

Λ -DOUBLET POPULATION INVERSION IN COLLISIONS OF OH, OD, CH, CD AND NH^+

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The results of a new approach to the problem of the collisional step in the pumping cycle for OH and CH masers are reported. Rotationally inelastic collisions of OH and CH with both open and closed shell collision partners are considered using an expression derived from scattering theory. It is shown how Λ -doublet population inversion may arise in OH and CH. H-atoms and H_2 may show opposite behaviour with CH, one partner cooling where collisions with the other lead to inversion. Implications for maser action are discussed and reveal excellent qualitative agreement with observation. Λ -doublet population inversion in OD, CD and NH^+ is also considered.

INTRODUCTION

This contribution is concerned with the collisional step in the mechanism by which population inversion may be induced within the Λ -doublets of OH and CH. Previous treatments have related collisional behaviour to the electronic structure of the isolated OH and CH radicals^{1,2}. Different cross-sections for rotational excitation have been assigned to pairs of Λ -doublets on the grounds that the spatial orientation of the unpaired electron differs within the doublets, leading to different interaction potentials and thus excitation probabilities.³ Whilst this model embodies an important element of the physics of the interaction, it contains only a partial description of the inelastic collisions of interest. We adopt the well-established scattering theoretic approach to rotationally inelastic collisions, and the present work is thus fundamentally different from that of previous authors. A further new element that we wish to introduce is that exchange forces between two open shell collision partners impart a strong anisotropy to the interaction potential. Calculated potentials³ show this clearly. In consequence collisions with H atoms have larger cross-sections than those with H_2 or He.

THE COLLISIONAL MODEL

We have extended standard scattering theory to include the case of rotational excitation of $^2\Pi$ -state molecules by open shell atoms^{4a,b}. The non-axially symmetric effective Hamiltonian, involving the electronic angle about the molecular axis, is essentially similar to that of Green and Zare⁵ but also now incorporates spin correlation between the collision partners.

The interaction potential is expressed as an expansion of a product of radial functions $V_{\lambda\mu}(R)$ and spherical harmonics $Y_{\lambda\mu}(\Omega_0)$ in the angles between the molecular axes and the collision partner. There are selection rules for collisional matrix elements:

$$J''(+) \rightarrow J'(+) \text{ and } J''(-) \rightarrow J'(-) : \lambda = \text{even only}$$

$$J''(+) \rightarrow J'(-) \text{ and } J''(-) \rightarrow J'(+) : \lambda = \text{odd only.}$$

For Π -states the projection μ down the molecular axis of the pole of interaction λ is limited to the values 0 and ± 2 . To develop an expression for excitation cross sections we have used the restricted distorted wave Born approximation. Experimental results on the analogous system $H + NH_2$ lend strong support to the validity of the method here.

We refer to any non-equality of the cross-sections for the excitation of pairs of transitions between Λ -doublets as 'parity discrimination'. Differences in excitation probabilities arise largely from terms involving $\lambda=2$ whereas terms for $\lambda=0$ or 1 do not contribute at this level of approximation. Experimental results^{4c} suggest that the expansion of the potential can be meaningfully truncated at $\lambda=2$. Parity discrimination is then determined by the interference between the radial integrals of $V_{20}(R)$ and $V_{22}(R)$. The absolute degree of discrimination is quite sensitive to the relative magnitudes of $\langle V_{20} \rangle$ and $\langle V_{22} \rangle$ but, more significantly, their relative sign determines the sense of the discrimination. By the 'sense' is conveyed which of the transitions $(+)\rightarrow(+)$ or $(-)\rightarrow(-)$ has the larger cross-section for a given pair of J levels. From the available potential surfaces, together with an empirical model of directed valence very much in the spirit of the original Gwinn and Townes model, the relative signs of V_{20} and V_{22} could be deduced. The sense of the parity discrimination is the same for OH or OD with H, H_2 and He. However for CH, CD and NH^+ H-atoms show an opposite sense of discrimination to H_2 or He.

DISCUSSION

Simple collisional radiative cycles are considered with a view to making some qualitative predictions of population inversion in various levels of OH, OD, CH, CD and NH^+ . Table 1 shows the favoured parities for the various transitions originating from the lowest rotational levels of OH and CH for collisions involving H atoms. Energy levels are shown in fig. 1. The radiative step in the cycle is known to have only a very small parity discrimination and thus the $\lambda=2$ contribution to the collisional step is all-important. There is no term in the interaction Hamiltonian which is dependent on nuclear spin: accordingly the eventual choice of hyperfine component that mases will be determined

by the properties of the cloud and the radiation field but not of the collision.

OH: Collisions of H, H₂ and He will preferentially populate the level of (-) symmetry of F₁(2½). Spontaneous emission results in inversion in the F₁(1½) ground state. The inversion predicted in F₁(2½) and (3½) may also lead to maser action in the levels. Populations of F₂(½) are cooled according to the present calculations. Inverted populations of F₂(½) may be formed by absorption of a resonant photon at 126 cm⁻¹ transferring the inverted population of F₁(1½) to F₂(½). Our calculations would therefore suggest that inversion in ground and excited states of OH would result from collisions in diffuse, intermediate and dense clouds in accord with observation.

CH: Let us first consider excitation by H atoms. The low temperature excitation of F₁(1½) results in the inversion of the ground state. At higher temperatures CH maser action may be quenched by excitation of F₂(1½). Collisions with H₂, He will tend to cool the ground state of CH at low temperature.

Our results predict collisional population inversion of the CH ground state in low temperature clouds in which hydrogen is at least partly atomic in form. Emission should be seen from the ground state only (see below). CH emission should not be seen from dense clouds. Further, CH emission should not be seen in diffuse or intermediate clouds accompanied by OH emission, on the grounds of excitation temperature. All these features are supported by observation.⁶ Our results would suggest that it would be worth searching for CH emission from the A-doublet transition in F₂(1½) of CH.

OD, CD, NH⁺: OD population inversion is predicted in precisely the same circumstances as OH. However OD is closer to Hund's case (a) and for this reason will show a weaker parity discrimination in collisions. The pattern for CD and NH⁺ inversion is identical to that of CH. CD emission is unlikely to be seen since isotopic fractionation enhancement should not be operative in diffuse or intermediate clouds.

Table 1: Parity Discrimination in collisions of OH and CH with H-atoms

OH	CH	Favoured Parity
F ₁ (1½) → F ₁ (2½)	F ₂ (½) → F ₂ (1½)	- → -
F ₁ (3½)	F ₂ (2½)	+ → +
F ₂ (½)	F ₁ (1½)	+ → +
F ₂ (1½)	F ₁ (2½)	- → -

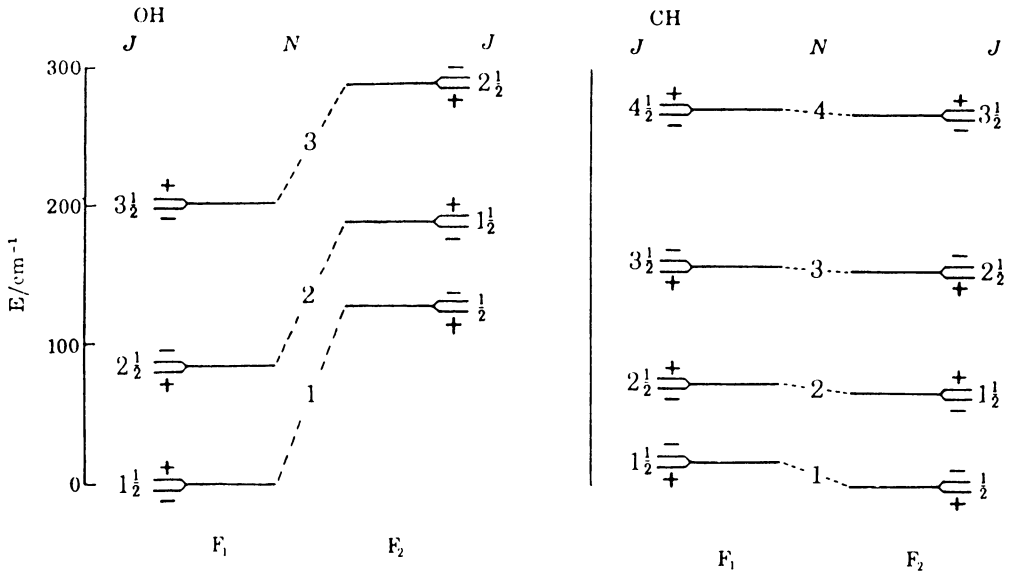


Fig. 1: Rotational Energy Levels of OH and CH

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DISCUSSION FOLLOWING FIELD

Robinson: We observe the $2\pi_{1/2}$ CH 9 cm triplet in *emission* and weakly masering in low density regions. As density increases towards the centres of clouds, the transitions are cooled, and the lines progressively change to *absorption*. This behaviour agrees qualitatively with your suggestion of collisional pumping of CH.

Field: My interpretation of the results presented in Zuckerman and Turner (1975, *Ap. J.* 197, 123) was precisely the same, and it is very nice to hear it confirmed in your work too.

Elitzur: If collisions with H_2 are so efficient in producing inversion, we have a problem with the observations. If your cross-sections are right the $^2\pi_{3/2}$ ($J=5/2$) state is sufficiently excited to lead to main-line inversion for temperatures larger than about 30 K. Main-line inversions are certainly not as widespread as that.

Field: I certainly appreciate this problem, and I hope that further experimental and theoretical investigation both in astrophysics and in the laboratory will serve to resolve it.

Hjalmarson: At which densities do you think we will be unable to observe CH maser inversion? At Onsala we see an indication of CH maser emission in the dust cloud L1500, by observations towards and around 3C123. The indication also seems to be confirmed by Effelsberg CH data taken in the same direction.

Field: Without accurate cross-sections and cloud parameters, it is difficult to say. A rough estimate might be made as follows: if the cross-section for excitation of CH by H is 5 to 10 times that for excitation by H_2 , perhaps when $[H]/[H_2]$ drops below .2 to .1, the CH $F_2(\frac{1}{2})$ Λ -doublet will begin to cool. This may be the case around a number density of 10^3cm^{-3} .

Goldreich: Non-LTE level populations occur under a wide variety of conditions if radiative rates are greater than or comparable to collisional rates. It is probably not worth making detailed models of pump cycles unless the maser has very special observational characteristics. It is only in this case that one might hope to obtain conclusive and unambiguous results. While it is admirable that people are working in this subject, their energies might be better spent in other ways.

Field: In the first place, the work I have presented is not a detailed pumping model but the most simple one that could be thought of. In the second place, there is no doubt whatsoever that collision cross-sections are data of the greatest value in astrophysics, and are eagerly awaited by many workers in the field. Before deciding on the critical parameters in a model for any particular maser, it is essential to have basic molecular data such as the collision cross-sections.

Irvine: Sume and I at Onsala searched for the $^2\pi_{3/2}$, $J=5/2$, Λ -doublet transition of CH at about 4.8 GHz. Unless the rest frequency is considerably outside the expected range, we can rule out any *strong* maser in several sources, but not a weak maser action like that seen in the ground state Λ -doublet (Astron. Astrophysics, published).

Field: That is certainly an interesting observation and seems to agree with our predictions.