H₂O MASER PUMPING BY SHOCK WAVES

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ABSTRACT. We discuss a simple H_2O maser pumping mechanism in which the population inversion of the masing levels takes place during the quick cooling of the gas behind a shock wave. The population of the rotational energy levels in the initial hot state and final cool state of the molecular gas, and the decay paths between levels are analysed to calculate the average number of 22 GHz photons emitted per H_2O molecule in the cooling process.

1.The model

1.1.Shock Waves

We describe briefly the effect of a shock wave propagating in a dense $(10^{10} \text{ cm}^{-3})$ molecular gas in a circumstellar or interstellar environment, with velocity 20-60 kms⁻¹. A sudden rise in temperature occurs at the shock front; the maximum temperature reached depends on the square of the velocity discontinuity, being about 8000 K for 20 kms⁻¹. Dissociation of molecules, excitation and even ionization of atoms occur, producing recombination lines emission.

The chemical reactions in the post-shock gas are almost independent of density, the chemical equilibrium between molecules being almost only a function of the temperature (Draine, 1984). Due to endothermic reactions envolving O and OH, H₂O becomes the most abundant molecule after H₂, reaching a relative abundance of about 3 10^{-4} . Because of its large electric dipole moment, H₂O radiation is also the dominant cooling agent (see Neufeld and Melnik ,1987, for the cooling efficiency of H₂O). According to Draine *et al.*(1983), about one half of the power is radiated by rovibrationnal H₂ emission, one half is radiated by H₂O, and less than 2% is radiated by CO, OH and OI.

Considering a reference frame moving with the shock front, we are concerned with what happens in a thin layer of the post-shock cooling region, in which the molecular gas enters at a temperature of about 1000 K and leaves at about 200 K, this being the temperature interval at which most of the 22 GHz H₂O masing effect takes place.

1.2. H_2O de-excitation

The rotational energy levels of the ground state of ortho $-H_2O$ are shown in figure 1 (this is a well known figure). Let us compute the fraction of H_2O molecules which pass through the 6_{16} state when the gas cools from 1000 K to 200 K. The fraction of H_2O molecules with $J \ge 6$ is:

$$\mathbf{f}(\mathbf{J} \geq \mathbf{6}) = \mathbf{Z} \ (\mathbf{J} \geq \mathbf{6}) \ / \ \mathbf{Z}$$

where

$$\mathbf{Z} = \Sigma \omega_i \, \mathrm{e}^{-Ei/ht}$$

is the partition function, $\omega = 2J+1$, and $Z(J \ge 6)$ is the partition function obtained with the summation performed only on the levels with $J \ge 6$. The fractions $f(J \ge 6)$ and $f(J \ge 7)$ are shown as a function of temperature in figure 2.

Since some levels of the J=6 and J=7 ladders can decay to J=5 levels without passing through 6_{16} , and conversely some J=5 levels can decay to 6_{16} , the fraction of molecules decaying through 6_{16} is given by:

$$f(6_{16}) = \Sigma \omega_i b_i e^{-Ei/kT}/Z$$

where b_i are branching ratios representing the probability of a given level to use a decay path passing through θ_{16} , taking into account the transition probabilities involved in each possible decay path.

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P. D. Singh (ed.), Astrochemistry of Cosmic Phenomena, 245–247. © 1992 IAU. Printed in the Netherlands. Once the θ_{16} level is reached, we need to know the fraction of molecules which take the θ_{16} - δ_{28} decay path, emitting a 22 GHz photon. The spontaneous transition rate strongly favors the θ_{16} - δ_{05} transition (the Einstein A coefficient is $10^{-9}s^{-1}$ for θ_{16} - δ_{28} and $10^{-1}s^{-1}$ for θ_{16} - δ_{05}). But:

-The radiative 6_{16} - 5_{05} decay is inhibited by the optical thickness of this line.

-Collisional 6_{16} - 5_{05} transitions in fact tend to transfer population from the lower to the upper level, in a short-lived pumping mechanism caused by the hot-H₂-cold H₂O situation. During the cooling process the population of the backbone levels is controlled by collisions with H₂.

-Due to stimulated emission, the effective 6_{16} - 5_{23} transition rate is much larger than the spontaneous emission rate. In the presence of population inversion, the maser emission grows exponentially until saturation is reached.

We make use of the following basic principle: in a hot H_2 -cold H_2O situation, all the available collisional transitions are used in the transfer of energy from H_2 to H_2O . The collisional transition rates depend on the population of the levels and on the electric dipole matrix elements, in a way similar to the radiative transition rates, so that in first approximation all the radiative transitions of H_2O are enhanced by a same factor, by the supply of energy from H_2 .

The very simple result of our calculations can be summarised as follows: on the average one H_2O molecule of the post-shock region emits about 600 photons in the δ_{16} - 5_{23} transition. In order to compute the output power of a maser, one has the to calculate the number of H_2O molecules reached by the shock. Even if they are dissociated by the shock, the molecules are formed again in the post-shock chemical reactions in about the same quantity.



Figure 1: Rotational energy levels of ortho- H_2O (for v=0).



Figure 2: The fraction of H_2O molecules which are in excited levels with $J \ge 6$ and with $J \ge 7$, as a funtion of excitation temperature. The "maser" line indicates the fraction of molecules which pass through the 6_16 level, when the temperature decreases to less than 200 K.

2. Comparison with observations

The sites in which the H_2O maser are found fall in three main categories: 1)envelopes of Miras and M supergiants 2) the vicinity of young stellar objects in star-forming regions 3) the circum-nuclear region of some galaxies. All the three categories of H_2O sources are well known to be permeated by shock waves. We have compared the observed photon emission rate in well studied objects of each category, and we find very good agreement with our model. This discussion will be presented elsewhere.

References

Draine, B.T., Roberge, W.G., Dalgarno, A., 1983, Ap.J. 264, 485 Neufeld, D.A., Melnik, G.J, 1987, Ap.J. 322,266