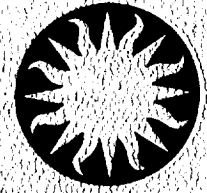




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## Implications of SWAS Observations for Interstellar Chemistry and Star Formation

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### ABSTRACT

A long standing prediction of steady state gas-phase chemical theory is that H<sub>2</sub>O and O<sub>2</sub> are important reservoirs of elemental oxygen and major coolants of the interstellar medium. Analysis of SWAS observations has set sensitive upper limits on the abundance of O<sub>2</sub> and has provided H<sub>2</sub>O abundances toward a variety of star forming regions. Based on these results, we show that gaseous H<sub>2</sub>O and O<sub>2</sub> are not dominant carriers of elemental oxygen in molecular clouds. Instead the available oxygen is presumably frozen on dust grains in the form of molecular ices, with a significant portion potentially remaining in atomic form, along with CO, in the gas phase.

H<sub>2</sub>O and O<sub>2</sub> are also not significant coolants for quiescent molecular gas. In the case of H<sub>2</sub>O, a number of known chemical processes can locally elevate its abundance in regions with enhanced temperatures, such as warm regions surrounding young stars or in hot shocked gas. Thus, water can be a locally important coolant. The new information provided by SWAS, when combined with recent results from the Infrared Space Observatory, also provide several hard observational constraints for theoretical models of the chemistry in molecular clouds and we discuss various models that satisfy these conditions.

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*Subject headings:* ISM: molecules – abundances – evolution; stars: formation; molecular processes

## 1. Introduction

Since the recognition that reactions between ions and molecules play a major role in molecular synthesis (Herbst & Klemperer 1973; Watson 1973; Dalgarno & Black 1976), it has long been proposed that H<sub>2</sub>O and O<sub>2</sub> are important species in the dense interstellar medium. Indeed steady-state gas-phase chemical theory predicts that H<sub>2</sub>O and O<sub>2</sub>, along with O and CO, constitute the gas-phase reservoirs of elemental oxygen in molecular gas that is well shielded from ultraviolet radiation (e.g., Millar 1990). As a consequence H<sub>2</sub>O and O<sub>2</sub> have been suggested as important coolants for dense gas (Goldsmith & Langer 1978; Hollenbach 1988; Neufeld, Lepp, & Melnick 1995).

Atmospheric obscuration has impeded direct observation of these two molecules and our overall understanding of interstellar oxygen chemistry has remained uncertain. Ground-based observations of isotopologs, such as H<sub>2</sub><sup>18</sup>O and O<sup>18</sup>O, have provided some information on their relative importance (e.g., Zmuidzinas et al. 1995; Maréchal et al. 1997) and the Infrared Space Observatory has recently provided direct observations of H<sub>2</sub>O in warm gas (cf. van Dishoeck et al. 1999). However, despite these efforts, over the past decade laboratory determinations of reaction rates and crucial branching ratios has reached the point that our knowledge of the chemical pathways theorized to create O<sub>2</sub> and H<sub>2</sub>O in cold (T < 50 K) gas has, surprisingly, surpassed our observational capabilities.

The Submillimeter Wave Astronomy Satellite (SWAS) has opened a new window on interstellar oxygen chemistry by conducting pointed observations in low energy transitions of ortho-H<sub>2</sub>O and O<sub>2</sub> toward numerous dense molecular cores. Some results from these observations have been presented in this issue where chemical abundances (and upper limits) relative to H<sub>2</sub> are derived. In this Letter we examine the consequences of these results on the chemistry of molecular clouds, on the potential of H<sub>2</sub>O and O<sub>2</sub> as coolants, and on the oxygen budget in the interstellar medium. In our analysis we assume the ortho/para ratio of water is 3:1.

## 2. Primary Oxygen Reservoirs

The total oxygen budget is constrained by observations of diffuse clouds where the amount of oxygen not locked inside the refractory cores of dust grains is  $\sim 6.4 \times 10^{-4}$  relative to H<sub>2</sub> (Meyer, Jura, & Cardelli 1998). About  $\sim 15\%$  is in gas phase CO (e.g., Sutton et al. 1984) and SWAS observations have demonstrated that in most regions, gas-phase water and molecular oxygen account for  $\ll 1\%$  of the available oxygen (Snell et al. 2000a,b,c; Goldsmith et al. 2000). Thus gaseous H<sub>2</sub>O and O<sub>2</sub> are *not* primary reservoirs of atomic oxygen.

In the solid state, a large portion of the oxygen budget is frozen on the surfaces of cold dust grains. Towards NGC7538 (IRS9)  $\sim 40\%$  is in the form of  $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{CH}_3\text{OH}$ , and  $\text{CO}_2$  ice (Whittet et al. 1996).<sup>1</sup> In the cold absorbing gas towards the background star Elias 16 molecular ices account for nearly 65% (Schutte 1999). Thus in star forming cores (NGC7538, OMC-1, Ceph A, etc.) gas and solid phase molecules account for  $\sim 55\%$  of the available oxygen (see also van Dishoeck et al. 1999). The remainder could be in the form of atomic oxygen, which has been found to be abundant towards a few sources (see Caux et al. 1999 and references therein). Another possibility is that there is higher depletion of elemental oxygen into refractory dust cores in denser regions as found for other elements (see Snow et al. 1998; Meyer et al. 1998).

### 3. Cooling

There have been several theoretical studies of the cooling from molecular emission (Goldsmith & Langer 1978; Hollenbach 1988; Neufeld, Lepp & Melnick 1995; hereafter GL78, H88, and NLM95), each focusing on the gas-phase chemistry and resulting cooling for specified conditions. In the case of  $\text{O}_2$ , GL78 assume an abundance of  $x(\text{O}_2) = 10^{-5}$  and find that  $\text{O}_2$  contributes  $\sim 30 - 40\%$  of the total cooling for  $n_{\text{H}_2} < 10^5 \text{ cm}^{-3}$  and  $T_{\text{gas}} = 10 - 20 \text{ K}$ . NLM95 used a higher  $\text{O}_2$  abundance of  $\sim 9 \times 10^{-5}$  and found that  $\text{O}_2$  accounts for  $\sim 20\%$  of the cooling for low density gas. Observations of  $\text{O}_2$  (e.g., Goldsmith et al. 2000) find  $x(\text{O}_2) < 10^{-6}$  in regions of high and moderate density ( $n_{\text{H}_2} > 10^3 \text{ cm}^{-3}$ ). Since  $\text{O}_2$  emission is optically thin the cooling rate will scale with abundance and therefore the contribution of molecular oxygen to the overall cooling must be  $< 1\%$ .

Both GL78 and NLM95 assume a water abundance of  $\sim 10^{-6}$  and for clouds with  $T_{\text{gas}} < 30 \text{ K}$   $\text{H}_2\text{O}$  is predicted to account for  $\sim 10\%$  of the total cooling, provided  $n_{\text{H}_2} \geq 10^5 \text{ cm}^{-3}$ . In regions with low UV intensities, and for  $T_{\text{gas}} > 400 \text{ K}$ , a series of neutral-neutral reactions with activation barriers will convert all of the atomic oxygen not locked in  $\text{CO}$  into  $\text{H}_2\text{O}$ . Under these conditions the abundance of water can be as high as  $\sim 3 \times 10^{-4}$  and water is a major coolant for molecular gas (H88, NLM95).

SWAS observations of water in extended gas in Orion and M17 (and other sources) show that the abundances in the cold,  $T < 50 \text{ K}$ , quiescent gas are only  $\sim 10^{-8}$  (Snell et al. 2000a,b,c). With this abundance, and using the cooling functions provided by NLM95, the total cooling rate for  $\text{o-H}_2\text{O}$  is a factor of 25 below the rate for  $x(\text{H}_2\text{O}) = 10^{-6}$ . *Thus, globally water emission is not an important coolant for molecular clouds.* However, locally the cooling of water can be quite important. The detection of  $\text{o-H}_2\text{O}$  emission in a beam size of  $3.3 \times 4.5$  by SWAS does not preclude the existence of regions smaller than the SWAS beam with high water abundance.

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<sup>1</sup> Assuming the total column density is  $N(\text{H}_2) \sim 5.0 \times 10^{22} \text{ cm}^{-2}$  from the  $^{13}\text{CO}$  observations of Mitchell et al. (1990),  $x(\text{CO}) = 2.0 \times 10^{-4}$  (Lacy et al. 1994), and  $^{12}\text{C}/^{13}\text{C} = 60$ .

Indeed, ISO observations have shown that water is found in high abundance both in hot shocked gas and in warm regions surrounding young stars (see van Dishoeck et al. 1999). For those conditions H<sub>2</sub>O emission is an important, if not the dominant coolant (Saraceno et al. 1999; Melnick et al. 2000).

#### 4. Observational and Theoretical Constraints on Chemical Models

In warm gas SWAS and ISO have demonstrated that chemical theory is in agreement with observations (van Dishoeck et al. 1999; Melnick et al. 2000; Neufeld et al. 2000). For cold quiescent gas we view SWAS observations and recent results from ISO as having set several hard observational constraints for chemical theory. We suggest that successful chemical models satisfy the following conditions:

1. Produce an abundance of molecular oxygen that is less than  $10^{-6}$  (Goldsmith et al. 2000).
2. Be able to account for the low water abundance ( $10^{-9} < x(\text{H}_2\text{O}) < \text{few} \times 10^{-8}$ ; Snell et al. 2000a,b,c; Ashby et al. 2000) found in star forming regions with the following physical properties ( $n_{\text{H}_2} \geq 10^5 \text{ cm}^{-3}$ ;  $T_{\text{gas}} = 20 - 50 \text{ K}$ ;  $T_{\text{dust}} \leq 50 \text{ K}$ ;  $A_V > 10 \text{ mag}$ ;  $G_0 = 1 - 10^5$ )<sup>2</sup> and for star-less cores (e.g., TMC-1) produce an water abundance  $< 7 \times 10^{-8}$  (for  $n_{\text{H}_2} \geq 10^4 \text{ cm}^{-3}$ ;  $T_{\text{gas}} = 10 \text{ K}$ ;  $T_{\text{dust}} < 15 \text{ K}$ ;  $A_V > 10 \text{ mag}$ ;  $G_0 = 1$ ).
3. Be capable of simultaneously reproducing the high water abundances ( $x(\text{H}_2\text{O}) \sim 10^{-6}$ ; Neufeld et al. 1999) found in the low density gas along the line of sight towards SgrB2 ( $n_{\text{H}_2} \lesssim 10^4 \text{ cm}^{-3}$ ;  $T_{\text{gas}} \sim 10 - 30 \text{ K}$ ).
4. Account for the co-existence in the gas phase of complex carbon-bearing species (e.g., HC<sub>3</sub>N, HCN, and CH<sub>3</sub>C<sub>2</sub>H) with that of simple and complex oxygen-bearing molecules, such as SO and CH<sub>3</sub>OH (Bergin et al. 1997).
5. Account for a water ice abundance of  $x(\text{H}_2\text{O})_{\text{ice}} \sim 1 \times 10^{-4}$  (Tielens et al. 1991; Schutte 1999). The appropriate physical conditions are not highly constrained, but are between  $n_{\text{H}_2} = 10^3 - 10^6 \text{ cm}^{-3}$  and  $T_{\text{gas}} \sim 10 - 50 \text{ K}$ .
6. Be consistent with other species (e.g., NH<sub>3</sub>) observed to have non-negligible concentrations in molecular gas and have similar sensitivities to the radiation field. For example, H<sub>2</sub>O, O<sub>2</sub>, and NH<sub>3</sub> have similar sensitivities to both internal and external radiation fields (van Dishoeck 1988; Sternberg & Dalgarno 1996). Therefore the low abundances found by SWAS cannot be the result of enhanced UV penetration.

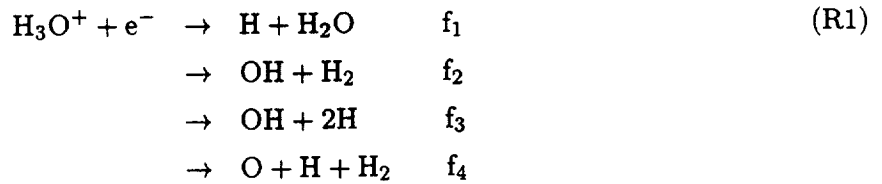
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<sup>2</sup> $G_0$  = enhancement factor above normal interstellar UV radiation field

## 5. Oxygen Chemistry in Molecular Clouds

### 5.1. Time Dependent Chemistry

The oxygen chemistry begins with the cosmic ray ionization of  $\text{H}_2$  which quickly leads to the formation of the trihydrogen ion ( $\text{H}_3^+$ ).  $\text{H}_3^+$  will react with O and a sequence of rapid reactions leads to the formation of the  $\text{H}_3\text{O}^+$  ion. The next step involves the dissociative recombination of  $\text{H}_3\text{O}^+$  with electrons:



where  $f_{1-4}$  are the branching ratios.<sup>3</sup> The formation of  $\text{O}_2$  follows through a reaction between O and OH. The destruction of both  $\text{H}_2\text{O}$  and  $\text{O}_2$  is dominated by the cosmic-ray induced photo-field and reactions with  $\text{H}^+$ ,  $\text{He}^+$ ,  $\text{C}^+$ , and  $\text{H}_3^+$  (and C in the case of  $\text{O}_2$ ).

Fig. 1 presents this current view of pure gas phase time-dependent chemistry for typical conditions. The initial conditions simulate diffuse cloud abundances and are taken from Millar et al. (1997). This model is somewhat limited in application in that it does not include dynamics and the initial conditions are an approximation. Nonetheless it is illustrative of the relative importance of the various species and the timescales involved under the assumption of constant density.

The predicted water abundance changes sharply depending on the assumed  $\text{H}_3\text{O}^+$  branching ratio; for  $f_1 \leq 0.05$  the water is mainly produced via proton-transfer reactions between  $\text{H}_3\text{O}^+$  and other molecular species (e.g., HCN,  $\text{NH}_3$ ). Examining the constraints listed in § 4, the model is consistent with SWAS  $\text{O}_2$  observations, provided the chemistry for *all* sources surveyed has evolved for  $t < 10^5$  yr. The model is also consistent with the high water abundance found along the line of sight towards SgrB2, provided  $f_1 > 0.3$ . If, for consistency with the SgrB2 observations, we adopt  $f_1 = 0.33$ , then the water abundances found in star forming regions place even greater strains on the theory, as the observations require ages  $< 1000$  yr.<sup>4</sup>

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<sup>3</sup>Vejby-Christensen et al. (1997) measured  $f_1 = 0.33$ ,  $f_2 = 0.18$ ,  $f_3 = 0.48$ , and  $f_4 = 0.01$ , while Williams et al. (1996) find  $f_1 = 0.05$ ,  $f_2 = 0.36$ ,  $f_3 = 0.29$ ,  $f_4 = 0.30$ . These two laboratory measurements differ sharply in the amount of water produced.

<sup>4</sup>The ages of molecular clouds and cloud cores are highly uncertain. Lower limits can be set using the free-fall timescale, which is  $\sim 10^5$  yr for typical densities ( $n_{\text{H}_2} = 10^5 \text{ cm}^{-3}$ ). The mean age of embedded protostars sets another lower limit. In Orion the mean age is  $\sim 1$  Myr (Hillenbrand & Carpenter 2000).



## 5.2. Alternate Solutions

One possible method to lower the water and molecular oxygen abundance is a change in the elemental C/O ratio above the solar value of 0.4. If the C/O ratio is raised to higher values (e.g., by depleting the elemental oxygen relative to that of carbon) then the amount of atomic oxygen available to form water and molecular oxygen is limited and relatively more carbon atoms and ions exist to destroy H<sub>2</sub>O and O<sub>2</sub>. Additional effects have been discussed in the literature (Terzieva & Herbst 1998 and references therein).

In Fig. 2 we show points defining the plane of O<sub>2</sub> and H<sub>2</sub>O abundances as a function of time and the assumed elemental C/O ratio. Clearly changing the C/O ratio has a dramatic effect on the abundance of both molecules. Consistency with SWAS observations of star forming cores (constraints #1 and #2) requires C/O > 0.9 and has the desired effect of allowing for H<sub>2</sub>O and O<sub>2</sub> abundances to agree at later, more relevant, timescales ( $t > 10^5$  yr). Changing the elemental C/O ratio above solar could be the result of variations in the interstellar medium due to different formation histories, supernovae or planetary nebula activity, and/or a direct by product of the gas-grain interaction.

In Fig. 3 we show a more complex gas-grain chemical model that demonstrates how the C/O ratio could be altered using a chemical mechanism outlined in d'Hendecourt, Allamandola, & Greenberg (1985). The first panel shows a gas grain model with no surface chemistry. In this model oxygen atoms deplete on grains, remain inert, and their abundance is maintained in the gas phase by thermal evaporation. The gas phase oxygen enables a chemistry similar to that shown in Fig. 1. In Fig. 3b we show a gas-grain model including two surface reactions ( $O + gr \rightarrow H_2O(gr)$  and  $C + gr \rightarrow CH_4(gr)$ ). Here most oxygen is trapped on grains in the form of water ice, which will only evaporate if  $T_{dust} > 90$  K. In contrast, volatile CH<sub>4</sub> is released back into the gas phase for  $T_{dust} > 23$  K and the carbon chemistry is enhanced (see also Brown and Charnley 1991; Nejad & Williams 1992).

This model, with simple and reasonable assumptions for the chemistry reproduces constraints (#1) and (#2) with low abundances of H<sub>2</sub>O and O<sub>2</sub> at physically relevant timescales, and also enhances the abundances of complex species as exemplified by HC<sub>3</sub>N (#4). Because the depletion timescales are longer at lower densities, the inclusion of grains into the chemistry also naturally allows for a difference between the high water abundances found along the SgrB2 line of sight and the low water abundances in star forming regions.

However, there are two potential problems with this model. First, the sulfur chemistry, especially the production of SO (which is observed to be reasonably abundant), is effectively halted by the gas-grain interaction (Bergin & Langer 1997; Ruffle et al. 1999). Second, observations of atomic oxygen in absorption towards similar regions find high oxygen column densities (e.g., Caux et al. 1999). If the oxygen absorption features are probing the entire line of sight (and not just cloud halos), then this would be in conflict with the depletion of oxygen in the form of water ice (Fig. 3b).

Both of these problems could be alleviated by the presence of significant unresolved chemical structure along the line of sight with pockets of undepleted molecular chemistry, such as might exist at the low density cloud edges or in the vicinity of embedded sources, coexisting (within the SWAS beam) with regions of high depletion. The spatial resolution of the SWAS instrument is insufficient to resolve such structure.

Other possibilities that must be considered are that shocks can alter the C/O ratio by creating water ice mantles, supplementing the products of surface chemistry (Bergin et al. 1998), bistability in chemical models (Le Boulot et al. 1993; see discussion in Goldsmith et al. 2000), and/or that the apparent chemical youthfulness of dense cores could be maintained by turbulence or cycling of material between low density to high density phases (Chièze & Pineau des Forêts 1989; Charnley et al. 1988; Xie, Allen, & Langer 1995). Indeed in these models the O<sub>2</sub> and H<sub>2</sub>O abundances can be lowered several orders of magnitude below steady state values as required by SWAS observations (Chièze & Pineau des Forêts 1989; Xie, Allen, & Langer 1995).

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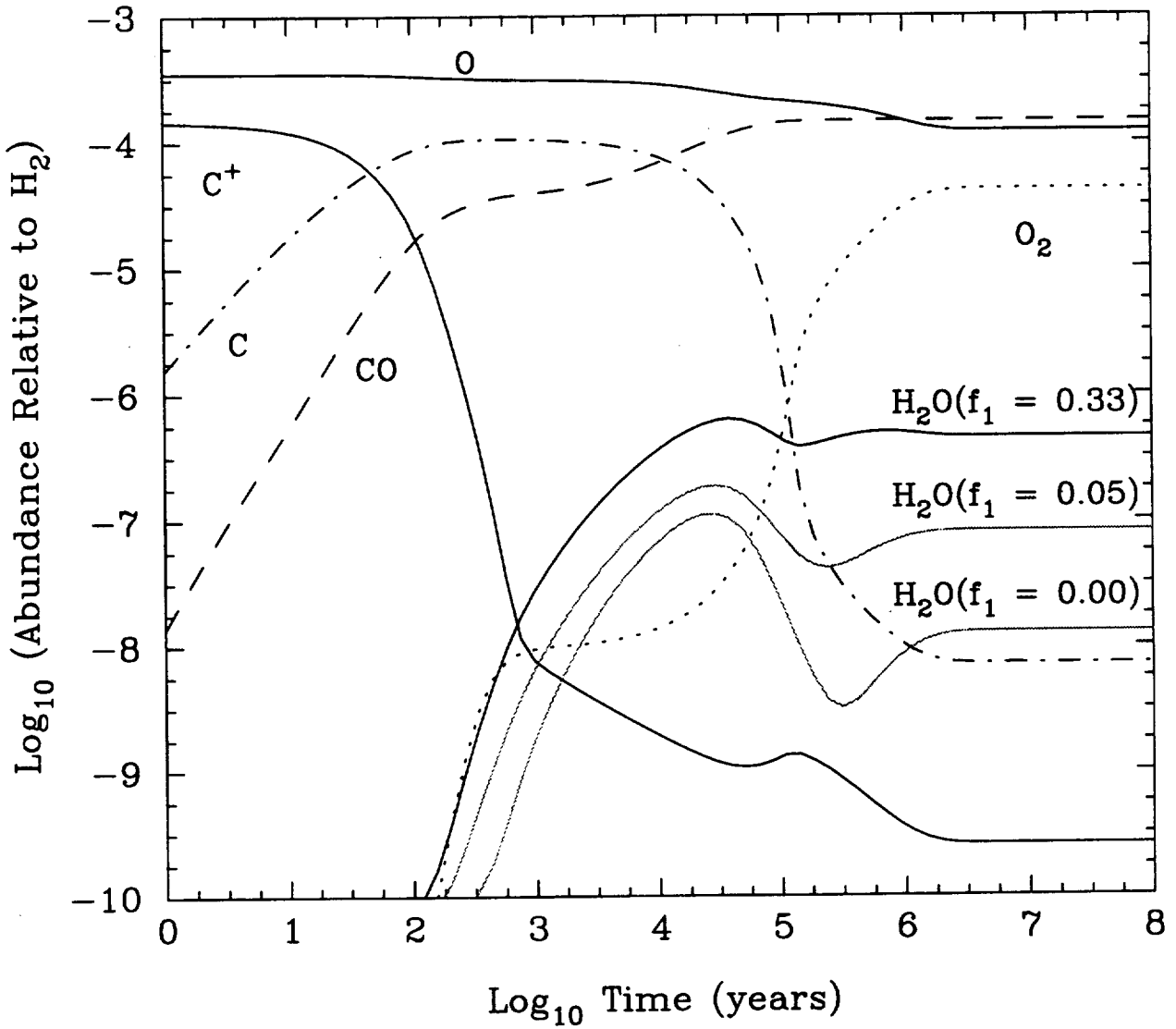


Fig. 1.— Time evolution of chemical abundances relative to H<sub>2</sub> for a solar C/O ratio of 0.4. The evolution of the H<sub>2</sub>O abundance is shown for different values of the H<sub>3</sub>O<sup>+</sup> branching ratio (discussed in § 5). The assumed physical conditions are:  $n_{H_2} = 10^5 \text{ cm}^{-3}$ ,  $T_{gas} = 30 \text{ K}$ , and  $A_V = 20^m$ . The chemical model used here has been described previously (e.g. Bergin & Langer 1997) and is similar to other current gas phase models (Lee et al. 1996).

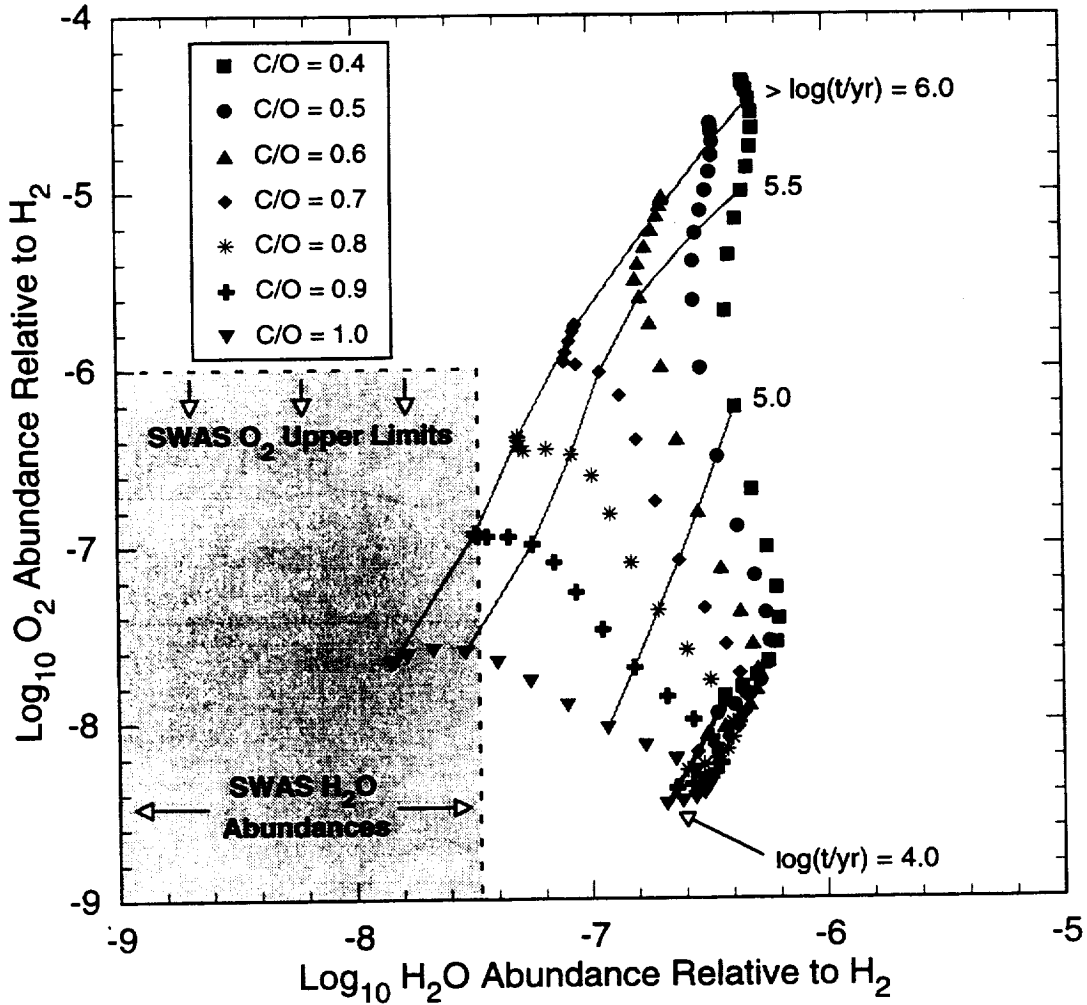


Fig. 2.— Plot of O<sub>2</sub> versus H<sub>2</sub>O abundances shown as a function of time and assumed elemental C/O ratio. The different point types delineate the various C/O ratios (a value of 0.4 is the solar ratio). The solid grey lines are isochrones of constant time. Models are run using  $n_{\text{H}_2} = 10^5 \text{ cm}^{-3}$ ,  $T_{\text{gas}} = 30 \text{ K}$ , and  $A_V = 20^m$ . The shaded area denotes the range of abundances implied by SWAS observations.

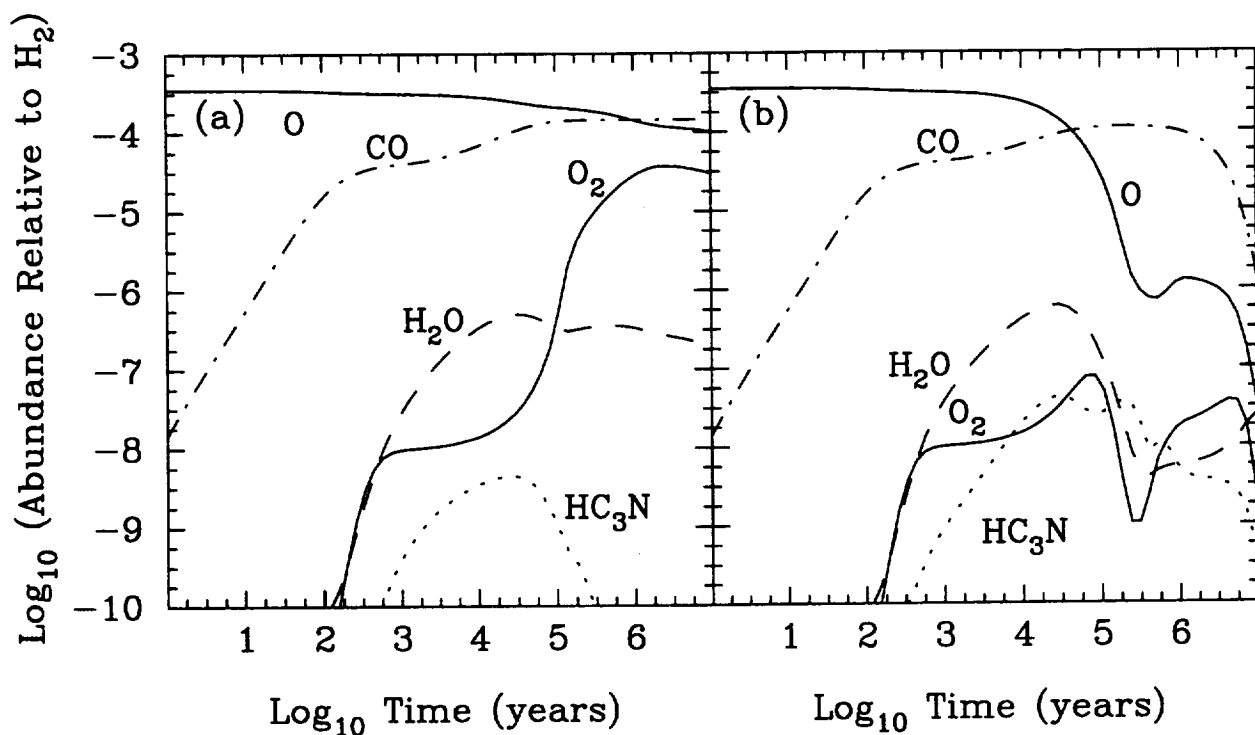


Fig. 3.— Abundances of CO, O<sub>2</sub>, H<sub>2</sub>O, and HC<sub>3</sub>N as a function of time for two models of the gas-grain chemistry. (a) Model including depletion and desorption onto grain surfaces, but no surface chemistry. (b) Model including depletion and desorption onto grains but with simple surface chemistry. Both models assume  $n_{H_2} = 10^5 \text{ cm}^{-3}$ ,  $T_{gas} = T_{dust} = 30 \text{ K}$ , and  $A_V = 20^m$ . The second model does not include any modifications to account for the discrete nature of grains (Caselli, Hasegawa, & Herbst 1998), but is nonetheless illustrative of the effects of the process.

