–$10^7$ yrs, the young object reaches the Class III phase with almost pure blackbody emission. The Class III sources are believed to be surrounded by debris disks from which
eventually planetary systems can further accrete.

Despite this evolutionary picture and physical understanding of low-mass star formation many details remain uncertain. For example, Class 0 objects may simply be surrounded by more massive envelopes than Class I sources and may not constitute a separate evolutionary state. The structure of the innermost region in Class 0/I objects is also not clear. Cavities (protostellar holes) are observed in envelopes around Class 0 objects with "300–600 AU radius in size (e.g., Jørgensen et al. 2005a). Whether such cavities are typical around the youngest objects remains uncertain. Related to this is the question of where the disk ends and the envelope begins, that is the size of the centrifugal radius. Once the star is born, it starts to illuminate its surrounding envelope, changing the physical and chemical composition. But what does this radiation look like? Are X-rays and/or ultraviolet (UV) photons already present at this stage? If so, what is the flux of these highly energetic photons at distances comparable to the innermost region of the envelope or on the surface of the young disk? The influence of X-ray and UV fluxes on the surrounding protostellar material will be studied in the Chapters 2, 3 and 4.

The picture is even less clear when it comes to the formation of high-mass stars \((M \gtrsim 8 \, M_\odot)\). The dividing line between high- and low-mass stars is set by two relevant timescales: the accretion timescale of the envelope \(t_{\text{acc}} = M_*/\dot{M}_{\text{acc}}\) and the contraction timescale of the protostar, the so-called Kelvin-Helmholtz timescale \(t_{\text{KH}} = GM_*^2/R_*L_*\). Here we have introduced with \(M_*, R_*, \) and \(L_*\) respectively the mass, radius and luminosity of the protostar, and with \(\dot{M}_{\text{acc}}\) the mass accretion rate. Low-mass stars have \(t_{\text{acc}} < t_{\text{KH}}\), the two timescales become equal for \(M_* \approx 8 \, M_\odot\), and for larger masses, \(t_{\text{acc}} > t_{\text{KH}}\) (e.g., Cesaroni 2005). High-mass stars thus reach the main sequence when they are still accreting matter, deeply embedded in their natal molecular cloud. The radiation pressure and copious UV flux emitted by O-B stars, however, are bound to halt the collapse and disrupt the surrounding environment, preventing further mass accretion. Massive stars \((M \gtrsim 8 \, M_\odot)\) should therefore never form and yet they are widely observed. Two different scenarios are currently believed to lead to massive stars. One scenario is that high-mass stars are formed like the lower mass stars via (non-spherical) accretion of ambient interstellar matter with sufficiently large accretion rates (e.g., Tan & McKee 2002). Others suggest that massive stars may be formed via coalescence of intermediate mass protostars \((M_* \lesssim 8 \, M_\odot; \text{c.g., Bonnell} \& \text{McKee} 2002)\).
1.2. Feedback processes

Bate (2002). However, observations of powerful bipolar outflows associated with rotating circumstellar disks support the scenario of the scaled version of low-mass star-formation with larger mass accretion rates (e.g., Churchwell 1997; Garay & Lizano 1999; Cesaroni 2005).

An evolutionary scenario based on the SED proves to be more complicated for high-mass objects. Deriving SEDs for individual protostellar sources is difficult mainly due to the larger distances of most high-mass objects \(d > 1\, \text{kpc}\) which leads to low spatial resolution. However, an evolutionary picture has been proposed where accreting High-Mass Protostellar Objects (HMPOs) evolve by the formation of a Hot Molecular Core (HMC), Hypercompact HII regions (HCHIIs, size < 0.01 pc), which eventually will form Ultracompact HII regions (UCHIIs, size < 0.1 pc) and finally an extended HII region (e.g., Churchwell 2002; Beuther et al. 2006). Protostellar disks are predicted to be evaporated by the central UV field (e.g., Yorke & Welz 1996) and planets may therefore never form around high-mass objects.

1.2 Feedback processes

The new born star irradiates its molecular environment at wavelengths from optical to X-rays. In addition, mass is ejected from the star-disk system, channeling energy and momentum to the outer medium. Such feedback processes lead to distinct regions with different temperatures, density and chemical compositions. Influence from outside the system comes mainly from cosmic rays, extremely energetic \(\approx 10-10^{14}\, \text{MeV}\) nuclei that penetrate everywhere, processing gas and dust through collisions. The feedback processes are discussed in the next sections. A summary is presented in Fig. 1.1 for a young high-mass object. The chemistry of such regions will be discussed in Sect. 1.3.

1.2.1 Outflows

Most, if not all, stars produce energetic outflows during their formation (e.g., Arce et al. 2006). The physical processes, however, that initially launch the outflowing material are not well understood. It is suggested that fast winds originating either at the star or at the accretion disk sweep up ambient molecular gas, forming two cavities perpendicular to
Figure 1.1: Feedback processes of a young stellar object on its surrounding envelope (not to scale). Also included are cosmic rays from outside the system (dashed-dotted line). "HH" refers to Herbig Haro object. The shaded shells mark regions with different temperatures, densities and sources of ionization. These regions are likely to be extended to larger distances from the protostar along the outflow walls (not shown in the figure). The distances given in the figure correspond roughly to those of high-mass objects. The scales in low-mass objects are up to an order of magnitude smaller. The innermost region (< 1000 AU) is usually not resolved with current instrumentation and provides the largest uncertainty.

the protostellar disk (e.g., Shu et al. 1994). Outflows interact with the molecular environment by injecting energy and momentum into the gas at distances ranging from a few AU to up to tens of parsecs away from the protostar. On impact, shocks occur, altering the density, temperature and thus the chemical composition of the gas.

Molecular outflows can be traced by CO line wings (e.g., Phillips et al. 1988). Observed outflow velocities are between 10–100 km s⁻¹ with mass outflow rates up to ≈ 10⁻⁶ M☉ yr⁻¹ in the low-mass objects and between ≈ 10⁻⁵–10⁻³ M☉ yr⁻¹ in the high-mass sources. The outflows evolve with the age of the protostar. The most powerful outflows with the largest degree of collimation are thus driven by the youngest embedded protostars (e.g., Nisini et al. 2002; Beuther & Shepher 2005).
1.2. Feedback processes

This is also the phase where protostellar jets are produced. The more collimated and faster jets are suggested to be the driving force of molecular outflows. They have temperatures of $\approx 10^4 \text{ K}$ and move away from the sources at speeds $\approx 100$–$500 \text{ km s}^{-1}$ (e.g., de Gouveia dal Pino 2005). Jets produce chains of knots that manifest themselves as Herbig Haro (HH) objects and are often observed in lines of neutral atoms and ions (e.g., [HI], [OI], [CI], [FeII], [SII]). HH objects are commonly observed towards low-mass young stellar objects. Although HH objects are also observed towards high-mass YSOs, optical manifestations of jets are hard to find there due to the large distances and heavy obscuration. Jet shocked regions are also the source of high energy radiation (e.g., Favata et al. 2002). The post-shock temperature is given by

$$T \approx 4 \times 10^6 \text{ K} \left( \frac{v_j}{500 \text{ km s}^{-1}} \right)^2$$

where $v_j$ is the jet velocity. The photon emission is therefore mainly in the EUV and soft X-ray regime for jet velocities in the range mentioned above.

The chemical properties of the envelope, however, can also be influenced indirectly by outflows: photons from the protostar are able to travel through the low-density outflow cavities and impact the outflow walls up to large distances from the central source. This will be further discussed in Chapter 5.

1.2.2 Radiation from the protostar

Radiation in the optical and ultraviolet wavelength range ($h\nu \gtrsim 1 \text{ eV}$) heats the dust in the surrounding envelope. After collapse, the dust temperature thus rises from $\approx 10 \text{ K}$ in the outer part of the envelope to $\gtrsim 1000 \text{ K}$ close to the protostar. At higher temperatures ($\gtrsim 2000 \text{ K}$), however, heavy elements return into the gas-phase until the dust particle is completely evaporated. In the inner part of the envelope, the dust and gas temperature are well coupled, while the gas temperature in the outer region can be below the one for dust due to CO rotational emission (Doty & Neufeld 1997).

Extreme UV (EUV; $h\nu \geq 13.6 \text{ eV}$) photons ionize atomic hydrogen. They are thus completely absorbed by hydrogen, forming HII regions around massive stars where the EUV is re-radiated at longer wavelengths.
This shields the molecules deeper inside the envelope from the EUV. The photons are typically absorbed within a few AU for hydrogen densities $n_H \gtrsim 10^6 \text{cm}^{-3}$.

Far UV (FUV; $6 \text{eV} < h\nu < 13.6 \text{eV}$) photons can penetrate the HII region and ionize atoms such as carbon and dissociate molecular hydrogen and CO. The dissociation process of these two important molecules occurs in an indirect way, where the initial absorption leads to a bound discrete excited state which then interacts with the continuum of a final dissociating state (e.g., van Dishoeck 1988). The molecules deeper inside the cloud, however, are shielded from the FUV by other species, dust and themselves (self-shielding). FUV irradiated regions are called Photon Dominated Regions (or Photo-Dissociation Regions; PDRs). At optical depths $A_V^1 \lesssim 1$, the gas is mainly in the form of H, C$^+$ and atomic oxygen. The transition H to H$_2$ and C$^+$ to CO occurs at $A_V$ of a few and O to O$_2$ at $A_V \approx 10$ (e.g., Hollenbach & Tielens 1999). The gas in PDRs is mainly heated by the photoelectric effect on dust grains and PAHs (polycyclic aromatic hydrocarbons) and far-ultraviolet pumping of H$_2$ (through collisional deexcitation). The gas temperature can reach up to a few 1000 K.

The production of UV photons is coupled to the effective temperature and bolometric luminosity of the source ($L_{\text{bol}} = 4\pi R_*^2 \sigma_B T_{\text{eff}}^4$, where $\sigma_B$ is the Stefan-Boltzmann constant). Following Wien's displacement law ($\lambda_{\text{max}} T_{\text{eff}} = 0.29 \text{cm K}$), a protostar with $T_{\text{eff}} = 10^4 \text{K}$ emits most energy in the ultraviolet wavelength range, assuming blackbody radiation. Massive O and B stars ($T_{\text{eff}} \gtrsim 10^4 \text{K}$) therefore produce much higher UV fluxes in comparison to the low-mass objects with typically $T_{\text{eff}} \lesssim 6000 \text{K}$. However, accretion can heat the gas in shocks and increase the bolometric luminosity to (Stahler & Palla 2005)

$$L_{\text{acc}} = \frac{G\dot{M}M_*}{R_*}$$
$$\approx 61L_\odot \left(\frac{\dot{M}}{10^{-5} \text{M}_\odot \text{yr}^{-1}}\right) \left(\frac{M_*}{1\text{M}_\odot}\right) \left(\frac{R_*}{5R_\odot}\right)^{-1}, \quad (1.2)$$

$^1A_V = 1$ corresponds to a hydrogen column density of $\approx 2 \times 10^{21} \text{cm}^{-2}$.
1.2. Feedback processes

with

\[
T_{\text{eff}} \approx \left( \frac{G M_* \dot{M}}{4\pi \sigma_B R_*^2} \right)^{1/4}
    \approx 7300 \, \text{K} \left( \frac{\dot{M}}{10^{-5} \, \text{M}_\odot \, \text{yr}^{-1}} \right)^{1/4} \left( \frac{M_*}{1 \, \text{M}_\odot} \right)^{1/4} \left( \frac{R_*}{5 \, \text{R}_\odot} \right)^{-3/4},
\]

assuming that all kinetic energy is converted to radiation and where \( G \) is the gravitation constant. Thus, a heavily accreting protostar with \( \dot{M} \approx 10^{-4} \, \text{M}_\odot \, \text{yr}^{-1} \) can have an effective temperature similar to those of high-mass objects. Such high accretion rates (\( \dot{M} \approx 5 \times 10^{-5} \, \text{M}_\odot \, \text{yr}^{-1} \)) have indeed been estimated for Class 0 objects (e.g., Bontemps et al. 1996; Schöier et al. 2002; Maret et al. 2002). The effect of UV radiation on the molecular surrounding depends also on the shape of the spectrum and on line emission (e.g., Bergin et al. 2003) which will be different in shock produced UV fields. The radiation field in shocks is predicted to have high contribution of Lyman \( \alpha \) radiation due to recombination and collisional excitation of atomic hydrogen. However, these subtleties are usually ignored and the strength of the FUV radiation field, \( G_0 \), is in general expressed in units of the Habing (1968) or Draine (1978) field. The difference between the two estimates of the interstellar radiation field intensity is typically within a factor of two (e.g., van Dishoeck 1988).

X-rays (\( \approx 0.1-100 \, \text{keV} \)) have smaller cross sections with increasing energy. Hard X-rays (\( \gtrsim \) a few keV) can penetrate clouds with up to \( A_V \approx 100 \). X-rays heat the gas and influence the chemistry. The dominant parameter controlling the condition of the gas in X-ray dominated regions (XDRs) is the ratio of the local energy deposition rate \( H_X \) to gas density (Maloney et al. 1996). \( H_X \) is given by

\[
H_X = \int \sigma(E) F(E) \, dE \quad [\text{erg s}^{-1}],
\]

where \( \sigma \) is the total X-ray absorbing cross section per hydrogen atom and \( F(E) \) is the local X-ray flux in erg s\(^{-1}\) cm\(^{-2}\).

A characteristic feature of XDRs is that the ionization rate of hydrogen is dominated by the so called secondary ionizations, i.e. the ionizations generated by the photoelectrons. This is due to the fact that the primary photoelectron carries the bulk energy of the X-ray photon (\( \sim \text{keV} \)) and can therefore efficiently ionize other species. At high ionization fractions (\( x_e \approx 1 \)), however, the energy of the primary photoelectron
Figure 1.2: X-ray luminosity vs. stellar (isochronal) age for the stars in the COUP sample (Preibisch & Feigelson 2005).

goes mainly into heating through Coulomb interactions with other electrons. The gas temperatures in XDRs with high $H_X/n$ ratios ($x_e \approx 0.1$) can get $\approx 10^4$ K. The gas then consists of H, C, O and C$. With decreasing $H_X/n$ values ($x_e \lesssim 10^{-3}$), the gas is molecular and the temperature $\lesssim 200$ K.

The X-ray luminosity observed towards young stellar objects (YSOs) is typically between $10^{28}-10^{33}$ erg s$^{-1}$ (e.g., Preibisch & Feigelson 2005; Ezoe et al. 2006). The emission is explained by a thermal plasma with temperatures $\gtrsim 1$ keV. Differences in luminosity and plasma temperature between low and high-mass YSOs are usually small (e.g., Nakajima et al. 2003). Observations of a large sample of low-mass protostars indicate that the average X-ray luminosity is correlated with the protostellar mass and anti-correlated with the stellar age (Fig. 1.2; Preibisch & Feigelson 2005), indicating that the youngest sources are the strongest X-ray emitters. Although it is generally agreed that magnetic activity causes the extremely high temperatures ($T \propto B^2$), the mechanisms at work are not
known. For low-mass objects, it is suggested that a turbulent convective dynamo in the stellar source builds up the magnetic energy that can be converted into heat (e.g., Preibisch & Feigelson 2005) or that field lines connecting the protostar with the circumstellar disk eventually lead to reconnection events where the gas is heated (e.g., Favata et al. 2005). A detailed review on this matter is given by Feigelson & Montmerle (1999). Strong winds and/or magnetic fields are believed to be the X-ray driving source in high-mass objects. X-rays emitted in shocks of strong winds can reach plasma temperatures of a few keV for wind velocities of 1000–2000 km s\(^{-1}\) (Eq. 1.1). Assuming the kinetic energy to be fully converted into X-rays, the X-ray luminosity of this diffuse emission can be as high as (Ezoe et al. 2006)

\[
L = \frac{1}{2} \dot{M} v_w^2 \\
\approx 10^{35} \text{erg s}^{-1}\left(\frac{\dot{M}}{10^{-7} \text{M}_\odot \text{yr}^{-1}}\right)\left(\frac{v_w}{2000 \text{ km s}^{-1}}\right)^2, \tag{1.5}
\]

where \(\dot{M}\) is the mass loss rate and \(v_w\) the wind velocity. Intermediate mass protostars on the other hand, have no convective zone and no strong winds. X-ray observations towards these sources are explained either by fossil magnetic fields or by an X-ray emitting companion low-mass protostar (e.g., Stelzer et al. 2005).

1.3 Chemistry in star-forming regions

The chemical composition of the gas alters dramatically during the process of star formation. The physical condition, that is the temperature, the density, the rate of ionization and the velocity structure can be probed by the observation of molecular lines. Detailed reviews on the chemistry near young stellar objects are given, for example, by van Dishoeck & Hogerheijde (1999), van Dishoeck (2003) and Caselli (2005).

The first chemically distinct stage in star-formation is set by dense, starless cores. In comparison to molecular clouds, prestellar cores have similar temperatures \(T \lesssim 20 \text{ K}\) but higher densities \((n \gtrsim 10^4 \text{ cm}^{-3})\). Regions in these cores exist where the density and temperature are high and low enough, respectively, that molecules like CO can (partially) freeze out
on grains (Jørgensen et al. 2005b). Other molecules (e.g., N$_2$H$^+$), however, remain in the gas-phase, allowing to study the density structure and cosmic ionization rate of the cores. During this prestellar phase, grain surface chemistry efficiently produces more complex molecules. Since hydrogen is the most abundant and "mobile" element, many hydrogenated species (e.g., H$_2$O, NH$_3$, CH$_4$, H$_2$CO, CH$_3$OH) are formed. Another important process on grains is the oxidation of species, that leads to (among others) CO$_2$.

After the core is collapsed, the surrounding dust and gas is heated by radiation and accretion events. Molecules formed on grains are liberated into the gas-phase following their desorption temperatures. Based on observations and chemical models, an onion like shell structure has been suggested to be around YSOs (e.g., van Dishoeck & Hogerheijde 1999). The evaporation of molecular ices together with an enriched chemistry due to hot gas temperatures leads to chemically rich hot molecular cores. Typical hot core species such as H$_2$CO, CH$_3$OH or CH$_3$CN have been observed towards several high and low-mass star-forming regions (e.g., Hatchell et al. 1998; Ceccarelli ct al. 2000a). While the hot core molecules are generally believed to trace the inner part of the envelope in high-mass sources, it is not clear where the complex molecules in low-mass objects come from. Since the envelope may not be hotter than $\approx$ 80 K by the presence of inner cavities, the organic molecules may as well trace the protostellar disk where the temperature can exceed 100 K (e.g., Schöier et al. 2005a).

The earliest stage after collapse is also the most powerful outflow phase. Outflows and shocks are commonly observed in YSOs (Sect. 1.2). Depending on the shock velocity, C-shocks and J-shocks can be distinguished. In C-shocks, the hydrodynamic fluid variables change smoothly and continuously. Shock velocities are $\lesssim$ 40 km s$^{-1}$. J-shocks have fluid variables that undergo a discontinuous jump and velocities are $>$ 40 km s$^{-1}$. Chemically, C-shocks are characterized by the liberation of volatile molecules (e.g., CH$_3$OH) from grains through sputtering erosion (e.g., Caselli et al. 1997) and by a hot gas chemistry ($T \approx$ 1000 K) which results in copious H$_2$O, SO and SO$_2$. J-shocks on the other hand can heat the gas up to $10^5$ K and produce large amounts of UV photons (Sect. 1.2), creating a molecule-free zone (e.g., Hollenbach & McKee 1989).

The impact of UV photons and X-rays originating from the central
1.3. Chemistry in star-forming regions

Figure 1.3: Fractional electron abundances (solid line) for the high-mass envelope model of AFGL 2591 without X-rays (black) and with X-rays (grey), assuming a central X-ray luminosity of $L_X = 10^{31}$ erg s$^{-1}$. The position is given as radial distance to the central source. In the X-ray models, $x_e$ is comparable within a factor of $\approx 2$ to the fractional HCO$^+$ abundance (dotted line). In the models without X-rays, $x_e$ is traced by HCO$^+$ in the cold outer part of the envelope ($T \lesssim 100$ K, $r \gtrsim 1000$ AU) and by H$_3$O$^+$ in the inner hot part. Other contributions to the ionization fraction are mainly from H$_3^+$, NH$_4^+$, HCS$^+$, HCNH$^+$. The impact of X-rays or FUV photons will lead to high fractions of ionization close to the protostar. The ionization fraction ($x_e$) can be

source or from shocks on the surrounding material leads to a distinct chemistry. PDRs typically show an enhanced carbon chemistry, ranging from atomic and ionized carbon to more complex carbon chains, depending on the incident FUV flux (e.g., Teyssier et al. 2004). Little has been known so far about the influence of X-rays on the chemistry around YSOs. In comparison to FUV photons ($h\nu < 13.6$ eV), X-rays are more energetic and can also ionize, for example, hydrogen, oxygen and nitrogen and even doubly ionize certain species. An enhanced nitrogen and oxygen chemistry can thus be expected (e.g., Lepp & Dalgarno 1996). Table 1.1 provides the ionization potential for a few species.

The impact of X-rays or FUV photons will lead to high fractions of ionization close to the protostar. The ionization fraction ($x_e$) can be
Chapter 1. Introduction

Table 1.1: Ionization potentials $E_{ip}$.

<table>
<thead>
<tr>
<th>Species</th>
<th>$E_{ip}$ (eV)</th>
<th>Species</th>
<th>$E_{ip}$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>13.60</td>
<td>Si</td>
<td>8.15</td>
</tr>
<tr>
<td>He</td>
<td>24.60</td>
<td>S</td>
<td>10.36</td>
</tr>
<tr>
<td>C</td>
<td>11.26</td>
<td>Fe</td>
<td>7.90</td>
</tr>
<tr>
<td>N</td>
<td>14.53</td>
<td>H$_2$</td>
<td>15.60</td>
</tr>
<tr>
<td>O</td>
<td>13.62</td>
<td>CO</td>
<td>14.10</td>
</tr>
</tbody>
</table>

traced in molecular envelopes by the observations of molecular ions as shown in Fig. 1.3. These ions are typically enhanced for moderate X-ray fluxes (Chapter 3). Typical ionization fractions in clouds or regions in the envelope that are dominated by cosmic-ray ionization are $x(e) \approx 10^{-9}$–$10^{-8}$. This fraction can be 10–100 times higher in the inner part of the envelope due to X-rays. The ionization fraction in PDRs, on the other hand, is comparable to the fractional C$^+$ abundance, since this is the most abundant ion under the influence of strong FUV fields. High FUV fluxes typically lead to $x(e) \approx 10^{-6}$–$10^{-4}$. The influence of FUV fields and X-rays from the central source on the surrounding protostellar envelope will be studied and discussed in the Chapters 2 and 3.

1.3.1 Chemical processes

Chemical processes that have to be considered in the gas-phase are listed in Table 1.2. The density in the gas around YSOs is low enough to assume all chemical reactions to be binary in nature and ternary processes can be neglected. Since reactions of molecules involve the breaking of chemical bonds, most reactions have appreciable activation energy ($E_a$) even if exothermic. Neutral-neutral reactions are therefore slow at cold temperatures. The most prominent reaction of that type is the formation of water through OH + H$_2$ → H$_2$O + H, which is only efficient at temperatures above $\approx 250$ K. The rate coefficient of such reactions can be expressed by the Arrhenius formula

$$k(T) = A(T)\exp(-E_a/k_BT) \quad [\text{cm}^3\text{s}^{-1}]$$

(1.6)

where $k_B$ is the Boltzmann constant, $T$ is the gas temperature and $A(T)$ is the preexponential factor, a weak function of the temperature (usually
approximated by a power-law \( \alpha T^\beta \). The reaction rate for a generic reaction \( A + B \rightarrow C + D \) is obtained by multiplying the rate coefficient with the densities of the reactants. This compares then to the rate at which a species is formed or destroyed, for example

\[
\frac{dn_A}{dt} = -n_A n_B k_{AB} \quad [\text{cm}^{-3} \text{s}^{-1}],
\]

\[
\frac{dn_C}{dt} = +n_A n_B k_{AB} \quad [\text{cm}^{-3} \text{s}^{-1}].
\]

Radiative association reactions are the only way to form molecular bonds in the gas-phase. However, these reactions are rather slow and formation of molecules on grain surfaces are usually more important. Especially \( \text{H}_2 \), the most abundant species in molecular gas, is believed to be formed on grains (e.g., Hollenbach & Salpeter 1971).

Important for the chemistry of cold gas are ion-molecule reactions (e.g., Herbst & Klemperer 1973). These reactions have no activation barrier. Due to the long-range attraction between the molecule and the ion, the reactions proceed relatively fast and the temperature-independent rate coefficient is given by

\[
k_L = 2\pi e \left( \frac{\alpha_p}{\mu_m} \right)^{1/2} \quad [\text{cm}^3 \text{s}^{-1}],
\]

the so called Langevin rate, where \( e \) is the electronic charge, \( \alpha_p \) is the polarizability \( [\text{cm}^3] \) and \( \mu_m \) is the reduced mass. Owing to the strong Coulomb interaction, recombination reactions tend to be rapid and are often dissociative.

Photodissociation and ionization are fast and can be even enhanced when the gas is exposed to a strong source of radiation. Ionization and dissociation can also occur by the impact of highly energetic photo-electrons (\( \gtrsim 1 \text{ eV} \)) originating from X-ray ionization of, for example, \( \text{H}_2 \).

### 1.4 Molecular excitation

Molecules can have electronic, vibrational or rotational energy transitions \( (E = E_{el} + E_{vib} + E_{rot}) \). A change in the electronic configuration, however, occurs only at \( \gtrsim 1 \text{ eV} \) \( (T \approx 10000 \text{K}) \), which corresponds to the visible
Table 1.2: Chemical gas-phase reactions.

<table>
<thead>
<tr>
<th>Type</th>
<th>Process</th>
<th>Rate coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutral-neutral</td>
<td>A + B → C + D</td>
<td>~10^{-9} cm^{3}s^{-1}</td>
</tr>
<tr>
<td>Radiative association</td>
<td>A + B → AB + h\nu</td>
<td>~10^{-16} cm^{3}s^{-1}</td>
</tr>
<tr>
<td>Ion-molecule</td>
<td>A^{+} + B → C^{+} + D</td>
<td>~10^{-9} cm^{3}s^{-1}</td>
</tr>
<tr>
<td>Charge transfer</td>
<td>A^{+} + B → A + B^{+}</td>
<td>~10^{-9} cm^{3}s^{-1}</td>
</tr>
<tr>
<td>Dissociative recombination</td>
<td>AB^{+} + e → A + B</td>
<td>~10^{-6} cm^{3}s^{-1}</td>
</tr>
<tr>
<td>Photodissociation</td>
<td>AB + h\nu → A + B</td>
<td>~10^{-9} cm^{3}s^{-1}</td>
</tr>
</tbody>
</table>

or ultraviolet wavelength regime. Vibrational motion of the nuclei requires typically \( \approx 0.1 \text{eV} \) \((T \approx 1000 \text{K})\). These transitions are observable at infrared wavelengths. The rotational levels, on the other hand, can already be excited in cold gas \((T \gtrsim 5 \text{K})\). For a rigid rotor, the rotational energy levels of linear molecules are given by \(E_J = BJ(J+1)\), where \(B\) is the rotational constant and \(J\) the rotational quantum number. The energy levels can be further split due to coupling between the various angular momenta. Important cases are the coupling between the electronic spin and the total angular momentum in molecules with \(^{>1}\Sigma\) (e.g., CN, SO), "\(\Lambda\)-Doubling" in molecules with a total electronic orbital momentum \(L = 1\) and non-zero total spin (e.g., NO, OH), and hyperfine splitting, where the nuclear spin couples to the rotation (e.g., CN, \(\text{N}_2\text{H}^+\)).

Molecules can be excited either by collisions or by radiation. The background radiation field \((T = 2.73 \text{K})\) is important in the millimeter regime for heavy molecules, since their energy levels are closely spaced. Dust emission in the infrared is more important for the lighter hydrides (e.g., CH, OH and \(\text{H}_2\text{O}\)). Since \(\text{H}_2\) is the most abundant species in the gas, collisional excitation is dominated by hydrogen. However, excitation through collisions with electrons can become important in regions with high ionization fractions \((x(e) \gtrsim 10^{-5}; \text{e.g., Jansen 1995})\).

Level populations \(n_i\) due to radiative and collisional processes are given by the statistical equilibrium equations

\[
n_i \sum_{j<i} A_{ij} + n_i \sum_{j} (B_{ij} \bar{J} + C_{ij}) = \sum_{j>i} n_j A_{ji} + \sum_{j} n_j (B_{ji} \bar{J} + C_{ji}), \quad (1.9)
\]

where \(A_{ij}\) and \(B_{ij}\) are the Einstein \(A\) and \(B\) coefficients for spontaneous and stimulated emission and absorption, \(\bar{J}\) is the intensity of radiation.
field averaged over all directions and integrated over the line profile, and $C_{ij}$ is the collisional rate between levels $i$ and $j$. $C_{ij}$ is the product of $n_{\text{col}}$, the density of the collision partner (e.g., $H_2$), and $K_{ij}$, the rate coefficient, which is the velocity integrated cross section. The upward and downward rate coefficients for an upper level $u$ and a lower level $l$ are related through $K_{lu} = K_{ul}(g_u/g_l)\exp(-hv/k_BT)$, where $g$ is the statistical weight. The Einstein coefficients are given by $g_lB_{lu} = g_uB_{ul}$ and

$$A_{ul} = \frac{2hv^3}{c^2} B_{ul} = \frac{64\pi^4\nu^3\mu^2 S_{ul}}{3c^3h} g_u,$$

where $\mu$ is the electric dipole moment and $S_{ul}$ is the transition strength. For transitions with $\Delta J \pm 1$ in linear molecules, the transition strength $S_{ul}$ is $g_l$.

Collisional processes are comparable to radiative processes if the two timescales are equal, that is $1/A_{ji} = 1/\sum_i C_{ji}$. This defines the critical density $n_{\text{crit}} = A_{ji}/\sum_i K_{ji}$ where level $i$ is substantially populated. Since $A_{ji} \propto \mu^2 \nu^3$, molecules with large dipole moments and transitions with high frequencies have higher critical densities. A large range of densities can therefore be probed by choosing the appropriate molecule and transition (e.g., Jansen 1995; van Dishoeck & Hogerheijde 1999). Molecular transitions contain therefore not only information about their abundance but also about the excitation condition, that is the temperature and gas density.

### 1.4.1 Radiative transfer

The averaged intensity of the radiation field $\bar{J}$ in Eq. (1.9) is related to the observed intensity $I_\nu$ through

$$\bar{J} = \frac{1}{4\pi} \int \int I_\nu \phi(\nu) d\Omega d\nu$$

where $\phi(\nu)$ is the line profile. The observed intensity $I_\nu$ of a transition is obtained by solving the radiative transfer equation

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + J_\nu$$
with $\alpha_\nu$ and $j_\nu$ being the absorption and emission coefficients, respectively. The relation between $I_\nu$ and $J$ couples the equations for the level population to the radiative transfer. However, the formal solution of Eq. (1.12) is the sum of the fraction of background emission and radiation emitted by the medium itself:

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} S(\tau_\nu')e^{-(\tau_\nu-\tau_\nu')} d\tau_\nu'.$$

(1.13)

The source function $S_\nu$ is the ratio $\alpha_\nu/j_\nu$ and $\tau_\nu$ is the optical depth defined by

$$\tau_\nu = \int_0^s \alpha_\nu(s')ds'.$$

(1.14)

Defining an excitation temperature $T_{\text{ex}}$, the source function can be expressed by the Planck function $B_\nu(T_{\text{ex}})$ and the general solution for a homogeneous medium with $I_\nu(0) = 0$ is

$$I_\nu = B_\nu(T_{\text{ex}})(1 - e^{-\tau_\nu}).$$

(1.15)

In the Rayleigh-Jeans limit, the radiation temperature can be defined by

$$T_R = \frac{c^2}{2k_B\nu^2}I_\nu.$$

(1.16)

In terms of observed temperatures at a telescope, $T_R$ states an upper limit since the size of the emitting source may be smaller compared to the beam width of the telescope. By introducing a beam filling factor $\eta_B$, the main beam temperature is $T_{\text{mb}} = \eta_B T_R$.

### 1.4.2 From models to observations to models

A growing number of (Sub-)millimeter and infrared telescopes (for example, the James Clerk Maxwell Telescope (JCMT), the Submillimeter Array (SMA), the Caltech Submillimeter Observatory (CSO), the IRAM telescopes, the Infrared Space Observatory (ISO), the Spitzer Space Telescope - just to name a few) provide important data of molecular and dust emission at various wavelengths and spatial resolution. However, the interpretation of these observations is not straightforward since it usually requires a prerequisite model of the region, that is the spatial distribution of density and temperature.
1.4. Molecular excitation

Many studies of star-forming cores or envelopes therefore start with an analysis of the spatial distribution of the submillimeter continuum emission from dust and its spectral energy distribution (e.g., van der Tak et al. 2000a; Jørgensen et al. 2002). The density profile as a function of radius \( n \propto r^{-p} \) and the dust temperature structure \( T_d(r) \) can be calculated self-consistently through continuum radiative transfer. The gas temperature can either be taken to be equal to \( T_d \) (as a good approximation, Doty & Neufeld 1997) or calculated from a detailed chemical model by solving the full thermal balance of the gas. The level populations, radiative transfer and line fluxes of molecular transitions can then be calculated for an assumed abundance \( x(r) = n_M(r)/n_{H_2}(r) \) until agreement is found between modeled and observed line flux. Observations of two or more transitions of one molecule allow to study the spatial distribution of the molecule. In these studies "jump" or "drop" profiles are considered in which the assumed fractional abundance is increased by a large factor in the inner warm region or lowered in the colder outer part of the envelope due to freeze-out effects (e.g., Schöier et al. 2002; Jørgensen et al. 2005b).

In full chemical models, the rate equations (Eq. 1.7) for a large set of species and chemical reactions are solved dependent on the radial distance to the central source. The calculated abundances can be compared to the observed abundances in order to constrain the chemical age (e.g., Doty et al. 2002), the ionization rate (e.g., Doty et al. 2004), dynamical properties (e.g., Ceccarelli et al. 1996; Rodgers & Charnley 2003) or simply estimate abundances of unobserved species. It should be mentioned, however, that large uncertainties exist in some rate coefficients and more theoretical and experimental studies on this subject are necessary in order to improve the accuracy of chemical models.

To study the influence of FUV fields and X-rays on the environment of YSOs, chemical models are constructed and compared to observations. This will be discussed in the Chapters 2, 3, and 4. In order to test the models and to find tracers for high-energy radiation from protostars, observations of several molecular lines are performed using the JCMT on Mauna Kea, Hawaii. They will be presented and discussed in Chapter 5.

Upcoming observatories such as the Atacama Large Millimeter Array (ALMA) or the Herschel Space Observatory (Fig. 1.4) will supply astronomers with thousands of terabytes of data that will eventually improve our current understanding of the physical and chemical properties of star-forming regions. ALMA will be able to spatially resolve the in-
Figure 1.4: ESA’s cornerstone Herschel Space Observatory will explore the universe in the far-infrared and sub-millimeter wavelength regime. Its mirror is 3.5 m – the largest mirror ever built for a space telescope. Herschel will be launched in 2008.

Figure 1.4: ESA’s cornerstone Herschel Space Observatory will explore the universe in the far-infrared and sub-millimeter wavelength regime. Its mirror is 3.5 m – the largest mirror ever built for a space telescope. Herschel will be launched in 2008.

nermost regions whereas Herschel observes the Universe at submillimeter and far-infrared wavelengths that are not accessible from ground based telescopes due to earth’s atmospheric absorption. The last section (Chapter 6) is dedicated to future observations with Herschel.
Chapter 2

Influence of UV radiation from a massive YSO on the chemistry of its envelope

ABSTRACT: We have studied the influence of far ultraviolet (UV) radiation ($6 < h\nu < 13.6$ eV) from a massive young stellar object (YSO) on the chemistry of its own envelope by extending the models of Doty et al. (2002) to include a central source of UV radiation. The models are applied to the massive star-forming region AFGL 2591 for different inner UV field strengths. Depth-dependent abundance profiles for several molecules are presented and discussed. We predict enhanced column densities for more than 30 species, especially radicals and ions. Comparison between observations and models is improved with a moderate UV field incident on the inner envelope, corresponding to an enhancement factor $G_0 \approx 10-100$ at 200 AU from the star with an optical depth $\tau \approx 15-17$. The chemical networks of various species are explored. Subtle differences are found compared with traditional models of Photon Dominated Regions (PDRs) because of the higher temperatures and higher gas-phase H$_2$O abundance caused by evaporation of ices in the inner region. In particular, the CN/HCN ratio is not a sensitive tracer of the inner UV field, in contrast with the situation for normal PDRs: for low UV fields, the extra CN reacts with H$_2$ in the inner dense and warm region and produces more HCN. It is found that the CH$^+$ abundance is strongly enhanced and grows steadily with increasing UV field. In addition, the ratio CH$^+$/CH is increased by a factor of $10^3$-$10^5$ depending on the inner UV flux. High-$J$ lines of molecules like CN and HCN are most sensitive to the inner dense
region where UV radiation plays a role. Thus, even though the total column density affected by UV photons is small, comparison of high-$J$ and low-$J$ lines can selectively trace and distinguish the inner UV field from the outer one. In addition, future Herschel-HIFI observations of hydrides can sensitively probe the inner UV field.

### 2.1 Introduction

A newly formed massive star in the earliest stages of evolution is surrounded by a dense envelope and is deeply embedded in its natal molecular cloud. Although highly obscured, these objects show signs of different stellar activity. Radio continuum observations reveal compact HII regions close to the young star (e.g., Churchwell 2002) and molecular outflows have been observed toward numerous massive star-forming regions (Shepherd & Churchwell 1996; Beuther et al. 2002a). Outflows and high energy photons from the YSO can strongly affect both the physical and chemical structure of the envelope. Observational studies of massive YSO environments reveal rich molecular spectra with a large variety of species (see e.g., Blake et al. 1987, 1996; Turner 1989; Helmich & van Dishoeck 1997; Gibb et al. 2000). This molecular complexity is thought to be associated with a specific stage in the evolution of a massive young star—the so-called ‘hot core’ phase—in which selected molecules have just evaporated off the grains and drive a rich high temperature chemistry. However, there are also massive YSOs which do not show this molecular complexity, but where energetic phenomena can still cause chemical changes. Indeed, chemistry may be a unique diagnostic of the relative importance of different physical processes that occur within the YSO envelope, and a good understanding of chemistry is therefore crucial to comprehend the birth and evolution of massive stars.

Much effort has been put into the quest of understanding the physical and chemical structure of massive YSO envelopes in recent years. Van der Tak et al. (1999, 2000), Mueller et al. (2002) and Beuther et al. (2002b) investigated the physical structure of the envelopes around several massive young stars on $100-10^6$ AU scales, using lines of the CS molecule and continuum data. Adopting the resulting density profiles as input, Doty et al. (2002) calculated detailed gas temperature and chemical models to test these physical structures and, in particular, to study
the chemical evolution of the high-mass star forming region AFGL 2591. Self-consistent models of the gas and dust thermal balance, chemistry, and radiative transfer within YSO envelopes have also been performed by Doty & Neufeld (1997) for high-mass objects and Ceccarelli et al. (1996) for low-mass sources. Most recently, Rodgers & Charnley (2003) have modeled the chemistry of gravitationally collapsing low-mass YSO envelopes considering spatial density variations and gradual heating of the gas as well as temporal chemical evolution.

All of these models do not consider a central source of UV radiation, and include (at most) an external radiation field comparable to the average interstellar radiation field. The only exception is the work by Ceccarelli et al. (1991), who modeled the chemistry around a low-mass YSO with central UV radiation and calculated radial abundances between \( \approx 1000-10^5 \) AU. Their assumed density profile was flat rather than a power-law, whereby UV photons can penetrate further. The results from such models resemble those from standard models of photon-dominated regions (PDRs), in which the UV radiation from a hot star impacts a nearby molecular cloud. In these regions the physical and chemical structure is determined by the incident FUV field (6 eV < \( h\nu \) < 13.6 eV; see e.g., Sternberg & Dalgarno 1995; Hollenbach & Tielens 1999). PDRs are characterized by bright atomic fine-structure lines, strong high-\( J \) CO emission, PAHs and specific molecules like CN, C2H or CO+ (e.g., Jansen et al. 1995b; Störzer et al. 1996). Thus, while there is no doubt that UV photons affect their surroundings in the later stages of massive star evolution when the envelope is being dispersed, their importance in the early stages is still unclear.

The question whether or not UV radiation plays a role in the chemistry of YSO envelopes has been a hotly debated subject for some time. Because of the limited penetration depth of UV photons (typically a few magnitudes of visual extinction \( A_V \)), the bulk of the envelope with \( A_V > 100 \) mag must be unaffected. However, the presence of certain solid-state features, in particular the XCN or OCN\(^-\) band at 4.62 \( \mu \)m, is often cited as an indicator of 'energetic processing' (e.g., Pendelton et al. 1999). Whether this indeed implies the presence of UV radiation or simply requires higher temperatures is still uncertain. Indeed, recent laboratory experiments by van Broekhuizen et al. (2004) indicate that similar production efficiencies of OCN\(^-\) can be obtained with thermal heating of HNCO-containing mixtures, reducing its diagnostic value. PAH emission
is not detected in the earliest embedded stages, but this could be due either to freezing out of the PAHs onto grains or to the high extinction at infrared wavelengths. The aim of this paper is therefore to find other diagnostics of the inner UV field, in particular from molecular tracers whose (sub-)millimeter emission can penetrate the entire envelope.

We study here the chemistry in YSO envelopes under the influence of UV radiation from the central source as well as from an outside interstellar FUV radiation field. For this purpose, we have extended the time- and position-dependent detailed chemical model of Doty et al. (2002) to allow the impact of a central UV field on the inner envelope. In addition, we have used the resulting abundance profiles to compute emission lines of selected species using the Monte Carlo code of Hogerheijde & van der Tak (2000), for direct comparison with observations. Although our applications are focused on high-mass YSOs, the results should be equally applicable to the envelopes around low-mass sources, albeit that the origin of the UV radiation may be slightly different.

This paper is organized as follows. In Sect. 2.2, the physical and chemical model is described. The model is then applied to the envelope around AFGL 2591 and the results are discussed. We examine the highly abundant molecules CO, H$_2$O and CO$_2$ in Sect. 2.3.1. In Sect. 2.3.2 we discuss the 'PDR-related' elements and ions C, O and C$^+$. The reactive ions CO$^+$, recently observed toward the high-mass star forming region W3 IRS5 by Stäuber et al. (2004b), SO$^+$, HCO$^+$ and HOC$^+$, which were also studied by Fuente et al. (2003) in PDRs, are examined in Sect. 2.3.3. Hydrides and ions like OH, OH$^+$, CH and CH$^+$ are discussed in Sect. 2.3.4. These are important species for future space-borne observatories like Herschel where they will be observable with the high resolution spectrometer HIFI (de Graauw & Helmich 2001). In Sect. 2.3.5, CN-bearing molecules are studied since they are thought to be sensitive to UV radiation and readily observable with existing instrumentation. Line emission of CN and HC$^{15}$N is calculated and the results are presented and discussed in Sect. 2.4. We conclude by summarizing our results in Sect. 2.5.

2.2 Model

In order to calculate the abundances of each species at a certain time and distance from the central object, a physical and thermal model of the
2.2. Model

Figure 2.1: Gas temperature distribution in the inner 200–250 AU for different UV fluxes $G_{0,\text{in}}$. The dust temperature $T_{\text{dust}}$ equals the gas temperature for low UV fields ($G_0 \leq 100$).

envelope is needed and initial conditions, i.e., initial abundances, have to be assumed. We adopt the values provided by Doty et al. (2002) and refer to that paper and references therein for more detailed information. However, a brief outline is given in this section.

2.2.1 Physical and thermal model

Van der Tak et al. (1999, 2000) fitted their observations of AFGL 2591 with a spherical power-law density distribution $n = n_0 (r_0/r)^\alpha$ ($n_0 = 5.8 \times 10^4 \text{cm}^{-3}$, $r_0 = 2.7 \times 10^4 \text{AU}$, $\alpha = 1.0$) by modeling CS emission lines over a large range of critical densities and fitting the continuum emission. Our model covers a region that extends from $(r_{\text{in}}, n_{\text{in}}) \approx (200 \text{AU}, 5.9 \times 10^6 \text{cm}^{-3})$ to $(r_{\text{out}}, n_{\text{out}}) \approx (29 \text{000 AU}, 4.2 \times 10^4 \text{cm}^{-3})$. The dust temperature profile was determined from a self-consistent solution of the continuum radiative transfer problem. As shown by Doty & Neufeld (1997) and Doty et al. (2002), the assumption that the gas and dust temperatures are equal, $T_{\text{gas}} \approx T_{\text{dust}}$, holds throughout most of the envelope because of the high density. However, at the inner edge, photoelectric heating and other heating processes proportional to the radiation field (e.g., collisional de-excitation of vibrationally excited H$_2$ pumped by FUV
radiation) can become important (Tielens & Hollenbach 1985; Sternberg & Dalgarno 1989). Comparison of these heating rates with the cooling rate due to gas-dust collisions (Hollenbach & McKee 1989) shows that the difference in gas and dust temperatures is only a few K for low FUV fields ($G_{0,\text{in}} \leq 100$; see Sect. 2.2.2 and 2.2.3 for definition). For higher FUV fields, the gas temperature becomes significantly higher, with values up to a few thousand K at the edge.

Figure 2.1 illustrates the gas temperature in the inner region computed taking the above-mentioned processes into account for values of $G_{0,\text{in}}$ up to $10^5$. The gas temperature drops quickly within $A_V \leq 1$ and equals the dust temperature further in the cloud. The dust temperature—in particular the freeze-out radius ($T_{\text{dust}} \approx 100$ K)—is not affected beyond $A_V \approx 1$, since the FUV photons are quickly re-distributed in frequency and the total luminosity of the system is unchanged (Doty & Leung 1994). The physical structure is kept constant with time. Following the arguments summarized in van der Tak et al. (1999), we assume a distance to AFGL 2591 of 1 kpc.

### 2.2.2 Chemical model

The chemical model is based upon the UMIST gas-phase chemical reaction network (Millar et al. 1997) and basically solves the equations for molecular evolution given by

$$\frac{dn(i)}{dt} = \sum_j k_{ij} n(j) + \sum_{j,k} l_{ijk} n(j)n(k), \quad (2.1)$$

where $n(i)$ is the number density of species $i$; $k_{ij}$ and $l_{ijk}$ are the rate coefficients for production and destruction of the given species. The main inputs of the model are the temperature and density distribution, the cosmic ray ionization rate $\zeta \approx 5.6 \times 10^{-17}$ s$^{-1}$ for AFGL 2591, and the strength of the FUV field $G_0$ with respect to the average interstellar flux at $6 < h\nu < 13.6$ eV of $1.6 \times 10^{-3}$ erg cm$^{-2}$ s$^{-1}$. The model then calculates the time- and depth-dependent chemistry for 395 species and 3865 reactions. The chemical abundances are calculated over a range of 34 radial grid points, providing a time- and space-dependent chemical evolution. The approximate effects of freeze-out onto dust grains are included by initially depleting certain species below 100 K. The effects of
changing the cosmic-ray ionization rate have been investigated by Doty et al. (2002) and are not further discussed in this paper.

2.2.3 UV radiation field

In our spherical model, the envelope can be irradiated by UV photons from the inside by a central source and from the outside by the interstellar radiation field (ISRF). The UV flux is characterized in units of $G_0$ (see Sect. 2.2.2). We therefore denote the enhancement factor due to the inner source $G_{0,\text{in}}$ and that connected to the ISRF $G_{0,\text{out}}$, assuming the same spectral energy distribution. The rates for the photodissociation and photoionization reactions can then be approximated by (see also van Dishoeck 1988)

$$k = G_{0,\text{in}}Ce^{-\gamma_{\text{in}}} + G_{0,\text{out}}Ce^{-\gamma_{\text{out}}} \ [s^{-1}], \quad (2.2)$$

where $C$ and $\gamma$ are fit parameters and $\tau_{\text{in}}$ and $\tau_{\text{out}}$ are the attenuation factors, approximated by $\tau \approx A_V$, the total visual extinction $A_V$. The values of $A_V$ at each depth are calculated from the total hydrogen column using the conversion factor $N(H_{\text{tot}}) = 2N(H_2) + N(H) \approx 1.86 \times 10^{21} A_V \text{ cm}^{-2}$, constrained from observations of translucent clouds by Rachford et al. (2002). For simplicity we start our model with an attenuation of $\tau_{\text{in}} = 0$ at 200 AU and vary the inner UV flux from $G_{0,\text{in}} = 0$ to $G_{0,\text{in}} = 10^5$. We have also carried out different models by varying $G_{0,\text{out}}$ from 0 up to 100 but the changes of the total radial column densities due to different ISRF fluxes are very small. The standard value for the ISRF flux in our models is therefore $G_{0,\text{out}} = 1$.

To obtain a rough indication of the inner UV field, we assume a luminosity of $2 \times 10^4 L_\odot$ and an effective temperature of $3 \times 10^4$ K for the central source as suggested by van der Tak et al. (1999). A large fraction of this luminosity may be due to accretion (Osorio et al. 1999). This luminosity and stellar temperature would yield $G_{0,\text{in}} \approx 2 \times 10^8$ at 200 AU in the absence of any absorption. Hence an estimated UV field strength of $G_0 \approx 10$ corresponds to a dust optical depth $\tau \approx 17$ at this distance. A first question is whether such a relatively low value for $\tau$ corresponds to a mass that is high enough to provide a typical mass accretion rate for high mass YSOs of $\approx 10^{-4} - 10^{-2} M_\odot \text{ yr}^{-1}$ (e.g., Behrend & Maeder 2001; McKee & Tan 2003). Using the relation between the total visual extinction and the hydrogen column density given
earlier in this Sect., $A_V \approx 17$ mag corresponds to a column density of $N(H_2) \approx 2 \times 10^{22}$ cm$^{-2}$ or a density of $n \approx 10^7$ cm$^{-3}$ at 200 AU. Assuming spherical free fall inflow and a central mass of $M_* = 10 M_\odot$, this density would be consistent with an accretion rate of (e.g., Shu et al. 1987) $M_{\text{acc}} = 4\pi pr^{3/2}(2GM_*)^{1/2} \approx 10^{-4} M_\odot \text{yr}^{-1}$. It is expected that these high accretion rates 'choke off' an incipient HII region (Walmsley 1995) and that the hydrogen-ionizing photons ($E > 13.6$ eV) cannot travel far from the protostar before being absorbed by infalling matter. The result would be a small Strömgren sphere around the central protostar, with the non-ionizing photons allowed to escape to larger distances. Both the luminosity and effective temperature of the radiation are actually expected to evolve during the protostellar stage (e.g., McKee & Tan 2003), but such detailed modeling is beyond the scope of this study. Note also that the geometry of this dust and inflowing material is not known and is therefore not included in our envelope model. If our model were extended inward to account for this extra material, only the first few radial positions in our grid up to $A_V \approx 1$ would change.

Our models are spherically symmetric and do not include geometrical effects like outflow cones or clumps in the central regions that could allow UV photons to travel further into the envelope. The effects of UV radiation escaping through outflow cones and scattering back on the surrounding envelope have been studied by Spaans et al. (1995) for the case of low-mass YSOs. Finally, it should be mentioned that the photoreaction rates (2.2) are fitted for plane parallel models but are applied to spherical models. In spherical symmetry, the FUV photons can penetrate further on average, but the gas temperature is somewhat lower assuming the same density structure (Störzer et al. 1996). The authors conclude that spherical geometry only becomes important for clouds with $n \approx 10^5$ cm$^{-3}$ exposed to FUV fields with intensities $G_0 \approx 10^3$ and a H$_2$ column density of less than $\approx 10^{22}$ cm$^{-2}$. We therefore neglect these effects.

### 2.3 Chemistry results

We have modeled the envelope around AFGL 2591 with different UV fluxes $G_{0,\text{in}}$ at the inner boundary and compared our results to those of Doty et al. (2002), representing the model $G_{0,\text{in}} = 0$ in this paper. Photodissociation and photoionization processes are generally fast for the
main species in the regions where they are significant \( \approx 10^{-8} \text{s}^{-1} \) so that the effects are not significantly different for \( 3 \times 10^3 \) and \( 3 \times 10^5 \) years. The results are therefore presented for \( t = 3 \times 10^4 \) years, the chemical age of AFGL 2591 as proposed by Doty et al. (2002). Total column densities for a selection of species are predicted in Table 2.1. The selection criteria are: (i) the species have a column density larger than \( N(X) = 10^{10} \text{cm}^{-2} \); (ii) the relative difference of the total column densities with and without an inner UV source is more than \( \approx 30\% \); and (iii) the species are observable with present or future instrumentation. In addition we show the abundances of the model predictions for basic molecules (other than \( \text{H}_2 \)) such as \( \text{CO}, \text{H}_2\text{O}, \text{CO}_2 \) and \( \text{N}_2 \) at the bottom of Table 2.1. In general, the species whose abundances are particularly enhanced are the same as those found in traditional PDR models, i.e., radicals and ions, and their chemically related species. The reason that most ratios given in Table 2.1 are \( > 1 \) is that small differences in very abundant species like \( \text{CO} \) or \( \text{H}_2\text{O} \) can make large differences in much less abundant species.

In Fig. 2.3, the column densities for various molecules as functions of \( G_{0,\text{in}} \) are presented, normalized to the values for \( G_{0,\text{in}} = 0 \). Figs. 2.4 to 2.7 show the depth-dependent fractional abundances for selected species in the inner 2500 AU. The radial scale is taken to be somewhat smaller in these plots than the full extent of the envelope (29000 AU, \( \log(r) = 17.6 \)) in order to emphasize the region which is influenced most by the inner UV field (see Doty et al. 2002 for variations in the outermost regions). Even for the highest values of \( G_{0,\text{in}} \), the effects of the UV radiation do not penetrate beyond the freeze-out radius at 100 K (\( \log(r) = 16.2 \)).

Several molecules shown in Figs. 2.4 to 2.7 have local minima or maxima at certain positions (for example \( \text{H}_2\text{O} \) at \( \log(r) \approx 15.5 \) for \( G_{0,\text{in}} = 10 \) or \( \text{HCO}^+ \) at \( \log(r) \approx 15.7 \) for \( G_{0,\text{in}} = 10^5 \)). These peaks are not caused by numerical artifacts but are due to different chemical affects, some of which are explained in the following sections.

Table 2.1 lists the radial column densities \( N_{\text{radial}} = \int n(r) \, dr \). For comparison of observed emission lines to model-predicted column densities, beam-averaged column densities defined by \( N_{\text{beam}} = \iint n(z,p) \, G(p) \, 2\pi \, p \, dp \, dz \, / \, \int G(p) \, 2\pi \, p \, dp \) have to be calculated, where \( p \) is the impact parameter and \( G(p) \) is the beam response function. Beam averages are centered on the source whereas the calculated radial column densities are through the cloud center. \( N_{\text{beam}} \) generally has slightly lower
Chapter 2. Influence of UV radiation

Figure 2.2: CN/HCN, HNC/HCN, CH\(^+\)/CH and HOC\(^+\)/HCO\(^+\) column density ratios as a function of \(G_{0,\text{in}}\).

values than \(N_{\text{radial}}\) for typical observing beams. Rather than calculating \(N_{\text{beam}}\), however, we have computed the actual line fluxes by solving the equations of molecular excitation and radiative transfer throughout the envelope and convolving the emerging emission with the telescope beam (see Sect. 2.4).
Table 2.1: Predicted total radial column densities $N_{\text{radial}}$ for different UV fluxes $G_{0,\text{in}}$.

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<th>Species</th>
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(a/b) means $a \times 10^b$.

The ratio is the enhancement relative to the model without an inner UV source, i.e. $N(G_{0,\text{in}} = 10^x)/N(G_{0,\text{in}} = 0)$. Continued on next page.
Table 2.1—continued from previous page.

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$N_{\text{a(b)}}$ means $a \times 10^b$.

The ratio is the enhancement relative to the model without an inner UV source, i.e. $N(G_{0,\text{in}} = 10^2)/N(G_{0,\text{in}} = 0)$. Continued on next page.
Table 2.1—continued from previous page.

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<th>(N\text{ [cm}^{-2}\text{]}) (G_{0,\text{in}} = 10)</th>
<th>Ratio</th>
<th>(N\text{ [cm}^{-2}\text{]}) (G_{0,\text{in}} = 100)</th>
<th>Ratio</th>
<th>(N\text{ [cm}^{-2}\text{]}) (G_{0,\text{in}} = 10^3)</th>
<th>Ratio</th>
<th>(N\text{ [cm}^{-2}\text{]}) (G_{0,\text{in}} = 10^5)</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOC(^+)</td>
<td>1.1(10)</td>
<td>27.0</td>
<td>3.4(10)</td>
<td>87.7</td>
<td>1.6(12)</td>
<td>4168.1</td>
<td>4.5(11)</td>
<td>1138.3</td>
</tr>
<tr>
<td>NO(^+)</td>
<td>2.6(12)</td>
<td>2.8</td>
<td>3.2(12)</td>
<td>3.5</td>
<td>1.9(12)</td>
<td>2.1</td>
<td>1.0(12)</td>
<td>1.1</td>
</tr>
<tr>
<td>HCS(^+)</td>
<td>1.9(12)</td>
<td>3.8</td>
<td>1.8(12)</td>
<td>3.5</td>
<td>9.5(11)</td>
<td>1.9</td>
<td>7.8(11)</td>
<td>1.5</td>
</tr>
<tr>
<td>SO(^+)</td>
<td>6.5(12)</td>
<td>24.3</td>
<td>1.3(13)</td>
<td>47.1</td>
<td>5.8(12)</td>
<td>20.8</td>
<td>1.4(12)</td>
<td>5.2</td>
</tr>
<tr>
<td>CO</td>
<td>3.9(19)</td>
<td>1.0</td>
<td>3.9(19)</td>
<td>1.0</td>
<td>3.8(19)</td>
<td>1.0</td>
<td>3.7(19)</td>
<td>1.0</td>
</tr>
<tr>
<td>H(_2)O</td>
<td>4.5(18)</td>
<td>1.1</td>
<td>4.2(18)</td>
<td>1.0</td>
<td>3.6(18)</td>
<td>0.8</td>
<td>3.0(18)</td>
<td>0.7</td>
</tr>
<tr>
<td>CO(_2)</td>
<td>1.2(18)</td>
<td>0.9</td>
<td>1.2(18)</td>
<td>0.9</td>
<td>1.1(18)</td>
<td>0.9</td>
<td>1.1(18)</td>
<td>0.9</td>
</tr>
<tr>
<td>(N(_2)</td>
<td>7.3(18)</td>
<td>1.0</td>
<td>7.3(18)</td>
<td>1.0</td>
<td>7.3(18)</td>
<td>1.0</td>
<td>7.2(18)</td>
<td>1.0</td>
</tr>
</tbody>
</table>

(a/b) means \(a \times 10^b\).

The ratio is the enhancement relative to the model without an inner UV source, i.e. \(N(G_{0,\text{in}} = 10^2)/N(G_{0,\text{in}} = 0)\).
2.3.1 Basic molecules: CO, H$_2$O, and CO$_2$

As seen in Table 2.1 and Fig. 2.4, the total radial column densities of the high abundance molecules CO, H$_2$O and CO$_2$ are not affected significantly by an inner UV field. The major destruction mechanism for these molecules is photodissociation. Measurable changes can only be seen for relatively high UV fields in the dense region within $\approx 500$ AU from the central source. For H$_2$O another efficient destructive reaction is the production of HCO$^+$ and HOC$^+$ through reactions with C$^+$. The slight increase in the relative abundance of H$_2$O at $r \approx 4 \times 10^{15}$ cm for $G_{0,\text{in}} = 10$ and $G_{0,\text{in}} = 100$ is caused by the protonation of HCN through H$_3$O$^+$ which leads to HCNH$^+$ and H$_2$O, and by the high-temperature reaction of molecular hydrogen with OH, also producing H$_2$O. All reactants are slightly increased by a moderate UV field, enough to speed up these reactions. At $\approx 5 \times 10^{15}$ cm the relative abundance of CO is the same for all UV fields. This is slightly closer to the star than the enhancement of OH for high UV fields (see also Fig. 2.6) and since CO + OH $\rightarrow$ CO$_2$ + H is the dominant reaction to produce gas-phase CO$_2$, the enhancement of OH leads to the small increase of CO$_2$ between $5-6 \times 10^{15}$ cm for $G_{0,\text{in}} \geq 10^3$. The sudden decrease of the H$_2$O and CO$_2$ abundances at $\approx 2 \times 10^{16}$ cm ($T \approx 100$ K) is due to the effects of their freeze-out onto grains (see Doty et al. 2002 for more information). The abundance minima of H$_2$O, CO and CO$_2$ for $G_{0,\text{in}} \geq 10^3$ are due to the higher gas temperature for these high FUV fields: the abundances are rising again toward the protostar.

CO$_2$ is a highly abundant molecule in our model with a column density of the order of $10^{18}$ cm$^{-2}$. Boonman et al. (2003a) derive a total column density of $2.6 \times 10^{16}$ cm$^{-2}$ for AFGL 2591 from observations with the Infrared Space Observatory. Even high UV fields do not reduce much CO$_2$. This overprediction of CO$_2$ has also been discussed by Doty et al. (2002), and our new models add little to this discussion: enhanced UV photodissociation does not solve the problem.

2.3.2 PDR-related species: O, C, and C$^+$

Figure 2.4 also shows the dominant line emitters, and thus coolants, in a PDR: O, C and C$^+$. Photodissociation of CO is the main source for both carbon and oxygen. The major destruction mechanism for carbon
in a low \((G_{0,\text{in}} = 10)\) UV field is the reaction with OH leading to CO and atomic hydrogen. Photoionization of carbon becomes important for higher UV fields and is the main production channel of \(\text{C}^+\). The somewhat unexpected jump of \(\text{C}^+\) at \(\approx 2 \times 10^{16} \text{ cm}^2\) can be explained by the freeze-out of \(\text{H}_2\text{O}\): the main destroyer of \(\text{C}^+\) at this distance is depleted onto grains below 100 K. The relatively high atomic oxygen abundance for \(T < 100 \text{ K}\) is due to our initial elemental abundance, consistent with Meyer et al. (1998) for diffuse clouds.

The main production channel for \(\text{O}^+\) is not the photoionization of atomic oxygen (which cannot occur for photon energies less than 13.6 eV) but the reactions \(\text{H}^+ + \text{O} \rightarrow \text{O}^+ + \text{H}\) and \(\text{C}^+ + \text{O}_2 \rightarrow \text{O}^+ + \text{CO}\).

The observed column density of atomic carbon toward AFGL 2591 \((N \leq 6.8 \times 10^{17} \text{ cm}^{-2}\), see Doty et al. 2002) can be reproduced with a UV field of \(G_{0,\text{in}} \geq 10\). The high \(\text{C}^+\) abundances \((N \leq 6.8 \times 10^{17} \text{ cm}^{-2}\)) are consistent with a UV field of \(G_{0,\text{in}} \geq 10^3\). However, as discussed in Sect. 2.4, the observed antenna temperatures require high abundances of \(\text{C}\) and \(\text{C}^+\) to be extended over a larger region than just the inner few hundred AU. Thus, these species likely trace the outer radiation field, \(G_{0,\text{out}} \approx 10 - 100\), rather than an inner UV field.

### 2.3.3 Reactive ions

From Table 2.1, it is seen that \(\text{HOC}^+\) is much more affected by the strength of the UV field than \(\text{HCO}^+\). The reason for this is that in our models \(\text{HOC}^+\) is basically formed by the two reactions \(\text{H}_3^+ + \text{CO} \rightarrow \text{HOC}^+ + \text{H}_2\) and \(\text{C}^+ + \text{H}_2\text{O} \rightarrow \text{HOC}^+ + \text{H}\), which are both highly dependent on the ionization fraction and thus on the incoming UV field. In contrast more production channels are possible for \(\text{HCO}^+\), e.g., \(\text{HOC}^+ + \text{H}_2 \rightarrow \text{HCO}^+ + \text{H}_2\), thus more \(\text{HCO}^+\) than \(\text{HOC}^+\) is produced. Another reason for the much higher abundances of \(\text{HCO}^+\) is the jump at \(T = 100 \text{ K}\) where \(\text{H}_2\text{O}\) freezes out: since \(\text{HCO}^+ + \text{H}_2\text{O} \rightarrow \text{H}_3\text{O}^+ + \text{CO}\) is the main destruction channel, much more \(\text{HCO}^+\) remains in the region below 100 K. Water is important, however, to produce \(\text{HOC}^+\), hence the \(\text{HOC}^+\) abundance is lower once water has depleted onto grains.

The \(\text{HCO}^+ / \text{HOC}^+\) abundance ratios predicted by our chemical models are in the range of \(\approx 10^2 - 10^6\) which is at the upper limit of the ratios observed toward PDRs. Fuente et al. (2003) reported ratios of 50–120
toward the reflection nebula NGC 7023 — the lowest ratio measured so far — up to 450 toward the planetary nebula NGC 7027. Our models only reproduce such low values for \( G_{0,\text{in}} \geq 10^3 \). However, the observed peak values of HOC\(^+\) toward several PDRs are in the range of the predicted column densities for \( G_{0,\text{in}} = 10^{-100} \).

Van der Tak et al. (1999) find HCO\(^+\) abundances of the order of \( \approx 10^{-8} \), which are well fitted by our models with \( G_{0,\text{in}} = 10 \). Unfortunately, there are no observations of HOC\(^+\) toward AFGL 2591 to date. The question therefore is whether these low ratios also hold in massive star-forming regions.

For low UV fields the reactive ion CO\(^+\) is produced mainly by \( \text{He}^+ + \text{CO}_2 \rightarrow \text{CO}^+ + \text{O} + \text{He} \) and \( \text{C}^+ + \text{CO}_2 \rightarrow \text{CO}^+ + \text{CO} \). For higher UV fields the reaction \( \text{C}^+ + \text{OH} \rightarrow \text{CO}^+ + \text{H} \) is the most efficient to build up CO\(^+\). Its destruction for all UV fields is mainly by reactions with H\(_2\). The most efficient pathway to SO\(^+\) is \( \text{S}^+ + \text{OH} \rightarrow \text{SO}^+ + \text{H} \). Its destruction is caused mainly by dissociative recombinations with electrons.

### 2.3.4 Hydrides

As in traditional PDR models, the abundances of unsaturated hydrides are strongly increased by UV radiation. OH and CH\(_3\) are the species that are the least affected by the inner UV field. CH\(^+\) on the other hand is enhanced by more than a factor of 10\(^4\) even for a moderate UV field and its column density grows steadily with increasing UV field strength. To date, there are observations only of OH for AFGL 2591 reporting \( N \geq 4.7 \times 10^{14} \) (see Doty et al. 2002). This column density is well fitted by our models for the region \( T < 100 \text{ K} \). Our models, however, produce much more OH in the warmer, inner region (see Fig. 2.6). Without UV radiation, OH is mainly produced through collisions of atomic oxygen with molecular hydrogen in the inner warm part. In the presence of a UV field, photodissociation of H\(_2\)O becomes the dominant production route. The OH destruction is primarily through C\(^+\), and for very high UV fields (\( G_{0,\text{in}} = 10^5 \)) the photodissociation of OH becomes important too. For UV fields with \( G_{0,\text{in}} \geq 10^3 \), CH\(^+\) is efficiently produced in the warm inner regions by reactions of C\(^+\) with molecular hydrogen. For smaller UV fields, CH\(^+\) is produced mainly by the reaction HCO\(^+\) + C \rightarrow CH\(^+\) + CO. For higher UV fields, photoionization of CH becomes the main mechanism for CH\(^+\) production. In all our models, CH\(^+\) is mainly
2.3. Chemistry results

destroyed in collisions with H₂.

For smaller UV fields, CH is mainly destroyed through CH + H₂ → CH₂ + H and built up by the reverse reaction. OH⁺ is primarily produced by collisions of singly ionized oxygen with molecular hydrogen. The jump at ≈ 2 × 10¹⁶ cm is due to the increase of atomic oxygen. Charge exchange reactions then enlarge the OH⁺ abundances, in particular the reaction H₃⁺ + O → OH⁺ + H₂. OH⁺ is most efficiently reduced in collisions with H₂. OH and OH⁺ play a crucial role in the gas-phase chemistry of water.

Several species such as C⁺ and CH⁺ are not only excellent tracers of enhanced UV fields but also of the strength G₀ since their abundances rise steadily with increasing field strengths. The fact that C⁺ can also be enhanced by an outer UV field reduces its value as a diagnostic, however. An alternative tracer is the CH⁺/CH ratio, which is 10⁵-10⁶ times higher if the inner UV is included. The column density ratio is shown in Fig. 2.2 as a function of G₀ in. Similar arguments hold for other hydrides such as CH₂ and CH₂⁺ which are less easily observable. Hydrides like CH and CH⁺ are also important for building complex hydrocarbons (see e.g., van Dishoeck & Hogerheijde 1999); indeed, a rich carbon chemistry has been observed in PDR layers (e.g., Hogerheijde et al. 1995; Teyssier et al. 2004).

It is somewhat surprising that CH₃ is much less affected by the inner UV field than, e.g., CH₂. This is only partly true since the production and destruction mechanisms of CH₃ do change by the impact of the inner UV field. Without the inner UV source CH₃ is efficiently built up by the reaction He⁺ + CH₃OH → OH⁺ + CH₃ + He. With the onset of an inner UV field, CH₃ is mainly the photodissociation product of species like CH₃CN, CH₄ and CH₃OH. CH₃ forms H₂CO when it reacts with O, which is the main destruction channel. Since an inner UV field clearly enhances atomic oxygen (see Fig. 2.4), this reaction is very efficient deeper in the cloud where CH₃ is destroyed fast. Thus, although CH₃ is first enhanced in the very inner region, it becomes less abundant deeper in the cloud. This leads to an average radial column density more or less equal to that where no inner UV radiation is considered.

2.3.5 CN-bearing species

The chemistry of CN and HCN is thought to be strongly affected by UV radiation and the CN/HCN ratio has been proposed to be a good tracer
Figure 2.3: Column densities of various species as functions of $G_{0,\text{in}}$, normalized to the value for $G_{0,\text{in}} = 0$.

of PDR chemistry (Fuente et al. 1995; Jansen et al. 1995b). Since our envelopes are more extended than normal PDRs, we predict lower CN/HCN ratios than those observed in PDRs where the ratio is typically $\approx 1$ in the shielded regions and $> 1$ in regions exposed to UV radiation. Observations of CN and HCN toward AFGL 2591 confirm these low ratios. The observed abundance of CN (see Doty et al. 2002) is well fitted with $G_{0,\text{in}} = 10$–100. The HCN chemistry is discussed in detail by Doty et al. (2002), especially the situation in the warm gas-phase ($T > 230$ K) region where a jump has been suggested from $x(\text{HCN}) = 10^{-8}$ to $x(\text{HCN}) = 10^{-6}$ by Boonman et al. (2001). The observed HCN column density is reproduced in our models for $G_{0,\text{in}} = 10$ within a factor of 2, whereas it is underproduced in models without an inner UV field. Alternatively, the model could be extended inward to the radius where high temperature chemistry may enhance the HCN abundances. However, a closer position to the star also means an increased UV field, and HCN is more vulnerable to photodissociation. UV radiation may therefore be an explanation for the relatively high observed HCN abundances. The CN/HCN ratio is only enhanced for $G_{0,\text{in}} \geq 10^3$. For lower UV fields, the ratio is even smaller than that without UV irradiation (see also Fig. 2.2). Hence, the CN/HCN ratio is not a good UV tracer for this high mass star-forming region, in contrast with the situation for PDRs.

Fig. 2.7 shows the radial dependences of the abundances of CN, HCN,
2.3. Chemistry results

Figure 2.4: Depth-dependent fractional abundances of the basic molecules CO, H$_2$O and CO$_2$ and the 'PDR-related' species O, C and C$^+$ for different UV fluxes.
Figure 2.5: Depth-dependent fractional abundances of HCO\(^+\), HOC\(^+\), CO\(^+\) and SO\(^+\) for different UV fluxes.

Figure 2.6: Depth-dependent fractional abundances of the hydrides OH, OH\(^+\), CH and CH\(^+\) for different UV fluxes.
2.3. Chemistry results

HNC and the reactive molecular ion HCNH$^+$. In the warm high density regime, the production of HCN through collisions of CN with H$_2$ is slightly more efficient than photodissociation of HCN, hence more HCN is produced than CN. Collisions of HCN with H$_3$O$^+$, however, produce water and HCNH$^+$, which can recombine to form HNC or CN. Since this is the main path to HNC in our models, more HCN is produced compared to HNC. CH$_3$CN is generated through H$_4$C$_2$N$^+$, whereas the association of CN with CH$_3$ plays a minor role. CH$_3$CN and HNC are also photodissociated to CN. No grain surface production and subsequent evaporation of CH$_3$CN are assumed. The following network is valid for UV-affected CN chemistry in our models:

$$
\begin{align*}
\text{CH}_3\text{CN} & \xleftarrow{h\nu} \text{CH}_3^+ / \text{H}_3\text{O}^+ \\
\text{CN} & \xleftarrow{h\nu} \text{H}_2 \\
\text{HNC} & \xleftarrow{H_3\text{O}^+ / \text{HCO}^+} \text{HCNH}^+
\end{align*}
$$

Figure 2.7: Depth-dependent fractional abundances of CN, HCN, HNC and HCNH$^+$ for different UV fluxes.
The HNC/HCN ratio is \( \approx 0.01-0.03 \) for low UV fields. The ratio is approximately unity for \( G_{0,\text{in}} = 0 \) and slightly higher (1.4) for high UV fields (\( G_{0,\text{in}} = 10^5 \)). The variation of the ratio is mainly due to the changing HCN abundances. The observed HNC/HCN ratio varies strongly from source to source but is generally < 1. For AFGL 2591, the observed ratio is HNC/HCN\( \approx 0.01 \), which is in good agreement with a low UV field.

### 2.4 Calculated line emission

The temperature, density and abundance profiles presented in Sect. 2.3 have been used as input to the excitation and Monte Carlo radiative transfer code of Hogerheijde & van der Tak (2000) to compute the emerging line intensities. The intrinsic (turbulent) line profile is taken to be a Gaussian with a Doppler parameter (1/e width) of 1.6 km s\(^{-1}\), independent of radius. The line profiles are convolved to an appropriate telescope beam size. The low-lying transitions trace primarily the low density outer YSO envelope whereas the higher-lying lines are only excited in the high density inner envelope. Thus, the intensities of the higher-lying transitions of species like CN or HCN, whose abundances are affected by UV irradiation, are expected to be enhanced and the effect on the lines ratios should be observable.

#### 2.4.1 CN and HCN emission lines

Fig. 2.8 shows emission lines of CN for different inner UV fields. While the lowest transition CN 1–0 line has the same intensity for all UV fields, the higher transitions show clear differences for different UV strengths. The CN 3–2 line intensity is increased by a factor of \( \approx 2 \) for \( G_{0,\text{in}} = 10 \) and \( G_{0,\text{in}} = 100 \). The enhancement is even more noticeable in the CN 4–3 transition. The lines for \( G_{0,\text{in}} = 10 \) and \( G_{0,\text{in}} = 100 \), respectively, are \( \approx 3 \) times stronger than that for \( G_{0,\text{in}} = 10^3 \), which in turn is approximately twice as strong as that for \( G_{0,\text{in}} = 10^5 \) and \( G_{0,\text{in}} = 0 \). Since these enhancements are clearly larger than the typical 30% observational errors, the impact of central UV photons on the inner envelope is predicted to have measurable consequences for higher CN transitions. The line ratios for \( G_{0,\text{in}} = 0 \) are CN 1–0/3–2/4–3 \( \approx 100/11/2 \), whereas for \( G_{0,\text{in}} = 10 \)
2.4. Calculated line emission

![Diagram of CN line profiles](image1)

**Figure 2.8:** CN line profiles calculated for different UV fields. Solid line: $G_{0,\text{in}} = 0$. Dashed line (small): $G_{0,\text{in}} = 10$. Dashed line (big): $G_{0,\text{in}} = 100$. Dotted line: $G_{0,\text{in}} = 10^3$. Dash-dotted line: $G_{0,\text{in}} = 10^5$. The CN 1–0 transition has a frequency of 113,491 MHz (convolved with a 33" Onsala beam), the CN 3–2 transition has a frequency of 340,248 MHz (convolved to a 14" JCMT beam) and the CN 4–3 transition has a frequency of 453,606 MHz (convolved to a 11" JCMT beam). The size of the source is approximately 30" (29,000 AU).

![Diagram of HC$^{15}$N line profiles](image2)

**Figure 2.9:** HC$^{15}$N line profiles calculated for different UV fields. Solid line: $G_{0,\text{in}} = 0$. Dashed line (small): $G_{0,\text{in}} = 10$. Dashed line (big): $G_{0,\text{in}} = 100$. Dotted line: $G_{0,\text{in}} = 10^3$. Dash-dotted line: $G_{0,\text{in}} = 10^5$. The HC$^{15}$N 1–0 transition has a frequency of 86 GHz (convolved to a 63" NRAO beam), the 3–2 transition has a frequency of 258 GHz (convolved to a 20" JCMT beam) and the 4–3 transition has a frequency of 344 GHz (convolved to a 14" JCMT beam). The size of the source is approximately 30" (29,000 AU).
they are approximately 100/18/12 and for $G_{0,\text{in}} = 100$ CN 1-0/3-2/4-3
$\approx 100/17/11$.

In Fig. 2.9, it is seen that the higher-lying HC$^{15}$N lines are similarly
enhanced for a moderate UV field with $G_{0,\text{in}} = 10$. The optically thin
HC$^{15}$N isotope is modeled, since the synthetic HCN lines are optically
thick and therefore not ideal to show the effects of inner UV enhancement
(see also the discussion by van der Tak et al. 1999 on HCN modeling).
The HCN/HC$^{15}$N ratio is taken to be 450 (Wilson & Rood 1994). The $J = 3-2$
line is enhanced by a factor of 7 and the $J = 4-3$ line a factor of
$\approx 26$ for moderate UV fields. For the lowest transition, all line intensities
are the same, except that for $G_{0,\text{in}} = 10$, which is approximately 9% higher
and thus not distinguishable from the other lines if calibration errors are
taken into account. The intensity ratios for $G_{0,\text{in}} = 0$ are HC$^{15}$N 1-0/3-
2/4-3 $\approx 10/10/4$, for $G_{0,\text{in}} = 10$ HC$^{15}$N 1-0/3-2/4-3 $\approx 10/64/103$ and
for $G_{0,\text{in}} = 100$ they are approximately 10/41/70.

Line intensities have also been calculated for an outer UV field of
$G_{0,\text{in}} = 10-100$. It is found, however, that the CN and HCN lines are
not very sensitive to the outer UV field due to the much lower densities
in those regions, with enhancements in line intensities of only 10–20%.
Thus, the CN and HCN lines trace the central UV field rather than the
outer interstellar radiation field. This is in contrast with species such as C
and C$^+$, whose transitions are readily excited at low densities in the outer
envelope (see below). High spatial resolution interferometry observations
of both low- and high-J CN and HCN lines should be able to directly
constrain the extent over which the inner and outer UV field affect the
chemistry.

### 2.4.2 C and C$^+$ emission lines

In addition to the molecular lines mentioned above, the line profiles of the
fine-structure transitions of C and C$^+$ have been calculated. Although
the abundances of both species are strongly enhanced by the inner UV
field, the resulting antenna temperatures are much lower than observed
by van der Tak et al. (1999). Thus, even though the column densities
including an inner UV field match those derived from observations, the
beam dilution of the inner region is so large that the resulting fluxes fall
short by 1–2 orders of magnitude. Therefore, models have also been run
in which the outer radiation field is enhanced above the average ISRF.
2.5 Summary and conclusions

Figure 2.10: The quality of the model fit to the observations as a function of $G_{0,\text{in}}$.

Such outer enhancements could be due to other nearby young stars. For example, for AFGL 2591 a nearby HII region (6000 AU projected distance) has been found (see e.g., van der Tak et al. 1999; Trinidad et al. 2003), whose exciting star could illuminate (part of) the outer AFGL 2591 envelope. An outer UV field with $G_{0,\text{out}} = 100$ and an enhanced gas temperature due to photoelectric heating matches the [C I] 492 GHz observations best. Since C$^+$ is mainly produced through photoionization of atomic carbon (ionization energy 11.26 eV), the same issue may be true for the [CII] line.

2.5 Summary and conclusions

We have extended the detailed chemical models of Doty et al. (2002) to study the influence of UV irradiation from AFGL 2591 on the chemistry in the surrounding envelope on 200–29 000 AU scales. From Figs. 2.4 to 2.7, it is seen that an inner UV flux affects only the region within 500–600 AU from the star. The species whose abundances are most enhanced are radicals and ions, similar to the case of normal PDRs. However, the chemistry differs from that in normal PDRs in various details owing to the higher temperature and higher H$_2$O abundance in the inner YSO envelope.

By comparing our results to those of Doty et al. (2002), we find
that agreement with the observed column densities is improved with a moderate UV field of $G_{0,\text{in}} = 10-100$. This is seen quantitatively in Fig. 2.10, which shows the absolute differences between the model results and the observations, $\Delta = \frac{1}{N} \sum_{i=1}^{N} |\log(N_{\text{obs}}) - \log(N_{\text{mod}})|$, summed over all species. Species like CN and HCN are particularly improved with a modest UV field. However, the high temperature chemistry of HCN in the inner region still needs further investigation. The CN/HCN ratio is found not to be a good tracer for $G_{0,\text{in}}$ for AFGL 2591. For low UV fields, the extra CN reacts with $\text{H}_2$ to HCN in the warm, dense region thus enhancing HCN more than CN, in contrast to typical PDRs. However, enhanced intensities of the 3–2 and 4–3 lines of CN and HC$^{15}$N are predicted compared with the lower $J = 1 - 0$ lines, which should be observable both with single dishes and with submillimeter interferometers. Another strong indicator for enhanced UV fields is the CH$^+$/CH ratio with values between $10^{-3}$ and $10^{-1}$. Neither species can readily be observed with ground based observatories, but are excellent targets for Herschel-HIFI.

Most other species have their maximum column density at lower UV fields (see Table 2.1). This is due to different preferred chemical networks for each strength of the UV field; in particular, many species are photodissociated away for very high UV fields. Like in Doty et al. (2002), the CO$_2$ column density is overpredicted by a factor of 40 in our model. In this sense, UV irradiation from the central star proves not to be an efficient destruction mechanism for CO$_2$. Impulsive heating events and X-ray chemistry may destroy carbon dioxide more efficiently.

Our model results indicate strongly that UV radiation from the high mass YSO AFGL 2591 cannot be neglected in the surrounding envelope chemistry. The inferred value of $G_{0,\text{in}} = 10-100$ for an inner UV field is reasonable for a young massive star like AFGL 2591 and the corresponding column density and dust opacity can be justified by the mass inflow rate even though we do not present a fully self-consistent model (see Sect. 2.2.3). Our models assume a spherical symmetry and neglect geometric effects. High spatial resolution data of species like CN should also be able to establish the importance of non-spherical effects, such as the escape of UV photons through the outflow cones.

In recent years it has become clear that YSOs are also strong X-ray emitters. The observed X-ray luminosities range from approximately $10^{28.5}$ to $10^{33}$ erg s$^{-1}$ (Feigelson & Montmerle 1999; Preibisch 1998). X-
2.5. Summary and conclusions

rays can also penetrate deeper into clouds than UV photons due to smaller absorption cross sections at high energies. Most recently Doty et al. (2004) suggested that X-rays may be responsible for a higher ionization rate in the low-mass hot core IRAS 16 293–2422. It is therefore important to also investigate the effects of X-rays on the chemistry in the envelopes of YSOs (see Stäuber et al. 2005, Chapter 3).
Chapter 3

X-ray chemistry in the envelopes around young stellar objects

ABSTRACT: We present chemical models of the envelope of a young stellar object (YSO) exposed to a central X-ray source. The models are applied to the massive star-forming region AFGL 2591 for different X-ray fluxes. Model results for this region show that the X-ray ionization rate with and without the effects of Compton scattering differs by only a few percent and the influence of Compton scattering on the chemistry is negligible. The total X-ray ionization rate is dominated by the 'secondary' ionization rate of H$_2$ resulting from fast electrons. The abundance profiles of several molecular and atomic species are shown to depend on the X-ray luminosity and on the distance from the source. The carbon, sulphur and nitrogen chemistries are discussed. It is found that He$^+$ and H$_3^+$ are enhanced and trigger a peculiar chemistry. Several molecular X-ray tracers are found and compared to tracers of the far ultraviolet (FUV) field. Like ultraviolet radiation fields, X-rays enhance simple hydrides, ions and radicals. In contrast to ultraviolet photons, X-rays can penetrate deep into the envelope and affect the chemistry even at large distances from the source. Whereas the FUV enhanced species cover a region of ≈ 200-300 AU, the region enhanced by X-rays is ≥ 1000 AU. We find that N$_2$O, HNO, SO, SO$^+$, HCO$,^+$, CO$^+$, OH$^+$, N$_2$H$^+$, SH$^+$ and HSO$^+$ (among others) are more enhanced by X-rays than by FUV photons even for X-ray luminosities as low as $L_X \approx 10^{30}$ erg s$^{-1}$. CO$_2$ abundances are reduced in the gas-phase through X-ray induced FUV photons. For
temperatures \( T \lesssim 230 \text{K} \), \( \text{H}_2\text{O} \) is destroyed by X-rays with luminosities \( L_X \gtrsim 10^{30} \text{ergs}^{-1} \). Best-fit models for AFGL 2591 predict an X-ray luminosity \( L_X \gtrsim 10^{31} \text{ergs}^{-1} \) with a hard X-ray spectrum \( T_X \gtrsim 3 \times 10^7 \text{K} \). This is the first time that the X-ray flux of a highly obscured source has been estimated by its envelope chemistry. Furthermore, we find \( L_X/L_{bol} \approx 10^{-6} \). The chemistry of the bulk of the envelope mass is dominated by cosmic-ray induced reactions rather than by X-ray induced ionization for X-ray luminosities \( L_X \lesssim 10^{33} \text{ergs}^{-1} \). The calculated line intensities of \( \text{HCO}^+ \) and \( \text{HCS}^+ \) show that high-\( J \) lines are more affected than lower \( J \) lines by the presence of X-rays due to their higher critical densities, and that such differences are detectable even with large aperture single-dish telescopes. Future instruments such as Herschel-HIFI or SOFIA will be able to observe X-ray enhanced hydrides whereas the sensitivity and spatial resolution of ALMA is well-suited to measure the size and geometry of the region affected by X-rays.

### 3.1 Introduction

Observational studies of star-forming regions show that some young stellar objects (YSOs) are very strong X-ray emitters. Typical X-ray luminosities range from approximately \( L_X = 10^{28} \text{ergs}^{-1} \) to \( L_X = 10^{33} \text{ergs}^{-1} \) in the 0.5–10 keV band (e.g., Hofner & Churchwell 1997; Carkner et al. 1998; Feigelson & Montmerle 1999). The heating of the X-ray emitting plasma is not well understood. In low-mass YSOs the emission may originate from powerful magnetic activity near the stellar surface or in the star-disk environment, whereas in high-mass YSOs wind instabilities and shocks may cause the high X-ray flux. In the earliest stage of evolution, the protostar is still deeply embedded in its natal molecular cloud (\( \text{A}_v > 100 \text{mag} \)). As a consequence, X-rays are not directly observable toward very young objects, and the onset of the high energy radiation remains a secret to this day. Indeed, X-ray observations toward massive star-forming regions are still rare, which may be due to absorption by the large hydrogen column densities toward these objects (Grosso et al. 2005).

Molecular gas exposed to X-rays forms an X-ray dissociation region (XDR) with a peculiar chemistry and physical structure. There has been a growing interest in XDRs in the past twenty years and several models
have been developed in order to study these regions. Krolik & Kallman (1983) investigated the influence of X-ray ionization on the Orion molecular cloud assuming a fixed density and temperature. Lepp & McCray (1983) presented constant gas pressure models to calculate the temperature and infrared line emission from an interstellar gas cloud containing a compact X-ray source. Maloney et al. (1996) studied the influence of X-rays on the physical and chemical state of neutral gas over a wide range of densities and X-ray fluxes. In addition, they discussed diagnostic line ratios to distinguish XDRs from shocks and photodissociation regions (PDRs). However, their chemical network focused primarily on carbon and oxygen, whereas nitrogen-bearing species, for example, were neglected. Calculations of molecular abundances for varying X-ray ionization rates in interstellar clouds were presented by Lepp & Dalgarno (1996). They mainly concentrated on HCO$^+$ and nitrogen-containing compounds. A thorough and more general treatment of the physics and chemistry in molecular clouds exposed to X-rays was done by Yan (1997). Tine et al. (1997) calculated the infrared response of H$_2$ in dense clouds. Other models concentrate on the X-ray ionization of protoplanetary disks (e.g., Glassgold et al. 1997; Aikawa & Herbst 1999; Markwick et al. 2002) or planetary nebulae (e.g., Natta & Hollenbach 1998). Most recently, Meijerink & Spaans (2005) presented a code for photodissociation and X-ray dissociation regions and discussed thermal and chemical differences between the two regions. They calculated four depth-dependent models for different densities and radiation fields that are typical in starburst galaxies and active galactic nuclei.

In this paper we study the influence of a central X-ray source on the chemistry in the envelopes around massive YSOs, using updated atomic and molecular data. The goal of this investigation is to find X-ray tracers that are observable with current or future telescopes in the (sub)millimeter or near-infrared range. The challenge is to distinguish between far ultraviolet (FUV) tracers (Stäuber et al. 2004a) and X-ray tracers, since both kinds of high-energy radiation tend to form ions and radicals. Further aims of this study are to estimate not only the X-ray flux emitted by highly obscured objects but also the ionization rate and ionization fraction in the envelopes around YSOs by carefully studying the chemistry. The ionization fraction of a cloud is an important parameter in the formation of a star as magnetic fields control the dynamics of ions. Ambipolar diffusion may support the molecular cloud and reg-
ulate the process of mass accretion. It may also influence disk viscosity and jet acceleration. Due to the small atomic and molecular cross sections at high energy (the total cross section summed over all species for a 1 keV photon is $\approx 2.5 \times 10^{-22} \text{cm}^2$ and decreases with energy as $\approx \lambda^3$), X-rays can penetrate deeper into the envelope than, for example, FUV photons and affect the gas-phase chemistry even at large distances from the source. In addition, the X-ray ionization rate may exceed the cosmic-ray ionization rate for a large part of the envelope. X-rays are therefore a plausible candidate for the ionization source in the inner, dense part of a YSO envelope.

We have extended the time- and position-dependent chemical model of Doty et al. (2002) to allow the impact of X-rays on the envelope. The physical and chemical models are described in Sect. 3.2 and Sect. 3.3. Our results are presented and discussed in Sect. 3.4. A selection of possible X-ray tracers is discussed in Sect. 3.5. In Sect. 3.6 best-fit models for AFGL 2591 are evaluated. To compare the modeled abundance profiles to observations and to show that the influence of X-rays on the chemistry is observable with (large) existing single-dish telescopes, we have calculated emission lines for a selection of species using the Monte Carlo radiative transfer code of Hogerheijde & van der Tak (2000). These results are shown in Sect. 3.7. Although our calculations are focused on high-mass YSOs, the qualitative results should be equally applicable to the envelopes around low-mass YSOs. Doty et al. (2004) showed that the chemical models of the low-mass source IRAS 16293–2422 required only minor modifications to their high-mass model. We summarize and conclude this paper in Sect. 3.8.

3.2 Model

The model is based on the detailed thermal and gas-phase chemistry models of Doty et al. (2002) and has been extended to allow the impact of X-rays on the envelope chemistry of young stellar sources.

3.2.1 X-ray flux

The observed X-ray spectra from high-mass YSOs are usually fitted with the emission spectrum of a thermal plasma (e.g., Hofner & Churchwell
The thermal X-ray spectrum can be approximated with

\[ F_{\text{in}}(E, r) = F_0(r)e^{-E/kT_X} \quad \text{[photons s}^{-1} \text{ cm}^{-2} \text{ eV}^{-1}] \]  

(3.1)

where \( F_{\text{in}}(E, r) \) is the incident X-ray flux per unit energy, and \( T_X \) is the temperature of the X-ray emitting plasma. If the X-ray luminosity \( L_X \) of the source is known, the factor \( F_0(r) \) can be evaluated from

\[ L_X = 4\pi r^2 F_X = 4\pi r^2 \int F_{\text{in}}(E)E dE \quad \text{[erg s}^{-1}] \]  

(3.2)

The column density between the source and our first calculated point is always \( N_{\text{H, in}} > 1/\sigma_p(1 \text{ keV}) \), where \( \sigma_p \) is the total photoabsorption cross section defined in eq. (3.3). It can therefore be assumed that all photons with energies below 1 keV are absorbed in the inner region. Photons at energies above 100 keV can be neglected as they contribute only minutely to the total integrated X-ray flux. Thus, we calculate the integral (3.2) over the energy range \( E_{\text{min}} = 1 \text{ keV} \) to \( E_{\text{max}} = 100 \text{ keV} \).

The local (i.e., attenuated) X-ray flux per unit energy is finally given by \( F(E, r) = F_{\text{in}}(E, r)e^{-\tau(E)} \), where \( \tau(E) \) is the total X-ray attenuation and \( F_{\text{in}} \) is the incident X-ray flux given by eq. (3.1). At lower energies \( (E \lesssim 10 \text{ keV}) \), X-rays lose their energy mainly through photoabsorption. Assuming that the photoabsorption cross section of a molecule or atom is equal to its photoionization cross section, the attenuation is given by

\[ \tau_p(E) = N_{\text{H}}\sigma_p(E) = N_{\text{H}} \sum x(i)\sigma_i(E), \]  

(3.3)

where,

\[ x(i) = \frac{n(i)}{n(\text{H}) + 2n(\text{H}_2)}, \]  

(3.4)

and \( N_{\text{H}} \) is the total hydrogen column density, \( \sigma_p \) the total photoabsorption cross section given by the sum of the ionization cross sections of each species in the cloud multiplied by its fractional abundance \( x(i) \). We have adopted the analytic fits of Verner et al. (1996) for the photoionization cross sections of atoms and ions and use the cross sections provided by Yan (1997) for \( \text{H}_2 \). To allow for the attenuation of X-rays by grains, the elemental abundances in the solid phase are added to eq. (3.3). The assumed total and gas-phase abundances are given in Table 3.1. The
values listed in Table 3.1 are taken from Doty et al. (2002) for the gas-phase abundances and from Yan (1997) for the total abundance.

For higher energies, X-rays also lose energy through inelastic Compton scattering, and Compton ionization becomes the dominant ionization source. The highly energetic X-ray photons interact mainly with free and bound electrons in the gas. Since molecular hydrogen is the most abundant species in our models, the total Compton cross section is dominated by hydrogen, rather than by heavy elements. We have fitted the values provided by the XCOM-NIST database (Berger et al. 1999) for hydrogen and assume that the Compton cross section of molecular hydrogen is twice that of atomic hydrogen. The energy loss of a Compton scattered photon is negligible compared to its initial energy, and attenuation through Compton scattering becomes important only for hydrogen column densities $N_H \gtrsim 10^{24}\,\text{cm}^{-2}$. However, since each scattering process leads to an ionization, the total (effective) cross section for ionizing $H_2$, $\sigma_{\text{eff}}$ (see Sect. 3.3.2), is the sum of the total photoabsorption cross section $\sigma_p$ and the cross section for Compton scattering $\sigma_s$. The attenuation of the X-rays is mainly through photoabsorption. Figure 3.1 shows the photoabsorption cross sections for the element abundances given in Table 3.1, the Compton cross section of molecular hydrogen, and the total (effective) ionization cross section $\sigma_{\text{eff}}$.

Model results for AFGL 2591 show that the X-ray ionization rate with and without the effects of Compton scattering differs by at most 20% and that the influence of Compton scattering on the chemistry is negligible. Nevertheless, we include attenuation and ionization due to Compton scattering, using a simplified radiative transfer method to calculate the incident radiation field.

Although eq. (3.1) approximates a thermal energy distribution, the X-ray spectrum of a thermal plasma has a more complex structure. In addition to the bremsstrahlung emission, line emission can become important. In order to evaluate the accuracy of the assumed X-ray spectrum, we have fitted the results of Raymond & Smith (1977) for an X-ray spectrum of a hot plasma. The results are very similar, leading to the same best-fit models (Sect. 3.6.1). The results in the following sections are therefore presented using the X-ray spectrum given by eq. (3.1).
### Table 3.1: Initial gas-phase and total abundances.

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All abundances are relative to total hydrogen. Only the abundances in the 2. and 3. column enter the chemistry. The total abundances $x(i)$ (4. column) are for the attenuation of the X-rays.

<sup>a</sup> van der Tak et al. (1999), <sup>b</sup> Boonman et al. (2003)<sup>b</sup>, <sup>c</sup> Boonman & van Dishoeck (2003), <sup>d</sup> see text, <sup>e</sup> Charnley (1997), <sup>f</sup> assumed to be frozen-out or absent in cold gas-phase, <sup>g</sup> taken to be $\sim$ consistent with Meyer et al. (1998), <sup>h</sup> assumed abundances, <sup>i</sup> Yan (1997).
3.2.2 Physical and thermal model

We have applied our model to the massive star-forming region AFGL 2591. AFGL 2591 is taken as a prototypical example of a deeply embedded high-mass YSO (a so-called high-mass protostellar object, HMPO) for which extensive observational data exist and for which reference models without X-rays are available (Doty et al. 2002; Stäuber et al. 2004a). No X-ray emission, however, has been observed to date toward this source. Assuming a distance of 1 kpc, the bolometric luminosity is $\sim 2 \times 10^4 L_\odot$ with a total mass of $\sim 10 M_\odot$ (van der Tak et al. 1999).

We adopt the temperature and power-law density distribution proposed by van der Tak et al. (1999) and Doty et al. (2002). The density structure of the envelope has been constrained from continuum observations of the dust and CS emission lines over a large range of critical densities. The dust temperature profile was determined from the self-consistent solution of the continuum radiative transfer problem. The gas temperature was calculated explicitly by Doty et al. (2002) who found that $T_{\text{gas}} \approx T_{\text{dust}}$. The influence of the X-rays on the gas temperature can be estimated by comparing the cooling rate due to gas-dust collisions.
3.2. Model

Figure 3.2: Physical and thermal structure of AFGL 2591. The power-law density distribution is adopted from the model of van der Tak et al. (1999). The gas temperature profile was calculated by Doty et al. (2002).

(Hollenbach & McKee 1989) and the X-ray heating rate provided by Maloney et al. (1996) \( n \Gamma_X \approx 3 \times 10^{-4} n H_X \text{ erg cm}^{-3} \text{s}^{-1} \), where \( H_X \) is the energy deposition rate per particle, defined by \( H_X = \int F(E, r) \sigma_{\text{eff}}(E) E \text{d}E \). Our first point of interest is at \( r \approx 200 \text{AU} \) from the central source where the density is already fairly high \( (n \approx 10^7 \text{cm}^{-3}) \) but \( H_X \) is low due to absorption and geometric dilution \( (H_X \approx 10^{-28} - 10^{-23} \text{erg s}^{-1}) \), for X-ray luminosities \( L_X \approx 10^{29} - 10^{33} \text{erg s}^{-1} \). The cooling rate at this point is \( \Lambda \approx 3.6 \times 10^{-18} \left( T_{\text{gas}} - T_{\text{dust}} \right) \text{erg cm}^{-3} \text{s}^{-1} \). Thus, in our modeled regions of AFGL 2591, a meaningful increase in the gas temperature \( (T_{\text{gas}} - T_{\text{dust}} \gtrsim 10 \text{K}) \) can only be expected for very high X-ray luminosities \( L_X \gtrsim 10^{33} \text{erg s}^{-1} \). For our best-fit models (Sect. 3.6.1), a difference of only 3 K at most is estimated between the gas and dust temperature. We therefore neglect additional heating of the gas through X-rays and assume \( T_{\text{gas}} \approx T_{\text{dust}} \) throughout the envelope. This is a reasonably good approximation as was shown by Doty & Neufeld (1997) and Doty et al. (2002). Figure 3.2 shows the adopted model for AFGL 2591. The model covers a region from \( r_{\text{in}} \approx 200 \text{AU} \) to \( r_{\text{out}} \approx 29000 \text{AU} \).
3.2.3 Chemical model

The chemical model is based upon the UMIST gas-phase chemical reaction network (Millar et al. 1997) and calculates the time-dependent number density $n(i)$ of each species at a certain distance from the source by solving the equations for molecular evolution given by

$$\frac{dn(i)}{dt} = \sum_j k_{ij}n(j) + \sum_{j,k} l_{ijk}n(j)n(k),$$

where $n(i)$ is the number density of species $i$; $k_{ij}$ and $l_{ijk}$ are the rate coefficients for production and destruction of the given species. The main inputs of the model are the temperature and density distribution, the cosmic ray ionization rate and the strength of the far ultraviolet (FUV) radiation field from the inside and outside, $G_{0,\text{in}}$ and $G_{0,\text{out}}$ respectively. They were discussed in detail by Doty et al. (2002) and Stäuber et al. (2004a). The new input parameters concerning the X-rays are the X-ray luminosity $L_X$, the plasma temperature $T_X$ and the inner hydrogen column density $N_{\text{H, in}}$, which is the column density between the source and the first innermost grid point of our envelope. In order to study the influence of X-rays on the chemistry, the chemical network has been extended by a number of species and reactions discussed in the following sections.

The assumed initial abundances given in Table 3.1 are taken to be consistent with the models of Doty et al. (2002) and Stäuber et al. (2004a). The initial gas-phase abundances allow us to reproduce many of the results of the hot core models of Charnley (1997). The effects of freeze-out onto dust grains are included by initially depleting certain species below 100 K. The temperature dependence of molecular depletion is discussed in detail by Boonman et al. (2003b) and Doty et al. (2004). The initial form of sulphur is not known. In our models we assume that sulphur is frozen out onto grains in the form of $\text{H}_2\text{S}$ and is evaporated into the gas-phase for $T > 100$ K. Solid $\text{H}_2\text{S}$ has not been detected, however (e.g., Boogert et al. 2000). On the other hand, Wakelam et al. (2004) have shown that it is likely that sulphur is in the icy mantles either as atomic S or in a form, perhaps polymerized S or $\text{S}_2$, that is soon converted into S. The dependence of our model results on the initial form of sulphur is discussed in Sect. 3.4.3.

For the total elemental abundances given in Table 3.1 we follow Yan
3.3. X-ray induced chemistry (1997). These abundances are the sum of the gas-phase elemental abundances and the abundances on the dust grains that do not enter the chemistry. In addition to the total hydrogen abundance, the total elemental abundances are important for the attenuation of the X-rays (see Sect. 3.2.1).

### 3.3 X-ray induced chemistry

#### 3.3.1 Direct X-ray ionizations and dissociations

X-rays ionize heavy elements preferentially by removing the K-shell electron. The vacancy is then filled by a cascade of radiative (fluorescent) and non-radiative Auger transitions. During this process other electrons and X-ray photons are emitted by the ion, leading finally to a multiply ionized species. The fluorescence probability is less than 10% for most species and approximately 30% for Fe (Dwek & Smith 1996). The contribution of the diffuse X-ray emission by fluorescence to the total X-ray flux can therefore be neglected.

We consider the ionization of atoms and atomic ions leading to a singly and doubly ionized state by calculating explicitly the cross sections according to Verner et al. (1996). The probability distribution for the number of ejected electrons for inner shell ionizations are taken from Kaastra & Mewe (1993). The (primary) X-ray ionization rate of species \( i \) at a point \( r \) is then simply given by

\[
\zeta_i = \int F(E, r)\sigma_i(E) dE \quad [\text{s}^{-1}],
\]

where \( \sigma_i(E) \) is the X-ray photoabsorption cross section of species \( i \) at energy \( E \) and \( F(E, r) \) is the local X-ray flux.

Little is known about the impact of X-rays on molecules. Although there are a few cross sections for photoabsorption in the literature, the destruction channels and branching ratios of the dissociated and ionized species are widely unknown. Following Maloney et al. (1996) we therefore consider only diatomic molecules for direct X-ray impact and assume that the molecule dissociates into singly charged ions after inner shell ionization. The cross sections for this process are calculated by adding the atomic cross sections. In general, primary X-ray ionization plays
only a minor role in the chemistry since the reactions are \( \approx 1000 \) times slower compared to the relevant chemical reactions and more than 10 times slower than electron impact ionizations for the case of our AFGL 2591 model parameters.

### 3.3.2 X-ray induced electron impact reactions

The fast photoelectrons and Auger electrons carry the bulk of the initial X-ray photon energy and are therefore very efficient in ionizing other species. The 'secondary' ionization rate dominates the total ionization rate in XDRs (e.g., Maloney et al. 1996). The electrons can also excite hydrogen and helium. The electronically excited states of H, He and H\( _2 \) decay back to the ground states by emitting UV photons. The internally generated ultraviolet photons can photoionize and photodissociate other species in the gas – similar to the case of cosmic-ray induced chemistry (e.g., Grede et al. 1989). Nearly all these secondary processes induced by electron impact are more important for the chemical network than the primary interaction of the X-rays with the gas.

**Ionizations**

Energy deposition of fast electrons in a gas is characterized by a mean energy per ion pair \( W(E) \) – the initial energy \( E \) of the electron divided by the number of produced ionizations, \( N(E) \), in the gas (e.g., Voit 1991; Dalgarno et al. 1999). To calculate \( W(E) \) and therefore the number of secondary electrons, we follow Dalgarno et al. (1999) for a H, He and H\( _2 \) gas mixture. An electron with an initial energy of 1 keV will then lead to \( \approx 27 \) ionizations. The 'secondary' ionization rate per hydrogen molecule at depth \( r \) can be calculated by

\[
\zeta(H_2) = \frac{\int F(E, r) \sigma_{\text{eff}}(E) \frac{E}{W(E)x(H_2)} dE}{[\text{s}^{-1}]},
\]

where \( x(H_2) \approx 0.5 \) is the fractional abundance of molecular hydrogen and \( \sigma_{\text{eff}} \) is the effective or total photoionization cross section at energy \( E \), including the cross section for Compton scattering, assuming that each scattering process will ionize a hydrogen molecule.

The electron impact ionization rates \( \zeta \) of other molecules or atoms can be calculated as a first approximation by multiplying the H\( _2 \) ionization
rate eq. (3.7) with the ratio of the electron impact cross sections of species $i$ to H$_2$ at a specific energy (Maloney et al. 1996). The average electron energy is taken to be 100 eV. The cross sections for the species were taken from Yan (1997), the NIST database (Kim et al. 2004) or estimated. The ratios for most molecules are between $\approx 2-8$. The error due to the energy dependence of the cross sections or to our estimations are therefore within a factor of a few but certainly $\lesssim 10 \times$.

UV photodissociations and photoionizations

The excited states in the Lyman-Werner bands of H$_2$ determine the internally generated FUV flux. The number of Ly$\alpha$ photons from H atoms are less important due to the relatively small fractional abundance of atomic hydrogen ($x(H) \lesssim 10^{-4}$). Following Gredel et al. (1989) the photodissociation and photoionization rate of species $i$ is given by

$$R_i = \frac{2x(H_2)\epsilon_{LyW}\zeta_{H_2}P_{i,LyW} + x(H)\epsilon_{Ly\alpha}\zeta_{H}P_{i,Ly\alpha}}{1 - \omega} \left[ \text{s}^{-1} \right],$$

where $\zeta_{H_2}$ and $\zeta_H$ are the H$_2$ and H ionization rate and $x(H_2)$ and $x(H)$ are the fractional H$_2$ and H abundances, respectively, $\omega$ is the grain albedo ($\omega \approx 0.6$) and $P_{i,LyW}$ and $P_{i,Ly\alpha}$ are factors that depend on the atomic or molecular photoabsorption cross sections (Gredel et al. 1989; Sternberg & Dalgarno 1995; Lepp & Dalgarno 1996). In eq. (3.8), $\epsilon_{LyW} \approx 1.4$ and $\epsilon_{Ly\alpha} \approx 1.2$ are the number of excitations per ionization calculated from the values provided by Dalgarno et al. (1999). For CO we follow Maloney et al. (1996) who fitted the self-shielding results of Gredel et al. (1987) and found

$$R_{CO} = 2.7x(CO)^{-1/2} \left( \frac{T}{1000 \, K} \right)^{1/2} x(H_2)\zeta_T \left[ \text{s}^{-1} \right],$$

where $x(CO)$ is the fractional CO abundance and $\zeta_T$ is the total ionization rate approximated by $\zeta_T \approx \zeta_{H_2} + \zeta_{cr}$, that is the sum of the H$_2$ ionization rate $\zeta_{H_2}$ and the cosmic-ray ionization rate $\zeta_{cr}$. The ‘primary’ X-ray ionization rate $\zeta_i$ can be neglected since it is in general much smaller than $\zeta_{H_2}$.

The He excited 2$^1$P state emits a 19.8 eV photon which ionizes mainly H$_2$, CO or H. The photoionization rate per He atom for these species is
\( R_{i,\text{He}} = \zeta_{\text{He}} \frac{x(\text{He})\sigma_i}{x(\text{H}_2)\sigma(\text{H}_2) + x(\text{H})\sigma(\text{H})} \) \text{ [s}^{-1}] \), \hspace{1cm} (3.10)

where \( \zeta_{\text{He}} \) is the He excitation rate and \( x(\text{He}) \) is the fractional He abundance, \( x(\text{H}_2), x(\text{H}), \sigma(\text{H}_2) \) and \( \sigma(\text{H}) \) are the \( \text{H}_2 \) and H fractional abundances, and the \( \text{H}_2 \) and H photoionization cross sections at \( \approx 20 \text{ eV} \) and \( \sigma_i \) is the photoionization cross section at \( \approx 20 \text{ eV} \) for H, \( \text{H}_2 \) and CO, respectively. The excitation rate of helium can be calculated similar to the \( \text{H}_2 \) ionization rate eq. (3.7) with the mean energy to excite a helium atom given by Dalgarno et al. (1999).

### 3.3.3 Other reactions

The electron recombination and charge transfer reactions of the doubly-ionized species are presented in Table 3.2 and Table 3.3. We consider only C, O, N, S, Fe, Ne and Si in the doubly-ionized state. Other ions in this state are neglected due to their low fractional abundances.

For the recombination of ions on grains we have adopted the treatment of Maloney et al. (1996) for all ions in the model. The grain surface recombination of \( \text{HCO}^+ \) is a critical reaction in dense regions (Aikawa et al. 1999) and important for the abundances of CO-bearing molecules. We follow the calculations of Aikawa et al. (1999) and assume branching ratios of 0.7 for the dissociative recombination and 0.3 for the radiative recombination reaction. However, our models for AFGL 2591 are not very sensitive to these values as long as the ratio dissociative/radiative recombination is \( > 1 \). For example, no noticeable differences were seen between models with ratios of 0.7/0.3 and 0.85/0.15, respectively. In addition, results of models without any grain recombination reactions of \( \text{HCO}^+ \) have shown no difference for species with fractional abundances \( x_i \gtrsim 10^{-10} \) and differences within only \( \approx 30\% \) for less abundant species. The recombination of \( \text{HCO}^+ \) in all our models is therefore dominated by electron recombination. Aikawa et al. (1999) further suggested that the dissociative recombination reaction might be more likely for most molecules. We have therefore assumed a branching ratio of 0.7/0.3 for all other molecules as well.

Aside from the grain surface recombination reactions we have ignored grain-surface chemistry, with the exception of the formation of \( \text{H}_2 \). In our
3.4. Results and discussion

Table 3.2: Electronic recombination reactions.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>a</th>
<th>b</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>O$^{2+}$ + e$^-$ → O$^+$ + h$\nu$</td>
<td>1.9E-11</td>
<td>-0.65</td>
<td>AP73</td>
</tr>
<tr>
<td>C$^{2+}$ + e$^-$ → C$^+$ + h$\nu$</td>
<td>2.2E-11</td>
<td>-0.65</td>
<td>AP73</td>
</tr>
<tr>
<td>N$^{2+}$ + e$^-$ → N$^+$ + h$\nu$</td>
<td>2.1E-11</td>
<td>-0.64</td>
<td>AP73</td>
</tr>
<tr>
<td>S$^{2+}$ + e$^-$ → S$^+$ + h$\nu$</td>
<td>2.0E-11</td>
<td>-0.69</td>
<td>MHT96</td>
</tr>
<tr>
<td>Fe$^{2+}$ + e$^-$ → Fe$^+$ + h$\nu$</td>
<td>2.1E-11</td>
<td>-0.84</td>
<td>MHT96</td>
</tr>
<tr>
<td>Si$^{2+}$ + e$^-$ → Si$^+$ + h$\nu$</td>
<td>1.6E-11</td>
<td>-0.79</td>
<td>MHT96</td>
</tr>
<tr>
<td>Mg$^{2+}$ + e$^-$ → Mg$^+$ + h$\nu$</td>
<td>1.7E-11</td>
<td>-0.84</td>
<td>AP73</td>
</tr>
<tr>
<td>Ne$^{2+}$ + e$^-$ → Ne$^+$ + h$\nu$</td>
<td>1.7E-11</td>
<td>-0.69</td>
<td>AP73</td>
</tr>
<tr>
<td>Ne$^+$ + e$^-$ → Ne + h$\nu$</td>
<td>3.1E-12</td>
<td>-0.76</td>
<td>AP73</td>
</tr>
</tbody>
</table>

Rate coefficients have the form $k = a(T/300)^b$ and $a$ is in units of cm$^3$s$^{-1}$. AP73 refers to Aldrovandi & Péquignot (1973). MHT96 refers to Maloney et al. (1996).

In the model, the rate is $R_{H_2} = 3 \times 10^{-17} n(H)n_H \text{cm}^{-3}\text{s}^{-1}$, where $n(H)$ is the atomic hydrogen density, and $n_H$ is the density of hydrogen nuclei. Other reactions that affect the H$_2$ network are the formation of the H$^-$ ion by radiative association H + e$^-$ → H$^-$ + h$\nu$ and the reaction H$^+$ + H → H$_2^+$ + h$\nu$. For these rates we have adopted the fits by Latter (1989). Since we are almost always in a pure molecular environment, these reactions play only a minor role in our models though.

3.4 Results and discussion

The chemistry in the envelope around AFGL 2591 under the influence of X-rays has been modeled assuming spherical symmetry. The parameters that were varied are the X-ray luminosity, the plasma temperature and the inner hydrogen column density. The inner hydrogen column density $N_{H,\text{in}}$ is the X-ray absorbing column density between the central source and the first calculated point at $r \approx 200$ AU (see also eq. (3.3)). Since only the total hydrogen column density is known, $N_{H,\text{in}}$ is treated as an unknown parameter.

The equilibrium timescale for X-ray induced chemistry is $t_{eq} \approx \zeta_{H_2}^{-1} \propto r^2/L_{X\gamma\text{r}}$. Thus, equilibrium may not be reached for most parts of the
### Table 3.3: Charge transfer reactions.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>a</th>
<th>b</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>O²⁺ + H → O⁺ + H⁺</td>
<td>7.7E-10</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>C²⁺ + H → C⁺ + H⁺</td>
<td>1.0E-12</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>N²⁺ + H → N⁺ + H⁺</td>
<td>8.6E-10</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>S²⁺ + H → S⁺ + H⁺</td>
<td>1.0E-14</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>Fe²⁺ + H → Fe⁺ + H⁺</td>
<td>1.6E-10</td>
<td>0.17</td>
<td>MHT96</td>
</tr>
<tr>
<td>Mg²⁺ + H → Mg⁺ + H⁺</td>
<td>9.0E-14</td>
<td></td>
<td>AR85</td>
</tr>
<tr>
<td>Ne²⁺ + H → Ne⁺ + H⁺</td>
<td>1.0E-14</td>
<td></td>
<td>AR85</td>
</tr>
<tr>
<td>Si²⁺ + H → Si⁺ + H⁺</td>
<td>1.8E-09</td>
<td>0.28</td>
<td>AR85</td>
</tr>
<tr>
<td>O²⁺ + H₂ → O⁺ + H⁺₂</td>
<td>1.0E-09</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>C²⁺ + H₂ → C⁺ + H⁺₂</td>
<td>1.0E-13</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>Fe²⁺ + H₂ → Fe⁺ + H⁺₂</td>
<td>1.0E-14</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>S²⁺ + H₂ → S⁺ + H⁺₂</td>
<td>1.0E-15</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>N²⁺ + H₂ → N⁺ + H⁺₂</td>
<td>3.4E-11</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>N²⁺ + He → N⁺ + He⁺</td>
<td>1.3E-10</td>
<td></td>
<td>Yan (1997)</td>
</tr>
<tr>
<td>C²⁺ + He → C⁺ + He⁺</td>
<td>1.0E-10</td>
<td></td>
<td>AR85</td>
</tr>
<tr>
<td>O²⁺ + He → O⁺ + He⁺</td>
<td>7.1E-12</td>
<td>0.95</td>
<td>AR85</td>
</tr>
<tr>
<td>Ne²⁺ + He → Ne⁺ + He⁺</td>
<td>1.0E-14</td>
<td></td>
<td>BD80</td>
</tr>
</tbody>
</table>

Rate coefficients have the form $k = a(T/300)^b$ and $a$ is in units of $\text{cm}^3\text{s}^{-1}$. MHT96 refers to Maloney et al. (1996). AR85 refers to Arnaud & Rothenflug (1985). BD80 refers to Butler & Dalgarno (1980).
### Figure 3.3: Ionization rates $\zeta_{H_2}$ for the X-ray models presented in Table 3.4 and a constant cosmic-ray ionization rate $\zeta_{cr} = 5.6 \times 10^{-17} \text{s}^{-1}$. The arrow indicates the distance out to which an inner UV field is effective.

### Table 3.4: Model parameters for AFGL 2591.

<table>
<thead>
<tr>
<th>Model</th>
<th>$L_X$ (erg s$^{-1}$)</th>
<th>$T_X$ (K)</th>
<th>$N_{H, in}$ (cm$^{-2}$)</th>
<th>$G_{0, in}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>1.0E+30</td>
<td>7.0E+07</td>
<td>3.0E+22</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1.0E+31</td>
<td>7.0E+07</td>
<td>3.0E+22</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>1.0E+32</td>
<td>7.0E+07</td>
<td>3.0E+22</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>1.0E+32</td>
<td>7.0E+08</td>
<td>5.0E+22</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>8.0E+31</td>
<td>1.0E+08</td>
<td>3.0E+22</td>
<td>10</td>
</tr>
<tr>
<td>6</td>
<td>6.0E+31</td>
<td>3.0E+07</td>
<td>3.0E+22</td>
<td>10</td>
</tr>
</tbody>
</table>
envelope. The results in this section are presented for \( t \approx 5 \times 10^4 \) years according to our best-fit models. This result is in good agreement with the chemical age of AFGL 2591 found by Doty et al. (2002). For simplicity, the luminosity was kept constant with time. For all models an outer standard FUV field \( G_{0,\text{out}} = 1 \) has been assumed to be consistent with Doty et al. (2002) and Stäuber et al. (2004a). The effects of an enhanced outer FUV radiation field will be discussed in Sect. 3.4.7.

Table 3.4 lists the models that are discussed in more detail in this paper. In addition to the best-fit models (Model 5,6,7), models with a plasma temperature \( T_X = 7 \times 10^7 \) K and an inner column density of \( N_{H,\text{in}} = 3 \times 10^{22} \) cm\(^{-2}\) are presented. Model 0 corresponds to the standard model of Doty et al. (2002) without any inner radiation field and Model 1 assumes an inner FUV radiation field with a field strength \( G_{0,\text{in}} = 10 \) according to the models of Stäuber et al. (2004a). The plasma temperature of Models 2–4 has been chosen as a mean value of the best-fit models (Sect. 3.6.1). The only parameter that has been varied for the plots of the Models 2–4 is the X-ray luminosity \( L_X \). This is useful since the energy deposition rate \( H_X \) is directly proportional to the X-ray luminosity and all the X-ray induced reactions therefore scale with \( L_X \). Results for different X-ray temperatures \( T_X \) and inner hydrogen column densities \( N_{H,\text{in}} \) are presented in Sect. 3.4.6.

Figure 3.3 shows the \( H_2 \) ionization rates \( \zeta_{H_2} \) for the different X-ray models. In addition, the cosmic-ray ionization rate \( \zeta_{\text{cr}} = 5.6 \times 10^{-17} \) s\(^{-1}\) is shown which is taken from van der Tak & van Dishoeck (2000). By taking the physical parameters given in Fig. 3.2, it can be estimated that half of the envelope mass is inside \( r \approx 3 \times 10^{17} \) cm. Comparison of \( \zeta_{H_2} \) and \( \zeta_{\text{cr}} \) in Fig. 3.3 therefore shows that the bulk of the envelope mass is dominated by the cosmic-ray ionization rate rather than by the X-ray ionization rate. X-ray luminosities \( L_X \geq 10^{33} \) erg s\(^{-1}\) are required for the X-ray ionization rate to dominate the cosmic-ray ionization rate. The influence of different cosmic-ray ionization rates on the chemistry is shown in Sect. 3.4.8.

Abundances of various species are presented in Fig. 3.4–3.6 for Models 0, 2–4 and Model 6. Since it is more common to compare number densities to the number density of molecular hydrogen rather than to the total hydrogen density, the following results are presented with fractional abundances \( \tilde{x}(i) = n(i)/n(H_2) \).
3.4. Results and discussion

3.4.1 CO, H$_2$O and CO$_2$

The CO abundance profile in Fig. 3.4 shows that the total abundance of this molecule is not significantly affected by X-rays. H$_2$O and CO$_2$ on the other hand are destroyed in the gas-phase. CO$_2$ is destroyed mainly by FUV photons induced through electron impact on H$_2$. The additional CO$_2$ at higher temperatures is primarily from the reaction of OH with CO. The bump at $r \approx 4 \times 10^{15}$ cm ($T \approx 300$ K) is due to the reaction of HCO$^+$ with CO which is slightly faster at this distance than the destruction of CO$_2$. HCO$^+$ is efficiently produced by the reaction of HCO$^+$ with OH. Detailed studies of Boonman et al. (2003a) showed that the fractional CO$_2$ abundance is $\tilde{x}(\text{CO}_2) \approx 1-2 \times 10^{-6}$ for $T \gtrsim 300$ K and $\tilde{x}(\text{CO}_2) \approx 10^{-8}$ for $T \lesssim 300$ K. This jump at $T \approx 300$ K is well produced by our models for relatively high X-ray luminosities $L_X \gtrsim 10^{31}$ erg s$^{-1}$. The models of Doty et al. (2002) for AFGL 2591 overpredicted the CO$_2$ abundance in the gas phase and Stäuber et al. (2004a) showed that an inner FUV flux does not destroy CO$_2$ significantly either. X-rays are therefore a possible explanation for the observed gas-phase CO$_2$ abundance profile.

H$_2$O is most efficiently destroyed by reactions with HCO$^+$ and H$_3^+$ for $T \gtrsim 100$ K. In the warm, inner region water is mainly produced by the reaction of OH with H$_2$. For temperatures $T \lesssim 230$ K, however, most of the gas-phase OH and O goes into O$_2$, thus H$_2$O is less abundant for these temperatures. H$_2$O has been observed and studied in detail towards AFGL 2591 by Boonman & van Dishoeck (2003). They derived a fractional abundance of $\tilde{x}(\text{H}_2\text{O}) \approx 10^{-4}$ for $T \gtrsim 100$ K (scenario 8 in Boonman & van Dishoeck 2003). Our models for high X-ray fluxes ($L_X \gtrsim 10^{30}$ erg s$^{-1}$) give such high abundances only at $T \gtrsim 230$ K and are therefore inconsistent with the observations of gas-phase water towards AFGL 2591. The low X-ray luminosity is in contradiction with the overall best-fit results (Sect. 3.6.1) and with the results for CO$_2$. One possible solution to this problem could be the evolution of water with time or related to this, the X-ray luminosity may not be constant with time. However, the destruction of H$_2$O starts already at $t \gtrsim 1000$ yrs which would imply an implausibly young age. Another possible origin of the discrepancy may be the chemical reaction coefficients that cause the production of O$_2$ rather than H$_2$O for 100 K $\lesssim T \lesssim 230$ K. In particular, the coefficients may depend on the populations of the fine-structure levels of atomic oxygen. A higher temperature from $r \approx 0.4-1.7 \times 10^{16}$ cm
Figure 3.4: Depth dependent fractional abundances for the models described in Table 3.4. The solid line corresponds to Model 0, the dotted line is Model 2, the dashed line is Model 3. The dashed-dotted line is Model 4 and the dashed-dotted-dotted line (Model 6) correspond to the best fitted X-ray model with an inner UV field of $G_{0,\text{in}} = 10$. 
3.4. Results and discussion

Figure 3.5: Depth dependent fractional abundances for the models described in Table 3.4. The solid line corresponds to Model 0, the dotted line is Model 2, the dashed line is Model 3. The dashed-dotted line is Model 4 and the dashed-dotted-dotted line (Model 6) correspond to the best fitted X-ray model with an inner UV field of $G_{0,\text{in}} = 10$. 
Figure 3.6: Depth dependent fractional abundances for the models described in Table 3.4. The solid line corresponds to Model 0, the dotted line is Model 2, the dashed line is Model 3. The dashed-dotted line is Model 4 and the dashed-dotted-dotted line (Model 6) correspond to the best fitted X-ray model with an inner UV field of \( G_{\text{in}} = 10 \).
would solve this problem as well.

3.4.2 Carbon: C, C\(^+\), CO\(^+\), HCO\(^+\) and HOC\(^+\)

In the models with X-rays, atomic carbon is particularly produced by the photodissociation of CO by FUV photons from H\(_2\) excited by electron impact. If a FUV field \(G_{0,\text{in}}\) is turned on, however, carbon is more efficiently created by the photons from the inner FUV field. By comparing the two reaction rates, it can be shown that the production of atomic carbon by dissociating CO is dominated by X-ray induced reactions if the total ionization rate is

\[ \zeta_T \gtrsim 3 \times 10^{-12} \left( \frac{x(\text{CO})}{10^{-4}} \right)^{1/2} \left( \frac{T}{300 \, \text{K}} \right)^{-1/2} G_0 e^{-2.5A_V} \, \text{s}^{-1}, \]  

(3.11)

where \(A_V\) is the total visual extinction. If we define the difference of a chemical photodissociation region (PDR) and an X-ray dominated region (XDR) by the way CO is photodissociated, eq. (3.11) allows to determine the physical boundary of the two regions through the visual extinction \(A_V\). For Models 4–7, that is the best-fit models, this is the case for \(A_V \approx 2\).

Neutral atomic carbon is mainly destroyed by ionization through FUV photons from either X-ray induced processes or from the inner FUV field. Further in the envelope (\(T \lesssim 100 \, \text{K}\)), carbon is primarily destroyed in reactions with O\(_2\) and HCO\(^+\). The most efficient way to produce C\(^+\) in the pure X-ray models is the reaction He\(^+\) + CO \(\rightarrow\) C\(^+\) + O + He. For high X-ray fluxes (\(L_X \gtrsim 5 \times 10^{31} \, \text{erg} \, \text{s}^{-1}\)), this reaction even dominates the photoionization due to an inner FUV field once \(A_V \gtrsim 2\). The production of C\(^+\) through the X-ray induced FUV photoionization of C or through the ‘primary’ X-ray ionization and dissociation of CO (Sect. 3.3.1) is approximately 10 times less efficient. The fastest destruction process for C\(^+\) is by reaction with H\(_2\)O. This is also the dominant production mechanism for HOC\(^+\). HCO\(^+\) on the other hand, is more efficiently produced by the reaction of H\(_3^+\) with CO. This is due to the fact that the production of HCO\(^+\) through this reaction is \(\approx 60\) times faster compared to the production of HOC\(^+\). The destruction of HCO\(^+\) and HOC\(^+\) is mainly through reactions with water in the inner part of the envelope and through electron recombination at larger distances from the source. HOC\(^+\) is also destroyed in reactions with H\(_2\) which form HCO\(^+\).
CO$^+$ is mainly produced by electron impact ionization of CO. Other important reactions are the charge exchange reaction of He$^+$ with CO$_2$ and the reactions of C$^+$ with OH and O$_2$, respectively. CO$^+$ is quickly destroyed by H$_2$ and forms HCO$^+$.

### 3.4.3 Sulphur chemistry

Fig. 3.4–3.6 show that sulphur and sulphur-bearing molecules are strongly enhanced by X-rays. The following (simple) network explains the relatively high fractional abundances of some of these species: The chemical sulphur network starts with the production of atomic sulphur through X-ray induced FUV photodissociation of H$_2$S. Sulphur reacts then with OH to form either SO or SH. SO reacts with atomic carbon and can therefore form CS. Reactions of CS with H$_3$O$^+$ and HCO$^+$ lead to HCS$^+$. SH$^+$ is efficiently produced by the reactions of atomic sulphur with H$_3^+$ or HCO$^+$. The dominant destruction channel for S in the innermost part of the envelope is the photoionization due to an inner FUV field or due to FUV photons from X-ray induced reactions. These are also the most important reactions to produce S$^+$. S$^+$ reacts with OH and O$_2$ and forms SO$^+$. X-rays can ionize atomic sulphur even at large distances and the abundances of S$^+$, SO$^+$ and HCS$^+$ are enhanced throughout the entire envelope.

In order to study the dependence of our model results on the form of the initial sulphur, we have run models assuming the initial sulphur to be atomic for $T > 100$ K instead of being in the form of H$_2$S with the following result: For the best fitted X-ray models (Sect. 3.6.1) all species have exactly the same abundances after a few 1000 yrs as in the models where the initial sulphur was assumed to be in H$_2$S. In models without X-rays, however, the results differ less than 20% once $t \gtrsim 5 \times 10^4$ yrs. For $t \approx 3 \times 10^4$ yrs, the chemical age of AFGL 2591 found by Doty et al. (2002), the column density of H$_2$S is $\approx 25$ times less in the model where the initial sulphur was in atomic form compared to the model where sulphur was in the form of H$_2$S. By comparing the two models without X-rays but with different initial forms of sulphur to observations of H$_2$S (van der Tak et al. 2003) it is seen that the model where sulphur is assumed to be initially in the form of H$_2$S fits the observations much better. Other species like S, SO$_2$, CS and H$_2$CS, however, differ less than 30% for $t \approx 3 \times 10^4$ yrs. Since we will compare our results to the models of Doty et al. (2002) and
3.4. Results and discussion

Stäuber et al. (2004a) we assume sulphur initially to be in the form of H$_2$S.

3.4.4 Nitrogen chemistry

Since the initial nitrogen in our models is in molecular form, the nitrogen chemistry starts with the photodissociation of N$_2$ by either an inner FUV field $G_{0\text{in}}$ or by X-ray induced FUV photons from excited H$_2$. Atomic nitrogen is then transformed into NO in reactions with OH. NO reacts with N and forms N$_2$, or it reacts with C to make CN. HCN is then efficiently produced by the reaction of CN with H$_2$. The destruction of N$_2$ by H$_3^+$ leads to N$_2$H$^+$ that is mainly destroyed by H$_2$O or by CO. The destruction of N$_2$H$^+$ by HCN leads to HNCH$^+$ which can recombine either back to HCN, HNC, or CN.

The bulk abundance of N$^+$ in the gas stems from the ionization of N$_2$ by He$^+$. For N$^+$, reactions with H$_2$ lead to NH$_2^+$ which dissociates into NH$_2$ and H$_2$ via electron recombination. NH$_2$ and O form HNO which on the other hand forms N$_2$O by reaction with O. From Fig. 3.6 it can be seen that both HNO and N$_2$O are greatly enhanced by X-rays.

3.4.5 Simple hydrides

Hydrides are strongly enhanced by X-rays as can be seen in Fig. 3.4–3.6. The hydrides SH and SH$^+$ have already been discussed in Sect. 3.4.3. X-ray enhanced CH reaches a fractional abundance of $\tilde{x}$(CH) $\approx$ few $\times$ 10$^{-10}$ for high X-ray fluxes ($\mathcal{L}_x \approx 10^{32}$ ergs$^{-1}$) and its abundance is almost constant in the entire envelope. CH is mainly produced by the reaction CH$_2$ + H → CH + H$_2$. CH$_2$ is efficiently produced in reactions of C with H$_2$ and by the X-ray induced photodissociation of CH$_4$. At larger distances of the source, electron recombination reactions of CH$_3^+$ become also important for the production of both CH and CH$_2$. CH is primarily destroyed in reactions with H$_2$. CH$^+$ is mainly formed in reactions of H$_3^+$ or HCO$^+$ with atomic carbon. The fractional abundance of CH$^+$ is also almost constant throughout the envelope for the higher X-ray flux models, but with $\tilde{x}$(CH$^+$) $\approx$ 10$^{-15}$–10$^{-13}$, $\tilde{x}$(CH$^+$) $<$ 10$^{-3}$ $\times$ $\tilde{x}$(CH). However, CH$^+$ is enhanced up to $\tilde{x}$(CH$^+$) $\approx$ 10$^{-13}$ in the innermost part of the envelope where it is $\approx$ 10$^5$ times more abundant in the best-fit models than in the
models without X-rays.

OH and OH$^+$ are both enhanced by X-rays through the destruction of water in the gas-phase. OH is the product of FUV photodissociation of H$_2$O whereas OH$^+$ is mainly produced in reactions of He$^+$ with H$_2$O or in reactions of H$_3^+$ with OH. Both, OH and OH$^+$ are destroyed primarily by H$_2$. For the best-fit models, OH reaches fractional abundances $\tilde{x}$(OH) $\approx$ 10$^{-8}$ in the outer part and $\tilde{x}$(OH) $\approx$ 10$^{-6}$ in the innermost part of the envelope. OH$^+$ has a fractional abundance of $\tilde{x}$(OH$^+$) $\approx$ 10$^{-14}$-10$^{-13}$ in the outer part and reaches $\tilde{x}$(OH$^+$) $\approx$ 10$^{-12}$ closer to the source.

Hydrides like SH, SH$^+$, CH, CH$^+$, OH and OH$^+$ are difficult to observe with ground based telescopes due to atmospheric absorption. These hydrides are therefore possible molecules to observe with the space-borne instrument Herschel-HIFI (de Graauw & Helmich 2001).

### 3.4.6 Varying $T_X$ and $N_{H,\text{in}}$

The influence of different X-ray temperatures $T_X$ and inner hydrogen column densities $N_{H,\text{in}}$ on the chemistry is shown in Fig. A.1 for six species for $L_X = 10^{32}$ erg s$^{-1}$. It can be seen that the results for $T_X = 3 \times 10^7$ K and $T_X = 7 \times 10^7$ K are very similar. A lower temperature of $T_X = 7 \times 10^6$ K, however, leads to lower abundances at larger distances from the source since the softer X-rays are more absorbed on their way through the envelope. The results for different inner column densities are even less distinctive. In general, higher absorbing hydrogen column densities lead to lower abundances. Comparison of the integrated column densities for all species for the different models shows that the results differ only a factor of 2 at most for the different X-ray temperatures, $T_X$, and absorbing inner hydrogen column densities, $N_{H,\text{in}}$. The influence of the X-ray temperature and the inner hydrogen column density on the chemistry is therefore not as strong as it is for the X-ray luminosity where the abundances of species like H$_3^+$ basically scale with the X-ray luminosity (see also Table 3.5 in Sect. 3.5). Indeed, it will be shown in Sect. 3.6.1 that the X-ray luminosity $L_X$ is the dominant parameter in our models.
3.4. Results and discussion

3.4.7 Influence of an enhanced outer FUV field

Regions of high-mass star formation often have FUV fields that are higher than the average interstellar radiation field. Evolved massive stars emit a copious amount of ultraviolet radiation. The immediate environment is ionized and a HII region is formed. The FUV photons (6< \( h\nu < 13.6 \) eV), however, penetrate the HII region and may influence the chemistry of a nearby cloud or the envelope of a young stellar object, forming a photon-dominated region (eg., Hollenbach & Tielens 1999). For AFGL 2591, a nearby HII region has been found (van der Tak et al. 1999; Trinidad et al. 2003) whose exciting star may have an influence on the outer part of the AFGL 2591 envelope.

Fig. A.2 shows a selection of species for different outer FUV fields \( G_{0,\text{out}} \). The influence of the outer FUV field is noticeable at \( r \gtrsim 2.5 \times 10^{17} \) cm from the source. The chemistry is that of a photon-dominated region (e.g., Sternberg & Dalgarno 1995). The chemical reaction network basically starts with the dissociation of CO and the ionization of C leading to an enhancement of atomic and ionized carbon. Other species that are enhanced by an outer FUV field are CH and CH\(^+\). In our models, CH is mainly produced by the dissociation of CH\(_4\) and CH\(_2\). Photoionization of CH leads to CH\(^+\). CO\(^+\) is enhanced through reactions of C\(^+\) with OH and CH\(^+\) with O. HOC\(^+\) is only enhanced for a low outer FUV field \( (G_{0,\text{out}} = 10) \). HOC\(^+\) is produced in reactions of water with C\(^+\).

Other molecules like HCO\(^+\), CN, HCN, HCS\(^+\) or SH\(^+\) that are enhanced by X-rays are destroyed by an outer FUV field. The increase of the electron abundance leads to relatively fast electron recombination reactions for HCO\(^+\), HCS\(^+\) and SH\(^+\). CN and HCN are efficiently photodissociated by the FUV field. Due to the lower density in the outer part of the envelope, however, these species differ less than 30% in the radial column density for the different outer FUV fields. C, C\(^+\), CH and CH\(^+\) on the other hand can be enhanced up to several orders of magnitude. Since the influence of the outer FUV field is limited to the outermost part of the envelope, spatially resolved data can distinguish between an abundance enhancement of these species due to an outer FUV field and due to X-rays or FUV photons from the inside. In addition, the excitation of these species is different in the inner part of the envelope where the density is higher than in the outer part of the envelope.
3.4.8 Influence of cosmic-ray ionization rate

Like X-rays, cosmic rays are able to produce He\(^+\) and H\(_3^+\) and trigger a peculiar chemistry (e.g., Lepp et al. 1987; Herbst 2000). The cosmic-ray ionization rate \(\zeta_{\text{cr}} = 5.6 \times 10^{-17}\) s\(^{-1}\) in our models was derived from observations of HCO\(^+\) by van der Tak & van Dishoeck (2000). In order to study the influence of different cosmic-ray ionization rates on our X-ray models we have run Model 5 with a \(\approx 5\) times higher and lower cosmic-ray ionization rate, respectively. Figure A.3 presents the result of this investigation for a few species. Comparison of Model 0 with \(\zeta_{\text{cr}} = 5.6 \times 10^{-17}\) s\(^{-1}\) and Model 5 with \(\zeta_{\text{cr}} = 10^{-17}\) s\(^{-1}\) and \(\zeta_{\text{cr}} = 5.6 \times 10^{-17}\) s\(^{-1}\) shows that the influence of the cosmic-ray ionization rate dominates the chemistry for \(r \gtrsim 8 \times 10^{16}\) cm from the source for \(L_X = 10^{32}\) erg s\(^{-1}\) in agreement with Fig. 3.3. Cosmic-ray ionization rates as high as \(\zeta_{\text{cr}} = 3 \times 10^{-16}\) s\(^{-1}\), however, are able to dominate the gas-phase chemistry for \(r \gtrsim 2 \times 10^{16}\) cm from the source, that is from where H\(_2\)O freezes out on dust grains. By comparing H\(^{13}\)CO\(^+\) observations to a simple chemical model with different cosmic-ray ionization rates van der Tak & van Dishoeck (2000) showed for seven high-mass sources that the ionization rate varies between \(\zeta_{\text{cr}} = 0.61 - 5.6 \times 10^{-17}\) s\(^{-1}\). In addition, ionization rates as high as \(\zeta_{\text{cr}} \approx 10^{-16}\) s\(^{-1}\) are not confirmed by our best-fit models (Sect. 3.6.1). The influence of the cosmic-ray ionization rate on the emission line profiles of H\(^{13}\)CO\(^+\) will be discussed in Sect. 3.7 (see also Doty et al. 2002).

3.5 X-ray tracers

In order to find species that trace X-rays in highly obscured regions we have to distinguish X-ray enhanced species from species that are enhanced by other mechanisms such as inner FUV fields from the source, outer FUV fields from nearby stars or from cosmic-ray induced chemistry. By focusing only on the innermost region of the envelope (\(r \lesssim 2000\) AU), the effects of the latter two mechanisms can be neglected. The only challenge then is to separate species that are enhanced by X-rays from species that trace more preferably the FUV field from the central source.
Table 3.5: AFGL 2591 predicted column densities (cm$^{-2}$) for different X-ray models in a 2" beam.

<table>
<thead>
<tr>
<th>Species</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
<th>Model 6</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N_{\text{beam}}$</td>
<td>$q_{2/0}$</td>
<td>$q_{2/1}$</td>
<td>$q_{3/0}$</td>
</tr>
<tr>
<td>H</td>
<td>3.1(16)</td>
<td>1.9</td>
<td>0.1</td>
<td>1.7(17)</td>
</tr>
<tr>
<td>C</td>
<td>7.5(13)</td>
<td>5.4</td>
<td>2.0(-2)</td>
<td>5.2(14)</td>
</tr>
<tr>
<td>N</td>
<td>8.3(15)</td>
<td>7.0</td>
<td>2.0</td>
<td>1.0(17)</td>
</tr>
<tr>
<td>O</td>
<td>3.6(17)</td>
<td>8.4</td>
<td>7.2</td>
<td>2.2(18)</td>
</tr>
<tr>
<td>S</td>
<td>4.1(14)</td>
<td>1.0</td>
<td>1.1</td>
<td>3.2(15)</td>
</tr>
<tr>
<td>CH</td>
<td>2.0(11)</td>
<td>0.4</td>
<td>0.2</td>
<td>1.9(11)</td>
</tr>
<tr>
<td>NH</td>
<td>4.0(12)</td>
<td>0.5</td>
<td>0.5</td>
<td>2.2(12)</td>
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<tr>
<td>NH$_2$</td>
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<td>0.9</td>
<td>1.1</td>
<td>1.2(13)</td>
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<tr>
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<td>8.8(14)</td>
<td>0.4</td>
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<td>2.0(14)</td>
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<tr>
<td>HCN</td>
<td>3.5(15)</td>
<td>9.3</td>
<td>0.8</td>
<td>6.0(15)</td>
</tr>
<tr>
<td>CN</td>
<td>3.9(11)</td>
<td>1.5</td>
<td>3.0(-2)</td>
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</tr>
<tr>
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<td>7.3</td>
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<tr>
<td>N$_2$O</td>
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<td>1.7</td>
<td>1.9(13)</td>
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<td>0.6</td>
<td>0.6</td>
<td>6.8(14)</td>
</tr>
<tr>
<td>HNO</td>
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<td>1.2</td>
<td>1.2</td>
<td>4.5(12)</td>
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<tr>
<td>SH</td>
<td>8.3(11)</td>
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<td>0.5</td>
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<tr>
<td>H$_2$S</td>
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<td>0.4</td>
<td>1.3(12)</td>
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<tr>
<td>SO</td>
<td>5.3(15)</td>
<td>6.7</td>
<td>6.6</td>
<td>2.0(16)</td>
</tr>
</tbody>
</table>

a(b) means $a \times 10^b$. The enhancement factor $q_{x/y}$ is defined by $N_{t,\text{Model}x}/N_{t,\text{Model}y}$ (see Table 3.4). 

Continued on next page.
Table 3.5—continued from previous page.

<table>
<thead>
<tr>
<th>Species</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
<th>Model 6</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>$N_{\text{beam}}$</td>
<td>$q_{2/0}$</td>
<td>$q_{2/1}$</td>
<td>$N_{\text{beam}}$</td>
</tr>
<tr>
<td>CS</td>
<td>4.2(13)</td>
<td>1.5</td>
<td>0.8</td>
<td>3.2(14)</td>
</tr>
<tr>
<td>H$^+$</td>
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<td>14.1</td>
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<tr>
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<td>2.1</td>
<td>6.8(11)</td>
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<tr>
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<td>0.1</td>
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</tr>
<tr>
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<td>2.0</td>
<td>2.0</td>
<td>7.9(7)</td>
</tr>
<tr>
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<td>7.0</td>
<td>2.2</td>
<td>1.6(8)</td>
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<tr>
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<td>8.2</td>
<td>1.0(-2)</td>
<td>4.2(12)</td>
</tr>
<tr>
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<td>2.9</td>
<td>6.9(12)</td>
</tr>
<tr>
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<td>1.2</td>
<td>1.1</td>
<td>3.6(13)</td>
</tr>
<tr>
<td>OH$^+$</td>
<td>5.3(7)</td>
<td>8.9</td>
<td>3.5</td>
<td>9.8(8)</td>
</tr>
<tr>
<td>CH$^+$</td>
<td>9.0(4)</td>
<td>28.3</td>
<td>4.0(-4)</td>
<td>6.3(6)</td>
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<td>CO$^+$</td>
<td>1.4(7)</td>
<td>3.1</td>
<td>1.1</td>
<td>5.9(7)</td>
</tr>
<tr>
<td>HCO$^+$</td>
<td>4.5(13)</td>
<td>25.8</td>
<td>9.9</td>
<td>3.4(14)</td>
</tr>
<tr>
<td>HOC$^+$</td>
<td>1.9(7)</td>
<td>1.4</td>
<td>2.0(-2)</td>
<td>7.9(7)</td>
</tr>
<tr>
<td>HCNH$^+$</td>
<td>4.3(12)</td>
<td>5.6</td>
<td>1.2</td>
<td>9.7(12)</td>
</tr>
<tr>
<td>N$_2$H$^+$</td>
<td>3.7(11)</td>
<td>3.8</td>
<td>3.8</td>
<td>2.2(12)</td>
</tr>
<tr>
<td>HCS$^+$</td>
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<td>5.1</td>
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<td>1.0(12)</td>
</tr>
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<td>SO$^+$</td>
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<td>4.4</td>
<td>1.4</td>
<td>3.1(12)</td>
</tr>
<tr>
<td>HSO$^+$</td>
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<td>145.2</td>
<td>143.2</td>
<td>3.4(13)</td>
</tr>
<tr>
<td>SH$^+$</td>
<td>3.0(9)</td>
<td>38.1</td>
<td>2.4</td>
<td>2.7(11)</td>
</tr>
</tbody>
</table>

(a/b) means $a \times 10^b$. The enhancement factor $q_{x/y}$ is defined by $N_{t,\text{Model } x}/N_{t,\text{Model } y}$ (see Table 3.4).
3.5. X-ray tracers

3.5.1 X-ray vs. FUV tracers

Figures 3.4–3.6 show that X-rays are capable of influencing the atomic and molecular abundances throughout almost the entire envelope. This is the main difference with the models of Stäuber et al. (2004a) where the influence of an inner FUV field has been examined. Due to their small cross sections, X-rays penetrate deeper into the envelope and affect the chemistry on large scales. The enhanced region due to a low inner FUV field \( G_{0,\text{in}} = 10 \) is \( \approx 300\text{-}500 \) AU (Stäuber et al. 2004a) whereas the X-ray enhanced region is often \( \gtrsim 1000 \) AU, even for relatively low X-ray fluxes \( L_x \approx 10^{30} \text{erg s}^{-1} \). Current and future (sub)millimeter interferometers like ALMA are able to resolve regions covering \( \lesssim 1\text{-}2'' \). At a distance of 1 kpc, this corresponds to a region of \( \approx 1000\text{-}2000 \) AU. However, it will be shown in Sect. 3.7 that the influence of X-rays and therefore the enhanced emission of several species can also be seen in much bigger single-dish beams.

X-rays and UV photons have similar effects on the chemistry. They both increase the abundances of ions and radicals. However, X-rays can ionize atoms with an ionization threshold \( E_{\text{th}} \geq 13.6 \text{eV} \) like hydrogen, helium, oxygen and nitrogen which is not possible for FUV photons \( (6 < h\nu < 13.6 \text{eV}) \) and can even doubly ionize many species. Reactions with ions like \( \text{He}^+ \) or \( \text{H}_3^+ \) can therefore become important in X-ray induced chemistry. For example, reactions of \( \text{He}^+ \) or \( \text{H}_3^+ \) with CO efficiently produce \( \text{C}^+ \) and \( \text{HCO}^+ \), respectively (Sect. 3.4.2). The main contribution to the \( \text{He}^+ \) abundance, however, is from electron impact ionization of \( \text{He} \), rather than direct X-ray ionization. \( \text{H}_3^+ \) is formed by the reaction of \( \text{H}_2^+ \) with \( \text{H}_2 \) where \( \text{H}_2^+ \) is also formed through electron impact ionization. Both \( \text{He}^+ \) and \( \text{H}_2^+ \) cannot be produced with FUV photons but with cosmic rays as discussed in Sect. 3.4.8.

Table 3.5 presents beam averaged column densities of Model 2, 3, 4 and Model 6 for a selection of species for the inner \( \approx 2000 \) AU, that is the region that can be resolved by interferometers. The enhancement factor \( q_{\text{Model } x / \text{Model } 0} \) in Table 3.5 is defined as the ratio of the column density of a species predicted by the X-ray model \( x \) and the column density of the model without any radiation field, that is Model 0. The enhancement factor \( q_{\text{Model } x / \text{Model } 1} \) is defined as the ratio of the calculated column density from X-ray model \( x \) and the column density of the model without X-rays but with an inner FUV field with a field strength \( G_{0,\text{in}} = 10 \) (Model 1).
Since the results for the best-fit models and Model 4 are similar, the column densities of Model 4 are representative of all best fitted models.

Most species presented in Table 3.5 are enhanced due to X-rays ($q_{\text{Model}x/\text{Model}0} > 1$) and may therefore serve as possible tracers. An enhancement factor $q_{\text{Model}x/\text{Model}1} > 1$, however, distinguishes X-ray tracers from species that are enhanced by an inner UV field. It can be seen in Table 3.5 that species like N$_2$O, HNO, SO, SO$^+$, HCO$^+$, CO$^+$, OH$^+$, N$_2$H$^+$, SH$^+$ and HSO$^+$ are more enhanced by X-rays than by FUV photons even for X-ray luminosities as low as $L_X \approx 10^{30}$ erg s$^{-1}$. In addition, the abundances for these species increase with increasing X-ray flux. Other species like CS, SH, HCN, CH or HCS$^+$ are enhanced either by X-rays or an inner FUV field, depending on the incident X-ray or FUV flux, respectively. Species like C or HOC$^+$ are more enhanced by an inner FUV field than by X-rays.

Table 3.5 and Fig. 3.6 show that HSO$^+$ is a remarkable tracer for X-rays. It is enhanced by more than a factor of 100 even for low X-ray fluxes with fractional abundance $\tilde{x}(\text{HSO}^+) \approx 10^{-10} - 10^{-9}$ in the inner $\approx 1000$ AU. In our models, HSO$^+$ is primarily produced by the reactions of H$_3^+$ and HCO$^+$ with SO. Unfortunately though, little is known about this molecule which has not been observed to date. In addition, spectral information is missing and laboratory work is needed before HSO$^+$ can be searched in molecular clouds. SH$^+$ is enhanced even more than 10000 times compared to Model 0 and more than 1000 times compared to Model 1 for the best-fit models. Four hyperfine lines of SH$^+$ have recently been measured by Savage et al. (2004). It was found that the best candidates for observations are the strongest lines near 526 GHz which requires instruments such as Herschel-HIFI or SOFIA.

### 3.5.2 Column density ratios

Ratios like CN/HCN or HOC$^+$/HCO$^+$ are of specific interest since they depend on the flux of FUV radiation (Fuente et al. 1995; Fuente et al. 2003; Stäuber et al. 2004a). Since X-rays affect the abundances of ions and radicals, these ratios may also depend on the incident X-ray flux. The ratios CN/HCN, HNC/HCN, CO$^+$/HCO$^+$ and HOC$^+$/HCO$^+$ of the radial column densities of the inner $\approx 2000$ AU are presented in Fig. 3.7. The ratios CO$^+$/HCO$^+$ and HOC$^+$/HCO$^+$ are effectively enhanced only by models containing an inner FUV field. The ratio HNC/HCN is higher...
3.5. X-ray tracers

Figure 3.7: Column density ratios for the inner \( \approx 2000 \text{ AU} \) (\( \approx 2'' \)) of the envelope. The models are described in Table 3.4.

for the X-ray models than for the FUV models but similar to the ratio of Model 0. The CN/HCN ratios depend strongly on the incident X-ray flux and vary within a factor of 100. Models with high X-ray luminosities \( (L_x \approx 10^{32} \text{ erg s}^{-1}) \) and models with X-rays and an inner FUV field, that is Model 6 and 7, are capable of increasing the CN/HCN ratio up to 0.01. Although the CN/HCN ratio increases with increasing X-ray flux (Models 2–4), the ratio is also enhanced by an inner FUV field without X-rays. In general, all these ratios give poor information about the X-ray flux, since they are enhanced more likely by an inner FUV flux rather than by X-rays. The crucial point for an enhanced CN/HCN ratio is the strength of the inner FUV field and therefore the inner column density \( N_{\text{H,in}} \). For column densities \( N_{\text{H,in}} \gtrsim 4 \times 10^{22} \text{ cm}^{-2} \), the optical depth \( A_V \) is \( \approx 20 \) and most FUV photons from the young star will be absorbed. The enhancement of the CN/HCN ratio is then more likely due to X-rays.

3.5.3 Previously suggested X-ray tracers

Earlier models of molecules exposed to an X-ray source predicted similar molecular X-ray tracers. Lepp & Dalgarno (1996) found that CN and NO are particularly enhanced by X-rays. The enhancement of CN is confirmed with our models. CN can be enhanced up to \( \approx 50 \) times in
the inner 2000 AU. The beam averaged column density of NO given in Table 3.5, however, is smaller for the X-ray models than for the models without X-rays. From Fig. 3.6 it can be seen that NO is enhanced in the outer parts of the envelope and in the innermost part of the envelope ($r \lesssim 500$ AU). The ‘cut-off’ of the bump in the middle part of the envelope causes the decreasing NO column density with increasing X-ray flux. The bump of the NO abundance profile is due to the evaporation of water at $T = 100$ K, a process not included by Lepp & Dalgarno (1996). For $T \gtrsim 100$ K, NO is efficiently produced by the reaction HNO$^+$ + H$_2$O $\rightarrow$ H$_3$O$^+$ + NO. In our X-ray models NO is enhanced up to fractional abundances $\tilde{x}(\text{NO}) \approx 10^{-7}$–$10^{-6}$ in the innermost part of the envelope. This is the same result found by Lepp & Dalgarno (1996). To observe the enhanced region of NO towards the inner $\approx 500$ AU of AFGL 2591 the sensitivity and spatial resolution of ALMA is needed. The model results of Krolik & Kallman (1983) for the Orion molecular cloud are generally in good agreement with our results. The enhancement factors they derive are comparable to those of Model 6. In particular, they also find that NO is not changing in models with high ionization rates.

### 3.6 AFGL 2591 models

#### 3.6.1 Best-fit models

To find the best fitting model for AFGL 2591 by varying the input parameters $L_X$, $T_X$, $N_{H,in}$ – the column density between the X-ray source and the first radial model point – and the inner UV field $G_{0,in}$, a $\chi^2$ statistic has been used defined by

$$\chi^2 = \sum_i w_i^2 \times \frac{(\log(N_{\text{model},i}) - \log(N_{\text{obs},i}))^2}{(\varepsilon_i \times \log(N_{\text{model},i}))^2}. \quad (3.12)$$

We follow the method and observational data provided by Doty et al. (2002). The weights $w_i$ are in favor of column densities that have been derived by a full non-LTE radiative transfer model ($w_i = 3$) rather than methods assuming LTE ($w_i = 2$). For the error we assume $\varepsilon_i = 0.6$ for all species except for those given either by an upper or a lower limit. For these, we assume $\varepsilon_i = 5$ when the model results are within the limit, since...
these observational results can have big errors due to, for example, non-detections. The ranking of the fits is not very sensitive to the assumptions on $\varepsilon_i$, though. Agreement of models to within a factor of a few compared to the observations can still be considered as good for chemical modeling. Thus, the ratios of the column densities are taken by calculating the difference of the modeled and observed logarithmic column densities. The value of $\chi^2$ has then a slightly different meaning, but the minimum of eq. (3.12) still provides the best-fit model since the ideal model would have $\chi^2 = 0$.

As a first approach models with only X-rays are considered: $L_X$ was varied from $10^{29} \text{ erg s}^{-1}$ to $7 \times 10^{32} \text{ erg s}^{-1}$, $T_X$ from $5 \times 10^6 \text{ K}$ to $3 \times 10^8 \text{ K}$ and $N_{\text{H,in}}$ from $10^{22} \text{ cm}^{-2}$ to $10^{24} \text{ cm}^{-2}$. The minimum and maximum values of the grid for the X-ray luminosity and plasma temperature are based on results of X-ray observations toward YSOs. The best fitted parameters out of $\approx 800$ calculated models are $L_X = 10^{32} \text{ erg s}^{-1}$, $T_X = 10^8 \text{ K}$, $N_{\text{H,in}} = 5 \times 10^{22} \text{ cm}^{-2}$ and $t \approx 5 \times 10^4 \text{ yrs}$ (Model 5). The X-ray luminosity and temperature are rather high and at the upper end of what has been observed toward star forming regions (e.g., Feigelson & Montmerle 1999; Hofner et al. 2002). If, however, the X-ray luminosity decreases
as the YSO evolves - like it does in low-mass YSOs (Feigelson & Montmerle 1999; Tsujimoto et al. 2002) - such high luminosities and plasma temperatures could be possible. The inner column density corresponds to \( A_V \approx 25 \) which is in good agreement with the results of van der Tak et al. (1999) for \( r < 175 \text{ AU} \).

As a second step in finding the best-fit X-ray model, an inner FUV field of \( G_{0,\text{in}} = 10 \) has been assumed with an inner column density of \( N_{\text{H,in}} = 3 \times 10^{22} \text{ cm}^{-2} \) in agreement with the models of Stäuber et al. (2004a). The parameters of the best fitted model are then \( L_X = 8 \times 10^{31} \text{ ergs}^{-1} \), \( T_X = 10^8 \text{ K} \) and \( t \approx 5 \times 10^4 \text{ yrs} \) (Model 6). Models with higher inner FUV fields in general lead to much higher \( \chi^2 \) values. The assumption of an inner FUV therefore yields a slightly lower X-ray luminosity.

Using a reduced \( \chi^2 \) statistic where each addend in eq. (3.12) is divided by the number of observed lines of that species, the best fitted model is \( L_X = 6 \times 10^{31} \text{ ergs}^{-1} \), \( T_X = 3 \times 10^7 \text{ K} \) with an inner column density of \( N_{\text{H,in}} = 3 \times 10^{22} \text{ cm}^{-2} \) and an inner FUV field \( G_{0,\text{in}} = 10 \) at \( t \approx 3 \times 10^4 \text{ yrs} \) (Model 7).

Considering only species that are influenced most by X-rays in eq. (3.12), the best fitted parameters are \( L_X = 10^{32} \text{ ergs}^{-1} \), \( T_X = 9 \times 10^7 \text{ K} \) and \( t \approx 4 \times 10^4 \text{ yrs} \) which is very similar to Model 5. The species considered are HCN, HNC, \( \text{H}_2\text{S} \), CS, CN, SO, HCO\(^+\), HCS\(^+\), \( \text{H}_3^+ \) and N\(_2\)H\(^+\). The lower (dotted) curve in Fig. 3.8 shows the results for this calculation whereas the upper (solid) curve corresponds to the \( \chi^2 \) values for all species.

In general all best-fit models have very similar \( \chi^2 \) values and the differences may be too small to elect the winner. The goodness of fit of the different parameters is further discussed in the next section. Table A.1 lists the column densities of the observed species and the modeled column densities for Model 6. Further shown are the parameters that fit each specific molecule best. It can be seen that the parameters \( L_X \), \( T_X \), \( N_{\text{H,in}} \) and time vary from species to species. Only two species, \( \text{H}_2\text{CO} \) and \( \text{C}_2\text{H}_2 \), are modeled best with Model 0, that is the model without any high energy radiation from the source. All other species seem to require a more or less strong X-ray flux from the source to match the observed column density.

O- and B-type main sequence stars emit X-rays due to shocks from
3.6. AFGL 2591 models

the radiation driven stellar winds with $L_X/L_{\text{bol}} \approx 10^{-7}$ (Berghoefer et al. 1997). A bolometric luminosity $L_{\text{bol}} = 2 \times 10^4 L_\odot$ for AFGL 2591 implies an X-ray luminosity $L_X \approx 8 \times 10^{30} \text{erg s}^{-1}$. If we assume that young massive stars emit rather more X-rays, this value could be regarded as a lower limit for the X-ray emission for AFGL 2591. The ratio of the luminosities for our best-fit models is $L_X/L_{\text{bol}} \approx 10^{-6}$.

As can be seen in Fig. 3.3, the $\text{H}_2$ ionization rates $\zeta_{\text{H}_2}$ for the best-fit models (5, 6, 7) differ only little throughout the envelope. The ionization rates of Model 5 and Model 6 are somewhat flatter in radial dependence than that for Model 7 due to the harder spectrum. However, since similar ionization rates lead to similar abundance profiles, the conclusion can be drawn that the X-ray induced chemistry depends mainly on the $\text{H}_2$ ionization rate $\zeta_{\text{H}_2}$.

Figure 3.9: $\chi^2$ contour plots for the species influenced most by X-rays. The parameters in each plot that were not varied have been fixed at $L_X = 10^{32} \text{erg s}^{-1}$, $T_X = 10^8 \text{K}$, $N_{\text{H},\text{in}} = 5 \times 10^{22} \text{cm}^{-2}$ and $t \approx 5 \times 10^4 \text{yrs}$ (Model 5). The contour levels are plotted for 0.7–2.4 in steps of 0.1.
Chapter 3. X-ray chemistry

3.6.2 Contour plots

To quantify the plausible ranges of the various parameters, contour plots of the $\chi^2$ values for the species influenced most by X-rays are shown in Fig. 3.9. It can be seen that the results are basically independent of $T_X$ and $N_{H,in}$ for different $L_X$. The plot of $L_X$ vs. $t$ shows that the results become independent of $t$ for high X-ray luminosities once $t \gtrsim 10^4$ yrs. $\chi^2$ does not change with time anymore, thus equilibrium is reached for the species in our statistical sample.

A region of confidence can be defined by the contours that are twice the minimum $\chi^2$ value, which is $\approx 0.6$. The constraint on the X-ray luminosity is then $L_X \gtrsim 10^{31}$ erg s$^{-1}$ with $t \gtrsim 10^4$ yrs. The plot of $T_X$ vs. $N_{H,in}$ in Fig. 3.9 shows that for low temperatures ($T_X \approx 10^7$ K), the column density is $N_{H,in} \lesssim 2 \times 10^{23}$ cm$^{-2}$. Higher temperatures allow higher column densities. However, the extra photons at higher energies are not efficiently absorbed by the inner column and the results become independent of the inner column density $N_{H,in}$.

Fig. 3.10 shows contour plots for $L_X$ vs. $G_{0,out}$ and $L_X$ vs. $\zeta_{cr}$. The plot for the different outer FUV fields shows that the results depend mainly on the X-ray luminosity $L_X$ rather than on the outer FUV field $G_{0,out}$. Models with higher FUV fields than the standard radiation field ($G_{0,out} = 1$) generally lead to higher $\chi^2$ values.

The values in the plot for the cosmic-ray ionization rate have been scaled by a factor of 100 in eq. (3.12) since only HCO$^+$ was considered. The cosmic-ray ionization rate is well constrained between $\zeta_{cr} \approx 2 \times$...
3.7 Calculated emission lines

$10^{-17}s^{-1}$ and $\zeta_{cr} \approx 10^{-16}s^{-1}$ in good agreement with the results of van der Tak & van Dishoeck (2000) and Doty et al. (2002). The X-ray luminosity is well constrained between $L_X \approx 2 \times 10^{30} \text{erg s}^{-1}$ and $L_X \approx 10^{31} \text{erg s}^{-1}$.

### Figure 3.11:
Calculated $^{13}\text{CO}^+$ line profiles for Model 0 (solid line), Model 1 (dotted line), Model 3 (short dashed line), Model 4 (dashed-dotted line) and Model 5 (long dashed line). The $^{13}\text{CO}^+$ 3–2 line (260 GHz) was convolved with a 18" JCMT beam, the $^{13}\text{CO}^+$ 4–3 line (347 GHz) was convolved with a 14" JCMT beam and the $^{13}\text{CO}^+$ 8–7 line (694 GHz) was convolved with a 8" JCMT beam.

### Figure 3.12:
Calculated HCS$^+$ line profiles for Model 0 (solid line), Model 1 (dotted line), Model 3 (short dashed line), Model 4 (dashed-dotted line) and Model 5 (long dashed line). The HCS$^+$ 6–5 line (256 GHz) was convolved with a 18" JCMT beam, the HCS$^+$ 8–7 line (341 GHz) was convolved with a 14" JCMT beam and the HCS$^+$ 10–9 line (427 GHz) was convolved with a 11" JCMT beam.
Table 3.6: Enhancement factors $q_{\text{Model } x/\text{Model } y} = f_{i,\text{Model } x}/f_{i,\text{Model } y}$ for different line transitions.

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<td>$q_{6/1}$</td>
<td>10</td>
<td>17</td>
<td>16</td>
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The values represent the ratios of the integrated line fluxes $f = \int T_{\text{mb}} dV$. The Models are described in Table 3.4 in Sect. 3.4.
3.7. Calculated emission lines

Figure 3.13: Calculated $^{13}$CO$^+$ line profiles for Model 0 (solid line) and Model 5 (dashed line) with a cosmic-ray ionization rate $\zeta_{cr} = 5.6 \times 10^{-17}\,\text{s}^{-1}$ and for Model 0 (dotted line) and Model 5 (dashed-dotted line) with a cosmic-ray ionization rate $\zeta_{cr} = 3 \times 10^{-16}\,\text{s}^{-1}$. The $^{13}$CO$^+$ 3–2 line (260 GHz) was convolved with a 18'' JCMT beam, the $^{13}$CO$^+$ 4–3 line (347 GHz) was convolved with a 14'' JCMT beam and the $^{13}$CO$^+$ 8–7 line (694 GHz) was convolved with a 8'' JCMT beam.

Molecules with high critical densities $n_{\text{crit}}$ are likely to probe the inner dense part of the envelope (see, e.g., van Dishoeck & Hogerheijde 1999 for a review). Since the critical density of a molecule is proportional to the Einstein $A$ coefficient for spontaneous transitions and therefore $n_{\text{crit}} \propto \nu^3$, higher frequency transitions have also higher critical densities. Stäuber et al. (2004a) show that enhancements of molecules due to an inner FUV field should already be detectable with single-dish telescopes having beam widths $\gtrsim 11''$. To show this for the case of X-ray enhanced molecules, the density profiles of HCO$^+$ and HCS$^+$ presented in Sect. 3.4 are used to compute the line intensities with the Monte Carlo radiative transfer code Hogerheijde & van der Tak (2000). The intrinsic (turbulent) line profile is taken to be a Gaussian with a Doppler parameter of $1.6\,\text{km}\,\text{s}^{-1}$, independent of radius. Molecular data are taken from the Leiden atomic and molecular database (Flower 1999; Schöier et al. 2005b). The line profiles are convolved to an appropriate telescope beam size. In order to avoid optical depth effects we have modeled the isotope $^{13}$CO$^+$. The assumed isotope ratio is $\text{HCO}^+ / ^{13}\text{CO}^+ = 60$ (Wilson & Rood 1994).

Figures 3.11 and 3.12 show that high-$J$ transitions are indeed sensitive to the different models and may therefore be used as tracers for high energy radiation. The enhancement factors for the higher transitions presented in Table 3.6 confirm the results of Sect. 3.4. $^{13}$CO$^+$ and HCS$^+$ are clearly enhanced by X-rays. The enhancement factors for the
H$^{13}$CO$^+$ $J = 8-7$ transition are between 2-43 compared to Model 0 and between 1-11 compared to the FUV Model 1. The $J = 10-9$ line of HCS$^+$ is enhanced between 2 and 169 times compared to the models without X-rays or FUV field and between 0.2 and 21 times compared to the FUV model. No influence is seen, however, from an enhanced outer FUV field in the emission lines of H$^{13}$CO$^+$ and HCS$^+$.

Figure 3.13 shows calculated H$^{13}$CO$^+$ lines for Model 0 and Model 5 with cosmic-ray ionization rates $\zeta_{cr} = 5.6 \times 10^{-17} \text{s}^{-1}$ and $\zeta_{cr} = 3 \times 10^{-16} \text{s}^{-1}$. As expected, the strongest line is that of Model 5 with $\zeta_{cr} = 3 \times 10^{-16} \text{s}^{-1}$. For the $J = 3-2$ and the $J = 4-3$ transitions Model 5 and Model 0 with $\zeta_{cr} = 3 \times 10^{-16} \text{s}^{-1}$ differ less than 30-50% and are therefore hardly distinguishable. At higher frequencies, however, the two lines of Model 5 clearly dominate the two lines of Model 0. The $J = 8-7$ transitions of Model 5 are enhanced by a factor of $\approx 5$ compared to that of Model 0 with the higher cosmic-ray ionization rate. Higher $J$ transitions of H$^{13}$CO$^+$ can therefore be used to distinguish between the effects of a central X-ray source and the effects of an enhanced cosmic-ray ionization. The X-ray luminosity, however, should be of the order of $\approx 10^{31} \text{erg s}^{-1}$ as can be seen in Fig. 3.11 to distinguish cosmic-ray ionization rates as high as $\zeta_{cr} = 3 \times 10^{-16} \text{s}^{-1}$ from the effects of X-rays.

### 3.8 Conclusion

We have extended the chemical models of Doty et al. (2002) to study the impact of X-rays from a central source on the chemistry of YSO envelopes. The models are applied to the massive star-forming region AFGL 2591 using the physical structure proposed by van der Tak et al. (1999) and Doty et al. (2002). Our major results are summarized below:

1. X-rays can penetrate deep into the envelope due to their small cross sections and affect the chemistry even at large distances from the source. The abundances of many species are enhanced by 2-3 orders of magnitude. Like FUV radiation, X-rays preferably enhance simple hydrides, ions and radicals. The region which is influenced most by X-rays is $\gtrsim 1000 \text{AU}$. Some species are enhanced throughout the entire envelope. The greater penetration of X-rays is the main difference to the models of Stäuber et al. (2004a) where the influence of an inner FUV field on YSO envelopes was studied (Sect. 3.4).
2. He$^+$ and H$_3^+$ have enhanced abundances up to a factor of 1000 in the innermost region compared to models without X-rays. These two ions trigger an X-ray characteristic chemistry which is similar to that induced by cosmic rays. Although the X-ray ionization rate exceeds the cosmic-ray ionization rate for a large part of the envelope, it is found that in the case of AFGL 2591 the chemistry of the bulk of the envelope mass is dominated by the cosmic-ray induced reactions rather than X-ray induced ionization (Sect. 3.4).

3. The X-ray ionization rate is dominated by the ‘secondary’ H$_2$ ionization rate resulting from fast electrons. The X-ray induced chemistry therefore depends mainly on the H$_2$ ionization rate $\zeta_{\text{H}_2}$ which is directly proportional to the X-ray luminosity (Sect. 3.4, Sect. 3.6.1).

4. Several molecules - among them N$_2$O, HNO, SO, SO$^+$, HCO$^+$, CO$^+$, OH$^+$, N$_2$H$^+$, SH$^+$ and HSO$^+$ - are pure X-ray tracers, that is they are more likely to be enhanced by X-rays than by FUV radiation (Sect. 3.5.1). The ratio CN/HCN increases with increasing X-ray flux whereas the ratios HNC/HCN, HOC$^+$/HCO$^+$ and CO$^+$/HCO$^+$ are not sensitive to the X-ray flux and trace the FUV field as confirmed by observations and models of PDRs by several authors. Whether the CN/HCN ratio is enhanced by an inner FUV field or by X-rays depends mainly on the FUV absorbing inner column density (Sect. 3.5.2).

5. SH$^+$ and HSO$^+$ are found to be excellent X-ray tracers. They are 100-10000 times more abundant in models with X-rays. Both are more likely to be enhanced by X-rays than by an inner FUV source. In addition, the abundance of SH$^+$ correlates with the X-ray flux. Only four hyperfine lines of SH$^+$ have so far been measured in the laboratory whereas no information is available for HSO$^+$. We would therefore like to encourage laboratories to further investigate these molecules (Sect. 3.5).

6. CO$_2$ abundances are reduced in the gas-phase through X-ray induced FUV photons. For temperatures $T \lesssim 230$ K, H$_2$O is destroyed by X-rays with luminosities $L_X \gtrsim 10^{30}$ erg s$^{-1}$ (Sect. 3.4.1).

7. An enhanced outer FUV field increases the column densities of C, C$^+$ and simple carbon-hydrides like CH and CH$^+$. The influence on the total column density of other species is minor, however (Sect. 3.4.7).

8. Comparison between observations and models is in general improved with models containing an inner X-ray source. Best-fit models for AFGL 2591 predict an X-ray luminosity $L_X \gtrsim 10^{31}$ erg s$^{-1}$ with a
hard X-ray spectrum $T_X \gtrsim 3 \times 10^7$ K. The ratio of the X-ray luminosity to the total luminosity is found to be $L_X/L_{bol} \approx 10^{-6}$. Best-fit models also confirm the chemical age $t \sim 10^4$ yrs of AFGL 2591 suggested by Doty et al. (2002). The results become independent of time at high X-ray luminosities once $t \gtrsim 10^4$ yrs (Sect. 3.6.1).

9. Previously proposed X-ray tracers like CN or NO are confirmed by our models. The enhancement of NO, however, is not obvious since it is only prominent in the inner $\approx 500$ AU of the envelope. Small ($0.5''-1''$) beams are therefore required to observe the enhanced region of NO (Sect. 3.5.3).

10. Calculated line intensities of $\text{H}^{13}\text{CO}^+$ and HCS$^+$ show that the enhancement due to X-rays is detectable for these species with single-dish telescopes. Due to the frequency dependence of the critical density, the influence of X-rays is more prominent in higher frequency transitions. High-$J$ lines of $\text{H}^{13}\text{CO}^+$ can be used to separate the effects of X-ray and cosmic-ray ionization for $L_X \gtrsim 10^{31}$ erg s$^{-1}$ and $\zeta_{cr} \lesssim 3 \times 10^{-16}$ s$^{-1}$ (Sect. 3.7).

11. The effects of Compton ionization on the chemistry are studied and compared to results of models without Compton scattering. It is found that the differences are minor and that the effects of Compton ionization can be neglected for column densities $N_H \lesssim 10^{24}$ cm$^{-2}$ (Sect. 3.2.1).

12. Future instruments like Herschel-HIFI, SOFIA and ALMA are needed to verify our models. In particular, Herschel-HIFI will be able to observe many hydrides whereas the sensitivity and spatial resolution of ALMA is well-suited to measure the size and geometry of the emitting region.
Chapter 4

Water destruction by X-rays in young stellar objects

ABSTRACT: We study the H$_2$O chemistry in star-forming environments under the influence of a central X-ray source and a central far ultraviolet (FUV) radiation field. The X-ray models are applied to envelopes around low-mass Class 0 and I young stellar objects (YSOs). The gas-phase water chemistry is modeled as a function of time, hydrogen density and X-ray flux. To cover a wide range of physical environments, densities between $n_H = 10^4$–$10^9$ cm$^{-3}$ and temperatures between $T = 10$–$1000$ K are studied. Three different regimes are found: For $T < 100$ K, the water abundance is of order $10^{-7}$–$10^{-6}$ and can be somewhat enhanced or reduced due to X-rays, depending on time and density. For $100$ K $\lesssim T \lesssim 250$ K, H$_2$O is reduced from initial abundance $x$(H$_2$O) $\approx 10^{-4}$ following ice evaporation to $x$(H$_2$O) $\approx 10^{-6}$ for $F_X \gtrsim 10^{-3}$ erg s$^{-1}$ cm$^{-2}$ ($t = 10^4$ yrs) and for $F_X \gtrsim 10^{-4}$ erg s$^{-1}$ cm$^{-2}$ ($t = 10^5$ yrs). At higher temperatures ($T \gtrsim 250$ K) and hydrogen densities, water can persist with $x$(H$_2$O) $\approx 10^{-4}$ even for high X-ray fluxes. Water is destroyed in both Class 0 and I envelopes on relatively short timescales ($t \approx 5000$ yrs) for realistic X-ray fluxes, although the effect is less prominent in Class 0 envelopes due to the higher X-ray absorbing densities there. FUV photons from the central source are not effective in destroying water. We conclude that X-rays reduce the water abundances especially in regions where the gas temperature is $T \lesssim 250$–$300$ K for fluxes $F_X \gtrsim 10^{-5}$–$10^{-4}$ erg s$^{-1}$ cm$^{-2}$. The affected regions can be envelopes, disks or outflow hot spots. The average water abundance in Class I sources for $L_X \gtrsim 10^{27}$ erg s$^{-1}$ is predicted to be $x$(H$_2$O) $\lesssim 10^{-6}$. Central UV fields have a negligible influence,
unless the photons can escape through cavities.

4.1 Introduction

The importance of water in star-formation is unquestioned. Water is found abundantly on dust grains as well as in the gas-phase of molecular clouds, cores, envelopes and protostellar disks. It is a key molecule in the hot \( T \gtrsim 100 \text{K} \) gas-phase chemistry and is one of the main gas coolants. The evolution over time of molecular cores influences the abundance of \( \text{H}_2\text{O} \) (Ceccarelli et al. 1996), making it sensitive to the chemical age of a source. Through its masing ability, water has been used to study dynamical properties of star-forming regions.

In cold gas \( (T < 100 \text{K}) \), water is mainly produced by ion-molecule reactions. At temperatures above 250 K, \( \text{H}_2\text{O} \) is largely produced in reactions of \( \text{O} \) and \( \text{OH} \) with \( \text{H}_2 \). Water is also efficiently generated on dust grains where it forms an icy mantle. Observed abundances of water ice arc typically \( x(\text{H}_2\text{O}) \approx 10^{-4} \) with respect to \( \text{H}_2 \) (Tielens et al. 1991; Boogert et al. 2004). At temperatures \( T \gtrsim 100 \text{K} \), \( \text{H}_2\text{O} \) evaporates into the gas-phase and has a major impact on the chemistry (van Dishoeck & Blake 1998; Doty et al. 2002). Water is also believed to be formed in shocked regions where it may be produced due to the high gas temperature and/or may be released from grains. Towards high-mass star-forming regions, hot \( (T \gtrsim 100 \text{K}) \) gas-phase water is usually observed with abundances \( x(\text{H}_2\text{O}) = 10^{-4} \), comparable to the ice abundance – whereas at temperatures below 100 K, it is found to be approximately 100 times less abundant (e.g., Boonman & van Dishoeck 2003; van der Tak et al. 2006). The observed water emission towards low-mass objects has been interpreted with similar jumps at \( T \approx 100 \text{K} \) (Ceccarelli et al. 2000b; Maret et al. 2002). Although the solid water abundances are comparable in low and high-mass regions, the hot gas-phase water in low-mass sources seems to be much less abundant than in the massive objects. In addition, a fraction of the emission is believed to arise in outflow regions, as inferred from observations both on and off source with the Long Wavelength Spectrometer (LWS) on board the Infrared Space Observatory (ISO) (Giannini et al. 2001; Benedettini et al. 2002). Nisini et al. (2002) compared the far-infrared spectra of both Class 0 and Class I sources. Water lines were found to be prominent in the spectra of Class 0 objects but they were not
detected toward Class I sources corresponding to an upper limit on the abundances of $x(\text{H}_2\text{O}) \lesssim 10^{-5}$.

Protostars are often found to be sources of strong X-ray fluxes (e.g., Casanova et al. 1995; Koyama et al. 1996; Imanishi et al. 2001). The observed X-rays are understood to be thermal emission from magnetic stellar activities or from the disk-star system (e.g., Feigelson & Montmerle 1999). Typical X-ray luminosities range from $L_X \approx 10^{28} - 10^{31}$ erg s$^{-1}$ in the 0.5 - 10 keV band with plasma temperatures between 0.6 - 7 keV (e.g., Imanishi et al. 2001). Flares can even lead to plasma temperatures temporarily exceeding $10^8$ K with luminosities higher than $L_X \approx 10^{32}$ erg s$^{-1}$. Within the Chandra Orion Ultradeep Project (COUP), Preibisch et al. (2005) found a ratio for the X-ray luminosity to the bolometric luminosity of $\log(L_X/L_{\text{bol}}) \approx -3.6$ for Class I and older protostars. No X-ray detection has been reported to date toward Class 0 objects (Hamaguchi et al. 2005a). However, this might be due to the large X-ray absorbing hydrogen and dust column densities found in these sources. The nature of the sources in recent reports of X-ray detections towards very young objects is poorly known and they could be either Class 0 or I objects (Hamaguchi et al. 2005b; Forbrich et al. 2005).

The influence of a central X-ray source on the envelope around young stellar objects has recently been studied by Stäuber et al. (2005). It was found that the ionization rate in the inner region of the surrounding envelope may be dominated by the ionizing X-ray flux rather than by an inner far ultraviolet (FUV) radiation field or the cosmic-ray ionization rate. The ionizing flux enhances $\text{H}_3^+$ and He$^+$ that trigger a distinct chemistry. It was also found that the $\text{H}_2\text{O}$ abundances in the gas-phase may be reduced due to X-rays. The abundance and behavior of $\text{H}_2\text{O}$ in both the solid and the gas-phase will be studied extensively with the upcoming Herschel Space Observatory. It is therefore timely to investigate the influence of X-rays and inner FUV fields on the abundances of gas-phase water in more detail.

In this paper, we first study the general influence of X-rays on gas-phase water. The time-dependent chemical X-ray models of Stäuber et al. (2005) are used and applied to different density and temperature regimes for different X-ray fluxes (Sect. 4.2). The densities and temperatures are chosen to cover a wide range of conditions that are applicable to cold molecular clouds, envelopes, protostellar disks and outflow hot spots. Regions with density and temperature gradients are modeled and
discussed in Sect. 4.3. These regions are representative of low-mass Class 0 and I envelopes. In addition to X-rays, central FUV fields are considered. The aim is to find systematic trends between the different type of sources. The results for the different envelopes are discussed in Sect. 4.4. The conclusions are drawn in Sect. 4.5.

4.2 General parameter study

The gas-phase water abundance is modeled as a function of time, hydrogen density \( n_H = n(H) + 2n(H_2) \) and X-ray flux. The results of this study can be applied to a wide range of different physical environments including protostellar envelopes and disks.

4.2.1 Chemical model

The X-ray chemistry models are described in detail by Stäuber et al. (2005). The models are an extension of the gas-phase chemical models of Doty et al. (2002, 2004) to allow the impact of X-rays from the central source on the surrounding molecular envelope. The input parameters for the model are the initial molecular or atomic abundances, the hydrogen density, the gas temperature, the X-ray luminosity, the X-ray emitting plasma temperature, the X-ray absorbing hydrogen column density, the cosmic-ray ionization rate and the enhancement of the inner and outer FUV field with respect to the average interstellar radiation field (ISRF).

The chemical model is based on the UMIST gas-phase chemical reaction network (Millar et al. 1997) and calculates the time-dependent number density \( n(i) \) of each species for a certain temperature and distance from the source. For the initial chemical abundances we follow the models of Doty et al. (2002, 2004) for the high-mass source AFGL 2591 and low-mass source IRAS 16293–2422. These models successfully reproduced many of the observed molecular lines. The effects of evaporation of a certain species into the gas-phase have been approximated by initially depleting this species below its evaporation temperature \( T_{ev} \). Specifically, all \( H_2O \) is assumed to evaporate at \( T > 100 \) K. No photodesorption of ice is taken into account. The initial abundances are listed in Table 4.1. The adopted cosmic-ray ionization rate is discussed in Sect. 4.3.1.
The gas temperature has been taken to be closely coupled to the dust temperature. Although the X-ray flux and the gas temperature are not fully independent, they have been treated as uncoupled variables in order to study the dependence of H$_2$O on each of them. To cover a wide range of different physical environments, the hydrogen density is varied between $n_H = 10^4$–$10^9$ cm$^{-3}$. At higher densities, the mean free path of X-rays becomes small (a few AU). Typical densities in the inner part of envelopes or protoplanetary disk atmospheres are between $n_H = 10^6$–$10^9$ cm$^{-3}$, whereas those for outflows are $n_H = 10^4$–$10^6$ cm$^{-3}$. The adopted gas temperature is between 10–1000 K. At higher temperatures ($T > 2000$ K), molecular hydrogen and water are dissociated due to H and H$_2$ collisions. The modeled X-ray fluxes are between $L_X = 10^{-6}$–$10^{-3}$ erg s$^{-1}$ cm$^{-2}$. The initial X-ray spectrum is reduced preferentially at low energies by the intervening hydrogen column density such that the local X-ray flux roughly scales with

$$F_X \approx \left( \frac{L_X}{10^{31} \text{erg s}^{-1}} \right) \left( \frac{N_H}{5.0 \times 10^{21} \text{cm}^{-2}} \right)^{-\gamma} \left( \frac{r}{56 \text{ AU}} \right)^{-2}$$

in erg s$^{-1}$ cm$^{-2}$, where $L_X$ is the original X-ray luminosity, $N_H$ the X-ray absorbing column density and $r$ is the distance from the source. The X-ray fluxes are accurate within 20% for $T_X = 3 \times 10^7$ K and $N_H = 5 \times 10^{21}$–$10^{23}$ cm$^{-2}$ with $\gamma = 0.3$, for $N_H = 2.5 \times 10^{22}$ cm$^{-2}$ with $\gamma = 0.4$ and for $N_H = 6 \times 10^{23}$–$10^{24}$ cm$^{-2}$ with $\gamma = 0.5$. A column density of $N_H = 5 \times 10^{21}$ cm$^{-2}$ absorbs all photons below $\approx 1$ keV (Stäuber et al. 2005). The X-ray spectrum is assumed to be thermal with a plasma temperature $T_X = 3 \times 10^7$ K (2.6 keV). The shape of the X-ray spectrum, however, has only little influence on the chemistry (Maloney et al. 1996; Stäuber et al. 2005). FUV fields are neglected.

All reaction rates that are relevant for the H$_2$O chemistry (Sect. 4.2.3) are given with a maximum uncertainty of 25% by the UMIST database$^1$. Self-shielding of CO has been included by using the shielding functions of Lee et al. (1996).

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$^1$http://www.rate99.co.uk
### Table 4.1: Initial abundances and cosmic-ray ionization rate.

<table>
<thead>
<tr>
<th>Species</th>
<th>Initial abundance</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
<td></td>
</tr>
<tr>
<td>CO</td>
<td>2.0E-04</td>
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</tr>
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<td>CO$_2$</td>
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<td>b</td>
</tr>
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</tr>
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</tr>
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<td>H$_2$CO</td>
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</tr>
<tr>
<td>CH$_4$</td>
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<td>e</td>
</tr>
<tr>
<td>C$_2$H$_4$</td>
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<td>c</td>
</tr>
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<td>e</td>
</tr>
<tr>
<td>S</td>
<td>0.0</td>
<td>e</td>
</tr>
<tr>
<td><strong>Initial abundances $T &lt; 100$ K</strong></td>
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<td></td>
</tr>
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</tr>
<tr>
<td>CH$_4$</td>
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</tr>
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<td>e</td>
</tr>
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<td>H$_2$CO ($60 &lt; T(K) &lt; 100$)</td>
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<td>d</td>
</tr>
<tr>
<td>H$_2$CO ($T(K) &lt; 60$)</td>
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<td>d</td>
</tr>
<tr>
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<td>d</td>
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<tr>
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<td>d</td>
</tr>
<tr>
<td>O</td>
<td>1.0E-04</td>
<td>d</td>
</tr>
<tr>
<td>S</td>
<td>6.0E-09</td>
<td>g</td>
</tr>
<tr>
<td>Cosmic-ray ionization rate $\zeta_{cr}$ ($s^{-1}$)</td>
<td>0.8E-17</td>
<td>h</td>
</tr>
</tbody>
</table>

All abundances are relative to molecular hydrogen. $^a$ Jørgensen et al. (2002), $^b$ Boonman et al. (2003a), $^c$ Boonman & van Dishoeck (2003), $^d$ Doty et al. (2004), $^e$ Charnley (1997), $^f$ assumed to be frozen-out or absent in cold gas-phase, $^g$ Doty et al. (2002), $^h$ see text.
4.2. General parameter study

4.2.2 Results

The model results for different X-ray fluxes and hydrogen densities are shown in Figs. 4.1 and 4.2 for \( t = 10^4 \) yrs and in Figs. 4.3 and 4.4 for \( t = 10^5 \) yrs. It can be seen in Figs. 4.1 and 4.3 that X-ray fluxes \( F_X \lesssim 10^{-6} \text{erg s}^{-1} \text{cm}^{-2} \) have no or minor influence on the water abundances for the densities considered. For higher X-ray fluxes, three characteristic regimes can be distinguished: 1. the regime at \( T < 100 \) K, where gas-phase water is mainly formed and destroyed in ion-molecule reactions \( (x(H_2O) \approx 10^{-7} - 10^{-6}) \), 2. the regime \( 100 \) K \( \lesssim T \lesssim 250 \) K, where water is released from grains, but destroyed by X-rays \( (x(H_2O) \approx 10^{-6}) \) and 3. the regime \( T \gtrsim 250 \) K, where the water abundance is \( x(H_2O) \gtrsim 10^{-4} \). The three regimes are discussed in some detail in the following paragraphs.

At \( t = 10^4 \) yrs, X-ray fluxes \( 10^{-5} \lesssim F_X \lesssim 10^{-2} \text{erg s}^{-1} \text{cm}^{-2} \) enhance the water abundance for temperatures \( T < 100 \) K compared to the model without X-rays. The reason for this is the increased \( H_3O^+ \) abundance due to X-rays. \( H_3O^+ \) can recombine quickly to \( H_2O \) in reactions with electrons. Note that net formation of \( H_2O \) at these fluxes can occur because \( H_3O^+ \) does not require \( H_2O \) in its formation. It is produced by ion-molecule reactions starting from \( \text{CO, CO}_2, \text{O, O}_2 \) and \( \text{OH} \), which exist in the gas phase. Higher X-ray fluxes, however, can enhance water only at densities \( n_H \gtrsim 10^7 \text{ cm}^{-3} \) for \( T < 100 \) K (Fig. 4.2). At \( t = 10^5 \) yrs, water is only enhanced at \( n_H = 10^6 \text{ cm}^{-3} \) in this temperature regime (Fig. 4.3). At higher densities, water is less abundant in models with X-rays compared to those without X-rays.

For \( 100 \) K \( \lesssim T \lesssim 250 \) K, the initial abundance of water is much higher due to ice evaporation but this high abundance rapidly decreases for \( F_X \gtrsim 10^{-3} \text{erg s}^{-1} \text{cm}^{-2} \) at \( t = 10^4 \) yrs and for \( F_X \gtrsim 10^{-4} \text{erg s}^{-1} \text{cm}^{-2} \) at \( t = 10^5 \) yrs. \( H_2O \) is mainly destroyed in reactions with \( \text{H}_3^+ \) and \( \text{HCO}^+ \) whose abundances are enhanced due to the X-rays. Another destruction mechanism is the dissociation of \( H_2O \) by FUV photons created locally by excited \( \text{H}_2 \). The rate for the X-ray induced FUV destruction of water is calculated with the method and numbers provided by Maloney et al. (1996). It is an adaption of the treatment of Gredel et al. (1989) for the effects of internally generated FUV photons by cosmic rays.

In the temperature regime \( T \gtrsim 250 \) K, the reaction \( \text{OH} + \text{H}_2 \rightarrow \text{H}_2O + \text{H} \) can become more efficient than the water destroying reactions and \( H_2O \) has abundances of the order of \( 10^{-4} \). At low densities (\( n_H = 10^4 \)-
10^5 \text{cm}^{-3})$, high X-ray fluxes lead to the destruction of water even for high temperatures. Although the gas temperature at these high fluxes may be more than 1000 K, water does not reach fractional abundances higher than $x(H_2O) \approx 10^{-7}$, since H$_2$O is destroyed in collisions with H and H$_2$ at higher temperatures. The water abundance is therefore $x(H_2O) \lesssim 10^{-10}$ for $F_X = 10 \text{ergs}^{-1} \text{cm}^{-2}$ and $n_H = 10^4 \text{cm}^{-3}$ and $x(H_2O) \lesssim 10^{-7}$ for $n_H = 10^5 \text{cm}^{-3}$, independent of the gas temperature. At higher densities, however, even high X-ray fluxes cannot destroy water in the regime $T \gtrsim 250 \text{K}$. At densities $n_H \gtrsim 10^7 \text{cm}^{-3}$, X-rays even enhance the water abundance ($x(H_2O) > 3 \times 10^{-4}$) for temperatures $T \gtrsim 300$–$600 \text{K}$ compared to models without X-rays. This enhancement is again mainly through recombination reactions of H$_3$O$^+$.

At later times ($t = 10^6 \text{yrs}$), water is destroyed in the regime 100 K $\lesssim T \lesssim 250 \text{K}$ for $F_X \gtrsim 10^{-5} \text{ergs}^{-1} \text{cm}^{-2}$. The other temperature regimes in the X-ray models resemble those at $t = 10^5 \text{yrs}$. The main differences with the models at $t = 10^5 \text{yrs}$, however, are the water abundances of the models without X-rays. H$_2$O is gradually destroyed in reactions with HCO$^+$ for temperatures $T \gtrsim 100 \text{K}$. In models without X-rays, HCO$^+$ is mainly formed by cosmic-ray induced reactions. At $t = 10^6 \text{yrs}$, water between $T \approx 100 \text{K}$ and $T \approx 200 \text{K}$ is destroyed down to abundances of a few $\times 10^{-7}$. The water abundances for $T < 100 \text{K}$ on the other hand, are slightly higher compared to the models at $t = 10^5 \text{yrs}$. This is due to the relatively slow ion-molecule reactions that need time to build up water.

### 4.2.3 Chemical reactions relevant for H$_2$O

Water is assumed to be initially frozen out on the dust grains for temperatures $T < 100 \text{K}$ and injected into the gas at $T = 100 \text{K}$ with a fractional abundance $x(H_2O) = 1.5 \times 10^{-4}$. In the presence of X-rays, water is then mainly destroyed in reactions with H$_3^+$ and HCO$^+$. Another destruction route is the dissociation of water due to X-ray induced FUV photons. To estimate the importance of this reaction on the H$_2$O abundance, models have been run for different X-ray luminosities ignoring this reaction. The resulting H$_2$O abundances vary by less than 15% in comparison to models where this reaction is included. It emphasizes that the main destruction reactions of H$_2$O are the ion-molecule reactions with H$_3^+$ and HCO$^+$, respectively. The bulk of the H$_2$O not evaporated from the grains stems from the reaction of OH with H$_2$, which becomes
4.2. General parameter study

Figure 4.1: Fractional water abundances as functions of the gas temperature and low X-ray flux ($F_X = 10^{-6}$ to $10^{-3}$ erg s$^{-1}$ cm$^{-2}$) for different densities (cm$^3$) at $t = 10^4$ yrs. The vertical line indicates the 250 K temperature mark.
Figure 4.2: Fractional water abundances as functions of the gas temperature and high X-ray flux ($F_X = 10^{-2} - 10^{-1}\text{ erg s}^{-1}\text{ cm}^{-2}$) for different densities ($\text{cm}^{-3}$) at $t = 10^4\text{ yrs}$. The vertical line indicates the 250 K temperature mark.
4.2. General parameter study

Figure 4.3: Fractional water abundances as functions of the gas temperature and low X-ray flux \( \left( F_X = 10^{-6} - 10^{-3} \text{erg s}^{-1} \text{cm}^{-2} \right) \) for different densities \( (\text{cm}^{-3}) \) at \( t = 10^5 \text{yrs} \). The vertical line indicates the 250 K temperature mark.
Figure 4.4: Fractional water abundances as functions of the gas temperature and high X-ray flux ($F_X = 10^{-2}$ $10$ erg s$^{-1}$ cm$^{-2}$) for different densities (cm$^3$) at $t = 10^5$ yrs. The vertical line indicates the 250 K temperature mark.
4.3 Applications to protostellar envelopes

In order to study the influence of X-rays on the gas-phase water abundance in more realistic environments, the models are applied to envelopes of Class I ($t \approx 10^5$–$10^6$ yrs) and Class 0 ($t \approx$ a few $\times 10^3$–$10^4$ yrs) low-mass stars.
YSOs. These regions may be characterized by a power-law density distribution and an increasing gas temperature towards the central protostar. Class 0 and I envelopes mainly differ in their total mass. Typical envelope masses of Class 0 objects are $M_{\text{env}} \gtrsim 0.5 \, M_{\odot}$ whereas Class I sources have less massive envelopes with $M_{\text{env}} \lesssim 0.5 \, M_{\odot}$ (e.g., Jørgensen et al. 2002, 2005c). Although spherical 1D models are an approximation to the real geometry of protostellar cores, they successfully explain many of the observed features of low-mass protostars from few hundred AU out to $10^4$ AU scales (e.g., Schöier et al. 2004; Jørgensen et al. 2002, 2005d) and provide a framework for discussing their overall chemical structure (e.g., Doty et al. 2004; Maret et al. 2004; Jørgensen et al. 2004). Inside a few hundred AU, however, the geometry is likely to be much more complex with cavities and a flattened protostellar disk in addition to the spherical inner envelope. Since no realistic physical models based on observations on those scales are yet available, we adopt the spherical models extrapolated to small radii as a starting point. Possible effects due to cavities and non-spherical symmetry are discussed throughout this section and in Sect. 4.4.

In the following models, the H$_2$O chemistry is assumed to be irradiated by X-rays and FUV photons from the central source. The FUV models have been described in detail by Stäuber et al. (2004a).

### 4.3.1 Class I envelope model

The density and temperature profiles adopted for a prototypical Class I source are presented in Fig. 4.6 and Table 4.2, based on the observations by Jørgensen et al. (2002). In that analysis, it was assumed that the gas temperature equals the dust temperature. X-rays and FUV fields, however, are able to increase the gas temperature due to photoelectric heating. The gas temperature has therefore been explicitly calculated for the different X-ray and FUV fluxes. The X-ray luminosity is varied between $L_X = 10^{26}$–$10^{32}$ erg s$^{-1}$ and the FUV field from the central source ($G_{0,\text{in}}$) at the inner radius from $10^5$ to $10^8$ with respect to the average ISRF. The heating rate due to X-rays is taken from Maloney et al. (1996), and for the FUV heating we follow Bakes & Tielens (1994). The heating rates are then compared to the cooling rate due to gas-dust collisions provided by Hollenbach & McKee (1989). At lower densities ($n_H \approx 10^5$ cm$^{-3}$) line cooling due to C$^+$, O and CO also becomes important (see also Doty
4.3. Applications to protostellar envelopes

Table 4.2: Model parameters for a prototypical Class I object.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_{bol}$</td>
<td>$0.66 L_{\odot}$</td>
</tr>
<tr>
<td>Envelope parameters:</td>
<td></td>
</tr>
<tr>
<td>Inner radius $r_{in}$ ($T = 250$ K)</td>
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</tr>
<tr>
<td>Outer radius $r_{out}$ ($T = 10$ K)</td>
<td>$4.3 \times 10^3$ AU</td>
</tr>
<tr>
<td>Density at 1000 AU, $n$(H$_2$)</td>
<td>$8.8 \times 10^4$ cm$^{-3}$</td>
</tr>
<tr>
<td>Density power-law index, $p$</td>
<td>1.6</td>
</tr>
<tr>
<td>Gas mass $M_{env}$ ($T = 10$ K)</td>
<td>0.034 $M_{\odot}$</td>
</tr>
<tr>
<td>Column density $N_{H_2}$</td>
<td>$6.9 \times 10^{22}$ cm$^{-2}$</td>
</tr>
</tbody>
</table>

& Neufeld 1997), but these effects are minor for our purpose since the densities in the regions of interest are always $n_H \gtrsim 10^6$ cm$^{-3}$.

It is found that only X-ray luminosities $L_X \gtrsim 10^{31}$ erg s$^{-1}$ lead to a noticeable increase in the gas temperature ($T_{gas} - T_{dust} \gtrsim 10$ K). The results for $L_X = 10^{31}$ erg s$^{-1}$ and $L_X = 10^{32}$ erg s$^{-1}$ are plotted in Fig. 4.6. The temperature of the gas is only affected in the inner $\approx 0.1$ AU by the central FUV field (not shown in Fig. 4.6). High FUV fields ($G_{0,in} \gtrsim 10^7$) are needed though to increase the gas temperature significantly above the dust temperature.

The effects of the outer FUV field can be neglected. The optical depth in the region of interest ($T \gtrsim 100$ K) is $A_V \approx 18$ and all FUV photons should be absorbed by the outer envelope for typical values of the ISRF. The outer FUV field is taken to be $G_{0,out} = 1$ according to the average ISRF.

The adopted value of the cosmic-ray ionization rate $\zeta_{cr} = 0.8 \times 10^{-17}$ s$^{-1}$ is based on the results of Stäuber et al. (2005) who showed that low-$J$ lines of HCO$^+$ tend to trace the cosmic-ray ionization rate, whereas high-$J$ lines are more sensitive to the ionizing inner X-ray flux. To constrain $\zeta_{cr}$, the rate is varied in our models in order to fit the HCO$^+$ 1–0 observations toward the low-mass star-forming region Taurus (TMC 1) of Hogerheijde et al. (1997). It is found that $\zeta_{cr} = 0.8 \times 10^{-17}$ s$^{-1}$ fits the observations best. This value is at the lower end of the rates found by van der Tak & van Dishoeck (2000) toward high-mass star-forming regions ($\zeta_{cr} = 0.61–5.6 \times 10^{-17}$ s$^{-1}$).
4.3.2 Results for the Class I model

X-ray models

The depth dependent water profiles for \( t = 5 \times 10^3 \) yrs to \( t = 10^6 \) yrs and for X-ray luminosities \( L_X = 10^{26} - 10^{28} \) erg s\(^{-1}\) are presented in Fig. 4.7. The inner FUV field is neglected in these models. It can be seen that an X-ray luminosity of \( L_X \gtrsim 10^{28} \) erg s\(^{-1}\) destroys the gas-phase H\(_2\)O within less than 5000 yrs from initial \( x(\text{H}_2\text{O}) \approx 10^{-4} \) down to \( x(\text{H}_2\text{O}) \approx 10^{-6} \) with respect to molecular hydrogen. For an X-ray luminosity of \( L_X \approx 10^{27} \) erg s\(^{-1}\) the timescale to destroy water is \( t \gtrsim 5 \times 10^4 \) yrs. In models with \( L_X \lesssim 10^{26} \) erg s\(^{-1}\), water has still high abundances \( (x(\text{H}_2\text{O}) \approx 10^{-4}) \) in the innermost part of the envelope. We therefore conclude that X-ray luminosities \( L_X \gtrsim 10^{27} \) erg s\(^{-1}\) destroy all gas-phase water down to fractional abundances of \( x(\text{H}_2\text{O}) \approx 10^{-6} \) on timescales \( t \approx 5 \times 10^4 \) yrs and \( L_X \gtrsim 10^{28} \) erg s\(^{-1}\) on a timescale of a few \( \times 10^3 \) yrs.

The water profile for \( t = 10^5 \) yrs and higher X-ray luminosities is shown in Fig. 4.8. The fractional abundances increase from \( x(\text{H}_2\text{O}) \approx 10^{-6} \) to \( x(\text{H}_2\text{O}) \approx 10^{-5} \) for increasing X-ray luminosities between \( L_X = 10^{29} - 10^{31} \) erg s\(^{-1}\), and \( x(\text{H}_2\text{O}) \) reaches even \( \gtrsim 10^{-4} \) in the innermost part.

Figure 4.6: Density and thermal structure for a prototypical Class I object adopted from the model results of Jørgensen et al. (2002) (solid lines). The dashed and dotted lines refer to the gas temperature for the models including an additional inner source of X-ray luminosity \( (L_X = 10^{31} \text{ erg s}^{-1} \) and \( L_X = 10^{32} \text{ erg s}^{-1} \), respectively). The arrow indicates the distance out to which X-rays dominate the H\(_2\) ionization rate over cosmic-rays \( (\zeta_{\text{cx}} = 0.8 \times 10^{-17} \text{ s}^{-1}) \) for \( L_X = 10^{30} \) erg s\(^{-1}\).
4.3. Applications to protostellar envelopes

of the envelope for $L_X = 10^{32}\,\text{ergs}^{-1}$. This effect can be explained by the fast electron recombination reaction of $\text{H}_3\text{O}^+$ that forms $\text{H}_2\text{O}$ and by the increasing gas temperature with increasing X-ray flux: The reaction of OH with $\text{H}_2$, that drives oxygen into $\text{H}_2\text{O}$, becomes faster than the destruction of water by X-rays at higher temperatures, hence more water is produced for higher X-ray fluxes. In the region $T < 100\,\text{K}$, $x(\text{H}_2\text{O})$ decreases with increasing X-ray luminosity for $t = 10^5\,\text{yrs}$, until $L_X \approx 10^{29}\,\text{ergs}^{-1}$. Higher X-ray luminosities lead to higher water abundances. This is again mainly due to the recombination of $\text{H}_3\text{O}^+$, which is more abundant in models with high X-ray fluxes (see also Sect. 4.2).

Fig. 4.8 shows that $x(\text{H}_2\text{O})$ increases from $\approx 4-5 \times 10^{-7}$ to $\approx 2 \times 10^{-6}$ with increasing X-ray luminosity ($L_X \gtrsim 10^{29}\,\text{ergs}^{-1}$). At early times, the recombination of $\text{H}_3\text{O}^+$ in the models with X-rays leads to even higher $\text{H}_2\text{O}$ abundances in the region $T < 100\,\text{K}$ compared with the model without X-rays (Fig. 4.7).

The OH abundance profiles for different X-ray luminosities at $t = 10^5\,\text{yrs}$ are given in Fig. 4.9. The OH densities are normalized by $n(\text{H}_2)$ (left) and by $n(\text{H}_2\text{O})$ (right), respectively. In the right part of Fig. 4.9 it can be seen that an X-ray luminosity $L_X = 10^{28}\,\text{ergs}^{-1}$ leads to

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**Figure 4.7:** Depth dependent temporal evolution of $\text{H}_2\text{O}$ for different X-ray luminosities. The solid line corresponds to the model without X-rays. X-ray luminosities are given in ergs$^{-1}$. The $T = 100\,\text{K}$ mark is at $r = 10\,\text{AU}$. 
Chapter 4. Water destruction by X-rays in young stellar objects

Figure 4.8: Depth dependent fractional abundances of H$_2$O for high X-ray luminosities and $t = 10^5$ yrs. The solid line corresponds to the model without X-rays. X-ray luminosities are given in erg s$^{-1}$.

$n$(OH)/$n$(H$_2$O) $\approx 10^{-2}$, whereas X-ray luminosities $L_X \gtrsim 10^{30}$ erg s$^{-1}$ can produce ratios of $n$(OH)/$n$(H$_2$O) $\approx 0.1$–1 in the innermost part of the envelope. The $n$(OH)/$n$(H$_2$O) ratio in the hot ($T > 100$ K) region of the envelope in the models without X-rays is only of the order of $\approx 10^{-4}$. X-rays therefore enhance the OH abundances as well as the OH to H$_2$O abundance ratio.

The high densities ($n_H > 10^8$ cm$^{-3}$) and temperatures ($T > 200$ K) in the model at $r < 10$ AU may be appropriate either to an inner envelope or to the inner regions of a circumstellar disk. However, there is also evidence for cavities in the inner few hundred AU (e.g., Jørgensen et al. 2005a). We have therefore also modeled an envelope where $r_{in}$ is assumed to be at 50 AU with a temperature $T = 100$ K. This corresponds to a source with $L_{bol} = 2 L_\odot$. The results for $t = 10^5$ yrs are presented in Fig. 4.10. H$_2$O is destroyed by the X-rays and has abundances $x$(H$_2$O) $< 10^{-5}$. At larger radii ($r_{in} > 50$ AU) the dust will not be heated above $T > 100$ K, i.e., the temperature where water evaporates into the gas phase, and the water abundances will stay below $x$(H$_2$O) $< 10^{-5}$.

**FUV models**

The H$_2$O profiles for different inner FUV fields ($G_{0, in} = 10^5$–$10^8$) are presented in Fig. 4.11. The X-ray emission has been neglected in these models. As can be seen, inner FUV fields affect the water abundances...
4.3. Applications to protostellar envelopes

Fractional abundances of OH (left: $x(\text{OH}) = n(\text{OH})/n(\text{H}_2)$, right: $x(\text{OH}) = n(\text{OH})/n(\text{H}_2\text{O})$) for the model without X-rays (solid line), for $L_X = 10^{28}\text{ergs}^{-1}$ (dotted line), for $L_X = 10^{30}\text{ergs}^{-1}$ (dashed line) and for $L_X = 10^{32}\text{ergs}^{-1}$ (dashed-dotted line).

only in the inner 0.2–0.3 AU. This is due to the high hydrogen densities ($n_H \approx 10^9 \text{cm}^{-3}$) in this region that absorb the FUV photons very quickly. Although the FUV photons from the central source can destroy $\text{H}_2\text{O}$ in the innermost region, even very high FUV fields ($G_{0,\text{in}} = 10^9$) cannot destroy $\text{H}_2\text{O}$ out to $r_{100K} = 10 \text{AU}$.

The FUV photons may reach distances in the envelope further away from the source by traveling through the outflow cones until they are scattered back into the envelope by dust grains (Spaans et al. 1995; Jørgensen 2004). However, the influence of the scattered photons is restricted to a small region around the outflow walls, since the FUV photons are absorbed quickly at these high densities and therefore water will not be destroyed on large scales.

Another possibility for the inner FUV field to affect larger distances might be a somewhat clumpy envelope. Models of clumpy photodissociation regions have shown that the FUV photons can travel deeper into the molecular cloud (Meixner & Tielens 1993). At large radii with lower densities, the FUV photons primarily heat the gas and not the dust. $\text{H}_2\text{O}$ desorption will therefore not be much affected - but $\text{H}_2\text{O}$ gas may be photodissociated. Spaans & van Dishoeck (2001) have shown that an inhomogeneous density distribution in molecular clouds lowers the column density of $\text{H}_2\text{O}$ by more than an order of magnitude compared with the homogeneous cloud model. The advent of ALMA or space-based far-infrared interferometers might help to investigate the possibility of
clumpy envelopes in more detail, since a spatial resolution of $\lesssim 1''$ is needed to resolve the region of interest.

Models where a central X-ray source and circumstellar FUV fields were combined showed similar results for the influence of the FUV photons. It is thus concluded that X-rays clearly dominate the chemistry of the envelope in comparison to FUV fields.

Other species

Depth dependent fractional abundances of the main species involved in the water reaction network are presented in Fig. 4.12 for $t = 10^5$ yrs. Atomic oxygen is mainly produced by the X-ray induced FUV dissociation of O$_2$ and the dissociative ionization of CO by He$^+$. Atomic oxygen reaches fractional abundances $x(O) \approx 10^{-4}$ in the inner warm ($T > 100$ K) region. The OH$^+$ abundance is dramatically increased by X-rays (see also Stäuber et al. 2005). The fractional abundance of OH$^+$ is $\approx 10^{-14}$ for $L_X = 10^{28}$ erg s$^{-1}$, $x$(OH$^+$) $\approx 10^{-12}$ for $L_X = 10^{30}$ erg s$^{-1}$ and $x$(OH$^+$) $\approx 10^{-10}$ for $L_X = 10^{32}$ erg s$^{-1}$ in the inner region of the envelope. It is mainly produced in the ion-molecule reactions of O with H$_3^+$, O$^+$ with H$_2$ and OH with H$^+$.

O$_2$ has fractional abundances $x$(O$_2$) $\approx 10^{-5}$, $10^{-4}$ in the models, much higher than observed. Molecular oxygen is efficiently produced in the reaction of atomic oxygen with OH. There is an uncertainty in the rate
of this reaction for O in the ground fine-structure level \((^3P_2)\), however, and the rate coefficient may be lower than that cited by UMIST (Sims et al. 2006). \(O_2\) is mainly destroyed in the reaction with \(H_3^+\) and by X-ray induced FUV photons. \(O_2\) has been searched with SWAS (e.g., Melnick 2004) and ODIN (e.g., Pagani et al. 2003) but has not been reported in the literature to date. Derived upper limits on \(O_2\) column densities are usually of the order of \(\approx a few \times 10^{15}\) cm\(^{-2}\) or \(x(O_2) \approx a few \times 10^{-7}\). Standard chemical models normally overestimate this value by 2–3 orders of magnitude (see Melnick 2004; Pagani et al. 2003 for a more detailed discussion). Our models are no exception. However, the 30ʺ averaged column density in the Class I models are \(N_{\text{beam}}(O_2) \lesssim 10^{15}\) cm\(^{-2}\), which is well within the upper limits derived by SWAS and ODIN. Oxygen could be frozen out on grains in some form at lower temperatures and therefore not seen with the big beams of ODIN (9ʺ) and SWAS (3.5ʹ × 5.0ʹ). Herschel might shed some light on this matter with its relatively small beam widths (8–35ʺ, depending on frequency).

\(H_3^+\) is a key molecule in the chemical reaction network of water and its abundance is greatly enhanced in the models including X-rays. Thus, observations of \(H_3^+\) in absorption at \(\approx 3.7\,\mu m\) (e.g., McCall et al. 1999) would allow a direct test of the models. The integrated radial column densities \(N_{\text{rad}}\) of \(H_3^+\) are therefore presented for the Class I X-ray models in Table 4.3. The values given in parenthesis are \(H_3^+\) column densities calculated for the model with \(r_{\text{in}} = 50\) AU, i.e. the model with a protostellar
Figure 4.12: Depth dependent fractional abundances of relevant species in the chemical H$_2$O reaction network for different X-ray luminosities and $t = 10^5$ yrs. The solid line corresponds to the model without X-rays or inner FUV fields. X-ray luminosities are given in erg s$^{-1}$.

4.3.3 Class 0 envelope model

Table 4.4 lists the main parameters for a prototypical Class 0 envelope model (Schöier et al. 2002). The crucial differences from the modeling point of view between the Class 0 and I envelope are the much higher bolometric luminosity, envelope mass and column density of the younger object, that lead to a different density and temperature distribution. The initial chemical abundances are again taken as given in Table 4.1. Freeze-out of CO is taken into account for temperatures $T < 20$ K. The increased gas temperature due to X-rays has been calculated as described in Sect. 4.3.1. The X-ray luminosity is varied between $L_X = 10^{28} - 10^{32}$ erg s$^{-1}$.

The results for H$_2$O are shown in Fig. 4.13 for $t = 10^4$ yrs and in Fig. 4.14 for $t = 10^5$ yrs. At $t = 10^4$ yrs, only high X-ray luminosities ($L_X > 10^{32}$ erg s$^{-1}$) lead to water abundances $x$(H$_2$O) $\lesssim 10^{-5}$. An X-ray luminosity of $L_X \gtrsim 10^{31}$ erg s$^{-1}$ destroys water between $\approx 40$–$80$ AU
Table 4.3: Radial column densities of $H_2^+$ for the Class I source.

<table>
<thead>
<tr>
<th>$\log(L_X)$</th>
<th>$N_{rad}$</th>
<th>$\log(L_X)$</th>
<th>$N_{rad}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\log(\text{ergs}^{-1} \text{ cm}^{-2})$</td>
<td>$\log(\text{ergs}^{-1})$</td>
<td>$\log(\text{ergs}^{-1})$</td>
<td>$\log(\text{ergs}^{-1})$</td>
</tr>
<tr>
<td>8.0E11 (2.0E09)</td>
<td>30</td>
<td>4.8E14 (4.2E11)</td>
<td></td>
</tr>
<tr>
<td>1.3E12 (2.5E09)</td>
<td>31</td>
<td>4.5E15 (3.9E12)</td>
<td></td>
</tr>
<tr>
<td>5.9E12 (6.5E09)</td>
<td>32</td>
<td>3.6E16 (2.9E13)</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.4: Model parameters for a prototypical Class 0 source.

<table>
<thead>
<tr>
<th>$L_{bol}$</th>
<th>27 $L_\odot$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Envelope parameters:</td>
<td></td>
</tr>
<tr>
<td>Inner radius $r_{in}$</td>
<td>32 AU</td>
</tr>
<tr>
<td>Outer radius $r_{out}$</td>
<td>$8 \times 10^3$ AU</td>
</tr>
<tr>
<td>Density at 1000 AU, $n(H_2)$</td>
<td>$6.7 \times 10^6$ cm$^{-3}$</td>
</tr>
<tr>
<td>Density power-law index, $p$</td>
<td>1.7</td>
</tr>
<tr>
<td>Mass $M_{\text{env}}$</td>
<td>5.4 $M_\odot$</td>
</tr>
<tr>
<td>Column density $N_{H_2}$</td>
<td>$1.6 \times 10^{24}$ cm$^{-2}$</td>
</tr>
</tbody>
</table>

with higher abundances ($x(H_2O) \approx \text{a few} \times 10^{-5}$) at $\approx 35$ AU and $\approx 100$ AU. Water is not significantly destroyed for X-ray luminosities $L_X \lesssim 10^{30}$ erg s$^{-1}$. Similar conclusions hold for $t = 10^5$ yrs although the region where $x(H_2O) \gtrsim 10^{-5}$ is less than 50 AU ($T \gtrsim 250$ K). Compared to the Class I models (after appropriate scaling of the X-ray flux $\propto L_X r^{-2}$), water is less destroyed by X-rays in the Class 0 envelope. The reason for this are the high densities ($n_H \gtrsim 10^9$ cm$^{-3}$) in the innermost region of the Class 0 source that absorb the X-ray flux.

4.4 Discussion

As discussed in Sect. 4.2, X-rays reduce the water abundance preferably in regions where the gas temperature is $T \lesssim 250$–$300$ K ($x(H_2O) \approx 10^{-6}$). At low densities ($n_H \lesssim 10^5$ cm$^{-3}$), the fractional water abundance is less than $\approx 10^{-7}$ for X-ray fluxes $F_X \gtrsim 10$ erg s$^{-1}$ cm$^{-2}$ even for high gas tempera-
Chapter 4. Water destruction by X-rays in young stellar objects

Figure 4.13: Depth dependent fractional abundances of H$_2$O for a Class 0 object for different X-ray luminosities and $t = 10^4$ yrs. The solid line corresponds to the model without X-rays. X-ray luminosities are given in erg s$^{-1}$.

Figure 4.14: Depth dependent fractional abundances of H$_2$O for a Class 0 object for different X-ray luminosities and $t = 10^5$ yrs. The solid line corresponds to the model without X-rays. X-ray luminosities are given in erg s$^{-1}$.
4.4. Discussion

For higher densities and temperatures $T \gtrsim 250$–300 K, water has fractional abundances $x(\text{H}_2\text{O}) \gtrsim 10^{-4}$ (nearly) independent of the X-ray flux. In the following, we discuss these findings in the context of protostellar envelopes and other models.

4.4.1 Envelope models

For high-mass YSOs, the observed water abundance can be successfully explained within the hot-core scenario in which the high temperatures in the inner envelope drive most of the oxygen into water and in which most of the water is frozen out onto grains in the outer region (e.g., Doty et al. 2002; Boonman et al. 2003b). Recent interferometer studies of $\text{H}_2^{18}\text{O}$ by van der Tak et al. (2006) towards the high-mass young stellar object (YSO) AFGL 2591 confirm the existence of a hot ($T > 100\,\text{K}$) compact central region with high abundant water ($x(\text{H}_2\text{O}) \approx 10^{-4}$) and a region with lower abundances in the colder outer part. Although X-ray models predict the destruction of water also in high-mass objects (Stäuber et al. 2005), these envelopes are likely to have regions with temperatures exceeding $T = 250\,\text{K}$ (van der Tak et al. 2000a). In addition, the distance from the central source to the region in the envelope where the gas temperature is $T = 100\,\text{K}$, is much larger in high-mass sources compared to low-mass objects due to their high bolometric luminosities. The X-ray flux decreases rapidly with $r^{-2}$ and may already be too low to destroy $\text{H}_2\text{O}$. Water can therefore have fractional abundances of the order of $10^{-4}$ in envelopes around high-mass YSOs despite their possible X-ray emission.

Similar jumps in the water abundances are also observed toward low-mass Class 0 sources, although the derived abundances in the inner part are usually much lower compared to the massive objects. Ceccarelli et al. (2000b) derived water abundances of $x_{\text{in}}(\text{H}_2\text{O}) = 3 \times 10^{-6}$ for the inner part of the envelope of the Class 0 source IRAS 16293–2422 and $x_{\text{out}}(\text{H}_2\text{O}) = 5 \times 10^{-7}$ for the outer part from detailed models of ISO observations. Maret et al. (2002) found $x_{\text{in}}(\text{H}_2\text{O}) = 5 \times 10^{-6}$ for the Class 0 object NGC1333–IRAS4 and $x_{\text{out}}(\text{H}_2\text{O}) = 5 \times 10^{-7}$. Within the spherical envelope models in Sect. 4.3.3, such jumps with relatively low inner water abundances occur for high X-ray luminosities $L_X = 10^{31}$–$10^{32}\,\text{ergs}\,\text{s}^{-1}$ and $t = 10^5\,\text{yrs}$ (Fig. 4.14). X-rays are therefore a possible explanation for the low water abundances found in these objects.
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Class I envelopes may have no or only a small region where the temperature exceeds $T \approx 250$ K. The inner part of the envelope may already have been dispersed by outflows or accreted onto the star/disk system. Water is therefore easily destroyed by X-rays. According to the models in Sect. 4.3.2, the average water abundance is predicted to be at most $x(H_2O) \approx 10^{-6}$ in Class I sources with X-ray luminosities $L_X \gtrsim 10^{27}$ erg s$^{-1}$. Note that the generic Class I model in Sect. 4.3.1 is considered as an extreme case where the gas temperature gets $T \approx 250$ K close to the protostar. If the inner envelope has cavities of any kind, the gas temperature of the envelope will be lower at the inner edge of the envelope ($r_{in}$), since this will be at a larger distance and since the dust temperature roughly falls with $r_{in}^{-0.4}$. Water will in that case be destroyed even more readily (Sect. 4.3.2, Fig. 4.10), unless there is some mechanism (e.g., photodesorption) that returns water ice to the gas phase.

4.4.2 Disks and outflows

As discussed in Sect. 4.3, the inner envelopes of Class 0 and I sources are likely to have a much more complex geometry than the spherical envelopes adopted here. If protostellar cavities or holes (Jørgensen et al. 2005a) are common, the emission from H$_2$O and other typical "hot core" species may be dominated by the protostellar accretion disk or outflow hot spots rather than by the envelope. Disks are known to be present (e.g., Brown et al. 2000; Looney et al. 2000) and can dominate over the hot core in terms of column density (Jørgensen et al. 2005d). From the chemical point of view, the disk and hot core scenario are difficult to distinguish since both have high densities and temperatures in their inner region. According to the results in Sect. 4.2, the X-ray flux of a protostar with $L_X = 10^{31}$ erg s$^{-1}$ and an absorbing column density of $N_H = 10^{24}$ cm$^{-2}$ at the outer part of a protostellar disk ($r \approx 400$ AU) is $F_X \approx 10^{-3}$ erg s$^{-1}$ cm$^{-2}$. Water at temperatures below $T \approx 250$ K is therefore destroyed from initial $x(H_2O) \approx 10^{-4}$ down to $x(H_2O) \approx 10^{-7}$–$10^{-6}$. High column densities and/or temperatures are needed for the water to persist at $x(H_2O) \approx 10^{-4}$ in protostellar disks. For comparison, the chemistry disk models including X-rays by Aikawa & Herbst (2001) have H$_2$O abundances below $\approx 10^{-8}$ at $r = 500$ AU from the central source. In the disk atmosphere models of Glassgold et al. (2004), water has fractional abundances $x(H_2O) < 10^{-5}$ at 1 AU from the source for
vertical column densities of less than a few $10^{23}$ cm$^{-2}$.

Recent results presented by Chandler et al. (2005) for the inner $\approx 1''$ of IRAS 16293−2422 suggest outflow shocks to be the origin for the hot core species. Giannini et al. (2001) and Nisini et al. (2002) pointed out the importance of outflows for the water abundances in Class 0 and I sources on larger scales. The results of Sect. 4.2 imply that the source of H$_2$O emission with $x(\text{H}_2\text{O}) \approx 10^{-4}$ from outflow regions with gas temperatures $100 \, \text{K} \lesssim T \lesssim 250 \, \text{K}$ has to be located at a certain distance $d(L_X)$ from the X-ray source in order to survive. Consider, for example, $t = 10^4$ yrs, typical outflow densities ($n_H = 10^4-10^6$ cm$^{-3}$) and an X-ray absorbing column density $N_H = 5 \times 10^{21}$ cm$^{-2}$. It can then be concluded from Figs. 4.1-4.4 (Sect. 4.2), that the H$_2$O emitting source would have to be at $d \gtrsim 170$ AU for $L_X = 10^{28}$ erg s$^{-1}$, at $d \gtrsim 550$ AU for $L_X = 10^{29}$ erg s$^{-1}$, at $d \gtrsim 1700$ AU for $L_X = 10^{30}$ erg s$^{-1}$ and at $d \gtrsim 5500$ AU for $L_X = 10^{31}$ erg s$^{-1}$. Larger hydrogen densities and X-ray absorbing column densities, however, decrease these distances. The physical quantities of the observed outflows by Benedettini et al. (2002) range between $300 \, \text{K} \lesssim T \lesssim 1400 \, \text{K}$ and $4 \times 10^4$ cm$^{-3} \lesssim n_H \lesssim 2 \times 10^6$ cm$^{-3}$. It is interesting to see, that the derived water abundances for $T > 300$ K by Benedettini et al. are a factor of $\approx 10$ higher than those at $T = 300$ K. This is in good agreement with the results in Sect. 4.2 where the X-ray models show a jump at these densities but where the models without X-rays show no jump at $T = 300$ K. X-rays are therefore also predicted to influence the water abundances in outflow hot spots. It should be noted that FUV fields from the central star may also influence the water abundances if the photons can impact the H$_2$O emission region relatively unhindered, e.g. through outflow cones. High FUV fields tend to destroy water even at high temperatures though (Sect. 4.3.2; Stäuber et al. 2004a).

4.5 Conclusion

The gas-phase water abundance is found to be critically dependent on time, gas temperature, hydrogen density and X-ray flux (Sect. 4.2). Three distinct regimes are identified: In the first regime ($T \lesssim 100$ K), the water abundance is $x(\text{H}_2\text{O}) \approx 10^{-7}-10^{-6}$ and can be somewhat enhanced or destroyed by X-rays in comparison to models without X-rays. In the second regime ($250 \, \text{K} \lesssim T \lesssim 100 \, \text{K}$), water is released from grains with
$x(\text{H}_2\text{O}) \approx 10^{-4}$ but quickly reduced by X-rays to fractional abundances $x(\text{H}_2\text{O}) \approx 10^{-6}$. The third regime ($T \gtrsim 250$ K) is characterized by high water abundances ($x(\text{H}_2\text{O}) \gtrsim 10^{-4}$) due to the efficient reaction of OH with molecular hydrogen. At low densities ($n_H \lesssim 10^5$ cm$^{-3}$) water is destroyed even at high temperatures for X-ray fluxes $F_X \gtrsim 10$ erg s$^{-1}$ cm$^{-2}$. In general, higher gas temperatures and higher hydrogen densities allow higher X-ray fluxes for H$_2$O to survive. Water is mainly destroyed in reactions with the X-ray enhanced species HCO$^+$ and H$_3^+$. It is also destroyed by internally created FUV photons.

The envelopes of both Class I (Sect. 4.3.1) and Class 0 (Sect. 4.3.3) objects were modeled under the influence of central X-ray and FUV emission. The results for the Class I envelope show that an initial warm gas-phase water abundance of $x(\text{H}_2\text{O}) \approx 10^{-4}$ is reduced to $x(\text{H}_2\text{O}) \approx 10^{-6}$ within $\approx 5000$ yrs for X-ray luminosities $L_X \gtrsim 10^{28}$ erg s$^{-1}$ and within $\approx 5 \times 10^4$ yrs for X-ray luminosities $L_X \gtrsim 10^{27}$ erg s$^{-1}$, consistent with reported upper limits for H$_2$O towards Class I sources. Water is also destroyed by X-rays in the Class 0 object, but higher X-ray fluxes are needed due to the higher densities in the inner region. The influence of a central FUV field is negligible in our models, unless the FUV photons can escape to larger distances (Sect. 4.3.2).

The current protostellar models are limited to spherical symmetry, which is obviously an approximation to the true geometry of the inner few hundred AU where cavities and flattened disks may be present. Nevertheless, the high densities and temperatures in the current models are representative of such regions. In particular, X-rays are predicted to regulate the H$_2$O abundances wherever the gas temperature is $T \lesssim 250$–300 K. This will not only be the case for H$_2$O originating from envelopes or disks in high-mass star-forming regions, but also for H$_2$O produced in outflow hot spots around low-mass objects. The presence of cavities or outflow cones will have the result that X-rays and/or FUV photons penetrate to larger radii in certain directions.

Future instruments such as Herschel Space Observatory will allow detailed studies of the water abundances in both high and low-mass YSOs. With its high resolution instrument HIFI (de Graauw & Helmich 2001), it will be possible to distinguish shock heated H$_2$O from H$_2$O in hot cores or disks from their line profiles. Observations of the optically thin isotope H$_2^{18}$O will help to sample the envelope, whereas optically thick lines may give information about outflow properties. PACS will delineate the water
4.5. Conclusion

abundances on 9" scale including maps of the outflows. ALMA, on the other hand, will be able to resolve the innermost region (< 0.1") of YSO envelopes and/or disks in order to study the chemistry and therefore its physical properties in molecules other than H$_2$O. Limited maps of H$_2^{18}$O on arcsec scale may be possible though with ALMA under exceptional conditions in the 203 GHz line. High-$J$ lines of CO will reveal the gas temperature in these regions whereas the observation of X-ray and FUV tracers (Stäuber et al. 2004a, 2005) may help to clarify the high-energy properties of young stellar objects. Together, these new facilities and models will reveal much about the physical and chemical structure of the inner regions of young stellar objects, which are currently poorly understood.
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Chapter 5

Tracing high energy radiation with molecular lines near deeply embedded protostars

**ABSTRACT:** Submillimeter lines of CN, NO, CO$^+$ and SO$^+$, and upper limits on SH$^+$ and N$_2$O are observed with the James Clerk Maxwell Telescope in two high-mass and up to nine low-mass young stellar objects. Constant fractional abundances derived from radiative transfer modeling of the line strengths are $x$(CN) $\approx$ a few $\times 10^{-11}$-$10^{-8}$, $x$(NO) $\approx$ $10^{-9}$-$10^{-8}$ and $x$(CO$^+$) $\approx$ $10^{-12}$-$10^{-10}$. SO$^+$ has abundances of a few $\times 10^{-11}$ in the high-mass objects and upper limits of $\approx 10^{-12}$-$10^{-11}$ in the low-mass sources. All abundances are up to 1–2 orders of magnitude higher if the molecular emission is assumed to originate mainly from the inner region ($\lesssim 1000$ AU) from the envelope. However, the CN abundances are well-fit with constant fractional abundances. The observed CN and SO$^+$ abundances can be explained by the influence of a central X-ray source. The observed CO$^+$ emission towards high-mass objects is best interpreted by a far ultraviolet (FUV) field irradiating the outflow walls on scales comparable to the observing beam. Chemical models show, however, that FUV fields efficiently produce CO$^+$ only for $T \gtrsim 300$ K. The CO$^+$ emission in low-mass objects is therefore thought to trace an X-ray enhanced region close to the protostar ($r \lesssim 500$ AU). Gas-phase chemical models produce more NO compared to observations, suggesting that NO is frozen out in the cooler outer part of the envelope. It is concluded that the observed CN, CO$^+$ and SO$^+$ abundances can only be explained with either enhanced X-rays or FUV fields from the central source. High-mass

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sources are predicted to have low opacity regions that allow the FUV photons to reach large distances from the central source. X-rays are suggested to be more effective than FUV fields in the low-mass sources. The observed abundances imply X-ray fluxes for the Class 0 objects at similar levels as observed from Class I protostars with \( L_X \approx 10^{29} - 10^{31} \text{ erg s}^{-1} \).

5.1 Introduction

The earliest phase of star-formation can only be probed through observations of molecular lines and dust continuum at (sub)millimeter and infrared wavelengths. Comparison of observations with detailed chemical models can put constraints on, for example, the ionization rate of the gas around young stellar objects (YSOs; e.g., Doty et al. 2004). Understanding the chemistry in these regions is therefore essential to gain knowledge of the physical processes involved at this stage.

The density and temperature distribution in envelopes around protostars can be derived by modeling the observed dust continuum. The chemical structure of the envelopes is constrained by molecular line observations, both in emission and absorption. To obtain molecular abundances, radiative transfer and line fluxes are calculated and compared to observations until agreement is found. This approach has been used successfully in high-mass (e.g., van der Tak et al. 2000a; Boonman et al. 2003b) as well as in low-mass YSOs (e.g., Schöier et al. 2002; Jørgensen et al. 2004).

The density distribution can also be taken as a starting point for a full chemical model of the envelope. The molecular abundances are calculated in a large chemical network as a function of density, temperature and radial position from the source. The models can then be used to determine the cosmic-ray ionization rate or to constrain the chemical time when compared to a large set of observations (e.g., Ceccarelli et al. 1996; Doty et al. 2002, 2004). In this way, Doty et al. (2004) found that an additional source of ionization was required for the low-mass Class 0 YSO IRAS 16293-2422, since the observations could only be interpreted with an unusually high cosmic-ray ionization rate. It was shown by Stäuber et al. (2004a, 2005), that FUV fields and X-rays from the central source provide supplementary ionizations and influence the chemistry of the inner envelope. These spherically symmetric envelope models
generally improved the model fits to observations. FUV fields were found to affect only the chemistry in the innermost part of the envelope whereas X-rays penetrate deeper into the cloud due to the small cross sections at higher energies. X-rays can easily dominate over cosmic rays in terms of ionization rates in the inner part of the envelope.

It is still an open question, whether the youngest low-mass objects (Class 0 YSOs) emit X-rays (e.g., Hamaguchi et al. 2005a; Forbrich et al. 2006). High optical depths ($A_V > 150$) prevent possible X-rays from the young protostar to penetrate the surrounding envelope. X-ray luminosities observed towards more evolved objects are typically between $L_x \approx 10^{28} - 10^{31} \text{erg s}^{-1}$ in the 0.5–6 keV band with a thermal spectrum 0.6–7 keV (e.g., Imanishi et al. 2001, Preibisch et al. 2005). High X-ray luminosities with hard spectra are also observed towards high-mass YSOs (e.g., Hofner et al. 2002). The X-ray luminosities typically observed towards low and high-mass sources are of the same order whereas the FUV fields from high-mass objects are expected to be much higher due to their higher stellar temperature. The amount of FUV photons emitted by young low-mass protostars is poorly known (e.g., Bergin et al. 2003). However, if the deeply embedded sources emit X-rays or FUV photons, the radiation might be traced by an enhanced chemistry. This is the goal of our investigation.

We present single-dish observations of molecular lines towards a sample of both low and high-mass YSOs (Sect. 5.2). The observed molecules are radicals and ions that are predicted to be enhanced by X-rays and FUV fields (Stäuber et al. 2004a, 2005). To sample the dense inner region of the envelope rather than the outer part or large scale outflow material, the lines are chosen to have high critical densities ($n_{H_2} \approx 10^6 - 10^7 \text{cm}^{-3}$). The source sample is mainly based on the studies of Jørgensen et al. (2004) with focus on Class 0 objects for the low-mass sources and van der Tak et al. (2000a) for the young high-mass objects. The FU Orionis source V1057 Cyg has been added to this list since it shows surprising emission of ionized nitrogen at 122 µm which might be another indicator of energetic radiation (Lorenzetti et al. 2000). The observations are presented and discussed in Sect. 5.3. Radiative transfer is calculated to determine the molecular abundances in Sect. 5.4. To put constraints on the X-ray or FUV flux, gas density and temperature, the molecular abundances are calculated as a function of these parameters. The observations are compared to chemical models in Sect. 5.5. The results are discussed
with focus on the inner source of radiation in Sect. 5.6. Other possible processes, such as shock chemistry, are not considered.

5.2 Observations

Heterodyne observations were carried out using the James Clerk Maxwell Telescope (JCMT) on Mauna Kea, Hawaii\(^1\) between August 2003 and December 2005. The B3 receiver at 315–370 GHz was used with the digital autocorrelation spectrometer (DAS) in setups with bandwidths ranging from 125 MHz to 250 MHz. The main-beam efficiency was \(\eta_{MB} = 0.63\) and the half-power beam width (HPBW) \(\approx 14''\). The observed molecules and frequencies are listed in Table 5.1, the sources in Table 5.2. The CN lines as well as the two CO\(^+\) lines were observed simultaneously in the upper and lower sideband, respectively. On source integration time was generally in the range of 1–3 hours and 10 hours for CO\(^+\) in N1333–I2. The data were converted to the main-beam antenna temperature scale and analyzed with the CLASS software. The final spectra have a resolution of \(\approx 0.27–0.55\) km s\(^{-1}\) and rms noise levels between \(\approx 11–50\) mK.

To derive the envelope structure of the FU Orionis object V1057 Cyg, continuum maps at 450 \(\mu\)m and 850 \(\mu\)m were obtained with the Submillimeter-User Bolometer Array (SCUBA) on the JCMT. The HPBW of SCUBA is \(\approx 8''\) at 450 \(\mu\)m and \(\approx 14''\) at 850 \(\mu\)m. The observations were performed in March 2004 with approximately one hour integration time.

5.3 Results

5.3.1 Line spectra

The observed spectra are presented in Figs. 5.1–5.4. CN was observed and detected in all sources listed in Table 5.2. CN was previously observed in the low-mass objects by Schöier et al. (2002) and Jørgensen et

\(^1\)The JCMT is operated by the Joint Astronomy Centre on behalf of the Particle Physics and Astronomy Research Council of the United Kingdom, the Netherlands Organization for Scientific Research, and the National Research Council of Canada.
Table 5.1: Observed lines.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Line</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN\textsuperscript{a}</td>
<td>3( \frac{5}{2} ) - 2( \frac{3}{2} )</td>
<td>340.035</td>
</tr>
<tr>
<td></td>
<td>3( \frac{7}{2} ) - 2( \frac{5}{2} )</td>
<td>340.247</td>
</tr>
<tr>
<td>NO</td>
<td>7( \frac{9}{2} ) - 5( \frac{7}{2} )</td>
<td>351.043</td>
</tr>
<tr>
<td></td>
<td>7( \frac{7}{2} ) - 5( \frac{5}{2} )</td>
<td>351.051</td>
</tr>
<tr>
<td>N\textsubscript{2}O</td>
<td>14 - 13</td>
<td>351.668</td>
</tr>
<tr>
<td>CO\textsuperscript{+}</td>
<td>3( \frac{5}{2} ) - 2( \frac{3}{2} )</td>
<td>353.741</td>
</tr>
<tr>
<td></td>
<td>3( \frac{7}{2} ) - 2( \frac{5}{2} )</td>
<td>354.014</td>
</tr>
<tr>
<td>SO\textsuperscript{+}</td>
<td>15( \frac{13}{2} )</td>
<td>347.740</td>
</tr>
<tr>
<td>SH\textsuperscript{+}</td>
<td>1( \frac{3}{2} ) - 0( \frac{1}{2} )</td>
<td>345.930</td>
</tr>
</tbody>
</table>

\textsuperscript{a} Hyperfine splitting observed.

al. (2004). Current data, however, have higher signal to noise ratios to detect weaker hyperfine components that allow to determine the optical depth. NO was observed and detected in both high-mass sources as well as in N1333–I2 and N1333–I4A. CO\textsuperscript{+} was observed towards all sources except L1489 but only detected in the high-mass sources, in IRAS 16293–2422 and in N1333–I2. SO\textsuperscript{+} was observed in all sources except in L483 and L1489 but only detected in the high-mass sources and tentatively in IRAS 16293–2422. The observed lines are all fairly Gaussian with no or only weak outflow components. No signs of shocks are seen in any of the lines. Line intensities and line widths were calculated by fitting a Gaussian to each line. The results are presented in the Tables 5.3–5.5. The lines are relatively narrow and are not broadened due to, for example, inflow motion in the inner region (e.g., van der Tak 2003). The lines could trace the static envelope or arise in a thin layer of gas. Such a gas layer, however, would have to be centered at the cloud velocity, since the lines are not shifted from the local standard of rest velocity of the corresponding source. Thin gas layers could exist close to the outflow cavity walls that are irradiated from the central source or in upper disk layers (see also Sect. 5.6). The influence of an outer FUV enhanced region can be excluded due to the high critical densities of the observed transitions.
and previous model results by Stäuber et al. (2004a, 2005).

In the case of non-detections, $3\sigma$ upper limits are given ($1\sigma = 1.2\sqrt{\delta V \Delta V \sigma_{\text{rms}}}$, where $\Delta V$ is the expected line width, $\delta V$ the channel width and $\sigma_{\text{rms}}$ is the rms noise in the observed spectra, Jørgensen et al. 2004). The calibration uncertainty is taken to be 20%. N$_2$O at 351.668 GHz was observed in W3 IRS5 and N1333–I2 but not detected. A $3\sigma$ upper limit of 0.06 K km s$^{-1}$ is derived for W3 IRS5 and N1333–I2. SH$^+$ was searched for in AFGL 2591 at 345.930 GHz. Unfortunately the line is blended with a $^{34}$SO$_2$ line at 345.929 GHz. The upper limit derived for SH$^+$ will be discussed in Sect. 5.3.1. Judging from the Tables 5.3–5.5, V1057 Cyg does not appear to be unusual in its chemistry in spite of its strong [NII] emission.
Table 5.2: Sample of sources.

<table>
<thead>
<tr>
<th>Source</th>
<th>RA (J2000) (hh mm ss)</th>
<th>Dec (J2000) (dd mm ss)</th>
<th>$V_{\text{LSR}}$ (km/s)</th>
<th>$L_{\text{bol}}$ ($L_\odot$)</th>
<th>Distance (pc)</th>
<th>$M_{\text{env}}$ (M_\odot)</th>
<th>$r_{\text{env}}$ (AU)</th>
<th>$N(H_2)$ (10^{23} cm^{-2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFGL 2591$^a$</td>
<td>20 29 24.7</td>
<td>+ 40 11 19</td>
<td>-5.5</td>
<td>$2 \times 10^4$</td>
<td>1000</td>
<td>44</td>
<td>27000</td>
<td>1.0</td>
</tr>
<tr>
<td>W3 IRS5$^a$</td>
<td>02 25 40.6</td>
<td>+ 62 05 51</td>
<td>-39.0</td>
<td>$1.7 \times 10^5$</td>
<td>2200</td>
<td>262</td>
<td>60000</td>
<td>6.6</td>
</tr>
<tr>
<td>IRAS 16293–2422$^b$</td>
<td>16 32 22.8</td>
<td>− 24 28 33</td>
<td>4.0</td>
<td>27</td>
<td>160</td>
<td>5.4</td>
<td>8000</td>
<td>16.0</td>
</tr>
<tr>
<td>N1333-I2$^c$</td>
<td>03 28 55.4</td>
<td>+ 31 14 35</td>
<td>7.0</td>
<td>16</td>
<td>220</td>
<td>1.7</td>
<td>21000</td>
<td>5.5</td>
</tr>
<tr>
<td>N1333-I4A$^c$</td>
<td>03 29 10.3</td>
<td>+ 31 13 31</td>
<td>7.0</td>
<td>6</td>
<td>220</td>
<td>2.3</td>
<td>24000</td>
<td>22.0</td>
</tr>
<tr>
<td>L1448-C$^c$</td>
<td>03 25 38.8</td>
<td>+ 30 44 05</td>
<td>5.0</td>
<td>5</td>
<td>220</td>
<td>0.93</td>
<td>15000</td>
<td>1.7</td>
</tr>
<tr>
<td>L483$^c$</td>
<td>18 17 29.8</td>
<td>− 04 39 38</td>
<td>5.2</td>
<td>9</td>
<td>200</td>
<td>1.1</td>
<td>32000</td>
<td>9.3</td>
</tr>
<tr>
<td>L723$^c$</td>
<td>19 17 53.7</td>
<td>+ 19 12 20</td>
<td>11.2</td>
<td>3</td>
<td>300</td>
<td>0.62</td>
<td>21000</td>
<td>3.4</td>
</tr>
<tr>
<td>SMM4$^d$</td>
<td>18 29 56.7</td>
<td>+ 01 13 15</td>
<td>7.9</td>
<td>11</td>
<td>250</td>
<td>5.8</td>
<td>9300</td>
<td>12.0</td>
</tr>
<tr>
<td>V1057 Cyg$^e$</td>
<td>20 58 53.7</td>
<td>+ 44 15 28</td>
<td>4.1</td>
<td>70</td>
<td>650</td>
<td>1.4</td>
<td>15000</td>
<td>0.5</td>
</tr>
<tr>
<td>L1489$^e$</td>
<td>04 04 43.0</td>
<td>+ 26 18 57</td>
<td>7.0</td>
<td>3.7</td>
<td>140</td>
<td>0.097</td>
<td>9400</td>
<td>1.0</td>
</tr>
</tbody>
</table>

The luminosity and envelope parameters are from $^a$ van der Tak et al. (1999, 2000a); $^b$ Schöier et al. (2002); $^c$ Jørgensen et al. (2002); $^d$ Pontoppidan et al. (2004); $^e$ this paper.

The H$_2$ column densities are radially integrated densities from the power-law envelope profiles ($N(H_2) = \int n(r) dr$).
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Figure 5.1: CN and NO $J = 3 - 2$ transitions for the high-mass sources. The first row shows the CN $3 \frac{5}{2} - 2 \frac{3}{2}$ hyperfine transitions around 340.035 GHz. The CN $3 \frac{7}{2} - 2 \frac{5}{2}$ lines around 340.247 GHz are presented in the second row. The NO lines are in the third row. The dotted lines indicate the $V_{LSR}$ position.

CN and NO

The CN lines in the high-mass sources (Fig. 5.1) look similar with almost identical main-beam temperatures and line widths (Tables 5.3 and 5.4). The strongest CN lines in W3 IRS5 show wings which indicate that some CN is at a different velocity, probably due to outflows.

The CN lines of the low-mass sources are presented in Figs. 5.2 and 5.3. The strongest CN lines among the low-mass sources are found in L483. The weakest lines are those of the Class I object L1489. The CN lines in SMM4 have blue shifted wings that may be due to outflows (e.g., Hogerheijde et al. 1999). The low-mass sources IRAS16293-2422 and L1489 have double-peaked line profiles (Fig. 5.2). A large rotating disk may cause the profile in L1489 (Hogerheijde et al. 2001) whereas selfabsorption effects may occur in IRAS 16293–2422 (e.g., van Dishoeck et al. 1995). A velocity structure in the envelope, however, could also lead to a double-peak. The line fluxes in these cases are calculated by summing the individual components.

The hyperfine structure of the CN lines allows to calculate the optical depth of these lines with the HFS method described within CLASS. The
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**Figure 5.2:** CN $3 \frac{5}{2} - 2 \frac{3}{2}$ hyperfine lines (340.035 GHz) for the low-mass sources. The spectrum of L1489 was multiplied by a factor of 5. The dotted lines indicate the $V_{LSR}$ position.

**Figure 5.3:** CN $3 \frac{7}{2} - 2 \frac{5}{2}$ hyperfine lines (340.247 GHz) for the low-mass sources. The spectrum of L1489 was multiplied by a factor of 5. The dotted lines indicate the $V_{LSR}$ position.
method assumes the same excitation temperature and line width for all components of the multiplet. The derived optical depths $\tau$ of CN are given in Tables 5.3 and 5.4. None of the CN lines appear to be highly optically thick since $\tau$ is $< 1$ for all lines.

The NO main-beam temperatures are $\approx 10\times$ lower than those of the strongest CN lines. The lines are presented in Fig. 5.1 for the high-mass objects and in Fig. 5.4 for the two N1333 sources.

**CO$^+$ and SO$^+$**

CO$^+$ is detected for the first time towards AFGL 2591, W3 IRS5 and N1333–I2. Previously, CO$^+$ has been observed towards PDRs, planetary nebulae (e.g., Latter et al. 1993; Fuente et al. 2003; Savage & Ziurys 2004) and tentatively towards the low-mass YSO IRAS16293–2422 (Ceccarelli et al. 1998). The CO$^+$ line at 353.741 GHz detected towards IRAS16293–2422 is surprisingly strong and has a similar peak temperature as the lines in the high-mass objects. The CO$^+$ profile at 354.014 GHz is found to be double-peaked similar to CN (Fig. 5.6). The detection of CO$^+$ at 353.741 GHz towards N1333–I2 is at the $3\sigma$ level with a main-beam temperature $T_{MB} = 0.04$ K. The line flux is even at $6\sigma$ (Table 5.5). However, the 354.014 GHz line is not seen in the spectrum and CO$^+$ is thus only tentatively detected towards N1333–I2. The 353.7/354.0 line ratio is estimated to be $\approx 0.8 - 1.2$ from radiative transfer calculations. The line at 353.7 GHz appears to be $\approx 2 - 3$ times stronger though in all observations, which could be due to different excitation mechanisms (Sect. 5.4.3). Another possibility is that the line at 353.741 GHz is blended with an unidentified line. The CO$^+$ spectra at
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**Figure 5.5:** CO\(^+\) and SO\(^+\) \(J = 3 - 2\) transitions for the high-mass sources. The CO\(^+\) \(J = 3 \frac{5}{2} - 2 \frac{3}{2}\) lines (353.741 GHz) are presented in the first row. The CO\(^+\) \(J = 3 \frac{7}{2} - 2 \frac{5}{2}\) (354.014 GHz) transitions are shown in the second row. SO\(^+\) is given in the third row. The SO\(^+\) spectrum of AFGL 2591 was multiplied by a factor of 9. The dotted lines indicate the \(V_{\text{LSR}}\) position.

**Figure 5.6:** CO\(^+\) IRAS 16293-2422 and N1333-I2. The N1333-I2 spectra are multiplied by a factor of 3. The \(J = 3 - 2\) transitions at 353.741 GHz are presented in the upper row, those at 354.014 GHz in the lower row. The features seen to the right of the CO\(^+\) lines are unidentified lines (see text). The dotted lines indicate the \(V_{\text{LSR}}\) position.
353.741 GHz of AFGL 2591, IRAS 16293–2422 and N1333–I2 show one or several lines at $\approx 353.730$ GHz. The lines could be due to emission of C$_3$H at 353.731 GHz and 353.733 GHz and CH$_3$OOH at 353.736 GHz. These features, however, are not seen in the spectrum of W3 IRS5, where the CO$^+$ 353.7/354.0 line ratio is also $\approx 2$. In addition, the observed sources are not extremely rich in complex molecules (no line confusion; e.g., Helmich & van Dishoeck 1997). The lines are therefore assumed to be real in the following sections.

The SO$^+$ line in W3 IRS5 is $\approx 9$ times as strong as that in AFGL 2591 (Fig. 5.5). This is most probably due to the unusually high sulphur abundance found in W3 IRS5 (e.g., van der Tak et al. 2003). When SO$^+$ was first detected towards the supernova remnant IC443 (Turner 1992), it was proposed as a tracer of dissociative shocks. When later surveys, however, showed large amounts of SO$^+$ towards dark clouds and star forming regions, it was suggested that SO$^+$ is not associated to shocks (Turner 1994). Indeed, the line profiles of the observed SO$^+$ lines do not indicate signs of shocked gas (Fig. 5.5). In the low-mass sample, SO$^+$ is tentatively detected towards IRAS16293–2422 (Fig. 5.7). Assuming the lines to be doubly peaked as is the case for CN and CO$^+$, the integrated SO$^+$ line fluxes are 0.08 K km s$^{-1}$ and 0.09 K km s$^{-1}$, corresponding to $\approx 4\sigma$ detections. Nevertheless, the lines are treated as upper limits due to the noisy spectrum (Table 5.5).

**SH$^+$**

SH$^+$ was searched for at 345.930 GHz (Savage et al. 2004) towards AFGL 2591. Unfortunately, the line is blended with the $^{34}$SO$_2$ ($J = 19_{1,18} - 18_{0,18}$)
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Figure 5.8: Spectrum at 345.930 GHz. The two dotted vertical lines indicate the frequencies 345.930 GHz (SH\(^+\)) and 345.929 GHz (\(^{34}\)SO\(_2\)), respectively, at the \(V_{\text{LSR}}\) of the source. The spectrum is overlaid with a Gaussian fit to be viewed as an upper limit for SH\(^+\).

A line at 345.929 GHz. Van der Tak et al. (2003) observed line fluxes between 1.0–1.2 K km s\(^{-1}\) for \(^{34}\)SO\(_2\) with line widths between 3.5–4.5 km s\(^{-1}\). A Gaussian fit of the observed \(^{34}\)SO\(_2\) line at 345.930 GHz leads to a line width \(\Delta V = 3.8 \text{ km s}^{-1}\) and an integrated flux of 0.5 K km s\(^{-1}\). The values of the line flux and width are well in the range of those observed for other \(^{34}\)SO\(_2\) transitions by van der Tak et al. (2003). Motivated by the fact that the two lines seen in Fig. 5.8 are exactly at 345.930 GHz and 345.929 GHz, an upper limit for the line flux of SH\(^+\) can be obtained by assuming the lines to be SH\(^+\) and \(^{34}\)SO\(_2\), respectively. The width of the SH\(^+\) line is assumed to be 1.5 km s\(^{-1}\). This might be too small but larger widths lead to poorer line fits. The Gaussian fit gives an integrated intensity of 0.23 K km s\(^{-1}\) for SH\(^+\) as an upper limit for AFGL 2591. It should be mentioned though, that SH\(^+\) has never been observed in the interstellar medium. A clear identification of the molecule therefore requires detections of at least two different transitions. This might be possible with the future Herschel Space Observatory, since the higher lying lines of SH\(^+\) are not detectable with ground based telescopes (Savage et al. 2004).
Table 5.3: Observed line fluxes ($F = \int T_{MB} \, dV$ in K km s$^{-1}$), line widths ($\Delta V$ in km s$^{-1}$) and opacities for the CN $3 \frac{5}{2} - 2 \frac{3}{2}$ transitions. The frequencies are given in GHz. Upper limits are at 3σ in line flux.

<table>
<thead>
<tr>
<th>Source</th>
<th>340.035</th>
<th></th>
<th>340.031</th>
<th></th>
<th>340.019</th>
<th></th>
<th>340.008</th>
<th></th>
</tr>
</thead>
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<tr>
<td></td>
<td>$F$</td>
<td>$\Delta V$</td>
<td>$\tau$</td>
<td>$F$</td>
<td>$\Delta V$</td>
<td>$\tau$</td>
<td>$F$</td>
<td>$\Delta V$</td>
</tr>
<tr>
<td>AFGL 2591</td>
<td>7.71</td>
<td>8.39</td>
<td>2.7</td>
<td>0.27</td>
<td>1.40</td>
<td>2.7</td>
<td>0.05</td>
<td>1.49</td>
</tr>
<tr>
<td>W3 IRS 5</td>
<td>8.34</td>
<td>9.04</td>
<td>3.1</td>
<td>0.27</td>
<td>1.52</td>
<td>3.1</td>
<td>0.05</td>
<td>1.36</td>
</tr>
<tr>
<td>IRAS 16293</td>
<td>1.14</td>
<td>0.92</td>
<td>1.0</td>
<td>0.53</td>
<td>0.12</td>
<td>1.0</td>
<td>0.10</td>
<td>&lt;0.06</td>
</tr>
<tr>
<td>N1333-12</td>
<td>0.61</td>
<td>0.59</td>
<td>1.0</td>
<td>0.06</td>
<td>0.16</td>
<td>0.8</td>
<td>0.02</td>
<td>&lt;0.10</td>
</tr>
<tr>
<td>N1333-14A</td>
<td>0.38</td>
<td>0.31</td>
<td>0.9</td>
<td>0.08</td>
<td>&lt;0.09</td>
<td>...</td>
<td>...</td>
<td>&lt;0.09</td>
</tr>
<tr>
<td>L1448-C</td>
<td>0.46</td>
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<td>0.06</td>
</tr>
<tr>
<td>L483</td>
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<td>1.28</td>
<td>1.3</td>
<td>0.09</td>
<td>0.19</td>
<td>1.2</td>
<td>0.01</td>
<td>0.29</td>
</tr>
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<td>0.40</td>
<td>1.3</td>
<td>0.03</td>
<td>&lt;0.06</td>
<td>...</td>
<td>...</td>
<td>&lt;0.06</td>
</tr>
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<td>0.22</td>
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<tr>
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<td>&lt;0.07</td>
<td>...</td>
<td>...</td>
<td>&lt;0.07</td>
</tr>
<tr>
<td>L1489</td>
<td>0.28</td>
<td>0.21</td>
<td>1.1</td>
<td>0.01</td>
<td>&lt;0.07</td>
<td>...</td>
<td>...</td>
<td>&lt;0.07</td>
</tr>
</tbody>
</table>
Table 5.4: Observed line fluxes \( F = \int T_{MB} dV \) in K km s\(^{-1}\), line widths \( \Delta V \) in km s\(^{-1}\) and opacities for the CN 3 \( \frac{7}{2} \) - 2 \( \frac{5}{2} \) transitions. The frequencies are given in GHz. Upper limits are at 3\( \sigma \) in line flux.

<table>
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<tr>
<th>Source</th>
<th>F (1.59)</th>
<th>( \Delta V ) (2.6)</th>
<th>( \tau ) (0.06)</th>
<th>F (1.36)</th>
<th>( \Delta V ) (2.7)</th>
<th>( \tau ) (0.05)</th>
<th>F (19.21)</th>
<th>( \Delta V ) (3.3)</th>
<th>( \tau ) (0.55)</th>
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</thead>
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<tr>
<td>AFGL 2591</td>
<td>1.59</td>
<td>2.6</td>
<td>0.06</td>
<td>1.36</td>
<td>2.7</td>
<td>0.05</td>
<td>19.21</td>
<td>3.3</td>
<td>0.55</td>
</tr>
<tr>
<td>W3 IRS 5</td>
<td>1.66</td>
<td>2.6</td>
<td>0.06</td>
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<td>20.68</td>
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<td>N1333-I2</td>
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<td>...</td>
</tr>
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<td>1.28</td>
<td>1.4</td>
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</tr>
<tr>
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<td>1.1</td>
<td>0.02</td>
<td>0.15</td>
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<td>0.01</td>
<td>2.78</td>
<td>1.7</td>
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<td>...</td>
<td>&lt;0.06</td>
<td>...</td>
<td>...</td>
<td>1.03</td>
<td>1.7</td>
<td>...</td>
</tr>
<tr>
<td>SMM4</td>
<td>0.23</td>
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<td>0.01</td>
<td>0.22</td>
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<td>0.01</td>
<td>2.86</td>
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<td>V1057 Cyg</td>
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<td>...</td>
<td>&lt;0.07</td>
<td>...</td>
<td>...</td>
<td>0.85</td>
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<td>...</td>
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<td>...</td>
<td>&lt;0.07</td>
<td>...</td>
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<td>0.72</td>
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<td>...</td>
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</table>
Chapter 5. Tracing high energy radiation

<table>
<thead>
<tr>
<th>Source</th>
<th>NO</th>
<th>CO⁺</th>
<th>NO</th>
<th>CO⁺</th>
<th>NO</th>
<th>CO⁺</th>
</tr>
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<tr>
<td></td>
<td>351.043</td>
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<td>353.741</td>
<td>354.014</td>
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<td>0.13</td>
<td>0.99</td>
<td>0.13</td>
</tr>
<tr>
<td>W3 IRS 5</td>
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<td>2.21</td>
<td>1.79</td>
<td>1.79</td>
</tr>
<tr>
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<td>1.10</td>
<td>1.10</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>N1333-12</td>
<td>0.13</td>
<td>0.13</td>
<td>0.24</td>
<td>0.24</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>L1448-C</td>
<td>0.13</td>
<td>0.13</td>
<td>0.24</td>
<td>0.24</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>L483</td>
<td>0.13</td>
<td>0.13</td>
<td>0.24</td>
<td>0.24</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>L723</td>
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<td>0.24</td>
<td>0.24</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>SM4</td>
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<td>0.24</td>
<td>0.24</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>V1057 Cyg</td>
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<td>0.13</td>
<td>0.24</td>
<td>0.24</td>
<td>0.13</td>
<td>0.13</td>
</tr>
</tbody>
</table>

Table 5.5: Observed line fluxes (in K km s⁻¹) and line widths (ΔV in kHz) for the NO, CO⁺ and SO⁺ transitions. The frequencies are given in GHz. Upper limits are at 3σ in line flux.
5.4 Molecular abundances

5.3.2 Continuum observations of V1057

The peak flux densities observed towards V1057 with SCUBA are 2.0 and 0.35 Jy beam$^{-1}$ at 450 and 850 μm, respectively. The result for 850 μm is comparable to the observations of Sandell & Weintraub (2001), who studied this source in detail.

V1057 was not included in the source sample of Jørgensen et al. (2002). A model is thus constructed for the envelope using the same approach reproducing SCUBA maps at 450 μm and 850 μm and the SED from 25 μm–850 μm from the literature (in particular, ISOPHOT measurements of Abraham et al. 2004). The V1057 envelope is found to be well-fit by a power-law density profile $n \propto r^{-p}$ with $p=1.3$ and $n_{H_2}(1000\text{AU}) = 2.9 \times 10^5 \text{cm}^{-3}$ for radii of 10 AU to 15000 AU and for a total luminosity of 70 $L_\odot$ (at a distance of 650 pc). Previously Kenyon & Hartmann (1991) modeled the SED of V1057 focusing primarily on the IRAS measurements; their results for the V1057 envelope are found to be similar to ours. The luminosity, envelope mass, $H_2$ column density and approximate size of the envelope (radius) are presented in Table 5.2.

5.4 Molecular abundances

5.4.1 Constant abundance models

In order to estimate molecular abundances, a radiative transfer analysis is performed by using the 1D Monte Carlo radiative transfer code by Hogerheijde & van der Tak (2000). The program solves for the molecular excitation as a function of radius. The principle input parameters of the code are the radial $H_2$ density and gas temperature distribution, which were derived from dust radiative transfer analysis described in Jørgensen et al. (2002), assuming $T_{\text{gas}} = T_{\text{dust}}$. For the high-mass sources we use the results of van der Tak et al. (1999, 2000a), for IRAS 16293–2422, the results of Schöier et al. (2002), for SMM4 we follow Pontoppidan et al. (2004), the results for V1057 Cyg are taken from Sect. 5.3.2. The parameters for all other low-mass sources are used from the studies of Jørgensen et al. (2002). The molecular abundances for the species of interest are assumed to be constant with respect to $H_2$. The result is integrated over the line of sight and convolved with a 14″ telescope beam.
Table 5.6: Inferred abundances from radiative transfer models assuming constant radial abundances.

<table>
<thead>
<tr>
<th>Source</th>
<th>CN</th>
<th>NO</th>
<th>CO⁺</th>
<th>SO⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFGL 2591</td>
<td>$2.3 \times 10^{-08}$</td>
<td>$3.1 \times 10^{-08}$</td>
<td>$1.6 \times 10^{-10}$</td>
<td>$5.8 \times 10^{-11}$</td>
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<tr>
<td>W3 IRS 5</td>
<td>$3.6 \times 10^{-09}$</td>
<td>$1.7 \times 10^{-08}$</td>
<td>$3.9 \times 10^{-11}$</td>
<td>$7.0 \times 10^{-11}$</td>
</tr>
<tr>
<td>IRAS 16293</td>
<td>$5.4 \times 10^{-11}$</td>
<td>...</td>
<td>$1.5 \times 10^{-12}$</td>
<td>$&lt; 3.0 \times 10^{-12}$</td>
</tr>
<tr>
<td>N1333-I2</td>
<td>$3.9 \times 10^{-10}$</td>
<td>$2.5 \times 10^{-09}$</td>
<td>$&lt; 7.5 \times 10^{-12}$</td>
<td>$&lt; 5.0 \times 10^{-12}$</td>
</tr>
<tr>
<td>N1333-I4A</td>
<td>$4.2 \times 10^{-11}$</td>
<td>$1.5 \times 10^{-09}$</td>
<td>$&lt; 1.3 \times 10^{-12}$</td>
<td>$&lt; 2.2 \times 10^{-12}$</td>
</tr>
<tr>
<td>L1448-C</td>
<td>$1.1 \times 10^{-09}$</td>
<td>...</td>
<td>$&lt; 2.0 \times 10^{-11}$</td>
<td>$&lt; 1.4 \times 10^{-11}$</td>
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<tr>
<td>L483</td>
<td>$1.5 \times 10^{-09}$</td>
<td>...</td>
<td>$&lt; 7.0 \times 10^{-12}$</td>
<td>...</td>
</tr>
<tr>
<td>L723</td>
<td>$9.2 \times 10^{-10}$</td>
<td>...</td>
<td>$&lt; 2.0 \times 10^{-11}$</td>
<td>$&lt; 4.3 \times 10^{-11}$</td>
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<tr>
<td>SMM4</td>
<td>$1.6 \times 10^{-10}$</td>
<td>...</td>
<td>$&lt; 1.0 \times 10^{-12}$</td>
<td>$&lt; 4.0 \times 10^{-12}$</td>
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<tr>
<td>V1057 Cyg</td>
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<td>...</td>
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<td>$&lt; 5.0 \times 10^{-11}$</td>
</tr>
<tr>
<td>L1489</td>
<td>$2.5 \times 10^{-09}$</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

Observed and synthetic line fluxes are then compared with a $\chi^2$ statistic to find the best-fit abundance. The individual hyperfine components of CN are modeled as separate lines and the integrated line fluxes are summed in case of overlapping lines (e.g., CN $3 \frac{7}{2} - 2 \frac{5}{2}$ and CN $3 \frac{9}{2} - 2 \frac{7}{2}$). The collisional rate coefficients for CN are obtained by scaling the coefficients of CO (Green & Chapman 1978). Estimates by Black (2004, private communication) are used for the CO⁺ coefficients. Molecules for which no collision rates are available (NO, N₂O, SO⁺ and SH⁺), the excitation is assumed to be thermalized at the temperature of each grid point of the model.

Table 5.6 lists the inferred abundances for CN, NO, CO⁺ and SO⁺. The upper limits for CO⁺ and SO⁺ correspond to $3\sigma$ in line flux (Table 5.5). Our CN abundances are consistent within a factor of two to those found by Jørgensen et al. (2004) and Schöier et al. (2002) for the same sources. CN was also observed by Helmich & van Dishoeck (1997) towards W3 IRS5. They derived a fractional abundance of $6.9 \times 10^{-10}$ for CN, which is $\approx 5$ times lower than ours. This is most probably due to the different methods used to derive the molecular abundance (radiative transfer modeling vs. escape probability method). The reduced $\chi^2$ values from 3 to 7 different CN transitions per source (see Tables 5.3 and 5.4) are $\lesssim 1$, indicating that the constant abundance models fit the observations.
well. The same is true for NO. In the case of CO$^+$, $\chi^2$ is between 1–2 for all sources. However, the number of lines are two at most for CO$^+$ and NO, providing rather poor statistics.

NO was first observed by Liszt & Turner (1978) towards the molecular cloud Sgr B2. They reported a fractional abundance of $\approx 10^{-8}$. Similar abundances were derived by Ziurys et al. (1991) towards other star-forming clouds. Our observed NO abundances towards the high-mass and the N1333 sources (Table 5.6) are comparable to these values.

For N$_2$O, an upper limit of $x(N_2O) \lesssim 5 \times 10^{-10}$ is derived for W3 IRS5 and $x(N_2O) \lesssim 7 \times 10^{-9}$ for N1333–I2. The relatively high upper limits are due to the rather low Einstein spontaneous transition coefficient for the observed emission ($A_{ul} \approx 6.3 \times 10^{-6}$ s$^{-1}$). The upper limit for SH$^+$ in AFGL 2591 is estimated to be $x$(SH$^+$) $\lesssim 4.1 \times 10^{-11}$.

SO$^+$ in W3 IRS5 was observed by Turner (1994) and Helmich & van Dishoeck (1997). Our derived fractional SO$^+$ abundance differs by only a factor of 2.7 compared to the results of Turner (1994). No SO$^+$ abundances were reported by Helmich & van Dishoeck (1997). Ceccarelli et al. (1998) inferred a CO$^+$ column density $N$(CO$^+$) $\approx 10^{11}$–$10^{12}$ cm$^{-2}$ - depending on the size of the CO$^+$ emitting region - from spectrally unresolved ISO observations towards IRAS 16293–2422 in a 90$''$ beam. Our observed column densities toward the low-mass sources are $N$(CO$^+$) $\approx 10^{12}$ cm$^{-2}$ for IRAS 16293–2422 and N1333–I2.

Fractional abundances of CO$^+$ and SO$^+$ observed toward photon-dominated regions (PDRs) are usually a few times $10^{-11}$–$10^{-10}$ with column densities between $10^{12}$–$10^{13}$ cm$^{-2}$ (Fuente et al. 2003). Our abundances observed towards the high-mass sources are thus of the order of those found towards PDRs, indicating that FUV fields from the central source may be important.

5.4.2 Jump abundance models

The envelope models for AFGL 2591 (Stäuber et al. 2005) suggest a jump in abundance for molecules like, for example, CO$^+$ and SO$^+$ at $T = 100$ K where water and H$_2$S evaporate into the gas-phase. The abundances can be several orders of magnitude higher in the inner hot region of the envelope due to the influence of the enhanced water and sulphur abundances. The CN, NO, CO$^+$ and SO$^+$ abundances towards AFGL 2591,
W3 IRS5 and IRAS 16293–2422 have therefore been calculated assuming
the observed molecular emission to originate mainly from the region with
$T \gtrsim 100$ K. Low and high-$J$ CN observations by Jørgensen et al. (2004)
towards a large sample of low-mass YSOs suggest, however, that CN has
constant abundances, or in some sources even larger abundances in the
outer part of the envelope. Also, our CN lines are in general well-fit with
constant abundances (Sect. 5.4.1). Nevertheless, we also calculate the
CN abundance assuming a jump at $T = 100$ K. This could happen, for
example, in an X-ray or FUV illuminated disk. The outer abundances
$x_{\text{out}}$ are assumed to be $10^{-8}$ for NO, $10^{-15}$ for CO$^+$ and $10^{-13}$ for SO$^+$. For CN we assume $x_{\text{out}} = 10^{-9}$ for the high-mass sources and $x_{\text{out}} = 10^{-11}$ for IRAS 16293–2422.

An enhancement in the envelope due to the influence of X-rays is
expected within the inner $\approx 1000$ AU from the central source for $L_X \approx 10^{30}–10^{31}$ erg s$^{-1}$ (Stäuber et al. 2005). Since the attenuation of X-rays
is dominated by geometric dilution rather than absorption (Stäuber et
al. 2006a), the X-ray dominated region will be of similar size for all
sources. We therefore also calculate the abundances assuming the jump
to be at 1000 AU. The influence of a strong inner FUV field is restricted
to $A_V \lesssim 10$. This is already achieved within a few hundred AU in the
high-mass envelopes and a few AU in the low-mass objects. Although
high-$J$ lines are sensitive to even such a small region, the produced line
fluxes are too small to account for the observed ones (see also Stäuber et
al. 2004a).

The inner abundances $x_{100\text{K}}$ and $x_{\text{XDR}}$ for the models assuming a jump
at $T = 100$ K and $r = 1000$ AU, respectively, are presented in Tables 5.7
and 5.8. Also listed in the tables are the average hydrogen density and
gas temperature in the regions of interest. The jump abundances can
be more than two orders of magnitude higher compared to the constant
abundances in Table 5.6. However, the jump and constant abundance
models are statistically not distinguishable since they produce similar $\chi^2$
values so that all scenarios remain plausible.
Table 5.7: Inferred inner abundances $x_{100K}$ from jump models assuming the emission to come from the region with $T \geq 100$ K. The average temperature $T_{av}$, hydrogen density $n_{H,av}$ and size (radius) of the inner 100 K region are also given.

<table>
<thead>
<tr>
<th>Source</th>
<th>$T_{av}$ (K)</th>
<th>$n_{H,av}$ (cm$^{-3}$)</th>
<th>Radius (AU)</th>
<th>CN</th>
<th>NO</th>
<th>CO$^+$</th>
<th>SO$^+$</th>
</tr>
</thead>
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<td>1100</td>
<td>$6 \times 10^{-07}$</td>
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<td>$1 \times 10^{-09}$</td>
<td>$2 \times 10^{-09}$</td>
</tr>
<tr>
<td>W3 IRS 5</td>
<td>210</td>
<td>$1 \times 10^7$</td>
<td>5400</td>
<td>$1 \times 10^{-08}$</td>
<td>$2 \times 10^{-07}$</td>
<td>$7 \times 10^{-11}$</td>
<td>$9 \times 10^{-10}$</td>
</tr>
<tr>
<td>IRAS 16293</td>
<td>160</td>
<td>$1 \times 10^9$</td>
<td>100</td>
<td>$3 \times 10^{-09}$</td>
<td>...</td>
<td>$6 \times 10^{-11}$</td>
<td>$\lesssim 1 \times 10^{-10}$</td>
</tr>
</tbody>
</table>
Table 5.8: Inferred inner abundances \( x_{\text{XDR}} \) from jump models assuming the emission to come from the X-ray dominated inner 1000 AU envelope. The average temperature \( T_{\text{av}} \) and hydrogen density \( n_{\text{H,av}} \) of the inner 1000 AU region are also given.

<table>
<thead>
<tr>
<th>Source</th>
<th>( T_{\text{av}} ) (K)</th>
<th>( n_{\text{H,av}} ) (cm(^{-3}))</th>
<th>CN</th>
<th>NO</th>
<th>CO(^+)</th>
<th>SO(^+)</th>
</tr>
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<td>( 3 \times 10^{-09} )</td>
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<td>...</td>
<td>( 2 \times 10^{-12} )</td>
<td>( &lt; 5 \times 10^{-12} )</td>
</tr>
</tbody>
</table>
5.4. Molecular abundances

5.4.3 CO⁺ anomalous excitation

A problem in the interpretation of the observed CO⁺ emission is the question of how the molecule is excited. CO⁺ reacts quickly ($\approx 10^{-9}$ cm$^3$ s$^{-1}$) with atomic or molecular hydrogen. Instead of being collisionally excited, CO⁺ is more likely to be destroyed on virtually every collision with H and H$_2$ (Black 1998). This is not the case for the other observed molecules. The reaction of SH⁺ with H$_2$, for example, is endothermic with an activation barrier of $\approx 6000$ K (Millar et al. 1986). Similar is likely to be true for SO⁺.

CO⁺ could be produced in an excited level and the observed emission may be coupled to its formation. If CO⁺ is not collisionally excited, however, the fractional abundances derived from the radiative transfer modeling do not represent those of CO⁺. The column densities are therefore calculated using the following expression that is independent of the excitation mechanism and can be obtained by simply integrating the standard radiative transfer equations assuming the line to be optically thin (Blake et al. 1987):

$$N = \frac{1.94 \times 10^5 \nu^2 Q(T_{ex})}{A_{ul}} e^{E_u/kT_{ex}} \int T_{MB} dV, \quad [\text{cm}^{-2}] \quad (5.1)$$

where $\nu$ is the line frequency in GHz, $Q(T_{ex})$ is the partition function at the excitation temperature $T_{ex}$, $A_{ul}$ is the Einstein spontaneous emission coefficient in s$^{-1}$, $E_u$ and $g_u$ are the upper energy level and statistical weight, respectively. The integrated intensity is in K km s$^{-1}$. The results are critically dependent on the excitation temperature, which we do not know. The excitation temperature derived in PDRs by Fuente et al. (2003) is $T_{ex}(\text{CO}^+) = 10$ K. Since our observed transitions are at higher frequencies with $\approx 10$ K higher upper energy levels, the excitation temperature is likely to be higher than that derived by Fuente et al. (2003). We therefore assume $T_{ex}(\text{CO}^+) = 20$ K, which is also consistent with the average excitation temperature derived from the radiative transfer models assuming constant fractional abundances. The results for the CO⁺($3 \frac{5}{2} - 2 \frac{3}{2}$) line at 353.741 GHz are presented in Table 5.9. The column densities for $T_{ex} = 10$ K are $\approx 3$ times higher and $\approx 30\%$ higher for $T_{ex} = 100$ K. They are $\approx 10$—$15\%$ lower for $T_{ex} = 30$—$50$ K. The fractional abundances are calculated using the integrated hydrogen column densities presented...
Table 5.9: Column densities $N(\text{CO}^+)$ and fractional abundances $x(\text{CO}^+)$ calculated with Eq. (5.1) assuming $T_{\text{ex}}(\text{CO}^+) = 20$ K. The upper limits correspond to $3\sigma$ in line flux.

<table>
<thead>
<tr>
<th>Source</th>
<th>$N(\text{CO}^+)$ $10^{12}$ cm$^{-2}$</th>
<th>$x(\text{CO}^+)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFGL 2591</td>
<td>1.0</td>
<td>$1.0 \times 10^{-11}$</td>
</tr>
<tr>
<td>W3 IRS 5</td>
<td>1.7</td>
<td>$2.5 \times 10^{-12}$</td>
</tr>
<tr>
<td>IRAS 16293</td>
<td>0.6</td>
<td>$3.9 \times 10^{-13}$</td>
</tr>
<tr>
<td>N1333-I2</td>
<td>0.2</td>
<td>$3.3 \times 10^{-13}$</td>
</tr>
<tr>
<td>N1333-I4A</td>
<td>&lt; 0.1</td>
<td>&lt; $6.0 \times 10^{-14}$</td>
</tr>
<tr>
<td>L1448-C</td>
<td>&lt; 0.1</td>
<td>&lt; $6.0 \times 10^{-13}$</td>
</tr>
<tr>
<td>L483</td>
<td>&lt; 0.1</td>
<td>&lt; $9.0 \times 10^{-14}$</td>
</tr>
<tr>
<td>L723</td>
<td>&lt; 0.1</td>
<td>&lt; $3.0 \times 10^{-13}$</td>
</tr>
<tr>
<td>SMM4</td>
<td>&lt; 0.1</td>
<td>&lt; $9.0 \times 10^{-14}$</td>
</tr>
<tr>
<td>V1057 Cyg</td>
<td>&lt; 0.1</td>
<td>&lt; $2.0 \times 10^{-12}$</td>
</tr>
</tbody>
</table>

in Table 5.2. $\text{H}_2$ column densities averaged over a 14" beam may be somewhat lower and the derived fractional abundances can thus be regarded as lower limits. The abundances in Table 5.9 are approximately an order of magnitude lower than those inferred from the radiative transport models (Table 5.6). In case of the low-mass YSO IRAS 16293–2422, the difference is only a factor of four.

5.5 Comparison to chemical models

In this section, we compare our observed abundances to those of chemical X-ray and FUV models. As for the case of $\text{H}_2\text{O}$ (Stäuber et al. 2006a), abundance results are presented for a general range of parameters. The general parameter study is useful because it covers the entire range of temperatures and densities expected in protostellar environments without assigning them to a specific component like the envelope, disk or dense outflows. Similarities and differences between our models and those previously published are discussed in Stäuber et al. (2004a, 2005). In particular, the presence of evaporated $\text{H}_2\text{O}$ at high abundances in the inner envelope results in different chemical characteristics compared with
traditional PDR and X-ray dominated region (XDR) models.

The initial chemical abundances for the general parameter study are listed in Table 5.10. They are taken to be the same as those in the models for IRAS 16293–2422 by Doty et al. (2004). Many species are taken to be initially frozen out onto grains in the cold part and assumed to evaporate instantaneously into the gas-phase at $T_{ev}$ (Table 5.10). However, no subsequent adsorption or desorption of gas-phase species is taken into account. The gas temperature is assumed to be coupled to the dust temperature and independent of the X-ray or FUV flux. The X-ray flux ($F_X \propto L_X r^{-2}$) is normalized in such a way that a typical protostellar X-ray luminosity of $L_X = 10^{31}$ erg s$^{-1}$ corresponds to an X-ray flux of $F_X = 1$ erg s$^{-1}$ cm$^{-2}$ at an arbitrary distance of $r \approx 56$ AU from the central star. The temperature for the thermal X-ray spectrum is assumed to be $3 \times 10^7$ K. The X-ray flux is further assumed to be attenuated by a hydrogen column density of $5 \times 10^{21}$ cm$^{-2}$. The FUV flux is varied between $G_0 = 0$–100 for $A_V = 0$.

We have also compared our inferred abundances with those of traditional dense PDR models such as those by Sternberg & Dalgarno (1995). Although such models can reproduce the abundances of selected species in narrow PDR zones, they generally underpredict the column densities.

### 5.5.1 CN

The observed constant fractional abundances are between a few $\times 10^{-11}$–$10^{-8}$ (Table 5.6) with an average abundance of $10^{-9}$ for the low-mass objects and $10^{-8}$ for the high-mass sources. The jump abundances $x_{100K}$ are between a few $\times 10^{-9}$–$10^{-7}$ (Table 5.7) and $x_{XDR}$ ranges from $8 \times 10^{-11}$ to $8 \times 10^{-7}$ (Table 5.8). Multiplying the constant fractional abundances with the H$_2$ column density (Table 5.2) for each source leads to CN column densities $N$(CN) $\approx 10^{14}$ cm$^{-2}$ for most low-mass sources and $\approx 10^{15}$ cm$^{-2}$ for the high-mass objects and the low-mass YSO L483.

For AFGL 2591, Stäuber et al. (2004a) studied the influence of FUV fields from the central source on the chemistry of the surrounding envelope, assuming a spherically symmetric geometry. They have shown that the CN abundance in the inner part of the envelope ($r \approx 200$ AU) can get as high as $x$(CN) $\approx 10^{-7}$ relative to H$_2$ even for low FUV fields ($G_0 \gtrsim 10$). The enhanced region, however, is too small to account for the observed
Table 5.10: Assumed initial abundances and cosmic-ray ionization rate for the chemical models (Figs. 5.9–5.18).

<table>
<thead>
<tr>
<th>Species</th>
<th>Initial abundance</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Initial abundances T &gt; 100 K</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H₂</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>CO</td>
<td>$2.0 \times 10^{-4}$</td>
<td>a</td>
</tr>
<tr>
<td>CO₂</td>
<td>$3.0 \times 10^{-5}$</td>
<td>b</td>
</tr>
<tr>
<td>H₂O</td>
<td>$1.5 \times 10^{-4}$</td>
<td>c</td>
</tr>
<tr>
<td>H₂S</td>
<td>$10^{-8}$</td>
<td>d</td>
</tr>
<tr>
<td>H₂CO</td>
<td>$8.0 \times 10^{-8}$</td>
<td>d</td>
</tr>
<tr>
<td>N₂</td>
<td>$7.0 \times 10^{-5}$</td>
<td>e</td>
</tr>
<tr>
<td>CH₄</td>
<td>$10^{-7}$</td>
<td>c</td>
</tr>
<tr>
<td>C₂H₄</td>
<td>$8.0 \times 10^{-8}$</td>
<td>e</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>$10^{-8}$</td>
<td>e</td>
</tr>
<tr>
<td>CH₃OH</td>
<td>$1.5 \times 10^{-7}$</td>
<td>d</td>
</tr>
<tr>
<td>O</td>
<td>0.0</td>
<td>e</td>
</tr>
<tr>
<td>S</td>
<td>0.0</td>
<td>e</td>
</tr>
<tr>
<td><strong>Initial abundances T &lt; 100 K</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H₂</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>CO</td>
<td>$2.0 \times 10^{-4}$</td>
<td>d</td>
</tr>
<tr>
<td>CO₂</td>
<td>0.0</td>
<td>f</td>
</tr>
<tr>
<td>H₂O</td>
<td>0.0</td>
<td>f</td>
</tr>
<tr>
<td>H₂S</td>
<td>0.0</td>
<td>f</td>
</tr>
<tr>
<td>N₂</td>
<td>$7.0 \times 10^{-5}$</td>
<td>e</td>
</tr>
<tr>
<td>CH₄</td>
<td>$10^{-7}$</td>
<td>e</td>
</tr>
<tr>
<td>C₂H₄</td>
<td>$8.0 \times 10^{-8}$</td>
<td>e</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>$10^{-8}$</td>
<td>e</td>
</tr>
<tr>
<td>H₂CO (60 &lt; T(K) &lt; 100)</td>
<td>$8.0 \times 10^{-8}$</td>
<td>d</td>
</tr>
<tr>
<td>H₂CO (T(K) &lt; 60)</td>
<td>0.0</td>
<td>d</td>
</tr>
<tr>
<td>CH₃OH (60 &lt; T(K) &lt; 100)</td>
<td>$1.5 \times 10^{-7}$</td>
<td>d</td>
</tr>
<tr>
<td>CH₃OH (T(K) &lt; 60)</td>
<td>0.0</td>
<td>d</td>
</tr>
<tr>
<td>O</td>
<td>$1.0^{-4}$</td>
<td>d</td>
</tr>
<tr>
<td>S</td>
<td>$6.0 \times 10^{-9}$</td>
<td>g</td>
</tr>
<tr>
<td>Cosmic-ray ionization rate $\zeta_{cr}$ (s⁻¹)</td>
<td>$0.8 \times 10^{-17}$</td>
<td>h</td>
</tr>
</tbody>
</table>

All abundances are relative to molecular hydrogen.  

- a Jørgensen et al. (2002),  
- b Boonman et al. (2003a),  
- c Boonman & van Dishoeck (2003),  
- d Doty et al. (2004),  
- e Charnley (1997),  
- f assumed to be frozen-out or absent in cold gas-phase,  
- g Doty et al. (2002),  
- h Stäuber et al. (2006a).  

Stäuber et al. (2006a).
column densities.

X-rays from the protostar may lead to \( x(CN) \approx 10^{-8} - 10^{-7} \) relative to \( H_2 \) in the inner part \( (r \approx 200 \text{AU}) \) and to \( x(CN) \approx 10^{-9} \) in the outer part of the high-mass AFGL 2591 envelope (Stäuber et al. 2005). These abundances are comparable to those observed for AFGL 2591.

The results of the general parameter study for CN are presented in Fig. 5.9 for the X-ray models and in Fig. 5.10 for different FUV fields for \( t = 5 \times 10^4 \text{yrs} \). Compared to models for \( t = 10^4 \text{yrs} \) and \( t = 10^5 \text{yrs} \), the difference in the CN abundances is minor. In general, the temperature dependence of CN is fairly small in the X-ray models for \( T \lesssim 400 \text{K} \). At higher temperatures and \( F_X < 1 \text{erg s}^{-1} \text{cm}^{-2} \), CN is destroyed by \( H_2 \), forming HCN. Models without X-rays have \( x(CN) < 10^{-10} \) for \( n_H = 10^6 - 10^8 \text{cm}^{-3} \). X-ray fluxes between \( 10^{-4} - 1 \text{erg s}^{-1} \text{cm}^{-2} \) lead to \( x(CN) \approx 10^{-10} - 10^{-7} \) – the approximate range of observed CN abundances. The \( x_{\text{XDR}} \) jump abundance of IRAS 16293-2422 can be modeled with \( F_X \gtrsim 10^{-3} \text{erg s}^{-1} \text{cm}^{-2} \). Such a flux can be achieved at 1000 AU from a central protostar with \( L_X \approx 10^{31} \text{erg s}^{-1} \). The XDR abundances in the high-mass sources, however, require high X-ray fluxes \( (F_X > 1 \text{erg s}^{-1} \text{cm}^{-2}) \), corresponding to luminosities \( \gtrsim 10^{33} \text{erg s}^{-1} \). X-rays can enhance the CN abundances up to three orders of magnitude compared to models without X-rays on scales of a few 100–1000 AU.

FUV fields produce CN abundances between \( 10^{-9} - 10^{-8} \) (Fig. 5.10) for temperatures \( T \lesssim 300 \text{K} \) and \( G_0 = 5-100 \). The abundances can be even higher for \( T \gtrsim 300 \text{K} \) at the relevant densities \( (10^6-10^7 \text{cm}^{-3}) \). Low FUV fields can thus enhance the CN abundances to similar values as high X-ray fluxes, if they can penetrate to large enough distances.

All models have \( x(CN) < 10^{-10} \) for \( n_H \gtrsim 10^6 \text{cm}^{-3} \) without the influence of X-rays or FUV fields. The observed constant fractional CN abundances for most sources, however, are \( > 10^{-10} \) (Table 5.6). CN is therefore a clear indicator of enhanced X-rays or FUV fields.

### 5.5.2 NO

Our observed NO abundances are of the order of \( 10^{-8} \) with respect to \( H_2 \) for the high-mass sources and \( 10^{-9} \) for the low-mass objects assuming constant fractional abundances (Table 5.6). In the jump models, the abundances of the high-mass sources are between \( 10^{-7} \) and a few times
Figure 5.9: Modeled CN abundances as a function of the X-ray flux (erg s\(^{-1}\) cm\(^{-2}\)), gas temperature and total hydrogen density (cm\(^{-3}\)). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of \(x_{100K}\). The square indicates \(x_{\text{XDR}}\) for AFGL 2591 at the position of the average temperature and density in this region (Table 5.8); the triangle represents W3 IRS5 and the diamond represents IRAS 16293–2422.

Figure 5.10: Modeled CN abundances as a function of the FUV radiation field \(G_0\), gas temperature and total hydrogen density (cm\(^{-3}\)). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of \(x_{100K}\).
10^{-6} (Tables 5.7 and 5.8). The observed NO column densities in the low and high-mass YSOs are \( N(\text{NO}) \approx 10^{15} - 10^{16} \text{ cm}^{-2} \).

The chemical models of Stäuber et al. (2005) for AFGL 2591 have shown that the NO abundance can get as high as \( \approx 10^{-7} - 10^{-6} \) in the inner part of the envelope and \( \approx 10^{-8} - 10^{-7} \) relative to \( \text{H}_2 \) in the outer part. The column densities are larger than \( 10^{16} \text{ cm}^{-2} \) in models with and without X-rays or inner FUV fields. The observed column density for AFGL 2591 is \( \approx 3 \times 10^{15} \text{ cm}^{-2} \). The abundances are thus all higher compared to the observations.

The dependence of NO on the gas temperature, hydrogen density and X-ray flux is shown in Fig. 5.11. The fractional NO abundance can get as high as \( 10^{-7} \) compared to total hydrogen in the models without X-rays for temperatures \( 300 \lesssim T(\text{K}) \lesssim 100 \) and densities \( n_\text{H} = 10^6 - 10^7 \text{ cm}^{-3} \). The fractional NO abundance in models without X-rays is between a few times \( 10^{-10} - 10^{-9} \) for \( T \lesssim 100 \text{ K} \) and \( n_\text{H} = 10^6 - 10^7 \text{ cm}^{-3} \). X-rays can enhance these values by three orders of magnitude. The observed constant fractional abundances are comparable to the models without X-rays or low X-ray fluxes. The jump model abundances \( x_{100K} \) (Table 5.7) are comparable to models with \( F_X \approx 10^{-3} - 1 \text{ erg s}^{-1} \text{ cm}^{-2} \), corresponding to X-ray luminosities \( \gtrsim 10^{31} \text{ erg s}^{-1} \). The XDR abundances require higher X-ray fluxes \( (F_X \gtrsim 1 \text{ erg s}^{-1} \text{ cm}^{-2}) \).

Models with low FUV fields (Fig. 5.12) show that the NO abundance is decreased to \( \approx 10^{-12} - 10^{-11} \) for temperatures \( \lesssim 300 \text{ K} \). NO is destroyed by photodissociation and in reactions with \( \text{C}^+ \). In the FUV models, NO is mainly produced in reactions of N with OH. OH is more abundant at high temperatures due to higher \( \text{H}_2\text{O} \) abundances there, leading also to higher NO abundances for \( T \gtrsim 300 \text{ K} \) in the FUV models. The observed NO abundances correspond to the model results with \( G_0 \gtrsim 5 \) and \( T \gtrsim 300 \text{ K} \).

The fact that chemical models without X-rays overestimate the NO abundance in the outer part of the envelope \( (n_\text{H} \lesssim 10^6 \text{ cm}^{-3}) \) for most sources suggests that either FUV fields are present that reduce the overall NO abundance or that NO is frozen out on grains at lower temperatures. Comparison of the observed abundances (Table 5.6) to the envelope mass for each source shows that NO follows the trend of having less abundances with increasing mass. Such a trend for CO was interpreted as an evolutionary freeze-out effect by Jørgensen et al. (2002, 2004). Depletion may therefore also play a role in the NO chemistry. Both X-rays and FUV, however, can produce the observed jump abundances.
Chapter 5. Tracing high energy radiation

Figure 5.11: Modeled NO abundances as a function of the X-ray flux (erg s\(^{-1}\) cm\(^{-2}\)), gas temperature and total hydrogen density (cm\(^{-3}\)). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of \(x_{100K}\). The square indicates \(x_{XDR}\) for AFGL 2591 at the position of the average temperature and density in this region (Table 5.8); the triangle represents W3 IRS5.

Figure 5.12: Modeled NO abundances as a function of the FUV radiation field \(G_0\), gas temperature and total hydrogen density (cm\(^{-3}\)). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of \(x_{100K}\).
5.5. Comparison to chemical models

5.5.3 \( \text{SO}^+ \)

Our observed \( \text{SO}^+ \) abundances in the high-mass objects are \( 5-7 \times 10^{-11} \) assuming constant fractional abundances with respect to \( \text{H}_2 \) (Table 5.6). The \( x_{100 \text{K}} \) jump abundance is \( 2 \times 10^{-9} \) for AFGL 2591 and \( 9 \times 10^{-10} \) for W3 IRS5. The XDR jump abundance for AFGL 2591 is \( 3 \times 10^{-9} \) and \( 3 \times 10^{-8} \) for W3 IRS5. Inferred \( \text{SO}^+ \) column densities are \( N(\text{SO}^+) \approx 10^{13} \text{cm}^{-2} \).

In the FUV models of Stäuber et al. (2004a), \( \text{SO}^+ \) can have abundances \( x(\text{SO}^+) \approx 10^{-8} \) in the innermost part of the envelope (\( r \approx 200 \text{ AU} \)) for \( G_0 = 10-100 \) and \( \approx 10^{-10} \) for \( G_0 = 10^5 \). Column densities are comparable to our observations for \( G_0 = 10-100 \).

High \( \text{SO}^+ \) abundances were also predicted for AFGL 2591 by the X-ray models of Stäuber et al. (2005). In these models, \( \text{SO}^+ \) can be enhanced to \( x(\text{SO}^+) \approx 10^{-9} \) in the inner part of the envelope (\( T > 100 \text{ K} \), \( r \approx 1000 \text{ AU} \)). This is comparable to the jump model abundances derived for AFGL 2591 (Table 5.7).

The \( \text{SO}^+ \) abundance is studied as a function of the gas temperature, the X-ray flux and the hydrogen density (Fig. 5.13). The temperature dependence of \( \text{SO}^+ \) is rather weak for \( T \lesssim 300 \text{ K} \). At higher temperatures, however, most oxygen is either in \( \text{CO} \) or \( \text{H}_2\text{O} \), and \( \text{SO}^+ \) is less abundant. The upper \( x_{\text{XDR}} \) limit derived for IRAS 16293-2422 is consistent with X-ray fluxes \( F_X \gtrsim 1 \text{ erg s}^{-1} \text{ cm}^{-2} \). Compared to the X-ray models for AFGL 2591 (Stäuber et al. 2005), much less \( \text{SO}^+ \) is produced. This is due to the much lower assumed initial sulphur abundance of only \( 10^{-8} \) for \( T > 100 \text{ K} \) compared to \( 1.6 \times 10^{-6} \) for AFGL 2591. For \( T < 100 \text{ K} \) the initial abundances are the same. The model results can thus be scaled by a factor of 160 for comparison with the high-mass sources at \( T > 100 \text{ K} \). High sulphur abundances \( (x(\text{S}) \gtrsim 10^{-6}) \), gas temperatures \( (T \gtrsim 100 \text{ K}) \) and X-ray fluxes \( (F_X \gtrsim 10^{-2} \text{ erg s}^{-1} \text{ cm}^{-2}) \) are therefore required to explain the \( \text{SO}^+ \) observations towards the high-mass objects.

The FUV models in Fig. 5.14 show that \( \text{SO}^+ \) is destroyed for temperatures lower than 300 K. In this temperature regime, the recombination of \( \text{SO}^+ \) is faster than its production. At higher temperatures, \( \text{SO}^+ \) can efficiently be produced in reactions of \( \text{OH} \) and \( \text{S}^+ \). The observed abundances of a few \( \times 10^{-11} \) are only achieved at high temperatures \( (T \gtrsim 300 \text{ K}) \). \( \text{SO}^+ \) is clearly enhanced either by X-rays or by FUV fields at high temperatures.
Figure 5.13: Modeled SO\(^+\) abundances as a function of the X-ray flux (ergs\(^{-1}\) cm\(^{-2}\)), gas temperature and total hydrogen density (cm\(^{-3}\)). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of \(x_{100K}\). The square indicates \(x_{\text{XDR}}\) for AFGL 2591 at the position of the average temperature and density in this region (Table 5.8); the triangle represents W3 IRS5 and the diamond represents the upper limit in IRAS 16293–2422.

Figure 5.14: Modeled SO\(^+\) abundances as a function of the FUV radiation field \(G_0\), gas temperature and total hydrogen density (cm\(^{-3}\)). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of \(x_{100K}\).
5.5.4 CO+

CO+ is observed with constant fractional H₂ abundances of \( \approx 10^{-11} - 10^{-10} \) in the high-mass objects and a few \( \times 10^{-12} \) in the low-mass sources (Table 5.6). Beam averaged column densities are \( \approx 10^{12} \text{cm}^{-2} \) for the high-mass objects and a few \( \times 10^{11} \text{cm}^{-2} \) for the low-mass YSOs, depending on the excitation temperature (Table 5.9). The \( x_{100\text{K}} \) jump abundances are \( \approx 10^{-10} - 10^{-9} \) for \( T \gtrsim 100 \text{K} \) (Table 5.7) and \( x_{\text{XDR}}(\text{CO}^+) \approx 10^{-12} - 10^{-9} \) (Table 5.8).

The FUV envelope models of Stäuber et al. (2004a) produce \( x(\text{CO}^+) \approx 10^{-13} \) for \( G_0 = 10 \) and \( x(\text{CO}^+) \approx 10^{-10} - 10^{-9} \) for \( G_0 = 100-1000 \) in the innermost envelope \( (r \approx 200 \text{AU}) \). Even small FUV fields are therefore able to produce the observed fractional CO+ abundances. The CO+ column densities in these models are all \( N(\text{CO}^+) < 10^{12} \text{cm}^{-2} \), however, and thus not consistent with the observations.

The X-ray models of Stäuber et al. (2005) predict fractional abundances of \( x(\text{CO}^+) \approx 10^{-14} - 10^{-13} \) in the inner part of the AFGL 2591 envelope and \( x(\text{CO}^+) \approx 10^{-15} - 10^{-14} \) in the outer part. This is several orders of magnitude smaller than observed.

It is well-known, that chemical models usually have difficulties in producing the observed CO+ column densities (e.g., Fuente et al. 2006). However, to study the general conditions in the gas to produce the observed CO+ abundances, they are calculated as functions of the X-ray flux, hydrogen density and gas temperature (Fig. 5.15). The CO+ abundances are fairly constant with temperature for \( T \lesssim 300 \text{K} \). At higher temperatures, most oxygen is driven into H₂O even for high X-ray fluxes (Stäuber et al. 2006a) and the CO+ abundance decreases. The observed constant fractional abundances of the order \( 10^{-12} - 10^{-11} \) are reached for densities \( n_H \lesssim 10^7 \text{cm}^{-3} \) and X-ray fluxes \( F_X \gtrsim 10^{-1} \text{erg s}^{-1} \text{cm}^{-2} \). The XDR jump abundances require X-ray fluxes exceeding \( F_X = 1 \text{erg s}^{-1} \text{cm}^{-2} \), corresponding to \( L_X \gtrsim 10^{33} \text{erg s}^{-1} \).

Figure 5.16 shows how the CO+ abundance depends on the FUV field strength. The fractional abundances are two orders of magnitude below the observed values for \( T \lesssim 300 \text{K} \). The fractional abundances can increase to \( x(\text{CO}^+) \approx 10^{-12} - 10^{-10} \) with respect to total hydrogen for gas temperatures \( \gtrsim 300 \text{K} \). CO+ is efficiently produced in reactions of C+ and OH with the latter being more abundant at higher temperatures due to dissociations of H₂O (see also Stäuber et al. 2004a). The
Figure 5.15: Modeled CO⁺ abundances as a function of the X-ray flux (ergs⁻¹ cm⁻²), gas temperature and total hydrogen density (cm⁻³). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of T<br>100K. The square indicates xₜₜ for AFGL 2591 at the position of the average temperature and density in this region (Table 5.8); the triangle represents W3 IRS5 and the diamond represents IRAS 16293-2422.

CO⁺ observations can thus be interpreted with either a high X-ray flux (Fx > 1 ergs⁻¹ cm⁻²) or an FUV flux (G₀ > 5) at high gas temperatures.

5.5.5 SH⁺ and N₂O

Our derived upper limit for SH⁺ in AFGL 2591 is 4.1 x 10⁻¹¹ with respect to H₂ assuming constant fractional abundances (Table 5.6) or ≈ 10⁻⁸ if we assume the SH⁺ emission to be from the inner part of the envelope (Table 5.7). The column density is N(SH⁺) < 4 x 10¹² cm⁻².

The X-ray models of Stäuber et al. (2005) have x(SH⁺) ≈ 10⁻¹⁰ for T > 100 K and x(SH⁺) ≈ 10⁻¹³–10⁻¹² for T < 100 K. The X-ray models are below the upper x(SH⁺) limits and no conclusion can be drawn on the X-ray flux.

The predicted N₂O abundances in the X-ray models for AFGL 2591
5.5. Comparison to chemical models

Figure 5.16: Modeled CO$^+$ abundances as a function of the FUV radiation field $G_0$, gas temperature and total hydrogen density (cm$^{-3}$). The light shaded region indicates the observed constant abundances. The dark shaded region indicates the range of $x_{100K}$.

are between $\approx 4 \times 10^{-11}$ in the outer region of the envelope and $\approx 10^{-9}$ in the inner envelope. The models are therefore well below the derived upper limits for the inner region for W3 IRS5 ($2 \times 10^{-7}$) and N1333-I2 ($4 \times 10^{-7}$).

5.5.6 Abundance ratios

In the following sections we discuss molecular abundance ratios and study their dependence on X-rays and FUV fields. The CN to HCN ratio, for example, is considered to be a good tracer for enhanced FUV fields. In the vicinity of strong FUV fields the CN/HCN ratio is observed to be $\gtrsim 1$ (e.g., Fuente et al. 1993) in good agreement with chemical PDR models (e.g., Jansen et al. 1995a; Sternberg & Dalgarno 1995). The CN/HCN, CN/NO, CO$^+$/HCO$^+$ and SO$^+$/SO abundance ratios for all observed sources are presented in Table 5.11. The fractional abundances are taken from the constant abundance models (Table 5.6). Those for HCN, HCO$^+$ and SO are from the literature and are presented in Table 5.12. All abundances were derived from radiative transfer models assuming constant fractional abundances as described in Sect. 5.4.1. Exceptions are the HCO$^+$ and HCN abundances towards W3 IRS5 which were derived from statistical equilibrium calculations at a single temperature and density using an escape probability mechanism (Helmich & van Dishoeck 1997).

It should be mentioned, however, that the compared species may not be co-existent. For example, since HCN is substantially produced at high
gas temperatures \((T \gtrsim 300\, \text{K})\), CN is likely to be more extended than HCN and may even be enhanced along the outflow regions as found by Jørgensen (2004) for the low-mass source L483. Also, species that are less sensitive to high energy radiation (or even destroyed by it) are bound to come from FUV and/or X-ray shielded regions in the envelope. Care should therefore be taken when interpreting the abundance ratios.

**CN to HCN ratios**

Our CN/HCN ratios are \(\gtrsim 1\) for both high-mass sources and for the Class I object L1489. The ratio is \(\approx 1\) for L483 and L723. All other sources have \(x(\text{CN}/\text{HCN}) < 0.2\) (Table 5.11).

The CN/HCN ratio is studied as a function of the X-ray flux, the gas temperature and the hydrogen density (Fig. 5.17). Ratios of the order \(\approx 0.1\) are reached for gas temperatures \(\lesssim 200\, \text{K}\), \(F_X = 10^{-3} - 10^{-2}\, \text{erg}\, \text{s}^{-1}\, \text{cm}^{-2}\), and \(n_H = 10^6 - 10^7\, \text{cm}^{-3}\). It can be seen that only high X-ray fluxes \((F_X \gtrsim 1\, \text{erg}\, \text{s}^{-1}\, \text{cm}^{-2})\) and gas temperatures \(T \lesssim 200\, \text{K}\) lead to CN/HCN ratios of \(\approx 1\) for densities \(n_H \gtrsim 10^7\, \text{cm}^{-3}\). The ratio can be \(\gtrsim 1\) for lower X-ray fluxes \((F_X \approx 10^{-2}\, \text{erg}\, \text{s}^{-1}\, \text{cm}^{-2})\) and lower densities. For a protostar with \(L_X = 10^{31}\, \text{erg}\, \text{s}^{-1}\), such high X-ray fluxes can be reached within \(r \approx 600\, \text{AU}\) from the central source.

The FUV model results are presented in Fig. 5.18. The CN to HCN ratio is between 1–100 for relatively low FUV fields \((G_0 \lesssim 100)\) and temperatures below \(\approx 200\, \text{K}\). The ratio decreases with increasing gas temperature. The observed ratios require gas temperatures \(T \gtrsim 300\, \text{K}\) for \(n_H = 10^6\, \text{cm}^{-3}\). For \(n_H = 10^7\, \text{cm}^{-3}\), the gas temperature can be lower for FUV fields \(G_0 \lesssim 10\). The observed ratios clearly indicate the presence of X-rays or FUV fields.

**Other ratios**

Our observed \(\text{CO}^+\) to \(\text{HCO}^+\) ratios are of the order \(10^{-3}\) in the low-mass objects and \(\approx 10^{-2} - 10^{-1}\) in the high-mass sources (Table 5.11). The X-ray models of Stäuber et al. (2005) predict \(\text{CO}^+\) to \(\text{HCO}^+\) ratios of \(\lesssim 10^{-6}\). The FUV envelope models of Stäuber et al. (2004a) show ratios between \(10^{-5} - 10^{-2}\) for \(G_0 = 10^{-5} - 10^5\). Our observed values are in the range of our FUV models.
5.6 Discussion

### Table 5.11:Observed abundance ratios assuming constant abundances.

<table>
<thead>
<tr>
<th>Source</th>
<th>CN/HCN</th>
<th>CN/NO</th>
<th>CO⁺/HCO⁺</th>
<th>SO⁺/SO</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFGL 2591</td>
<td>1.15</td>
<td>0.74</td>
<td>0.016</td>
<td>0.006</td>
</tr>
<tr>
<td>W3 IRS 5</td>
<td>1.80</td>
<td>0.21</td>
<td>0.066</td>
<td>0.007</td>
</tr>
<tr>
<td>IRAS 16293</td>
<td>0.05</td>
<td>...</td>
<td>0.001</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>N1333-I2</td>
<td>0.20</td>
<td>0.16</td>
<td>0.002</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>N1333-I4A</td>
<td>0.12</td>
<td>0.03</td>
<td>&lt; 0.002</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>L1448-C</td>
<td>0.20</td>
<td>...</td>
<td>&lt; 0.002</td>
<td>&lt; 0.007</td>
</tr>
<tr>
<td>L483</td>
<td>0.75</td>
<td>...</td>
<td>&lt; 0.004</td>
<td>...</td>
</tr>
<tr>
<td>L723</td>
<td>0.92</td>
<td>...</td>
<td>&lt; 0.005</td>
<td>&lt; 0.017</td>
</tr>
<tr>
<td>SMM4</td>
<td>0.08</td>
<td>...</td>
<td>&lt; 0.001</td>
<td>...</td>
</tr>
<tr>
<td>L1489</td>
<td>3.85</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

The SO⁺/SO ratio for the high-mass objects is $6-7 \times 10^{-3}$. The upper limit for the low-mass YSOs is $\approx 10$ times less. The X-ray envelope models of AFGL 2591 have SO⁺/SO $\approx 10^{-3}$, comparable to the observations. Our PDR models predict ratios between $\approx 1-10^3$ in the innermost region, for $G_0 = 10-10^4$. If the observed SO⁺ abundance was from a PDR, the SO emission would thus have to come from a region that is not affected by the strong FUV radiation. Assuming that they originate from the same region, only X-rays can explain the observations.

### 5.6 Discussion

All molecular lines are observed within a HPBW of 14". The critical densities of the main transitions are estimated to be between $n_{\text{H}_2} \approx 10^6-10^7$ cm$^{-3}$. Comparison of observations with chemical models indicate that FUV and/or X-rays from the central star may be responsible for the relatively high observed CN, CO⁺ and SO⁺ abundances. Table 5.13 summarizes the results found in the general parameter study (Sect. 5.5). X-rays can produce in principle all observed abundances for high enough X-ray fluxes, except the constant fractional abundances of NO (i.e., NO at $T \lesssim 100$ K). X-rays overestimate its abundance possibly due to freeze out effects at lower temperatures. FUV fields can produce the observed CN abundances. The CO⁺ and SO⁺ abundances can only be explained
### Table 5.12: Observed fractional abundances from literature.

<table>
<thead>
<tr>
<th>Source</th>
<th>HCN $\times 10^{-9}$</th>
<th>HCO$^+$ $\times 10^{-9}$</th>
<th>SO $\times 10^{-9}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFGL 2591</td>
<td>20.0$^a$</td>
<td>10.0$^a$</td>
<td>10.0$^b$</td>
</tr>
<tr>
<td>W3 IRS 5</td>
<td>2.0$^c$</td>
<td>0.73$^c$</td>
<td>10.0$^b$</td>
</tr>
<tr>
<td>IRAS 16293</td>
<td>1.1$^d$</td>
<td>1.4$^d$</td>
<td>4.4$^d$</td>
</tr>
<tr>
<td>N1333-I2</td>
<td>2.0$^e$</td>
<td>3.3$^e$</td>
<td>3.4$^e$</td>
</tr>
<tr>
<td>N1333-I4A</td>
<td>0.36$^e$</td>
<td>0.43$^e$</td>
<td>4.6$^e$</td>
</tr>
<tr>
<td>L1448-C</td>
<td>5.4$^e$</td>
<td>9.1$^e$</td>
<td>1.4$^e$</td>
</tr>
<tr>
<td>L483</td>
<td>2.0$^e$</td>
<td>2.0$^e$</td>
<td>0.29$^e$</td>
</tr>
<tr>
<td>L723</td>
<td>1.0$^e$</td>
<td>4.1$^e$</td>
<td>2.4$^e$</td>
</tr>
<tr>
<td>SMM4</td>
<td>2.0$^f$</td>
<td>1.0$^f$</td>
<td>...</td>
</tr>
<tr>
<td>L1489</td>
<td>0.65$^e$</td>
<td>18.0$^e$</td>
<td>2.0$^e$</td>
</tr>
</tbody>
</table>

$^a$ van der Tak et al. (2000a); $^b$ van der Tak et al. (2003) $^c$Helmich & van Dishoeck (1997); $^d$ Schöier et al. (2002); $^e$ Jørgensen et al. (2004); $^f$ Hogerheijde et al. (1999)

#### Figure 5.17: Modeled CN/HCN ratio as functions of the X-ray flux (erg s$^{-1}$ cm$^{-2}$), gas temperature and total hydrogen density (cm$^{-3}$). The shaded region indicates the observed ratios (Table 5.11).
5.6. Discussion

Figure 5.18: Modeled CN/HCN ratio as functions of the FUV field strength, gas temperature and total hydrogen density (cm$^{-3}$). The shaded region indicates the observed ratios (Table 5.11).

by FUV fields with $T \gtrsim 300$ K.

5.6.1 Processes

So far only the conditions of the gas have been set to explain the observed abundances, providing a range of X-ray or FUV fluxes and gas temperatures (Table 5.13). Are these conditions comparable to those in spherical envelopes? It was already mentioned that FUV fields are absorbed within a few hundred AU from the source, affecting too small a region to account for the observed line fluxes of CN, CO$^+$ and SO$^+$. Also, some molecules require high X-ray fluxes that cannot be achieved at large distances from the source with typical X-ray luminosities ($L_X \lesssim 10^{32}$ erg s$^{-1}$). A region of enhanced X-rays or FUV fields may thus be needed at larger radii to explain some of the observations.

FUV fields from the protostar can only explain our observations if there is a low-opacity region in the envelope that allows the FUV photons to escape and impact the envelope on large scales. This could be possible for example due to scattering of FUV photons in outflow cavities as suggested by Spaans et al. (1995). Assuming a geometry as presented in Fig. 5.19, the FUV photons could also impact the envelope directly on large scales without being scattered. In this scenario, the protostar is surrounded by a (flaring) disk and low density outflows. Such a geometry would be expected in the presence of disk-driven winds (e.g., Shu et al. 1994). A region in the envelope with low optical depth was also suggested
for AFGL 2591 by van der Tak et al. (1999). Images from the Spitzer Space Telescope of high-mass objects also show a patchy structure with regions through which FUV photons can escape (e.g., Curchwell et al. 2004).

The same scenario could be possible for X-rays. X-rays, however, do not depend on geometry as much as FUV fields due to the smaller absorbing cross sections. An X-ray absorbing column density of $N(\text{H}_2) \lesssim 10^{23} \text{cm}^{-2}$ reduces the X-ray flux only by a factor of a few but not by orders of magnitude (Stäuber et al. 2005, 2006a). The main reducing parameter for the X-ray flux is the geometrical dilution ($F_X \propto r^{-2}$). The X-ray enhanced cavity walls are thus of minor importance compared to the quiescent bulk envelope irradiated by X-rays.

X-rays could also be powered by fast winds or jets from the embedded protostar. In this scenario, the source of X-ray emission would be shocks shifted from the central position which could even be multiple in nature. X-rays can then impact the envelope on large scales with luminosities between $L_X \approx 10^{29} - 10^{33} \text{erg s}^{-1}$ (e.g., Favata et al. 2002; Ezoe et al. 2006). The thermal X-ray spectrum is given by the temperature of the shocked gas ($\approx 1 \text{keV} (v/1000 \text{km s}^{-1})^2$). An ionized wind with $v \approx 500 \text{km s}^{-1}$ has been observed in the [SII] $\lambda 6731$ line towards AFGL 2591 by Poetzel et al. (1992). Such a velocity would lead to the emission of soft X-rays ($\approx 3 \times 10^6 \text{K}$) on large scales if it came to a shock with the surrounding material. However, further investigation of this scenario is beyond the scope of this paper.

The possible scenarios are further discussed separately for the high and low-mass objects in the next two sections. A summary of the processes that we believe are traced by each molecule for the low and high-mass objects is presented in Table 5.14.

### 5.6.2 High-mass objects

While the chemical X-ray models for AFGL 2591 can explain the observed CN and SO$^+$ abundances within a factor of a few for high X-ray luminosities ($L_X \gtrsim 10^{32} \text{erg s}^{-1}$), they cannot reproduce the observed CO$^+$ abundance. Only high X-ray fluxes ($F_X \gtrsim 0.1 \text{erg s}^{-1} \text{cm}^{-2}$) enhance CO$^+$ to abundances $> 10^{-12}$. Such high fluxes imply $L_X \approx 10^{33} - 10^{34} \text{erg s}^{-1}$ (Sect. 5.5.4) – an extraordinary high X-ray luminosity. The predicted X-
5.6. Discussion

Table 5.13: Summary of the results from the general parameter study$^a$.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>X-rays ($F_X$)</th>
<th>FUV ($G_0$) (T \lesssim 300) K</th>
<th>FUV ($G_0$) (T \gtrsim 300) K</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN (const.)</td>
<td>$\gtrsim 10^{-4}$</td>
<td>$\gtrsim 5$</td>
<td>$\gtrsim 5$</td>
</tr>
<tr>
<td>CN (jump)</td>
<td>$\gtrsim 10^{-3}$</td>
<td>$\gtrsim 5$</td>
<td>$\gtrsim 5$</td>
</tr>
<tr>
<td>NO (const.)</td>
<td>$0 \cdot 10^{-2}$</td>
<td>-</td>
<td>$\gtrsim 5$</td>
</tr>
<tr>
<td>NO (jump)</td>
<td>$\gtrsim 10^{-3}$</td>
<td>-</td>
<td>$\gtrsim 5$</td>
</tr>
<tr>
<td>SO$^+$ (const.)</td>
<td>$\gtrsim 10^{-3}$</td>
<td>-</td>
<td>$\gtrsim 5$</td>
</tr>
<tr>
<td>SO$^+$ (jump)</td>
<td>$\gtrsim 10^{-2}$</td>
<td>-</td>
<td>$\gtrsim 5$</td>
</tr>
<tr>
<td>CO$^+$ (const.)</td>
<td>$\gtrsim 10^{-1}$</td>
<td>-</td>
<td>$\gtrsim 5$</td>
</tr>
<tr>
<td>CO$^+$ (jump)</td>
<td>$&gt; 1$</td>
<td>-</td>
<td>$\gtrsim 5$</td>
</tr>
</tbody>
</table>

$^a$ The lower limit or range of X-ray and FUV fluxes for each molecule corresponds to the values that either fit the observed constant fractional abundances or the jump abundances \(x_{100K}, x_{XDR}\). NO, SO$^+$ and CO$^+$ cannot be modeled with \(G_0 \gtrsim 5\) and \(T \lesssim 300\) K.

Table 5.14: Summary of processes predicted to be involved in the formation of each molecule.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>high mass YSOs</th>
<th>low-mass YSOs</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN</td>
<td>FUV cavity walls</td>
<td>X-rays</td>
</tr>
<tr>
<td></td>
<td>X-rays</td>
<td></td>
</tr>
<tr>
<td>NO</td>
<td>X-rays</td>
<td>X-rays</td>
</tr>
<tr>
<td></td>
<td>freeze out</td>
<td>freeze out</td>
</tr>
<tr>
<td></td>
<td>FUV cavity walls</td>
<td></td>
</tr>
<tr>
<td>SO$^+$</td>
<td>FUV cavity walls</td>
<td>X-rays</td>
</tr>
<tr>
<td></td>
<td>X-rays</td>
<td></td>
</tr>
<tr>
<td>CO$^+$</td>
<td>FUV cavity walls</td>
<td>inner region X-rays</td>
</tr>
<tr>
<td></td>
<td></td>
<td>inner region FUV</td>
</tr>
</tbody>
</table>
ray luminosity for AFGL 2591 is more than an order of magnitude lower (Stäuber et al. 2005) and more than two orders compared to ASCA X-ray observations towards W3 (Hofner et al. 2002). X-rays from the central source are therefore not a plausible explanation to account for the observed CO$^+$ emission.

The observations could be explained with FUV fields ($G_0 \gtrsim 5$) and high gas temperatures ($T \gtrsim 300$ K) on large scales such as in the outflow cavity scenario (Fig. 5.19). Such a scenario would also explain the observed high CN to HCN ratios towards these objects. The question is whether a source like AFGL 2591 can maintain high FUV fields and gas temperatures out to large distances from the protostar. To estimate the FUV flux for AFGL 2591 at $r_{\text{beam}} = \text{HPBW}/2 \approx 7000$ AU, we assume a black body spectrum with a stellar temperature $T = 3 \times 10^4$ K and $L_{\text{bol}} = 2 \times 10^4 L_\odot$ (van der Tak et al. 1999). This corresponds to $G_0(r_{\text{beam}}) \approx 2 \times 10^5$ ($G_0 = 1$ corresponds to $1.6 \times 10^{-3} \text{erg s}^{-1} \text{cm}^{-2}$, Habing 1968). Material in the outflows and geometric dilution due to a non-perpendicular impact angle will reduce this FUV flux by a factor of $\approx 10$--1000, depending mainly on the outflow density. However, the effective FUV flux at $r_{\text{beam}}$ can still be between $G_{0,\text{eff}} \approx 10$--$10^4$. If the heating of the gas along the outflow walls is provided by FUV, a temperature of $\approx 300$ K requires $G_0 \approx 10^4$ (e.g., Sternberg & Dalgarno 1995). This implies $A_V \lesssim 2$ at $r_{\text{beam}}$ and the material in the outflow is therefore suggested to have a density of $\lesssim 4 \times 10^4 \text{cm}^{-3}$.

To further test whether the FUV scattering scenario of Spaans et al. (1995) is possible for the high-mass objects, the Spaans et al. model is scaled to the luminosity and radial size of AFGL 2591. A 3D model of the region is constructed with a spherical envelope and an outflow cavity, assuming a 30 degree opening angle. This leads to a region of high FUV fields ($G_0 \approx 1000$) and $T \gtrsim 100$ K out to $r_{\text{beam}}$ along the outflow walls. By convolving this envelope model with the JCMT beam for different angles of telescope pointing relative to the direction of outflow, it is seen that $6$--$43\%$ of the volume is in the high FUV region, assuming the molecular line emission to be optically thin. Applying this result to the fractional abundances from the FUV model results of Stäuber et al. (2004a) leads to $x(\text{CN}) \approx 6 \times 10^{-9} - 4 \times 10^{-8}$, $x(\text{NO}) \approx 6 \times 10^{-9} - 4 \times 10^{-8}$, $x(\text{SO}^+) \approx 6 \times 10^{-11} - 4 \times 10^{-10}$, $x(\text{CO}^+) \approx 6 \times 10^{-11} - 4 \times 10^{-10}$. These values are in good agreement to those observed towards AFGL 2591. The observed column densities can easily be achieved if we assume the density profiles
in the outflow walls to be the same as that in the envelope \( n \propto r^{-1} \); van der Tak et al. 1999). If the species trace an FUV enhanced region at few \( A_V \) away from the outflow cavity wall, the center velocity can be expected to be the one of the system. In addition, such a relatively thin layer of gas would lead to the observed narrow lines (Sect. 5.3.1). This simple model shows that strong FUV fields from high-mass objects can explain the observed features if the FUV photons travel through the outflow cavities and affect the envelope at large distances either due to scattering or direct impact.

If the species indeed trace FUV enhanced regions along the outflow walls, the question is then whether or not X-rays are important for the chemistry in envelopes around high-mass protostars. In the case of our sample of species, approximately 80–90% of the emission can be attributed to the influence of FUV. This is not likely to be the case for pure X-ray tracers. Stäuber et al. (2005) found that a large sample of the molecules were better fitted in models assuming a central X-ray source. Only a few species among them, however, were tracers of the FUV field. Other species like \( \text{N}_2\text{H}^+ \) or \( \text{HCO}^+ \), for example, are reduced in FUV enhanced regions (eg., Jansen et al. 1994) but were well fitted within the X-ray models. Thus, X-rays are still necessary even in the FUV enhanced outflow cavity scenario. Spatially resolved data are needed to distinguish between outflow enhanced regions and the FUV shielded envelope.

5.6.3 Low-mass objects

To explain the observed abundances in the low-mass objects, a similar scenario is possible as suggested for the high-mass sources, where \( \text{CO}^+ \) and CN are enhanced in regions along the outflow walls. While high-mass objects emit large amounts of UV photons, this may not be the case for low-mass sources due to lower stellar temperatures. However, accretion can heat the gas to high temperatures and the FUV flux could be increased. Taking this into account, the FUV flux is estimated to be \( G_0 \lesssim 10^4 \) at 100 AU for a source with \( L_{\text{bol}} \approx 20 L_\odot \) and an effective temperature of \( T \approx 7000 \text{K} \). Bergin et al. (2003) argued that \( G_0 \) may be only a few hundred, albeit at later stages, and the estimated value above can be regarded as an upper limit for \( G_0 \) at 100 AU. Considering absorption in the outflows and geometric dilution, the effective FUV field at \( r_{\text{beam}} \) is \( G_{0,\text{eff}} \lesssim \) a few. Also, to explain the observed \( \text{CO}^+ \) (and \( \text{SO}^+ \))
abundance with enhanced FUV fields, the gas temperature would have to be $\gtrsim 300\,\text{K}$. Such high temperatures are not predicted by the models of Spaans et al. (1995).

CN appears to be a different case. Observations towards the Class 0 object L483 by Jørgensen (2004) indicate an extended CN emission morphology which is suggestive of FUV enhancement along the cavity walls. It has been shown that low FUV fluxes can already enhance CN by more than an order of magnitude (Fig. 5.10). In fact, the FUV radiation field of low-mass YSOs may not have enough UV photons at wavelengths $< 1100\,\text{Å}$ required to photodissociate CN so that its abundance may be even higher than predicted by our models. On the other hand, outflows in young low-mass objects appear to be more collimated than in high-mass objects, so that the outflow cavity walls may contribute only a few percent to the observed emission in a $14''$ beam, depending on the line of sight. The bulk CN emission would thus still have to come from the X-ray enhanced envelope in some sources. High spatial resolution observations of high-excitation CN lines are needed to further investigate this question.

CO$^+$ and CN could in principle trace an FUV enhanced gas in the protostellar hole region, in the inner edge of the envelope or in the disk ($r \lesssim 500\,\text{AU}$). The temperature requirement of $T \gtrsim 300\,\text{K}$ for CO$^+$, however, is not consistent with the dust radiative transfer models for the
5.6. Discussion

low-mass sources (Jørgensen et al. 2002; Schöier et al. 2002). To provide the additional heating through FUV photons at $n_H = 10^6 - 10^7 \text{ cm}^{-3}$ (comparable to upper disk layers), requires $G_0 \gtrsim 10^4$ (e.g., Sternberg & Dalgarno 1995), at the upper limit of what is likely.

If the species trace X-rays from the central source, the protostellar X-ray luminosity can be estimated from the model results (Sect. 5.5) and the observed abundances (Table 5.6). Since the high densities in the inner region of the continuum envelope models (Table 5.2) may be due to disk contributions and since protostellar holes exist in some of the sources, $n_H$ is assumed to be $\approx n(r_{\text{beam}})$. The gas temperature is assumed to be $T \lesssim 100 \text{ K}$. Table 5.15 shows the results of this comparison for CN. Since X-rays will be attenuated by the gas between the protostar and $r_{\text{beam}}$, the X-ray luminosities in Table 5.15 are given as lower limits. To explain the constant fractional CO$^+$ abundances, the X-ray luminosities would have to be at least two orders of magnitude higher. Any flattening of the inner envelope region will allow the X-rays to impact the surrounding envelope relatively unabsorbed at large distances, lowering the requirement on $L_X$. If we assume the observed emission to originate from upper disk layers or gas in the protostellar hole region ($r \lesssim 500 \text{ AU}$) of IRAS 16293 and N1333–I2, the X-ray luminosity would have to be $L_X \approx 10^{30} - 10^{32} \text{ erg s}^{-1}$ to account for the observed CN and CO$^+$ emission. The fact that even smaller densities ($n_H \lesssim 10^6 \text{ cm}^{-3}$) in the inner protostellar hole region lead to higher CO$^+$ abundances with similar X-ray luminosities (Fig. 5.15), supports the idea that CO$^+$ may indeed trace the innermost region.

We conclude that CN is tracing the X-ray enhanced envelope since the observations are better fitted with constant abundances (Sect. 5.4.2; Schöier et al. 2002; Jørgensen et al. 2004) and since FUV enhanced outflow walls may contribute only a few percent to the observed emission. CO$^+$ on the other hand, is more likely to trace the inner region ($r \lesssim 500 \text{ AU}$) following the arguments stated above. Due to the required high gas temperatures in the FUV scenario, CO$^+$ is suggested to be enhanced by X-rays. The estimated luminosities in all X-ray scenarios are between a few $\times 10^{29} - 10^{31} \text{ erg s}^{-1}$ which is in good agreement to observations of Class I or older protostars. Class 0 objects may therefore emit X-rays on similar scales as later type YSOs.
Table 5.15: Estimates of the X-ray luminosity in low-mass objects from the observed CN abundances.

<table>
<thead>
<tr>
<th>Source</th>
<th>( r_{\text{beam}} ) AU</th>
<th>( n_H(r_{\text{beam}}) ) cm(^{-3} )</th>
<th>X-ray luminosity ( L_X ) erg s(^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRAS 16293</td>
<td>1120</td>
<td>( 10^7 )</td>
<td>( 4 \times 10^{29} )</td>
</tr>
<tr>
<td>N1333-I2</td>
<td>1540</td>
<td>( 10^6 )</td>
<td>( 7 \times 10^{29} )</td>
</tr>
<tr>
<td>N1333-I4A</td>
<td>1540</td>
<td>( 10^7 )</td>
<td>( 7 \times 10^{29} )</td>
</tr>
<tr>
<td>L1448-C</td>
<td>1540</td>
<td>( 10^6 )</td>
<td>( 7 \times 10^{30} )</td>
</tr>
<tr>
<td>L483</td>
<td>1400</td>
<td>( 10^6 )</td>
<td>( 6 \times 10^{30} )</td>
</tr>
<tr>
<td>L723</td>
<td>2100</td>
<td>( 10^6 )</td>
<td>( 1 \times 10^{31} )</td>
</tr>
<tr>
<td>SMM4</td>
<td>1750</td>
<td>( 10^6 )</td>
<td>( 1 \times 10^{30} )</td>
</tr>
<tr>
<td>V1057 Cyg</td>
<td>4550</td>
<td>( 10^5 )</td>
<td>( 6 \times 10^{30} )</td>
</tr>
<tr>
<td>L1489</td>
<td>980</td>
<td>( 10^5 )</td>
<td>( 8 \times 10^{29} )</td>
</tr>
</tbody>
</table>

5.7 Conclusion

Several molecular ions and radicals that are thought to trace FUV and/or X-rays have been observed and detected towards both low and high-mass star-forming regions. For the FU Orionis object V1057 Cyg, continuum SCUBA observations have been carried out and the results were used to constrain the one dimensional physical structure of the envelope. The fractional molecular abundances are estimated through Monte Carlo line radiative transfer modeling. Chemical models are presented and compared to the observed abundances. The main conclusions are:

1. CN and NO \( J = 3 - 2 \) lines are detected towards all observed sources. The NO fluxes are typically an order of magnitude lower compared to the strongest CN lines, but its abundance is up to an order of magnitude higher. CO\(^+\) is detected towards both high-mass sources that were observed (AFGL 2591 and W3 IRS5) and towards two low-mass sources (IRAS 16293–2422 and N1333–I2). SO\(^+\) is detected towards the two high-mass objects and tentatively towards the low-mass YSO IRAS 16293–2422. SH\(^+\) has been searched for in AFGL 2591 with no clear detection, possibly due to \(^{34}\)SO\(_2\) blending. N\(_2\)O has been searched for in W3 IRS5 and N1333–I2 but was not detected (Sect. 5.3.1).

2. CN can in general be well fitted with constant fractional abundances. \( x(\text{CN}) \) is a few \( \times 10^{-9} \)–\( 10^{-8} \) in the high-mass objects and a few
Conclusion

\(10^{-11} - 10^{-9}\) in the low-mass YSOs. NO has abundances of the order \(10^{-8}\) in the high-mass sources and \(\approx 10^{-9}\) in the low-mass objects assuming constant fractional abundances (Sect. 5.4.1). In jump models, these abundances can be increased by up to two orders of magnitude in the inner region of the envelope (Sect. 5.4.2). The jump models are statistically not distinguishable from the constant abundance models.

3. The fractional abundances of CO\(^+\) are \(\approx 10^{-11} - 10^{-10}\) in the high-mass objects and \(\approx 10^{-12}\) in the low-mass sources if CO\(^+\) is assumed to have constant abundances with respect to H\(_2\) (Sect. 5.4.1). Jump models have 2–10 times higher abundances in the inner region of the envelope (Sect. 5.4.2). Beam averaged column densities of CO\(^+\) are \(\approx 10^{12}\) cm\(^{-2}\) in the high-mass objects and a few \(\times 10^{11}\) cm\(^{-2}\) in the low-mass YSOs (Sect. 5.4.3).

4. SO\(^+\) has constant fractional abundances of a few \(\times 10^{-11}\) in the high-mass objects and \(x(\text{SO}^+) \lesssim 3 \times 10^{-12}\) in IRAS 16293–2422 (Sect. 5.4.1). The abundances can be 10–30 times higher in the jump models (Sect. 5.4.2).

5. Comparison to chemical models suggest that X-rays cannot explain the observed CO\(^+\) abundances in the high-mass objects. The features could be explained by the influence of FUV fields with \(G_0 \gtrsim 10\) and \(T \gtrsim 300\) K. Low opacity regions such as outflow cavities allow the FUV photons to illuminate the surrounding envelope on large scales (Sects. 5.5 and 5.6.2).

6. The observed abundances imply X-ray fluxes for Class 0 objects at similar levels as more evolved protostars. The presence and influence of FUV fields in low-mass objects cannot be ruled out, however.
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Chapter 6

Herschel's view of X-rays

ABSTRACT: The chemistry of envelopes surrounding typical Class 0, Class I and high-mass young stellar objects is modeled assuming a central source of X-ray emission. Hydride abundances are modeled independently of geometry as functions of the X-ray or FUV flux, hydrogen density and gas temperature. Line strengths of H$_3$O$^+$ and OH are calculated for the envelope models for different X-ray luminosities. Model results show that neutral and ionized hydrides are enhanced by X-rays in spherical envelopes. CH, OH, NH and H$_3$O$^+$ are found to have abundances $\gtrsim 10^{-12}$ throughout the envelope. SH, SH$^+$ and OH$^+$ have such high abundances only in the innermost part of the envelope. A general parameter study shows that CH and CH$^+$ are enhanced by FUV fields with $G_0 \gtrsim 50$ to $x$(CH) $\approx 10^{-7}$ and $x$(CH$^+$) $\approx 10^{-11}$, respectively. Only high X-rays fluxes ($F_X \gtrsim 1$ erg s$^{-1}$ cm$^{-2}$) lead to similarly high abundances. OH, OH$^+$, SH$^+$, H$_3$O$^+$ and H$_2$O$^+$ are enhanced by FUV fields only for temperatures $T \gtrsim 300$ K, whereas X-rays cause high abundances also at lower temperatures. X-ray fluxes of the order $F_X = 1$ erg s$^{-1}$ cm$^{-2}$ lead to $x$(NH) $\approx 10^{-8}$ and $x$(NH$^+$) $\approx 10^{-12}$. FUV fields can enhance these species only for $T \gtrsim 500$ K but the fractional abundances for $G_0 = 1000$ are 1–2 orders of magnitude lower compared to the X-ray models. SH is enhanced by X-rays and FUV fields for $T \lesssim 100$ K and reduced for higher temperatures compared to models without X-rays or FUV fields. Estimates from the general parameter study show that CH, CH$^+$, OH, OH$^+$ and H$_2$O$^+$ can have abundances $\approx 10^{-12}$–$10^{-6}$ with respect to the H$_2$ column densities in AFGL 2591 and IRAS 16293. The strongest H$_3$O$^+$ lines observable with Herschel are predicted to have fluxes between 0.2–0.4 K km s$^{-1}$ for AFGL 2591 and $\gtrsim 1$ K km s$^{-1}$ for IRAS 16293–2422. Similar fluxes are predicted
for OH. It is concluded that NH and NH\(^+\) are more sensitive to X-rays than to FUV fields. CH and CH\(^+\), on the other hand, are good tracers for FUV fields. The oxygen bearing hydrides and SH\(^+\) trace X-rays rather than FUV fields in regions with \(T \lesssim 300\) K. A Herschel detection of OH\(^+\) or H\(_2\)O\(^+\) in gas with temperatures \(T \lesssim 300\) K would imply the presence of X-rays since these species are several orders of magnitude enhanced compared to models without X-rays.

### 6.1 Introduction

Atmospheric water vapor makes ground based observations in the submillimeter band difficult. The atmosphere is essentially opaque between approximately 500–600 GHz, 700–800 GHz and above 900 GHz. However, many rotational molecular lines – in particular those of light hydrides – can be found in this frequency regime. The upcoming Herschel Space Observatory enables imaging photometry and spectroscopy in the far infrared and submillimeter wavelength range (e.g., Pilbratt 2003). The Heterodyne Instrument for the Far-Infrared (HIFI) on board the satellite is a very high resolution (0.3–300 km s\(^{-1}\)) spectrometer that will allow to disentangle the expected ‘forest of lines’ and to study dynamically evolving regions (de Graauw & Helmich 2001). HIFI will observe frequencies between 480–1910 GHz (157–625 \(\mu\)m) with half power beam widths (HPBW) of \(\approx 13'' - 39''\). HIFI is therefore well suited to study hydrides at high frequencies with a HPBW that is comparable to those of typical ground based single dish telescopes. Another instrument on board the Herschel satellite is the Photodetector Array Camera & Spectrometer (PACS). It operates either as an imaging photometer or an integral field spectrometer over the spectral band from 57 \(\mu\)m to 210 \(\mu\)m (\(\approx 1428–5360\) GHz). The spectrometer allows simultaneous observations at 57–105 \(\mu\)m and 105–210 \(\mu\)m over a field of view of 47'' \(\times\) 47'', resolved into 5 \(\times\) 5 pixels, with a spectral resolution of \(\approx 75–300\) km s\(^{-1}\) (e.g., Poglitsch et al. 2005). The third instrument carried by Herschel is the Spectral and Photometric Imaging Receiver (SPIRE; e.g., Griffin et al. 2005). SPIRE allows spectral and photometric imaging between 200–670 \(\mu\)m (\(\approx 450–1500\) GHz).

Observations of hydrides are important for understanding the chemistry of molecular clouds and star-forming regions as they are the initial products of the ion-molecule reaction network and therefore potential
building blocks of larger molecules. In addition, simple hydrides such as CH and OH and in particular their ions are predicted to be sensitive tracers of the far ultraviolet (FUV; \(6 \text{ eV} < h\nu < 13.6 \text{ eV}\)) field and X-rays (e.g., Stäuber et al. 2004a, 2005). The probably most abundant hydride ion that will be observed with Herschel is \(\text{H}_3\text{O}^+\) (hydronium), the protonated version of \(\text{H}_2\text{O}\). Ground-based observations by Phillips et al. (1992) have confirmed the relatively high fractional abundance of \(\text{H}_3\text{O}^+\) (\(\approx 10^{-9}\) relative to \(\text{H}_2\)) towards several star-forming regions. \(\text{H}_3\text{O}^+\) is a key ion in the oxygen chemistry since its dissociative recombination leads to \(\text{OH}\) and \(\text{H}_2\text{O}\) (e.g., Herbst & Klemperer 1973). Water itself is one of the most abundant molecules (after \(\text{H}_2\) and \(\text{CO}\)) in the interstellar medium (ISM). The influence of X-rays and FUV fields on water in star-forming environments was most recently studied by Stäuber et al. (2006a). The water abundance was shown to depend strongly on the X-ray flux, and \(\text{H}_3\text{O}^+\) was found to play an important role in the water chemistry since its abundance can be enhanced by the influence of X-rays.

The goal of this paper is to find X-ray tracing hydrides that are observable with Herschel. We study first the radial abundances of simple hydrides in X-ray exposed spherical envelopes of typical Class 0, Class I and high-mass young stellar objects (Sect. 6.2). To distinguish the effects of X-rays and FUV fields, the abundances are studied as a function of temperature for different hydrogen densities, and X-ray and FUV fluxes in Sect. 6.3. The FUV and X-ray models are compared and diagnostics for each type of radiation are discussed. In order to predict line intensities of \(\text{H}_3\text{O}^+\) and \(\text{OH}\) for Herschel, radiative transfer models are used in Sect. 6.4 to calculate line profiles of \(\text{H}_3\text{O}^+\) and \(\text{OH}\) for the different X-ray envelope models found in Sect. 6.2.

### 6.2 Envelope models

The hydrogenated species of carbon, oxygen, sulphur, nitrogen and silicon are studied in envelopes around young stellar objects (YSOs). Protonated and ionized water (\(\text{H}_3\text{O}^+\) and \(\text{H}_2\text{O}^+\)) is also considered. The envelope profiles correspond to those of the high-mass source AFGL 2591, the Class 0 object IRAS 16293–2422 and the Class I source TMC 1. The objects differ in their bolometric luminosity, envelope mass and optical depth and cover a wide range of envelope parameters. Table 6.1 lists the
Table 6.1: Physical parameters of the sources.

<table>
<thead>
<tr>
<th>Source</th>
<th>$L_{bol}$ ($L_\odot$)</th>
<th>Dist. (pc)</th>
<th>$M_{env}$ ($M_\odot$)</th>
<th>$r_{env}$ (AU)</th>
<th>$N$(H$_2$) ($10^{23}$ cm$^{-2}$)</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFGL 2591$^a$</td>
<td>$2 \times 10^4$</td>
<td>1000</td>
<td>44</td>
<td>27000</td>
<td>1.0</td>
<td>HMPO</td>
</tr>
<tr>
<td>IRAS 16293–2422$^b$</td>
<td>27</td>
<td>160</td>
<td>5.4</td>
<td>8000</td>
<td>16.0</td>
<td>Class 0</td>
</tr>
<tr>
<td>TMC 1$^c$</td>
<td>0.66</td>
<td>140</td>
<td>0.034</td>
<td>4300</td>
<td>0.69</td>
<td>Class 1</td>
</tr>
</tbody>
</table>

The luminosity and envelope parameters are from $^a$ van der Tak et al. (1999); $^b$ Schöier et al. (2002); $^c$ Jørgensen et al. (2002). The H$_2$ column densities are radially integrated densities from the power-law density envelopes ($N$(H$_2$) = $\int n(r) \, dr$).

The density and thermal structure of the AFGL 2591 and IRAS 16293–2422 envelopes are taken from the dust continuum models by van der Tak et al. (1999) and Schöier et al. (2002), respectively. For TMC 1, we follow the model results of Jørgensen et al. (2002). The inner structure of these envelopes is poorly known. The density profile in the innermost part is usually obtained by extrapolating the structure of the outer region. Observations by Jørgensen et al. (2005a) imply that the envelope of IRAS 16293–2422 may have a large ($\approx 400–600$ AU radius) hole near the protostar. To study the influence of such a cavity on the X-ray enhanced chemistry, an additional envelope of IRAS 16293–2422 is modeled, assuming a protostellar hole with a radial size of 400 AU. The initial chemical abundances for IRAS 16293–2422 and TMC 1 are taken to be consistent with the models of Doty et al. (2004), those for AFGL 2591 are the same as in Doty et al. (2002). The cosmic-ray ionization rate is varied in the models for each source until the model output was in agreement with the

6.2.1 X-ray models

The density and thermal structure of the AFGL 2591 and IRAS 16293–2422 envelopes are taken from the dust continuum models by van der Tak et al. (1999) and Schöier et al. (2002), respectively. For TMC 1, we follow the model results of Jørgensen et al. (2002). The inner structure of these envelopes is poorly known. The density profile in the innermost part is usually obtained by extrapolating the structure of the outer region. Observations by Jørgensen et al. (2005a) imply that the envelope of IRAS 16293–2422 may have a large ($\approx 400–600$ AU radius) hole near the protostar. To study the influence of such a cavity on the X-ray enhanced chemistry, an additional envelope of IRAS 16293–2422 is modeled, assuming a protostellar hole with a radial size of 400 AU. The initial chemical abundances for IRAS 16293–2422 and TMC 1 are taken to be consistent with the models of Doty et al. (2004), those for AFGL 2591 are the same as in Doty et al. (2002). The cosmic-ray ionization rate is varied in the models for each source until the model output was in agreement with the
observed HCO$^+$ 1–0 abundance in that source. The adapted cosmic-ray ionization rates are $\zeta_{\text{cr}} = 5.6 \times 10^{-17} \text{s}^{-1}$ for AFGL 2591, $7 \times 10^{-17} \text{s}^{-1}$ for IRAS 16293 and $0.8 \times 10^{-17} \text{s}^{-1}$ for TMC 1.

The X-ray flux can be modeled by assuming an X-ray luminosity $L_X$ of the central source and a thermal X-ray spectrum with a temperature $T_X$. The X-rays may be absorbed by some unknown amount of material $N_{\text{in}}(\text{H})$ between the source and the inner edge of the envelope. For the Class 0 and I models, $T_X$ is assumed to be $3 \times 10^7 \text{K}$ and $N_{\text{in}}(\text{H}) = 5 \times 10^{21} \text{cm}^{-2}$. For AFGL 2591 the values are taken to be $7 \times 10^7 - 1 \times 10^8 \text{K}$ and $3 \times 10^{22} \text{cm}^{-2}$, according to the results of Stäuber et al. (2005).

### 6.2.2 Results

The hydride abundances for different X-ray luminosities are presented in Figs. 6.1-6.4. The results of AFGL 2591 and IRAS 16293 are presented for the chemical ages found in previous models by Schöier et al. (2002) and Doty et al. (2002, 2004). For TMC 1 we assume $t = 10^5 \text{yrs}$, appropriate for Class I sources. The figures show the radial abundances out to $\approx 20''$, which is half of Herschel’s biggest HPBW.

The qualitative distribution of the hydrides with position is in general similar in the different envelopes. In models without X-rays, the abundance decreases towards the dense and warm center where more complex molecules are formed. X-rays cause dissociations and ionizations that lead to the enhancement of the simple hydrides in the inner part of the envelope. Some neutral hydrides (e.g., OH and SH) may also be reduced at $T \gtrsim 100 \text{K}$, depending on the central X-ray luminosity. AFGL 2591 and TMC 1 have less dense inner regions than IRAS 16293–2422 ($n(\text{H}_2) < 10^9 \text{cm}^{-3}$) and X-rays can penetrate more easily into the envelope and enhance species at large distances for lower X-ray luminosities.

Comparison of the two IRAS 16293–2422 models shows that X-rays with luminosities $L_X \gtrsim 10^{31} \text{erg s}^{-1}$ can enhance the species out to a radial distance of $\approx 600–1000 \text{AU}$ in the envelope without an inner cavity (Fig. 6.1) and throughout the whole envelope in the model with a protostellar hole (Fig. 6.2). Owing to the presence of circumstellar disks in the inner 400–600 AU, however, the X-rays will be shielded in the direction of the disks. The protostellar hole model is therefore only valid for less shielded parts of the envelope.
The abundance jump in some of the species close to the protostar (≈ 100 AU for IRAS 16293, ≈ 1000 AU for AFGL 2591 and ≈ 10 AU for TMC 1) is due to the evaporation of water from dust grains into the gas phase that alters the chemistry (e.g., Doty et al. 2002). This jump cannot be seen in the models for IRAS 16293 with an inner cavity (Fig. 6.2) since the temperature there does not exceed ≈ 40 K and most water remains depleted on grains. A similar jump can be noticed in the outer part of the low-mass envelopes due to the freeze out of CO at ≈ 30 K (≈ 1000 AU). This effect is not included in the AFGL 2591 models.

The usual detection limit within 2.5 hours of integration for species with critical densities between $10^6$–$10^7$ cm$^{-3}$ and Einstein $A$ coefficients of the order $10^{-3}$ s$^{-1}$ for these sources is $x(i) < 10^{-13}$–$10^{-12}$ with ground based telescopes with beams of ≈ 14″ (e.g., Stäuber et al. 2006b). Such abundances are only reached by CH, OH, NH and H$_3$O$^+$. SH, SH$^+$ and OH$^+$ have abundances of this order only in the innermost region of the envelope. These species may also be strongly enhanced, for example, along outflow walls. Estimates for such a scenario will be presented in Sect. 6.3.1. SiH has abundances $\lesssim 10^{-14}$. The abundances of SiH and SiH$^+$, however, are very uncertain. The silicon abundance in the gas is poorly known. The initial abundance in our model is $x(\text{Si}) = 2 \times 10^{-8}$ relative to H$_2$. Silicon can have abundances up to a few $\times 10^{-5}$ on grains that can be released into the gas in shocked region (e.g., Martín-Pintado et al. 1992; Garay et al. 2002), altering locally the gas-phase Si abundance. Such effects were not included in our models.

### 6.3 General parameter study

The abundances of neutral and ionized CH, OH, SH and NH as well as H$_2$O$^+$ and H$_3$O$^+$ are studied as functions of the gas temperature, hydrogen density ($n_H = n(\text{H}) + 2n(\text{H}_2)$) and X-ray or FUV flux. The gas temperature covers 30–1000 K. The density is taken to be constant at $n_H = 10^6$ and $10^7$ cm$^{-3}$, respectively. The X-ray flux is varied between $F_X = 10^{-4}$–$1$ erg s$^{-1}$ cm$^{-2}$. The FUV flux is between $G_0 = 10$–$1000$ at $A_V = 0$. Evaporation of H$_2$O from dust at 100 K is taken into account. Other model parameters are taken to be consistent with the H$_2$O models of Stäuber et al. (2006a). It should be mentioned, however, that the initial sulphur abundance is taken to be $10^{-8}$ for $T > 100$ K which corresponds
Figure 6.1: Radial abundances for the prototypical Class 0 YSO IRAS 16293-2422 without an inner hole for different X-ray luminosities $L_X$ (ergs$^{-1}$). The solid line corresponds to the model without X-rays.
Figure 6.2: Radial abundances for IRAS 16293-2422 assuming a protostellar hole of the size 400 AU for different X-ray luminosities $L_X$ (erg s⁻¹). The solid line corresponds to the model without X-rays.
Figure 6.3: Radial abundances for the high-mass source AFGL 2591 for different X-ray luminosities $L_X$ (erg s$^{-1}$). The solid line corresponds to the model without X-rays.
Figure 6.4: Radial abundances for the Class I object TMC 1 for different X-ray luminosities $L_X$ (ergs$^{-1}$). The solid line corresponds to the model without X-rays.
6.3. General parameter study

The low-mass models of Doty et al. (2004). The sulphur abundance in AFGL 2591 is $160 \times$ higher. The results are presented in Figs. 6.5–6.9 for $t = 5 \times 10^4$ yrs. Table 6.2 provides a summary of the results found in the general parameter study.

CH and CH$^+$ can be enhanced to fractional abundances $\approx 10^{-7}$ and $\approx 10^{-11}$, respectively, for FUV fields $G_0 \gtrsim 50$ (Fig. 6.5). To reach similar abundances with X-rays requires $F_X \gtrsim 1$ erg s$^{-1}$ cm$^{-2}$. The reason for this is that FUV fields can efficiently dissociate CO and ionize carbon (ionization potential $E_{ip} = 11.26$ eV). Following a series of hydrogenation forming CH$^+$, CH$_2^+$ etc., C$^+$ can be quickly transformed into carbon hydrides. Large chains of C and H can build up as often observed in photodissociation regions (PDRs; e.g., Fuente et al. 2003). A general parameter study for C$_2$H and C$_3$H$_2$ shows that these species can indeed be enhanced to $x$(C$_2$H) $\approx 10^{-8}$ and $x$(C$_3$H$_2$) $\approx 10^{-10}$–$10^{-8}$ for $G_0 \lesssim 1000$. However, the larger molecules can also be photo-dissociated to form CH or CH$^+$.

OH and OH$^+$ are largely produced by X-rays and can be enhanced to $x$(OH) $\approx 10^{-6}$ and $x$(OH$^+$) $\approx 10^{-11}$ for $F_X = 1$ erg s$^{-1}$ cm$^{-2}$ (Fig. 6.6).

Figure 6.5: Temperature dependent fractional abundances of CH and CH$^+$ for $n_H = 10^6$ cm$^{-3}$ and $n_H = 10^7$ cm$^{-3}$. The upper figures show the abundances for different X-ray fluxes: $F_X = 10^{-4}$ erg s$^{-1}$ cm$^{-2}$ (dotted line), $F_X = 10^{-3}$ erg s$^{-1}$ cm$^{-2}$ (dashed line), $F_X = 10^{-2}$ erg s$^{-1}$ cm$^{-2}$ (dashed-dotted line), $F_X = 1$ erg s$^{-1}$ cm$^{-2}$ (dashed-dotted-dotted line). The FUV models are in the lower figures with $G_0 = 10$ (dotted line), $G_0 = 50$ (dashed line), $G_0 = 100$ (dashed-dotted line) and $G_0 = 1000$ (dashed-dotted-dotted line). The solid line corresponds to the models without X-rays or FUV fields.
Figure 6.6: Temperature dependent fractional abundances of OH and OH$^+$ for $n_H = 10^6 \text{ cm}^{-3}$ and $n_H = 10^7 \text{ cm}^{-3}$. The upper figures show the abundances for different X-ray fluxes: $F_X = 10^{-4} \text{ erg s}^{-1} \text{ cm}^{-2}$ (dotted line), $F_X = 10^{-3} \text{ erg s}^{-1} \text{ cm}^{-2}$ (dashed line), $F_X = 10^{-2} \text{ erg s}^{-1} \text{ cm}^{-2}$ (dashed-dotted line), $F_X = 1 \text{ erg s}^{-1} \text{ cm}^{-2}$ (dashed-dotted-dotted line). The FUV models are in the lower figures with $G_0 = 10$ (dotted line), $G_0 = 50$ (dashed line), $G_0 = 100$ (dashed-dotted line) and $G_0 = 1000$ (dashed-dotted-dotted line). The solid line corresponds to the models without X-rays or FUV fields.

FUV fields can enhance the species only for $T \gtrsim 300 \text{ K}$. The same is true for H$_3$O$^+$ and H$_2$O$^+$. X-rays can efficiently ionize H$_2$ ($E_{\text{ip}} = 15.4 \text{ eV}$) and produce large amounts of H$_2^+$ which is quickly turned into H$_3^+$. H$_3^+$ reacts with oxygen and forms OH$^+$. Successive hydrogenation leads first to H$_2$O$^+$ and then to H$_3$O$^+$ which in turn can recombine to OH. FUV fields can produce large amounts of atomic oxygen by the dissociation of CO, but cannot ionize O since the threshold is slightly above 13.6 eV ($E_{\text{ip}} = 13.62 \text{ eV}$). FUV fields produce orders of magnitude more electrons per path length than X-rays with comparable fluxes ($x(e^-) \approx 10^{-4}$ for $G_0 = 1000$ and $x(e^-) \approx 10^{-6}$ for $F_X = 1 \text{ erg s}^{-1} \text{ cm}^{-2}$). H$_3$O$^+$ is reduced by FUV fields for $T \lesssim 300 \text{ K}$ due to fast electron recombination reactions. At temperatures $T \gtrsim 300 \text{ K}$, water can be efficiently produced leading to higher abundances of the oxygen bearing hydrides through photoionization and dissociation of H$_2$O. H$_3$O$^+$ is then mainly formed by H$_2$O$^+ + \text{H}_2 \rightarrow \text{H}_3\text{O}^+ + \text{H}$.

The nitrogen hydrides are clearly more enhanced by X-rays than by FUV fields (Fig. 6.7). With $F_X = 1 \text{ erg s}^{-1} \text{ cm}^{-2}$, they have fractional abundances of $x(\text{NH}) \approx 10^{-8}$ and $x(\text{NH}^+) \approx 10^{-12}$. Nitrogen has an
ionization potential above 13.6 eV ($E_{\text{ip}} = 14.53 \text{ eV}$) and can thus not be ionized by FUV photons. The reaction of N$^+$ with molecular hydrogen is, however, the main production process of NH$^+$. NH and NH$^+$ can be enhanced by FUV fields only at temperatures $T > 400 \text{ K}$. But even at high temperatures FUV fields of the order $G_0 = 1000$ do not produce as much NH and NH$^+$ as X-rays. The nitrogen hydrides are therefore excellent tracers for X-rays. The main mechanism to produce NH in the FUV models at high temperatures is the temperature dependent reaction of nitrogen with H$_2$. Once NH is formed, it can be ionized by FUV photons to produce NH$^+$ ($E_{\text{ip}} = 13.49 \text{ eV}$).

The dependence of SH and SH$^+$ on X-rays and FUV fields is somewhat more complex since there is a strong temperature dependence for $T > 100 \text{ K}$. SH can only be enhanced for temperatures below $T < 100 \text{ K}$. SH$^+$, on the other hand, can be enhanced up to $\approx 10^{-12}$ with X-rays for all temperatures ($T = 30 - 1000 \text{ K}$). FUV fields produce such abundances only for $T > 800 \text{ K}$, making SH$^+$ also a valuable species to distinguish X-rays from FUV fields. In the X-ray models, SH$^+$ is mainly produced in reactions of atomic sulphur and H$_3^+$ for $T > 300 \text{ K}$. At higher tem-
Figure 6.8: Temperature dependent fractional abundances of SH and SH$^+$ for $n_H = 10^6 \text{ cm}^{-3}$ and $n_H = 10^7 \text{ cm}^{-3}$. The upper figures show the abundances for different X-ray fluxes: $F_X = 10^{-4} \text{ erg s}^{-1} \text{ cm}^{-2}$ (dotted line), $F_X = 10^{-3} \text{ erg s}^{-1} \text{ cm}^{-2}$ (dashed line), $F_X = 10^{-2} \text{ erg s}^{-1} \text{ cm}^{-2}$ (dashed-dotted line), $F_X = 1 \text{ erg s}^{-1} \text{ cm}^{-2}$ (dashed-dotted-dotted line). The FUV models are in the lower figures with $G_0 = 10$ (dotted line), $G_0 = 50$ (dashed line), $G_0 = 100$ (dashed-dotted line) and $G_0 = 1000$ (dashed-dotted-dotted line). The solid line corresponds to the models without X-rays or FUV fields.

At temperatures, the reaction of $S^+$ with molecular hydrogen is the dominant production source of SH$^+$. Since sulphur has an ionization potential of $E_{\text{ip}} = 10.36 \text{ eV}$, it can be ionized by FUV fields too. At lower temperatures in the FUV models, SH$^+$ is mainly produced in reactions of $\text{H}_2S^+$ with oxygen or hydrogen. The fast electron recombinations, however, quickly reduce the SH$^+$ abundances.

6.3.1 Estimates of fractional hydride abundances in AFGL 2591 and IRAS 16293–2422

The general parameter study has shown that nitrogen hydrides trace X-rays rather than FUV fields and SH$^+$ and the oxygen hydrides trace X-rays in regions with $T \lesssim 300 \text{ K}$. The presence of FUV fields as low as $G_0 = 10$, on the other hand, enhances the carbon hydrides to high abundances, making them excellent tracers for FUV fields.

To disentangle FUV fields and X-rays in regions with $T \gtrsim 300 \text{ K}$ will be difficult though and may only be possible by the detection of
6.3. General parameter study

Figure 6.9: Temperature dependent fractional abundances of H$_3$O$^+$ and H$_2$O$^+$ for $n_{\text{H}} = 10^6$ cm$^{-3}$ and $n_{\text{H}} = 10^7$ cm$^{-3}$. The upper figures show the abundances for different X-ray fluxes: $F_X = 10^{-4}$ erg s$^{-1}$ cm$^{-2}$ (dotted line), $F_X = 10^{-3}$ erg s$^{-1}$ cm$^{-2}$ (dashed line), $F_X = 10^{-2}$ erg s$^{-1}$ cm$^{-2}$ (dashed-dotted line), $F_X = 1$ erg s$^{-1}$ cm$^{-2}$ (dashed-dotted-dotted line). The FUV models are in the lower figures with $G_0 = 10$ (dotted line), $G_0 = 50$ (dashed line), $G_0 = 100$ (dashed-dotted line) and $G_0 = 1000$ (dashed-dotted-dotted line). The solid line corresponds to the models without X-rays or FUV fields.

highly abundant NH or NH$^+$. It should be mentioned, however, that FUV photons are absorbed in the innermost part of the envelope in the spherical models (Stäuber et al. 2004a) and FUV fields from the central source may only be probed along the outflow walls of the young stellar objects. Such a scenario was suggested by Stäuber et al. (2006b) to explain the observed CO$^+$ abundances in high-mass young stellar objects. It was found that FUV (or X-ray) enhanced outflow walls may contribute $\approx 6 - 40\%$ of the emission observed in a $14''$ beam. The hydrides may thus be observed with much higher fractional abundances than predicted in the spherical models in Sect. 6.2.2 if they are enhanced in or along the outflows.

In case of the low mass objects, observations of CO$^+$ and CN were interpreted as the result of an X-ray enhanced chemistry and CO$^+$ was suggested to trace a region with $n_{\text{H}} \approx 10^6$ cm$^{-3}$ and $T \gtrsim 100$ K close to the protostar. Outflows were thought to be less important for the low-mass sources. Applying the FUV field strength and X-ray flux found by Stäuber et al. (2006b) from fitting the observations towards AFGL 2591 and IRAS 16293–2422 to the hydride models in this section, allows to
### Table 6.2: Molecular tracers for enhanced X-ray and FUV fluxes\(^a\).

<table>
<thead>
<tr>
<th>Molecule</th>
<th>X-rays</th>
<th>FUV ((T \lesssim 300, \text{K}))</th>
<th>FUV ((T \gtrsim 300, \text{K}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH</td>
<td>x</td>
<td>xx</td>
<td>xx</td>
</tr>
<tr>
<td>CH(^+)</td>
<td>x</td>
<td>xx</td>
<td>xx</td>
</tr>
<tr>
<td>OH</td>
<td>x</td>
<td>xx</td>
<td>xx</td>
</tr>
<tr>
<td>OH(^+)</td>
<td>x</td>
<td>xx</td>
<td>xx</td>
</tr>
<tr>
<td>NH</td>
<td>(\text{xx}^b)</td>
<td>(\text{x}^c)</td>
<td>(\text{x}^c)</td>
</tr>
<tr>
<td>NH(^+)</td>
<td>(\text{xx})</td>
<td>(\text{x}^c)</td>
<td>(\text{x}^c)</td>
</tr>
<tr>
<td>SH</td>
<td>(\text{xx}^d)</td>
<td>(\text{x}^d)</td>
<td>(\text{x}^d)</td>
</tr>
<tr>
<td>SH(^+)</td>
<td>xx</td>
<td>xx</td>
<td>xx</td>
</tr>
<tr>
<td>H(_3)O(^+)</td>
<td>xx</td>
<td>xx</td>
<td>xx</td>
</tr>
<tr>
<td>H(_2)O(^+)</td>
<td>x</td>
<td>xx</td>
<td>xx</td>
</tr>
</tbody>
</table>

\(^a\) "x" means that the species can be enhanced in comparison to models without X-rays or FUV, respectively, and "xx" means that the highest abundances are reached here; \(^b\) preferably enhanced for \(T \lesssim 100\, \text{K}\); \(^c\) only enhanced for \(T \gtrsim 500\, \text{K}\); \(^d\) only enhanced for \(T \lesssim 100\, \text{K}\).

estimate the fractional hydride abundances in these sources in a more realistic way. The results of this simple estimate are presented in Table 6.3.

Predictions of SH, NH, NH\(^+\) and H\(_3\)O\(^+\) towards AFGL 2591 are difficult in the FUV enhanced outflow cavity wall scenario since their abundances can be reduced by the presence of FUV fields. These species probably trace FUV shielded regions in the envelope (Sect. 6.2.2). The derived H\(_3\)O\(^+\) abundance for IRAS 16293–2422 is an upper limit since only X-rays but no FUV fields were considered, which are likely to be present in the innermost region of the envelope. For comparison, the H\(_3\)O\(^+\) abundance in the FUV models is only \(\approx 10^{-12}\). To study the H\(_3\)O\(^+\) abundance under the influence of both X-rays and FUV fields, additional models have been run with \(G_0 = 100 - 1000\) and \(F_X = 10^{-2}\, \text{erg s}^{-1}\, \text{cm}^{-2}\). They show that the H\(_3\)O\(^+\) abundance is \(\approx 10^{-10}\) for temperatures below \(\approx 300\, \text{K}\). H\(_3\)O\(^+\) may therefore not trace regions close to the protostar or outflow walls where FUV fields are likely to be present but may trace the cosmic-ray ionization rate and X-ray flux in the FUV shielded envelope. This will be further investigated in Sect. 6.4.1, where H\(_3\)O\(^+\) lines are calculated for the
AFGL 2591 spherical X-ray envelope models (Sect. 6.2.2) and compared to the outflow cavity wall scenario. SH is also difficult to predict, since its abundance can be enhanced for $T \lesssim 100$ K and reduced for higher temperatures. A mean value derived from Fig. 6.8 at high X-ray fluxes and/or FUV fields is $\lesssim 10^{-12}$ relative to H$_2$ for both objects.

Comparison of the CH, CH$^+$, OH, OH$^+$ and H$_2$O$^+$ fractional abundances in Table 6.3 to those of the envelope models in Sect. 6.2.2 shows that higher abundances (between $10^{-12}$ to $10^{-6}$) are expected to be observed with Herschel than predicted by the envelope models. It should be mentioned, however, that the estimated abundances in Table 6.3 are – strictly speaking – only valid if they are assumed to be constant relative to H$_2$ in a spherical envelope seen by a 14" (JCMT) beam since this is how the CO$^+$ and CN abundances were derived before compared to the general parameter study models. No conclusion can be drawn on abundances outside the JCMT beam. If the abundances dropped significantly at $> 14"$, the beam dilution for a 39" beam would be a factor of $\approx 8$.

### 6.3.2 H$_3$O$^+$ to H$_2$O abundance ratio

H$_3$O$^+$ can quickly ($\approx 10^{-7}$ cm$^3$s$^{-1}$) recombine to H$_2$O. Knowing the electron fraction and the recombination rate therefore allows to estimate the water abundance in star-forming regions from H$_3$O$^+$ observations. The H$_3$O$^+$ to H$_2$O ratio was estimated to be $\approx 10^{-3}$ by Phillips et al. (1992) from CSO observations of H$_3$O$^+$ at frequencies between $\approx 300 - 400$ GHz using a simple chemical model.

To study the H$_3$O$^+$ to water ratio in X-ray enhanced environments, the ratio is calculated as a function of temperature for different X-ray fluxes and densities between $10^5 - 10^8$ cm$^{-3}$. The results are presented in Fig. 6.10. It can be seen that $x(\text{H}_3\text{O}^+)/x(\text{H}_2\text{O}) \approx 10^{-3}$ only holds for $n_\text{H} = 10^5$ cm$^{-3}$ and $T \geq 100$ K in models without X-rays. With higher densities, the recombination of H$_3$O$^+$ to OH and H$_2$O proceeds faster and the ratio decreases. The ratio increases with increasing gas temperature in models without X-rays. The ratio is generally higher in the models with X-rays for temperatures $T \gtrsim 300$ K compared to lower temperatures. The X-ray models lead to ratios between $10^{-3} - 10^{-1}$, depending on temperature and X-ray flux. At high densities ($n_\text{H} = 10^8$ cm$^{-3}$), the ratio increases gradually with increasing X-ray flux. At this density, the ratio is $\approx 10^{-6}$ in the models without X-rays and $\approx 10^{-3}$
Table 6.3: Predicted fractional abundances $x(i)$ relative to H$_2$ due to FUV enhanced regions along the outflow walls for AFGL 2591 and X-ray enhanced regions for IRAS 16293–2422.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>$x(i)^a$</th>
<th>$x(i)^b$</th>
</tr>
</thead>
<tbody>
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<td>$10^{-8}$</td>
</tr>
<tr>
<td>CH$^+$</td>
<td>$10^{-10}$</td>
<td>$10^{-12}$</td>
</tr>
<tr>
<td>OH</td>
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<td>$10^{-7}$</td>
</tr>
<tr>
<td>OH$^+$</td>
<td>$10^{-11}$</td>
<td>$10^{-11}$</td>
</tr>
<tr>
<td>NH</td>
<td>$&lt; 10^{-11}$</td>
<td>$10^{-8}$</td>
</tr>
<tr>
<td>NH$^+$</td>
<td>$&lt; 10^{-14}$</td>
<td>$&lt; 10^{-13}$</td>
</tr>
<tr>
<td>SH</td>
<td>$&lt; 10^{-12}$</td>
<td>$&lt; 10^{-12}$</td>
</tr>
<tr>
<td>SH$^+$</td>
<td>$10^{-13}$</td>
<td>$10^{-13}$</td>
</tr>
<tr>
<td>H$_3$O$^+$</td>
<td>$10^{-9}$</td>
<td>$&lt; 10^{-8}$</td>
</tr>
<tr>
<td>H$_2$O$^+$</td>
<td>$10^{-11}$</td>
<td>$10^{-11}$</td>
</tr>
</tbody>
</table>

$^a$ The fractional abundances refer to a total hydrogen column density for AFGL 2591 of $N$(H$_2$) = $10^{23}$ cm$^{-2}$. $^b$ The fractional abundances refer to a total hydrogen column density for IRAS 16293–2422 of $N$(H$_2$) = $1.6 \times 10^{24}$ cm$^{-2}$. $^c$ The species are difficult to predict due to their different behavior in X-ray and FUV enhanced regions (see text).

in models with $F_X \gtrsim 10^{-1}$ erg s$^{-1}$ cm$^{-2}$. The ratio is also calculated for the FUV models and it is seen that the ratio is $\gtrsim 10^{-3}$ only for temperatures $T \gtrsim 300$ K. At lower temperatures, the ratio is $\approx 10^{-8}$. High H$_3$O$^+$ to water ratios ($\gtrsim 10^{-3}$) in regions with $n_H \gtrsim 10^6$ cm$^{-3}$ and $T \lesssim 300$ K therefore indicate the presence of X-rays.

6.4 Radiative transfer modeling

6.4.1 H$_3$O$^+$

H$_3$O$^+$ submillimeter lines that are accessible from ground based telescopes were observed towards several star-forming regions by Wootten et al. (1991) and Phillips et al. (1992). Typical abundances were found to be
6.4. Radiative transfer modeling

Figure 6.10: Temperature dependent fractional abundances of H$_3$O$^+$ relative to H$_2$O for different densities (cm$^{-3}$) and X-ray fluxes (ergs$^{-1}$cm$^{-2}$) for $t = 5 \times 10^4$ yrs.

a few $\times 10^{-10}$–$10^{-9}$ with respect to H$_2$. Goicoechea & Cernicharo (2001) observed H$_3$O$^+$ towards the Sagittarius B2 molecular cloud in the far-infrared with the Infrared Space Observatory (ISO). They derived an abundance $x$(H$_3$O$^+$) $\approx 10^{-9}$, consistent with the submillimeter results. The ortho to para ratio was found to be $\approx 1$.

Phillips et al. (1992) observed H$_3$O$^+$ lines at 307 GHz, 364 GHz and 396 GHz towards star-forming regions (including IRAS 16293–2422) with the CSO. The lines towards IRAS 16293–2422, however, were not detected. The upper limit in the main beam temperature at 396 GHz was $T_{\text{mb}} \approx 0.13$ K. The lines at 396 GHz and 364 GHz were detected towards, e.g., W3 IRS5 with line fluxes (and $T_{\text{mb}}$) of 2.2 K km s$^{-1}$ (0.6 K) and 0.74 K km s$^{-1}$ (0.2 K), respectively. Upper limits for the H$_3$O$^+$ 364 GHz line towards several massive star-forming regions (including AFGL 2591) were reported by van der Tak et al. (2006) with $T_{\text{mb}} \lesssim 0.13 - 0.21$ K.

H$_3$O$^+$ is thought to trace the X-ray and cosmic ray ionization rate in FUV shielded envelopes (Sect. 6.3). To test this and to compare the X-ray model results of AFGL 2591 and IRAS 16293–2422 (Sect. 6.2.2) to the observations of Phillips et al. (1992) and van der Tak et al. (2006) and
also to predict line intensities for Herschel HIFI, the line profiles of \( \text{H}_3\text{O}^+ \) are calculated using the radiative transfer code by Hogerheijde & van der Tak (2000). Molecular data for calculating the excitation of \( \text{H}_3\text{O}^+ \) is taken from the LAMDA database\(^1\). These collisional rate coefficients have been computed by Offer & van Hemert (1992) using a model potential based on that of \( \text{NH}_3-\text{H}_2 \) but with the appropriate long-range terms for interaction of \( \text{H}_2 \) with an ion. The brightness distribution is integrated in the line of sight and convolved with an appropriate beam size. The beam widths at 307 GHz, 364 GHz and 396 GHz are 21", 20" and 18", respectively, corresponding to CSO beam widths. The beam sizes for the higher frequencies (984–1663 GHz) correspond to those of Herschel's HIFI (21" and 13", respectively). The \( \text{H}_3\text{O}^+ \) ortho to para ratio is assumed to be 1. The Doppler parameter (1/e width) is assumed to be 1.6 km s\(^{-1}\) for AFGL 2591 and 0.8 km s\(^{-1}\) for IRAS 16293-2422. The \( \text{H}_3\text{O}^+ \) abundances for the outflow cavity wall model were assumed to be enhanced by FUV fields only in the region with \( T \gtrsim 300 \) K. In this region, \( x(\text{H}_3\text{O}^+) \) is taken to be between \( 10^{-9} \) and \( 10^{-7} \) according to Fig. 6.9.

The line intensities and profiles of AFGL 2591 are presented in Fig. 6.11 for the ortho \( \text{H}_3\text{O}^+ \) lines and in Fig. 6.12 for the para lines. Since some of the lines show strong non-Gaussian features, the line flux is calculated by integrating the intensity from \(-10 \) km s\(^{-1}\) to \( 10 \) km s\(^{-1}\) rather than fitting a Gaussian profile to the lines. The results are presented in Table 6.4 for AFGL 2591. The strongest \( \text{H}_3\text{O}^+ \) line in AFGL 2591 detectable with HIFI (≥ 480 GHz) is at 1663 GHz. The line fluxes generally increase with increasing X-ray luminosity. The highest flux ratio of models with X-rays compared to models without X-rays has the line at 1616 GHz with an enhancement factor of \( F(L_X = 8 \times 10^{31})/F(L_X = 0) \approx 15 \). It can also be seen in Table 6.4 that the FUV enhanced outflow cavity wall scenario leads to smaller line fluxes than the X-ray models with \( L_X = 8 \times 10^{31} \) erg s\(^{-1}\). In general, lines with higher excitation temperatures have higher abundances compared to models with \( L_X = 0 \). For example, the lines with the highest ratio \( F(\text{FUV})/F(L_X = 0) \) are the lines at 1031 GHz and 1616 GHz. Both have excitation temperatures \( T_{\text{ex}} > 200 \) K. Thus, these lines trace regions with high temperatures.

To compare the 364 GHz line to the upper limits observed by van der Tak et al. (2006), the line for the \( L_X = 8 \times 10^{31} \) erg s\(^{-1}\) model is also

\(^1\)www.strw.leidenuniv.nl/~moldata/
Table 6.4: Modeled H$_3$O$^+$ line fluxes [K km s$^{-1}$] in AFGL 2591 for different X-ray luminosities $L_X$ [ergs$^{-1}$].

<table>
<thead>
<tr>
<th>Otho H$_3$O$^+$</th>
<th>$J_K$</th>
<th>$L_X$</th>
<th>$L_X$</th>
<th>$L_X$</th>
<th>$L_X$</th>
<th>FUV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0</td>
<td>10$^{30}$</td>
<td>10$^{31}$</td>
<td>8 $\times 10^{31}$</td>
<td></td>
</tr>
<tr>
<td>396$^a$</td>
<td>$3^+_0-2^-_0$</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>1.2</td>
<td>0.2</td>
</tr>
<tr>
<td>984$^b$</td>
<td>$0^-_0-1^+_0$</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.09</td>
<td>0.05</td>
</tr>
<tr>
<td>1031$^b$</td>
<td>$4^+_3-3^-_3$</td>
<td>0.03</td>
<td>0.03</td>
<td>0.05</td>
<td>0.2</td>
<td>0.07</td>
</tr>
<tr>
<td>1616$^c$</td>
<td>$4^-_3-4^-_3$</td>
<td>0.002</td>
<td>0.003</td>
<td>0.007</td>
<td>0.03</td>
<td>0.009</td>
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<tr>
<td>1663$^c$</td>
<td>$3^-_3-3^-_3$</td>
<td>0.1</td>
<td>0.1</td>
<td>0.2</td>
<td>0.4</td>
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</table>

<table>
<thead>
<tr>
<th>Para H$_3$O$^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$307^b$</td>
</tr>
<tr>
<td>$364^d$</td>
</tr>
<tr>
<td>$388^c$</td>
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<td>$1632^c$</td>
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<td>$1655^c$</td>
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<tr>
<td>$1657^c$</td>
</tr>
</tbody>
</table>

$^a$ Convolved to a beam size of 18", $^b$ 21", $^c$ 13", $^d$ 20" and $^e$ 19", respectively.

The line flux is then 0.59 K km s$^{-1}$ with $T_{mb} = 0.23$ K. The main beam temperature is slightly higher compared to the upper limit. However, assuming a similar line width ($\Delta V = 5.4$ km s$^{-1}$) as observed by Phillips et al. (1992) towards W3 IRS5 for this line, the main beam temperature of the 364 GHz line is 0.08 K and therefore well below the upper limit. The line fluxes at 364 GHz and 396 GHz for $L_X = 8 \times 10^{31}$ erg s$^{-1}$ are comparable to those observed by Phillips et al. (1992) towards W3 IRS5.

The results for IRAS 16293–2422 are presented in Figs. 6.13 and 6.14 and in Table 6.5. The strongest H$_3$O$^+$ lines in IRAS 16293–2422 detectable with HIFI are those at 984 GHz and 1663 GHz, depending on the X-ray luminosity. The line with the highest flux ratio of models with X-rays compared to models without X-rays is at 1616 GHz with $F(L_X = 10^{30})/F(L_X = 0) \approx 20$. Compared to the line fluxes predicted for AFGL 2591 (Table 6.4), the lines are in general stronger in the IRAS 16293 models. This is due to the high critical densities of these lines.
Figure 6.11: Line profiles of the ortho $\text{H}_3\text{O}^+$ lines for the AFGL 2591 X-ray envelope models (Fig. 6.3). The solid line corresponds to the model without X-rays, the dashed line is $L_X = 10^{30}\text{erg}\text{s}^{-1}$, the dotted line is $L_X = 10^{31}\text{erg}\text{s}^{-1}$ and dashed-dotted line corresponds to $L_X = 8 \times 10^{31}\text{erg}\text{s}^{-1}$.
Figure 6.12: Line profiles of the para H$_2$O$^+$ lines for the AFGL 2591 X-ray envelope models (Fig. 6.3). The solid line corresponds to the model without X-rays, the dashed line is $L_X = 10^{30}$ ergs$^{-1}$, the dotted line is $L_X = 10^{31}$ ergs$^{-1}$ and dashed-dotted line corresponds to $L_X = 8 \times 10^{31}$ ergs$^{-1}$.
Table 6.5: Modeled H$_3$O$^+$ line fluxes [K km s$^{-1}$] in IRAS 16293–2422 for different X-ray luminosities.

<table>
<thead>
<tr>
<th>Otho H$_3$O$^+$</th>
<th>$J_K$</th>
<th>beam</th>
<th>$L_X$</th>
<th>$L_X$</th>
<th>$L_X$</th>
</tr>
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<td>0</td>
<td>10$^{29}$</td>
<td>10$^{30}$</td>
</tr>
<tr>
<td>396</td>
<td>$3^+_0 - 2^-_0$</td>
<td>18</td>
<td>0.2</td>
<td>0.2</td>
<td>0.4</td>
</tr>
<tr>
<td>984</td>
<td>$0^-_0 - 1^+_0$</td>
<td>21</td>
<td>0.9</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>1031</td>
<td>$4^+_3 - 3^-_3$</td>
<td>21</td>
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($n_{\text{crit}} > 10^6 \text{cm}^{-3}$). The region with high densities is smaller in AFGL 2591 than in IRAS 16293–2422 and therefore more beam diluted.

It can be seen in Fig. 6.13 for the 396 GHz line, that only the models with $L_X \lesssim 10^{29}$ erg s$^{-1}$ are within the upper limit ($T_{mb} \lesssim 0.13$ K) observed by Phillips et al. (1992). The model with $L_X = 10^{30}$ erg s$^{-1}$ has $T_{mb} = 0.25$ K, which is already a factor of two above the upper limit. However, large uncertainties exist in the line fluxes due to the collisional rate coefficients and due to the assumption of a spherically symmetric envelope. The upper limit for $L_X$ may therefore be higher.

The ortho and para H$_3$O$^+$ lines are also calculated for the Class I envelope of TMC 1 using the X-ray models of Sect. 6.2.2. The results are presented in Table 6.6. Since the lines are weak, the line fluxes are multiplied by 1000. The strongest lines are at 1663 GHz ($T_{mb} = 25$ mK) and at 984 GHz ($T_{mb} = 17$ mK) for the model with $L_X = 10^{31}$ erg s$^{-1}$. The highest enhancement due to X-rays can again be seen in the fluxes of the 1616 GHz line where an enhancement up to a factor of $\approx 4500$ is possible for $L_X = 10^{31}$ erg s$^{-1}$.
Figure 6.13: Line profiles of the ortho $\mathrm{H_3O^+}$ lines for the IRAS 16293–2422 X-ray envelope models without a protostellar hole (Fig. 6.1). The solid line corresponds to the model without X-rays, the dashed line is $L_X = 10^{29}\,\text{erg s}^{-1}$ and the dotted line is $L_X = 10^{30}\,\text{erg s}^{-1}$. The dashed horizontal line in the 396 GHz spectrum indicates the upper limit observed by Phillips et al. (1992).
Chapter 6. Herschel's view of X-rays

Figure 6.14: Line profiles of the para H$_3$O$^+$ lines for the IRAS 16293–2422 X-ray envelope models without a protostellar hole (Fig. 6.1). The solid line corresponds to the model without X-rays, the dashed line is $L_X = 10^{29}$ erg s$^{-1}$ and the dotted line is $L_X = 10^{30}$ erg s$^{-1}$. 
Table 6.6: Modeled H$_3$O$^+$ line fluxes [10$^{-3}$ K km s$^{-1}$] in TMC 1 for different X-ray luminosities and for the FUV outflow cavity wall scenario without X-rays.

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6.4.2 OH

Pure rotational lines of OH were observed in star-forming regions with ISO (e.g., Ceccarelli et al. 1998; Giannini et al. 2001; Goicoechea et al. 2006). Typical derived abundances are $\approx 10^{-6}$ to $10^{-5}$ with respect to H$_2$ (see van Dishoeck 2004 for a detailed review).

OH lines are calculated for AFGL 2591 and IRAS 16293–2422 using the molecular data provided by the LAMDA database. The collisional rate coefficients were calculated by Offer et al. (1994). The Doppler parameter is assumed to be 0.8 km s$^{-1}$ for IRAS 16293–2422 and 1.6 km s$^{-1}$ for AFGL 2591. The lines at 1800 GHz are convolved with a 13$''$ beam appropriate for HIFI. The lines at higher frequencies (> 2000 GHz) are convolved with a 9.4$''$ beam corresponding to one pixel in the PACS field of view.

The line intensities and profiles for AFGL 2591 are presented in Fig. 6.15 and Fig. 6.16 for the HIFI and PACS lines, respectively. The lines for IRAS 16293–2422 are shown in Figs. 6.17 and 6.18. In addition to the X-ray envelope models from Sect. 6.2.2, models are calculated using the estimates from Sect. 6.3.1 based on the general parameter study. The
constant fractional abundance is $10^{-6}$ for AFGL 2591 and $10^{-7}$ for IRAS 16293−2422.

The lines show strong self-absorption features. The most dramatic being those at 2509 GHz ($^{2}\Pi_{3/2} J = 5/2^{-} - 3/2^{-}$) and 2514 GHz ($^{2}\Pi_{3/2} J = 5/2^{-} - 3/2^{+}$). These are also the strongest lines for both sources. The critical density of some lines is $\gtrsim 10^9 \text{cm}^{-3}$ which is the reason why they are very weak in AFGL 2591 (Fig. 6.16). In addition, the upper energy levels are $> 400 \text{K}$ (e.g., lines at 4209 GHz, 4212 GHz, 4592 GHz and 4602 GHz). These lines are not easily excited.

The main beam peak temperatures and line fluxes for the strongest PACS line (2514 GHz $^{2}\Pi_{3/2} J = 5/2^{-} - 3/2^{+}$) are 0.2 K (0.4 K km s$^{-1}$) for AFGL 2591 with $x(\text{OH}) = 10^{-6}$ and 1.2 K (1.6 K km s$^{-1}$) for IRAS 16293−2422 with $x(\text{OH}) = 10^{-7}$. The values for the strongest HIFI line (1834 GHz $^{2}\Pi_{1/2} J = 3/2^{-} - 1/2^{+}$) are 0.1 K (0.4 K km s$^{-1}$) for AFGL 2591 with $x(\text{OH}) = 10^{-6}$ and 0.9 K (3.0 K km s$^{-1}$) in IRAS 16293−2422 with $x(\text{OH}) = 10^{-7}$, respectively. The 1834 GHz (163.35 μm) was observed with a flux of $1.5 \times 10^{-19} \text{W cm}^{-2}$ by Ceccarelli et al. (1998). A correction factor of $1.7 \times 10^{-7}$ for an extended source (Gry et al. 2003), yields a modeled line flux for the $x(\text{OH}) = 10^{-7}$ models of $3 \times 10^{-19} \text{W cm}^{-2}$, comparable to the observations of Ceccarelli et al. (1998).
Figure 6.16: Profiles of OH lines in the PACS frequency regime for the AFGL 2591 X-ray envelope models (Fig. 6.3). The solid line corresponds to the model without X-rays, the dashed line is \( L_X = 10^{30}\) erg s\(^{-1}\) and the dotted line is \( L_X = 8 \times 10^{31}\) erg s\(^{-1}\). Also shown are the models for \( x(\text{OH}) = 10^{-6}\) (dashed-dotted line). The frequencies are given in GHz.
Figure 6.17: Profiles of OH lines in the HIFI frequency regime for the IRAS 16293–2422 X-ray envelope models without a protostellar hole (Fig. 6.1). The solid line corresponds to the model without X-rays, the dashed line is $L_X = 10^{29}$ erg s$^{-1}$ and the dotted line is $L_X = 10^{30}$ erg s$^{-1}$. Also shown are the models for $x'(OH) = 10^{-7}$ (dashed-dotted line).

6.5 Discussion and conclusion

The spherical envelope models in Sect. 6.2 and the general parameter study in Sect. 6.3 have shown, that hydride abundances can be enhanced several orders of magnitude by the presence of X-rays. It was also shown in Sect. 6.3, however, that in some cases FUV fields may lead to similar abundances. The effects of FUV fields and X-rays are difficult to distinguish in particular for gas temperatures $\gtrsim 300$ K. Only high abundances of NH ($\approx 10^{-8}$) and NH$^+$ ($\approx 10^{-12}$) at $n_H = 10^8 - 10^7$ cm$^{-3}$ clearly indicate the presence of X-rays. Both species are in the frequency range observable with the Herschel Space Observatory. Detections of NH$^+$ would also allow to estimate the X-ray flux and hence the protostellar X-ray luminosity since its abundance increases gradually with increasing X-ray flux.

However, the oxygen bearing hydrides and SH$^+$ are enhanced by FUV fields only at high temperatures ($T \gtrsim 300$ K). These species therefore also trace X-rays in cold gas. If FUV photons provide the heating, FUV fluxes of the order $G_0 \approx 10^4$ are required to heat gas with $n_H = 10^6$ cm$^{-3}$ to such temperatures (e.g., Sternberg & Dalgarno 1995). Low-mass YSOs are not likely to produce such high FUV fields on large scales (e.g., Spaans et al. 1995; Bergin et al. 2003), except in the inner 100 AU where high FUV fields and temperatures above $\approx 300$ K are possible. High-mass YSOs are
Figure 6.18: Profiles of OH lines in the PACS frequency regime for the IRAS 16293–2422 X-ray envelope models without a protostellar hole (Fig. 6.1). The solid line corresponds to the model without X-rays, the dashed line is $L_X = 10^{29}$ erg s$^{-1}$ and the dotted line is $L_X = 10^{30}$ erg s$^{-1}$. Also shown are the models for $x$(OH) $= 10^{-7}$ (dashed-dotted line). The frequencies are given in GHz.
in principle able to illuminate outflow cavities and their immediate surrounding with FUV fields of the order $10^3$–$10^4$ (e.g., Stäuber et al. 2006b). If OH, OH$^+$, H$_3$O$^+$, H$_2$O$^+$ or SH$^+$ are used as X-ray tracers, it is essential to observe transitions with low ($\lesssim 180 \text{ K}$) excitation temperatures to probe the gas at $T \lesssim 300 \text{ K}$.
Chapter 7

Summary and outlook

7.1 Summary and outlook

The influence of FUV and X-ray fluxes from the central source on the molecular protostellar environment has been studied. It was shown that FUV fields can enhance several species out to distances of a few hundred AU in the spherically symmetric envelope of the high-mass object AFGL 2591. Compared to traditional models of photon-dominated regions (PDRs), subtle differences were found because of higher temperatures and higher gas-phase water abundance caused by evaporation of ices in the inner region. In contrast to the FUV photons, X-rays were found to penetrate deeper into the envelope due to their smaller cross sections with higher energy. It was also shown that X-rays can dominate the ionization rate over cosmic rays in large parts of the envelope (out to distances of a few thousand AU from the central source). X-rays and FUV photons generally enhance similar species, mainly simple hydrides, radicals and ions. Due to a different chemical network and differences in the size of the enhanced region, however, tracers were predicted that distinguish the effects of FUV fields and X-rays in spherical envelopes.

Observations of FUV and X-ray tracers towards two high-mass and nine low-mass objects confirmed the model predictions since the observations could only be interpreted by the influence of high-energy radiation from the central source. However, they also showed that – especially in the case of the high-mass objects – irradiated outflow cavity walls cannot be neglected. The influence of FUV photons is strongly dependent on geometry with a major impact on the abundances of many species (in
particular CO$^+$) if they can irradiate the outflow cavity walls. X-rays are less dependent on geometry since the effects of photoabsorption in the envelope are generally small (a factor of a few in X-ray flux) and the enhancement along outflow walls is thus of minor importance. X-rays are predicted to be important in the FUV shielded envelope. Low-mass objects may have cavities in the innermost region (protostellar holes) that allow FUV photons and X-rays to impact the envelope relatively unhindered at large distances from the source. In regions that are not shielded by the inner disk, the chemistry in the envelope is predicted to be dominated by X-rays on scales of a few thousand AU.

To further distinguish the effects of X-rays and FUV fields, the abundances of simple hydrides were calculated for different conditions in the gas. It was found that carbon hydrides generally trace enhanced FUV fluxes whereas nitrogen hydrides are more sensitive to X-rays. Oxygen and sulphur hydrides trace X-rays rather than FUV fields in gas with $T \lesssim 300$ K. FUV photons can enhance these species only at higher gas temperatures.

Chemical models showed that the water abundance is critically dependent on the X-ray flux. At temperatures $\lesssim 300$ K water will be destroyed by X-rays. Higher temperatures, however, increase the efficiency of building up water in gas-phase reactions and water can persist at high abundances, nearly independent of the X-ray flux.

Water and other hydrides will be observed with the upcoming Herschel Space Observatory. A careful abundance and excitation study of these species will allow to trace X-rays and FUV fields from the central source. Two dimensional chemical and radiative transfer models will allow such detailed studies. The central X-ray and FUV flux can then be estimated. This is important, since the evolution of the innermost region, that is the protostellar disk and thus the formation of planets, depends on the impinging X-ray and FUV flux. Fortunately, Herschel is not the only observatory in the near future that allows to study star-forming regions in more detail. Another important upcoming observatory (among others) is the Atacama Large Millimeter Array (ALMA) which will resolve the innermost region and also the structure of the surrounding envelope.

Improved chemical and radiative transfer models together with high spatial resolution observations with ALMA as well as observations in the sub-millimeter and far-infrared regime with Herschel will reveal directly or indirectly the face behind the mask of star-forming regions. This will
improve our current knowledge about the process of star-formation from molecular clouds to the formation of habitable planets.
Appendix
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Appendix A

X-ray chemistry in AFGL 2591

The following figures and tables belong to Chapter 3. In Sect. A.1, depth dependent fractional abundances are shown for different X-ray temperatures $T_X$, inner column densities $N_{\text{H, in}}$, outer FUV fluxes and different cosmic-ray ionization rates. Sect. A.2 provides a detailed comparison to observations for the X-ray models of AFGL 2591.
A.1 Influence of $T_X$, $N_{H,\text{in}}$, an outer FUV field and cosmic rays

![Graphs showing depth dependent fractional abundances for different X-ray temperatures $T_X$ with $L_X = 10^{32}\text{ ergs}^{-1}$ and $N_{H,\text{in}} = 5 \times 10^{22}\text{ cm}^{-2}$ (upper 6 figures) and for different inner column densities $N_{H,\text{in}}$ with $L_X = 10^{32}\text{ ergs}^{-1}$ and $T_X = 7 \times 10^7\text{ K}$ (lower 6 figures).]

**Figure A.1:** Depth dependent fractional abundances for different X-ray temperatures $T_X$ with $L_X = 10^{32}\text{ ergs}^{-1}$ and $N_{H,\text{in}} = 5 \times 10^{22}\text{ cm}^{-2}$ (upper 6 figures) and for different inner column densities $N_{H,\text{in}}$ with $L_X = 10^{32}\text{ ergs}^{-1}$ and $T_X = 7 \times 10^7\text{ K}$ (lower 6 figures).
A.2. Comparison to observations

The observation type is listed in Table A.1. Infrared absorption lines are observed along the line of sight toward the central source. The column densities can therefore be compared to the radial column density $N_{\text{radial}} = \int n(r)dr$. For centrally condensed envelopes, the column density is dominated by the interior.

Emission lines on the other hand arise from throughout the envelope. The column densities for the emission lines in Table A.1 are calculated from the fractional abundances that were determined through detailed, non local thermodynamic equilibrium (NLTE) radiative transfer modeling (eg., van der Tak et al. 1999). For a density distribution like that of
Figure A.3: Depth dependent fractional abundances for different cosmic-ray ionization rates for Model 0 with $\zeta_{cr} = 5.6 \times 10^{-17}\,s^{-1}$ (solid line), for Model 5 with $\zeta_{cr} = 5.6 \times 10^{-17}\,s^{-1}$ (dotted line), for Model 5 with $\zeta_{cr} = 10^{-17}\,s^{-1}$ (dashed line) and for Model 5 with $\zeta_{cr} = 3 \times 10^{-16}\,s^{-1}$ (dashed-dotted line).

AFGL 2591 (Sect. 3.2.2), the mass is dominated by the outer part of the envelope and emission measurements often probe the exterior (see also Doty et al. 2002 for a detailed discussion).
Table A.1: Comparison of best-fitting models with observed radial column densities for AFGL 2591.

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<td>0</td>
<td>3.2(5)</td>
<td></td>
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<tr>
<td>HCN</td>
<td>2.0(16)</td>
<td>2.5(16)</td>
<td>IR-ISO Bm03</td>
<td>3.0(32)</td>
<td>3.0(7)</td>
<td>3.0(22)</td>
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<td>2.4(5)</td>
<td></td>
<td></td>
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<tr>
<td>HCN</td>
<td>1.9(15)</td>
<td>9.6(14)</td>
<td>mm-JCMT vdT03</td>
<td>6.0(31)</td>
<td>1.0(8)</td>
<td>3.0(22)</td>
<td>10</td>
<td>2.4(5)</td>
<td></td>
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<tr>
<td>HCN</td>
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<td>4.5(15)</td>
<td>mm-JCMT Do</td>
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<td>5.0(7)</td>
<td>5.0(22)</td>
<td>0</td>
<td>1.8(4)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*a(b) means \(a \times 10^b\). Continued on next page.*
Table A.1—continued from previous page.

<table>
<thead>
<tr>
<th>Species</th>
<th>Model 6 [cm$^{-2}$]</th>
<th>Observed [cm$^{-2}$]</th>
<th>Data</th>
<th>Ref.</th>
<th>$L_X$ [erg s$^{-1}$]</th>
<th>$T_X$ [K]</th>
<th>$N_{H,in}$ [cm$^{-2}$]</th>
<th>$G_{0,in}$</th>
<th>Time [yrs]</th>
<th>[cm$^{-2}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>OCS</td>
<td>8.8(14)</td>
<td>9.6(14)</td>
<td>mm-JCMT</td>
<td>vdT03</td>
<td>6.0(31)</td>
<td>5.0(7)</td>
<td>3.0(22)</td>
<td>0</td>
<td>1.4(5)</td>
<td></td>
</tr>
<tr>
<td>NH$_3$</td>
<td>5.7(15)</td>
<td>1.9(15)</td>
<td>cm-Effelsb.</td>
<td>Do</td>
<td>5.0(30)</td>
<td>1.0(8)</td>
<td>7.0(22)</td>
<td>0</td>
<td>1.0(4)</td>
<td></td>
</tr>
<tr>
<td>N$_2$H$^+$</td>
<td>4.9(13)</td>
<td>4.7(13)</td>
<td>mm-JCMT</td>
<td>St</td>
<td>7.0(31)</td>
<td>1.0(8)</td>
<td>3.0(22)</td>
<td>0</td>
<td>1.0(4)</td>
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<tr>
<td>SO</td>
<td>1.8(16)</td>
<td>9.6(14)</td>
<td>mm-JCMT</td>
<td>vdT03</td>
<td>Mod. 1</td>
<td></td>
<td></td>
<td>10</td>
<td>5.6(4)</td>
<td>(1.6(15))</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>2.7(15)</td>
<td>1.9(14)</td>
<td>mm-JCMT</td>
<td>vdT03</td>
<td>5.0(32)</td>
<td>3.0(7)</td>
<td>3.0(22)</td>
<td>0</td>
<td>1.0(4)</td>
<td>(6.9(14))</td>
</tr>
<tr>
<td>NS</td>
<td>2.4(12)</td>
<td>4.7(11)</td>
<td>mm-JCMT</td>
<td>vdT03</td>
<td>6.0(31)</td>
<td>3.0(7)</td>
<td>3.0(22)</td>
<td>10</td>
<td>5.6(3)</td>
<td>(2.0(12))</td>
</tr>
</tbody>
</table>

a(b) means $a \times 10^b$. The column density of a model with the parameters $L_X$, $T_X$, $N_{H,in}$, $G_{0,in}$ and time in columns 6–10 match the observed column density. If no model was found to give a good fit, the best fitted model is presented with the column density given in brackets at the end of the line.

References: BmOl Boonman et al. (2001), Bm03 Boonman et al. (2003b), Bmv Boonman & van Dishoeck (2003), Do Doty et al. (2002), LvD Lahuis & van Dishoeck (2000), Mc McCall et al. (1999), St Stark et al. (1999), vdT99 van der Tak (1999), vdT00 van der Tak (2000), vdT03 van der Tak (2003).
Curriculum Vitae

Name Pascal Stäuber
Date of birth October 4, 1971
Place of birth Lucerne, Switzerland
Nationality Swiss

1978 - 1987 Primary and secondary school in Horw, Lucerne
1987 - 1991 Berufsschule in Emmen and apprenticeship as Elektrozeichner in Lucerne
1988 - 1991 Berufsmittelschule in Emmen
1991 - 1993 Technischer Sachbearbeiter for Schindler Aufzüge AG in Ebikon
1993 - 1994 Handels- und Verwaltungsschule in Lucerne
1994 Harven School of English in Woking, England
1995 - 1996 Kaufmännischer Sachbearbeiter for Landis & Gyr AG
1995 - 1998 Maturitätsschule für Erwachsene in Lucerne
1998 Matura Typus C ("Maths and Physics")
1998 - 2003 Physics studies at ETH in Zurich
2003 Dipl. Phys. ETH
2003 - 2006 Research assistant at the Radio Astronomy and Plasma Physics Group, Institute of Astronomy, ETH Zurich
2006 Doctoral thesis:
The Impact of High-Energy Radiation on the Chemistry of Star-Forming Regions
Thesis supervisor: Prof. Dr. A. O. Benz
List of Publications

Publications in Refereed Journals

• Subarcsecond observations of the high-mass protostar AFGL 2591 with the Submillimeter Array
  Arnold O. Benz, Pascal Stäuber, Tyler L. Bourke, Floris, F.S. van der Tak, Ewine F. van Dishoeck

• Starburst dominated warm molecular ISM in deeply obscured galactic nuclei
  Fred Lahuis, Henrik W.W. Spoon, Steven D. Doty, Lee Armus, Jim R. Houck, Pascal Stäuber, Xander G.G.M. Tielens, Ewine F. van Dishoeck

• Tracing high energy radiation with molecular lines near deeply embedded protostars
  Pascal Stäuber, Arnold O. Benz, Jes K. Jørgensen, Ewine F. van Dishoeck, Steven D. Doty,

• Water destruction by X-rays in star-forming environments
  Pascal Stäuber, Jes K. Jørgensen, Steven D. Doty, Ewine F. van Dishoeck, Arnold O. Benz,

• X-ray chemistry in envelopes around young stellar objects
  Pascal Stäuber, Steven D. Doty, Ewine F. van Dishoeck, Arnold O. Benz,
• Influence of UV radiation from a massive YSO on the chemistry of its envelope
Pascal Stäuber, Steven D. Doty, Ewine F. van Dishoeck, Jes K. Jørgensen, Arnold O. Benz,
2004, Astronomy and Astrophysics, 425, 577

Publications in Conference Proceedings

• X-ray chemistry in the envelopes around young stellar objects
Pascal Stäuber, Arnold O. Benz, Steven D. Doty, Ewine F. van Dishoeck
2004, Proceedings of the dusty and molecular universe: a prelude to Herschel and ALMA, Paris, ed. A. Wilson, 413

• High-energy radiation probes of protostellar envelopes
Pascal Stäuber, Arnold O. Benz, Steven D. Doty, Ewine F. van Dishoeck, Jes K. Jørgensen
Acknowledgments

"You'll never walk alone" is an old song that has become a standard, sung by graduation classes and football crowds all over the world. What does this have to do with my thesis? Well, the song is sung to give courage in bad times as well as to celebrate the good times. Completing this thesis was not always a "breeze" but, fortunately, I never had to walk alone. I therefore wish to express my gratitude to all who supported me during this time.

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Bibliography


Caselli, P., 2005, Proceedings of the meeting "Cores to Clusters", Porto, Portugal


de Gouveia dal Pino, E.M., 2005, Advances in Space Research, 35, 908

de Graauw, T., & Helmich, F.P., 2001, in Proc. ESA Symp., The Promise of the Herschel Space Observatory, ESA SP-460, 45


Forbrich, J., Preibisch, T., Menten, K., 2005, Star Formation in the Era of Three Great Observatories
BIBLIOGRAPHY


Griffin, M., Swinyard, B., Vigroux, L., 2005, The Dusty and Molecular Universe: A Prelude to Herschel and ALMA, 17

Gry, C., et al., 2003, ESA Special Publication, 1262


Herbst, E., 2000, Astronomy, physics and chemistry of H$_3^+$, 358, 2523


Jansen, D.J., 1995, Ph.D. Thesis

Kim, Y.K., et al., 2004, Electron-Impact Ionization Cross Section for Ionization and Excitation Database (version 3.0). National Institute of Standards and Technology, Gaithersburg, MD


Latter, W.B., 1989, Ph.D. Thesis


Melnick, G. J., 2004, Advances in Space Research, 34, 511


Pilbratt, G.L., 2003, ESA SP-511: Exploiting the ISO Data Archive. Infrared Astronomy in the Internet Age, 31


Poglitsch, A., et al., 2005, The Dusty and Molecular Universe: A Prelude to Herschel and ALMA, 11


Schöier, F.L. et al., 2005a, IAU Symposium, 231, 138


van Dishoeck, E.F., 1988, in Rate Coefficients in Astrochemistry, ed. T.J. Millar & D.A. Williams (Kluwer), 49


Yan, M., 1997, Ph.D. Thesis
