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On the spatial coincidence of hydroxyl and methanol masers

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ABSTRACT
We argue that purely gas-phase chemical models for the production of OH in hydroxyl masers around ultracompact H II regions such as W3(OH) cannot account for the CH_3OH in the methanol masers that are found to coincide with the hydroxyl masers in these sources. We suggest that the CH_3OH in the masers is injected into the gas phase by evaporation of the grain mantles, the grains being heated by the passage of weak shocks. Gas evaporation also injects H_2O into the gas. Photodissociation of H_2O, CH_3OH and OH occur at similar rates, and substantial abundances of CH_3OH and OH coexist.

Key words: masers - molecular processes - H II regions - radio lines: ISM.

1 INTRODUCTION
Interstellar hydroxyl masers in the vicinities of H II regions have higher abundances of OH than can be maintained by low-temperature, gas-phase chemical schemes. To explain the enhanced OH abundances, Elitzur & de Jong (1978) invoked heating behind shocks, driven into the ambient molecular media by the expansion of the H II regions, and subsequent exposure to strong radiation fields. Speeds higher than 10 km s^{-1} are required for the temperatures in MHD shocks propagating into ambient media with number densities in excess of 10^4 cm^{-3} to be high enough to drive the neutral particle O, OH, H_2O chemistry (Draine, Roberge & Dalgarno 1983). However, Reid et al. (1980) and Garay, Reid & Moran (1985) pointed out that the line-of-sight velocities of hydroxyl maser spots are shifted by less than 10 km s^{-1} relative to the mean line-of-sight velocities of the associated H II regions. Hartquist & Dalgarno (1982) speculated that the OH is formed in regions heated by ion-neutral drift in the precursors of MHD shocks and exposed to radiation capable of photodissociating H_2O and H_2. In their model the neutral gas in a precursor would not be accelerated much, the heating would give rise to sufficient temperatures to drive chemical reactions that are slow at low temperatures, and the photodissociating radiation would prevent the gas-phase reactions from concentrating the gas-phase oxygen into H_2O and CO. However, because the radiation field would give rise to significant S^+ and C^+ production, resulting in an effective coupling of the ion and neutral motions, such a precursor bathed by a strong radiation field would probably be too narrow to be the site of a hydroxyl maser.

Hartquist (1986) suggested the alternative of static, equilibrium, photon-dominated region models for hydroxyl masers. Hartquist & Sternberg (1991) found that such regions are heated sufficiently by the radiation fields at the boundaries of compact H II regions for a warm chemistry to proceed. The OH column densities for some such models are in harmony with those required in models of hydroxyl maser pumping (cf. Guilloteau, Baudry & Walmsley 1985; Cesaroni & Walmsley 1991; Gray, Doel & Field 1991; Gray, Field & Doel 1992). We argue later that, because of photodissociation, adequate amounts of CH_3OH cannot be produced in the gas phase in photon-dominated regions.

Menten et al. (1992) have shown from VLBI data that many methanol masers and hydroxyl masers observed toward the ultracompact H II region W3(OH) appear to be spatially coincident. In the present paper, we examine the viability of various hydroxyl maser models in view of these observations. The observational evidence for high methanol abundances in the molecular envelopes of ultracompact H II regions is summarized in Section 2. In Section 3, we argue that high abundances of CH_3OH cannot exist in the photon-dominated regions considered by Hartquist & Sternberg (1991). In Section 4, we show that CH_3OH is unlikely to be produced copiously by gas-phase chemistry in shocks like the one that exists around the H II region in W3(OH). In Section 5, we examine the possibility that irradiation of gas containing CH_3OH and H_2O liberated from grain surfaces by the passage of a weak shock is responsible for the coexistence of high abundances of both CH_3OH and OH in the maser regions. This final possibility is fully consistent with the model of 'cometary' compact H II regions as wind-blow bubbles around stars moving with respect to the molecular
media around them (Van Buren et al. 1990) and with recent proper motion results for hydroxyl maser spots in W3(OH) (Bloemhof, Reid & Moran 1992).

2 OBSERVATIONAL BACKGROUND

Very strong maser emission from various transitions of the methanol molecule has been detected toward numerous regions of high-mass star formation (Menten 1991a). So-called Class II methanol masers arise from the immediate vicinity of ultracompact H II regions and seem to be closely related to hydroxyl masers. Virtually all known Class II methanol maser sources show maser action in OH, with the emissions observed in both species always covering similar velocity ranges (Menten 1991b). VLBI observations of several sources show directly that many methanol and hydroxyl masers are spatially coincident and have similar velocity structure on scales smaller than about 500 au (Menten et al. 1988). The best-studied is the archetypal ultracompact H II region W3(OH), for which detailed milliarcsecond-resolution maps are available in several OH and CH$_3$OH transitions (Moran et al. 1978; Reid et al. 1980; Menten et al. 1988, 1992).

Absorption of far-infrared radiation emitted by warm dust around the H II region is a likely pumping mechanism for OH (Guilloteau et al. 1985) and also for Class II CH$_3$OH masers (Menten 1991a; Cragg et al. 1992). Thus the coexistence of masers in both species is understandable from their excitation requirements. However, while the maser observations do not allow a direct determination of the CH$_3$OH abundance, an estimate for the W3(OH) envelope can be obtained from the quasi-thermal methanol absorption observed against the H II region continuum background in a number of centimetre-wave lines (Menten et al. 1986). VLA observations show that this absorption extends over the same part of the continuum source as the methanol and hydroxyl masers, although almost certainly with a much larger filling factor (Wilson, Johnston & Mauersberger 1991). The total methanol column density in the absorbing material was estimated to lie between 2 $\times$ 10$^{17}$ and 2 $\times$ 10$^{18}$ cm$^{-2}$, translating into a CH$_3$OH/H$_2$ abundance ratio between 10$^{-6}$ and 10$^{-5}$ (Menten et al. 1985, 1986). There are major sources of uncertainty in this estimate, introduced by the poorly known source filling factor and methanol excitation mechanism; nevertheless, the derived CH$_3$OH/H$_2$ ratios are several orders of magnitude higher than values produced in gas-phase reaction schemes at temperatures below several hundred degrees (Herbst & Leung 1989; Millar et al. 1991).

3 METHANOL IN PHOTON-DOMINATED REGIONS

Hartquist & Sternberg (1991) found that, in a photon-dominated region with a total hydrogen number density $n_H$ equal to or greater than 10$^6$ cm$^{-3}$ exposed to an intense radiation field, the OH fractional abundance reaches 10$^{-3}$ in a limited zone where the temperature is near 1000 K. The radiation field intensity must be a factor $\chi$ of 10$^4$ or greater than the standard interstellar radiation field for such a zone to exist. The H$_2$O abundance is of the same order as OH, or somewhat higher. In a hot gas, CH$_3$OH can be produced in the endothermic reactions

\[
\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{OH} + \text{H},
\]

which has an endothermicity of 6500 K (Wagman et al. 1968), and

\[
\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{OH} + \text{H},
\]

which has an endothermicity of about 14 700 K (Wagman et al. 1968), of which the former is more effective. The main destruction mechanism is photodissociation. We use laboratory data of Burton et al. (1992) and follow the procedures described by Roberge et al. (1991) to calculate the interstellar photodissociation rates. In terms of the visual extinction $A_V$, the photodestruction rate corresponding to the standard interstellar radiation field of Draine (1978) enhanced by a factor $\chi$ is given by

\[
\Gamma = 6.00 \times 10^{-10} \, \text{s}^{-1} \times \chi \exp (-2.508 A_V + 4.896 \times 10^{-2} A_V^2).
\]

The branching ratios for the individual product channels are listed in Table 1.

Photodissociation of CH$_3$OH proceeds at a similar rate to the photodissociation of H$_2$O, and the radiation field necessary in a photon-dominated region to heat the gas and to produce OH from H$_2$O will be efficient in destroying CH$_3$OH and, through the photodissociation of CH$_4$, limiting the pathways by which it is formed. In the absence of a radiation field, large abundances of CH$_3$OH can be created in a gas at temperatures near 2000 K, but in photon-dominated regions the abundance of CH$_3$OH is small.

4 METHANOL PRODUCTION IN DARK SHOCKED GAS

Van Buren et al. (1990) have suggested that ‘cometary’ compact H II regions, of which W3(OH) may be one, are stellar-wind-blown bubbles which are moving relative to the ambient molecular media at speeds greater than the sound speed in them. According to Van Buren et al., hydroxyl masers around a ‘cometary’ compact H II region form in gas

<table>
<thead>
<tr>
<th>Process</th>
<th>Unattenuated Rate $\alpha$</th>
<th>One-sided Model with $A_\nu = 100$ $\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Photodestruction</td>
<td>1.88(09)</td>
<td>6.00(10)</td>
</tr>
<tr>
<td>Total Photodissociation*</td>
<td>1.52(09)</td>
<td>5.09(-10)</td>
</tr>
<tr>
<td>CH$_3$OH $\rightarrow$ CH$_3$OH + e</td>
<td>2.48(-10)</td>
<td>8.33(11)</td>
</tr>
<tr>
<td>CH$_3$OH $\rightarrow$ CH$_3$O* or CH$_3$OH*</td>
<td>1.03(-10)</td>
<td>3.93(11)</td>
</tr>
<tr>
<td>CH$_3$OH $\rightarrow$ CH$_3$OH* or OH*</td>
<td>2.01(-12)</td>
<td>7.46(-11)</td>
</tr>
<tr>
<td>CH$_3$OH $\rightarrow$ CO* or COH</td>
<td>1.81(-13)</td>
<td>6.65(-14)</td>
</tr>
<tr>
<td>CH$_3$OH $\rightarrow$ CH$_3$* or CH$_2$</td>
<td>1.23(-13)</td>
<td>4.51(-14)</td>
</tr>
</tbody>
</table>

*The neutral products are uncertain. A major channel is likely to be CH$_3$ + OH.

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that has passed through the bow shock propagating into the molecular material near the leading edge of the wind-blown bubble. Maser spots in gas that has passed through such a bow shock have a distribution of proper motion velocities with magnitudes that range up to a large fraction of the speed of the bubble velocities for maser spots in W3(OH) which are in harmony with the Van Buren et al. model and which limit the relative speed between the bubble and the ambient medium to less than about 10 km s\(^{-1}\).

In W3(OH) and possibly most other ultracompact H\(_II\) regions, the observed small differences between the velocities of the ionized gas and the maser material imply that the maximum post-shock temperature anywhere in the molecular gas cannot be high. Indeed, because the magnitude of its velocity component parallel to the normal to the bow shock is considerably less than 10 km s\(^{-1}\) over much of the bow shock surface, a large fraction of the shocked gas will not be heated to 1000 K. Our discussion is restricted to situations in which gas in the bow shock is heated to \(T \lesssim 1 \times 10^3\) K; the temperature lies above this range in some parts of the bow shock around the ‘cometary’ compact H\(_II\) region found by Van Buren & MacLow (1992) to be associated with a star moving at about 20 km s\(^{-1}\) relative to neutral material around it, and the chemical conclusions drawn in this section may not apply to that source.

In low-temperature, purely gas-phase, dark-cloud chemical schemes the only species, other than CO, that ever contains much of the carbon is C (cf. Millar 1990). Thus, if the CH\(_2\)OH in the masing region were produced as a consequence of purely gas-phase chemistry, its most probable formation sequence in warm shocked dark-cloud gas would be initiated by

\[
\text{C} + \text{H}_2 \rightarrow \text{CH} + \text{H}. \tag{4}
\]

Further hydrogen abstraction reactions, culminating in

\[
\text{CH}_3 + \text{H}_2 \rightarrow \text{CH}_4 + \text{H}, \tag{5}
\]

give rise to CH\(_3\) and CH\(_4\) production. OH is formed in shocked gas by

\[
\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H} \tag{6}
\]

and removed by

\[
\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}. \tag{7}
\]

Reactions (1) and (2) are the major gas-phase sources of CH\(_2\)OH in shocked gas, but they are not very productive. At 1000 K in a shocked dense gas, most of the oxygen is taken up as H\(_2\)O. However, reaction (2) proceeds very slowly at 1000 K because of the large endothermicity. Reaction (1) is also an inefficient source of CH\(_2\)OH, because the CH\(_4\) production is limited by the endothermicity of reaction (4) and there is little OH available.

5 WEAK SHOCKS AND GRAIN-MODERATED CHEMISTRY

The CH\(_2\)OH in methanol masers that are coincident with hydroxyl masers cannot be produced by purely gas-phase chemical processes. As an alternative, we propose that evaporation of methanol ice off icy dust grain mantles is the source of the masing methanol. The injection of H\(_2\)O from grains into the gas phase occurs simultaneously.

Convincing evidence for methanol ice as a substantial constituent of interstellar dust grain mantles has been accumulated with infrared spectroscopy of various star-forming regions. Absorption features at wavelengths around 3.1, 3.5 and 6.87 \(\mu\)m have been attributed to different vibrational bands of solid methanol (Grim et al. 1991; Allamandola et al. 1992; Skinner et al. 1992). For some sources high solid CH\(_3\)OH abundances have been derived, ranging up to 0.5 times the abundance of solid H\(_2\)O, which appears to be the dominant interstellar grain mantle component. The CH\(_3\)OH may be formed on the grain surfaces by hydrogenation of CO accreted from the gas phase (Tielens 1989; Brown & Charnley 1991; Charnley, Tielens & Millar 1992; Hasegawa, Herbst & Leung 1992). Several of the sources showing methanol ice features, such as Mon R2, W33A and AFGL 2136, are strong methanol and hydroxyl maser sources (Koo et al. 1988; Menten 1991b). Most ultracompact H\(_II\) regions are embedded in warm, dense dusty envelopes, which radiate most effectively at far-infrared wavelengths, while at 3 and even 6 \(\mu\)m, very high extinction attenuates the near-infrared radiation emitted by the hot inner regions of the envelope, making absorption spectroscopy difficult. 3.1- and 3.3-\(\mu\)m absorption data have not been reported for W3(OH), which is a weak near-infrared source with a 3.5-\(\mu\)m flux density of \(\approx 0.2\) Jy (Wynn-Williams, Becklin & Neugebauer 1972). Prominent 3-\(\mu\)m sources, such as W33A, are either surrounded by less circumstellar material or have special geometries, allowing observations of hotter material closer to the embedded objects. With present technology, infrared absorption measurements even toward weaker sources, such as W3(OH), are feasible and highly desirable.

The injection of CH\(_2\)OH and H\(_2\)O may be induced by the propagation of a weak shock. Pilipp & Hartquist (1994) have constructed a model of a steady MHD shock propagating into a medium with \(n_\text{H} = 10^7\) cm\(^{-3}\) at a speed of 2.3 km s\(^{-1}\). They found that the neutral temperature is about 70 K, which is probably sufficient to drive evaporation. At such a high density, the neutral and dust temperatures are well coupled, unless at least one of them exceeds several hundred degrees (e.g. Guillemont et al. 1985). The evaporation rate of any particular ice in a mantle is a sensitive function of temperature when \(T > 100\) K, and increases by orders of magnitude to become rapid compared to gas-phase chemical and dynamical time-scales when the temperature rises by only tens of degrees above the critical melting temperature, which is generally less than 100 K (Watson & Salpeter 1972; Nakagawa 1980). Pilipp & Hartquist (1994) calculated the width of the 70-K region to be roughly \(3 \times 10^{15}\) cm, through which the visual extinction is several tens of magnitudes. In contrast, Hartquist & Sternberg (1991) showed that, at only several magnitudes of visual extinction into a photon-dominated region with density \(n_\text{H} = 10^7\) cm\(^{-3}\), heated only by photoabsorption of the radiation from an early-type star at a distance of 0.01 pc, the temperature is below 70 K. Thus the shock dissipation zone extends far beyond the region heated significantly by photoabsorption, and evaporation of grain mantles is driven by the shock.

As in the Elitzur–de Jong model, once in the gas phase, H\(_2\)O is photodissociated to produce OH. Because of their similar photodissociation rates, H\(_2\)O, CH\(_3\)OH and OH possess substantial abundances simultaneously in gas irradi-
ated after the injection of large amounts of H₂O and CH₃OH. If we were to neglect differences between the OH, H₂O and CH₃OH photodestruction rates, we would find that the OH and H₂O abundances are comparable to one another over a length, δ, corresponding to roughly one magnitude of visual extinction near the point at which the visual extinction satisfies

\[ \delta = \frac{u}{C"} \exp(a A' + \beta A"'), \tag{8} \]

with

\[ \delta = \frac{N_{\text{H}}}{{A}' n_{\text{H}}}, \tag{9} \]

where \( C", a \), and \( \beta \) are given in Table 1, \( N_{\text{H}} = 2 \times 10^{21} \ A' \) cm⁻² is the column density of hydrogen nuclei to the star, and \( u \) is the speed of the gas relative to the star. The corresponding column density of OH is of the order of

\[ N(\text{OH}) = \frac{1}{2} n_{\text{w}}(\text{H}_2\text{O}) \delta = \frac{1}{2} \frac{n_{\text{w}}(\text{H}_2\text{O})}{n_{\text{H}}} \frac{N_{\text{H}}}{10^{17} \text{ cm}^{-2}} \frac{n_{\text{w}}(\text{H}_2\text{O})}{10^{-4} n_{\text{H}}}, \tag{10} \]

where \( n_{\text{w}}(\text{H}_2\text{O}) \) is the number density of H₂O in gas that has been shock-heated but has not approached the ionization front. The column density of H₂O is comparable to \( N(\text{OH}) \), and the column density of methanol in that region is of the order of \( N(\text{OH}) n_{\text{w}}(\text{CH}_3\text{OH})/n_{\text{w}}(\text{H}_2\text{O}) \), where \( n_{\text{w}}(\text{CH}_3\text{OH}) \) is the number density of CH₃OH in gas that has been shock-heated but has not approached the ionization front.

The absence of water masers in W₃(OH) is probably a consequence of unsuitable physical, rather than chemical, conditions for water masering. Specifically, if the H₂O enters the gas phase by evaporation from mantles, rather than being produced by high-temperature, gas-phase chemistry, the temperature may be too low for water maser pumps to operate. Elitzur, Hollenbach & McKee (1989), Menten et al. (1990) and Neufeld & Melnick (1991) have argued that temperatures at around 400 K typify and seem to be required to pump collisionally high-velocity interstellar water masers. Water maser spots might be found in the vicinities of hydroxyl maser spots around compact 'cometary' H II regions surrounding stars that move at speeds higher than 10 km s⁻¹ with respect to their associated ambient molecular gas. Swept-up molecular gas around such higher speed cometary H II regions would reach temperatures equal to and exceeding those required by water-maser pumping models. However, it is possible that the density, radiation field and temperature regimes in which water and hydroxyl maser pumps operate do not overlap.

Because kinematic studies of hydroxyl masers in W₃(OH) indicate that the shocks associated with them are too slow for high-temperature, gas-phase chemistry to occur behind them, and that in any case injection of CH₃OH into the gas phase is better able to account for the existence of methanol masers in W₃(OH), we conclude that injection from grain mantles plays a major role in the production of hydroxyl masers as well as methanol masers in W₃(OH).

Thus hydroxyl and methanol masers may exist around compact H II regions propagating at only a few km s⁻¹ with respect to the surrounding ambient medium.

More generally, injection of molecular grain mantle material heated by weak shocks or embedded objects is likely to be an important mechanism for producing high gas-phase abundances of molecules in star-forming regions. Evaporation of grain mantles into 100-K gas has been suggested to account for the abundances of oxygen-bearing organic molecules in the Orion Compact Ridge (Blake et al. 1987; Charnley et al. 1992). Injection from grain mantles may also produce the CH₃OH in Class I methanol masers. These sources are fundamentally different from the W₃(OH)-type Class II methanol masers. Class I sources are found to be distinctly offset (up to several pc) from ultracompact H II regions and OH or H₂O masers. They show maser action in different transitions, none of which is masering in Class II sources and vice versa (Menten 1991a). For the Class I source DR21-β, the interferometric observations of Plambeck & Menten (1990) show that the maser emission arises from the interface region between a prominent molecular outflow and an ambient dense molecular clump. Our results support their speculation that shock heating by the molecular outflow leads to evaporation of methanol from grain mantles, creating the methanol abundance necessary for the observed masers.

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