THE FAR-INFRARED SPECTRUM OF THE SAGITTARIUS B2 REGION: EXTENDED MOLECULAR ABSORPTION, PHOTODISSOCIATION, AND PHOTOIONIZATION

JAVIER R. GOICOECHEA, NEMESIO J. RODRÍGUEZ-FERNÁNDEZ, and JOSÉ CERNICHARO

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ABSTRACT

We present large-scale 9′ × 27′ (~25 pc × 70 pc) far-IR observations around Sgr B2 using the Long-Wavelength Spectrometer (LWS) on board the Infrared Space Observatory (ISO). The spectra are dominated by the strong continuum emission of dust, the widespread molecular absorption of light hydrides (OH, CH, and H2O), and the fine-structure lines of [N ii], [O iii], [C ii], and [O i]. The widespread dust emission is reproduced by a cold component (T_d ≈ 13–22 K) together with a warm component (T_d ≈ 24–38 K), representing ≤10% of the dust opacity. The fine-structure line emission reveals a very extended component of ionized gas. The [O ii] 52 μm/88 μm and [N ii] 57 μm/[N ii] 122 μm line intensity ratios show that the ionized gas has an average electron density of ~240 cm⁻³. The ionizing radiation can be characterized by a hard but diluted continuum, with effective temperatures of ~36,000 K and a Lyman continuum photon flux of ~10^50.4 s⁻¹. The spatial distribution of the ionizing sources with respect to the extended cloud and the clumpiness of the medium determine the large-scale effects of the radiation. Photodissociation regions (PDRs) can be numerous at the interface of the ionized and neutral gas. The analysis of the [C ii] 158 μm and [O i] 63 and 145 μm lines indicates a far-UV radiation field of G_0 ≈ 10⁻²⁻¹⁰⁴ and a density of n_H = 10⁵–10⁴ cm⁻³ in these PDRs. The widespread OH lines are produced by nonlocal radiative transfer models for clouds of moderate volume density (n_H ≈ 10³–10⁴ cm⁻³) at T_d ≈ 40–100 K. PDR models can explain the enhanced column density of species such as H2O, OH, and O³. However, they fail to reproduce the observed NH₃/NH₂/NH ≈ 100/10/1 abundance ratios. For N-bearing species, it seems that shock chemistry has to be invoked. The molecular richness in the outer layers of Sgr B2 is probed by the ISO/LWS Fabry-Pérot (~35 km s⁻¹) detections toward Sgr B2(M), where more than 70 lines from 15 molecular and atomic species are observed at high signal-to-noise ratios.

Subject headings: Galaxy: center — H II regions — infrared: ISM — ISM: individual (Sagittarius B2) — ISM: lines and bands — ISM: molecules

1. INTRODUCTION

The Sagittarius B (Sgr B) complex is located in the inner 400 pc of the Galaxy, sometimes referred to as the “Central Molecular Zone” (Morris & Serabyn 1996), at l ≈ 0°6 ± 0°2 Galactic longitude. It contains the well-known Sgr B2 and B1 and G0.6–0.0 radio sources (see Fig. 1a). Sgr B1 lies to the south of the complex and opposite Sgr B2; it is dominated by extended radio features (see Mehringer et al. 1992). The G0.6–0.0 region is situated between Sgr B2 and B1. The velocity of the ionized gas in G0.6–0.0 is between that of Sgr B1 and B2, suggesting that these regions are physically associated. Large-scale continuum studies show that Sgr B2 is associated with the brightest emission (Pierce-Price et al. 2000) and is the most massive cloud of the Galactic center (GC) region (10⁶ M☉; Lis & Goldsmith 1990). In the following, we assume that it is situated at ~100 pc from the dynamical center of the Galaxy for a distance of 8.5 kpc (Kerr & Lynden-Bell 1986).

Figure 1a shows a schematic representation of the main components within Sgr B2. In the central region there are three dust condensations, labeled as Sgr B2 north (N), middle (M), and south (S), which are situated in an imaginary north-south line of 2″ (~5 pc). They contain all the tracers of ongoing star formation: ultracompact H II regions created by the UV field of newly born OB stars (e.g., Benson & Johnston 1984; Gaume & Claussen 1990), X-ray sources associated with H II regions, X-ray sources with neither a radio nor an IR counterpart (Takagi, Murakami, & Koyama 2002), hot cores of dense material (T_k = 150–300 K; n_H ≈ 10³ cm⁻³) and embedded protostars (e.g., Vogel, Genzel, & Palmer 1987; Lis et al. 1993), molecular maser emission in H2O, OH, H2CO, CH3OH, and SiO (e.g., Mehringer & Menten 1997 and references therein), and high far-IR luminosity (≈7 × 10⁸ L☉; Thronson & Harper 1986). These components are embedded in a moderate-density (n_H ≈ 10³–10⁴ cm⁻³) cloud of ~10 pc in size (Lis & Goldsmith 1991; Hüttemeister et al. 1993). The temperature in the moderate-density cloud decreases with distance from 80 to 40 K, except in a ring structure of warm gas (T_k = 100–120 K) with a radius of ~4 pc (de Vicente, Martín-Pintado, & Wilson 1997). These internal regions are surrounded by an extended lower density (n_H ≤ 10² cm⁻³) envelope (~15″), hereafter the Sgr B2 envelope, of warm gas (T_k ≥ 100 K; Hüttemeister et al. 1995).

The origins of the observed rich chemistry in the Sgr B2 envelope and its heating mechanisms are far from settled, and several scenarios have been proposed. Low-velocity shocks have traditionally been invoked to explain the enhanced gas-phase abundances of molecular species such as SiO or NH₃ and the differences between gas and dust temperatures in the Sgr B2 envelope (Martín-Pintado et al. 1997; Flower, Pineau...
The origins of shocks in Sgr B2 have been associated with either large-scale cloud-cloud collisions (Hasegawa et al. 1994) or small-scale wind-blown bubbles produced by evolved massive stars in the envelope itself (Martínez-Pintado et al. 1999).

The effect of the radiation in the Sgr B2 envelope has traditionally been ruled out because of differences in the gas and dust temperature, the unusual chemistry, and the absence of thermal radio-continuum and ionized gas outside the H ii regions and hot cores within the central condensations. The Infrared Space Observatory (ISO) observations presented here reveal the presence of an extended component of ionized gas detected by its fine-structure line emission. The presence of widespread UV and X-ray fields illuminating large portions of Sgr B2 could trigger the formation of photodissociation regions (PDRs) and X-ray–dominated regions in the interface between the ionized gas and the self-shielded neutral layers and could influence the selective heating of the molecular gas. The complexity of the region possibly allows a combination of different scenarios and excitation mechanisms to coexist within the whole complex.

In this paper we study the large-scale properties of the Sgr B2 region and the effect of the far-UV radiation by analyzing its far-IR spectrum (43–197 μm). In § 2 we summarize the ISO observations and the data reduction. The resulting spectra are presented and analyzed in the following sections: dust emission (§ 3), fine-structure lines (§ 4), and molecular lines (§ 5). Several techniques have been used in the analysis: graybody fitting, photoionization models, molecular radiative transfer models, and comparisons with PDR models. A general overview and a brief summary are given in § 6.

2. OBSERVATIONS AND DATA REDUCTION

The far-IR wavelength range covers the spectral signature of several interesting phenomena that are difficult to observe from ground-based telescopes. These include the fine-structure lines of atoms and ions, the high-J/fundamental rotational lines of heavy/light molecules, the low-energy bending modes of carbon clusters, and the continuum emission peak for the bulk of star-forming regions. Therefore, we proposed to use the Long-Wavelength Spectrometer (LWS; Clegg et al. 1996) on board ISO (Kessler et al. 1996) to study the large-scale distribution of the dust, the ionized gas, and the neutral gas and molecular content around the Sgr B2 region.

The present study includes the observations of our open-time programs in different positions within the Sgr B complex. In addition, we also present some LWS observations retrieved from the public ISO Data Archive (IDA) observations. The main observations are a 9° × 27° raster map that targets 19 individual positions within the complex (see Fig. 1b). The crosslike LWS grating map is centered near the Sgr B2(M) position at α = 17h44m10.61s, δ = −27°22.30′ (B1950.0). Offsets between consecutive positions are 90″, except for north-south points with |Δδ| ≥ 450″ for which a 180″ spacing was selected. The central position of our maps, Sgr B2(M), has been widely studied at higher resolution by different LWS Fabry-Pérot (FP) observations (see the references in Tables 4 and 5).

2.1. LWS Astronomical Observation Template L01 Observations

The crosslike map was made during 1996 August and 1997 February (target dedicated time numbers [TDTs] 28702130, 28702131, 46900233, and 46900234) using the Astronomical Observation Template (AOT) L01 with a spectral resolution of 0.29 μm for the 43–93 μm range (detectors SW1–SW5) and 0.6 μm for the 80–197 μm range (detectors LW1–LW5). It uses all 10 LWS detectors with beam sizes (Ω_LWS) around 80″. The typical flux accuracy varies from 10% to 50% depending on the source geometry, the source flux, and the particular

See http://www.iso.vilspa.esa.es/ida.
detector (Gry et al. 2003). Based on the overlapping regions, the agreement in the flux measured by different detectors is found to be better than 10%. Shifting factors of \( \leq 10\% \) have been applied in some selected detectors to yield a smoothed and aligned continuum spectrum (Fig. 2). Only detector LW2 showed intensities too high by \( \sim 20\% \) relative to the neighboring detectors and had to be scaled by a factor of 0.8. The spectra were oversampled at one-fourth of a resolution element. The long-wavelength data have been dereddened for the interference pattern systematically seen in the AOT L01 spectra of extended sources or point sources that are offset from the optical axis (Swinyard et al. 1996, Fig. 2b).

Depending on the position in the cross-raster, the far-IR spectrum exhibits several OH, CH, and H\(_2\)O rotational lines and several fine-structure lines. We have clearly detected the \([\text{O} \text{ I}] 63, 145 \mu\text{m} \) and \([\text{C} \text{ II}] 158 \mu\text{m} \) lines in all positions, except in Sgr B2(M). In addition, lines coming from higher excitation potential\(^5\) ions such as \([\text{N} \text{ II}] 122, [\text{N} \text{ III}] 57, \) and \([\text{O} \text{ III}] 52 \) and 88 \( \mu\text{m} \) are also detected. The OH (\( \sim 79 \mu\text{m} \)), \([\text{O} \text{ I}] 63, [\text{N} \text{ III}] 57, \) and \([\text{O} \text{ III}] 88 \mu\text{m} \) lines lie in the overlapping regions of two different LWS detectors. Since fluxes agreed within \( \sim 15\% \), we averaged both determinations. Line fluxes were extracted by fitting Gaussians after removing a polynomial baseline for each detector coverage. Emission-line fluxes are listed in Table 1.

### 2.2. LWS Astronomical Observation Template L04 Observations

The LWS/FP instrument has been used to investigate the atomic and molecular features in Sgr B2(M) at a higher spectral resolution (\( \sim 35 \text{ km s}^{-1} \)). The majority of detected lines (see Fig. 8) have been observed in our AOT L04 ISO proposals. The TDTs are 32201428, 32701751, 47600907, 47600908, 47600909, 47601001, 47601002, and 46900332. However, an extensive inspection and reduction of about more than 50 TDTs\(^6\) from the public IDA have been carried out in order to add some detections and average all available lines (see Polehampton 2002 for the AOT L03 detections). The LWS/FP spectrum of Sgr B2(M) includes the \([\text{O} \text{ I}], [\text{C} \text{ II}], \) and \([\text{O} \text{ III}] \) lines (see Figs. 3a and 3b) also detected at lower resolution in the LWS gratings. In the case of the \([\text{O} \text{ III}] 52 \) and 88 \( \mu\text{m} \) lines, their clear LWS/FP identification confirms the doubtful detection made in the gratings and shows the importance of increasing spectral resolution. A declination raster (TDT 32201429) of some molecular lines was also carried out up to \( \Delta\delta = \pm 270\arcmin \). Figure 4a shows the raster in the \(^{16}\text{OH} 119.442 \mu\text{m} \) line. The richness of the LWS/FP spectrum of Sgr B2(M) suggests that the far-IR spectra of other observed sources can also be much richer than that observed at the grating resolution.

### 2.3. Data Reduction

AOT L04 products have been processed and compared through the Off-Line Processing (OLP) pipeline, versions 6.0–10.1. There are no major differences except that recent pipelines produce less than 10% less absorption in some lines because of continuum level differences from one OLP pipeline.

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\(^5\) The excitation potentials of the observed ionic species are \( \text{in eV} = 11.26 \) (\( \text{CN} \)), 14.53 (\( \text{N} \text{ II} \)), 29.60 (\( \text{N} \text{ III} \)), and 35.12 (\( \text{O} \text{ II} \)).

\(^6\) The additional AOT L04 observations analyzed were taken by ISO during orbits 498, 494, 467, 464, 462, 326, 327, 326, and 322, while the additional AOT L03 observations were taken during orbits 849, 847, 845, 838, 836, 509, 508, 507, 506, 504, and 476.

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3. WIDESPREAD FAR-IR CONTINUUM EMISSION: RESULTS

All positions around Sgr B2(M) ([0\arcsec, 0\arcsec]) present their continuum emission peak between 90 and 100 \( \mu\text{m} \) (Fig. 2), indicating that the bulk of observed dust has a relatively cold temperature. The far-IR luminosity in the map is \( L_{\text{IR}} \approx 8.5 \times 10^6 \text{ L}_\odot \). The strongest IR positions are Sgr B2(M) and (N) \( \sim 0\arcsec, 90\arcmin \)); they contribute \( \sim 28\% \) and \( \sim 14\% \) to \( L_{\text{IR}} \), respectively. The rest of the positions show decreasing continuum fluxes with increasing distance from Sgr B2(M). For the same distance from Sgr B2(M), the southern points of the cloud have larger fluxes than the northern ones, while the dust emission in the east-west direction is more symmetrical.

In order to estimate and better constrain the dust temperature and the associated column density of material, we have modeled the observed continuum spectrum as a sum of two graybodies. A single graybody crudely fits the observed emission in any position. The total continuum flux in the model is given by

\[
S_\delta = \left( 1 - e^{-\tau_0} \right) B_{\delta}(T_\delta) \Omega_w + \left( 1 - e^{-\tau_\delta} \right) B_\delta(T_\delta) \Omega_c ,
\]

where \( c/w = i \) stands for cold/warm dust components, \( B_\delta(T_\delta) \) is the Planck function at a temperature \( T_\delta \), \( \tau_\delta \) is the continuum opacity, and \( \Omega_i \) is the solid angle subtended by the \( i \) dust component. We have expressed \( \tau_\delta \) at far-IR wavelengths as a function of the 30 \( \mu\text{m} \) opacity using a power law with exponent \( \beta \) \( \tau_\delta = \tau_{30} (30/\lambda)^\beta \). In addition, \( \tau_{30} \) can be written as a function of the visual extinction \( (A_V) \) as \( \tau_{30} = 0.014 A_V \) (Draine 1989). Thus, \( \tau_\delta \) is given by

\[
\tau_\delta^{c/w} = 0.014 A_V (30/\lambda)^\beta .
\]

Taking into account the large extension of the dust emission in the region, we have considered that both dust components fill the beam for all the observed positions \( \Omega_i = \Omega_{\text{L,WS}} \). Note that equation (1) applies for all positions but not for Sgr B2(M) and (N), which is discussed below.

We have tried to fit the continuum emission with \( \beta \) between 1.0 and 2.0, which are the expected emissivity exponents for silicates and graphite grains (Spitzer 1978). We obtain satisfactory fits in this range of \( \beta \)-values. However, fits obtained for \( \beta \sim 1 \) are slightly better (\( \chi^2 \) is 2 times lower). In
Fig. 2.—Raster map obtained with the LWS grating between 43 and 197 μm, with a spectral resolution of ~1000 km s$^{-1}$. In each box, offset positions are given in arcseconds with respect to the (0°, 0°) central position at $\alpha = 17^h 44^m 10^s.61$, $\delta = -28^\circ 22' 30.0''$ (B1950.0). The intensity scale corresponds to the flux (in units of $10^{-16}$ W cm$^{-2}$ μm$^{-1}$) and the abscissa to the wavelength in μm. (a) Average continuum flux of each LWS detector and graybody best fits (black lines) for some selected positions. The dotted lines correspond to the warm component and the solid gray lines to the cold component. The error bars correspond to 30% flux uncertainty. (b) Top: Observed fringing in the long-wavelength detectors. Bottom: Continuum level after defringing the spectra. (c, d) Comparison of LWS grating spectra of Sgr B2(M) (0°, 0°) (black lines) and an average of (90°, 0°) + (0°, -90°) + (0°, -180°) adjacent positions (gray lines). A polynomial baseline has been removed. The main assigned features are labeled.
addition, the visual extinction derived for $\beta \sim 2$ is more than a factor of 10 larger than the extinction expected from the molecular column densities. Thus, $\beta \gtrsim 2$ seems unrealistic for far-IR wavelengths, whereas $\beta$-values between 1 and 1.5 are in agreement with those derived from ISO observations of other GC clouds by Lis & Menten (1998). Note that $\beta \sim 2$ has been obtained from the optically thin emission at 350 and 800 $\mu$m around Sgr B2 (Lis & Carlstrom 1994; Dowell et al. 1999). However, the central regions of the cloud ($\leq 180''$) are characterized by $\tau_{100} \gtrsim 1$, so the continuum is optically thick in most of the far-IR wavelengths. Hence, the dust emission observed by ISO basically arises in the external layers of the cloud, i.e., the extended envelope that veils the dense star-forming regions, while a considerable fraction of the submillimeter emission comes from the dense regions of Sgr B2. In addition, the extended dust component observed by ISO is partially filtered out by the beam-switching submillimeter observations. Thus, far-IR and submillimeter observations could trace different dust components. In the following, all calculations have been carried out for $\beta$-values in the range 1.0–1.5.

Table 2 lists the lower and upper limits to the visual extinction. The extinction varies from $A_V \gtrsim 250$ mag for the positions within a radius of $90''$ ($\sim 4$ pc) to $A_V \gtrsim 50$ mag for positions within $270''$ ($\sim 10$ pc).

Table 3 gives the dust temperatures (unlike the visual extinction, $T_d$ is only weakly dependent on $\beta$). The spectral energy distributions are best fitted with a dust component with a temperature of $13–22$ K and a warmer component with a temperature of $24–38$ K. The higher dust temperatures are those measured in the southern regions. The warmer component contributes less than 10% to the total extinction. For comparison, Gordon et al. (1993) derived $T_d \approx 19$ K for a smaller region ($95'' \times 270''$) using millimeter observations and gray-body analysis, while they obtained IRAS $100 \mu$m/$60 \mu$m color temperatures of $\sim 35$ K. The IRAS observations are more sensitive to the GC diffuse dust (Gordon et al. 1993). The properties of this diffuse component (temperature and opacity) agree with those derived for the warm component in our fits to the far-IR emission of Sgr B2.

3.1. Sgr B2(M) and Sgr B2(N)

One of the main properties of the Sgr B2 central region is the tricky Sgr B2 (N)/(M) continuum flux ratio ($N/M$) as a function of the observed wavelength. The observational evidence that $N/M < 1$ at 53 $\mu$m (Harvey, Campbell, & Hoffmann 1977), while $N/M > 1$ at 1300 $\mu$m (Goldsmith, Snell, & Lis 1987), can be explained if Sgr B2(N) is embedded behind the dust and gas envelope of Sgr B2(M). Thus, the Sgr B2(N) line of sight will have a larger column density of dust producing a greater emission at millimeter wavelengths. However, at far-IR wavelengths, part of the warm dust emission from Sgr B2(N) will be absorbed by the cooler foreground dust associated with Sgr B2(M), resulting in an $N/M < 1$ ratio (Thronson & Harper 1986; Goldsmith et al. 1990). From the present LWS observations of Sgr B2(M) and (N), we found $N/M = 0.3$ at 57 $\mu$m and $N/M = 0.7$ at 178 $\mu$m. These ratios confirm the importance of dust opacity even at $\sim 180 \mu$m. Because of the large dust opacity in the obscured Sgr B2(M) and (N) positions, we have only fitted a single graybody to extract the average dust temperature and opacity. From the fits we infer $\tau_{100} \approx 3.8 \pm 0.4$ ($T_d \approx 31 \pm 1$ K) and $\approx 5.3 \pm 0.6$ ($T_d \approx 26 \pm 1$ K) for Sgr B2(M) and (N), respectively (see Fig. 2a).
Fig. 3.—Raster map obtained with the LWS grating of the [O i] 63, [O iii] 88, and [C ii] 158 μm lines. In each box, offset positions are given in arcseconds with respect to the (0°, 0°) central position at α = 17h44m10s, δ = −28°22′30″ (B1950.0). The intensity scale corresponds to the line flux and the abscissa to the wavelength. (a) [C ii] and [O iii] lines detected with the LWS/FP at (0°, 0°). (b) [O i] lines detected with the LWS/FP at (0°, 0°). (c) Main features of the grating raster map labeled. (d) Raster map positions with the clearest [O iii] 52 μm detections.
Fig. 4.—Raster map obtained with the LWS grating between 115 and 121 $\mu$m. In each box, offset positions are given in arcseconds with respect to the (0$''$, 0$''$) central position at $\alpha = 17^\mathrm{h}44^\mathrm{m}10^s$, $\delta = +22^\circ23'20''$ (B1950.0). The intensity scale corresponds to the continuum normalized flux and the abscissa to the wavelength. (a) LWS/FP declination raster of the $^{16}$OH $119.442\mu$m line. (b) Top: Fundamental OH A-doublet detected with the LWS/FP at (0$''$, 0$''$) around $119\mu$m. Bottom: o- and p-NH$_2$ lines detected with the LWS/FP at (0$''$, 0$''$) around 117 and 126 $\mu$m. The NH$_2$ 117 $\mu$m triplet may contribute to the U117 line observed at much lower resolution. (c) Main features of the grating raster map labeled. (d) Raster map positions with clear [N ii] 57 $\mu$m detections.
4. FINE-STRUCTURE LINES: RESULTS

4.1. Extinction Corrections

The large H$_2$ column densities (up to $10^{25}$ cm$^{-2}$) found across the Sgr B2 region suggest that even in the far-IR, fine-structure lines can suffer appreciable extinction. In addition, the average interstellar extinction toward the GC, with $A_V$ $\approx$ 25 mag (e.g., Schultheis et al. 1999), also contributes to the attenuation of atomic emission. In this work we estimate limits to the extinction in each position by using two approximations. A lower limit to the extinction can be obtained using the $[O\,\text{iii}]$ 52 $\mu$m$–[O\,\text{iii}]$ 88 $\mu$m (hereafter [O iii] 52/88) line intensity ratios. This ratio cannot be lower than $\sim$0.55, which is the value obtained in the low electron density limit if lines are optically thin. For those positions where the [O iii] 52/88 ratios are lower than the lower limit, we derive a minimum visual extinction of $\sim$20 mag for positions very distant ($\gtrsim$7.5) from Sgr B2(M), while a minimum extinction of $\sim$100 mag inside the 15$''$ diameter cloud has been found.

A more direct estimation of the prevailing extinction was obtained from the continuum analysis (§ 3). Note that the lower limit to $A_V$ derived from the [O iii] 52/88 ratios is consistent with that derived from the dust models (Table 2). In the subsequent discussion we have corrected the line intensities by the extinction limits presented in Table 2.

4.2. The Ionized Gas

The [O iii] lines shown in Figure 3 (see also Fig. 4 for the [N ii] and [N iii] lines) reveal an extended component of ionized gas in the southern and eastern regions of Sgr B2. In particular, the [O iii] 88 $\mu$m emission extends $\sim$13.5$''$ ($\sim$35 pc) to the south of Sgr B2(M). The smooth decrease of the [O iii] 88 $\mu$m intensity as a function of the distance to Sgr B2(M) suggests that the major contribution to the observed flux arises in an extended component of ionized gas rather than in compact sources. We also note that the G0.6–0.0 and Sgr B1 radio sources could contribute to the ionization in the southern positions.

To study the properties of the ionized gas we have analyzed the [O iii] 52/88 and the [N iii] 57 $\mu$m$–[N\,\text{ii}]$ 122 $\mu$m (hereafter [N iii]/[N ii]) line intensity ratios. Table 2 lists both ratios for all positions after correcting for extinction.

4.2.1. Electron Densities

We have used the [O iii] 52/88 ratio to estimate the electron density in the observed sources (see Rubin et al. 1994). The [O iii] 52/88 ratio derived from our observation varies between $\sim$3 for the central sources to $\sim$0.5 for positions located far from Sgr B2(M). Comparing these [O iii] ratios with Figure 1 of Rubin et al., one finds electron densities ranging from $\sim$10$^3$ to $\sim$50 cm$^{-3}$ for the sources located close to and far from Sgr B2(M), respectively. The average electron density in all observed positions is 240 cm$^{-3}$.

For Sgr B2(M) itself, the [O iii] lines are hardly detected with the LWS in grating mode. Nevertheless, Figure 3a shows their unambiguous LWS/FP detections toward Sgr B2(M). Both [O iii] lines appear centered at $v_{LSR}=\pm 50 \pm 15$ km s$^{-1}$ and, as could be expected, do not show emission/absorption at more negative velocities produced by the foreground gas in the line of sight. From the LWS/FP [O iii] line intensities and by correcting the [O iii] 52/88 line intensity ratio by the $\sim$1000 mag of visual extinction derived for Sgr B2(M), we found an electron density of $\sim$10$^{3.4\pm 1.3}$ cm$^{-3}$. As expected, the densest ionized material seen in the far-IR is located in the central star-forming regions of Sgr B2.

Mehringer et al. (1993), from 20 cm interferometric observations ($26'' \times 15''$ in resolution), detected a $\sim$7$''$ ($\sim$20 pc) halo of diffuse emission around Sgr B. The [O iii] 88 $\mu$m line emission in Figure 3 spreads beyond the radio recombination line contours of Mehringer et al.
4.2. Radiation Temperatures

We have used the [N\textsc{ii}] 57 and [N\textsc{ii}] 122 \textmu m line intensities and followed the method described in Rubin et al. (1994) for ionization-bounded nebulae to derive the effective temperature of the ionizing radiation \(T_{\text{eff}}\). For each position, we have determined the volume emissivities of both the [N\textsc{ii}] 57 and [N\textsc{ii}] 122 \textmu m lines, which are derived from the [O\textsc{ii}] 52/88 line intensity ratio. From these emissivities, it is possible to derive the actual N\textsuperscript{++}/N\textsuperscript{+} abundance ratio. We have used the results of Rubin et al. (see their Fig. 4) and from the [N\textsc{ii}] 57 and [N\textsc{ii}] 122 \textmu m line intensities, it is possible to derive \(T_{\text{eff}}\). Table 2 gives the derived values at several positions. The largest \(T_{\text{eff}}\) is obtained toward the central positions (~36,000 K).

It has been pointed out by Shields & Ferland (1994) that the fine-structure line ratios observed in the GC can be reproduced with a higher \(T_{\text{eff}}\) and a lower incident flux of ionizing photons (low ionization parameters). This would be the case if the ionizing radiation were diluted, i.e., if the medium were clumpy and inhomogeneous and/or the ionizing sources were located far from the ionized nebulae. Indeed, this is the situation in the Radio Arc region by Rodríguez-Fernández, Martín-Pintado, & de Vicente (2001), also in the GC, where an extended (40 pc \times 40 pc) gas component is ionized by hot (~35,000 K) diluted radiation arising from the Quintuplet and the Arches clusters. They concluded that the radiation reaches large distances because of the inhomogeneity of the medium. If this also applies to the Sgr B2 envelope, then the \(T_{\text{eff}}\) derived above should be considered as a lower limit.

In this work it is possible to perform a detailed study of the geometry of the region because of the limited angular and spectral resolution of the ISO data. Instead, we have performed some simple photoionization model calculations using the MPE IDL CLOUDY Environment (MICE), which was developed by H. Spoon at the Max-Planck-Institut für extraterrestre Physik\textsuperscript{8} (MPE) and uses CLOUDY 94 (Ferland 1996). To determine the shape of the continuum illuminating the nebulae, we have taken the stellar atmospheres modeled by Schaerer & de Koter (1997). First, we have modeled the Sgr B2 cloud as a sphere with a density law taken from Lis & Goldsmith (1990):

\[
7 \times 10^5 \text{ cm}^{-3} \quad \text{for } 0.3 < R < 1.25, \quad (3)
\]

\[
\left[ \left( \frac{7 \times 10^5}{R} \right) \left( \frac{1.25}{R} \right)^2 + 2000 \right] \text{ cm}^{-3} \quad \text{for } 1.25 < R < 22.5, \quad (4)
\]

where \(R\) is the radius in parsecs. We have considered an ionizing source in the center of this sphere emitting a Lyman continuum photon flux, \(Q(H)\), of \(10^{50.3} \text{ s}^{-1}\) [approximately equal to the total \(Q(H)\) in Sgr B2(M) and (N); see Gaume et al. 1995]. To define the shape of the ionizing continuum, we have used a 37,800 K atmosphere (similar to the maximum \(T_{\text{eff}}\) derived with the nitrogen lines ratio). The results show that the radius of the [N\textsc{ii}] region would not be larger than 1 pc. The same is true for models with \(Q(H) = 10^{51.3} \text{ s}^{-1}\) and a 41,700 K atmosphere. With such a dense and homogeneous model, it is not possible to explain the large extension of the ionized gas component observed with ISO. However, if the cloud around the newly born OB stars is inhomogeneous and clumpy enough, the UV radiation field can illuminate several surfaces along the line of sight (Tauber & Goldsmith 1990). This scenario was required in the past to explain the first extended [C\textsc{ii}] and [C\textsc{i}] observations in molecular clouds (e.g., Phillips & Huggins 1981). Moreover, the poor correlation between the HC\textsubscript{3}N and C\textsubscript{18}O extended emission found around Sgr B2 suggests that both the envelope and the dense regions are clumpy and/or fragmented (Lis & Goldsmith 1991; Goldsmith et al. 1992).

Instead of making a complex three-dimensional inhomogeneous density model, we have used the different observed positions as independent nebula located at a distance from Sgr B2(M) equal to their projected distance in the plane of the sky. The model assumes that the medium is inhomogeneous and that the radiation can reach all the observed positions, but, of course, it takes into account the dilution caused by the distance of the different sources from Sgr B2(M). This is done by means of an ionization parameter \(U\), defined as \(U = Q(H)/4\pi n_e c D^2\), where \(n_e\) is the electron density, \(c\) is the speed of light, and \(D\) is the distance of the nebula to the ionizing source. We take \(n_e = 240 \text{ cm}^{-3}\) (the average density derived from the [O\textsc{ii}] lines) for all positions.

Figure 5 illustrates the results of some of these models in terms of the [N\textsc{ii}]/[N\textsc{ii}] ratio versus the distance in arcseconds from Sgr B2(M) for the north-south raster. Black lines show that the observed line ratios can be reproduced with \(Q(H) \approx 10^{50.3} \text{ s}^{-1}\) arising from the center of the cloud and \(T_{\text{eff}}\) between 35,500 (dashed lines) and 36,300 K (dotted lines). Unfortunately, the large error bars due to the extinction uncertainties make a more precise analysis difficult. However, it seems that the [N\textsc{ii}]/[N\textsc{ii}] ratios in the southernmost positions are somewhat higher than would be expected from the points closer to Sgr B2(M) and from model calculations. This should be an effect of the presence of additional ionizing sources in the Sgr B1 area. We have tried to model the effect of Sgr B1 assuming that the effective temperature of the radiation arising from these sources is similar to that arising from Sgr B2 and to estimate a total ionization parameter defined as

\[
U = \frac{1}{4\pi n_e c} \left[ \frac{Q(H)_2}{D_2^2} + \frac{Q(H)_1}{D_1^2} \right], \quad (5)
\]

\(n_1\) being the electron density, \(c\) the speed of light, and \(D_1\) and \(D_2\) the distances from the Sgr B2 cloud and Sgr B1 cloud to the ionizing source.

\begin{table}[h]
\centering
\caption{Dust Temperatures Derived by Fitting the Far-IR Continuum Emission with Two Graybodies and Luminosities in the LWS Range}
\begin{tabular}{llll}
\hline
Map Position & \(T_{\text{dust}}\) & \(T_{\text{dust}}\) & \(L_{\text{LWS}}\) \\
 & (K) & (K) & (L\_\odot) \\
\hline
(0, 810) & 30–33 & 17–20 & 6.91E04 \\
(0, 630) & 30–33 & 17–20 & 9.57E04 \\
(0, 450) & 31–35 & 18–22 & 1.37E05 \\
(0, 270) & 25–29 & 13–20 & 1.86E05 \\
(0, 180) & 26–35 & 16–20 & 2.56E05 \\
(0, -90) & 27–30 & 17–19 & 6.20E05 \\
(0, -180) & 32–36 & 18–21 & 4.74E05 \\
(0, -270) & 34–38 & 18–22 & 3.61E05 \\
(0, -450) & 36–38 & 17–20 & 3.17E05 \\
(0, -630) & 32–34 & 18–21 & 1.91E05 \\
(0, -810) & 34–37 & 18–22 & 1.20E05 \\
(270, 0) & 25–27 & 14–19 & 2.63E05 \\
(180, 0) & 29–32 & 17–20 & 2.90E05 \\
(90, 0) & 31–34 & 18–20 & 5.21E05 \\
(-90, 0) & 24–26 & 15–19 & 5.07E05 \\
(-180, 0) & 24–26 & 13–19 & 2.60E05 \\
(-270, 0) & 24–25 & 13–19 & 2.24E05 \\
\hline
\end{tabular}
\end{table}
where \( Q(H)_2 \) and \( Q(H)_1 \) are the Lyman continuum photons arising from Sgr B2 and Sgr B1, respectively, and \( D_2 \) and \( D_1 \) are the distance of the observed sources from Sgr B2 and Sgr B1, respectively. The gray lines in Figure 5 show the results of some of these combined models with \( Q(H)_1 = 10^{49} \) or \( 10^{49.5} \text{ s}^{-1} \). Including the effect of Sgr B1 helps to explain the observed ratios in the \((0^\circ, -450^\circ)\) and \((0^\circ, -630^\circ)\) positions, but the measured ratio in \((0^\circ, -810^\circ)\) is still higher than expected. Hence, additional ionizing sources in the southern region of Sgr B2 cannot be ruled out.

In any case, it is important to remark that even taking into account the simplicity of the model and the dust extinction uncertainties, the agreement of the model with the observations is fairly good. All measured ratios lie between the 35,500 and 36,300 K curves (see Fig. 5). We conclude that the whole Sgr B complex is permeated by hot radiation arising mainly from Sgr B2. There is also a contribution to the large-scale ionization from sources located in the vicinity of Sgr B1. A minor contribution from additional ionizing sources cannot be ruled out. The long-range effects of the ionizing radiation can only be understood if the medium is clumpy and inhomogeneous, but also only if the location and geometric distribution of the ionizing sources are appropriate for predominantly ionizing the southern and eastern regions.

### 4.3. Photodissociation Regions

The detection of a widespread component of ionized gas suggests that numerous PDRs can exist in the interface between this ionized material and the molecular gas throughout the cloud. Furthermore, the prevailing far-UV radiation field and the X-ray emission can also be important in the heating and chemistry of the neutral gas. In the following sections we analyze the fine-structure emission related to the PDRs and the molecular content of Sgr B2 as seen by far-IR spectroscopy.

#### 4.4. The [N II] versus [C II] Correlation

The chemistry and the heating of a PDR are basically controlled by the hydrogen gas density \((n_H)\) and the far-UV \((6 \text{ eV} < h\nu < 13.6 \text{ eV})\) radiation field. The main coolants in a PDR are the far-IR continuum emission of dust and the [C II] and [O I] fine-structure lines. Thus, their relative intensities can be used as a diagnostic of the PDR conditions. Hence, the first step is to find a way to distinguish the diffuse ionized gas from that of the PDR.

If ionized and neutral/PDR phases exist and/or are associated, [C II] emission can arise from both components (Heiles 1994). For positions with [N II] detections, the [C II] emission coming from the diffuse gas should scale with the [N II] lines, because the bulk of N\(^{++}\) emission arises in the low-density ionized gas (~75%, according to Malhotra et al. 2001). Figure 6 shows the good correlation found in the Sgr B2 region. The lack of [C II] emission in the grating spectra of Sgr B2(M) and (N) is the combined effect of extinction, self-absorption in foreground clouds, and absorption of the continuum by C\(^+\) in low-excitation diffuse clouds (see the absorption in Fig. 3a). Those observations were not included in the correlation. However, the line is well detected farther from the central position, where the extinction is less considerable and there is less background continuum to be absorbed by the diffuse component. The resulting observational correlation is

\[
I(C^+)_{-11} \approx 5.2 I(N^{+})_{-11} + 6.4 , \tag{6}
\]

where \( I(C^+)_{-11} \) and \( I(N^{+})_{-11} \) are the 158 and 122 \text{ m\m} line intensities, respectively, in units of \( 10^{-11} \text{ W cm}^{-2} \text{ sr}^{-1} \). A crude approximation to the [C II] emission arising in PDR gas can be estimated by assuming that the second term in relation (6) represents the average [C II] emission in PDRs. For comparison, Malhotra et al. (2001) derived the theoretical scaling \( I(C^+) = 4.3 I(N^{+}) + I(C^+)_{\text{PDR}} \)

Fig. 6.—Correlation between the [N II] 122 \text{ m\m} and [C II] 158 \text{ m\m} lines. Each source position has been corrected for its minimum visual extinction derived from far-IR continuum fits (see Table 2). Sgr B2(M) and (N) positions are not included (see text).
4.5. PDR Diagnostics

Once we have estimated the amount of [C ii] arising from PDRs, we can compare the usual far-IR diagnostics, [C ii] 158 and [O i] 63 and 145 µm lines and continuum emission with theoretical PDR models, to estimate the gas density and the far-UV incident field.

Because of the prominent foreground absorption in the [C ii] 158 and [O i] 63 µm lines observed toward Sgr B2(M), we have omitted the (M) and (N) positions in the following discussion (see Vastel et al. 2002). Figure 7 shows PDR model predictions of the [C ii]/[O i] ratio versus the [C ii]/[Si i] far-IR ratio in terms of the density $n_H$ and the far-UV incident flux $F_{10}$ (in units of the local interstellar value) taken from Wolfire, Tielens, & Hollenbach (1990, hereafter WHT90). Nevertheless, Simpson et al. (1997) emphasized that Si is highly depleted in WTH90 models so that the effect of the unobserved [Si i] line across the region can be neglected. The experimental points in Figure 7 do not include the [Si i] 35 µm line, because only the central position has been observed by Goicoechea & Cernicharo 2002, hereafter GC02). The uncorrected line intensity ratio in Sgr B2(M) is [C ii] 158 µm/[Si i] 35 µm $\approx 10$, with the [C ii] intensity coming from the emission component (see Fig. 3a for the LWS/FP line).

Squares and triangles in Figure 7 show the parameter space occupied by Sgr B2. Dark gray triangles represent line ratios that consider all the observed [C ii] intensity at each position, and light gray squares show ratios that consider only the mean PDR [C ii] emission derived from the correlation with [N ii]. The different points show the intensity ratios corrected for the minimum (filled symbols) and maximum (open symbols) visual extinction (see Table 2). The data scatter over the $G_0 \approx 10^{-8} - 10^{-10}$ and $m_H \approx 10^{-6} - 10^{-3}$ cm$^{-2}$ curves. The expected PDR surface temperature for those values is $\approx 300$ K (WHT90), and it can reach $\approx 500$ K if heating by photoelectrons ejected from polycyclic aromatic hydrocarbons and very small grains is included in the models (Kaufman et al. 1999).

The possible errors in the PDR parameters are influenced by the $A_\lambda$ uncertainty of each line of sight, the estimation of the PDR [C ii] emission, and optical depth effects, such as the [C ii] absorption seen in Figure 3a. Additional uncertainty is due to the [O i] 63 µm line intensity used as a PDR diagnostic in Figure 7. The line intensity can be larger if cold foreground gas absorbs part of the emission associated with Sgr B2 that is outside the (M) and (N) lines of sight. The line can also be weaker (relative to the [O i] 145 µm line) if the emission is saturated because of a high optical depth. Finally, the line intensity can also be overestimated if the majority of the emission arises from other inner regions (mainly molecular) of the cloud and not from the PDRs. In such a case, and assuming that the [O i] 63 µm line emission is very thick across Sgr B2, it is difficult to estimate the different contributions to the measured line intensity. Therefore, the main properties of the widespread PDRs in Sgr B2 derived from Figure 7 should be considered to cover the range of densities $n_H \approx 10^4 - 10^6$ cm$^{-3}$ and the far-UV incident flux $G_0 = 10^2 - 10^4$.

The ionized component shown in Figure 3 proves the presence of an extended far-UV radiation field. Although the PDR models can explain the fine-structure line intensities, we have also considered the role of shocks in the excitation of [O i] and [C ii] lines. Such shocks are known to be present in Sgr B2 (Hüttemeister et al. 1995; Martin-Pintado et al. 1997).

The ratio of the integrated line emission ([O i] 63 µm + [C ii] 158 µm) to the integrated far-IR emission in PDRs cannot be larger than $\sim 10^{-2}$ because of the low efficiency of the photoelectric heating mechanism. On the other hand, this ratio is at least of order magnitude larger if the lines arise in shocked gas (Hollenbach & McKee 1989). Thus, the observational ratios in Figure 7 show that the extended [C ii] and [O i] emission is dominated by the PDR scenario.

The absolute intensities can also be compared with PDR and shock models in the range $n_H = 10^2 - 10^4$ cm$^{-3}$. The intensity of the [C ii] 158 µm line associated with PDRs estimated from the [N ii] versus [C ii] correlation is $\approx 6.4 \times 10^{-11}$ W cm$^{-2}$ sr$^{-1}$, which we found to be consistent with the PDR model predictions of Hollenbach, Takahashi, & Tielens (1991) for $G_0 \approx 10^3$. Only J-shock models (Hollenbach & McKee 1989) predict some [C ii] emission, but it is orders of magnitude weaker than that observed, unless high shock velocities ($\approx 100$ km s$^{-1}$) occur. These velocities are not inferred from the line widths derived from large-scale molecular observations at radio wavelengths (see Hüttemeister et al. 1993 for NH$_3$ lines). In addition, the average absolute intensity of the [O i] 145 µm line, $\approx 2 \times 10^{-11}$ W cm$^{-2}$ sr$^{-1}$ (Sgr B2(M) and (N) not included), agrees within a factor of $\sim 2$ with the PDR model predictions. Finally, the low-velocity ($\approx 10$ km s$^{-1}$) C-shock models of Draine, Robarge, & Dalgarno (1983) predict weaker [O i] 145 µm line intensities. Comparing these two model predictions with the observed intensity, we estimate that the shock contribution to the [O i] emission in Sgr B2 is $10\% - 30\%$.

5. THE MOLECULAR GAS

Most pure rotational lines of light molecules appear in the far-IR and submillimeter domains. The search for these species provides a crucial insight into the chemical pathways...
leading to the observed richness in molecular clouds. Besides, the far-IR absorption measurements allow the tracing of gas that is more extended and of lower density (i.e., the envelopes) than that observed in collision-excited emission surveys. The majority of line surveys in Sgr B2 have been concentrated in Sgr B2(M) and (N) and in the millimeter domain (Cummins, Thaddeus, & Linke 1986; Sutton et al. 1991; Nummelin et al. 1998), but less or nothing is known about the possible extended distribution of the light molecular species.

5.1. Sgr B2(M)

The spectral resolution of the grating observations is rather limited (~1000 km s\(^{-1}\)) and produces strong dilution in the search for molecular features in most interstellar medium (ISM) sources. In order to have an idea of the line density and molecular carriers, we have performed a search with the LWS/FP (~35 km s\(^{-1}\)) in Sgr B2(M). Figure 8 shows the most abundant species that can be detected with ISO in the far-IR and gives insights into which could be detected with the grating in other positions. Tables 4 and 5 list the observed transitions and their corresponding references in the literature. Molecular features include several rotational lines of light O-bearing molecules such as H\(_2\)O, H\(_2\)CO, OH, and H\(_2\)O\(^+\); N-bearing molecules such as NH, NH\(_2\), and NH\(_3\); other diatomic species such as CH, HD, or HF; and low-energy bending modes of nonpolar carbon chains such as C\(_2\) or C\(_3\) (only in the grating). The list of detected molecules could still increase, since several weak features remain unidentified (see Polehampton [2002]). Atomic features include the fine-structure lines of [O \(i\)], [O \(ii\)], and [C \(i\)]. In § 5.2 we analyze the main molecular lines producing widespread absorption in LWS grating maps at lower resolution: OH, CH, and H\(_2\)O.

5.2. Widespread OH, H\(_2\)O, and CH Absorption

Although the spectral resolution in the grating is limited, the broad line widths observed toward the GC (~30 km s\(^{-1}\)), with the use of Figure 8, could help in the detection of the most abundant molecular species at a large scale. In Sgr B2 we have confidently detected prominent absorption from the ground-state rotational lines of OH (\(\sim 79\) and \(\sim 119\) \(\mu m\), CH (\(\sim 149\) \(\mu m\)), H\(_2\)O (\(\sim 179\) \(\mu m\)), and H\(_2\)O\(^+\) (\(\sim 181\) \(\mu m\); Cernicharo et al. 1997; possibly contaminated by H\(_2\)O\(^+\), see Goicoechea & Cernicharo 2001) in almost all positions (see Figs. 2c and 2d). This implies that light hydrides are present in a region as large as 25 pc \(\times\) 70 pc. Other molecular features produce less extended absorption/emission, and their definitive assignment will require better spectral resolution. This second group of molecular lines includes H\(_2\)O (\(\sim 180\), \(\sim 175\), \(\sim 108\), and \(\sim 101\) \(\mu m\), NH\(_2\) (\(\sim 170\) and \(\sim 166\) \(\mu m\)), OH (\(\sim 163\), \(\sim 84\), and \(\sim 53\) \(\mu m\)), and C\(_2\) or C\(_3\)H (\(\sim 58\) \(\mu m\); Cernicharo, Goicoechea, & Benalil 2002). The rest of the absorption features not present in Sgr B2(M) should be considered with caution. Note that no far-IR rotational line of CO was successfully assigned in any position at the signal-to-noise ratio (S/N) of the grating spectra. However, we have detected the CO \(J = 7\rightarrow 6\) line toward Sgr B2(M) with an emission peak at \(\sim +50\) km s\(^{-1}\) (Goicoechea, Cernicharo, & Pardo 2003). This and the LWS/FP H\(_2\)O lines from the warm molecular gas in front of Sgr B2(M) will be discussed in a forthcoming paper (J. Cernicharo et al. 2004, in preparation).

Another striking result of the cross-raster map is the presence of an unidentified absorption feature at \(\sim 117\) \(\mu m\) (U117) in all positions near the OH 119 \(\mu m\) line (see Fig. 4). This feature has a nearly constant absorption depth of \(\sim 4\%\) independent of the distance to the central position and is present in all individual scans. Prompted by this detection, we inspected the public IDA observations taken with the LWS/FP in this wavelength range. A tentative carrier is presented in § 5.3.

5.2.1. Large-Scale OH Absorption

According to the chemical models, the hydroxyl radical, OH, is an important intermediary in the formation of many molecules present in both the dense (\(n_\text{H}_2\) \(\sim 10^4\) \(\text{cm}^{-3}\); Bergin, Langer, & Goldsmith 1995) and the diffuse (\(n_\text{H}_2\) \(\sim 10^2\) \(\text{cm}^{-3}\); van Dishoeck & Black 1986) gas. The typical OH abundance in dense molecular clouds is \((0.1\rightarrow 1) \times 10^{-7}\). Enhanced abundances are predicted in molecular regions under C-shock activity (Draine et al. 1983) and in the outer layers of PDRs, where H\(_2\)O is being photodissociated (Sternberg & Dalgarno 1995). When applied to Sgr B2(M), the C-shock models (Flower et al. 1995) cannot reproduce the large OH/H\(_2\)O abundance ratio found in the warm envelope, which seems more consistent with the PDR scenario (GC02). The less self-shielded PDR layers are also a source of [O \(i\)] by means of the OH photodissociation. Although in PDRs [O \(i\)] can exist deeper in the cloud than OH (Sternberg & Dalgarno 1995), a correlation between the emission/absorption of both species is expected in the outer layers of the cloud and could be used to follow the ionized-PDR–molecular gas relation.

The present crosslike grating maps show the OH \(2\Pi_{1/2} J = 5/2 \rightarrow 3/2\) ground-state line at \(\sim 119\) \(\mu m\) (Fig. 4) and the \(2\Pi_{1/2} \rightarrow 2\Pi_{3/2} J = 1/2 \rightarrow 3/2\) cross-ladder line at \(\sim 79\) \(\mu m\) (Fig. 10) over the \(\sim 25\) pc \(\times 70\) pc region. Both lines may be blended with their \(18\text{OH}\) and \(17\text{OH}\) isotopomers because of the low resolution of the spectra. The individual OH A-doubling line components cannot be distinguished (only possible at the FP resolution; see the OH lines in Fig. 8). The \(\sim 119\) \(\mu m\) line is detected in absorption in all directions and remains strong throughout the map. The mean line absorption depth of \(\sim 20\%\) is consistent with saturated OH lines. On the other hand, the \(\sim 79\) \(\mu m\) absorption is observed below the northern \(\Delta\delta = 630''\) position, but its intensity is more sensitive to the position in the map (see Figs. 9 and 10). In fact, the \(\sim 79\) \(\mu m\) line absorption depth seems to be tracing the dust continuum variations through the region, but not necessarily OH abundances, so that OH column densities are correlated with far-IR emission (Fig. 9, top). The absorption produced by the OH \(2\Pi_{1/2} \rightarrow 2\Pi_{3/2} J = 3/2 \rightarrow 3/2\) line at \(\sim 53\) \(\mu m\) is only clearly detected toward Sgr B2(M) and (N), absorbing \(\sim 3\%\) of the dust continuum emission. The low S/N of the spectra makes the identification rather difficult in other positions. Finally, an emission line centered at \(\sim 163\) \(\mu m\) has been found in almost all positions (see Fig. 10). The line intensity, \(2\%\) of the continuum, appears to be constant across the region. The emission line probably arises from the OH \(2\Pi_{1/2} J = 3/2 \rightarrow 1/2\) line, which has been clearly detected in Sgr B2(M) with the FP (Fig. 8). Hence, it is plausible that a fluorescence mechanism (absorption of photons in the \(\sim 53\) \(\mu m\) cross-ladder line and emission in the \(2\Pi_{1/2}\) line at \(\sim 163\) \(\mu m\)) similar to that found toward Sgr B2(M) by GC02 also operates in the whole region favored by the low density of the Sgr B2 envelope and by the large far-IR continuum emission.
For these lines, a considerable fraction of the absorption is produced by the low-excitation clouds in the line of sight (see Neufeld et al. 2000). The $\Delta \delta = \pm 270''$ FP declination raster of the OH 119.442 $\mu$m line (Fig. 4a) reveals that in all observed positions, the absorption is dominated by the cold foreground gas at negative velocities, which is not associated with Sgr B2. The line almost completely absorbs the continuum emission and covers a broad velocity range, $\Delta v_{\text{FWHM}} \approx 200$ km s$^{-1}$, much larger than the FP resolution. Lines are thus saturated and imply high opacities.

Another FP line declination raster was carried out in the OH $^2\Pi_{3/2}, J = 7/2 \leftarrow 5/2$ excited state at 84.597 $\mu$m in order to follow up the excitation of the warm OH gas. This line was confidently detected only toward Sgr B2(M) and (N). This time, both lines were strictly centered at Sgr B2 velocities without appreciable foreground absorption.

The interpretation of the molecular absorption in the Sgr B2 envelope is not obvious, and realistic radiative transfer models taking into account both dust and molecular emission are needed. The dust emission plays a significant role because photons emitted by dust grains can excite the far-IR rotational transitions of molecules such as OH. In Sgr B2(M) and (N) the dust grains can also absorb the photons emitted by the molecules. For prominent molecular clouds such as Sgr B2, where the far-IR continuum emission and opacity are substantial, these conditions mean that the external envelope can absorb both the dust emission and the molecular line emission from the inner regions of the cloud (if any emission escapes the core).

The present observations have been modeled with the same nonlocal radiative transfer code (see González-Alfonso & Cernicharo 1993) that we used in the analysis of the OH lines toward Sgr B2(M) at higher resolution (GC02). Since few OH rotational lines are clearly detected in the grating spectra, we tried to estimate the approximate physical conditions leading to the observed OH extended emission/absorption. The excitation temperature in the cross-ladder and $^2\Pi_{3/2}$ lines has to be lower than the dust temperature (Table 3) in order to see the lines in absorption. In addition, the $\sim 163$ $\mu$m emission cannot be very prominent, while the $\sim 84$ $\mu$m line must be almost insignificant outside Sgr B2(M) and (N) positions (at the limited grating resolution). From this information we found that the widespread OH component has a moderate density, $n(H_2) = 10^2$–$10^4$ cm$^{-3}$, with lower limit temperatures in the range of 100 K [Sgr B2(M) and (N)] to 40 K (extended envelope). For a given temperature, larger densities give asymmetrical profiles in the $\Lambda$-doubling lines, and emission lines are also apparent in the cross-ladder transitions (not observed at the FP resolution, Fig. 8). These calculations show that the PDR diagnostics and the OH nonlocal models yield similar physical conditions for the outer layers of Sgr B2.
in the external regions of the PDR. The good [O i] 145 μm versus OH ~79 μm correlation confirms that a large fraction of the warm [O i] is produced by the photodissociation of OH and/or that it arises in the same warm OH layers.

### 5.2.2. Large-Scale H₂O and CH Absorption

Besides the OH absorption discussed in § 5.2.1, the fundamental lines coming from the rotational ground states of CH at ~149 μm and ortho-H₂O (o-H₂O) at ~179 μm (see also Cernicharo et al. 1997) are also detected in the crosssilk spectrum (Fig. 10). Therefore, in addition to the widespread ionized gas and dust emission, the Sgr B2 envelope can be characterized by its extended molecular content.

The H₂O ~179 μm map represents further evidence that water vapor is extended in molecular clouds (e.g., Cernicharo et al. 1994, 1997; Snell et al. 2000; Neufeld et al. 2003). In addition, the FP observations of the ~179 μm line (Cernicharo et al. 1997; lower panel in Fig. 10b) showed that water is present in Sgr B2 but also in the clouds in the line of sight (see also

### Table 4

| Species          | Transition | \( \lambda_{\text{tot}} \) (μm) | References |
|------------------|------------|---------------------------------|------------|
| H₂O(1,1)         | 1−1        | 1.80                            | 1          |
| H₂O(1,0)         | 2−1        | 1.80                            | 1, 2, 3    |
| H₂O(1,1)         | 2−1        | 1.80                            | 3          |
| H₂O(1,1)         | 3−1        | 1.80                            | 3          |
| NH₃(3,2)         | 1−0        | 167.68                          | 5          |
| NH₃(3,2)         | 2−1        | 165.60                          | 4          |
| OH(2−1)          | 3/2−1/2    | 163.40                          | 6          |
| OH(2−1)          | 3/2−1/2−1/2 | 163.12                          | 6          |
| C₃(2−1)          | 1−0        | 158.06                          | 5          |
| C₃(2−1)          | 2−1        | 157.74                          | 7, 8       |
| C₃(2−1)          | 3−1        | 156.19                          | 3          |
| C₃(2−1)          | 4−2        | 156.19                          | 5          |
| C₃(2−1)          | 5−3        | 153.34                          | 5          |
| C₃(2−1)          | 6−4        | 153.30                          | 5          |
| C₃(2−1)          | 7−5        | 151.70                          | 7          |
| CH(1−2)          | 3/2−1/2−1/2 | 149.39                          | 7, 10      |
| CH(1−2)          | 3/2−1/2−1/2 | 149.09                          | 7, 10      |
| C₃(2−1)          | 4−2        | 148.04                          | 5          |
| O³(2−1)         | 3P₂−1P₁     | 145.53                          | 7, 8       |
| C₃(2−1)          | 6−4        | 143.88                          | 5          |
| H₂O(1,1)         | 3−1         | 135.83                          | 3          |
| NH₃(3,2)         | 1−0        | 127.11                          | 4          |
| NH₃(3,2)         | 3−1        | 126.80                          | 7          |
| NH₃(3,2)         | 5−3        | 124.80                          | 4          |
| HF(2−1)          | J = 2−1    | 121.70                          | 11         |
| ¹⁰OH(2−1)        | 3/2−1/2−1/2 | 120.17                          | 6, 12      |
| ¹⁰OH(2−1)        | 3/2−1/2−1/2 | 119.97                          | 6, 12      |
| ¹⁰OH(2−1)        | 3/2−1/2−1/2 | 119.83                          | 13         |
| ¹⁰OH(2−1)        | 3/2−1/2−1/2 | 116.62                          | 13         |

### References

1. Goicoechea & Cernicharo 2001; 2. Cernicharo et al. 1995; 3. J. Cernicharo et al. 2004, in preparation; 4. Ceeccarelli et al. 2002; 5. Cernicharo et al. 2000; 6. GC02; 7. This paper; 8. Vastel et al. 2002; 9. Giesen et al. 2001 (with KAO); 10. Stacey et al. 1987 (with KAO); 11. Neufeld et al. 1997; 12. Lugten, Stacey, & Genzel 1986 (with KAO); 13. Polehampton et al. 2003.

### Table 5

| Species          | Transition | \( \lambda_{\text{tot}} \) (μm) | References |
|------------------|------------|---------------------------------|------------|
| OH(2−1)          | 3P₂−1P₁     | 119.44                          | 1, 2, 3    |
| OH(2−1)          | 3P₂−1P₁     | 119.23                          | 2, 3       |
| NH₃(2−1)         | 1−0        | 117.79                          | 4          |
| NH₃(2−1)         | 3−2        | 117.38                          | 4          |
| NH₃(2−1)         | 5−3        | 117.07                          | 4          |
| H₂O(1,1)         | 1−0        | 113.54                          | 5          |
| H₂O(1,1)         | 2−1        | 108.07                          | 5          |
| H₂O(1,1)         | 4−3        | 102.01                          | 5          |
| NH₃(1,0)         | (4,4)−(3,3) | 101.53                          | 7          |
| NH₃(1,0)         | (4,4)−(3,3) | 100.98                          | 5, 8       |
| NH₃(1,0)         | (6,5)−(5,5) | 100.87                          | 8          |
| NH₃(1,0)         | (6,6)−(5,5) | 100.58                          | 8          |
| NH₃(1,0)         | (5,3)−(4,3) | 100.11                          | 7          |
| NH₃(1,1)         | (4,5)−(4,4) | 99.95                           | 7          |
| OH(2−1)          | 3P₂−1P₁     | 98.74                           | 2          |
| OH(2−1)          | 3P₂−1P₁     | 89.99                           | 5          |
| NH₃(2−1)         | 3P₂−1P₁     | 88.36                           | 4          |
| OH(2−1)          | 3P₂−1P₁     | 84.60                           | 1, 2       |
| NH₃(2−1)         | (6,5)−(5,5) | 84.54                           | 2          |
| OH(2−1)          | 3P₂−1P₁     | 84.42                           | 2          |
| NH₃(2−1)         | (6,5)−(5,5) | 83.43                           | 7          |
| OH(2−1)          | 3P₂−1P₁     | 79.18                           | 2          |
| OH(2−1)          | 3P₂−1P₁     | 79.12                           | 2          |
| H₂O(1,1)         | 3−1        | 75.38                           | 5          |
| NH₃(1,1)         | (7,6)−(6,6) | 72.44                           | 7          |
| NH₃(1,1)         | (6,7)−(6,6) | 71.61                           | 7          |
| H₂O(1,1)         | 3−1        | 67.09                           | 5          |
| NH₃(2−1)         | (7,8)−(7,8) | 66.44                           | 5          |
| OH(2−1)          | 3P₂−1P₁     | 63.38                           | 7          |
| NH₃(1,1)         | (8,7)−(7,7) | 63.18                           | 9, 10      |
| OH(2−1)          | 3P₂−1P₁     | 62.73                           | 7          |
| NH₃(1,1)         | (9,8)−(8,8) | 56.34                           | 7          |
| OH(2−1)          | 3P₂−1P₁     | 53.35                           | 2          |
| OH(2−1)          | 3P₂−1P₁     | 53.26                           | 2          |
| O³(2−1)         | 3P₂−1P₁     | 51.82                           | 4          |

### References

1. Cernicharo et al. 1997; 2. GC02; 3. Storey, Watson, & Townes 1981 (with KAO); 4. This paper; 5. J. Cernicharo et al. 2004, in preparation; 6. Polehampton et al. 2002; 7. Ceeccarelli et al. 2002; 8. Goicoechea & Cernicharo 2001; 9. Lis et al. 2001; 10. Vastel et al. 2002.
the CH 2 \(J = 1/2\) ground level (Lien 1984). Therefore, the CH \(\sim 149 \mu m\) line is analogous to the fundamental OH \(2 \Sigma^+ J = 5/2 \rightarrow 3/2\) intraladder line at \(\sim 119 \mu m\). The \(\Delta\)-doubling lines are only resolved in the FP spectrum (Fig. 10d). Stacey, Lugten, & Genzel (1987) detected the CH \(\sim 149 \mu m\) lines with the Kuiper Airborne Observatory (KAO) only toward Sgr B2(M). ISO observations show that CH is present in the whole region. Furthermore, the line profile obtained with the FP toward Sgr B2(M) is very similar to that observed with KAO (at a resolution of 62 km s\(^{-1}\) and a beam of 55\(^{\circ}\)). The lines have the same broad profiles seen in fundamental lines of H\(_2\)O and OH produced by the foreground clouds not associated with Sgr B2. Two distinct absorption peaks at \(\approx 0\) and \(\approx +50\) km s\(^{-1}\) are clearly detected.

For each position in the crosslike map, the CH column density in the ground state has been estimated considering a single unresolved rotational line. The rotational line strength we have used is the sum of each \(\Lambda\)-doubling line strength calculated from the individual hyperfine transitions. The absorption across the extended region is proportional to the total CH column density. We found column densities for the \(2 \Sigma^+ J = 1/2\) ground level at \((0.8\text{-}1.8) \times 10^{15} \text{ cm}^{-2}\), with the larger values centered around Sgr B2(M) and (N). Using the FP observations (Fig. 10d), we derive a column density of \(1.7 \times 10^{15} \text{ cm}^{-2}\) for Sgr B2(M), similar to the value obtained by Stacey et al. (1987). We have also searched for several excited CH rotational lines at \(\sim 180 \mu m\), but aside from OH, no other lines have been detected (see Cernicharo et al. 1999 for undetected FP line spectra). The lack of absorption from other lines of CH rather than those connecting with the ground level suggest that the molecule is only abundant in the foreground clouds and the external layers of Sgr B2, where collisional excitation is unimportant. Thus, the above column densities can be a good approximation to the total CH column density. Only higher spectral resolution maps of the CH \(\sim 149 \mu m\) line will allow the accurate division of these column densities into the different foreground clouds. In the case of the Sgr B2(M) line of sight, only \(\sim 30\%\) of the total column density arises from Sgr B2 (Stacey et al. 1987). The lack of CH detections in excited rotational states confirms that this species predominantly appears in low-density clouds. Because of the large continuum opacity at \(\sim 149\) and \(\sim 180 \mu m\), the CH emission coming from the inner and denser regions does not contribute much to the far-IR observations. Such CH emission is observed at radio wavelengths (Stacey et al. 1987).

5.3. Far-IR Detection of NH\(_2\) and NH

In this section we report the far-IR detection of amidogen, NH\(_2\), and imidogen, NH, key radicals toward Sgr B2(M). It is the first time that the \(\alpha\)-NH\(_2\) species have been observed in the ISM. We also analyze in more detail the first detection of NH in the dense ISM (Cernicharo, Goicoechea, & Caux 2000).

NH\(_2\) is a light and floppy molecule thought to be an important reactant intermediate in the production/destruction of N-bearing molecules such as ammonia. NH\(_2\) is an asymmetrical molecule with a \(2B_1\) ground electronic state characterized by an intricaterotational spectrum. Because of the two equivalent H nuclei, ortho and para modifications can be distinguished. The spin-rotation interaction caused by the unpaired electron splits each rotational level into two sublevels, which are further split by hyperfine interactions caused by the \(14\)N nuclear spin. Additional splitting occurs in the ortho levels because of the resulting proton spin. Although its presence as a photodissociation product of NH\(_3\) in cometary spectra has been known since the early 1940s (Swings, McKellar, & Minkowski 1943), its interstellar detection had to wait 50 years until the detection of the \(1_{10} - 1_{01}\) lines of para-NH\(_2\) (p-NH\(_2\)) at millimeter wavelengths toward Sgr B2 (van Dishoeck et al. 1993). This is the only detection of the molecule reported in the ISM. Several far-IR spectral features have been recently observed in the laboratory (Gendriesch et al. 2001 and references therein). Here we report the ISM detection of some of them.
Fig. 10.—Raster map obtained with the LWS grating of the OH (~79 μm), CH (~149 μm), and H2O (~179 μm) lines. Detections of an emission feature at ~163 μm are also presented. In each box, offset positions are given in arcseconds with respect to the (0°, 0°) central position at α = 17°44′10″.61, δ = −28°22′30″ (B1950.0). The intensity scale corresponds to the continuum normalized flux and the abscissa to the wavelength. (a) NH lines detected with the LWS/FP at (0°, 0°) around ~153 μm. (b) Top: H2O 2_{12}−1_{01} apparent opacity in the north-south declination raster with main source positions labeled. Bottom: Fundamental o-H16 2 O line detected with the LWS/FP at (0°, 0°) around ~179 μm. (c) Main features of the grating raster map labeled. (d) CH and OH λ-doublets detected with the LWS/FP at (0°, 0°) around ~149 and ~79 μm, respectively.
Figure 4b (lower panel) shows the three spin-rotational components of the o-NH$_2$ 2$_{0}$=1$_{11}$ transition at ~117 $\mu$m, while only one spin-rotational component of the p-NH$_2$ 2$_{21}$=1$_{10}$ transition at ~126 $\mu$m has been detected. No more low-excitation NH$_2$ rotational lines with $E_I < 100$ K have been found. The lines are centered at Sgr B2 velocities, without absorption at negative velocities from the foreground clouds. The different spin-rotational line strengths were calculated by adding the individual hyperfine-structure line strengths that are listed in the Cologne Database for Molecular Spectroscopy catalog for NH$_2$ (Müller et al. 2001). However, ortho and para species were analyzed as two different molecules, and the energies of the para levels were referred to the lowest para level that we assign to 0 K energy. The two different spin-rotational partition functions were then computed. The theoretical line strength ratio for the three o-NH$_2$ 2$_{0}$=1$_{11}$ spin-rotational lines is 10.0/5.6/1.1 ($S_{117.8}/S_{117.4}/S_{117.1}$), while the optical depth ratio derived from FP observations is 10.0/7.3/1.7. This suggests that the $J = 5/2$–3/2 line (117.792 $\mu$m) is moderately thick. With this ratio we can compute the total opacity of the rotational transition and estimate the o-NH$_2$ column density.

Assuming a Boltzmann population of the rotational levels and excitation temperatures between 20 and 30 K ($T_{ex} \leq T_K$), we found $N$(o-NH$_2$) = (1.2 ± 0.3) $\times$ 10$^{15}$ cm$^{-2}$. We have only detected the more intense spin-rotational component of the p-NH$_2$ 2$_{21}$=1$_{10}$ transition at ~126.8 $\mu$m. The theoretical line strength ratio for the three lines is 10.0/5.5/1.1 ($S_{26.8}/S_{26.4}/S_{26.0}$). Because of the high continuum level measured by the LWS/FP in TDT 50601112 at ~126 $\mu$m and the fact that only three scans were available (low S/N), the other two components are expected to be under the detection limit of the AOT L03 observations. No definitive assignment has been done. Assuming that the component at ~126.8 $\mu$m is optically thin, we derive $N$(p-NH$_2$) ~ 4 $\times$ 10$^{14}$ cm$^{-2}$. Van Dishoeck et al. (1993) derived $N$(p-NH$_2$) = (1.3 ± 0.3) $\times$ 10$^{15}$ cm$^{-2}$ from escape probability calculations. Hence, this value has to be considered as an upper limit to the para column density if both the submillimeter (ground state) and far-IR (excited) lines arise from the same gas. It is also possible that far-IR NH$_2$ rotational lines trace a warmer component of lower column density material. Taking into account both observations, we estimate a total (ortho + para) NH$_2$ column density of (1.5–3.0) $\times$ 10$^{15}$ cm$^{-2}$. The upper limit reflects the p-NH$_2$ column density derived from submillimeter observations, while the lower limit is an estimation of $N$(p-NH$_2$) based on far-IR observations.

We have finally explored the possibility that the unidentified feature U117 at ~117.1 $\mu$m observed in all positions of the raster map (see Fig. 4) arises from the three spin-rotational components of the o-NH$_2$ 2$_{0}$=1$_{11}$ transition observed at higher resolution toward Sgr B2(M) (Fig. 4b). In that case, the widespread absorption corresponds to a nearly constant o-NH$_2$ column density of ~2 $\times$ 10$^{15}$ cm$^{-2}$. However, the unresolved NH$_2$ line in the gratings should be centered at ~117.6 $\mu$m, which prevents a definitive assignment to NH$_2$. In addition, we have studied other possible molecular contributors with significant line strength. In particular, the U117 line could also arise from several $b$-type transitions of slightly asymmetrical species such as HNO, HNCO, or HOCO$^+$, or it could be the $Q$-branch of a low-energy bending mode of a carbon chain. For example, theoretical calculations predict a 117–125 $\mu$m wavelength for the $\nu_{11}$ bending mode of C$_7$H, but no laboratory bands have ever been attributed (Kurtz & Adamowicz 1991; Martin, El-Yazal, & François 1995).

Also related to the formation/destuction of the widely observed NH$_3$ molecule is the NH radical. The NH (X$^3\Sigma^-$) rotational spectrum is also complicated by the different angular couplings between the rotation, the electronic spin, and the H and $^{14}$N nuclear spin momenta (e.g., Klaus, Takano, & Winnelisser 1997). Before our far-IR detection in Sgr B2, NH detections had only been reported in diffuse and translucent clouds (Meyer & Roth 1991). The enhanced NH column densities found in these environments have been used to support the position that N chemistry is dominated by grain-surface reactions instead of gas-phase reactions (Wagenblast et al. 1993).

The LWS/FP can only resolve different spin-rotational components of a rotational line. The two detected lines (Fig. 10a) arise from the $N = 2 \leftarrow 1$ rotational transition with the lower energy level at ~45 K. These lines peak at Sgr B2 velocities. The $N = 2 \leftarrow 1$ lines arise from Sgr B2(M) and represent the first detection of this species in a dense molecular cloud. Future observations of the $N = 1 \leftarrow 0$ transition from the fundamental ground state at ~1 THz will provide a signature of NH present in the diffuse molecular clouds of the line of sight and will complement the observations of NH in translucent clouds through its electronic spectrum. We have computed the spin-rotational line strengths from the individual hyperfine-structure line strengths listed in the JPL catalog for NH (Pickett et al. 1998). An analysis of line structure similar to that done with NH$_2$ was carried out to extract the opacity from the NH 2$_{3}$–1$_{2}$/2$_{1}$–1$_{1}$ optical depth ratio. Assuming an excitation temperature of 20–30 K, we derive $N$(NH) = (4 ± 2) $\times$ 10$^{14}$ cm$^{-2}$.

5.3.1. Nitrogen Chemistry and Shocks

The ISO observations of Sgr B2(M) have given the opportunity to observe simultaneously the NH$_3$, NH$_2$, and NH species. These molecules represent the best signature of the prevailing N-chemistry in the outer regions of the cloud. Far-IR NH$_3$ lines have been analyzed by Ceccarelli et al. (2002). Their large velocity gradient calculations showed the NH$_3$ column density in the warm absorbing layers to be (3.0 ± 1.0) $\times$ 10$^{16}$ cm$^{-2}$. Assuming that NH$_3$ far-IR and radio (Hüttemeister et al. 1995) lines arise in the same region, they derived large temperatures ($T_K \sim 700$ K), similar to those obtained from radio observations. However, the ammonia observed in absorption against the radio continuum is dominated by the molecular gas in front of the H II regions. Because of the large opacity in the far-IR, the bulk of the gas sampled by ISO refers only to the Sgr B2 envelope enclosing the star formation regions.

There is strong evidence that both the NH$_3$ heating and the observed metastable column densities can be reproduced if grain-surface formation and sputtering by low-velocity shocks are taken into account (Flower et al. 1995). In fact, the same shock models satisfactorily explain the recent NH$_3$ (Ceccarelli et al.) and NH$_2$ (this work) column densities derived from ISO observations.

The special formation conditions of gas-phase NH$_3$ (grain chemistry and mantle erosion) and its survival conditions (easily photodissociated) suggest that studies of the neutral gas in Sgr B2 by means of NH$_3$ absorption are only sensitive to its specific conditions.

We found that the observational NH$_3$/NH$_2$/NH ~ 100/10/1 column density ratio cannot be explained in terms of dark cloud models; these predict NH$_3$/NH$_2$ < 3 (Millar et al. 1991), and this ratio would be even smaller if photodissociation of
NH$_3$ were included. In addition, Sternberg & Dalgarno (1995) derived an NH$_3$/NH column density ratio of more than 2 $\times 10^3$ in the region where the incident far-UV field is completely attenuated. A PDR contribution to the observed N-bearing radicals may be possible as photodissociation products of NH$_3$. However, current models predict NH$_2$/NH $< 1$ and NH$_3$/NH $< 1$ column density ratios in the regions affected by the far-UV radiation field ($A_V < 5$ mag; Sternberg & Dalgarno 1995), which are not observed, at least in the average picture given by the large ISO/LWS beam. The large column densities of warm ammonia found in the Sgr B2 envelope (Ceccarelli et al. 2002) can still be compatible with its photodissociation if a notable enhancement in the NH$_3$ grain-surface formation and an efficient mantle erosion mechanism dominate the ammonia chemistry. Such processes occur in the widespread low-velocity shocks that liberate large amounts of NH$_3$ from the grains and also heat the NH$_3$ in the gas phase.

The chemistry in Sgr B2 is a challenging issue, since the same shock models that apparently reproduce the N-chemistry (Flower et al. 1995) fail to reproduce the O-chemistry traced by far-IR observations. The predicted H$_2$O column density is almost 2 orders of magnitude larger than that observed by ISO (Goicoechea & Cernicharo 2001; J. Cernicharo et al. 2004, in preparation), while the predicted OH column density is an order of magnitude lower than that observed (GC02). Thus, the large OH abundance seems more related to the photodissociation of H$_2$O. Recent analysis of the extended H$_2$O $1_{10} - 1_{01}$ absorption observed by the Submillimeter Wave Astronomy Satellite around Sgr B2 (Neufeld et al. 2003) and of the HDO absorption toward Sgr B2(M) and (N) (Comito et al. 2003) support the above (ISO) column densities for the water vapor. Finally, the OH absorption is correlated with the warm [O i] emission, and this could be related to the OH photodissociation in the outer layers.

6. SUMMARY

The present far-IR continuum and spectral observations of the Sgr B2 region have revealed a new perspective of the less-known extended envelope of the complex. The ISO observations show the presence of an extended component of ionized gas reaching very large distances from the regions of known massive star formation. Photoionization models show that high effective temperatures are possible if the ionization parameter is low. We found that the radiation can be characterized by a hard ionizing continuum typical of an O7 star ($T_{\text{eff}} \approx 36,000$ K) and that the ionization of the Sgr B complex is dominated by Sgr B2.

We suggest that the whole region must be highly clumped and/or fragmented, so that the diffusion of the far-UV radiation field allows the ionized/neutral (warm)/neutral (cold and dense) material to exist throughout the cloud. However, the exact three-dimensional locations of the ionization sources relative to the extended cloud are not clear, but the regions preferably illuminated by the UV radiation are determined (southern and eastern regions). It is plausible that the moderate-density cloud around Sgr B2(M) and (N) blocks the ionization radiation in the northern and western directions.

Another possibility is the presence of evolved stars and/or young massive stars in the envelope of Sgr B2 itself, so that the UV field on the extended cloud is the average interstellar field. The observed X-ray emission could also play a role in the large-scale ionization, but the effects on the neutral gas are more difficult to determine. In any case, we have presented observational evidence that gas is photochemically active far from the ionizing sources. This is reflected in the neutral gas heating and in the column densities of some molecules.

In addition, molecular tracers and atomic fine-structure tracers do not show evidence of high-velocity shocks. Hence, the ionized gas cannot be explained in terms of high-velocity dissociative shocks. It seems that the well-established, widespread, low-velocity shocks (Hüttemeister et al. 1995; Martín-Pintado et al. 1997) are not the only mechanism heating the gas to temperatures higher than those of the dust. The coexistence of mechanical- and radiative-type heating mechanisms based on the effects of a UV radiation field that permeates an inhomogeneous medium seems to be the rule in Sgr B2 and also in the bulk of GC molecular clouds observed by ISO (N. J. Rodríguez-Fernández et al. 2004, in preparation).

According to the extended distribution of molecular species such as H$_2$O, OH, and CH and the large column density of key molecular species detected in the Sgr B2(M) position, Sgr B2 is one of the richest and most peculiar clouds in the Galaxy. The geometrical properties of Sgr B2 (clumped structure, extended envelope, centrally condensed hot cores, and compact H ii regions), its physical conditions (high average densities, widespread warm gas, cool dust, turbulence, and an enhanced interstellar radiation field), and its chemical complexity (some molecules detected only toward Sgr B2 and nowhere else in the Galaxy, extended emission of refractory molecules, etc.) mimic a miniature Galactic center with only a $\sim$15$^\circ$ extent. Therefore, Sgr B2 provides a good template for studying the main physical and chemical processes in a galactic nucleus with enough spatial resolution, from the developing clusters of hot stars to the regions without significant luminous internal heating sources that are exposed to the mean GC environmental conditions.

The actual far-IR spectral and spatial resolutions make a similar analysis of other galactic nuclei rather speculative. However, it seems tempting that extrapolating the far-IR spectrum of $\approx 10^3$ Sgr B2 clouds to a distance of a few megaparsecs yields a spectrum similar to those of normal and IR galaxies, such as Arp 220. Recent application of PDR models to different samples of galaxies observed in the far-IR shows that the physical conditions of extragalactic PDRs do not differ much from the values derived for Sgr B2 (WHT90; Malhotra et al. 2001). Hence, Sgr B2 also plays a template role for extragalactic ISM studies.

To summarize, we have carried out medium-resolution ($\sim 1000$ km s$^{-1}$) mapping from 43 to 197 $\mu$m of the Sgr B2 region ($9' \times 27'$) and have observed the Sgr B2(M) central source at high resolution ($\sim 35$ km s$^{-1}$). The main conclusions of this work are as follows:

1. The far-IR spectra show an extended region of strong dust emission ($L_{\text{IR}} \approx 10^7 L_{\odot}$). The observed continuum emission is best fitted with a dust component with a temperature of 13–22 K and a warmer component with a temperature of 24–38 K. The warmer component contributes less than 10% to the total optical depth.

2. The [O iii], [N iii], and [N ii] fine-structure line emission has revealed an extended component of ionized gas. The average electronic density is $\sim 240$ cm$^{-3}$. The ionizing radiation can be characterized by $T_{\text{eff}} \approx 36,000$ K but with a low ionization parameter. The total number of Lyman photons needed to explain such a component is approximately equal to that of the H ii regions within Sgr B2. The southern regions of the Sgr B...
The H$_2$/OH/O$^0$ chemistry in the envelope seems dominated by photodissociation processes, while the NH$_3$/H$_2$/NH $\sim 100/10/1$ column density ratios are still better explained by low-velocity shock activity.

Future far-IR heterodyne instruments, such as the Heterodyne Instrument for the Far Infrared on board the Herschel Space Observatory, will observe the Sgr B2 region and other galactic nuclei with larger spatial and spectral resolution than ISO. A direct observation of the inhomogeneous nature of the ionized gas, the warm PDRs, and the shocked regions will then be possible.

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