Astrochemistry: Recent Successes and Current Challenges
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Chemistry as a Probe of the Structure and Processes in Massive YSO Envelopes

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Abstract. The distribution and composition of the dust and gas surrounding Young Stellar Objects (YSOs) is of continuing interest. Fortunately, rapid advances in observational capabilities have led to data of high spatial and spectral resolution, as well as the opportunity to observe in previously unavailable windows using satellites. Such high-quality data have motivated enhancements in theoretical models. Key to these models is the chemical evolution of the gas. Since the chemical evolution depends upon temperature, density, and time, the state and history of the source is encoded in the spatial distribution of the chemical abundances.

It is possible, using both parametric and detailed physical-chemical modeling, to constrain many source properties, and identify potential reactions of further laboratory interest. Using specific examples, I discuss some successes toward constraining the source properties, as well as challenges posed by current problems. Finally, I discuss the potential effect of infall dynamics and recent laboratory measurements of temperature programmed desorption of ices from grains on inferring source properties.

Keywords. astrochemistry — ISM: abundances — ISM: molecules — stars: formation

1. Introduction

Star formation is of significant and continuing interest. Not only does it give us insight into the dominant form of luminous matter in the universe, but it also helps provide connections between an understanding of the general interstellar medium on the large scale, and planet formation on the small scale. The scenario for formation of low-mass stars is relatively well understood in at least general terms (see, *e.g.*, Shu, 1997). However, the same is not true for massive star formation. While the timescales are presumably shorter than for low-mass star formation, the triggering, evolution, and structure of high-mass star forming regions is unclear.

In this paper I discuss the construction of detailed, self-consistent models of the envelopes surrounding massive young stellar objects (YSOs). These models are compared with observations to constrain the source structure. By way of example, these comparisons are used to point out recent successes and future challenges in understanding massive YSO envelopes.

2. The Challenge

From an astronomical perspective, the challenges are great. Can we understand the chemical and physical structures, the evolution, and origin of massive YSOs? To attempt to answer some of these questions requires detailed knowledge of the history and evolution of the region. Fortunately, the chemical structure of the envelope (in principal) encodes the evolution of the temperature and density of each parcel of gas. Since both the chemical evolution and molecular excitation/radiative transfer are temperature and density dependent, it may be possible to infer the source structure and evolution from

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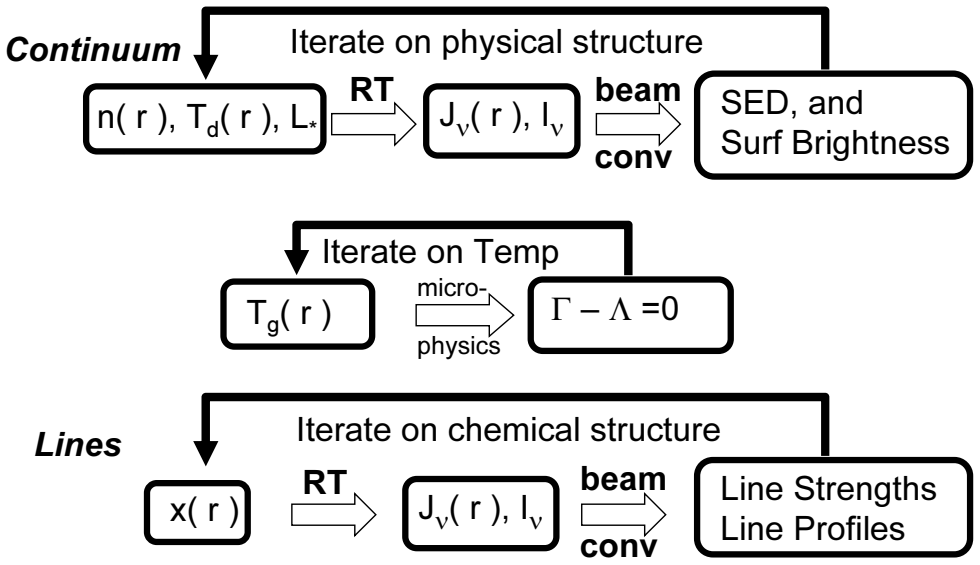

Figure 1. Schematic of comprehensive modeling. The inputs and unobservable internal source properties are on the left, the processes in the middle, and the outputs for comparison with observations are on the right.

multi-wavelength molecular line observations spanning a wide range of densities and temperatures.

From a modeling perspective, the challenges are also great. The temperature ranges from roughly ~ 10 K in the cool exterior to > 300 K in the warm interior. The densities vary from $< 10^4\,\mathrm{cm}^{-3}$ in the exterior to $> 10^8\,\mathrm{cm}^{-3}$ in the interior. Grains may hold, process, and liberate molecules from their mantles. Radiation from the ultraviolet to the X-ray may be present to process the gas. In short, the chemistry must respond to a wide range of physical conditions.

These two situations – together with recent (*e.g.*, SWAS, ODIN, ISO, JCMT, Spitzer, SMA) and upcoming (*e.g.*, SOFIA, ALMA, Herschel) observatories—suggest the need for detailed, comprehensive models of massive YSOs. The goal is to consider the combined effects of physical, thermal, and chemical structure as well as radiative transfer. A schematic of the modeling process is shown in Figure 1.

In this figure, the inputs/unobservable internal properties are on the left, and the outputs for comparison with observations are on the right. This is an important point. In particular, significant physics can be simulated between chemical evolution and detection of a signal at the telescope. Given the wide range of processing that can occur, it is preferable to compare simulations and direct observables such as line strengths and profiles, rather than intermediate quantities such as fractional abundances and column densities which require uncertain assumptions to infer directly from observations. In our modeling, we attempt to compare exclusively to line strengths and profiles. In cases where the column densities or abundances are presented, they have almost always been confirmed by radiative transfer models and simulated observations.

As can be seen, the physical structure is normally constrained by the dust continuum radiation. Likewise, the thermal and chemical structures are constrained by molecular line observations. Together this yields a comprehensive picture of the envelope.

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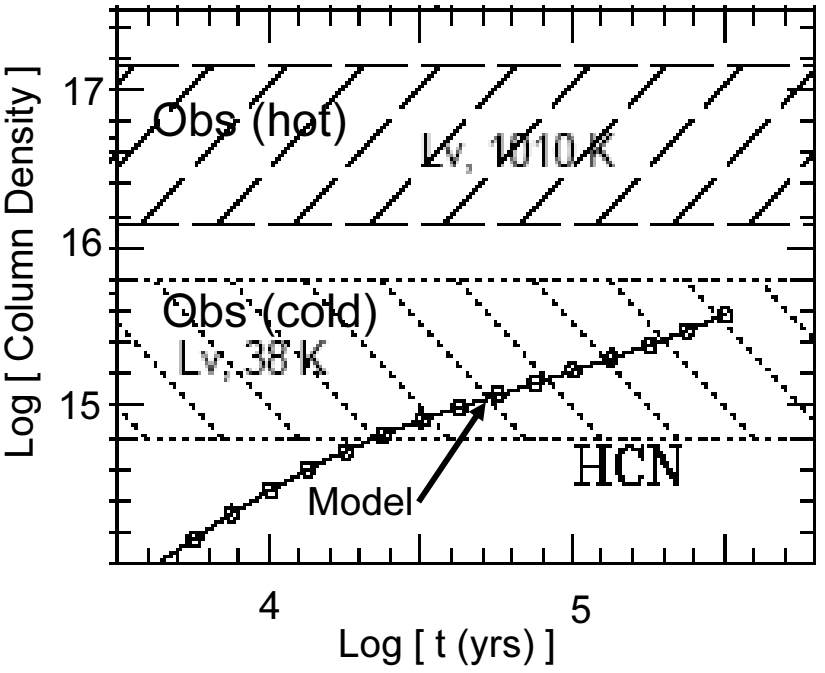

Figure 2. Comparison of predicted (line + symbols) and observed (shaded regions) column densities of HCN toward AFGL 2591. Notice that the cold HCN can be reproduced, but that the model cannot reproduce the hot HCN.

3. Discussion

3.1. *AFGL 2591*

AFGL 2591 is a massive YSO toward Cygnus X. It lies at a distance of approximately 1 kpc, though this is uncertain. AFGL 2591 has the advantage that it is a relatively isolated region of massive star formation, with far less influence from surrounding sources than other massive YSOs. While there exist broad wings in CO lines, the volume is not shock dominated. Most importantly, it has been well observed, with 29 molecular species detected. As a result, it is a good region in which to test our ability to understand the comprehensive chemistry and physics necessary to constrain the structures and processes in massive YSOs. In the following subsections, I discuss three sets of diagnostic species: HCN, sulphur-bearing species, and water.

3.2. *HCN*

HCN is observed toward AFGL 2591 with two apparent components: a cold ($T \sim 38$ K) less dense component, and a warm ($T \sim 1000$ K) and more dense component. The comparison of models with observations is shown in Figure 2. The modeling can explain the cold HCN abundance, but underproduces the hot HCN.

Radiative transfer modeling suggests an inner (warm) abundance of $x(\mathrm{HCN}) >$ few $\times$ 10^{-6} for $r < 4 \times 10^{15}$ cm ($T > 400$ K). Normal hot gas-phase chemistry based upon the UMIST (Millar *et al.*, 1997) reaction network cannot produce this level of HCN, even for very high temperatures (~ 800 K) and long times ($\sim 3 \times 10^5$ yrs).

However, Staeuber *et al.* (2005) recently considered the potential for X-ray driven chemistry. In this scenario, X-rays produce fast secondary electrons which drive an

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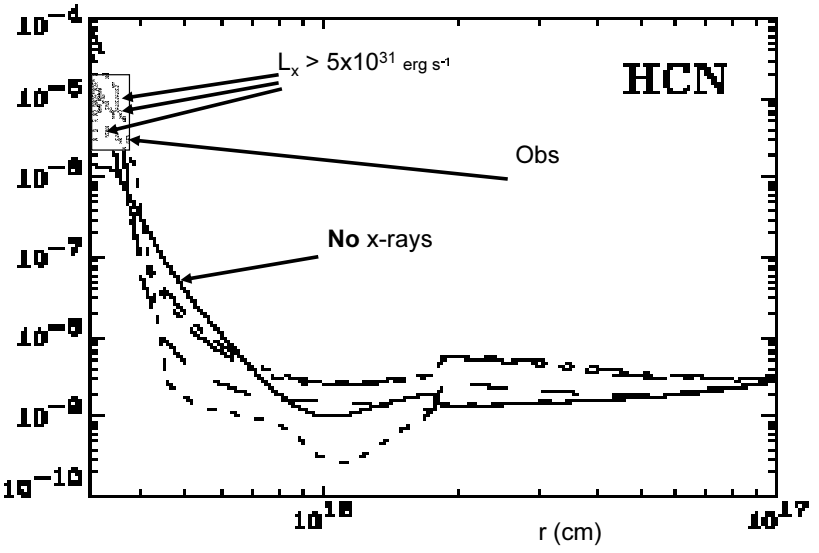

Figure 3. Comparison of model (lines) and observed (shaded region) HCN abundance as a function of position in the envelope. Notice that models with X-rays (broken lines) can enhance the HCN abundance to the observed level, while normal gas-phase chemistry (solid line) cannot.

efficient ion-molecule chemistry deep into the envelope at short times. They found that the inclusion of X-rays meaningfully improved the fit of models to observations. The case of HCN is shown in Figure 3.

In this figure, the broken lines signify different amounts of X-ray luminosity. The solid line is for a model without X-rays. Notice that including X-rays at a level $L_X > 5 \times 10^{31}$ erg s^{-1} produces sufficient HCN to reproduce the observations.

Combined, these results suggest that our current molecular databases have an incomplete description of HCN chemistry. In particular, other pathways (if HCN is driven by "normal" gas-phase chemistry) or processes (such as X-rays) must be considered in these interior regions.

3.3. *Sulphur Species*

Sulphur chemistry is generally regarded to be somewhat uncertain. As a result, we consider only those species which contain a significant fraction of the sulphur independent of the specific rates adopted. Such a sensitivity analysis with respect to reaction rates and initial state of the sulphur suggests that CS contains at least 25% of the sulphur in the cold ($T < 100$ K) gas phase. Above 100 K, much of the sulphur is shuttled into SO_2.

Radiative transfer modeling of CS and SO_2 lines suggest that $x(\mathrm{CS}) \sim 3 \times 10^{-9} - 10^{-8}$ throughout the envelope. Similar modeling requires $x(\mathrm{SO_2}) \sim 10^{-6}$ for $T > 100$ K. These abundances correspond to a jump of over 2 order of magnitude near $T \sim 100$ K in the dominant forms of sulphur.

This suggests that the cold sulphur is tied up in the ice mantles. Once $T > 100$ K, the mantles evaporate, liberating the sulphur into the gas phase. What is unclear, however, is the specific initial form of the cold sulphur (*e.g.*, H_2S, OCS, etc.) This is an open question, and will probably require more detailed and sophisticated gas-grain chemistry to answer.

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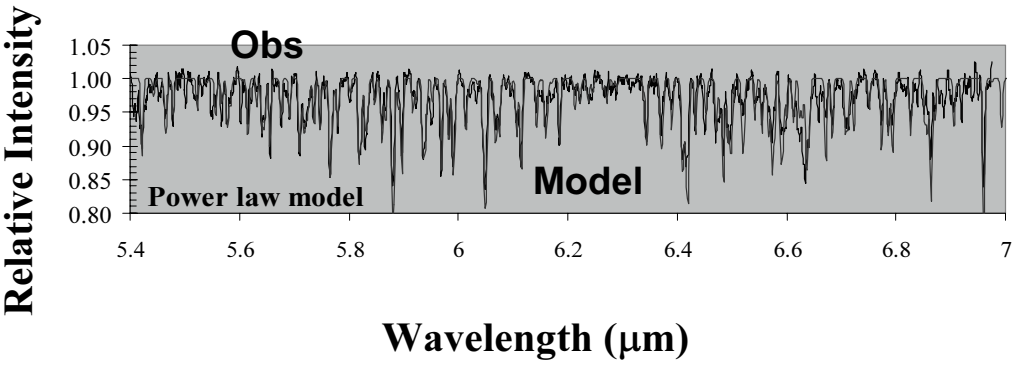

Figure 4. Comparison of observed (thick line) and model (thin line) ro-vibrational spectrum of water toward AFGL 2591. The rms deviation is less than a few percent.

3.4. *Water*

Water is well known as an important astrophysical molecule, due to both its role in thermal balance and as an important oxygen reservoir. It also can be a significant test of structure due to its wide range of excitable energy levels as well as its solid/gas phase-change at $T \sim 100$ K at astrophysical pressures.

Utilizing the model above together with detailed radiative transfer and parameterization of the water abundance throughout the envelope, Boonman *et al.* (2003) fit multi-wavelength observations of water toward AFGL 2591.

The upper limits on a range of ISO-LWS lines (and in particular the 108 μm $2_{21} - 1_{10}$ transition) requires that there be little cold gas-phase water to absorb against the warm central source. The strength of the SWAS 557 GHz line limits the cold water abundance, as well as the effective size of the warm inner region where water evaporates from grain surfaces. Finally, the 6 μm ro-vibrational absorption lines constrain the relative warm/cold water abundance. The fit for the 6 μm ro-vibrational lines is given in Figure 4.

The resulting best-fit water abundances are shown in Figure 5. As can be seen, the observational data constrain the water abundance in three ways: (1) a warm region having $x(\mathrm{H_2O})_{\mathrm{warm}} \sim 2 \times 10^{-4}$, (2) a cold region having $x(\mathrm{H_2O})_{\mathrm{cold}} < 10^{-8}$, and (3) a jump-like transition at $T \sim 100$ K. These results are consistent with recent laboratory data Fraser *et al.* (2001), showing that water ice evaporates from grain mantles near $T \sim 100$ K.

3.5. *Age Dating*

The comparison of model results and observations can be extended over the 29 species detected toward AFGL 2591. Since the physical and chemical models link the evolution of all species, it is possible to attempt to simultaneously age-date the envelope since protostellar turn-on. In Figure 6 the quality of fit over all species is shown as a function of time.

Note the best fit for $t \sim 1-3 \times 10^4$ yrs. The limits on the early and late times are shown in the figure. Note that both the early and late times are constrained by multiple species. This provides some confidence of the approximate age dating in the face of uncertainties in the reaction rates for any single species.

3.6. *Infall & Realistic Mantle Evaporation*

Last, Doty *et al.* (2005) consider the potential effects of stellar evolution and mantle evaporation. The protostellar evolution is taken from the recent model of McKee & Tan

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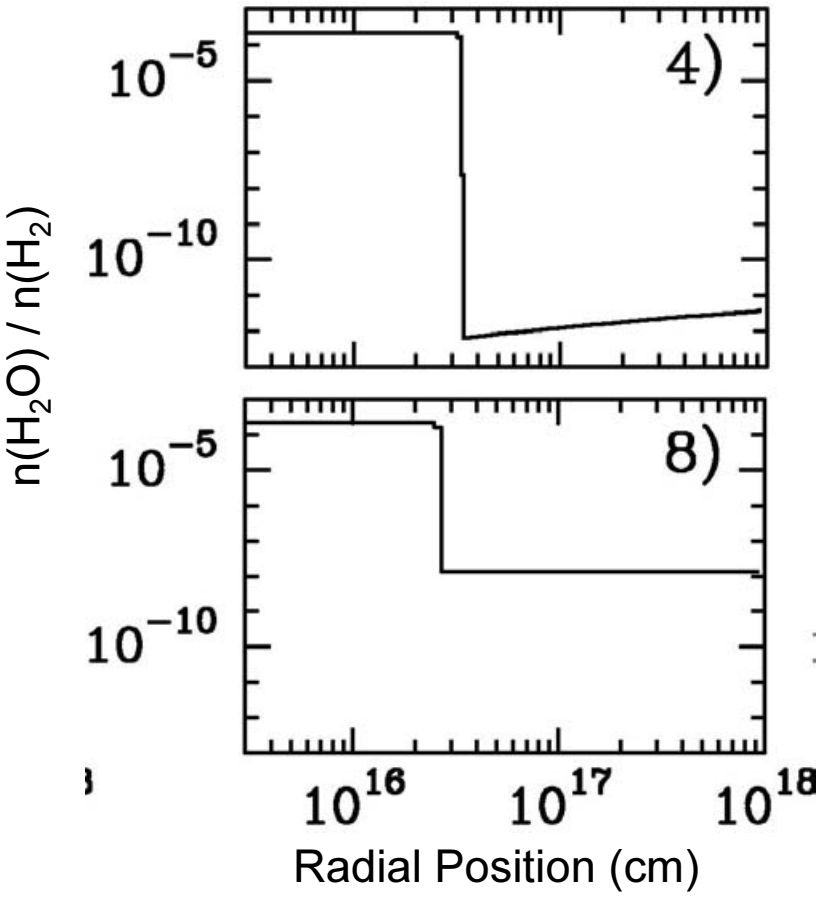

Figure 5. Best-fit water abundance profiles for AFGL 2591, based upon multi-wavelength observations of water lines.

(2003), which allows a determination of the stellar luminosity (and thus temperature distribution throughout the envelope) as a function of time. The stellar evolution is coupled with material infall. Likewise, we have removed the simple water abundance parameterization, and replaced it with laboratory-based Temperature Programmed Desorption studies of water by Fraser *et al.* (2001). As a result, we follow the gas and dust as it infalls into the warming envelope, and treat the mantle evaporation in detail.

The resulting gas-phase water abundance profiles are shown in Figure 7. Notice that the step function distribution that was inferred parametrically from the water line observations is naturally reproduced. As the protostar heats the envelope, a 'warming front' moves outward. The grain mantles evaporate nearly instantaneously on the timescale of the infall and protostellar evolution, leading to a near Heaviside-Lorentz abundance profile. While this is quite encouraging for water, it would be essential to be able to perform similar analyses for other grain mantle components.

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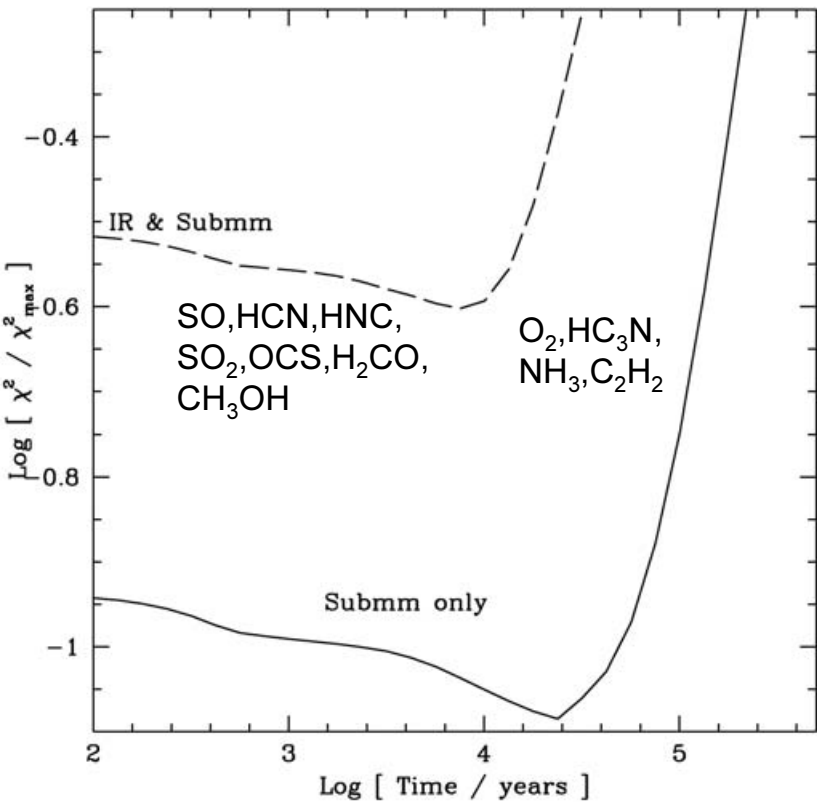

Figure 6. Quality of fit between models and observations for all 29 species observed toward AFGL 2591 as a function of time. The species best constraining the upper and lower times are noted.

4. Conclusions

Detailed, coupled, physical-chemical models of the envelopes of evolved stars have been constructed, and compared to observations with good success. We find that it is possible to simultaneously match many of the observed abundances in the envelope, and thus constrain the physical, thermal, and chemical structure, as well as (potentially) the source age. However, a number of open questions remain. In particular, is the high-temperature hydrocarbon chemistry incomplete? Are X-rays important? What is the low-temperature reservoir of solid-phase sulphur? To what extent can a better understanding of realistic grain surface chemistry aid the modeling process? Each of these questions will play key roles in any attempt to extend coupled, detailed models to the warmer interiors, earlier times, and/or more complicated regions.

Acknowledgements

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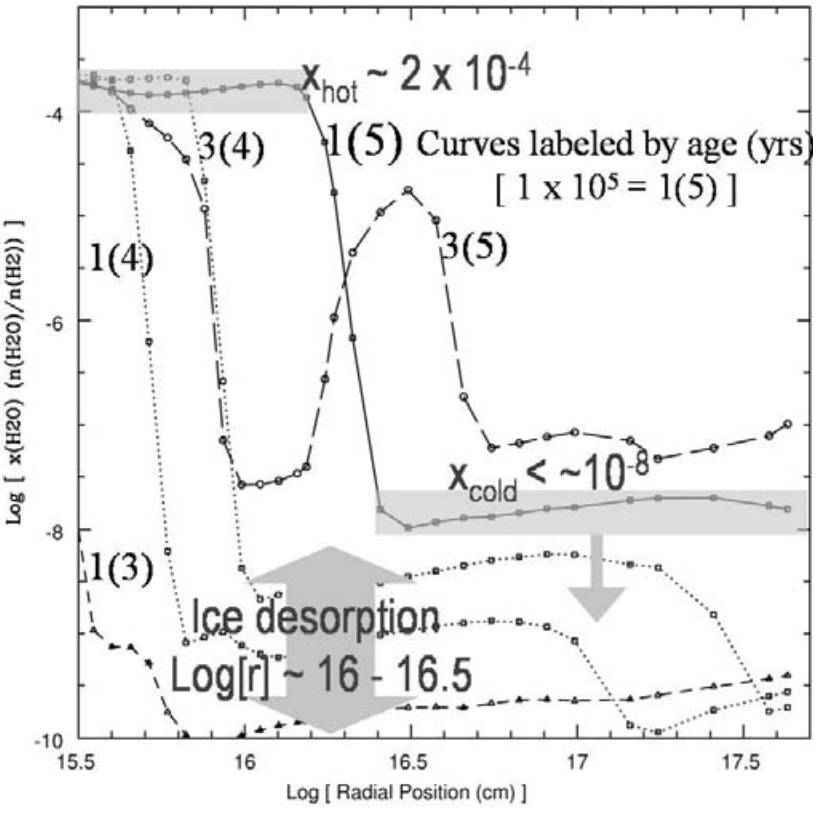

Figure 7. Water abundance profiles where the effects of protostellar evolution, infall, and exact water desorption model are included. Note that the step-function distribution inferred from the water line observations is naturally reproduced.

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Discussion

BAUCHTER: In an attempt to understand the erosion of graphite files of fusion reactor walls, Thomas Zedro and co-workers from the group of Prof. Kippers at Bayreuth University, and the Max-Planck Institute of Plasma Physics in Garching, conducted surface science experiments which shows carbon hydride formation at hydrogenated carbonaceous surfaces. In their TPD (Temperature Programmed Description) experiments they observed that light carbon hydrides are desorbed from edge related defect sites on a HOPG graphite surface (HOPG: highly oriented pyrolitically grown graphite) at

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temperatures above 700 K on a laboratory time scale. Did you include the possibility of carbon hydride formation on carbonaceous grains in your model?

DOTY: The experiment you describe is interesting. In our current model, we do not include carbon hydride formation on such surfaces. We also do not include surface erosion yet, though this may be of some importance in such high radiation field environments, especially if X-rays do play a role.

WALMSLEY: Is it possible that there exists a disk and that this may help explain the warm HCN?

DOTY: We do not include disks, so such a thing *may* be possible. However, to be consistent with linewidths, I would imagine it would have to be very face-on, and I am not sure this is consistent with the outflow geometry.

HUNTER: This object, AFGL 2591, was observed a dozen years ago in a VLA survey of massive protostellar water masers. There is a compact H II region that is many arc seconds in diameter. So, clearly, X-rays are present. How does this fit into your models?

DOTY: Unfortunately, to my knowledge X-rays have not yet been directly measured toward massive YSOs. The radio sources observed by Campbell and Trinidad *et al.* seem to lie within an ∼5 arsecond region. This corresponds to 5000 AU at 1 kpc. In our model, the central envelope is relatively transparent to X-rays, with enough column to be X-ray opaque occurring in the 3000–10,000 AU region. Therefore, so long as any X-ray source(s) is/are within this transparent center, our results should be reasonably valid.

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