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A SEARCH FOR INTERSTELLAR H_2O^+ IN DIFFUSE CLOUDS[1]

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ABSTRACT

Searches for H_2O^+ toward HD 187982, ζ Oph, *o* Per, and ζ Per have yielded significant upper limits for H_2O^+ when compared with existing models for similar lines of sight. Using available oscillator strength data, the column density for HD 187982, for example, cannot exceed 3×10^{12} cm^{-2} H_2O^+ molecules. Our most sensitive measurement for H_2O^+ toward ζ Oph is apparently limited by a blend with upper atmospheric H_2O^+, which is also present in the HD 187982 spectrum.

Subject headings: interstellar: abundances — interstellar: molecules

I. INTRODUCTION

In the oxygen family of molecules formed in diffuse interstellar clouds, the initial step is charge exchange

$$H^+ + O \rightarrow O^+ + H ,$$

rapidly followed by reactions with the abundant H_2 molecule:

$$O^+ \rightarrow OH^+ \rightarrow H_2O^+ \rightarrow H_3O^+ .$$

Cosmic ray ionization of hydrogen produces the necessary H^+. Neutral products arise through dissociative electron recombination of H_3O^+. Many thorough examinations of these reactions have been published recently; in particular, Glassgold and Langer (1976) have predicted column densities for these oxygen-bearing species. For the main cloud toward each of the stars, *o* Per, ζ Per, and ζ Oph, their work indicates $N(H_2O^+) \sim N(OH^+) \lesssim 10^{12}$ cm^{-2}.

Of the four ionic species, OH^+ and H_2O^+ can be observed via electronic transitions at wavelengths detectable from the ground. In this study, we searched for absorption due to H_2O^+. We made measurements toward ζ Oph and HD 187982 at the wavelengths for the doublet near 6147 Å (Lew 1976). These transitions have the least apparent interference from known terrestrial features (H_2O, O_2, etc.) and are as favorable as any other features in the H_2O^+ $\tilde{A}$–$\tilde{X}$ transition because of a rather broad maximum in the Franck-Condon factors from the ground to the excited state. Toward *o* Per, ζ Per, and ι Ori, the doublet near 6970 Å (Lew 1976) was observed, but because of telluric contamination, only the $J = N + \frac{1}{2}$ line was analyzed.

Herzberg (1980) tentatively identified H_2O^+ emission from the λ6147 transition in the upper atmosphere of the Earth. We were not aware of this possible identification at the time of our observations, so interference of terrestrial H_2O^+ may have occurred in the spectrum for ζ Ophiuchi. This was due to a coincidence of the redshifted heliocentric velocity with the blueshifted local standard of rest velocity of the molecules in the dominant neutral cloud in the direction of ζ Oph. In any case, we also observed upper atmosphere H_2O^+ molecules in the course of the search for interstellar molecules.

II. OBSERVATIONS

a) HD 187982 and ζ Oph

The observations toward HD 187982 and ζ Oph were obtained during portions of a single night using the NASA Infrared Telescope Facility. The servo-controled Fabry-Perot interferometer, SPIFI (Smith 1981), was placed at the Cassegrain focus (f/36) and was operated with a spectral resolving power of 120,000, or a full width at half-maximum (measured) of 52 mÅ at 6150 Å (2.5 km s^{-1} velocity resolution). We used a single etalon with a three-period interference filter having a 2.7 Å bandpass to block side orders. The finesse of the etalon near 6150 Å was over 70 with a measured free spectral range of 3.61 Å. The detector was an RCA C31034 A04 PMT with a dark count of less than one count per second at −78°C and with a quantum efficiency of about 25% at the observed wavelengths. The filter was tracked in tandem with the etalon to yield a flat instrumental function over about 5 Å of spectrum. Data were acquired in a rapid scan mode with the scans coherently added in the memory of the controlling computer. A total of 45,000 and 590,000 counts per spectral sampling element were detected, respectively, in the spectra of HD 187982 and ζ Oph. By scanning a portion of the lunar spectrum, we were able to check our wavelength calibration taken from internal rare gas discharge lamps as well as the wavelength scale over the range of our scans. The wavelength scale and calibration are correct to better than one spectral sample element across our scan range.

At the time of observation, HD 187982 had a heliocentric velocity of −8.4 km s^{-1}, while according to Herbig and Soderblom (1982), the local-standard-of-rest velocity for the

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dominant cloud in that direction lies at -7.2 km s^{-1} so that the features of H_2O^+ should lie at -15.6 km s^{-1} or 0.32 Å shortward of the laboratory rest frame wavelength. For ζ Oph at the time of observation, the heliocentric velocity was $+15.6$ km s^{-1} while the major cloud in the line of sight toward ζ Oph lies at -14 km s^{-1}. The result is that only 1.6 km s^{-1} in differential velocity existed at the time of observation. Thus, any interstellar lines in the ζ Oph line of sight would blend, within our spectral resolution, with any terrestrial H_2O^+ features present at the time of observation.

The data were reduced in several steps. The observations were processed by first coherently summing the several data scans. Individual scans were taken over 15 minute integrations to avoid losses due to the occasional power glitches encountered at the telescope. Second, the continua of HD 187982 and ζ Oph were not flat over the observed wavelength region. Because of the large rotational width of stellar features, however, we were certain that the sharp features seen did not originate in the stellar spectra. The stellar features were removed by fitting the spectra with a low-order polynomial which also partially suppressed a weak channel spectrum due to the interference filter. The data then were Fourier analyzed according to the scheme of Brault and White (1971).

b) *o Per*, *ζ Per*, *and ι Ori*

The directions toward o Per and ζ Per were observed because their interstellar absorption-line spectra are similar to that for ζ Oph, while ι Ori was observed as a check on telluric contamination. The line of sight to ι Ori has few H_2 molecules and, therefore, should not show any H_2O^+ absorption.

Measurements of H_2O^+ absorption for these directions were made with the 2.7 m telescope at McDonald Observatory. The photodiode Reticon detector at the coudé spectrograph (Vogt, Tull, and Kelton 1978) was used to obtain the spectra. A dispersion of 1.14 Å mm^{-1} (0.029 Å per diode) was achieved with an echelle grating. The resolving power of the spectrograph for the measurements was set at 60,000 for the wavelength region near 6970 Å (velocity resolution of 5 km s^{-1}). A narrow band interference filter blocked out unwanted echelle orders. Telluric water lines were used to set the wavelength scale. Only the $J = N + \frac{1}{2}$ line of H_2O^+ at 6973.720 Å was measurable because the $J = N - \frac{1}{2}$ line at 6970.152 Å was contaminated with telluric features.

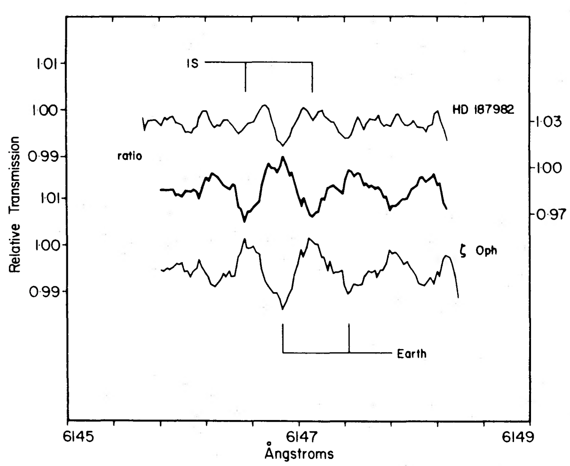

FIG. 1.—The region of H_2O^+ absorption at 6147 Å for HD 187982 (*upper curve*), for HD 187982 divided by the ζ Oph spectrum (*middle curve*), and for ζ Oph (*lower curve*). The apparent H_2O^+ terrestrial features are substantially diminished, while the apparent features at the expected interstellar velocity for HD 187982 are enhanced in the ratioed spectrum.

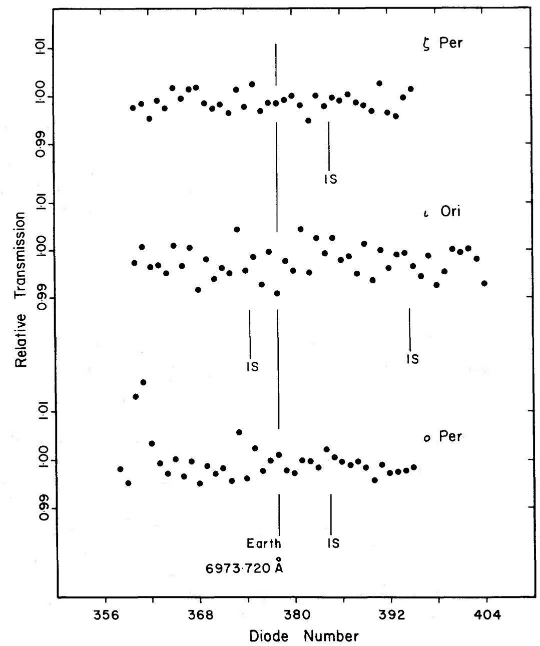

FIG. 2.—The region of H_2O^+ absorption at 6973 Å for ζ Per, ι Ori, and o Per. The wavelength scale is 0.029 Å per diode. In the spectrum of o Per, a cosmic ray event is present near diode 360.

The Reticon data were reduced in the usual manner. After being processed by the Reticon software package (Vogt, Tull, and Kelton 1978), the stellar spectra were divided by a flat lamp spectrum, which was taken after each measurement, to remove any variation in instrumental profile. The final step in the reduction of the data was a linear least squares fit to produce a flat continuum across the whole spectrum.

III. RESULTS

The rest wavelengths for the H_2O^+ transitions are marked on Figures 1 and 2, as well as the expected positions for the interstellar features. The signal-to-noise ratios (S/N) achieved and the spectral resolution along with the velocity distribution of absorption in the line of sight (Hobbs 1973) may be used to specify a detection limit for the H_2O^+ lines according to the prescription of Jenkins *et al.* (1973) where the detectable equivalent width (1 σ) is given by

$$W_\lambda(1\ \sigma) = M^{1/2}\Delta\lambda/\sigma\ .$$

M is the number of spectral elements in which a line may fall, $\Delta\lambda$ is the spectral resolution, and σ is the rms S/N in the continuum. The resultant detectable equivalent width (1 σ), along with the parameters for the stars observed, are listed in Table 1.

For ζ Oph, where we have the best S/N, the apparent blend of the terrestrial H_2O^+ with the interstellar lines unfortunately prevents our reaching the intrinsic detectivity for H_2O^+ given

TABLE 1

PROGRAM STARS

Star	α(2000)	δ(2000)	Spectral Type	m_V	$E(B-V)$	S/N	$W_\lambda(1\ \sigma)$ (mÅ)
HD 187982	$19^h51^m01^s$	+24°59′	A1	5.6	0.68	200	0.35
ζ Oph	16 37 09	−10 34	O9.5	2.6	0.32	800	0.10
o Per	03 44 19	+32 17	B1	3.8	0.30	600	0.30
ζ Per	03 54 08	+31 53	B1	2.8	0.33	600	0.30
ι Ori	05 35 26	−05 55	O9	2.8	0.07	300	0.60

in Table 1. For HD 187982, the greater expected absorption depth compensates for the poorer S/N, and the visibility of any interstellar features can be enhanced by dividing the spectrum of HD 187982 by that for ζ Oph. This reduces the influence of any residual channel spectrum and also divides out the terrestrial features to a high degree. As seen in Figure 1, the apparent terrestrial features do diminish while the features at the position of the dominant diffuse cloud for HD 187982 become more prominent. Nonetheless, for such marginal features, we are not claiming a detection but prefer to specify an upper limit of 0.7 mÅ (2 σ) for the features. Our upper limit is not an extreme upper limit (taking all parameters at their value which maximizes the upper limit) but a probable value consistent with the marginal features seen in the spectra. From the spectral parameters, we estimate that a 2 σ upper limit for ζ Oph of $\lesssim 0.2$ mÅ would have been obtained, if it were not for the blend with the apparent terrestrial features.

Detections of absorption features at the correct velocities satisfy only the necessary condition for the presence of H_2O^+ in the line of sight. The presence of the doublet reinforces the likelihood that the features are real and due to H_2O^+. We can readily improve the measurements of the terrestrial H_2O^+ features by observing a brighter star such as Vega, which we normally use to establish the instrumental transmission function. Under the present observing conditions, we detected over 60,000 counts per second for Vega.

For *o* Per and ζ Per, the rms continuum error is 0.0018, while the spectral resolution is 60,000. These numbers imply an upper limit (2 σ) of 0.6 mÅ for the H_2O^+ features near 6970 Å. The presence of terrestrial features is especially troublesome here, as noted above.

IV. INTERPRETATION OF THE SPECTRA

Interpretation of the observational data in terms of column densities depends on oscillator strengths for the observed transitions. Lifetime data for H_2O^+ was interpreted by Curtis and Erman (1977). The measured lifetimes were dependent on the experimental conditions and, hence, are less reliable than is often the case. We take a conservative position in that the actual lifetime of the state is midway between the extremes measured over the range of experimental conditions described by Curtis and Erman, i.e., 1.9 ± 1.1 μs. Using the vibrational transition probabilities implied by the photoelectron data of Brundle and Turner (1968), which yields a Franck-Condon factor of 0.10 for the $(v_1 v_2 v_3) = (0, 8, 0)$–$(0, 0, 0)$ transition, and the line strengths given by Lew (1976), the line oscillator strength for the $J_{K_{-1}K} = 1_{10}$–0_{00} doublet of the ${}^rR_{0,N}$ branch of the above vibrational transition of the $\tilde{A}\ {}^2A_1$–$\tilde{X}\ {}^2B_1$ electronic transition is found to be $4.3 \pm 2.5 \times 10^{-4}$. Due to the $q_{v'v''}\lambda^2$ dependence of the *f*-values on vibrational transition probabilities and on wavelength, the same *f*-value is computed for the corresponding rotational transition in the (0, 6, 0)–(0, 0, 0) band. The major possible error in this *f*-value is due to the lifetime uncertainty.

The pair of features possibly seen toward HD 187982, weighted by $2^{-1/2}$, indicates that H_2O^+ may be present with a column density not exceeding 3×10^{12} cm^{-2}. Because the H_2O^+ molecule has a large dipole moment, relaxation probably is fast enough so that only the lowest rotational level need be considered. Such a column density is not inconsistent with what might be expected toward this star. The models which refer to clouds more like the *o* Per, ζ Per, and ζ Oph lines of sight would predict about 5×10^{11} cm^{-2} for H_2O^+ compared with our upper limits of 2×10^{12} cm^{-2} for the Perseus stars. A comparison between atomic and diffuse interstellar bands in the various observed lines of sight (see, for example, Herbig 1968; Smith *et al.* 1981; and Herbig and Soderblom 1982) indicates that a factor of 3–5 increase in equivalent width (and column density) toward HD 187982 is quite reasonable for unsaturated features. The line of sight toward HD 187982 has not been modeled to date, while those toward *o* Per, ζ Per, and ζ Oph have been the subject of extensive efforts to understand the interstellar spectrum (e.g., Black and Dalgarno 1977; Black, Hartquist, and Dalgarno 1978). HD 187982 is a particularly interesting star in that it appears to have a very rich molecular spectrum while being quite bright ($V = 5.6$) and reddened [$E(B-V) = 0.68$] and having a single dominant cloud in the line of sight (Smith *et al.* 1981; Herbig and Soderblom 1982). Since the detectability of features increases, relatively, for the deeper features seen in such more reddened, but fainter stars, searches for new molecules, etc., may be at least as sensitive in these lines of sight as in the more traditional lines of sight like that toward ζ Oph. Many such stars are of sufficiently early spectral type that space observations will soon establish line-of-sight parameters needed for effective modeling.

Although the *f*-values are uncertain by a factor of 2 for the observed transitions, as described above, we have reached statistical levels in our observations which permit significant tests of model predictions, including current ideas of ionization rates. The H_2O^+ abundances from our data cannot greatly exceed the theoretical predictions. Confirming observations are indicated, certainly, and should be extended to include OH^+ which has a predicted abundance similar to that for H_2O^+ and which has considerably larger *f*-values for the transitions accessible to ground-based astronomy. OH^+ and H_2O^+ are suitable targets for a serious test of the ion-molecule schemes for the formation of molecules in diffuse interstellar clouds.

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Note added in proof.—Dr. J. Black has brought to our attention another set of lifetime measurements for the $\tilde{A}$–$\tilde{X}$ transition in H_2O^+ (D. Möhlmann *et al.* 1978, *Chem. Phys.*, **31**, 273). The lifetimes determined by Möhlmann *et al.* are approximately a factor of 10 longer than those of Curtis and Erman (1977). The use of longer lifetimes in our analysis results in significantly larger upper limits for the H_2O^+ column densities reported here. Additional laboratory measurements are required to establish the appropriate lifetimes necessary for an accurate determination of $N(H_2O^+)$.

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