

POSSIBLE OH^+ SUBMILLIMETER EMISSION IN ORION - KL

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RESUMEN. El ión molecular OH^+ no fue detectado en nubes interestelares hasta ahora, debido a que la posible detección de OH^+ en Orión-KL sería una confirmación independiente de las ondas de choque moleculares con o sin campos magnéticos (MHD y disociativas), es estudiada la estructura rotacional fina e hiperfina de este ión. El propósito de la comunicación es dar valores de probabilidades de transición para emisión espontánea e intensidades para frecuencias infrarojas medidas en laboratorio, los cuales deben hacer más fácil la tarea observacional de búsqueda de esta especie iónica.

ABSTRACT: The OH^+ molecular ion has not been detected in interstellar clouds so far. Since a possible detection of OH^+ in Orion-KL would be an independent confirmation of molecular shock waves with or without the presence of magnetic fields (MHD and dissociative), the fine and hyperfine rotational structure of this ion is studied. It is the purpose of the present communication to provide values of transition probabilities for spontaneous emission and intensities for laboratory measured infrared frequencies which should make easier the observational task to search for this ionic specie.

Key words: INTERSTELLAR-MOLECULES — TRANSITION PROBABILITIES

. INTRODUCTION

Few molecular species have been detected in interstellar clouds so far, through their transitions in emission in the far infrared (FIR) and submillimetric (SMM) regions of the electromagnetic spectrum (Viscuso et al., 1985a,b; Watson et al., 1985a; Melnick, 1986; Ziurys, 1988). A detailed study of these hyperfine transitions may reveal details of the physical conditions in regions where these molecules are located. In particular in Orion-KL, the nearest among the giant molecular clouds, which provides an unique source of heterogeneity in physical conditions and chemical abundances within a relatively small spatial region and where many of the chemical differences among the sub-sources seem to be directly related to processes of star formation generating shock fronts. Orion-KL emits strongly in the infrared and this radiation can be used as a diagnostic probe for the physical conditions in the interior of this region (Hayakawa, 1988; Nakada, 1988).

I. THEORETICAL FORMALISM AND NUMERICAL RESULTS

II.1 The Electric Dipole Transitions

Several laboratory studies have shown that the fundamental electronic state of OH^+ is $X^3\Sigma^-$ (see for instance Merer et al., 1975). For a molecule with state $X^3\Sigma^-$, the electron orbital angular momentum in the nuclear axis is zero ($\Lambda=0$) and the electron spin interactions with the molecular rotation obey the following expressions of rotational energy: $F_1(J=N+1)$, $F_2(J=N)$ and $F_3(J=N-1)$ (Dixon, 1959), where N is the rotational quantum number, excluding the electron spin and J is the total rotational quantum number including the molecular rotation with the electron spin S ($J=|N+S|$ to $|N-S|$).

For electric dipole transitions in state $X^3\Sigma^-$ (see Figure 1), with coupling belonging to

Hund's case b, the selection rules are $\Delta N = \pm 1$ and $\Delta J = 0, \pm 1$ (Somerville, 1978) and the emissions of OH^+ ($N=1 \rightarrow 0$) in level $v=0$ may occur in (Bekooy et al., 1985):

$$\begin{aligned} \nu_1 &= F_3'(0) - F_1''(1) = 909121.07 \text{ MHz} \\ \nu_2 &= F_1'(2) - F_1''(1) = 971811.77 \text{ MHz} \\ \nu_3 &= F_2'(1) - F_1''(1) = 1033078.37 \text{ MHz} \end{aligned} \quad (1)$$

The line strength (H^{Hnl} - London factors) of these rotational transitions are giving by (Somerville, 1978):

$$\begin{aligned} S_J(J' = 0 \rightarrow J''=1) &= \frac{1}{J(2J-1)(2J+1)} \\ S_J(J' = 2 \rightarrow J''=1) &= \frac{J(2J+3)}{2J+1} \\ S_J(J' = 1 \rightarrow J''=1) &= \frac{1}{J} \end{aligned} \quad (2)$$

which for $J=1$ assume values $1/2$, $5/3$ and 1 for ν_1 , ν_2 and ν_3 , respectively. This clearly shows that ν_2 corresponds to the strongest rotational transition between the $N=1 \rightarrow 0$ transitions in the $v=0$ level of the $X^3\Sigma^-$ state of OH^+ ion and holds $\sim 56\%$ of $N=1 \rightarrow 0$ total intensity. It should be noted that these three rotational transitions are localized in the wavelength range of $290 \mu\text{m}$ - $330 \mu\text{m}$ and consequently in the SMM region of the electromagnetic spectrum.

The Einstein transition probability for spontaneous emission of a rotational line is given by (Somerville, 1978):

$$A(J+1 \rightarrow J) = 1.16395 \times 10^{-38} \nu^3 \mu^2 \frac{S_J}{g_2} \quad (\text{s}^{-1}) \quad (3)$$

where ν is the rotational frequency in Hz, $\mu = 2.32$ Debye (Werner et al., 1983) is the electric dipole moment for OH^+ , S_J is the corresponding line strength for ν and $g_2 = 2J+1$ is the statistical weight of the upper level.

The emission in FIR is optically thin. For an optically thin line, the emission intensity in the FIR or SMM regions is given by (Watson, 1985a; Melnick, 1986; Sternberg, 1988):

$$I_{j \rightarrow i} = \frac{h}{4\pi} \nu_{ij} A_{ji} \int f_j n_{\text{ion}} d\ell,$$

or

$$I_{j \rightarrow i} = \frac{h}{4\pi} \nu_{ij} A_{ji} f_j [n_{\text{ion}} \ell] \quad (\text{erg s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1}) \quad (4)$$

where h is Planck's constant, ν_{ij} is the frequency of the observed transition, A_{ji} is the Einstein transition probability for spontaneous emission, f_j is the fraction of all the ions in the upper level j , n_{ion} is the volumetric density of the ionic species, ℓ is the length of the emitting region along the line of sight and the product $[n_{\text{ion}} \ell] \equiv [N] = \text{cm}^{-2}$. For a kinetic temperature $T_K = 70\text{K}$ which is appropriate for Orion-KL we have a fractional population f_j (Herzberg, 1950) of OH^+ ions in different rotational levels $N=0, 1$ and 2 for $v=0$ level of the $X^3\Sigma^-$ state as $f_0 = 0.338$, $f_1 = 0.516$ and $f_2 = 0.223$. This clearly shows that for $T_K = 70\text{K}$ the maximum OH^+ fractional population is in $N=1$ level and $\text{OH}^+(N=1 \rightarrow 0)$ transition occur in emission and with $N_{\text{OH}^+} = 1.8 \times 10^{13} \text{ cm}^{-2}$ produced by a dissociative shock propagating with a velocity $v_s = 60 \text{ km s}^{-1}$ in a dense gas cloud of density $n = 10^5 \text{ cm}^{-3}$ (Neufeld and Dalgarno, 1989) results in the following intensity values.

TABLE 1 - Values for $N=1 \rightarrow 0$ in level $v=0$ electric dipole moment transitions of $\text{OH}^+(X^3\Sigma^-)$ ion in Orion-KL

$\nu(\text{MHz})$	$J' - J''$	$S_{J', J''}$	$g_2 = 2J+1$	$A \times 10^{-2} (\text{s}^{-1})$	$I \times 10^{-5} (\text{cgs})$
909121.07	0 - 1	0.333	1	1.569	6.986
971811.77	2 - 1	1.667	5	1.917	9.124
1033078.37	1 - 0	1.000	3	2.302	11.647

II.2 The Hyperfine Rotational Structure

The nuclear spin of OH⁺ ion is 1/2, due to the hydrogen nucleus ($\vec{I}=1/2$). Thus the total angular momentum F of the molecule is given by

$$F = J + I \quad (5)$$

where J is the rotational quantum number including the electron spin and F can assume values from $|J+I|$ to $|J-I|$. Due to the nuclear spin, each level of spin-rotation will be split in several components. These hyperfine transitions are shown in Figure 1.

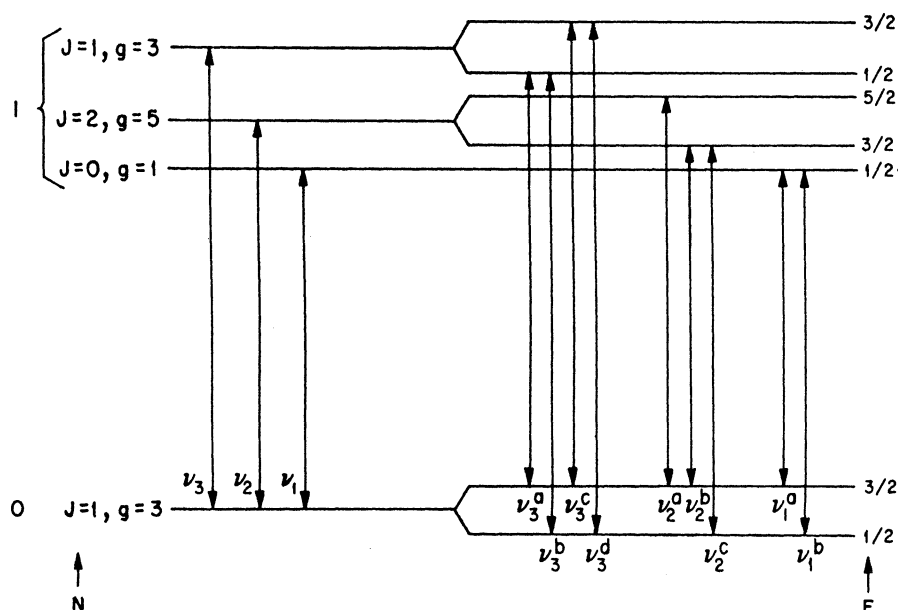


Figure 1 - Hyperfine transitions for $N=1 \rightarrow 0$ in level $v=0$ of $^{16}\text{O}^1\text{H}^+$ ion in state $X^3\Sigma^-$.

For the electric dipole transitions such as $\nu_2(N'=1, J'=2 \rightarrow N''=0, J''=1)$, we will have the corresponding hyperfine transitions ν_2^a, ν_2^b and ν_2^c with $(\Delta F=0, \pm 1)$. The frequencies of these hyperfine transitions (Table 2) were measured in laboratory with great accuracy by Bekooy et al. (1975)

$$\nu_2^a(J'=2, F'=5/2 \rightarrow J''=1, F''=3/2) = 971803.8 \text{ MHz}$$

$$\nu_2^b(J'=2, F'=3/2 \rightarrow J''=1, F''=3/2) = 971919.2 \text{ MHz} \quad (6)$$

$$\nu_2^c(J'=2, F'=3/2 \rightarrow J''=1, F''=1/2) = 971805.3 \text{ MHz}$$

The Hönl-London factors for these hyperfine transitions can be determined through the following formulas, adopted from Condon and Shortley (1959):

$$[(J'=2, F'=5/2) - (J''=1, F''=3/2)] = \frac{(F+J-I-1)(F+J-I)(I+J+F+1)(I+J+F)}{4F} S_J(J'=2 \rightarrow J''=1)$$

$$[(J'=2, F'=3/2) - (J''=1, F''=3/2)] = \frac{(2F+1)(F+I-I)(F+I-J+1)(I+J+1+F)(I+J-F)}{4J(F+1)} S_J(J'=2 \rightarrow J''=1)$$

$$[(J'=2, F'=3/2) - (J''=1, F''=1/2)] = \frac{(F+J-I-1)(F+J-I)(I+J+F+1)(I+J+F)}{4F} S_J(J'=2 \rightarrow J''=1)$$

(7)

where $S_J(J'=2 \rightarrow J''=1)=5/2$ (Eq.(2)) is the H δ n1-London factor corresponding to $\nu_2 = F'_1(2) - F''_1(1) = 971811,77$ MHz. Giving adequate values to F , J and I one will find the following values of H δ n1-London factors for the hyperfine transitions ν_2^a , ν_2^b , ν_2^c : 3, 1/3 and 5/3, respectively. The H δ n1-London factors for the other hyperfine transitions corresponding to ν_1 and ν_3 were evaluated in a similar way (see Condon and Shortley, 1959) and its values are given in Table 2. The H δ n1-London factors corresponding to ν_2 shows that the line ν_2^a is the strongest between the three hyperfine transitions coming from ν_2 and all of them (as well as the other hyperfine transitions coming from ν_1 and ν_3) fall in the SMM region of the electromagnetic spectrum since their wavelengths are localized also in the range $290 \mu\text{m} - 330 \mu\text{m}$.

It was said above that the probability for a rotational transition $A(J+1 \rightarrow J)$ is given by Eq. (3) and now with $g_2 = 2F'+1$ the emission intensities I (Eq.(4)) were evaluated for these hyperfine transitions and their values are shown in Table 2.

TABLE 2 - Values of hyperfine transitions for $N=1 \rightarrow 0$ in level $v=0$ in state $X^3\Sigma^-$ of OH^+ ion.

Frequency (MHz)	$N', J' \leftarrow N'', J''$	$F' \leftarrow F''$	ν	$g_2 = 2F'+1$	$S_{J', J''}$	$A \times 10^{-2} (\text{s}^{-1})$	$I \times 10^{-5} (\text{cgs})$
909 045,2	1,0 - 1,0	1/2-1/2	ν_1^b	2	0.333	0.785	3.495
909 158.8	1,0 - 1,0	1/2-3/2	ν_1^a	2	0.667	1.569	6.986
971 803.8	1,2 - 1,0	5/2-3/2	ν_2^a	6	3.000	2.875	13.683
971 805.3	1,2 - 1,0	3/2-1/2	ν_2^c	4	1.666	2.395	11.399
971 919,2	1,2 - 1,0	3/2-3/2	ν_2^b	4	0.334	0.479	2.280
1 032 997,9	1,1 - 1,0	1/2-1/2	ν_3^b	2	0.667	2.302	11.646
1 033 004.4	1,1 - 1,0	3/2-1/2	ν_3^a	4	0.333	0.575	2.909
1 033 111,8	1,1 - 1,0	1/2-3/2	ν_3^c	2	0.333	1.151	5.824
1 033 118,6	1,1 - 1,0	3/2-3/2	ν_3^b	4	1.667	2.879	14.567

III. DISCUSSION

Fast dissociative shocks in molecular clouds can produce detectable radio, optical and infrared recombination lines (McKee and Hollenbach, 1987). The FIR and SMM regions are not explored in an extension comparable to the radio region so far (see for instance Melnick, 1986). Observations in this part of the spectrum is important to interstellar gas-phase chemistry since many radicals and molecular ions have their fundamental transitions there.

The chemistry of Orion-KL region is governed mainly by molecular shock waves and consequently this fact can contribute, so that the abundance of a given molecular specie be enhanced by several times in this source due to high temperature chemistry, if compared with the rest of the Orion molecular cloud. The low temperature ion-molecule chemistry was discussed by Singh and Almeida (1980) and Almeida and Singh (1981). Recently, Neufeld and Dalgarno (1989) showed that the dissociative "J" type shocks (where the magnetic field is not important and the molecule is dissociated by a shock with velocity $v_s \geq 50 \text{ km s}^{-1}$ (Hollenbach and McKee, 1979; Chernoff et al., 1982)), propagating in dense gas clouds can produce the OH^+ ion in the hot post-shock cooling gas behind the fast dissociative "J" type shock with an abundance $N \geq 1.5 \times 10^{13} \text{ cm}^{-2}$ for a shock propagating with a velocity $v_s = 80 \text{ km s}^{-1}$ in a gas of density $n = 10^5 \text{ cm}^{-3}$. Plus, between the various FIR and SMM molecular lines presently detected at $\lambda < 350 \mu\text{m}$, mainly in Orion-KL region, that require observations in airborne spectrometers (for instance NASA's Gerald P. Kuiper Airborne Observatory - KAO), we note the presence of the transitions in the hydrides: Para - $\text{H}_3\text{O}^+ : J_K = 1_0 \rightarrow 0_0$ in $304.5 \mu\text{m}$ and $\text{NH}(X^3\Sigma^-) : N=1 \rightarrow 0$ in $307.6 \mu\text{m}$ (Watson, 1985b), which are localized also in the interval of $290 \mu\text{m} - 330 \mu\text{m}$ of the OH^+ ion SMM transitions.

Thus, the indication seems to be that OH^+ SMM emission may yield detectable with a gas kinetic temperature $T_K \gtrsim 50\text{K}$ with the largest column density $N = 3.0 \times 10^{13} \text{ cm}^{-2}$, which corresponds to a gas density $n = 10^6 \text{ cm}^{-3}$ and a shock velocity $v_s = 100 \text{ km s}^{-1}$, though weak in the hot shocked gas region in Orion-KL (Neufeld and Dalgarno, 1989) that is, measured in the post shock material of the quiet and hot ($v_{\text{LSR}} \sim 9 \text{ km s}^{-1}$; $\Delta v \sim 4 \text{ km s}^{-1}$) region (this sub-region was previously called the compact "ridge") (Ohishi et al., 1986).

Future balloon-platform observatories and space experiments such as the NASA's Space Infrared Telescope Facility (SIRTF) with a 2-700 μm multiband imaging photometer should be capable of detecting these emission lines, thus serving as an unambiguous indicator of high temperature or shock waves chemistry.

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REFERENCES

- Welnick, G., 1986, in *Astrochemistry*, IAU Symposium n^o 120, (eds.) M.S. Vardya and S.P. Tarafdar, p.137.
- Viscuso, P.J., Stacey, G.J., Fuller, C.E., Kurtz, N.T. and Hartwit, M., 1985a, *Ap.J.*, 296, 142.
- Viscuso, P.J., Stacey, G.J., Harwitt, M., Haas, M.R., Erickson, E.F. and Duffy, P.B., 1985b, *Ap.J.*, 296, 149.
- Watson, D.M., Genzel, R., Townes, C.H. and Storey, J.W.V., 1985a, *Ap.J.*, 298, 316.
- Ziurys, L.M., 1988, *Ap.J.*, 324, 544.
- Merer, A.J., Malm, D.N., Martin, R.W., Horani, M. and Rostas, J., 1975, *Can. J. Phys.*, 53, 251.
- Dixon, R.N., 1959, *Can. J. Phys.*, 37, 1171.
- Somerville, W.B., 1978, *Atomic and Mol. Phys.*, 13, 383.
- Bekooy, J.P., Verhoeve, P. Meerts, W.L. and Dymanus, A., 1985, *J. Chem. Phys.*, 82, 3868.
- Werner, H.-J., Rosmus, P. and Reinsch, E.-A., 1983, *J. Chem. Phys.*, 79, 905.
- Hollenbach, D., and McKee, C.F. 1979, *Ap. J. Suppl.*, 41, 555.
- Herzberg, G., 1950, *Spectra of Diatomic Molecules*, 2nd ed., Van Nostrand Co., Princeton, N.J., p. 125.
- Neufeld, D.A. and Dalgarno, A., 1989, to appear in *Ap. J.*
- Condon, E.U. and Shortley, G.H., 1959, *The Theory of Atomic Spectra*, Cambridge University Press.
- Watson, D.M., 1985b, *Phys. Ser.*, T11, 33.
- Singh, P.D. and Almeida, A.A., 1980, *Astron. Astrophys.*, 84, 177.
- Almeida, A.A. and Singh, P.D., 1981, *Astron. Astrophys.*, 95, 383.
- Nakada, Y., 1988, *Publ. Astron. Soc. Japan*, 40, 331.
- Ohishi, M., Kaifu, N., Suzuki, H., and Morimoto, M., 1986, *Astroph. Space Sc.*, 118, 405.
- Hayakawa, S., 1988, *Astroph. Sp. Sc.*, 144, 629.
- Chernoff, D.F., Hollenbach, D.J., and McKee, C.F., 1982, *Ap.J. (Letters)*, 259, L97.
- McKee, C.F. and Hollenbach, D.J., 1987, *Ap. J.*, 322, 275.
- Sternberg, A., 1988, *Ap. J.*, 332, 400.

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