COLLISIONAL INVERSION OF THE POPULATIONS OF Λ-DOUBLETS IN CH AND OH:
A CRITICAL STUDY

D.R. Flower
Physics Department, University of Durham, DH1 3LE, England

ABSTRACT

     Astronomical studies of the CH and OH masers have been based on
the hypotheses of both radiative and collisional pumping. The mechanism
of collisional inversion of the ground state Λ-doublets by neutral
perturbers was first described by Bertojo et al. (1976) who made a semi-
quantitative analysis of the collision process, based on calculations
of potential energy curves. More recent work (Kaplan and Shapiro, 1979;
Dixon and Field, 1979; Flower, 1980) has, however, been critical of
some of the assumptions made by Bertojo et al. Consideration of the
symmetry and the form of the interaction of CH and OH with the
spherically symmetric perturbers para-H_2 and He shows that current
knowledge of the interaction potential is insufficient for quantitative
results to be obtained.

     Studies of the interstellar CH and OH masers, based upon the
assumption of collisional inversion by neutral perturbers, generally
derive from the work of Bertojo et al. (1976). These authors calculated
the relevant potential energy curves for a perturber approaching
perpendicular to the intramolecular axis, and deduced the sense and the
magnitude of the inversion produced by H, H_2 and He. However, the
analysis, particularly of the collision process, was based on a number
of assumptions, and certain of these have been criticised in the recent
literature (Kaplan and Shapiro, 1979; Dixon and Field, 1979; Flower,
1980). For example, the implicit assumption that the whole of the
interaction energy can give rise to rotational excitation is invalid;
only the anisotropic part of the potential can contribute to rotationally
inelastic scattering, and the magnitude of the corresponding terms must
be determined before the efficiency of the collisional pumping
mechanism may be assessed.

     This fact may most simply be illustrated by considering the
interaction between an atom and a rigid diatomic molecule. In this case,
the potential may be expanded in terms of Legendre polynomials, $P_\lambda(\cos\theta)$,

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which are functions of the angle θ between the inter- and intramolecular axes:

$$V(\rho,\theta) = \sum_{\lambda} v_{\lambda}(\rho)\, P_{\lambda}\,(\cos\theta),$$

where ρ is the distance of the atom from the centre of mass of the molecule. Retaining terms in the expansion up to $\lambda = 2$, which are likely to be the most important, we obtain

$$V(\rho,\theta) = v_0(\rho) + v_1(\rho)\,\cos\theta + v_2(\rho)\,\frac{3\cos^2\theta - 1}{2}$$

(In the case of CH and OH, there are additional second order terms, arising from the interaction of the atom with the unpaired electron; see Flower, 1979).

Bertojo et al. made calculations of $V(\rho,\theta)$ for $\theta = \pi/2$. In this case,

$$V(\rho,\pi/2) = v_0(\rho) \;-\; v_2(\rho)/2.$$

In order to determine the contributions of v_1 and v_2 to the anisotropy of the potential, the interaction energy must also be known for collinear approaches of the perturber:

$$V(\rho,0) = v_0(\rho) + v_1(\rho) + v_2(\rho),$$

$$V(\rho,\pi) = v_0(\rho) - v_1(\rho) + v_2(\rho).$$

Potential energy calculations are planned for the additional collision geometries which will enable quantitative conclusions to be drawn regarding the efficiency of H_2 as a collisional pumping agent. In the meantime, only qualitative statements may be made regarding the relative efficiency of the different perturbers. In the case of para $-\,H_2$, the interaction with the radical is likely to become more rapidly repulsive with ρ for collinear than for perpendicular approaches, owing to the greater extent of the electron charge distribution along the internuclear axis of the radical. Under these circumstances, it may be shown that the degree of selective excitation of a given Λ-doublet component will be relatively small. Similar remarks apply to He. However, H is intrinsically different, in that one of the singlet state potential energy curves is attractive at intermediate range. For these reasons, H, but not para $-\,H_2$ or He, may be expected to induce significant departures of the level populations of the radical from their values in LTE

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