Non-equilibrium $\text{H}_2$ ortho-to-para ratio in two molecular clouds of the Galactic Center

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Abstract. We present ISO observations of the S(0), S(1), S(2), and S(3) rotational lines of molecular hydrogen from two molecular clouds near the Galactic Center (GC). We have also measured continuum dust emission at infrared wavelengths with ISO and the rotational radio lines $J=1–0$ of $^{13}\text{CO}$ and $^{18}\text{O}$ and $J=2–1$ of $^{18}\text{O}$ with the IRAM-30m telescope. Using the dust continuum spectra and the CO lines we derive a total visual extinction of $\sim 1, 250$ K and the column densities of warm gas are $\sim 2 \times 10^{21}$ cm$^{-2}$. This is the first direct measure of the $H_2$ column densities of the warm component; with this, we estimate an NH$_3$ abundance in the warm gas of $\sim 2 \times 10^{-7}$. The column density of warm gas is, at least, a factor of 100 larger than the corresponding column densities derived from the warm dust. The observed ortho-to-para ratio (OTPR) is $\sim 1$, clearly below the local thermodynamical equilibrium (LTE) OTPR for gas at $250$ K of $\sim 3$. Low velocity shocks ($\sim 10$ km s$^{-1}$) are the most likely explanation for the column densities of warm gas and dust and the non-LTE $H_2$ OTPR.

Key words: ISM: clouds – ISM: molecules – ISM: dust, extinction – Galaxy: center – Infrared: ISM: continuum – Infrared: ISM: lines and bands

1. Introduction

The central $\sim 6^\circ$ of our galaxy exhibit a large accumulation of molecular material which is forming big molecular clouds whose masses and sizes are so large as $10^6$ M$_\odot$ and 15 pc, respectively. These clouds are denser (average densities of $10^4$ cm$^{-3}$ ), more turbulent (line widths of $\sim 20$ km s$^{-1}$ ), and hotter (with a warm component with temperatures, $T$, up to 200-300 K) than the clouds of the disk of the galaxy (see e.g. Morris & Serabyn 1996). The high temperatures in Galactic Center (GC) clouds were known basically by observations of NH$_3$ inversion lines over limited regions (Giusti et al. 1982, Mauersberger et al. 1986). Hüttemeister et al. (1993) analyzed 36 molecular clouds distributed all along the Central Molecular Zone and the “Clump 2” complex; they showed that high kinetic temperatures are a general characteristic of the GC clouds and not only of those located close to Sgr A and Sgr B2. In the disk of the galaxy, kinetic temperatures higher than 100 K are associated with infrared sources, that is, embedded stars which heat the dust and subsequently the gas by collisions with the dust grains. The typical sizes of such regions are less than 1 pc. The high kinetic temperatures in the GC clouds are found in regions of $\sim 10$ pc, where one measures large column densities of cold dust ($T < 30$ K, Odenwald & Fazio 1984, Cox & Laureijs 1985). This rules out gas-dust collisions as a possible heating mechanism of the warm component. Dissipation of turbulence due to shocks induced by the rotation of the galaxy could be the main heating mechanism in the GC clouds (Wilson et al. 1982).

Unfortunately the NH$_3$ abundance in the warm component was unknown since one could not estimate the warm $H_2$ column densities. The Infrared Space Observatory (ISO; Kessler et al. 1996), has allowed us, for the first time, to measure directly the total column density of warm gas by observing pure-rotational lines of $H_2$. These trace gas with temperatures of a few hundreds Kelvin. ISO has also allowed us to study the $H_2$ ortho-to-para ratio (OTPR), which can help determine the possible heating
mechanism and the origin of this molecule. Before ISO, the H$_2$ OTPR had been studied in regions with temperatures of ~ 2000 K, using the vibrational lines. In such shock-excited sources, one measures an OTPR of ~ 3 (Smith et al. 1997), which is the local thermodynamical equilibrium (LTE) value for $T \geq 200$ K. In contrast, for regions heated mainly by ultraviolet (UV) radiation (Photodissociation regions [PDRs]), the vibrational lines give OTPRs in the range of 1.2-2 (see e.g. Chrysostomou et al. 1993). However, these low OTPRs might not be a consequence of an actual non-LTE ortho-to-para abundances ratio but a result of optical depth effects in the fluorescence-pumping of the ortho-H$_2$ (Sternberg & Neufeld 1999). Using these considerations, one can explain why the PDR in S140 exhibits an OTPR ~ 2 in the vibrational states but 3 in the lowest rotational levels.

There are two cases of non-equilibrium OTPR measured from the pure-rotational lines: the shock excited source HH54 (Neufeld et al. 1998) and the PDR associated with the reflection nebula NGC 7023 (Fuente et al. 1999). The first case has been explained using the shocks model of Timmermann (1998), which involves transient heating by low velocity shocks. To explain the non-LTE OTPR in NGC 7023, it was necessary to invoke a dynamic dissociation front.

To investigate the thermal balance of the GC clouds we have selected 18 clouds from the samples of Hüttemeister et al. (1993) and Martín-Pintado et al. (1997) and we have observed them with the ISO satellite. In this paper we present H$_2$ observations toward two sources which show similar characteristics (also shown in the NH$_3$ studies of Hüttemeister et al. 1993), indicating that their heating mechanisms are also very similar. In particular, they show a non-LTE OTPR. The detection of OTPRs out of equilibrium in the GC clouds gives us new insights into the heating mechanism, since the gas must be heated to several hundreds K almost without changing the OTPR of cold gas.

In Sects. 2 and 3, we present observations and results, respectively, and in Sect. 4 we discuss the possible heating mechanism and the origin of the non-equilibrium OTPR.

2. Observations and data reduction

2.1. ISO observations

We observed the pure-rotational H$_2$ lines S(0), S(1), S(2), and S(3) with the Short Wavelength Spectrometer (SWS; de Graauw et al. 1996) on board ISO toward two molecular clouds. The galactic coordinates and ISO beam sizes are given in Table 1. These sources are among the farthest from the dynamical center of the galaxy in our sample. M+3.06+0.34 [$\alpha$(2000) = 17$^\circ$ 51′ 26″.4, $\delta$(2000) = -26°08′29.4″] is located in the “Clump 2” complex (Stark & Bania 1988), while M+1.56−0.30 [$\alpha$(2000) = 17$^\circ$ 50′ 26″.6, $\delta$(2000) = -27°45′29.5″] belongs to the “l=175-complex” (Bally et al. 1998). The observations were made during orbits 313 (S(0) and S(3) lines), and 467 (S(1) and S(2) lines). The wavelength bands were scanned in the SWS02 mode with a typical on-target time of 100 s. The spectral resolution ($\lambda/\Delta \lambda$) of this mode is ~ 1000-2000 corresponding to a velocity resolution of ~ 150-300 km s$^{-1}$. All the lines have broader profiles than those expected for a point source by a factor 1.3-1.5, indicating that the sources are extended in the direction perpendicular to the slit (see Valentijn & Van der Werf 1999). The flux calibration is believed to be accurate to 30%, 20%, 25%, and 25% for the S(0), S(1), S(2), and S(3) lines, respectively (Salama et al. 1997). Data reduction was carried out with version 6 of the SWS Interactive Analysis at the ISO Spectrometer Data Center at MPE. Further analysis has been made using the ISAP software package. All lines have been rebinned to one fifth of the spectral resolution of the instrument. Fig. 1a-b shows the spectra, and the observed parameters are given in Table 1. The errors in the radial velocities of the H$_2$ lines listed in this table have been estimated from the Gaussian fits. The wavelength calibration uncertainties, expressed in velocities, are typically of 20-40 km s$^{-1}$ for $\lambda > 12 \mu$m and ~ 25-60 km s$^{-1}$ for $\lambda < 12 \mu$m (Valentijn et al. 1996). Thus, the calibration uncertainties usually dominate the global error in the radial velocities. When one takes into account the errors from the Gaussian fits and the wavelength calibration uncertainties, the central velocities of the H$_2$ lines are in agreement with those measured from the CO lines (section 2.2). It is noteworthy that, the higher the signal-to-noise ratio of the H$_2$ lines (S(1) lines), the better the agreement of the H$_2$ radial velocities with those of CO.

We also present Long Wavelength Spectrometer (LWS; Clegg et al. 1996, Swinyard et al. 1996) observations of these sources in grating mode (43-196.7 $\mu$m, $\lambda/\Delta \lambda \sim 200$). Fig. 1c-f shows the LWS spectra. The spectral resolution was 0.29 $\mu$m for the 43-93 $\mu$m range and 0.6 $\mu$m for the 80-196 $\mu$m range. The LWS aperture was ~ 80′′ × 80′′. The roll angle, which gives the orientation of the apertures, was 90° ± 2° for both the SWS and the LWS observations. Data were taken during orbits 315 and 318 and processed through the LWS Pipeline Version 7. The individual detector scans were calibrated to within 10% of each other, based on overlapping detectors. Post-pipeline analysis (including shifting the different detectors using dark currents and defringing) was performed with ISAP.

2.2. IRAM 30-m observations

The J=1−0 line of $^{13}$CO and C$^{18}$O and the J=2−1 line of C$^{18}$O were observed simultaneously with the IRAM 30-m

1 The ISO Spectral Analysis Package (ISAP) is a joint development by the LWS and SWS Instrument Teams and Data Centers. Contributing institutes are CESR, IAS, IPAC, MPE, RAL and SRON.
telescope (Pico Veleta, Spain) in May 1997. We used two SIS receivers at 3 and 1.3 mm connected to two 512 × 1 MHz channel filter banks. This configuration provided a velocity resolution of 2.7 and 1.4 km s⁻¹ for the J=1–0 and J=2–1 lines respectively. Typical system temperatures were ∼ 250 K for the J=1–0 line and ∼ 500 K for the J=2–1 line. The receivers were tuned to single side band with rejections always larger than 10 dB that were checked against standard calibration sources. The beam size of the 30-m telescope was 22″ and 11″ at 3 and 1.3 mm respectively. Pointing and focus were monitored regularly. Pointing corrections were always found to be smaller than 3″. Calibration of the data was made by observing a hot and cold loads with known temperatures, and the line intensities were converted to main beam brightness temperature, TMB, using main beam efficiencies of 0.74 and 0.48 at 3 and 1.3 mm respectively. The spectra are shown in Fig 1c-d and the observed parameters as derived from Gaussian fits are listed in Table 2.

3. Analysis

In Fig. 2 we show the H$_2$ rotational diagrams for the two sources. The open squares correspond to the column densities as measured with ISO, without any correction for the different apertures in the different lines and for the dust extinction. The rotational diagrams for the two sources show a zig-zag distribution since the column densities in the ortho-H$_2$ levels J=3 and 5 are lower than those expected from the para-H$_2$ levels for the LTE OTPR. For the typical temperatures involved in these transitions (∼ 200 K), the LTE OTPR is ∼ 3. Similar rotational diagrams derived from the H$_2$ pure-rotational lines have been previously found in HH54 by Neufeld et al. (1998) and in NGC7023 by Fuente et al. (1999). For these sources where extinction is known to be low, the immediate conclusion was that the OTPR was not in LTE.

The H$_2$ emission has been detected in all sources of our sample indicating that the H$_2$ emission in the GC must be relatively widespread and extended (Martín-Pintado et al. 1999b). This is also suggested from the measured linewidths of the H$_2$ lines (see Section 2). Anyhow, even in the extreme case that the H$_2$ emission were point-like, the corrections for the different apertures would be small and would not affect substantially the conclusions about the OTPR. For a point-like source the S(0) line will be more diluted than the S(1) and S(2) lines because of the larger beam (20″ × 27″ instead of 14″ × 27″). The situation for the S(3) line will be the opposite since the aperture at this wavelength is 14″ × 20″. Therefore, in this limit case, the column densities in the level J=2 (derived from the S(0) line) averaged in a beam of 14″ × 27″ would be larger by a factor of 1.4, while on the opposite, the beam-averaged column density in the J=5 level would be smaller by a factor of 1.4. Hence, the correction for different apertures, cannot explain the zig-zag distribution in the rotational diagram.

A more critical correction is that for the extinction produced by the foreground material. As described by Martín-Pintado et al. (1999b), the weakness of the S(3) line in the GC clouds should be due to the extinction produced by the silicate feature at 9.7 μm in the foreground dust clouds. In clouds with a LTE H$_2$ OTPR, one can use the intensity of the S(3) line to estimate the visual extinction once the relative value for the opacity at 9.7 μm to the 0.55 μm opacity is known. One could, in principle, apply corrections for increasing extinctions until the column density in the J=5 level is consistent with the column densities derived for other levels, i.e., until the rotational plot is a straight line (in the case of a Boltzmann distribution with one source temperature) or a smooth curve (in the case of a temperature gradient). In clouds with a non-equilibrium OTPR one could use an equivalent method using only ortho-H$_2$ levels, but obviously more than two levels are needed. The effect of foreground extinction on the rotational diagram is illustrated in Fig. 2 where the observed fluxes have been corrected for 30 (filled triangles) and 60 mag (filled circles) of visual extinction, using the extinction law of Draine & Lee (1984). Visual extinctions larger than 60 mag are needed for consistency between the S(1) and S(3) line intensities and a LTE OTPR. In this case, the curvature of the rotational plots suggests the presence of a large temperature gradient in the H$_2$ emitting region. To constrain the visual extinction toward these sources, in the following sections we will estimate the total column densities of dust and gas from measurements of the continuum dust emission, 13CO, and C$^{18}$O with a similar resolution to that of the SWS aperture.

3.1. H$_2$ column densities from C$^{18}$O and 13CO observations

We applied the Large Velocity Gradient (LVG) approximation to our data, to derive the physical conditions and the column densities of molecular gas from the emission of the J=2-1 line of C$^{18}$O and the J=1-0 lines of C$^{18}$O and 13CO. The lines toward the two sources show complex profiles with two velocity components. From the line intensity ratios one can see that these components have slightly different physical conditions. The C$^{18}$O J=2-1 to J=1-0 line ratio is 1.0–1.4 in M+3.06+0.34 and cannot be determined for the other source. The J=1-0 13CO to C$^{18}$O ratio ranges between 5 and 14 in M+3.06+0.34 and is > 7 in M+1.56–0.30. To within a factor of 2, these values are in agreement with the typical isotopic abundances found in the GC for carbon and oxygen (see Wilson & Matteucci 1994) indicating that the 13CO lines are optically thin. From the C$^{18}$O J=2-1 to J=1-0 ratio we derive for M+3.06+0.34 the H$_2$ densities given in Table 3 for two cases: high kinetic temperature $(T_k=100 \text{ K})$ and low kinetic temperature $(T_K=20 \text{ K})$. For those H$_2$ densi-
ties we have constrained the total column densities using the $^{13}$CO line intensities. When the C$^{18}$O lines were not detected the range of possible $^{13}$CO(1-0) column densities was obtained by changing the H$_2$ density between $10^3$ and $10^4$ cm$^{-3}$ for $T_K=100$ K and between $10^3.5$ and $10^{4.5}$ cm$^{-3}$ for $T_K=20$ K (see Hüttemeister et al. 1998). In the case of cold gas and even higher H$_2$ densities, the $^{13}$CO column densities will increase only in a factor of 1.3 since for low temperatures and densities $>10^4$ the J=1–0 transition of $^{13}$CO is thermalized. The H$_2$ column densities, $N_{H_2}$, in Table 3 have been derived from the $^{13}$CO column density and a fractional abundance with respect to H$_2$ of 5 $10^{-6}$. They are typically of a few $10^{22}$ cm$^{-2}$, in good agreement with the values given by Hüttemeister et al. (1998). With these column densities, we have derived the total visual extinction, $A_v$, using the standard conversion factor: $N_{H_2}$(cm$^{-2}$)= $A_v$(mag) $\times 10^{21}$. Thus the extinctions toward the two GC sources studied in this paper are typically of 15-20 magnitudes.

3.2. Dust column densities and temperatures

From the LWS data we can make a direct estimate of the dust temperature and the dust column densities toward both sources. Though the aperture of the LWS is larger than that of the SWS, the dust emission in the GC is relatively smooth (Odenwald & Fazio 1984) and one does not expect large variations within the LWS aperture. The spectra for the two sources have very similar shapes with the maximum of the emission at $\sim$ 100 $\mu$m, indicating that the bulk of the dust is relatively cold with temperatures below 30 K, in agreement with previous estimates (Odenwald & Fazio 1984, Gautier et al. 1984).

The data cannot be fitted with only one gray body. For simplicity, we have considered a model with two gray bodies of temperatures $T_1$ and $T_2$. The total flux, $S_\lambda$, is given by:

$$S_\lambda = \Omega [B(T_1,\lambda)(1-e^{-(1-f)\tau(\lambda)})+B(T_2,\lambda)(1-e^{-f\tau(\lambda)})]$$

(1)

where $\Omega$ is the solid angle of the continuum source, $B(T)$ is the Planck function, $f$ is the fraction of the opacity due to the warmer component ($T_2$), and $\tau(\lambda)$ is the total opacity at wavelength $\lambda$. In this model, the ratio of the visual extinction, $A_v$, to the total optical depth at 30 $\mu$m is taken from the Draine & Lee (1984) extinction law and the opacity for $\lambda > 30$ is given by:

$$\tau(\lambda) = 0.014 A_v (30 \mu m/\lambda)^\alpha$$

(2)

where $\alpha$ is the spectral index of the dust emission. In accordance with previous estimates for the envelope of Sgr B2 (Martín-Pintado et al. 1999a) and for the GC background of the core GCM 0.25+0.11 (Lis & Menten 1998), we have taken $\alpha \approx 1$. We have assumed extended emission ($\Omega = \Omega_{\text{LWS}}$) and then we have fitted the continuum spectrum with $f$, $A_v$, $T_1$, and $T_2$ as free parameters. As an example, we show in Fig. 3 the best fit to the LWS spectra towards M+1.56−0.30 obtained with $A_v$=40, $T_1$=15 K, $T_2$=27 K and $f$=0.1.

Table 4 lists the results of the parameters for the best fits for the two sources. The visual extinctions derived for the two sources are 30 and 40 mag. These values are in agreement, to within a factor of 2, with those derived from the CO data.

The dust emission is dominated by the cool ($T \sim$ 15 K) component ($\tau_2 \sim (1-f)\tau_1$), while the slightly warmer component ($T \sim$ 30 K) contributes only 10%-20% to the total optical depth ($\tau_1 \sim f\tau_2$). We can also fit the spectra with larger spectral indexes by increasing the dust column densities. For instance, an spectral index of 1.5 will increase the visual extinction to 50-100 mag. These high values of $A_v$ are very unlikely since they are almost one order of magnitude higher than the estimates made from CO (see Table 3).

Since the extinction derived from CO and the continuum accounts for the total gas and dust along the line of sight, they must represent an upper limit to the extinction to the H$_2$ emitting region. Considering the uncertainties introduced by the unknown spectral index and the many free parameters in the dust column density determination, in the following discussion we will assume that upper limits to the visual extinction of the H$_2$ emitting region are those derived from the CO emission, namely, 16 magnitudes for M+3.06+0.34 and 20 mag for M+1.56−0.30. These values are within a factor of two of estimates obtained from the total dust column density.

3.3. Warm H$_2$: ortho-to-para ratio and column densities.

As discussed at the beginning of Sect. 3 the H$_2$ OTPR depends on the correction for extinction. In the previous sections we have estimated the extinction for the two clouds and Fig 3 shows the H$_2$ rotational diagrams for M+3.06+0.34 and M+1.56−0.30 corrected for the estimated extinctions. The error bars take into account the errors in the Gaussian fits of the lines and the calibration uncertainties. From these data, we derive an ortho rotational temperature, $T_o$, from the ortho-H$_2$ levels J=3 and J=5. In the same way, one can define a para rotational temperature, $T_p$, derived from the para-H$_2$ levels J=2 and J=4, and an ortho-para temperature, $T_{op}$, derived from the ortho level J=3 and the para level J=2. These temperatures are listed in Table 5. As we see, $T_p$ is $\sim$ 250 K for both sources while $T_o$ is slightly higher (~270 K) indicating the presence of a moderate temperature gradient. This effect is more definite in other sources of our sample, where the S(4) and S(5) lines, which trace clearly higher temperatures, have also been observed (Martín-Pintado et al. 1999b). For the present sample, $T_{op}$ is $\sim$ 160 K, much smaller than $T_p$ and $T_o$ indicating a non-LTE OTPR. In
terms of these temperatures, the OTPR measured from our data will be given by:

$$\text{OTPR} = \text{OTPR}_{\text{LTE}}(T) \exp \left( \frac{1}{T_p} - \frac{1}{T_{\text{op}}} \right)$$

(3)

where OTPR\(_{\text{LTE}}(T)\) is the LTE OTPR at temperature \(T\). As mentioned before, OTPR\(_{\text{LTE}}\) is \(\sim 3\) for \(T \geq 200\) K. Using Eq. (3), one finds an OTPR of \(\sim 1\) for both sources (see Table 5). Increasing the extinction will make the H\(_2\) OTPR closer to the equilibrium value, however extinctions > 70 mag will be required to give an LTE OTPR ratio. Such large visual extinctions are very unlikely from the molecular line and continuum data discussed in the previous sections. We therefore conclude that for the two sources the H\(_2\) OTPR is not in equilibrium. Since the estimated error is \(\sim 0.4\), we can take \(\sim 1.4\) as a conservative upper limit for the OTPR in these two sources.

Extrapolating the populations in the \(J=2\) and \(J=3\) levels to the \(J=0\) and \(J=1\) levels, respectively, as two different species at temperature \(T_p\), one finds that the total column densities of warm H\(_2\) are \(\sim 2 \times 10^{21}\) cm\(^{-2}\). This must be considered as a lower limit to the actual warm H\(_2\) column density since the populations of the lowest levels (\(J=0\) and \(J=1\)) can be increased significantly by colder, though still warm (\(\sim 100\) K) gas. Of course, if extinction is higher column densities will also increase. This implies that the measured ratio of warm H\(_2\) to cold gas traced by CO is at least 15%.

High gas kinetic temperatures in these two clouds are known to be present from the NH\(_3\) observations of Hüttemeister et al. (1993). The rotational temperatures derived from the (4,4) and (5,5) metastable inversion lines of NH\(_3\) are in good agreement with the temperatures derived in this paper using the lowest H\(_2\) pure-rotational lines. Extrapolating the populations in the (4,4) and the (5,5) NH\(_3\) levels to lower levels with the rotational temperature derived for each source by Hüttemeister et al. (1993) one finds a column density of warm NH\(_3\) of \(\sim 7 \times 10^{14}\) cm\(^{-2}\) in both sources. Taking into account the warm H\(_2\) column densities given above, we find a NH\(_3\) abundance of \(2 \times 10^{-7}\), similar to the value obtained by Martín-Pintado et al. (1999a) in the expanding shells of the envelope of Sgr B2. A similar abundance is also obtained when we compare the column densities of cold (\(\sim 20\) K) NH\(_3\) (Hüttemeister et al. 1993) and the H\(_2\) column densities derived by our \(^{13}\)CO and O\(^{18}\)O data.

3.4. Warm dust column densities

If the gas and dust are coupled, one expects that the dust associated with the warm H\(_2\) component would be an intense continuum emitter in the mid- and far-IR. There is no hint of such dust component in our data, as shown in Fig. 3, where we represent (as a dotted line) the emission of a gray body with a temperature of 250 K and the size of the SWS aperture attenuated by the total column density of the cold component. The equivalent H\(_2\) column density of warm dust used to simulate the emission in Fig. 3 is only \(5 \times 10^{18}\) cm\(^{-2}\). Even this small column density should have been detected. Hence, we can rule out a dust component coupled to the warm gas with a column density larger than \(2 \times 10^{-3}\) times that of the warm H\(_2\). On the other hand, the comparison of CO emission with the cold dust emission shows agreement with the standard gas-to-dust ratio within a factor of two.

4. Discussion

4.1. Heating of the warm component

The large column densities of warm H\(_2\) and the low column densities of associated warm dust require a heating mechanism that heats selectively the gas maintaining the dust at much lower temperatures. A PDR with an incident far-ultraviolet (FUV) flux \(G_0\) of \(\sim 100\) (measured in units of \(1.6 \times 10^{-3}\) ergs cm\(^{-2}\) s\(^{-1}\)) can heat the gas via photoelectric effect in the grains to temperatures of 100-200 K in the external layers of the cloud without heating the dust to temperatures above 30 K (see Hollenbach et al. 1991). However, the large gas phase NH\(_3\) abundance, as derived in Sect. 3.3, is not possible in such a PDR scenario. The evaporation temperature of NH\(_3\) is \(\sim 75\) K, therefore it cannot be evaporated from grain mantles at only 30 K. Even in the case that evaporation occurs, the UV radiation that heats the dust would destroy the fragile NH\(_3\) molecule. This is the behavior found in NGC 7023 where the NH\(_3\) abundance is \(\sim 10^{-8}\) in the well shielded region and decreases by more than a factor of 30 towards the region where the UV radiation increases and the dust temperature is \(\sim 70\) K (Fuente et al. 1990).

Shocks have been invoked as an important heating mechanism for the GC clouds (Wilson et al. 1982; Martín-Pintado et al. 1997; Hüttemeister et al. 1998). In fact, M+1.56–0.30 belongs to the “l =1:5-complex”, where Hüttemeister et al. (1993) derived the highest SiO abundance within their sample, while the CS abundance (which traces all dense gas, not just the part that has been subjected to shocks) is not enhanced. They interpreted the SiO enhancement to be produced by large scale dynamic effects, proposing that in this complex, gas sprayed from the intersection of the \(x_1\) and \(x_2\) orbits is crashing into material that is still on \(x_1\) orbits in the context of a bar morphology. In our sample, M+1.56–0.30 is also the source with the highest SiO to CS ratio. Furthermore, Dahmen et al. (1997), studying the HNCO emission in this region, found evidence for collisional excitation by shocks.

On the other hand, M+3.06+0.34 is located close to one of the CS cores detected by Stark & Bania (1986) in the “Clump 2” complex. These dense cores are gravitationally bound but most of the CO is emitted from the lower density gas, not bound to the cores. Stark & Bania (1986) suggested that this material is the result of tidal
stripping of the cores. It is definite that shocks can play a role to explain the large column densities of warm H$_2$ and the relatively large abundances of NH$_3$, as well as the high kinetic temperatures in these clouds. In addition, transient heating by shock waves provides a natural explanation for H$_2$ OTPRs out of equilibrium.

We have compared the results of the model calculations for slow shocks by Timmermann [1998] with our H$_2$ data. Interpolating the H$_2$ line strengths predicted by the model for a preshock OTPR=1 as a function of density, we found that a shock with velocity of 10 km s$^{-1}$ and a preshock H$_2$ density of ~ 2 $10^5$ cm$^{-3}$ reproduces the observed line intensities. The results are displayed in Fig. 2 in the form of rotational plots. Open squares are the predicted column densities, while filled circles are the values derived from observations after correcting for extinction. Though the observed flux in the S(0) seems to be slightly larger than in the model, the agreement is excellent, and calibration errors can account for the discrepancies. The preshock density seems somewhat high but it is plausible since the S(3) line is apparently thermalized, which implies a lower limit to the H$_2$ density of ~ 10$^4$ cm$^{-3}$. In any event, the widespread distribution of the HCN emission (Jackson et al. 1996) shows that densities of ~ 10$^5$ cm$^{-3}$ are common in the GC.

4.2. The ortho-to-para ratio

The main processes that affect the OTPR of H$_2$ are proton exchange collisions with H$^+$ and reactive collisions with H atoms. Ortho-para conversion in grain surfaces is thought to be less efficient. The rate coefficient for the proton exchange reaction

$$H_2(\text{ortho}) + H^+ \rightleftharpoons H_2(\text{para}) + H^+ + 170.5 \text{ K}$$

is ~ 3 $10^{-10}$ cm$^3$ s$^{-1}$ (Gerlich 1996). The analogous reactions with H$_3^+$ and H$_3$O$^+$ may also occur at a similar rate (see e.g. Le Bourlot et al. 1999). This rate gives an ortho-para conversion timescale, $\tau_{\text{conv}}$, of ~ 100/n$(^+)$ yr, where n$(^+)$ represent the density of H$^+$, H$_3^+$ or H$_3$O$^+$ in cm$^{-3}$. One should note that the actual conversion time can be a factor of 10 larger than $\tau_{\text{conv}}$ (see Flower and Watt 1984).

The rate coefficient for the reactive collisions with H atoms

$$H_2(\text{ortho}) + H \rightleftharpoons H_2(\text{para}) + H + 170.5 \text{ K}$$

is ~ 8 $10^{-11} e^{(3900/T)}$ cm$^3$ s$^{-1}$ (see e.g. Le Bourlot et al. 1999). Due to the high activation barrier of this reaction (3900 K), in cold and dense molecular clouds the dominant process will be proton exchange collisions. This is also true for low velocity shocks of ~ 10 km s$^{-1}$ since the maximum temperature achieved in the post-shock region is only ~ 300 K. If the H$^+$ and H$_3^+$ densities (n(H$^+$), n(H$_3^+$)) in the postshock region of a 10 km s$^{-1}$ shock were as high as ~ 10$^{-3}$ cm$^{-3}$ (see Timmermann 1998), $\tau_{\text{conv}}$ would be ~ 10$^5$ yr. It is worth-noting that recent models for ortho-para conversion in shocks by Wilgenbus et al. 2003 find much lower H$^+$ and H$_3^+$ densities in the postshock region. In this case, the timescale for ortho-para conversion would be > 10$^5$ yr. On the other hand, the time needed for the passage of the proposed 10 km s$^{-1}$ velocity shock, from the point where the neutral gas starts to heat up to the point where the gas has reached interstellar temperatures again, is < 10$^4$ yr (see Timmermann 1998). However the timescales in which the neutral gas is at high temperatures are much shorter. Hence, if the initial OTPR was lower than 3, the heating-cooling of the gas is too fast for the OTPR to reach the equilibrium at the temperatures of the shocked material.

Shocks with velocities > 20 km s$^{-1}$ heat the gas to temperatures > 700 K. Then, collisions with H would be the main ortho-to-para conversion mechanism, and indeed, the ortho-para conversion timescale would be low enough to obtain at least some conversion in the shock timescale as in the source HH54 (Neufeld et al. 1998). However, the lines ratios in M+1.56-0.30 and M+3.06+0.34 cannot be explained with a preshock OTPR of < 1 and a shock with velocity >10 km s$^{-1}$. Therefore, the observed OTPR in these clouds must be approximately the preshock OTPR. This conclusion is independent of any shock model since the low temperatures involved by a 10 km s$^{-1}$ shock are not sufficient for the H$_2$-H reactive collisions to be effective and, even for the largest predicted H$^+$ and H$_3^+$ abundances, the proton exchange reactions are not fast enough to give ortho-para conversion in the shock timescale.

If the OTPR of the preshock gas was in equilibrium at the gas temperature, the temperature should be ~ 80 K. In this case, the preshock gas should have been already heated before the shock front compresses and heats the gas to 250 K. However, there is no strong reason to believe that the preshock OTPR should be in equilibrium at the preshock temperature. The H$_2$ molecule is formed mainly on the grain surfaces by a highly exothermic reaction. Thus, if it is rapidly ejected to gas phase the OTPR will be the typical OTPR at high temperature, i.e., 3. On the other hand, if it is not evaporated immediately from the grain there will be ortho-to-para conversion by collisions with radicals, impurities or defects and the OTPR could reach the equilibrium value at ~ 30 K (dust temperature) of ~0.01. In our case, the preshock OTPR of ~ 1 suggests that the H$_2$ molecules were ejected from the grains with OTPR > 1. Afterwards, this ratio could decrease due to proton exchange processes.

The equilibrium proton abundance in dense ($n$(H$_2$) ~ 10$^5$ cm$^{-3}$) clouds, where photoprocesses are not important, depends mainly on the ionization by cosmic rays and on charge exchange reactions with neutral molecules. Modeling the chemistry of dense PDRs, Sternberg and Dalgarno (1997) found $n$(H$^+$) of ~ 10$^{-5}$ cm$^{-3}$ in the well UV-shielded region for a cosmic ray ionization rate ($\zeta$) of
pose the following scenario. H$_2$ is formed in the grain surfaces and ejected to gas phase with OTPR $\leq$ 3. After $\sim 10^6$ years, the time required to reach the preshock OTPR = 1, a low velocity shock heated the gas to the observed temperatures of 250 K, but the OTPR was almost unaltered because the timescale for the passage of such a shock is much shorter than the ortho-to-para conversion timescale. Taking into account the shock timescale this occurred less than $10^4$ yr ago. It is interesting to note that the timescale of the cloud’s galactic rotation period is also $\sim 10^6$ years. This fact suggests that the origin of the shocks can be related to large scale dynamics of the GC region.

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In their model these proton densities were obtained with \( \zeta = 10^{-17} \) to \( 10^{-18} \) s$^{-1}$ using a simplified chemical network.
Table 3. Derived physical conditions for the $^{13}\text{CO}$ and C$^{18}$O lines for $T_K=20$ K and $T_K=100$ K

| Source | $T_K$ | log($n(H_2)$) | $N_{^{13}\text{CO}}$ | $N_{H_2}$ |
|--------|-------|---------------|---------------------|-----------|
|        | K     | cm$^{-3}$     | $10^{16}$ cm$^{-2}$ | $10^{21}$ cm$^{-2}$ |
| M+3.06$+0.34$ | 100 | 3.8 | 5.8 | 8 | 12-16 |
| M+3.06$+0.34$ | 20 | $>3.3$ | $\leq 8$ | $\leq 16$ |
| M+1.56$-0.30$ | 100 | 3-4$^a$ | 2.8-10.2 | 5.7-20 |
| M+1.56$-0.30$ | 20 | 3.5-4.5$^a$ | 2.8-8.1 | 5.6-16.2 |

$^a$ When C$^{18}$O is not detected, we have used, following Hüttemeister et al. (1998), $n(H_2) \sim 10^{3-4}$ cm$^{-3}$ when $T_K=100$ K and, $n(H_2) \sim 10^{5-5.5}$ cm$^{-3}$ when $T_K=20$ K.

$^b$ Contains the contribution from both velocity components. Dispersion in the column densities are due to errors from the Gaussians fits to the spectra.

Table 4. Parameters of the best fits to the LWS spectra with two gray bodies assuming $\alpha=1$ and $\Omega = \Omega_{\text{LWS}}$: Temperatures, ratio of the opacity in the warmer component to the total opacity, and total visual extinction. Numbers in parentheses are 1$sigma$ errors of the last significant digit.

| Source | $T_1$ | $T_2$ | $f$ | $A_v$ |
|--------|-------|-------|-----|-------|
| M+3.06$+0.34$ | 14(4) | 24(2) | 0.2(2) | 30(20) |
| M+1.56$-0.30$ | 15(4) | 27(3) | 0.1(1) | 40(20) |
Fig. 1. Spectra of the two sources: a-b H$_2$ spectra taken with the SWS. c-d IRAM-30m spectra of the C$^{18}$O(1–0), $^{13}$CO(1–0), and C$^{18}$O(2–1) lines. e-f LWS full grating spectra. Note the different radial velocities ranges in Fig. 1a-b and Fig. 1c-d.

Table 1. Observational parameters of the H$_2$ lines. Fluxes in units of $10^{-20}$ W cm$^{-2} \cdot$ Hz$^{-1}$, Heliocentric velocities ($v_{\text{lsr}}$) in km s$^{-1}$. Numbers in parenthesis are 1σ errors of the last significant digit of the Gaussian fits.

| Wavelength | Aperture | Flux | $v_{\text{lsr}}$ | Flux | $v_{\text{lsr}}$ | Flux | $v_{\text{lsr}}$ | Flux | $v_{\text{lsr}}$ |
|------------|----------|------|----------------|------|----------------|------|----------------|------|----------------|
| M+3.06+0.34 | 20'×27' | 6.9(6) | -13(7) | 19.6(6) | 3(4) | 16(3) | -30(20) | 1.6(5) | 80(20) |
| M+1.56–0.30 | 8.1(9) | -80(10) | 19(1) | -43(4) | 14(3) | -50(20) | 1.1(4) | -30(20) |
Fig. 2. Rotational plots. The results are displayed for three different values of the visual extinction: 0, 30, and 60 mag. We can see the typical zigzag distribution of a non-LTE OTPR. Extinctions higher than 60 mag are needed to have the smooth characteristic curve of emission arising from gas with an equilibrium OTPR and a temperature gradient.

Fig. 3. The LWS spectrum of M+1.56−0.30. The thick solid line is the best fit with two components of temperatures 15 K (dashed line) and 27 K (dot-dashed line). The solid line is the total emission for an equivalent column density of $N_{\text{H}_2} = 5 \times 10^{18} \text{ cm}^{-2}$ of hot (250 K) dust with $\Omega = 20' \times 20'$ (dotted line) located behind the cold dust. We have assumed that the hot component is extincted by the cold component.
**Fig. 4.** Rotational plots after correcting for the most probable extinctions. The slope of the lines is proportional to the inverse of the temperature. $T_p$ is the rotational temperature between the para-H$_2$ levels, $T_o$ between the ortho-H$_2$ levels, and $T_{op}$ between the ortho-level $J=3$ and the para-level $J=2$. Error bars take into account the calibration uncertainties and the errors in the Gaussian fits.

**Fig. 5.** Filled circles and error bars as in Fig. 4 Empty squares are the expected column densities using the model of Timmermann (1998) with preshock density $\sim 2 \times 10^5$ cm$^{-3}$, shock velocity 10 km s$^{-1}$, and preshock OTPR=1.
Table 2. Observational parameters of the C$^{18}$O and $^{13}$CO lines. Digits in parentheses are the errors in the last significant digits (rms of the Gaussian fits). For C$^{18}$O(2–1) linewidths were fixed, when detected, to that of the C$^{18}$O(1–0) lines.

| Source       | Position $v_{lsr}$ $^{13}$CO km s$^{-1}$ | C$^{18}$O(1–0)$^{a}$ $^{b}$ | C$^{18}$O(2–1)$^{a}$ | $^{13}$CO(1–0) $^{a}$ |
|--------------|----------------------------------------|-----------------------------|---------------------|---------------------|
|              | $\Delta v$ km s$^{-1}$ $T_{MB}$ K     | $\Delta v$ km s$^{-1}$ $T_{MB}$ K | $\Delta v$ km s$^{-1}$ $T_{MB}$ K | $\Delta v$ km s$^{-1}$ $T_{MB}$ K |
| M+3.06+0.34  | 10.5(4) 6(1) 0.80(5) 6(0) 0.8(2) 10(1) 2.3(2) |
| M+1.56−0.30  | -51(1)  8(3) 0.44(5) 8(0) 0.6(2) 18(2) 2.6(2) |
|              | -24.1(6) 8(3) 0.44(5) 8(0) 0.6(2) 18(2) 2.6(2) |

$^{a}$ Limits are 3σ assuming the same $\Delta v$ than that for the $^{13}$CO.

Table 5. Para, ortho, and ortho-para rotational temperatures, OTPR and H$_2$ column densities. Numbers in parentheses are 1σ errors.

| Source       | $T_p$ (K) | $T_o$ (K) | $T_{op}$ (K) | OTPR | $N_{H_2}$ ($10^{21}$ cm$^{-2}$) |
|--------------|-----------|-----------|--------------|------|-------------------------------|
| M+3.06+0.34  | 260(30)   | 280(20)   | 160(20)      | 0.9(0.4) | 2.6(1.0) |
| M+1.56−0.30  | 250(20)   | 270(20)   | 160(20)      | 1.0(0.4) | 2.1(0.8) |