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A SEARCH FOR VIBRATIONALLY EXCITED INTERSTELLAR H_2^+

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ABSTRACT

The 1000 foot (305 m) Arecibo telescope has been used to search for radio-frequency hyperfine transitions of vibrationally excited orthohydrogen ions. The sources observed were two of the shocked molecular clouds in the supernova remnant IC 443 and the interstellar clouds in the line of sight to the Crab Nebula. The best upper limits to the column densities in the observed transitions were $\sim 10^{16}$ cm^{-2}, implying a ratio of H_2^+ to H_2 of less than $\sim 5 \times 10^{-4}$.

Subject headings: interstellar: abundances — interstellar: molecules — nebulae: supernova remnants

I. INTRODUCTION

H_2^+, the simplest molecule, consists of two protons bound by one electron. When the proton spins are aligned (orthohydrogen ions), magnetic dipole hyperfine radio-frequency transitions are possible, closely analogous to the familiar 21 cm "spin flip" transition in atomic hydrogen.

The H_2^+ ion is expected to be produced from H_2, either through ionization by UV photons or by collision with cosmic-ray particles. In either case it is likely to be formed in excited vibrational states ($v = 1$–9) because, in accordance with the Franck-Condon principle, excitation to these states involves the least change in the separation of the two protons (Stecher and Williams 1969; Dalgarno and Black 1976). The H_2^+ ion is very reactive and forms H_3^+ when it collides with H or H_2. The cross section for the latter process decreases somewhat with increasing v (Chupka, Russel, and Refaey 1968), resulting in a greater lifetime for vibrationally excited H_2^+. In dense clouds the time scale for the conversion of H_2^+ to H_3^+ by collisions is expected to be $\sim 10^6$ s, which is similar to the radiative decay time by electric quadrupole transitions to a lower vibrational state. For the above reasons it is expected that there will be very few ions in the ground vibrational state, $v = 0$, and, following the suggestion of Somerville (1977), a search for the radio-frequency transitions of vibrationally excited H_2^+ was made.

The sequence of reactions $H_2 \rightarrow H_2^+ \rightarrow H_3^+$ is the starting point of gas phase ion-molecule reaction chemistry in interstellar molecular clouds (Watson 1978). This chemistry describes the formation of almost all the detected interstellar molecules. Accordingly, a measurement of the abundance of H_2^+, or even the determination of a stringent upper limit to its abundance, would provide important constraints on the physical conditions within molecular clouds, such as the flux of ionizing photons and particles, and on the rate of formation of molecules by gas phase reactions.

Previous published searches for H_2^+, all of which have been unsuccessful, have been directed at the hyperfine transitions (F_2, F): (3/2, 3/2–1/2, 3/2) and (3/2, 5/2–1/2, 3/2) at frequencies 1412.24 MHz and 1404.35 MHz (Somerville 1977) in the $N = 1$ rotational state, $v = 0$ vibrational state (Penzias *et al.* 1968; Shuter and Sloan 1969; Jefferts *et al.* 1970; Encrenaz and Falgarone 1971). They were conducted using receivers with considerably higher system noise temperatures than are available today, with relatively large antenna beams, and generally the sources chosen tended to be H II regions and quiescent molecular clouds. One of the best of such searches (Jefferts *et al.* 1970) had receiver system temperatures in the range 200–250 K and antenna beamwidths in the range 22′–26′. In contrast to this, in this work the system temperatures of the dual polarization receivers were typically 60 K, and the antenna beamwidth was $\sim 4'.5$. For the compact shocked molecular regions studied in this work, the signal-to-noise ratio available from the equipment was about two orders of magnitude greater than that of the Jefferts *et al.* (1970) search.

The sources chosen for this search were the shocked molecular regions B and C immersed in the supernova remnant IC 443 (DeNoyer 1979; DeNoyer and Frerking 1981). The reasons for this choice were that in these clouds the observed enhanced abundance of HCO^+ has been attributed to an enhanced cosmic-ray energy density (Elitzur 1983). Further, we felt that the ionization fronts associated with the shocks would also be effective in producing an enhancement of the H_2^+ abundance. The receivers and feeds at Arecibo Observatory could be tuned to the frequencies of the H_2^+ transitions from $v = 0$ to 3. We also searched for transitions in $v = 4$ and 5 in absorption against Taurus A. Although these high vibrational states were considerably lower in frequency than the nominal tuning range of the feed used, antenna temperatures from Taurus A were greater than 1000 K, so that an effective "source-noise–limited" search could be made. The reason for this choice is that we expected these levels to be the most highly populated, both from a consideration of the potential energy curves of H_2 and H_2^+ (Sharp 1971) and from the direct laboratory measurements of Jefferts (1969), who was only able to detect transitions in the vibrational levels $v = 4$–9.

The frequencies of the radio frequency transitions in the (3/2, 5/2–1/2, 3/2) hyperfine states for $v = 0$ through $v = 3$, which had the largest transition probabilities, were determined by polynomial extrapolation from the laboratory measurements. They are similar to those given by Somerville (1977). Additionally, we have independently calculated the frequencies of the $v = 0$ states using the molecular constants derived theoretically by Ray (1977). The method of Dixon and Woods (1977) was used to numerically diagonalize the doublet sigma Hamiltonian. The difference in frequency between the calculated values for the main $v = 0$ line and the value extrapolated from Jefferts (1969) is 0.26 MHz. Thus the frequency range covered in the present search (1.22 MHz) covers this possible uncertainty. The uncertainties in the extrapolated frequencies of the $v = 1, 2$, and 3 lines are progressively smaller. Somerville (1977) also lists the transition probabilities (A-values) for all transitions of interest, and these have been used to estimate limits to the column density of H_2^+ in the transitions observed.

II. OBSERVATIONS

A total of nine observing periods of $\sim 2\frac{1}{3}$ hr each were obtained at the Arecibo Observatory[1] in 1984 March and November. All observations were made using dual receivers connected to left- and right-hand circularly polarized line feeds. The system temperature in each polarization was ~ 60 K, of which 40 K was contributed by the receivers. The continuum antenna temperatures from IC 443 and Taurus A were respectively ~ 22 K and ~ 1200 K. Antenna temperatures have been converted to brightness temperatures, using multiplying factors of 1.43 for IC 443 and 4.8 for Taurus A. Each receiver was connected to a 504 channel autocorrelator bank, and our final spectra represent an average over both senses of circular polarization. Frequency-switching within the spectrometer bandpass and folding was used to enhance the signal-to-noise ratio. When the spectral baselines were reasonably flat, this resulted in a frequency coverage of ~ 610 kHz (134 km s^{-1} at $v = 1$) at optimum signal-to-noise ratio, and double this range with the signal-to-noise ratio a factor of 2 worse. When the spectral baselines were poor, the frequency coverage was somewhat less. The spectral resolution used throughout this work was 4.88 kHz (1.07 km s^{-1} at $v = 1$). To aid in interpretation, all results in this work have been scaled to give upper limits to the equivalent brightness temperature or optical depth expected in a 1.0 km s^{-1} bandwidth. The same data were also smoothed to an effective resolution of 12.5 km s^{-1}, which is more representative of the line widths expected from shocked molecular clouds, and upper limits were also determined for this resolution. An attempt was made to observe the (3/2, 5/2–1/2, 3/2) transition in $N = 1$, $v = 2$ at 1332.247 MHz in IC 443 B, but this was frustrated by severe radar interference from San Juan International Airport. We checked to see whether any of the tabulated recombination lines of atomic hydrogen and helium (Lilley and Palmer 1968) were close in frequency to the H_2^+ transitions studied here, and this was not the case. In fact, we were able to confirm that the equipment was operating properly by observing the H171α line at 1303.718 MHz in the Rosette Nebula. A summary of our observational results is given in Table 1.

[1] The Arecibo Observatory is part of the National Astronomy and Ionosphere Center, which is operated by Cornell University under contract with the National Science Foundation.

III. ANALYSIS

For H_2^+ in emission (expected if the H_2^+ ions were largely behind the continuum emission in IC 443),

$$N(H_2^+)_{\rm hf} = 1.94 \times 10^{18}(g_u + g_l)/g_u(\nu/\mathrm{GHz})^2 \times (A/10^{-15})^{-1} \int T_B\, dv \ \mathrm{cm}^{-2}\,. \quad (1)$$

Here, $N(H_2^+)_{\rm hf}$ is the total column density of H_2^+ in the

TABLE 1

OBSERVATIONAL RESULTS

PARAMETER	IC 433 B		IC 433 C	TAURUS A	
	$v = 1$	$v = 3$	$v = 1$	$v = 4$	$v = 5$
Position (1950.0):					
R.A.	$6^h15^m15^s$		$6^h14^m42^s$	$5^h31^m31^s$	
Decl.	$+22°27'50''$		$+22°23'30''$	$+21°59'17''$	
Hyperfine transition frequency[a] (MHz)	1366.935	1300.170	1366.935	1270.550	1243.251
A[b]($\times 10^{-15}$ s^{-1})	3.37	2.90	3.37	2.71	2.54
Velocity range of search[c] (km s^{-1}):					
Full sensitivity	+67 to −67	+113 to −92	+27 to −107	+37 to −37	+38 to −38
50% sensitivity	+134 to −134	...	+94 to −174	...	...
Integration time on source (minutes)	180	360	72	120	80
3 σ upper limits:					
In 1.0 km s^{-1} band:					
T_B(mK)	49	70	77	1345	1239
$N(H_2^+)_{\rm hf}$ (cm^{-2})	**8.8E16**	**1.3E17**	**1.4E17**	**2.6E18**	**2.4E18**
τ ($\times 10^{-3}$)	1.4[d]	2.0[d]	2.8[e]	0.60	0.69
$N(H_2^+)_{\rm hf}$ (cm^{-2})	**2.5E16**	**3.8E16**	**5.0E16**	**1.2E16**	**1.4E16**
In 12.5 km s^{-1} band:					
T_B(mK)	20	29	34	314	224
$N(H_2)_{\rm hf}$ (cm^{-2})	**4.5E17**	**6.8E17**	**7.6E17**	**7.6E18**	**5.5E18**
τ ($\times 10^{-3}$)	0.58[d]	0.84[d]	1.3[e]	0.14	0.13
$N(H_2^+)_{\rm hf}$ (cm^{-2})	**1.3E17**	**2.0E17**	**2.9E17**	**3.4E16**	**3.2E16**

[a] $F_2 F$: (3/2, 5/2–1/2, 3/2); $N = 1$ rotational state.
[b] Somerville 1977.
[c] With respect to VLSR = 0 km s^{-1}.
[d] Calculated from measured continuum $T_B = 34.6$ K.
[e] Calculated from measured continuum $T_B = 27.1$ K.

observed hyperfine transition, g_u and g_l are the statistical weights of the upper and lower levels ($= 2F + 1$), ν is the transition frequency in GHz, A is the A-coefficient in s^{-1}, T_B is the brightness temperature in K, and v is the velocity in km s^{-1}.

However, if the H_2^+ ions in IC 443 or Taurus A were largely in front of the continuum emission, and observed in absorption, then

$$N(H_2^+)_{hf} = 1.94 \times 10^{18}(g_u + g_l)/g_u(\nu/\mathrm{GHz})^2 \times (A/10^{-15})^{-1} \int \tau(v) T_s \, dv \ \mathrm{cm}^{-2} . \qquad (2)$$

Here, $\tau(v)$ is the absorption optical depth, and T_s is the excitation, or spin temperature of the hyperfine levels.

We did not detect any spectral features near the expected transition frequencies for H_2^+, in either emission or absorption toward either IC 443 or Taurus A. In Table 1 we present 3 σ upper limits to the column density for each observed transition in both 1.0 and 12.5 km s^{-1} bands, calculated from equations (1) and (2). For the purpose of the table we have adopted $T_s = 10$ K in our determination of the absorption upper limits, but as we shall indicate this value is extremely uncertain.

IV. INTERPRETATION

The observational upper limits to the column densities for individual transitions of H_2^+ presented in Table 1 are subject to a number of uncertainties.

The first is the value for spin temperature used in determining the absorption upper limits. We adopted $T_s = 10$ K, which is roughly equal to the kinetic temperature in dense molecular clouds. However, the energy difference between the upper and lower level of each hyperfine transition is much smaller than the energy released in the formation of H_2^+, and it would be reasonable to expect that at the time H_2^+ is formed, all hyperfine levels would be populated according to their statistical weights—i.e., all hyperfine transitions would have an infinite spin temperature. The lifetime of the H_2^+ molecular ion is short, $\sim 10^6$ s in a molecular region before it is converted to H_3^+ by collisions with hydrogen molecules, and $\sim 10^{10}$ s in atomic regions before being converted to H_3^+ by the same process, or being dissociated by photons or by collisions with hydrogen atoms or electrons. During this time there is typically only one collision or fewer. In most cases there is insufficient time for the spin temperature to equilibrate to the kinetic temperature. We therefore think that the spin temperature could range from a very large value to one as low as the kinetic temperature of the gas in which the H_2^+ is formed. The former seems more likely, and if this is true the absorption limits quoted are gross underestimates. However, in this case the emission limits, which are independent of the spin temperature, remain valid and do not depend on whether the H_2^+ is behind or in front of the continuum source. A final possibility is that the spin temperature may be negative, signifying inverted populations of the hyperfine levels and maser action. If this is the case the emission limits may be grossly overestimated.

The second uncertainty is the line width to be expected. We have quoted limits in a 1.0 km s^{-1} band, a typical value for a cold cloud, and for a 12.5 km s^{-1} band, more appropriate for a shocked region. The latter are $\sim$3–5 times higher than the former. The narrow band would be appropriate for the preshock gas in IC 443, the latter for the postshock gas. In the case of the clouds toward Taurus A, the appropriate choice would depend on whether the H_2^+ was formed with significant kinetic energy.

The third uncertainty is the partition function, required to estimate the total column density of H_2^+ from the column density in a single hyperfine transition. This has four components: a multiplying factor of 4/3 to account for the presence of parahydrogen ions, a factor of 3.4 to account for the distribution among all hyperfine levels in a given rotational state (assuming that all levels are populated according to their statistical weights), and factors to account for partitioning between the rotational states in a given vibrational level and for partitioning between the vibrational levels. We have adopted a factor of 12 to account for partitioning between four vibrational levels (as were readily detected in the laboratory measurements of Jefferts 1969) and three rotational states of orthohydrogen ions in each vibrational level, but again this number is quite uncertain. The product of these four terms is ~ 50, and multiplying the limits quoted in Table 1 by this factor gives upper limits to the total column density of H_2^+ toward IC 443 in the range 1.2×10^{18}–3.8×10^{19} cm^{-2}, and 6×10^{17}–3.8×10^{20} cm^{-2} toward Taurus A.

The quantity of interest in interstellar chemistry is the ratio of column densities of H_2^+ to H_2. We have estimated the total column density of H_2^+ in the shocked regions of IC 443 as follows: from the data of DeNoyer and Frerking (1981), the column density for ^{12}CO in $J = 0$ for IC 443 B is taken to be $\sim 6 \times 10^{16}$ cm^{-2} for an excitation temperature T_x of 10 K. Multiplying by the partition function $2kT_x/h\nu$ ($= 3.62$) gives the total ^{12}CO column density as 2.17×10^{17} cm^{-2}. Dividing by 40 gives the expected column density of ^{13}CO as 5.43×10^{15} cm^{-2}, and multiplying this by 7.2×10^5 (Dickman 1985) gives the column density of hydrogen molecules as $N(H_2) = 3.9 \times 10^{21}$ cm^{-2}. This gives upper limits to $N(H_2^+)/N(H_2)$ in the range 3×10^{-4} to 10^{-2}. Toward Taurus A we have adopted a value for $N(H_2)$ of 10^{21} cm^{-2}, giving upper limits to $N(H_2^+)/N(H_2)$ in the range 6×10^{-4} to 0.4.

The expected values of $N(H_2^+)/N(H_2)$ have been estimated. Solomon and Werner (1971) indicate that in a standard dense molecular cloud $N(H_2^+)/N(H_2)$ is $\sim 4 \times 10^{-10}$. In a shocked supernova remnant such as IC 443, the formation rate for H_2^+ is expected to be enhanced by one to three orders of magnitude, giving $N(H_2^+)/N(H_2)$ in the range 4×10^{-7} to 4×10^{-9}. For the more diffuse clouds in the direction of Taurus A, using the reaction rates of Black (1978), we have determined that the ratio $N(H_2^+)/N(H_2)$ should be $\sim 10^{-10}$ to 10^{-11}. All these values are several orders of magnitude lower than our observed upper limits.

V. CONCLUDING REMARKS

We have undertaken a deep search for the radio frequency hyperfine transitions of H_2^+. In spite of the fact that our search was much more sensitive than any previous one, the upper limits we have placed on the abundance of H_2^+ are several orders of magnitude greater than those predicted using standard rate coefficients of interstellar chemistry. H_2^+ might have been detected in this search if one of the hyperfine transitions studied had had an inverted population and been amplified by maser action. Our observations cannot rule out population inversion but show that this is insufficient to lead to detectable lines in the sources we studied. It would be difficult to make a significant improvement on this search, in terms of either signal-to-noise ratio or beam dilution, and it therefore appears that the best hope for detecting interstellar H_2^+ would be to search for its UV transitions, as detailed by Heap and Stecher (1981).

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