

CHEMISTRY IN INTERSTELLAR HYDROXYL MASER REGIONS

T.W. Hartquist

Max-Planck-Institut für Physik und Astrophysik, Institut
für extraterrestrische Physik, 8046 Garching, F.R.G.
Astronomy Program, University of Maryland, College Park,
Maryland 20742, U.S.A.

ABSTRACT. The pumping of the upper levels of the ${}^2\Pi_{3/2}$ $J=3/2$ state of OH at sufficient rates to account for the observed strengths of interstellar hydroxyl masers requires that OH contains a substantial fraction of the oxygen. Shocks have been suggested as the sites of the OH production, but a better understanding of OH photodissociation and observations of hydroxyl maser kinematics have led to the realization that the original hydroxyl maser shock model must be revised. The possibility that interstellar hydroxyl masers occur in dense molecular photodissociation zones, heated by photoabsorption and perhaps by ion-neutral friction in the magnetic precursor of a shock, is considered. Possible infrared line emission from interstellar hydroxyl maser regions is mentioned.

1. INTRODUCTION

The ground state of OH is a ${}^2\Pi_{3/2}$ $J=3/2$ state having four nearly degenerate levels split by Λ doubling and hyperfine interactions. In order of increasing energy the levels have the following parities and total angular momentum, F : (+, 1), (+, 2), (-, 1), and (-, 2). Transitions in which F does not change are called main line transitions and are at 1665 MHz for (-, 1) \rightarrow (+, 1) and at 1667 MHz for (-, 2) \rightarrow (+, 2). Transitions in which F does change are called satellite transitions and are at 1612 MHz for (-, 1) \rightarrow (+, 2) and at 1720 MHz for (-, 2) \rightarrow (+, 1). Correct parity assignments have been made only recently (Andresen et al. 1984b). Interstellar hydroxyl masers have been detected in all of the main lines and satellite lines of ${}^2\Pi_{3/2}$ $J=3/2$ as well as in lines from transitions in the ${}^2\Pi_{3/2}$ $J=5/2$ and ${}^2\Pi_{1/2}$ $J=1/2$ states (Reid and Moran 1981).

2. PUMPING OF HYDROXYL MASERS

The fractional concentration of OH in the interstellar hydroxyl masers can be estimated by specifying a pumping mechanism and determining the OH column density and the total density required for models based on that pumping mechanism to reproduce observational data.

The correct assignment of quantum numbers to the different $2\pi_{3/2}$ $J=3/2$ levels is required before an investigation of pumping models can be made. For the moment ignore hyperfine splitting and consider Λ -doubling only. Studies (Andresen et al. 1984b) of the photodissociation of water through the 1B_1 state showed that the product OH is preferentially in the upper Λ doublet level; the polarization of the OH was determined and the unpaired electron orbital was found to be more frequently perpendicular to the rotational plane than parallel. In contrast to earlier expectations (c.f. Bertojo, Cheung, and Townes 1976) the levels of lowest energy have even parity.

Andresen et al. (1984b) have suggested that an important mechanism for populating the upper Λ doublet levels of OH in masers is the photodissociation of H_2O . To attain significant population inversion, H_2O would then have to be reformed by the reaction of OH with H_2 to form water at rates approaching those for Λ doublet deexcitation by collisions of OH and H_2 ; the deexcitation rate coefficient is around 10^{-10} cm^3s^{-1} (Dewangen and Flower 1982).

Inversion of levels in $2\pi_{3/2}$ $J=3/2$ OH may occur if collisionally induced rotational excitation favors the production of those levels in the rotationally excited molecules that, because of parity selection rules, radiatively decay to produce $2\pi_{3/2}$ $J=3/2$ OH in the upper Λ doublet levels (Bertojo, Cheung, and Townes 1976). If the correct parity assignments are used calculations (Dewangen and Flower 1982) and measurements (Andresen, Häusler, and Lülfi 1984) of the rotational excitation rates show that inversion is not achieved by the selective behavior of rotational excitation rates (see also Andresen et al. 1984a).

Inversion of levels in $2\pi_{3/2}$ $J=3/2$ OH can be obtained if line overlap decreases the escape probability of photons emitted in the decay of excited rotational levels to $2\pi_{3/2}$ $J=3/2$ OH in the lower Λ doublet level (Guilloteau, S., Lucas, R., and Omont, A. 1981). Overlap effects can lead to inversion because the hyperfine structure of Λ doublet levels depends on the parity of the level, resulting in differences between overlap effects for transitions differing only by the parity of the states that they connect. Line overlap can be important only for a certain range of OH column densities; for very low ones the escape probability is nearly unity while for very high ones, complete thermalization occurs. Guilloteau, Baudry, and Walmsley (1985) have included radiative transfer effects in a statistical level model for OH in the presence of collisions with H_2 and dust with a temperature equal to the gas temperature. They explained observed inversions and anti-inversions of a number of rotationally excited OH levels in W3 (OH) as well as the inversion of $2\pi_{3/2}$ $J=3/2$ OH with models in which $n(H_2) \approx 10^7$ - $10^{7.5}$ cm^{-3} and $T=160$ K. They concluded that the column density of OH is about 5×10^{16} cm^{-3} corresponding to $n(OH)$ being in the range of tens or hundreds cm^{-3} , depending on the assumed length of the masers.

Collisions probably produce the excited rotational levels whose selective decay in optically thick regions can lead to the population inversion in the $2\pi_{3/2}$ $J=3/2$ state. In principle, the absorption of infrared photons emitted in the vicinity of the masers also can populate the rotationally excited levels, but the flux of infrared photons in the vicinity of W3 (OH) seems to be too low to provide sufficient pumping (Wynn-Williams, Becklin, and Neugebauer 1972; Elitzur and de Jong 1978).

Johnston (1967) and Elitzur (1979) have suggested that inversion of the Λ doublet levels occurs when collisions that lead to doublet excitation and deexcitation with electrons and ions having anisotropic velocity distributions are rapid. While ambipolar diffusion is rarely fast enough to lead to significant anisotropy in the electron distribution, it can create anisotropy in the ion distribution. However, evaluation of the ambipolar diffusion speed in masers (Black and Hartquist 1979) gives that it is probably so low that estimates for the cross sections based on simple theories may be unreliable (Elitzur 1977). Even so, one can conclude that if pumping by anisotropic ion collisions with OH is important, OH must contain at least ten percent of the oxygen.

3. PRODUCTION OF THE OH

From models of the pumping of OH, one concludes that $n(\text{OH})/n(\text{H}_2) \geq 10^{-6}$ in hydroxyl masers. Standard low temperature gas phase model OH fractional abundances are about 10^{-8} for high density dark regions (de Jong, Dalgarno, and Boland 1980; Prasad and Huntress 1980).

Elitzur and de Jong (1978) suggested that high concentrations of OH exist in masers because they lie behind shocks expanding away from the early-type stars with which they are associated. Immediately behind a shock H_2O is formed and contains most of the oxygen. Further behind the shock photodissociation of H_2O by the stellar UV radiation occurs forming OH which also is photo-dissociated. At the time of their work, OH was thought to be dissociated efficiently only by photons significantly bluer than those that photodissociate H_2O . Elitzur and de Jong concluded that the size of hydroxyl maser spots is determined by the difference in the stopping length of the photons that dissociate H_2O and OH. Subsequently, van Dishoeck and Dalgarno (1984) showed that the $1^2\Sigma^-$ channel is important for OH photodissociation implying that the OH photodissociation rate remains large to much greater depths than previously assumed. Forward scattering affects the depth dependences of photodissociation rates (e.g. Roberge, Flannery, and Dalgarno 1981) and interstellar chemists now recognize that uncertainties in grain properties prevent good estimates of the depth dependence.

The Elitzur-deJong model of hydroxyl maser chemistry is constrained severely by observations of the kinematics of maser spots (Reid et al. 1980; Garay, Reid, and Moran 1985). They show that OH maser spots do not have velocities that are shifted enough from the centroid velocity of the central HII region in W3 OH to lie behind an outwardly propagating hydrodynamic shock.

Hartquist and Dalgarno (1982) have suggested that OH masers lie in H_2 photodissociation zones, which need not have high material velocities. The nature of high density photodissociation zones differs from that of the low density photodissociation regions studied by Shull (1978) and by Tielens and Hollenbach (1985). The calculations of Shull showed that the column density of vibrationally excited H_2 increases with density. In high density regions it should become sufficient for self-shielding to become important leading to large column densities of vibrationally excited H_2 . In addition, the temperatures of high density dissociation zones lie above several hundred degrees

and collisions also produce vibrationally excited H_2 . The creation of significant populations in higher levels causes the photodissociation rate of H_2 to remain high even in those parts of the region where the lower levels are moderately optically thick. Hartquist and Dalgarno (1982) have estimated the thickness of a photodissociation region with a density typical of a hydroxyl maser to be comparable to the size of a maser spot.

Temperatures attained in the dissociation regions can induce the formation of OH and H_2O which are destroyed by photons. The internal energy of excited molecular hydrogen can drive reactions (Stecher and Williams 1974; Williams 1974) like $O+H_2 \rightarrow OH+H$ and $OH+H_2 \rightarrow H_2O+H$ (Glass and Chaturvedi 1981) even at relatively low temperatures.

Hydrodynamic studies of dissociation zones have shown that a shock preceding an ionization front eventually overtakes the dissociation zone (Hill and Hollenbach 1978; London 1978). At earlier stages of evolution the "magnetic precursor" (Draine 1980) of the shock is probably coincident with the dissociation zone and Hartquist and Dalgarno (1982) have speculated that ion-neutral friction may contribute to the heating of a dissociation zone even before substantial acceleration of the neutral gas occurs; if so, shocks can help heat maser regions to high enough temperatures to drive chemistry without producing velocities that are inconsistent with observations.

4. SOME OBSERVATIONAL DIAGNOSTICS

If hydroxyl maser regions are at temperatures of several hundred degrees observable H_2 (Black and Hartquist 1979) and OH (Flower, Guilloteau, and Hartquist 1982) infrared line emission may originate in the hydroxyl masers and in chemically and physically similar gas that surrounds the stars. H_2 emission appears to have a local maximum in the vicinity of the hydroxyl maser in Orion (e.g. Genzel et al. 1982). Ideally, very high velocity resolution H_2 observations would show whether the peak is associated with gas in the maser region itself, but scattering of the infrared emission in Orion is known to occur (Axon 1985) and may confuse the interpretation of data. Evidence is beginning to accumulate that infrared continuum sources with associated maser emission have a good probability of being detectable H_2 emission sources (Mountain 1985), but the maser regions themselves may not be the line sources.

The narrowness of the maser lines may suggest that the temperatures are less than about 200 K, but nonlinear radiative transfer effects may produce widths narrower than those characteristic of thermal Doppler broadening. Guilloteau et al. (1984) have deduced temperatures for hydroxyl maser regions of less than 200 K by deriving rotational populations from observations of transitions between Λ doublet levels in rotationally excited states; as described in section 2, Guilloteau, Baudry, and Walmsley (1985) suggested that hydroxyl masers in W3 (OH) have $T \approx 160$ K. However, the derivation of rotational level populations from observations of lines in which anomalous radiative transfer effects may be important is not straight forward and the existing uncertainties in maser pumping models complicate temperature determinations.

Hopefully, infrared observations will prove capable of giving insight into the hydroxyl maser phenomena in the near future.

5. ACKNOWLEDGEMENTS

Dr. H. Böhringer and Ms. G. Dirnberger provided great assistance in the preparation of the final manuscript. The author benefitted from an enjoyable conversation with Dr. C.M. Walmsley on interstellar masers.

6. REFERENCES

- Andresen, P., Häusler, D. and Lülff, H.W. 1984, J. Chem. Phys. **81**, 571.
Andresen, P., Häusler, D., Lülff, H.W. and Kegel, W.J. 1984a, Astron. Astrophys. **138**, L17.
Andresen, P., Ondrey, G.S., Titze, B. and Rothe, E.W. 1984b, J. Chem. Phys. **80**, 2548.
Axon, D. 1985, private communication.
Bertojo, A., Cheung, A.C. and Townes, C.H. 1976, Astrophys. J. **208**, 914.
Black, J.H. and Hartquist, T.W. 1979, Astrophys. J. (Letters) **232**, 179.
Dewangen, D.P. and Flower, D.R. 1983, J. Phys. B **16**, 2157.
van Dishoeck, E.F. and Dalgarno, A. 1984, Astrophys. J. **277**, 576.
Draine, B.T. 1980, Astrophys. J. **241**, 1021.
Elitzur, M. 1977, Astron. Astrophys. **57**, 179.
Elitzur, M. 1979, Astron. Astrophys. **73**, 322.
Elitzur, M. and de Jong, T. 1978, Astron. Astrophys. **67**, 323.
Flower, D.R., Guilloteau, S. and Hartquist, T.W. 1982, Mon. Not. R. astr. Soc. **200**, 55p.
Garay, G., Reid, M.J. and Moran, J.M. 1985, Astrophys. J. **289**, 681.
Genzel, R., Reid, M.J., Moran, J.M., Downes, D. and Ho, P.T.P. 1982, in Symposium on the Orion Nebula to Honor Henry Draper, ed. by Glassgold, A.E., Huggins P.J. and Schucking, E.L., Ann. N.Y. Acad. Ses. **395**, 142.
Glass, G.P. and Chaturvedi, B.K. 1981, J. Chem. Phys. **75**, 2749.
Guilloteau, S., Baudry, A., Walmsley, C.M., Wilson, T.L. and Winnberg, A. 1984, Astron. Astrophys. **131**, 45.
Guilloteau, S., Baudry, A. and Walmsley, C.M. 1985, Astron. Astrophys., in press.
Guilloteau, S., Lucas, R. and Omont, A. 1981, Astron. Astrophys. **97**, 347.
Hartquist, T.W. and Dalgarno, A. 1982, ESA Spec. Pub. **192**, 29.
Hill, J. and Hollenbach, D. 1978, Astrophys. J. **225**, 390.
Johnston, I.D. 1967, Astrophys. J., **150**, 33.
de Jong, T., Dalgarno, A. and Boland, W. 1980, Astron. Astrophys. **91**, 68.
London, R. 1978, Astrophys. J. **225**, 405.
Mountain, C.M. 1985, private communication.
Prasad, S.S. and Huntress, W.T., Jr. 1980, Astrophys. J. Suppl. Ser. **43**, 1.
Reid, M.J., Maschick, A.D., Burke, B.F., Moran, J.M., Johnston, K.J. and Swanson, G.W. 1980, Astrophys. J. **239**, 89.
Reid, M.J. and Moran, J.M. 1981, Ann. Rev. Astron. Astrophys. **19**, 231.

- Roberge, W.G., Dalgarno, A. and Flannery, B.P. 1981, Astrophys. J. **243**, 817.
- Shull, J.M. 1978, Astrophys. J. **219**, 877.
- Stecher, T.P. and Williams, D.A. 1974, Mon. Not. R. astr. Soc. **168**, 51 p.
- Tielens, A.G.G.M. and Hollenbach, D. 1985, Astrophys. J. **291**, 722.
- Williams, D.A. 1974, The Observatory **94**, 66.
- Wynn-Williams, C.G., Becklin, E.E. and Neugebauer, G. 1972, Mon Not R. astr. Soc. **160**, 1.

DISCUSSION

TURNER: The assignment of parity to the OH Λ -doublet levels, and the conclusion that collisional propensity rules will lead to anti-inversion of the ground state Λ -doublet might be of relevance to the problem of CH, which observationally seems to exhibit universal population inversion in its ground state Λ -doublet. This is because CH has a single $p\pi$ electron while OH has 3 $p\pi$ electrons which is equivalent to a single $p\pi$ electron hole (4 $p\pi$ electron makes a closed shell). Thus the semi-classical arguments advanced originally by Gwinn et al. (Ap.J., 179, 789, 1973) and pursued later by Bertojo et al. would imply that, whatever the assignment of parity for OH, those for CH should be opposite. Thus the assignments for CH should lead to population inversions in the ground Λ -doublet, in accordance with observation. CH is regarded as optically thin in its ground state 9 cm lines, so radiative pumping would appear difficult. Thus an explanation in terms of simple rotational collisional excitation would seem most attractive.

HARTQUIST: I would be suspicious of any semiclassical arguments as they fail for OH. However, Jura and Mayer have made optical absorption observations that show that the level populations in CH are inverted.

TATUM: In what way does the hyperfine structure depend on the parity?

HARTQUIST: The energy difference between hyperfine sublevels of the even parity level is less than the difference between sublevels of the odd parity level.