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NASA CR- 170601

WASHINGTON UNIVERSITY

DEPARTMENT OF EARTH AND PLANETARY SCIENCES

NASA Grant NSG 5187

Final Technical Report

Submitted By:

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Final Technical Report for NASA Grant NSG 5187

The above named grant resulted in a paper on the abundances of OH and H_2O in the interstellar toward the chosen stars. The Copernicus observations were successfully carried out, the data were reduced, and analysed. We found that the lower limits for the OH/H_2O ratio are, at present, consistent with the theoretical models. The effort we made here has led to a better understanding of the validity of the molecule producing mechanisms towards diffuse clouds, and has uncovered through continued laboratory study, even more favorable transitions of H_2O with which to establish the interstellar abundance of H_2O in diffuse clouds. The enclosed paper has now been submitted for publication.

I would like to thank NASA for their support in this program.

Invention Report

No inventions were made during the course of this research.

COPERNICUS OBSERVATIONAL SEARCHES FOR OH AND H$_2$O

IN DIFFUSE CLOUDS

by

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ABSTRACT

An intensive search for OH and H$_2$O in the directions of σ Sco, α Cam, and o Per was undertaken with the Copernicus satellite. Multiple scans were carried out over the wavelength region for the expected absorption features due to the OH D-X and H$_2$O $\tilde{C}$-$\tilde{X}$ transitions. The feature due to OH was detected marginally towards σ Sco, and only an upper limit can be given towards α Cam. H$_2$O was not detected in any of the stars at the signal level accumulated. The OH abundance towards σ Sco and the respective lower limits for the OH/H$_2$O ratios are discussed with regard to the extant models for the steady state abundances of OH and H$_2$O, and shown not to be inconsistent with ion-molecule schemes.

*Guest Investigator with the Princeton University telescope on the Copernicus satellite, which is sponsored and operated by the National Aeronautics and Space Administration.

I. INTRODUCTION

The effectiveness of molecule-producing processes in diffuse clouds can hardly be questioned. The molecules observed to date include H_2, CO, OH, CH, CH^+, CN and C_2. Reviews of possible formation mechanisms have been given by Watson (1975), Herbst and Klemperer (1973), and Dalgarno and Black (1976), among others. In spite of the amount of information already in hand and the formation models calculated, with the exception of molecular hydrogen (Hollenbach and Salpeter, 1971), there is not yet a fully understood formation mechanism for any given molecule. While schemes can be devised which produce large amounts of any of the above molecules, the lack of adequate laboratory data on relevant processes usually requires the use of poorly-supported estimates for various rate constants. A possible exception to this situation may be found in the ion-molecule scheme for the formation of OH and H_2O, where the abundances and ratios of OH/H_2O are determined by processes which would appear to be relatively well understood. Both molecules have transitions from the ground state in the ultraviolet. Observation of OH and H_2O in various lines-of-sight then offers a possibly significant test for that particular ion-molecule formation scheme.

Since a few lines-of-sight have already been investigated (Crutcher and Watson, 1976; Chaffee and Lutz, 1977;

Snow, 1976a, 1976b, 1977), it is known that OH frequently
exists at detectable levels and the H_2O is less abundant.
We have therefore obtained very extensive new data on σ Sco
and α Cam for both molecules and also have carried out
further scans of the H_2O transition in the spectrum of
o Per. After a brief discussion of the ion-molecule scheme
for OH and H_2O production, we will detail our observations
and the conclusions derived from them.

II. ION-MOLECULE REACTION FORMATION OF OH AND H_2O

Using the terminology of Dalgarno and Black (1976), we may write the following reaction scheme for OH and H_2O. First, the charge exchange

$$H^+ + O \rightarrow O^+ + H$$
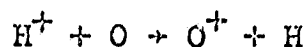
(Field and Steigman, 1971) initiates the reaction scheme. The O^+ thus formed is removed by reaction with H_2 in several successive reactions which are interrupted by recombination with ambient electrons, and hence are very sensitive to the depletion of elements producing the electrons. Two reactions ultimately produce H_2O and OH:

$$H_2O^+ + e^- \rightarrow OH + H \qquad \text{and}$$

$$H_3O^+ + e^- \rightarrow H_2O + H \text{ or } OH + H_2.$$
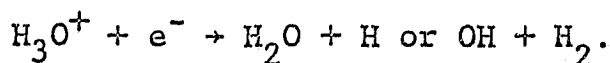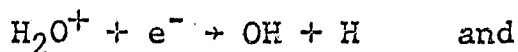
The branching ratio for this latter reaction has recently been given as approximately 10 in favor of OH by Herbst (1978), rather than the value of 1 assumed by many earlier studies (Watson, 1975; Herbst and Klemperer, 1973; Smith and Zweibel, 1976; and Glassgold and Langer, 1975). Destruction processes for OH and H_2O have been studied by Smith and

Zweibel and by Smith and Stella (1975). For a typical cloud of 100 H atoms cm^{-3} with a depletion factor f of 0.2, and an obscuration of 2 magnitudes at 950 $\overset{o}{A}$, the ratio of OH to H_2O is given by

$$n(OH)/n(H_2O) = (\frac{\beta_{H_2O}}{\beta_{OH} + \lambda_{OH}}) \frac{1}{(1-\alpha)(1-f)}$$

which has been simplified from Equation 10 of Smith and Zweibel (1976). In this equation β_{H_2O} and β_{OH}, the photo-dissociation rates, are given by Smith and Zweibel in their Table 1, and λ_{OH} is given by Herbst and Klemperer (1973) as 1.6×10^{-9} cm^3/sec times n_{ct}. According to Herbst (1978), the branching ratio α can be as high as 10, while the commonly adopted value 1 is actually a lower limit. The higher ratio in favor of OH increases $n(OH)/n(H_2O)$ by a factor of 5, or in the above simplified equation, gives $n(OH)/n(H_2O)$ as about 25, probably accurate to within a factor of 2 considering the approximations involved.

IV. RESULTS AND CONCLUSIONS

In Table 1 we summarize the extant ultraviolet observations of OH and searches for H_2O in various directions, including some earlier results and cloud parameters. Although the transitions of both molecules are well characterized as to wavelength, the strengths of the features have been the subject of considerable discussion in the literature since we initiated these observations. The OH D-X transitions' line strengths have been calculated and subsequently measured indirectly. Ray and Kelly (1975) computed an f-value of 0.0015, while Chaffee and Lutz (1977) derived an f-value for the 1220 Å line from their observation of the near ultraviolet transitions of OH near 3078 Å and the equivalent width for the OH D-X lines measured by Snow towards ζ Per. The recommended f-value for the transition is 0.0052 from the observational results. This value is much smaller than expected for an allowed Rydberg transition. The situation with regard to the f-value for the H_2O Rydberg transition near 1239 Å is also rife with uncertainty. Smith and Zweibel (1976) estimated from literature data an f-value which was believed to be correct to within a factor of 2. The f-value was 0.018. Very recently, Smith and Parkinson (1978) found an upper limit to the line f-value of 0.023, consistent with the earlier estimate. For the present, f = 0.018 is adopted.

The OH/H_2O limits given in the last column of Table 1 are consistent with the models, but only if Herbst's (1978) branching ratio strongly favoring the production of OH is correct. Hence, the present data appear to substantiate a high value for this branching ratio. These limits, however, refer only to the ground rotational state. For $T_{kin} \leq 16^\circ K$ (Snow, 1978), most of the molecules will be in this state, so this should not introduce much error. In any case, there is insufficient data available on collisional excitation cross-sections, radiative lifetimes, and the exact kinetic temperature to make any evaluation of rotational excitation very reliable.

Another factor which comes into play was recently discussed by Sandell (1977); _viz_. the shielding of molecules by the grains may be much less efficient than has previously been supposed. Grains as described by Lillie and Witt (1976) will have strongly forward scattering phase functions allowing the star light to penetrate much further into obscured clouds than would be assumed for isotropically scattering grains. In this case, the fact that longer wavelengths of light are much more effective in photodisso-ciating H_2O than OH will result in larger OH/H_2O ratios. In order to treat this problem correctly, the transfer of radiation must be handled as indicated by Sandell. Overall, the theoretical situation has evolved to the point that predictions are extremely model-dependent. Our upper limits

then are of considerably reduced value although at least indicative. A ray of hope exists that detection of H_2O may yet be possible through the features accessible to the Copernicus satellite. A stronger Rydberg series near 1115 Å may contain features sharp and strong enough for such observations (Johns, 1978). A careful search there could increase the lower limit of the ratio to allow a significant test of model predictions.

Table 1. OH and H$_2$O Observations

HD	E(B-V)	log N(H)* cm^{-2}	N(H$_2$)/N(H)*	n$_H^+$ cm^{-3}	OH WΛ(mA)	No. Scans	H$_2$O WΛ(mA)	No. Scans	N(OH)/N(H$_2$O)**
ir 23180	0.32	21.21	0.50	10^3:	Q: 5.8±2.0 P: ≤ 2.0	32	≤ 0.90	87	≥ 23.0
ir 24398	0.33	21.20	0.59	10^3:	Q: 3.6±1.7	31	—	—	—
am 30614	0.32	21.09	0.35	——	Q: ≤ 1.8	33	≤ 1.7	60	—
co 147165	0.40	21.37	0.05	740	Q: 0.71±.6	120	≤ .37	120	≥ 6.9
ph 149757	0.32	21.15	0.63	120	Q: 3.5±.42 P: 2.3±.42	30	≤ .76	30	≥ 16.4

drogen column densities are from Savage et al. (1977).

nsity of hydrogen nuclei are from CO rotational equilibrium analyses by Snow (1976b, 1977); Smith, Stecher, and Krishna vamy (1978); and Snow and Jenkins (1978).

The ratio N(OH)/N(H$_2$O) given here refers only to the ground rotational state.

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FIGURE CAPTIONS

Figure 1 - Average of 87 scans of the H_2O feature in the spectrum of o Per. The error envelope represents the 2σ uncertainty due to photon statistics. The expected position of the line is indicated.
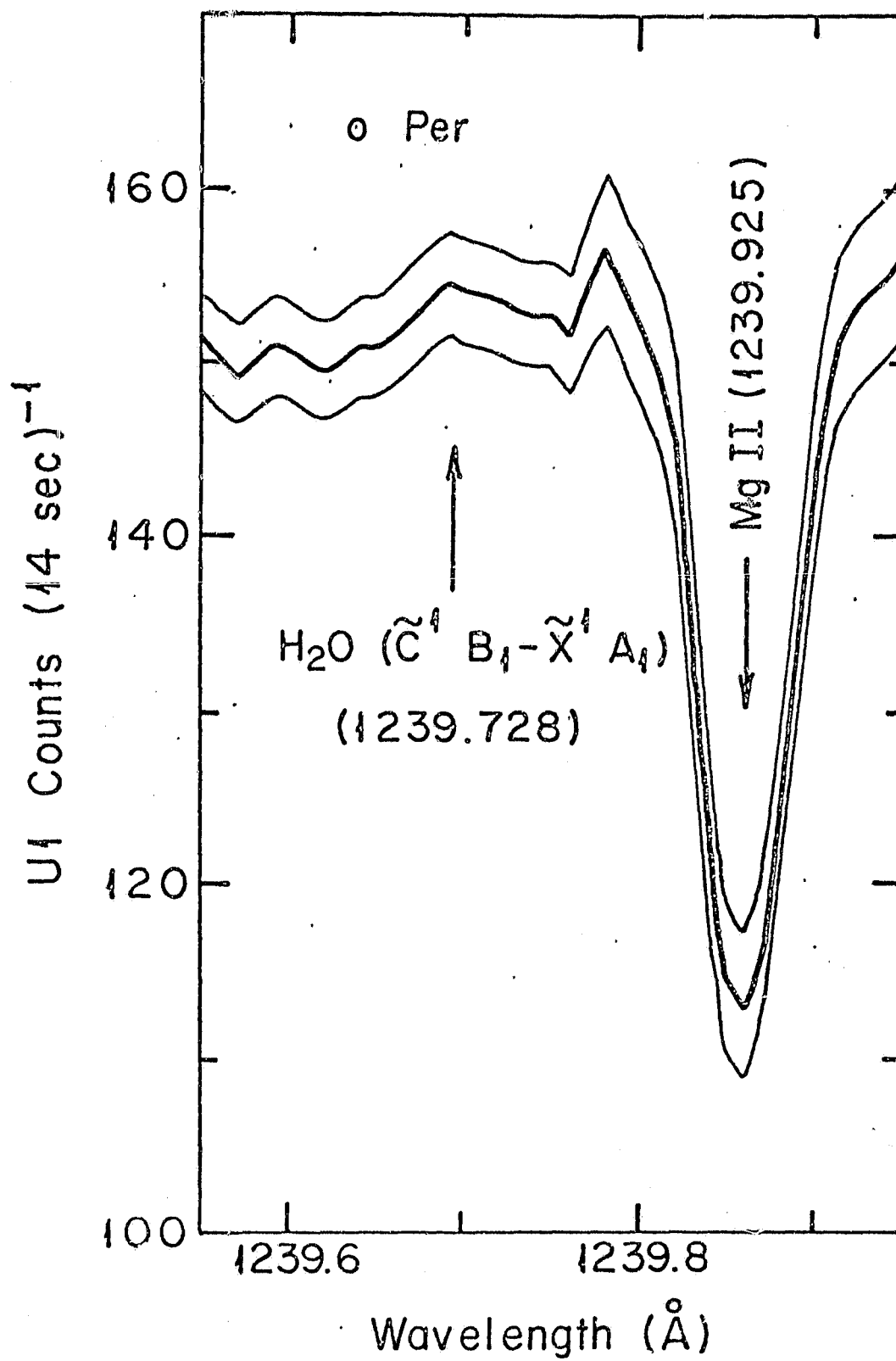
Figure 2 - The averaged OH data on α Cam.
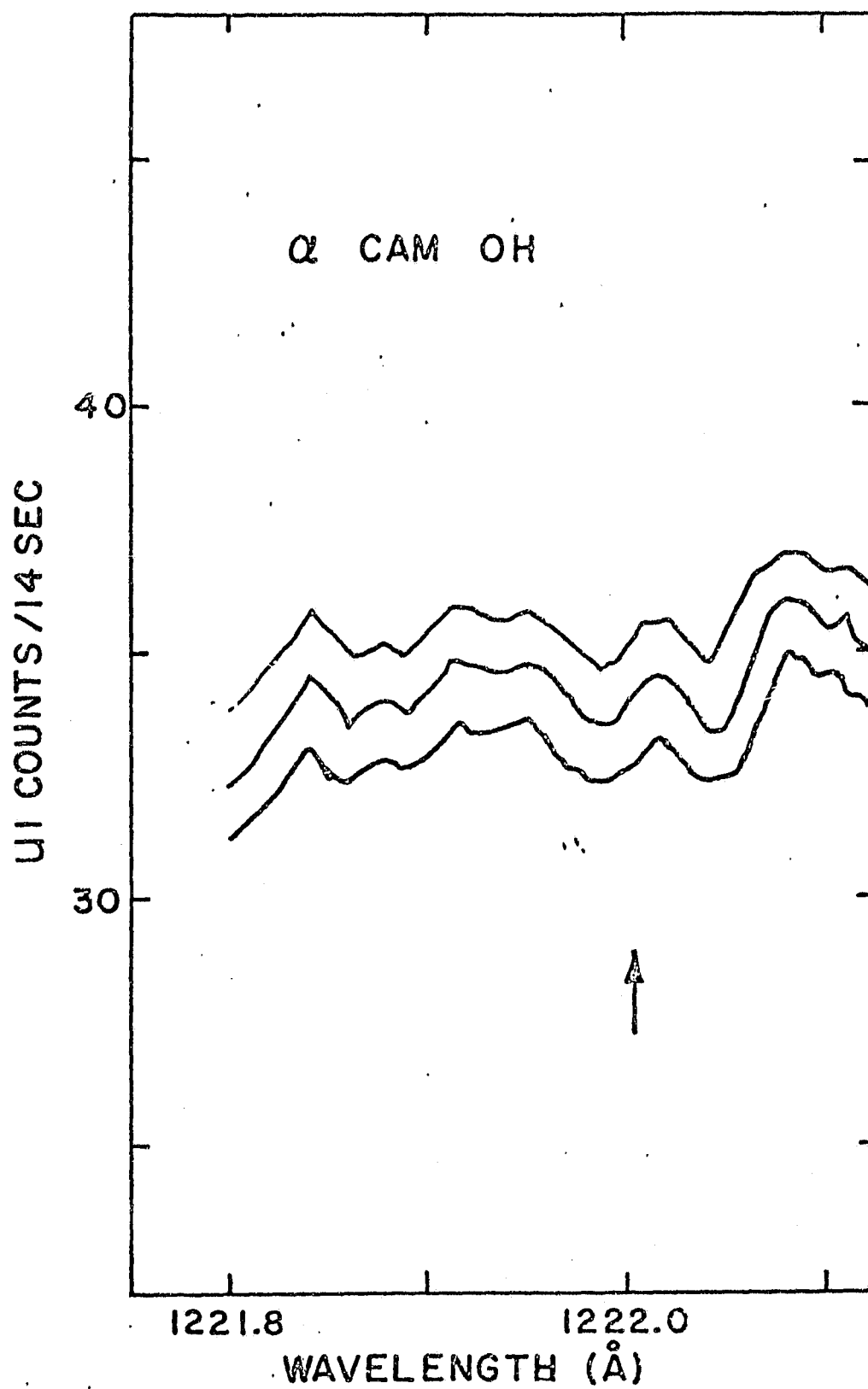
Figure 3 - The averaged H_2O data on α Cam.

Figure 4 - The averaged OH data on σ Sco. The feature is marginally present.
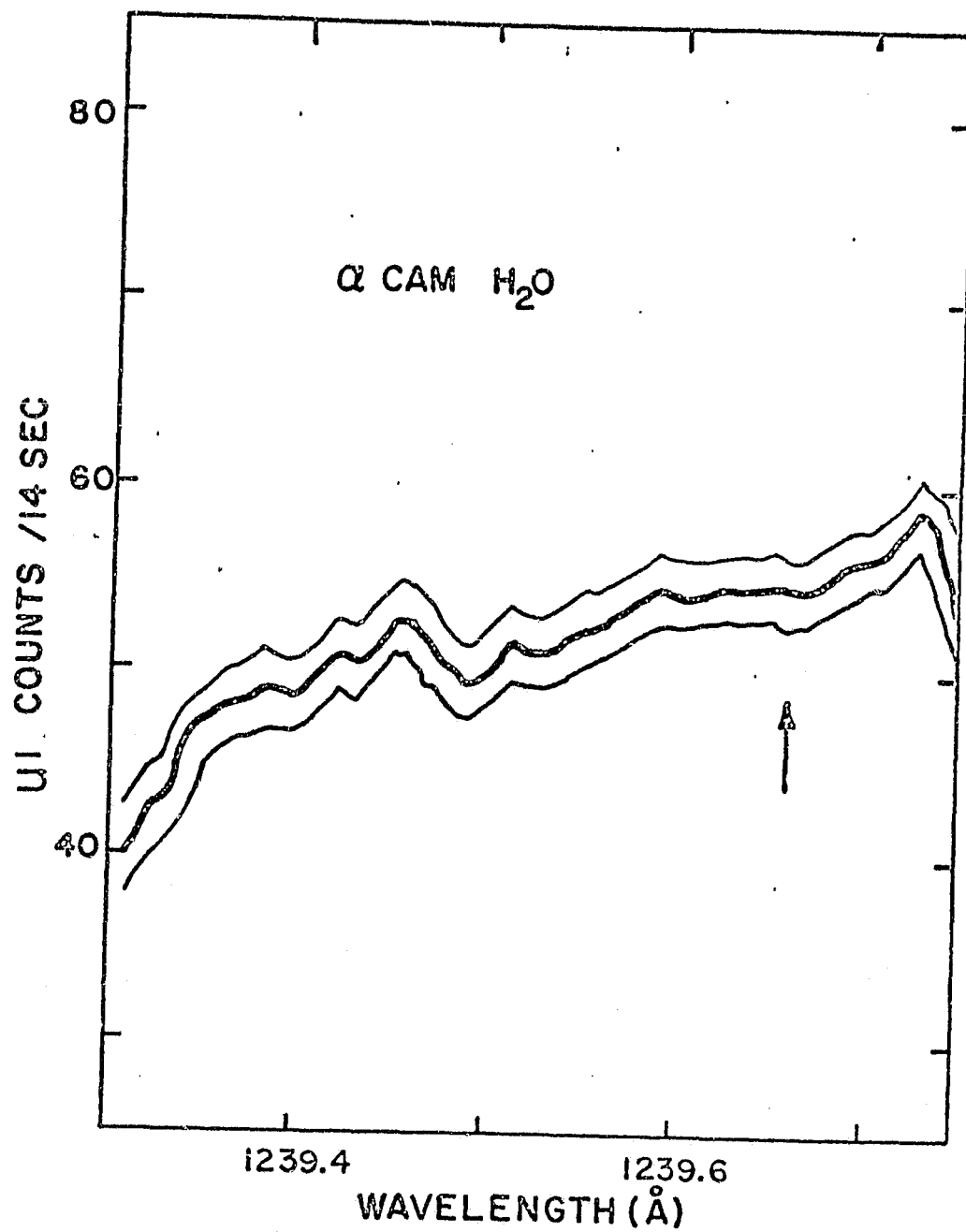
Figure 5 - The averaged H_2O data on σ Sco.

o Per

H_2O $(\tilde{C}^1 B_1 - \tilde{X}^1 A_1)$
(1239.728)

Mg II (1239.925)

α CAM OH

α CAM H_2O

σ SCO OH

σ SCO H₂O