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Collisional depolarization of molecular lines. Application to the SiO+H isotropic collisions

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ABSTRACT

This paper reports the first theoretical study on the collisional depolarization and polarization transfer for rovibrational levels of diatomic molecules in the infinite-order-sudden approximation. As an application, we compute depolarization and polarization transfer rates for rotational levels $J = 1,..., 99$ within the vibrational quantum numbers $v = 0, 1, 2, 3$ of the SiO molecules in collisions with neutral hydrogen atoms for temperatures $400 \leq T \leq 1500$ K. Analytical expressions of the collisional depolarizing rates of rovibrational levels as a function of local temperature and rotational number J are obtained. We note that the collisional depolarization rates decrease when J increases and that the fractional effect of the collisions on the J-levels can be characterized by a simple ratio. Especially for high J values, we find that alignment and population transfer rates between J to $J + 1$ inside the same vibrational number v are higher than the elastic depolarizing rates. This work might help to gain more understanding of the role of isotropic collisions in the formation of the very interesting polarized lines of C_2 and MgH observed in the solar photosphere.

Key words. molecular processes – line: formation – polarization – molecular data

1. Introduction

Scattering processes of incident anisotropic radiation fields can produce linear polarization in spectral lines without the need for magnetic fields. The line polarization reflects the fact that the Zeeman sublevels of the emitting atomic system are unevenly populated and they are characterized by definite coherence factors. The linear polarization degree and its direction can be modified by the presence of magnetic fields via their Hanle effect, which occurs when the Zeeman splitting is the order of the natural line width.

It is through the interpretation of observations related to polarimetric measurements that we can learn about the anisotropies and magnetic fields of a number of astrophysical objects. The linearly polarized spectrum observed close to the solar limb (second solar spectrum) is as rich in spectral structures as the ordinary intensity spectrum but differs in appearance and information content. Looking at the whole second solar spectrum, one remarks that more interesting lines to investigate are associated with complex atoms like Ti I, Fe I, Cr I, etc., with ions like Ce II, Nd II, Ba II, etc., and with diatomic molecules like MgH and C_2 (e.g. Gandorfer 2000). In another astrophysical context there are interesting possibilities for investigations based on the circumstellar SiO maser polarization (see Asensio Ramos et al. 2005). Interpretation of polarized radiation consists in solving a non local thermodynamic equilibrium (NLTE) general radiative-transfer problem, i.e. for which the unknown is not a scalar quantity (the intensity) but the Stokes vector (e.g. the recent review by Trujillo Bueno 2003a).

In order to properly interpret polarized radiation, it is necessary to know the rates of all the microscopic processes intervening in the polarized line formation. An important category of these processes involves collisional interactions of the emitting atomic systems with nearby perturbers like H I, He I atoms and H_2 molecules in cold astrophysical environments or protons, electrons, and H I atoms in solar conditions. In particular, isotropic elastic collisions tend to equalize populations of the Zeeman sublevels inside a given atomic level and to destroy their coherences, i.e. partially destroy the atomic polarization of the level. Collisional depolarization and polarization transfer rates should be taken into account to realistically simulate the formation of the polarized lines of the Sun and of other stars.

Over the last few years Derouich, Sahal-Bréchot, and Barklem have developed a general semi-classical theory that allows, for the first time, sufficiently accurate computation of the needed depolarizing and polarization transfer rates for

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levels of complex atoms in the second solar spectrum (Derouich et al. 2003a,b, 2004a,b, 2005a,b). However these rates are *completely unknown* in cases of diatomic molecules.

The problem of formulating and calculating the depolarizing and polarization transfer rates of rovibrational molecular levels is addressed in this paper. We show that these rates can be written as a linear combination of the so-called generalized infinite-order-sudden (IOS) rates. We calculate depolarization and polarization transfer rates for rotational levels $J = 1,..., 99$ within the vibrational quantum numbers $v = 0, 1, 2, 3$ of the *SiO molecule in isotropic collisions with neutral hydrogen*. These calculations are based on the vibrational close-coupling rotational IOS (VCC-IOS) cross sections available in electronic format in the EPAPS home page (cited as EPAPS in the references). The VCC-IOS cross sections are computed by Palov et al. (2002), who adopts accurate ab initio H-SiO interaction potential surfaces (see Jimeno et al. 1999; and Palov et al. 2002). We find that it is possible to make a good fit to the depolarizing rates as a function of J and T. Furthermore, we show that the fractional effect of the elastic collisions on the J-levels can be characterized by a simple ratio $\mathcal{R}$. In addition, our results show that the elastic depolarizing rates can be lower than the transfer rates of alignment and population from J to $J+1$. Transfer rates vary slowly with J and converge to asymptotic values for high J. This work would permit discussion of how important isotropic collisions with neutral hydrogen in the formation of the very interesting polarized lines of MgH and C_2 are, still an open question in the solar physics comminity (Mohan Rao & Rangarajan 1999; Faurobert & Arnaud 2002, 2003; Trujillo Bueno 2003b; Trujillo Bueno et al. 2004; Berdyugina & Fluri 2004; Asensio Ramos & Trujillo Bueno 2005; Bommier et al. 2005).

2. Theory and definitions

Observed polarization of molecular lines is due to population imbalances and quantum interferences (or coherences) among the Zeeman sublevels (vJM_J) pertaining to the upper and/or lower levels involved in the line transitions, where v is the vibrational quantum number, J the rotational number, and M_J its projection. Elastic collisions of emitting/absorbing molecules with hydrogen atoms induce transitions between degenerate Zeeman sublevels (vJM_J). When the hydrogen atoms follow an isotropic velocity distribution, these collisions have a depolarizing effect: they tend to reestablish thermodynamical equilibrium between the Zeeman sublevels (vJM_J) of a given level and to destroy their coherences. The overall population of the level J is not affected by elastic collisions. Inelastic collision processes can alter the population of a J-level and the polarization of the line by inducing transitions from $(vJM_J) \rightarrow (v'J'M'_J)$.

Physical interpretation of the observed polarization requires the solution of the coupling between NLTE polarized radiative transfer and statistical equilibrium equations. In such a situation, description of the internal states of the emitting/absorbing molecule in the density matrix formalism expressed on the basis of irreducible tensorial operators ${}^{vJ,v'J'}T^k_q$ is shown as the most suitable (e.g. Sahal-Bréchot 1977; and the book of Landi Degl'Innocenti & Landolfi 2004). The contribution of the isotropic collisions to the statistical equilibrium equations is:

$$\left(\frac{\mathrm{d}\,{}^{vJ}\rho^k_q}{\mathrm{d}t}\right)_{\mathrm{coll}} = -D^k(vJ,T)\,{}^{vJ}\rho^k_q - {}^{vJ}\rho^k_q \sum_{J'\neq J} \zeta(vJ \rightarrow vJ',T) + \sum_{J'\neq J} D^k(vJ' \rightarrow vJ,T)\,{}^{vJ'}\rho^k_q. \quad (1)$$

The quantities to be computed are the density matrix elements ${}^{vJ}\rho^k_q$, while $D^k(vJ,T)$ are the depolarization rates of the level (vJ) due to elastic collisions and $D^k(vJ \rightarrow vJ',T)$ are the polarization transfer rates between the levels $(vJ) \rightarrow (vJ')$. k is the tensorial order where $0 \leq k \leq 2J$ for $J = J'$, and, for $J \neq J'$, $0 \leq k \leq k_{\max}$ where $k_{\max} = 2J$ if $J < J'$ (or if $J > J'$ then $k_{\max} = 2J'$). Even though $-k \leq q \leq k$, the depolarization and polarization transfer rates are q-independent due to the isotropy of the collisions with hydrogen. Here $\zeta(vJ \rightarrow vJ',T)$ are the rotational excitation rates.

$D^k(vJ,T)$, $D^k(vJ' \rightarrow vJ,T)$, and $\zeta(vJ \rightarrow vJ',T)$ should be calculated independently to enter the statistical equilibrium equations. The cross sections, and hence, the rate coefficients for vibrational relaxation are much smaller than those for pure rotational relaxation by about three orders of magnitude. With very good approximation, one can neglect the transfer of polarization between different vibrational states.

2.1. Close coupling formulation

Let us consider binary collisions in the close coupling (CC) scattering formalism between diatomic molecule with rotational angular momentum $\boldsymbol{J}$ and a bath of neutral hydrogen atoms in their ground state having an angular momentum $\boldsymbol{j_2}$ ($j_2 = 1/2$). By $\boldsymbol{j_{12}} = \boldsymbol{j_2} + \boldsymbol{J}$ one can denote the angular momentum of the hydrogen atom + the molecule and couple $\boldsymbol{j_2}$ and $\boldsymbol{l}$ to obtain $\boldsymbol{j_p}$, where $\boldsymbol{l}$ is the relative angular momentum. Then $\boldsymbol{J_T} = \boldsymbol{j_{12}} + \boldsymbol{l}$ is the total angular momentum of the system (molecule + hydrogen + relative motion)[1].

One remark is that, formally in the CC, the above quantum mechanical formulation of the problem of atom-molecule scattering is similar to that of atom-atom scattering. Then, the depolarization and polarization transfer rates of rovibartional molecular levels (vJ) have the same form as those developed for *electronic atomic levels* by Reid (1973) in the case of a structureless perturber ($j_2 = 0$ like neutral Helium) and generalized by Kerkeni et al. (2000) for $j_2 \neq 0$ cases (like neutral hydrogen). In fact, one should only carry out formal substitution between the electronic state of the perturbed atom and the rovibartional state of the molecule.

[1] For more details, a description of the quantum close coupling method for limiting cases where the diatomic molecule collides with structureless rare gases can be found in Arthurs & Dalgarno (1960), and a general case where the perturbers have arbitrary angular momentum is in Launay (1977).

Consequently, using our notations, the spherical tensor components $\zeta^k(vJ \to vJ', T)$ are given by:

$$\zeta^k(vJ \to vJ', T) = n_{\rm H}\sqrt{\frac{8}{\pi\mu}}(kT)^{-\frac{3}{2}}\int_0^\infty E_{k_J}\exp\left(-\frac{E_{k_J}}{k_{\rm B}T}\right) \times\sum_g(-1)^{J+J'+k+g}(2g+1)\left\{\begin{array}{ccc} J' & J' & k \\ J & J & g\end{array}\right\}B(JJ',g) \tag{2}$$

where the expression of the Grawert parameter $B(JJ', g)$ is given in Reid (1973) for $j_2 = 0$ and Kerkeni et al. (2000) when $j_2 \neq 0$, $k_{\rm B}$ is the Boltzmann constant, μ the reduced mass of the system, E_{k_J} the collision energy, and k_J the wave number. T and $n_{\rm H}$ are the local temperature and the hydrogen perturber density respectively.

2.2. Introduction of the infinite-order-sudden (IOS) approximation

The number of the CC equations that one must solve in order to obtain the transition matrix and the Grawert parameter $B(JJ', g)$ increases nonlinearly with the highest rotational number $J_{\rm max}$. Thus, for large $J_{\rm max}$, attempted when the collision energy increases (which is especially the case for solar temperatures of about 5000−6000 K), the number of the CC equations soon becomes very large and therefore computationally costly. One then needs to resort to more approximate dynamical treatments, like those discussed often in the literature (see Kouri 1979, Atom-Molecule Collision Theory, Chap. 9). The most popular approximate dynamical methods are the coupled states (CS) or "centrifugal decoupling" method and the infinite-order-Sudden or IOS approximation. The CS method introduced by McGuire & Kouri (1974) assumes that in the space of the body-fixed coordinate system the centrifugal potential conserves the projection of the rotational angular momentum on the axis perpendicular to the plane of the collision. One can further simplify the coupling dynamics if the sudden approximation to the rotation of the diatomic molecule is also applicable; that is, the rotational excitation energies are smaller than the collision energy. When combined with the above CS scheme, the sudden approximation gives rise to the IOS approximation, which therefore considers that all important events in an atom-molecule encounter occur on much smaller time scales than that characterizing the rotation of the molecule (Goldflam et al. 1977).

In the framework of the IOS decoupling approximation, the transition probability, obtained after summing over final projections of the rotation number and averaging over initial projections, is given by (Goldflam et al. 1977, see also Parker & Pack 1978):

$$|\langle Jl|T(k)|J'l\rangle|^2 = \sum_L(2J'+1)\left(\begin{array}{ccc} J & L & J' \\ 0 & 0 & 0\end{array}\right)^2|\langle l|T_L(k)|l\rangle|^2 \tag{3}$$

where L is the order of the Legendre polynomials used to expand the IOS T-matrix and the interaction potential. The expression of the Grawert parameter $B(JJ', g)$ in the IOS approximate scattering method is obtained by carrying out the IOS coupling sheme, namely $J = 0$ and $J' = L$, and by replacing the CC transition probability by its expression in the IOS approximation (Eq. (3)). Then, from the CC Grawert parameter expression we derive the IOS expression:

$$\begin{aligned} B^{\rm IOS}(JJ', g) &= \delta_{g,L}\frac{(2J'+1)(2J+1)}{(2L+1)}\left(\begin{array}{ccc} J & L & J' \\ 0 & 0 & 0\end{array}\right)^2 \\ &\quad\times\frac{\pi}{k^2(2L+1)}\sum_l(2l+1)|\langle l|T_L(k)|l\rangle|^2 \\ &= \delta_{g,L}\quad\frac{(2J'+1)(2J+1)}{(2L+1)}\left(\begin{array}{ccc} J & L & J' \\ 0 & 0 & 0\end{array}\right)^2\sigma(0\to L)\end{aligned} \tag{4}$$

where $\sigma(0 \to L)$ is the so-called generalized IOS cross section and is given by:

$$\sigma(0\to L) = \frac{\pi}{k^2(2L+1)}\sum_l(2l+1)|\langle l|T_L(k)|l\rangle|^2. \tag{5}$$

We derive the depolarizing rate of the level $|vJ\rangle$ at a temperature T of the medium:

$$\begin{aligned} D^k(vJ,T) &= \zeta^0(vJ,T) - \zeta^k(vJ,T) \\ &= (2J+1)\sum_{L=0}^{2J}\left(\begin{array}{ccc} J & L & J \\ 0 & 0 & 0\end{array}\right)^2\zeta(v0\to vL) \\ &\quad-\sum_{L=0}^{2J}(2J+1)^2(-1)^{2J+k+L}\left\{\begin{array}{ccc} J & J & k \\ J & J & L\end{array}\right\} \\ &\quad\times\left(\begin{array}{ccc} J & L & J \\ 0 & 0 & 0\end{array}\right)^2\zeta(v0\to vL).\end{aligned} \tag{6}$$

We notice that owing to the selection rules on the $3j$-coefficients $\left(\begin{array}{ccc} J & L & J' \\ 0 & 0 & 0\end{array}\right)$, the summation over L vanishes identically unless $J + J' + L$ is of even parity, so the factor $(-1)^{J+J'+L} = 1$ ($J = J'$ and $J \neq J'$). Equation (6) is then reduced and we can express the depolarization rates as:

$$\begin{aligned} D^k(vJ,T) &= \sum_{L>0}^{2J}(2J+1)\left[1-(2J+1)(-1)^k\left\{\begin{array}{ccc} J & J & k \\ J & J & L\end{array}\right\}\right] \\ &\quad\times\left(\begin{array}{ccc} J & L & J \\ 0 & 0 & 0\end{array}\right)^2\zeta(v0\to vL).\end{aligned} \tag{7}$$

The polarization transfer rates from $|vJ\rangle$ to $|vJ'\rangle$ ($J \neq J'$) are given by:

$$\begin{aligned} D^k(vJ\to vJ') &= \zeta^k(vJ\to vJ') \\ &= \sum_{L>0}^{J+J'}(2J+1)(2J'+1)(-1)^k\left\{\begin{array}{ccc} J' & J' & k \\ J & J & L\end{array}\right\} \\ &\quad\times\left(\begin{array}{ccc} J & L & J' \\ 0 & 0 & 0\end{array}\right)^2\zeta(v0\to vL).\end{aligned} \tag{8}$$

Thus, we have succeeded in expressing the depolarization and polarization transfer rates in terms of rotational excitation rates for scattering out from $J = 0$ to $J' = L$ (Eqs. (7) and (8)). This is the most important consequence of using the IOS approximation as it allows us to rapidly calculate the depolarizing rates if the usual generalized IOS rates are known.

It is of interest to notice some properties which can be inferred from Eqs. (7) and (8). First of all, an interesting thing to note is that the $L = 0$ term does not contribute to the sum giving $D^k(vJ, T)$ and $D^k(vJ \to vJ', T)$ which is physically understandable because $L = 0$ corresponds to an isotropic part of the potential and cannot induce any change in the polarization of the level. Of course this result is not specific to the use of the IOS method, and one can also find it in the CC calculations. However, the tensorial component $\zeta^0(vJ)$ describing the elastic scattering of the hydrogen atom on the diatomic molecule is sensitive to the order $L = 0$, which leads to $\zeta^0(vJ)$ being clearly bigger than $D^k(vJ)$ and $D^k(vJ \to vJ')$ since the $L = 0$ component contributes most to the interaction potential. From Eq. (8) one obtains:

$$D^0(vJ \to vJ', T) = \sqrt{\frac{2J+1}{2J'+1}} \sum_{L>0} (2J'+1) \begin{pmatrix} J & L & J' \\ 0 & 0 & 0 \end{pmatrix}^2 \times \zeta(v0 \to vL, T). \quad (9)$$

On the other hand, $D^k(vJ \to vJ', T)$ can be written as a linear combination of $\zeta(vJM_J \to vJ'M'_J, T)$:

$$D^k(vJ \to vJ', T) = (2k+1) \sum_{M_J, M'_J} (-1)^{J+J'-M_J-M'_J} \times \begin{pmatrix} J & k & J \\ -M_J & 0 & M_J \end{pmatrix} \begin{pmatrix} J' & k & J' \\ -M'_J & 0 & M'_J \end{pmatrix} \times \zeta(vJM_J \to vJ'M'_J, T), \quad (10)$$

which in particular gives:

$$D^0(vJ \to vJ', T) = \sqrt{\frac{2J+1}{2J'+1}}\, \zeta(vJ \to vJ'). \quad (11)$$

By identification of Eqs. (9) and (11), we retrieve Eq. (42) of Goldflam et al. (1977):

$$\zeta(vJ \to vJ', T) = (2J'+1) \sum_{L>0} \begin{pmatrix} J & L & J' \\ 0 & 0 & 0 \end{pmatrix}^2 \times \zeta(v0 \to vL, T), \quad (12)$$

obtained in another way and widely used in the IOS calculations of rovibrational excitation rates. From Eqs. (4) and (12), we obtain:

$$\zeta(vJ \to vJ', T) = n_{\rm H} \sqrt{\frac{8}{\pi\mu}} (kT)^{-\frac{3}{2}} \int_0^\infty E_{k_J} \exp\left(-\frac{E_{k_J}}{k_{\rm B}T}\right) \times \sum_L \frac{2L+1}{2J+1} B^{\rm IOS}(JJ', L), \quad (13)$$

which is the same relationship as that given in Eq. (8) of Kerkeni et al. (2003) by full CC treatment of atom-atom collisions. The expression of the polarization transfer rate $D^k(vJ \to vJ', T)$ (Eq. (8)) is equal to the so-called Fano's generalized relaxation rate given by Eq. (31) of Goldflam et al. (1977), if multiplied by $\sqrt{\frac{2J'+1}{2J+1}}$.

3. Results

As an application of the theoretical formulation described above (Eqs. (7) and (8)), we have studied the variation of depolarization and polarization tarnsfer rates as a function of rotational levels J and temperature T. The calculations were possible in the case of the SiO molecules in collisions with neutral hydrogen, because generalized IOS cross sections $\sigma(0 \to L)$ are listed by Palov et al. (2002) on the EPAPS home page for collision energy range 200−9600 K (92 K $\simeq$ 64 cm^{-1}). We notice that our calculations are expected to be less accurate for high J ($J > 50$) because the rotational energy is comparable to the kinetic energy, so that the IOS approximation is not satisfied. Palov et al. (2002) have performed calculations up to $J > 100$, accuracy of our calculations depends on the Palov et al. results.

The depolarization and polarization transfer rates follow from integration of the corresponding cross-sections over a Maxwellian distribution of kinetic energies of the hydrogen atom for a local temperature T. The convergence was achieved for $\sim 400 \leq T \leq \sim 1500$ K, and J takes integral values 0, 1, 2, ..., 99 for each one of the vibrational quantum numbers $v = 0$, 1, 2, 3. The J-dependence of the depolarization rates are reported in Fig. 1 for each vibrational level where the temperatures $T = 500$ K, 1000 K, and 1500 K. In Fig. 2, we show the curves for the depolarization rates as a function of the local temperature T for the rotational number levels $J = 9$, 18, and 27. Population and alignment transfer rates between levels $J \to J+1$, $D^0(vJ \to v\ J+1, T)$ and $D^2(vJ \to v\ J+1, T)$, are presented in Fig. 3 as a function of J ($1 \leq J \leq 98$). Interestingly, for rather high J-values ($J > 6$), the transfer rates $D^0(vJ \to v\ J+1, T)$ and $D^2(vJ \to v\ J+1, T)$ are higher than the depolarizing rate $D^2(vJ, T)$. For example, for $J = 20$, $v = 0$ and $T = 1500$ K, $D^2(vJ, T)/n_{\rm H} = 1.42 \times 10^{-11}$ s^{-1}, $D^0(vJ \to v\ J+1, T)/n_{\rm H} = 10.71 \times 10^{-11}$ s^{-1}, and $D^2(vJ \to v\ J+1, T)/n_{\rm H} = 9.55 \times 10^{-11}$ s^{-1}. Moreover, unlike electric dipole radiative transitions, collisional processes do not obey strong selection rules[2]: for instance collisional transfer rates between $J \to J+2$ can efficiently alter the polarization of the J-level. The collisional transfer rates between different J should be taken into account to realistically models the contribution of the collisions in the polarized line formation (Eq. (1)).

For $v = 0$, it is possible to make a good least square fit, with a correlation coefficient $R > 0.9$, to the alignment destruction rates ($k = 2$) as a function of the local temperature T and for $J \geq 6$:

$$D^2(v = 0; J,\ T) = n_{\rm H}\ \sqrt{2}\ T^{0.3}\ (J)^{-1.5} \times 10^{-10}\ {\rm s}^{-1}. \quad (14)$$

Then, the ratio of the fractional effect of the elastic collisions on given J_1 and J_2 levels is:

$$\mathcal{R} = \left(\frac{J_1}{J_2}\right)^{-1.5}. \quad (15)$$

[2] We note however that for collisions involving homonuclear diatomic molecules (C_2, O_2, H_2, ...), only the L-even terms are non-vanishing in the Legendre expansion of the interaction potential. As $J + J' + L$ is of even parity, collisional transitions between even and odd J-levels are forbidden.

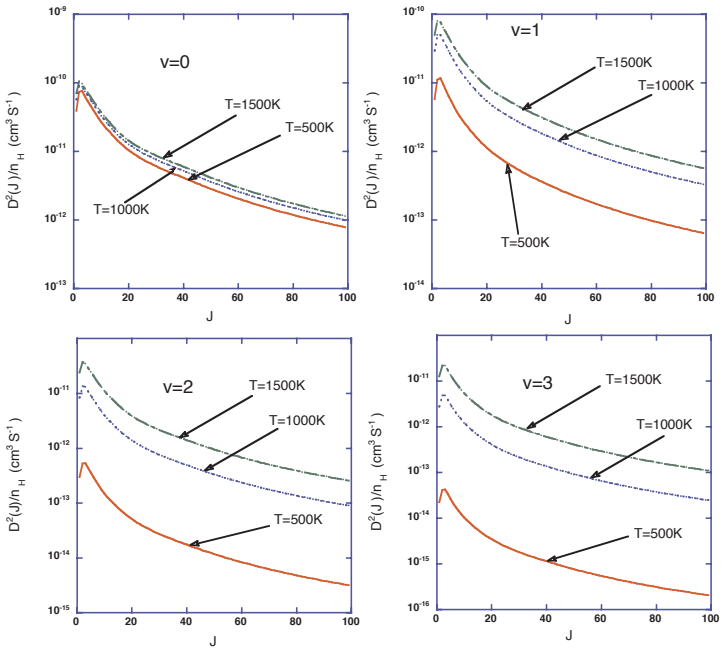

Fig. 1. A log-scale plot of the alignment destruction rates ($k = 2$) per unit H-atom density as a function of J for $v = 0$, 1, 2 and 3. The rates are calculated for the temperatures $T = 500$ K, 1000 K, 1500 K and given in cm^3 s^{-1}.

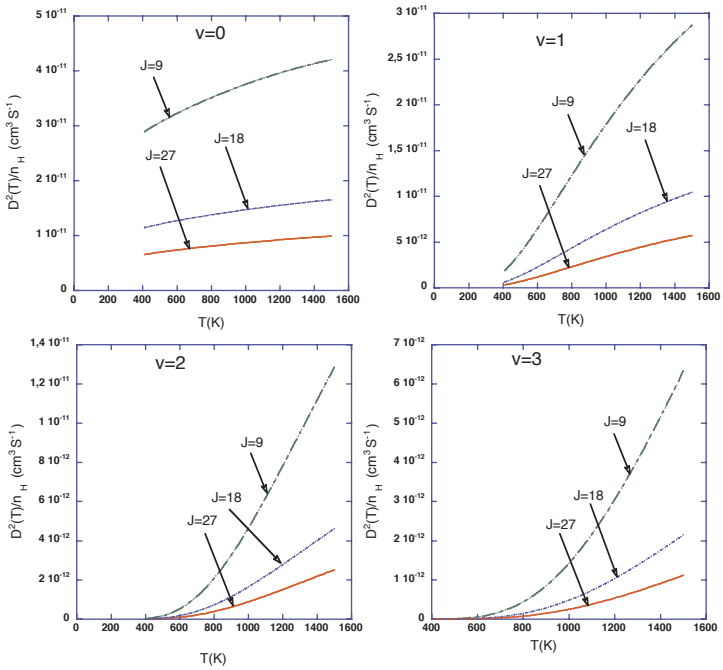

Fig. 2. Destruction rates of alignment per unit H-atom density as a function of the temperature for $J = 9$, 18 and 27. The rates are given in cm^3 s^{-1}.

Also, for $v = 1$, one can get an analytical expression of the destruction rates of alignment ($k = 2$) in s^{-1}:

$$D^2(v=1; J,\ T) = n_{\rm H}\Big(-0.58 + 1.57\ T \times 10^{-3} - 0.22\ T^2 \times 10^{-6}\Big)(J)^{-\frac{5}{3}} \times 10^{-10}\ {\rm s}^{-1}. \quad (16)$$

The depolarizing and polarization transfer rates given in this section are obtained with the most recent and accurate available H-SiO interaction potentials (see Jimeno et al. 1999; and Palov et al. 2002). Variation laws such as those given by Eqs. (14) and (16) for $v = 0$ and 1 can be easily implemented in a modeling of the maser SiO polarization, such as discussed by Asensio Ramos et al. (2005). Numerical values of these rates may be obtained on request from the author. Results obtained here for SiO molecule can provide a useful first-order approximation for cases of other diatomic molecules in their ground electronic states. This is because, as shown for problems involving rotational excitation (see Eq. (2.80) of Flower 1990),

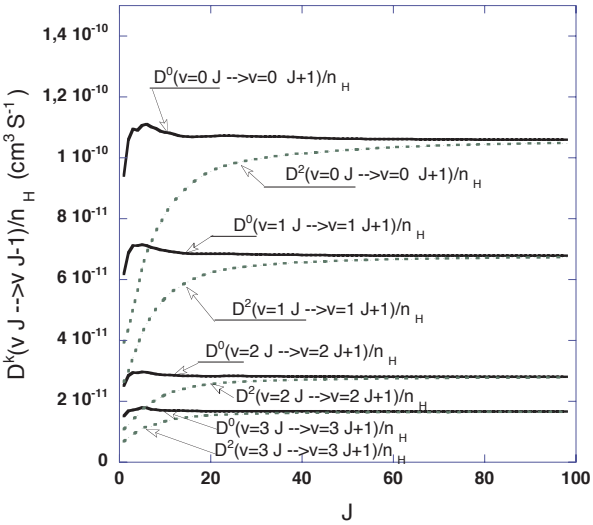

Fig. 3. Population ($k = 0$) and alignment ($k = 2$) transfer rates per unit H-atom density as a function of J for $T = 1500$ K. The rates are given in $\mathrm{cm}^3\,\mathrm{s}^{-1}$.

the depolarizing rates of diatomic molecules in a given electronic level have the same order of magnitude. To gain some understanding of the physical conditions in the formation of the MgH and C_2 lines, one could get a crude estimation of n_H from which the alignment of the electronic *ground* states of MgH and C_2 could be destroyed by comparing depolarizing and polarization transfer rates of SiO to the appropriate Einstein coefficients.

The depolarizing and polarization transfer rates are given within the IOS approximation as the sum of inelastic cross section $\sigma(0 \rightarrow L)$ multiplied by spectroscopic coefficients (Eqs. (14) and (16)). The spectroscopic coefficients are independent of the interaction potentials, so they are independent on the electronic state of the molecule. Besides, the magnitudes of successive coefficients in the expansion of the interaction potential tend to decrease as L increases, and $\sigma(0 \rightarrow L)$ becomes smaller independent of whether it is a ground or excited electronic state. Physically, the behavior of the decrease of $\sigma(0 \rightarrow L)$ for a ground electronic state should not be very different from the one for an excited electronic state.

According to these considerations, we think that the behavior of the depolarizing and polarization transfer rates with the rotational number J for a given vibrational number is approximately the same for the ground or excited electronic states of diatomic molecules. The variation law of the depolarizing rates associated to rotational levels inside the $v = 0$ vibrational level in excited electronic state of MgH or C_2 would have approximately the same J-dependence as the one obtained here for SiO. Obviously, this does not mean that the values of depolarizing rates of excited electronic states of MgH and C_2 are comparable to these of ground electronic state of SiO.

Sensitivity to the elastic collisions varies with the total angular momentum number J according to the ratio $\mathcal{R}$ (Eq. (15)). For example in the second solar spectrum of C_2, depolarizing rates for levels of the triplet R1(14), R2(13), R3(12) at 5140 Å are ~6 times (i.e. $\mathcal{R} \sim 6$) higher than these of the P-triplet at 5141.2 Å P1(42), P2(41), P3(40). We think that the higher the rotational number J, the smaller the difference between depolarizing rates involving different diatomic molecules. This is because collisional rates of levels with rather high J-values are less sensitive to the difference between interaction potentials than are levels with low J-values (e.g. Balakrishnan et al. 2002); the rotational excitation rates obtained using different interaction potentials can be very different at low J but converge to rather similar values when J increases. As a result, in the approximation that depolarizing rates are the same for MgH and C_2 for rather high J-values, one can estimate depolarizing rates of any J-level for C_2 if at least one depolarizing rate of J-level is known for MgH and vice versa.

The J-dependance obtained in this section might be a useful constraint to empirical calculations of depolarizing and polarization transfer rates based on interpretations of spectropolarimetric observations (Mohan Rao & Rangarajan 1999; Asensio Ramos & Trujillo Bueno 2005; Bommier et al. 2005).

4. Conclusion

This paper is an introduction to the problem of collisional depolarization and polarization transfer for rovibrational levels of diatomic molecules. Equations (7) and (8) allow direct determinations of the depolarizing and polarization transfer rates via the usual calculations of the IOS rates $\zeta(v0 \rightarrow vL, T)$. We compute depolarizing and polarization transfer rates of rotational levels $J = 1,..., 99$ for vibrational numbers $v = 0, 1, 2, 3$ associated to the maser SiO polarization. We think that these calculations constitute accurate data for the SiO molecule and give useful order of magnitude indications for rates of other diatomic molecules. A J-dependence of collisional depolarization rates is found and characterized by a simple ratio $\mathcal{R}$, which might be included in modeling of the scattering polarization in diatomic molecular lines. We find that the transfer rates of population and alignment between different J-levels inside the same vibrational number v can be larger than the elastic depolarizing rates especially for high J values.

In rather hot astrophysical environments, such as the solar atmosphere, molecules like MgH and C_2 present a linearly polarized light originating from transitions between ground and *excited* electronic states. Preliminary conclusions regarding the role of collisions in the formation of the very interesting polarized lines of C_2 and MgH observed in the solar photosphere are given in this paper. In the future, self-quantum chemistry collisional calculations concerned with MgH and C_2 molecules in their *excited* electronic states are needed to accurately interpret the spectropolarimetric observations. As far as we know, since the observed molecules in the interstellar medium are often in their ground states, calculations concerned with diatomic molecules in *excited* electronic states in collisions with neutral hydrogen have never been done.

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