SUBMILLIMETER SPECTROSCOPY OF INTERSTELLAR HYDRIDES

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ABSTRACT We discuss airborne observations of rotational transitions of various hydride molecules in the interstellar medium, including H$_2^{18}$O and HCl. The detection of these transitions is now feasible with a new, sensitive submillimeter receiver which has been developed for the NASA Kuiper Airborne Observatory (KAO) over the past several years.

INTRODUCTION

Atmospheric water vapor is responsible for the generally poor atmospheric transmission in the submillimeter band (300-3000 GHz). In particular, even for observatories located on dry high-altitude sites such as Mauna Kea, the atmosphere is essentially opaque between 500-600 GHz and 700-800 GHz because of the very strong water lines at 547 GHz and 752 GHz. In addition, ground-based submillimeter observations are impossible above 900 GHz. Nonetheless, these portions of the spectrum are very interesting astronomically because they contain many fundamental rotational transitions of hydride molecules, such as CH at 532 and 536 GHz, H$_2^{18}$O at 547 and 745 GHz, NH$_3$ at 572 GHz, HCl at 626 GHz, CH$_2$ at 945 GHz, and H$_3$O$^+$ at 985 GHz. Observations of these molecules are important for testing our understanding of the chemistry of molecular clouds, since the hydrides are the initial products of the ion-molecule reaction network which is thought to be responsible for the synthesis of more the more complex molecules commonly observed at radio and millimeter wavelengths.

In addition, hydrides may play a crucial role in the energetics of molecular clouds, particularly at the high densities found in star-forming cores, because their large rotational level spacings and large dipole moments make them very effective coolants. In fact, it is possible that cooling due to hydrides, especially H$_2$O, plays a decisive role in establishing the rate at which molecular clouds collapse, and thus ultimately controls the efficiency of star formation.

The Kuiper Airborne Observatory (KAO) is the only platform at present which allows observations of the transitions listed above (with perhaps the
exception of HCl, which can be observed from Mauna Kea in extremely good weather). Although some of these molecules can also be observed through transitions at radio wavelengths, airborne observations of the fundamental rotational transitions can often give essential information regarding the abundance and excitation of these species.

In this paper, we discuss studies of interstellar H$_2^{18}$O and HCl we have been pursuing over the past two years. We have also detected the CH transitions at 532 and 536 GHz in Orion, W51, M17, and other sources, but these observations will not be discussed in this paper due to the limited space. The observations which we present were obtained with a new submillimeter heterodyne receiver developed for the KAO, which at present operates over the 500-750 GHz band, which is described in a paper elsewhere in this volume (Zmuidzinas et al. 1994b).

Figure 1. Solid line: detection of the 626 GHz HCl line in absorption toward Sgr B2. Dashed line: spectrum predicted by our radiative transfer model for a fractional abundance of HCl/H$_2 = 1.1 \times 10^{-9}$.

HCl IN ABSORPTION IN SGR B2

The abundance of atomic chlorine in diffuse interstellar clouds has been studied using ultraviolet absorption lines by Jura & York (1978), Harris & Bromage (1984), and Harris, Gry, and Bromage (1984). These studies have shown that the depletion of chlorine (on dust grains) in diffuse clouds is not severe, with
abundances at most a factor of 2-3 below the solar value of Cl/H ≈ 2 × 10⁻⁷ (Anders & Grevesse 1989), although there is some indication that the depletion increases with density. It would be very interesting to study the depletion in denser regions; however, ultraviolet studies of dense clouds are obviously impossible. The submillimeter rotational transitions of HCl may be a useful probe of the chlorine depletion in dense molecular clouds, since gas-phase chemical models predict that a substantial fraction (> 10%) of chlorine will be in the form of HCl (Jura 1974; Dalgarno et al. 1974; Blake, Anicich, & Huntress 1986; Schilke, Phillips, & Wang 1994).

The 626 GHz J = 1 → 0 line was first detected in OMC-1 from the KAO by Blake, Keene, and Phillips (1985). The observed emission line (T_A ~ 0.7 K) was interpreted to give HCl/H_2 ~ 0.5 - 5.0 × 10⁻⁸, which corresponds to a probable range of chlorine depletion of 3-30 (below solar). The lower end of this range could be consistent with the chlorine depletion in diffuse clouds, but Neufeld and Green (1994) have recently reanalyzed this data using improved collisional excitation rates and a more detailed radiative transfer model, and argue that in fact the abundance may be only 2 × 10⁻⁹. Hence, it is likely that chlorine is either heavily depleted or the fraction of chlorine in HCl is much smaller than the predictions of the chemical models.

During a June 1993 KAO deployment to Hickam AFB in Honolulu, HI, we detected the 626 GHz line in absorption against the submillimeter continuum from the Sgr B2 (N) and (M) dust cores (Figure 1). It is not entirely surprising that the line is in absorption, given the fact that this is a ground-state transition which has a very large critical density of n_{cr} = 4 × 10⁷ cm⁻³. Furthermore, Sgr B2 has an extended envelope of moderate density, relatively cool molecular gas which could produce the absorption. However, Sgr B2 is also known to have very massive, dense, and hot cores, which might have been expected to produce an emission line instead.

To clarify the situation, we created a detailed radiative transfer model. The model assumes a spherical cloud whose density and temperature (dust and gas) vary with radius as

\[ n(r) = 2.2 \times 10^3 + 8.6 \times 10^4 \left( \frac{r}{1 \text{ pc}} \right)^{-2} \text{ cm}^{-3} \]

and

\[ T(r) = 40 \left( \frac{r}{1 \text{ pc}} \right)^{-0.5} \text{ K}. \]

This simple cloud model is based on the work of Lis, Goldsmith and collaborators, and is consistent with a map of C^{18}O(1 - 0) (Lis & Goldsmith 1989) and with a large variety of dust continuum observations ranging from 4'' OVRO interferometer measurements at \( \lambda = 1.3 \text{ mm} \) to the continuum intensity we observe in our 2' KAO beam at \( \lambda = 479 \mu \text{m} \) (Zmuidzinas et al. 1994a). Our radiative transfer program subdivides this model cloud into 200 radial shells, and self-consistently solves for the level populations and radiation intensities in each shell using an accelerated lambda-iteration method (Rybicki & Hummer 1991). This model treats collisional and radiative excitation of the molecular levels up to \( J = 11 \), and includes emission and absorption of radiation by both molecules and dust.
The model is successful in predicting our observed absorption line (Figure 1). The abundance needed to obtain the measured line to continuum ratio is HCl/H$_2$ $\approx 1.1 \times 10^{-9}$; hence, it appears that the chlorine is depleted by a factor of 50-180 below the solar abundance, if in fact HCl represents 10-30% of the gas-phase chlorine as predicted by the chemical models. This conclusion is fairly robust, since the same HCl fractional abundance can be obtained by comparing an HCl column density of $1.6 \times 10^{14}$ cm$^{-2}$ derived from the integrated optical depth (determined from the line to continuum ratio), to an H$_2$ column density of $1.5 \times 10^{23}$ cm$^{-2}$ for the absorbing envelope (determined from the C$^{18}$O map of Lis & Goldsmith 1989). The radiative transfer model verifies that the assumptions inherent in this simple calculation are correct, and that the absorption line is indeed formed in the cool, presumably quiescent outer layers of the cloud, corresponding to $r > 5$ pc, $n \sim 6 \times 10^3$ cm$^{-3}$, and $T_{\text{dust}} \sim 20$ K. An interesting prediction of our model is that dust continuum radiation dominates the excitation of the rotational levels of HCl throughout the cloud; this is quite plausible since Sgr B2 is a very bright continuum source and since the critical density of the 626 GHz transition is very large, $n_{\text{cr}} = 4 \times 10^7$ cm$^{-3}$.

![Figure 2](image_url)

**Figure 2.** The 547 GHz H$_2^{18}$O transition detected in absorption in Sgr B2. The dashed line is the prediction of a simple model consisting of a background continuum source ($T_A^* \approx 0.7$ K) and a foreground cloud with two velocity components. The minimum H$_2^{18}$O column density capable of producing this absorption is about $1.1 \times 10^{14}$ cm$^{-2}$.
Oxygen is the third most abundant element, and yet surprisingly little is understood about the chemistry of oxygen in molecular clouds. Potentially abundant oxygen-bearing species include O, O₂, and H₂O, but ground-based observations of these species are obviously difficult. Although the 22 GHz H₂O masers are very well known, the energy levels of the 6₁₆ → 5₂₃ transition lie about 640 K above the ground state. In fact, this is why the 22 GHz transition is observable from the ground, and partially explains why the masers are thought to arise from very dense and hot clumps of gas rather than the more ordinary regions of molecular clouds. If it is abundant, water may also be the major coolant of dense star-forming regions, since the water molecule has a strong asymmetric rotor spectrum with transitions throughout the submillimeter and far-infrared.

**Figure 3.** Detection of the 1₁₀ – 1₀₁ 547 GHz ground-state transition of ortho-H₂¹⁸O in Orion-KL.

To probe the abundance of water in a more general way, one must observe lower lying transitions which are more likely to be populated under the typical conditions found in interstellar clouds. However, absorption by atmospheric H₂O precludes this approach, unless one takes advantage of the fact that the lines of H₂¹⁸O are slightly shifted in frequency due to the somewhat larger moments of inertia. However, the isotopic ratio is ¹⁶O/¹⁸O ≈ 500, so the H₂¹⁸O lines are weak. Nonetheless, we have recently detected the 547 GHz ground-state transition and the 745 GHz transition (E_lower ≈ 100 K) in Orion-KL using our SIS receiver on
the KAO. We have also detected the 547 GHz line in absorption toward Sgr B2. Using the Caltech Submillimeter Observatory (CSO), we have followed up the airborne observations with detections of the 391 GHz transition ($E_{\text{lower}} \approx 300 \, K$) in Orion-KL, Sgr B2, and several other sources as well.

The 547 GHz H$_2^{18}$O absorption line in Sgr B2 is shown in Figure 2. This detection can be analyzed in the same manner as the HCl absorption line, since the critical densities and $A$-coefficients of these two ground-state transitions are similar. The integrated optical depth determined from the line to continuum ratio implies a minimum H$_2^{18}$O column density of $1.1 \times 10^{14}$ cm$^{-2}$. As in the case of HCl, we suspect that this is the actual column density in the low excitation molecular envelope that we are sampling. Thus, we arrive at a fractional abundance of H$_2^{18}$O/H$_2 \approx 7 \times 10^{-10}$, again taking the relevant H$_2$ column density to be $1.5 \times 10^{23}$ cm$^{-2}$ for the absorbing envelope. Since the isotopic ratio near the center of the galaxy is thought to be $^{16}$O/$^{18}$O $\approx 250$, we obtain H$_2$O/H$_2 \approx 1.7 \times 10^{-7}$. This value is low, but within the range predicted by current chemical models.

**Figure 4.** Detection of the $2_{11} - 2_{02}$ 745 GHz transition of para-H$_2^{18}$O in Orion-KL. The energy of the lower level in this transition is about 100 K.

H$_2^{18}$O may have previously been detected in Orion-KL through the 203 GHz and 321 GHz transitions using ground-based telescopes. However, these observations are badly confused by strong nearby SO$_2$ lines which hampers their interpretation. As Figures 3 and 4 show, we have unambiguously detected the 547 and 745 GHz lines from the KAO. In addition, we have obtained a solid
detection of the 391 GHz line from the CSO. All of these H$_2^{18}$O observations of Orion-KL are summarized in the table below.

**H$_2^{18}$O LINES DETECTED IN OMC-1**

<table>
<thead>
<tr>
<th>Telescope</th>
<th>$\nu$ (GHz)</th>
<th>Line</th>
<th>$E_{\text{lower}}$ (K)</th>
<th>$\theta_{\text{beam}}$ (arcsec)</th>
<th>$T^*_A$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NRAO $^a$</td>
<td>203</td>
<td>$3_{13} \rightarrow 2_{20}$</td>
<td>194</td>
<td>30</td>
<td>0.9</td>
</tr>
<tr>
<td>CSO $^b$</td>
<td>322</td>
<td>$5_{15} \rightarrow 4_{22}$</td>
<td>452</td>
<td>20</td>
<td>0.6</td>
</tr>
<tr>
<td>CSO $^c$</td>
<td>391</td>
<td>$4_{14} \rightarrow 3_{21}$</td>
<td>303</td>
<td>17</td>
<td>2.5</td>
</tr>
<tr>
<td>KAO $^c$</td>
<td>547</td>
<td>$1_{10} \rightarrow 1_{01}$</td>
<td>0</td>
<td>150</td>
<td>0.55</td>
</tr>
<tr>
<td>KAO $^c$</td>
<td>745</td>
<td>$2_{11} \rightarrow 2_{02}$</td>
<td>101</td>
<td>110</td>
<td>0.65</td>
</tr>
</tbody>
</table>

$^a$ Jacq et al. 1988; blended with SO$_2$ 120,12 $\rightarrow$ 111,11.

$^b$ Menten et al. 1990; blended with SO$_2$ 344,30 $\rightarrow$ 335,29.

$^c$ Zmuidzinas et al. 1994.

We have attempted a simple rotation diagram analysis of these lines, which yields H$_2$O abundances in the 10$^{-7}$ range, but the large variation in beamwidths makes the results fairly sensitive to the assumed source size. In addition, the 547 GHz line appears to be weaker than what one would extrapolate from the higher-lying transitions, and furthermore, the line profile of the 547 GHz transition does not seem to be consistent with either the 745 or 391 GHz profiles. Thus, we speculate that there may be foreground lower excitation gas which partially absorbs the 547 GHz radiation and distorts the line shape. We hope to learn more about the spatial distribution of H$_2^{18}$O by mapping the 391 GHz transition at the CSO, and perhaps by mapping the 203 GHz transition with the OVRO interferometer. This could give us the source size and therefore reduce the ambiguity in the rotation diagram analysis. In addition, these maps might tell us whether the “hot core” or “low-velocity outflow” component is primarily responsible for the H$_2^{18}$O emission, and therefore whether evaporation from radiatively heated dust grains or shock chemistry is leading to a substantial enhancement of the H$_2^{18}$O abundance. We have some hint of the answer from the linewidths of the H$_2^{18}$O transitions that we observe, which seem to be more consistent with the “low-velocity outflow” source than with the “hot core”, but the inconsistency in the observed line profiles points to several emission (or absorption) components.

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