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DISCOVERY OF INTERSTELLAR HYDROGEN FLUORIDE[1]

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ABSTRACT

We report the first detection of interstellar hydrogen fluoride. Using the Long Wavelength Spectrometer of the *Infrared Space Observatory* (*ISO*), we have detected the 121.6973 μm $J = 2–1$ line of HF in absorption toward the far-infrared continuum source Sagittarius B2. The detection is statistically significant at the 13 σ level. On the basis of our model for the excitation of HF in Sgr B2, the observed line equivalent width of 1.0 nm implies a hydrogen fluoride abundance of $\sim 3 \times 10^{-10}$ relative to H_2. If the elemental abundance of fluorine in Sgr B2 is the same as that in the solar system, then HF accounts for ~2% of the total number of fluorine nuclei. We expect hydrogen fluoride to be the dominant reservoir of gas-phase fluorine in Sgr B2, because it is formed rapidly in exothermic reactions of atomic fluorine with either water or molecular hydrogen; thus, the measured HF abundance suggests a substantial depletion of fluorine onto dust grains. Similar conclusions regarding depletion have previously been reached for the case of chlorine in dense interstellar clouds. We also find evidence at a lower level of statistical significance (~5 σ) for an emission feature at the expected position of the $4_{32}–4_{23}$ 121.7219 μm line of water. The emission-line equivalent width of 0.5 nm for the water feature is consistent with the water abundance of 5×10^{-6} relative to H_2 that has been inferred previously from observations of the hot core of Sgr B2.

Subject headings: infrared: ISM: lines and bands — ISM: individual (Sagittarius B2) — ISM: abundances — ISM: molecules — molecular processes

1. INTRODUCTION

Molecules are a ubiquitous component of the dense interstellar medium (ISM). To date, about 100 distinct species have been detected in the interstellar gas (Ohishi 1997); they range from simple diatomic molecules to complex species containing as many as 13 atoms. The wide variety of interstellar molecules demonstrates the thermodynamic tendency of most elements to form molecules under the conditions present in the dense interstellar medium. Although most of the interstellar molecules that have been detected previously contain elements[5] of cosmic abundance greater than 10^{-5}, a few molecules containing elements of lower abundance have also been detected. For example, chlorine, with a solar system abundance of only 2×10^{-7} relative to hydrogen (Anders & Grevesse 1989), was detected more than a decade ago in the form of hydrogen chloride (Blake, Keene, & Phillips 1985).

Recent estimates (Neufeld & Green 1994; Schilke, Phillips, & Wang 1995; Zmuidzinas et al. 1995a) of the HCl abundances implied by observations of the HCl $J = 1–0$ line toward Sgr B2 (Zmuidzinas et al. 1995a) and the Orion molecular cloud 1 (OMC-1; Blake et al. 1985; Schilke et al. 1995) have yielded results for $n(\mathrm{HCl})/n(\mathrm{H_2})$ in the range $(0.3–2) \times 10^{-9}$. If the elemental abundance of chlorine in these sources is the same as that in the solar system, then HCl accounts for only 0.1%–0.7% of the total number of chlorine nuclei. Theoretical models for the chemistry of chlorine-bearing molecules (Schilke et al. 1995) predict that HCl will account for ~30% of gas-phase chlorine. Thus, the observed abundance of HCl can be understood only if the chlorine depletion in the dense ISM is large. The required depletion factors of $\gtrsim 10^2$ greatly exceed the values inferred for the *diffuse* ISM from UV absorption-line studies (e.g., Harris, Gry, & Bromage 1984).

Prior to the observations reported in this Letter, HCl was the only known interstellar molecule containing a halogen element.[6] Motivated by the earlier observations of HCl, by the fact that the solar system abundance of fluorine lies only a factor of 6 below that of chlorine (Anders & Grevesse 1989), and by the large H–F bond strength that suggests that hydrogen fluoride is likely to be a major reservoir of gas-phase fluorine, we have undertaken a search for interstellar hydrogen fluoride toward the strong far-infrared continuum source Sgr B2. Such a search would provide a unique probe of the chemistry of interstellar fluorine and of the fluorine depletion in the dense interstellar medium. Because of its large rotational constant—the largest of any diatomic molecule other than molecular hydrogen or $\mathrm{HeH^+}$—HF possesses a rotational spectrum that lies entirely shortward of the atmospheric windows within which most molecules show a rotational spectrum. Observations of HF rotational transitions are therefore possible only from airborne or space-based observatories. We have made use of the Long Wavelength Spectrometer (LWS; Clegg et al. 1996) on board the *Infrared Space Observatory* (*ISO*; Kessler et al. 1996) to search for hydrogen fluoride. The $J = 1–0$ transition of HF lies longward of the wavelength range to which the photoconductive detectors used in LWS are sensitive, so we have carried out observations of the $J = 2–1$ line at 121.6973 μm. These observations are described in § 2 below. Our results are presented in § 3 and discussed in § 4. The detection of hydrogen fluoride reported here marks the first discovery of

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[5] Viz., hydrogen, oxygen, carbon, nitrogen, sulphur, and silicon.

[6] Note, however, that NaCl, KCl, AlCl, and AlF have been detected in the circumstellar envelope of IRC +10216 (Cernicharo & Guélin 1987; Ziurys, Apponi, & Phillips 1994) and that HF lines have been widely observed in the spectra of cool stars (e.g., Jorissen, Smith, & Lambert 1992).

an interstellar molecule containing the element fluorine and the first time that a new astrophysical molecule has been identified by means of observations in the far-infrared (30–300 μm) spectral region.

2. OBSERVATIONS AND DATA REDUCTION

Using the LWS of *ISO* in Fabry-Perot mode at a resolving power $\lambda/\Delta\lambda$ of 9600, we observed the $J = 2$–1 line of HF toward the source Sgr B2 on 1997 March 28. The rest frequency of the line is 2463428.11 ± 0.21 MHz (Nolt et al. 1987), which corresponds to a vacuum wavelength of 121.6973 μm. Unlike HCl, HF shows no electric quadrupole moment, and the magnetic hyperfine splitting is far smaller than the intrinsic width of any astrophysical absorption line. The *ISO* beam, with an approximate diameter of 70″ FWHM, was centered midway between Sgr B2(M) and Sgr B2(N), at coordinates $\alpha = 17^{\rm h}47^{\rm m}20\overset{\rm s}{.}0$, $\delta = -28^\circ22'41\overset{''}{.}3$ (J2000). The observation, which covered the wavelength range 121.63–121.80 μm, was carried out in fast scanning mode with eight spectral samples per resolution element. The total integration time was 2549 s.

The initial data reduction was carried out with version 6.1 of the *ISO* pipeline software. The ISAP software package was then used to remove bad data points, to co-add the individual spectral scans, and to derive estimates of the likely statistical error for each flux measurement from the variance of the individual scans. The resultant spectrum showed a continuum flux level that varied by ~13% over the narrow wavelength range covered. This behavior, which has been widely observed in LWS Fabry-Perot spectra, is caused by the grating that is used as an order sorter for the Fabry-Perot etalon. Because of errors in the grating setting, the grating wavelength is sometimes offset slightly from the central wavelength of the Fabry-Perot scan, thereby superposing an asymmetric envelope on the measured spectrum and compromising the absolute flux calibration. That envelope was fitted with a second-order polynomial, and the absolute flux calibration was obtained from a spectrum taken in the grating mode of LWS immediately after the Fabry-Perot scan.

3. RESULTS

Figure 1 shows the LWS spectrum observed toward Sgr B2, normalized with respect to the measured continuum flux of 4.8×10^4 Jy. We used a χ^2 analysis to fit the observed spectrum and assess the statistical significance of lines that we detected. Our analysis makes the implicit assumption that the errors in the fluxes measured at each spectral point are Gaussian and independent. We approximated the spectral response function of the Fabry-Perot instrument as a Lorentzian with a width corresponding to the nominal resolving power $\lambda/\Delta\lambda$ of 9600 (Trams, Clegg, & Swinyard 1996), and we assumed that the astrophysical absorption feature was narrow compared to the instrumental profile, as suggested by the intrinsic line widths measured for HCl (Zmuidzinas et al. 1995a).

Fitting a single absorption feature to the spectrum, and with a quadratic fit to continuum as described in § 2 above, we obtained an absorption-line equivalent width of 1.0 nm and a central LSR velocity of 67 km s^{-1} for the 121.6973 μm HF line. The measured LSR velocity is in excellent agreement with the centroid velocity observed by Zmuidzinas et al. (1995a) for the HCl $J = 1$–0 line in Sgr B2. Our detection of an absorption feature is statistically significant at the 13 σ level.

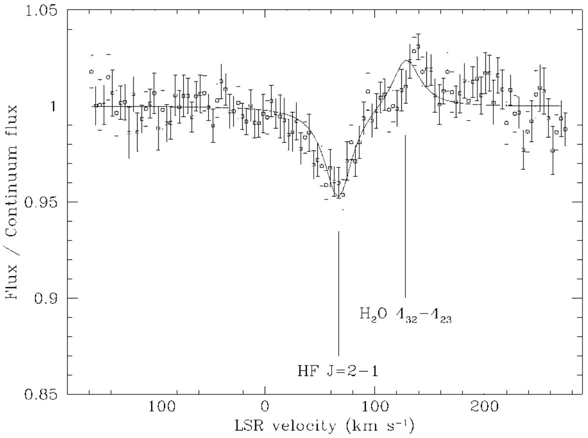

FIG. 1.—*ISO* LWS Fabry-Perot spectrum of the HF $J = 2$–1 line toward Sgr B2. The *ISO* beam, with an approximate diameter of 70″ FWHM, was centered midway between Sgr B2(M) and Sgr B2(N), at coordinates $\alpha = 17^{\rm h}47^{\rm m}20\overset{\rm s}{.}0$, $\delta = -28^\circ22'41\overset{''}{.}3$ (J2000). The flux has been normalized relative to the continuum flux of 4.8×10^4 Jy. The LSR velocity plotted on the horizontal axis applies to the HF $J = 2$–1 line at 121.6973 μm (rest wavelength). The solid line shows the fit obtained from the fitting procedure described in the text. The location of the $H_2^{16}O$ 4_{32}–4_{23} line in that fit is shown for the case $v_{\rm LSR} = 67$ km s^{-1}.

In addition to the absorption feature that we attribute to HF, we find evidence at a lower level of statistical significance (~5 σ) for an emission feature near the expected position (for $v_{\rm LSR} = 67$ km s^{-1}) of the 4_{32}–4_{23} line of water, which has a rest wavelength of 121.7219 μm (Toth 1991). The emission-line equivalent width is 0.5 nm. With the water emission line included in the fit, the reduced χ^2 is 0.98 (with 108 degrees of freedom).

4. DISCUSSION

Our identification of the absorption feature in Figure 1 with HF $J = 2$–1 is based on (1) the excellent agreement of the observed line position with the expected position of the HF line and (2) the absence of any other astrophysically plausible candidate in available line catalogs. Notwithstanding these considerations, the detection of additional HF lines would be desirable as a confirmation of this identification. Unfortunately, according to the excitation model discussed below, we do not expect absorption lines higher than $J = 2$–1 to be strong enough to be detected by the *ISO* spectrometers. Furthermore, the $J = 1$–0 transition near 243.2 μm lies longward of the spectral region that is observable with the photoconductive detectors used in LWS. Fortunately, the Earth's atmosphere permits observations of HF $J = 1$–0 from airplane altitude: that line, with a large predicted equivalent width of ~18 nm, will therefore be a prime target for observations with instrumentation for longer wavelengths that has been proposed for the Stratospheric Observatory of Infrared Astronomy (SOFIA). Observations of HF $J = 1$–0 will also be possible with instrumentation proposed for the Far Infrared and Submillimetre Telescope (FIRST).

In deriving a hydrogen fluoride abundance from the observed equivalent width of the $J = 2$–1 line, we have made use of an excitation model to determine the fractional level populations as a function of position in the source. Our model is essentially identical to that used by Zmuidzinas et al. (1995a) to model the excitation of HCl in Sgr B2. The temperature and H_2 density in the source are assumed to vary with the radial coordinate

$r = r_{pc}$ pc according to

$$T = 40 r_{pc}^{-1/2}\ \mathrm{K},$$

$$n(\mathrm{H_2})/\mathrm{cm^{-3}} = 8.6 \times 10^4 r_{pc}^{-2} + 2.2 \times 10^3.$$

For an assumed dust opacity that varies with wavelength as $\lambda^{-1.5}$, these temperature and density profiles yield a predicted dust continuum spectrum that is in excellent agreement with the observations. Because of the large dipole moment (1.826 D; Muenter 1972) and large rotational constant (20.54 $\mathrm{cm^{-1}}$) of the HF molecule, the critical density at which collisional processes become important in the excitation of HF $J = 1$ is very much larger ($\sim 10^9$ $\mathrm{cm^{-3}}$) than the density of the gas [$n(\mathrm{H_2}) \sim 10^5$ $\mathrm{cm^{-3}}$] that we sampled in our observations of Sgr B2. Thus, the excitation of HF is dominated by the effects of radiative pumping by dust continuum radiation. The radiative transfer was treated with the method of accelerated lambda iteration (Rybicki & Hummer 1991), and the line equivalent width was obtained as a function of the HF abundance. In the absence of available collisional data for HF, we adopted as the rate coefficients for collisional de-excitation those computed previously for the de-excitation of HCl by He (Neufeld & Green 1994); fortunately, because radiative pumping dominates the excitation of HF in Sgr B2, our results are almost entirely independent of the assumed collisional rate coefficients. On the basis of this model, we found that the observed equivalent width of 1.0 nm corresponds to an abundance $n(\mathrm{HF})/n(\mathrm{H_2}) \sim 3 \times 10^{-10}$. The predicted equivalent width shows a nearly linear dependence on the assumed HF abundance (equivalent width $\propto$ abundance$^{0.85}$) for abundances in the range (1–6) $\times 10^{-10}$. Figure 2 shows the fractional level populations in $J = 0$, 1, 2, and 3 as a function of radial coordinate for a hydrogen fluoride abundance of 3×10^{-10}. Observations of the $J = 2$–1 absorption line sample the region exterior to an effective photosphere at $r_{pc} \sim 0.6$.

We also modeled the excitation of the $\mathrm{H_2O}$ 4_{32}–4_{23} line that is evident in the spectrum at a lower level of statistical significance. For the case of water, an excitation model had previously been developed to account for the observed strengths (Zmuidzinas 1995b; Gensheimer, Mauersberger, & Wilson 1996) of the 4_{14}–3_{21} and 3_{13}–2_{02} emission lines of $\mathrm{H_2^{18}O}$ and the 1_{10}–1_{01} absorption line of $\mathrm{H_2^{18}O}$ toward Sgr B2. The temperature and $\mathrm{H_2}$ density profiles assumed in that model were identical to those adopted for the HF and HCl excitation models. To fit the measured fluxes of all three lines, a variable water abundance must be assumed, with a smaller water abundance of $n(\mathrm{H_2^{16}O})/n(\mathrm{H_2}) = 3.3 \times 10^{-7}$ in the cooler outer parts of the source ($T < 90$ K; $r_{pc} > 0.2$) and a larger water abundance of 5×10^{-6} in the warmer inner regions (i.e., the "hot core" with $T \geq 90$ K; $r_{pc} < 0.2$). A variation in the water abundance of this nature could be explained by the vaporization of water ice from grain mantles in the warmer parts of the source. Water abundances $\gtrsim 10^{-5}$ have previously been inferred from observations of $\mathrm{H_2^{18}O}$ and $\mathrm{H_2^{16}O}$ in other warm dense molecular regions (Jacq et al. 1988; Cernicharo et al. 1994; Gensheimer et al. 1996; van Dishoeck & Helmich 1996). Without the adjustment of any model parameter, our excitation model for water predicts that the 4_{32}–4_{23} line of $\mathrm{H_2^{16}O}$—which is excited primarily in the hot core where the assumed water abundance is 5×10^{-6}—will be an emission line with an equivalent width of 0.4 nm, in good agreement with the observations.

To interpret our detection of HF, we have constructed a simple model for the steady state chemistry of interstellar fluorine.

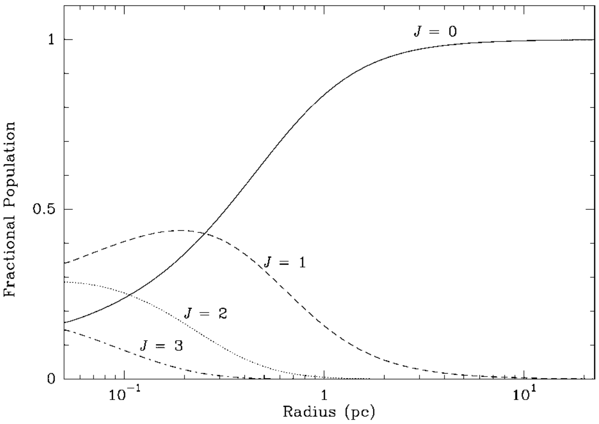

FIG. 2.—Fractional level populations for rotational states of HF, as a function of radius, obtained with the excitation model described in the text.

Fluorine is qualitatively different in at least one important respect from all the other elements of which hydrides have been detected in the interstellar medium:[7] atomic fluorine reacts exothermically with $\mathrm{H_2}$ via the reaction

$$\mathrm{H_2 + F \rightarrow HF + H}. \tag{1}$$

Fluorine also undergoes an exothermic reaction with water:

$$\mathrm{H_2O + F \rightarrow HF + OH}. \tag{2}$$

Both reactions have been well studied in the laboratory, although only at temperatures greater than 200 K. For reaction (1), measurements by three independent groups have yielded results for the rate coefficient at 298 K in the narrow range $(2.3-3.0) \times 10^{-11}$ $\mathrm{cm^3\ s^{-1}}$ (Wurzberg & Houston 1980; Heidner et al. 1980; Stevens, Brune, & Anderson 1989). The temperature dependence of the measured rate coefficient implied the presence of a relatively small activation energy barrier that was variously estimated as $E_a/k = 595 \pm 50$, 433 ± 50, and 470 ± 30 K in these three studies. We adopted Atkinson et al.'s (1992) review value of $k_{\mathrm{H2}} = 1.4 \times 10^{-10} \exp(-500\ \mathrm{K}/T)$ $\mathrm{cm^3\ s^{-1}}$ for the rate coefficient for reaction (1). For reaction (2), Stevens et al. (1989) obtained a rate coefficient $k_{\mathrm{H2O}} = (1.6 \pm 0.3) \times 10^{-11}$ $\mathrm{cm^3\ s^{-1}}$ with no detectable variation over the temperature range 240–373 K; the implied limit on any activation energy barrier was -28 ± 42 K. For a water abundance of 3.3×10^{-7}, these rate coefficients imply that reaction (1) dominates the formation of HF at temperatures $\gtrsim 30$ K. At the $\mathrm{H_2}$ densities present in Sgr B2, both reactions are expected to dominate ion-neutral reaction networks as a source of HF.

Once formed, HF is destroyed only very slowly. HF is more strongly bound than any of the species CF, CH, OF, OH, NF, NH, SF, SH, $\mathrm{SF^+}$, SiF, SiH, or $\mathrm{SiF^+}$: thus, reactions of HF with C, O, N, S, $\mathrm{S^+}$, Si, and $\mathrm{Si^+}$ are all endothermic. HF has a smaller proton affinity than $\mathrm{H_2O}$, CO, or $\mathrm{N_2}$: thus, reactions with $\mathrm{H_3O^+}$, $\mathrm{HCO^+}$, and $\mathrm{N_2H^+}$ are likewise endothermic. Destruction of HF takes place slowly by means of cosmic ray–induced photodissociation and as a result of reactions with species of low abundance such as CH, $\mathrm{He^+}$, $\mathrm{H_3^+}$, and $\mathrm{C^+}$.

Considering these formation and destruction processes for hydrogen fluoride, we find that over a wide range of densities

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[7] Viz., oxygen, carbon, nitrogen, sulphur, silicon, and chlorine.

and temperatures, including those probed by our observations of HF $J = 2–1$ in Sgr B2, HF accounts for more than 99% of all fluorine nuclei in the gas phase. In comparison with the ion-neutral reaction routes responsible for the formation of other interstellar hydrides, the neutral-neutral reactions (1) and (2) are extremely effective in producing HF. Given our theoretical expectation that HF is the dominant reservoir of gas-phase fluorine along the line of sight to Sgr B2, the assumption that the elemental abundance of F is the same as that measured in the solar system (3×10^{-8} relative to H; Anders & Grevesse 1989), and the observed HF abundance of $\sim 3 \times 10^{-10}$ relative to H_2, we conclude that a depletion factor of ~50 results from the depletion of fluorine onto dust grains in Sgr B2. This is somewhat smaller than the depletion factors inferred by Zmuidzinas et al. (1995a) and Schilke et al. (1995) for chlorine in Sgr B2 and in OMC-1.

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