AN INFRARED SEARCH FOR HDO IN COMETS

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ABSTRACT

We searched for HDO emission in our infrared database of six Oort Cloud comets (C/2002 C1 (Ikeya-Zhang), C/2001 A2 (LINEAR), C/2000 WM1 (LINEAR), C/1999 H1 (Lee), C/1999 S4 (LINEAR), and C/1999 T1 (McNaught-Hartley)). Spectral lines of the ν_1 fundamental vibrational band of HDO were sampled using high resolution infrared spectra acquired with both CSHELL at NASA's IRTF and NIRSPEC at the W.M. Keck Observatory. Of these comets, the recent apparition of the bright Comet Ikeya-Zhang, with its high gas production rate and good geocentric Doppler shift, provided an exceptional opportunity to search for minor constituents such as HDO. We report tentative detections of HDO in three Oort Cloud comets with upper limits determined for the remaining three. These data, combined with future observations, will be used to test models of nebular chemistry and delivery of water and organics to the early Earth.

Key words: HDO; comet; infrared.

1. INTRODUCTION

Cometary bodies contain a large percentage of volatile material and are thought to represent the most pristine material in the solar system. However, their composition does not necessarily reflect that of the natal molecular cloud material from which the solar system formed. Infalling material is subject to several processes that can alter the chemical composition. Shocks from infalling gas and dust impacting the dense circumstellar disk material will evaporate ice mantles in regions closer than ∼30 AU (Neufeld & Hollenbach 1994; Chick & Cassen 1997). While in the gas phase, evaporated material may undergo neutral-neutral or ion-molecule reactions before recondensing on the grain surface. Additional grain-surface reactions may also alter natal ice compositions. Turbulence and inward radial migration will transport matter within the nebula. These processes complicate any interpretation of chemical composition and diversity among cometesimals, as the material comprising a single comet may have diverse origins within the protoplanetary nebula. The extent to which these conditions affect the chemistry in the giant-planets region of the solar nebula and hence comet formation is still unknown.

Recent infrared and radio studies of cometary chemistry have shown that comets vary significantly in composition. Hale-Bopp, Hyakutake, and Halley have similar volatile compositions that may indicate formation in the Neptune region of the protoplanetary disk. Since these comets were observed, six other comets have been studied in detail, and the chemical diversity that is expected if comets formed throughout the giant-planet region is becoming evident. Deuterated species should also display variations among the comet population and should be representative of the physical conditions prevalent in the regions from which a cometary nucleus acquired its volatile components.

To date, radio transitions of deuterated species have only been detected in a small number of comets. Even then, only single lines have been detected, giving rise to large uncertainties in production rates. The abundance ratio (HDO/H_2O) was found to be similar in Halley, Hyakutake, and Hale-Bopp (Eberhardt et al. 1995; Bockelée-Morvan et al. 1998; Meier et al. 1998), at about twice that of the standard mean ocean water (SMOW) value of $3{\times}10^{-4}$. This is about an order of magnitude greater than the local interstellar medium D/H value of $1.5{\times}10^{-5}$ and the protosolar D/H ratio of $2.1{\times}10^{-5}$ (Geiss & Gloeckler 1998). HDO/H_2O has also been measured in several regions of massive star formation known as hot cores. These dense, warm regions have a gas phase composition that may be strongly influenced by evaporation of icy grain mantles. These objects usually exhibit HDO/H_2O ratios of $3\text{–}6{\times}10^{-4}$, consistent with or greater than the values reported in comets thus far. A maximum D/H ratio of 0.004–0.01 was reported in Orion IRc2 (Pardo et al. 2001). Such high abundances are probably indicative of fractionated icy material that has evaporated from dust mantles.

In section 2, we discuss the observations and data analysis. Section 3 shows our tentative detections of HDO in three comets, and in section 4 we discuss results and future plans.

Table 1. Observation

Comet	Date (UT)	Instrument	t_{int} (s)	ν_0 (cm^{-1})
IZ	22 Mar 2002	CSHELL	3360	2692.741
		CSHELL	2640	2680.756
A2	09 Jul 2001	NIRSPEC	1680	2753.542
		NIRSPEC	1680	2767.269
A2	10 Jul 2001	NIRSPEC	2280	2753.542
		NIRSPEC	2280	2767.269
WM1	23 Nov 2001	NIRSPEC	3600	2708.172
Lee	19 Aug 1999	NIRSPEC	480	2753.542
		NIRSPEC	480	2708.172
Lee	20 Aug 1999	NIRSPEC	1440	2708.172
S4	12 Jul 1999	NIRSPEC	960	2708.172
McNH	14 Jan 2000	NIRSPEC	1440	2708.172

2. OBSERVATIONS AND DATA ANALYSIS

The data for this study were taken with the echelle spectrometers CSHELL at NASA's IRTF and NIRSPEC at the W.M. Keck Observatory, both located at Mauna Kea, Hawaii. Both instruments are high dispersion cryogenic spectrometers with sensitivity in the 1–5.5 μm spectral region. For the comet observations with CSHELL, a 1-arcsec wide slit was used while a 3 pixel (0.42-arcsec) slit was used at NIRSPEC, allowing the acquisition of high resolution data in both the spectral ($\lambda/\Delta\lambda \sim 25000$) and spatial dimensions. A summary of the observations is given in Table 1. Flux calibration was based on observations of standard stars through a 4-arcsec slit. Observing and reduction procedures are discussed in detail in Dello Russo et al. (1998, 2000, 2001); DiSanti et al. (1999, 2001); Magee-Sauer et al. (1999).

Most of the data used in this study was part of a general study of overall cometary chemistry rather than a targeted search for HDO. Hence, the lines sampled do not always represent the ideal transitions for which to search for HDO. Also, the moderate productivity of most of these comets, coupled with observatory time constraints, often did not allow for sufficient time to perform sensitive searches for HDO. The available data set was searched for HDO transitions and the strongest expected line was used to place the most stringent upper limits possible. Three comets have an emission feature at the expected doppler shifted position of the strongest HDO transition observed. However, we note that other unidentified emission features are present in these spectra (see Figure 1), thus we claim these as tentative detections. In the case of comet A2, the emission feature is present on two dates and gives comparable abundances, lending confidence to the reality of the feature and robustness of the extraction process. When an emission feature is present, upper limits of the HDO abundance are also calculated using the next strongest transition. The upper limits are found to be consistent with the derived abundances.

The 3-sigma upper limits reported in Table 2 are based on the stochastic noise of the data. Our study is biased towards higher D/H ratios but with current technology, it should be possible to push the detection limit to 1 SMOW or less in dedicated searches in future bright comets, particularly with NIRSPEC. This instrument has the added advantage that the larger spectral coverage and higher sensitivity permits simultaneous targeting of multiple lines of HDO as well as other species, including water. This removes many sources of systematic error such as calibration errors, short-term variability, and possible jet activity that are generally difficult to quantify.

3. RESULTS

Of the six comets investigated in this study, we report tentative detections of HDO in three: A2 (LINEAR), Lee, and Ikeya-Zhang. In each case, a different transition was observed. A firm detection of HDO has not been possible as multiple transitions have not been observed in a single comet. However, the derived production rates for the observed transitions are consistent with the 3-sigma upper limits derived from weaker HDO transitions that were not detected (see Table 2). The HDO transitions in Tables 1 and 2 are not coincident with emission features from any other known molecule, though there are many unidentified lines in the infrared spectra of comets so a misidentification of one or more of the observed transitions cannot currently be ruled out.

Production rates (in molecules s^{-1}) are derived by assuming a spherically symmetric outflow at a uniform velocity. With strong lines, a symmetric Q curve is constructed by taking the mean emission intensity to either side of the nucleus measured in 1-arcsec intervals along the spatial direction of the slit. Our Q-curves increase with distance from the nucleus to a terminal value, which we take to be the "global" production rate (Dello Russo et al. 2002; Magee-Sauer et al. 2002; DiSanti et al. 2002). This method was used to derive the water production rates in these comets. A weak line due to a molecule like HDO, however, does not exhibit emission off the nucleus-centered position, and so it is not possible to construct a Q-curve in this manner. We calculate the production rate for HDO on the nucleus-centered position in this case using

$$Q = \frac{4\pi\Delta^2 F_i}{g_i \tau(hc\nu) f(x)} \tag{1}$$

where Δ is the geocentric distance in meters, $hc\nu$ is the energy (J) of a photon with wavenumber ν (cm^{-1}), $f(x)$ is the fraction of molecules expected in the sampled region, and F_i is the flux (W m^{-2}) from line i incident on the terrestrial atmosphere. τ is the photodissociation lifetime (s) and g_i is the line fluorescence efficiency (photons s^{-1} molecule^{-1}), both of which are calculated for a heliocentric distance of 1 AU.

Table 2. Tentative Detections and Upper Limits

Comet	$Q(H_2O)$ (10^{28} mol s^{-1})	HDO transition	ν_0	T_{rot} (K)	Q(HDO) (10^{26} mol s^{-1})	HDO/H_2O (SMOW)
IZ	80–100	2_{12}-3_{13}	2692.741	140	<31	<10–13
		1_{01}-2_{02}	2680.756	140	26(5)	~10(2)
A2 (Jul 09)	5.07	2_{02}-1_{01}	2753.542	70	2.9(1.3)	19(9)
		3_{03}-2_{02}	2767.269	70	<3.0	<20
A2 (Jul 10)	5.07	2_{02}-1_{01}	2753.542	70	0.11(0.06)	14(8)
		3_{03}-2_{02}	2767.269	70	<3.0	<20
WM1	3.05	0_{00}-1_{01}	2708.172	70	<0.11	<7.5
Lee (Aug 19)	12.6	2_{02}-1_{01}	2753.542	70	<13	<35
		0_{00}-1_{01}	2708.172	70	<8.4	<22
Lee (Aug 20)	12.6	0_{00}-1_{01}	2708.172	70	3.3(1.9)	10(5)
S4	6.38	0_{00}-1_{01}	2708.172	50	<1.9	<10
McNH	8	0_{00}-1_{01}	2708.172	70	<11	<44

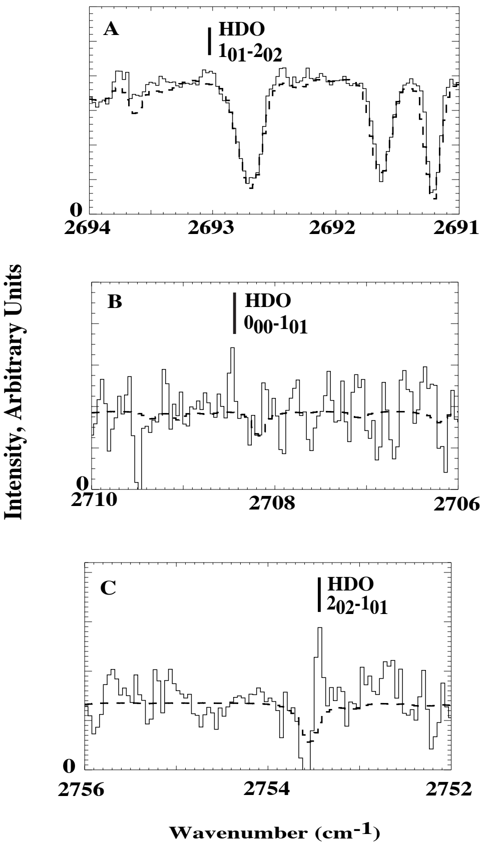

Figure 1. The three spectra showing tentative detections of HDO in A) C/Ikeya-Zhang (2002 C1), B) C/Lee (1999 H1), and C) C/2001 A2 (LINEAR). The dashed line shows the atmospheric model fit. The vertical line shows the doppler shifted position of the expected HDO transition.

To give the global production rate, this value for the nucleus centered production rate is then multiplied by the ratio between the terminal and nucleus centered values for the dust emission in that setting or, if the dust was weak or asymmetric, from a stronger emission feature within the order if such a feature is present. This value is usually around 2–3 for NIRSPEC and 3–4 for CSHELL and is consistent with the ratio determined in other orders. The rotational temperature of HDO was assumed to be the same as that derived from multiple lines of CO (DiSanti et al. 2001), HCN, and in some cases H_2O. These values are consistent with the temperatures determined by other groups (Biver et al. 1999, 2000).

4. DISCUSSION AND FUTURE WORK

Preliminary results of this study suggest that some comets may have HDO abundances greater than the value of about 2 SMOW found in Halley, Hyakutake, and Hale-Bopp (Eberhardt et al. 1995; Bockelée-Morvan et al. 1998; Meier et al. 1998). Though the uncertainties are large, abundances of ~10–15 SMOW are found for the Oort Cloud comets A2, Lee, and Ikeya-Zhang. These high HDO abundances are not unreasonable when compared to measurements of HDO/H_2O gas in hot cores. It is also interesting to note that when Blake et al. (1999) mapped HDO emission in comet Hale-Bopp using the Owens Valley Radio Observtory (OVRO), they found that D/H was enhanced in a jet of material offset from the nucleus. In fact, they estimate that the D/H value in the jet was over 20 times SMOW! This could indicate survival and incorporation of a substantial reservoir of presolar volatile material within comets formed in the outer solar system. Larger beam radio observations would not detect this since the jet material is emitted from a small region and is mixed with material sublimating from the rest of the nucleus.

Further, the work of Aikawa et al. (1999) suggests that cosmic ray ionization in the protoplanetary disk beyond 10 AU, coupled with inward radial migration of material, can lead to HDO/H_2O ratios of $\sim 6\times10^{-4}$ to $\sim 1.5\times10^{-3}$ (2–5 SMOW), depending on the ionization rate and temperature within the disk. However, Aikawa et al. (1999) do not include an initial enrichment in HDO from icy mantles or grain-surface reactions that may further enhance HDO/H_2O. Their ratio increases monotonically with time and increases as the temperature decreases so the maximum ratio may be even higher than 5 SMOW in the outer solar system. According to the Aikawa et al. (1999) model, cosmic rays would not have penetrated the disk material in the Jupiter-Saturn region of the protoplanetary disk, and hence the ion-molecule reactions would not have been efficient, resulting in a lower expected HDO/H_2O ratio. This has not yet been tested as HDO has not been observed in a sufficiently bright comet that is thought to have formed in the inner giant-planet region of the solar system.

All of the comets in which HDO has been detected to date are Oort Cloud objects that probably formed in the outer giant-planet region of the solar nebula. Temperature indications suggest that Hale-Bopp, Hyakutake, and Halley all formed in the Neptune region or beyond at temperatures consistent with ~30 K (Crovisier et al. 1997; Meier et al. 1998; Bockelée-Morvan et al. 1998). It is at these temperatures and distances that HDO is predicted to be enhanced, by either chemistry within the protoplanetary nebula or pre-existing enhancement of presolar material. Since the surface density of the protoplanetary disk declined with distance as $\sim 1/r^{1.5}$ (Weidenschilling & Cuzzi 1993), most of the cometary material formed closer to the Sun, near Jupiter-Saturn. According to dynamical models, Jupiter would likely have gravitationally slung most of this material out of the solar system entirely with anywhere from 15-40% of Oort Cloud objects originating in the Jupiter-Saturn region (Weissman 1999). Hence the Oort Cloud material could under represent Jupiter class objects, which would be expected to have lower D/H ratios (Drouart et al. 1999). Measuring the D/H ratio in water among a variety of comets is vital for testing these models of planet formation and disk chemistry.

The high (2 SMOW) D/H ratio observed in comets has been used in models and calculations to limit the contribution of cometary material, including that of biogenic importance, to the early Earth (Meier et al. 1998). We believe this to be premature as the comets sampled thus far have compositions consistent with low formation temperatures and origins in the outer giant-planet region of the protoplanetary disk. They do not appear to represent the class of comets that formed in the warmer region near Jupiter and Saturn and which may have contributed a greater percentage of material to the early Earth. Further discussion of cometary contribution of water and organics to the early Earth requires a larger sample of bright comets for which the abundances of HDO and other minor volatile constituents can be measured. In particular, it is important to observe comets for which upper limits of 1 SMOW or less can be measured.

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