SPITZER OBSERVATIONS OF HH 54 AND HH 7–11: MAPPING THE H$_2$ ORTHO-TO-PARA RATIO IN SHOCKED MOLECULAR GAS

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ABSTRACT

We report the results of spectroscopic mapping observations carried out toward the Herbig-Haro objects HH 7–11 and HH 54 over the 5.2–37 μm region using the Infrared Spectrograph on the Spitzer Space Telescope. These observations have led to the detection and mapping of the S(0)–S(7) pure rotational lines of molecular hydrogen, together with emissions in fine-structure transitions of Ne$^+$, Si$^+$, S, and Fe$^+$. The H$_2$ rotational emissions indicate the presence of warm gas with a mixture of temperatures in the range 400–1200 K—consistent with the expected temperature behind nondissociative shocks of velocity ~10–20 km s$^{-1}$—while the fine-structure emissions originate in faster shocks of velocity ~35–90 km s$^{-1}$ that are dissociative and ionizing. The H$_2$ ortho-to-para ratio is quite variable, typically falling substantially below the equilibrium value of 3 attained at the measured gas temperatures. The nonequilibrium ortho-to-para ratios are characteristic of temperatures as low as ~50 K, and are a remnant of an earlier epoch, before the gas temperature was elevated by the passage of a shock. Correlations between the gas temperature and H$_2$ ortho-to-para ratio show that ortho-to-para ratios <0.8 are attained only at gas temperatures below ~900 K; this behavior is consistent with theoretical models in which the conversion of para- to ortho-H$_2$ behind the shock is driven by reactive collisions with atomic hydrogen, a process that possesses a substantial activation energy barrier ($E_A/k$ ~ 4000 K) and is therefore very inefficient at low temperature. The lowest observed ortho-to-para ratios of only ~0.25 suggest that the shocks in HH 54 and HH 7 are propagating into cold clouds of temperature ≤50 K in which the H$_2$ ortho-to-para ratio is close to equilibrium.

Subject headings: ISM: abundances — ISM: clouds — ISM: molecules — molecular processes — shock waves

1. INTRODUCTION

Stars have a profound effect on the interstellar medium (ISM) that surrounds them. Stellar radiation heats—and sometimes photoionizes and photodissociates—the interstellar gas, while supersonic outflows associated with stellar birth (in protostellar outflows) and death (in supernova remnants) send shock waves propagating through the ISM. In regions of high-mass star-formation—such as the Orion Molecular Cloud, for example—many of these processes operate simultaneously, making their separate effects hard to disentangle and elucidate. In Herbig-Haro objects and supernova remnants, by contrast, the effects of shock waves can be studied in relative isolation in an environment where the stellar radiation field is not greatly enhanced.

Over more than three decades, the physics and chemistry of interstellar shock waves have been the subject of intensive study, both theoretical and observational, the results of which have been summarized in several review articles (e.g., Walmsley & Pineau Des Forêts 2005; Draine & McKee 1993). When shock waves propagate within molecular clouds, the shock velocity and magnetic field determine the fate of the gas. Fast shocks (with propagation velocities $v_g \gtrsim 40$ km s$^{-1}$ given interstellar magnetic fields of typical strength) are dissociative: they destroy molecules and may ionize the resultant atoms. Slow shocks ($v_g \lesssim 40$ km s$^{-1}$), by contrast, are nondissociative: they heat and compress the molecular gas through which they pass, and may modify its chemical composition, but molecules survive their passage. The chemical changes wrought by nondissociative shocks typically result from elevated gas temperatures or the phenomenon of ion-neutral drift (crucially important in nondissociative shocks), which can drive chemical processes that are negligibly slow in cold clouds because they are endothermic or possess activation energy barriers. The result of these processes depends critically on the timescale for key chemical reactions relative to the period of time for which shock elevates the temperature and ion-neutral drift velocities. In a previous study of HH 54 carried out with the Infrared Space Observatory (ISO), Neufeld et al. (1998, hereafter NMH98) argued that the H$_2$ ortho-to-para ratio, observed to lie significantly below its equilibrium value (~3) in the warm ($T \sim 650$ K) shocked gas in HH 54, provided a valuable probe of the relevant timescales.

The Infrared Spectrograph (IRS) on board the Spitzer Space Telescope is a powerful tool for the study of shocked interstellar gas. With a wavelength coverage of 5.2–37 μm, Spitzer IRS provides access to the S(0)–S(7) pure rotational lines of H$_2$, as well as fine-structure emissions of several atoms and ions produced in fast, dissociative shocks: Ne$^+$, Si$^+$, S, and Fe$^+$. The great sensitivity of Spitzer IRS, together with the multiplex advantage inherent in long-slit spectroscopy, allows large regions to be mapped rapidly.

In this paper we report the results of spectral line mapping in HH 54 and HH 7–11, two well-studied Herbig-Haro objects known to contain warm molecular gas. HH 7–11 is a chain of Herbig-Haro objects in the Perseus molecular cloud, associated with NGC 1333 (Snell & Edwards 1981). These objects lie in the blueshifted part of a CO outflow that originates near the protostar SVS 13. HH 7–11 has been studied extensively through observations of optical emission lines (Hartigan et al. 1989), near-IR...
emission lines of [Fe ii] (Stapelfeldt et al. 1991; Gredel 1996), H$_2$ vibrational emissions (Noriega-Crespo et al. 2002; Khanzadyan et al. 2003), far-infrared atomic and molecular lines (Molinari et al. 2000); and through high-resolution studies of CO emission (Bachiller et al. 2000). One key result to emerge from previous studies is that the hot H$_2$ emission exhibits a classic bow-shaped morphology in HH 7, with an emission peak offset from the peak emission of atomic fine-structure lines. Observations of the HH 7–11 flow have proven valuable in constraining detailed models for shock excited gas (e.g., Hartigan et al. 1987; Smith et al. 2003).

TABLE 1

| Source                  | Date       | Module | Observing Time (s) | Map Center           | Map Size (arcsec) |
|-------------------------|------------|--------|--------------------|----------------------|-------------------|
| HH 7–11 field 1         | 2004 Feb 15| SL     | ...                | 03 29 3.71           | +31 16 01.9       | 58 × 57           |
| HH 7–11 field 1         | 2004 Feb 15| SH     | ...                | 03 29 3.66           | +31 16 03.6       | 58 × 76           |
| HH 7–11 field 1         | 2004 Feb 15| LH     | 10243$^a$          | 03 29 3.66           | +31 16 03.6       | 61 × 77           |
| HH 7–11 field 2         | 2004 Feb 16| SL     | ...                | 03 29 8.61           | +31 15 26.6       | 58 × 57           |
| HH 7–11 field 2         | 2004 Feb 16| SH     | ...                | 03 29 8.56           | +31 15 28.3       | 58 × 76           |
| HH 7–11 field 2         | 2004 Feb 16| LH     | 10246$^a$          | 03 29 8.56           | +31 15 28.3       | 61 × 77           |
| HH 54                   | 2004 Apr 7 | SL     | 1133               | 12 55 51.52          | −76 56 19.1       | 47 × 64           |
| HH 54                   | 2004 Apr 7 | SH     | 3260               | 12 55 50.87          | −76 56 19.3       | 47 × 52           |
| HH 54                   | 2004 Apr 7 | LH     | 931                | 12 55 50.82          | −76 56 18.0       | 44 × 67           |

Note.—Units of right ascension are hours, minutes, and seconds, and units of declination are degrees, arcminutes, and arcseconds.

$^a$ Total for SL, SH, and LH modules.

**Fig. 1.**—H$_2$ S(0)–S(3) emission-line intensities observed toward HH 54. Logarithmic contours are shown, in steps of 0.1 dex, with the lowest contours corresponding to line intensities of $3 \times 10^{-7}$, $2 \times 10^{-6}$, $3 \times 10^{-5}$, and $1 \times 10^{-4}$ erg cm$^{-2}$ s$^{-1}$ sr$^{-1}$, respectively, for H$_2$ S(0), S(1), S(2), and S(3). The straight lines demark the regions within which each transition was mapped. The horizontal and vertical axes show the right ascension ($\Delta \alpha \cos \delta$) and declination ($\Delta \delta$) offsets in arcseconds relative to $\alpha = 12^h 55^m 53^s 40, \delta = -76^\circ 56^\prime 20^\prime 5$ (J2000.0).
The distance to HH 7–11 is a matter of debate; we adopt the value of 250 pc used by Enoch et al. (2006; see discussion in that paper, which refers to Černis 1993; Černis & Straizys 2003; Belikov et al. 2002). HH 54 is located in the Chamaeleon II molecular cloud at an assumed distance of 200 pc (Hughes & Hartigan 1992), and is known to have a large column of warm (>2000 K) shocked molecular and atomic gas (Schwartz & Dopita 1980; Gredel 1994). While it is less well studied than HH 7–11, HH 54 is notable because of an unusually large abundance of water vapor (Liseau et al. 1996) and H$_2$ ortho-to-para ratios that are below the equilibrium value expected at the observed gas temperature.

Our observations and data reduction methods are discussed in §2 and Appendix A, and the results are presented in §3. The implications of these results for our understanding of interstellar shock waves are discussed in §4. A brief summary follows in §5.

2. OBSERVATIONS AND DATA REDUCTION

One field in HH 54, and two fields in HH 7–11—one centered on HH 7 and one on the protostar SVS 13—were observed using the IRS as part of the IRAC Guaranteed Time program. The Short-Low (SL), Short-High (SH), and Long-High (LH) modules were used to provide complete spectral coverage over the wavelength range available to IRS. Maps covering fields of size $\sim$1′ × 1′ were obtained by stepping the slit perpendicular, and, in the case of SH and LH, parallel to its long axis. The observational details are provided in Table 1.

The data were processed at the Spitzer Science Center (SSC), using version 12 of the processing pipeline, and then reduced further using the SMART software package (Higdon et al. 2004), supplemented by additional routines that we have developed. The key capabilities provided by these additional routines were the removal of bad pixels in the LH and SH data, the calibration of fluxes obtained for extended sources, the extraction of individual spectra at each position sampled by the IRS slit, and the creation of spectral line maps from the set of extracted spectra.

Details of our data reduction method, as well as the various tests we performed to validate the additional routines that we developed, are discussed in Appendix A.

3. RESULTS

3.1. Spectral Line Maps

Widespread rotational emissions from molecular hydrogen, along with fine-structure emissions from atomic sulfur and several singly ionized species, were detected in each of the two sources we mapped. In Figures 1 and 2 we present maps of the...
H$_2$ line emissions detected in HH 54. The straight lines demark the regions within which each transition was mapped. The $S(1)$ through $S(7)$ lines all show morphological similarities, with most maps showing local maxima close to clumps E and K and to clump C (in the designation of Sandell et al. 1987). However, real differences in the spatial distribution of the various transitions are apparent and provide key information about the spatial variation of the H$_2$ excitation and ortho-to-para ratio; these variations are discussed in detail in § 4.2 and § 4.4 below.

Emissions in several fine-structure transitions have also been detected in HH 54. Figure 3 shows the distribution of the four fine-structure emission lines that are strong enough to map: [Ne ii] $12.8 \mu$m, [Fe ii] $26 \mu$m, [S i] $25 \mu$m, and [Si ii] $35 \mu$m transitions. The straight lines demark the regions within which each transition was mapped. The horizontal and vertical axes show the right ascension ($\Delta\alpha$ cos $\delta$) and declination ($\Delta\delta$) offsets in arcseconds relative to $\alpha = 12^h55^m53^s40$, $\delta = -76^\circ56^\prime20^\prime\prime$ (J2000.0).

Fig. 3.—Fine-structure emission-line intensities observed toward HH 54. Logarithmic contours are shown, in steps of 0.1 dex, with the lowest contours corresponding to line intensities of $1 \times 10^{-5}$, $1 \times 10^{-4}$, $5 \times 10^{-4}$, and $2 \times 10^{-3}$ ergs cm$^{-2}$ s$^{-1}$ sr$^{-1}$, respectively, for the [Ne ii] $12.8 \mu$m, [Fe ii] $26 \mu$m, [S i] $25 \mu$m, and [Si ii] $35 \mu$m transitions. The straight lines demark the regions within which each transition was mapped. The horizontal and vertical axes show the right ascension ($\Delta\alpha$ cos $\delta$) and declination ($\Delta\delta$) offsets in arcseconds relative to $\alpha = 12^h55^m53^s40$, $\delta = -76^\circ56^\prime20^\prime\prime$ (J2000.0).

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3.2. Average Spectra

We have averaged the observed spectra over several regions within the HH 54 and HH 7–11 fields, thereby obtaining substantial improvements in the signal-to-noise ratio (S/N). The resultant
spectra, plotted in Figure 8, are the averages of all spectra within a series of circular regions, the contributing spectra being weighted by a Gaussian taper (half-power beam width [HPBW] of 15″) from the center of each synthesized beam. The position of each synthesized beam is demarcated by the dotted circles in Figure 7, and the central positions are given in the caption to Figure 8.

In HH 54, we obtained average spectra for circular regions centered on the peak of the [Ne ii] emission and two peaks of the H2 emission. We denote the three circular beams HH 54FS (the peak of the [Ne ii] emission), HH 54C (the northern of the two H2 peaks, being roughly coincident with clump C identified by Sandell et al. 1987), and HH 54E+K (the southern H2 peak, roughly coincident with clumps E and K). In HH 7–11, we obtained the average spectrum for a circular region centered on the HH 7 bow shock.

The spectra plotted in Figure 8 all show very weak continua, leading to large line-to-continuum ratios even in the low-resolution module (Short-Low, with \( \lambda / \Delta \lambda \) of only \( \approx 60 \); left panel). A fairly rich spectrum of H2 rotational lines and low-excitation fine-structure lines is apparent in each case.

A total of eight H2 rotational lines and eight fine-structure lines of Ne++, Si++, S, and Fe+ (five transitions) have been detected at one or more such region. Table 2 lists the detected lines together with the mean frequency-integrated intensities for each circular region. As discussed in § 4.1, the H2 line ratios and intensities are typical of slow nondissociative shocks, while the fine-structure line intensities are in good agreement with those expected from fast dissociative shocks.

No fewer than five [Fe ii] fine-structure lines are clearly detected toward position HH 54FS. The observed spectra are shown in Figure 9, and the transitions detected are marked on the Grotrian diagram in Figure 10. The strength of the higher excitation transitions originating in the \( ^4F \) term, relative to the lower transitions within the \( ^6D \) term, is expected to be an increasing function of temperature. As discussed in § 4.1, the [Fe ii] line ratios provide a valuable probe of the physical conditions in the emitting region.

Upper limits are also obtained for two rotational transitions of water vapor that lie within the LH band and are discussed in § 4.3 below. In addition, the \( R(3) \) and \( R(4) \) rotational lines of HD have
been tentatively detected and discussed elsewhere (Neufeld et al. 2006).

4. DISCUSSION

4.1. Fast and Slow Shocks

In both sources that we observed, clear offsets between the fine-structure emissions and the molecular hydrogen emissions are evident. Similar offsets have also been observed toward Herbig-Haro objects in the GGD 37 (Cepheus A West) region (Raines 2000). The fine-structure emissions in HH 7 are offset by \( \sim 5'' \) from the bow shock, corresponding to a projected distance of \( \sim 2 \times 10^{16} \) cm for an assumed distance to the source of 250 pc. Such an offset has been observed previously in HH 7 (Stapelfeldt et al. 1991), where near-infrared emissions from \([\text{Fe} \ ii] \) and \( \text{H}_2 \) have been mapped at subarcsecond resolution by Noriega-Crespo et al. (2002) using the Hubble Space Telescope. Noriega-Crespo et al. interpreted the \([\text{Fe} \ ii] \) emissions as emerging from a “Mach disk,” in which the collimated supersonic outflow is decelerated and heated in a fast shock. In this picture, the fast shock is offset from a slower nondissociative bow shock that is driven into the ambient molecular medium, the latter giving rise to the molecular hydrogen emissions observed from HH 7. Our mid-infrared observations indicate that the \([\text{Si} \ ii] \) and \([\text{Si} \ i] \) fine-structure emissions—like the \([\text{Fe} \ ii] \) emissions—also emerge from a region offset from the bow shock. The morphology of the \([\text{Si} \ ii] \) map is most similar to the \([\text{Fe} \ ii] \) map. These observations support the two-shock picture in which the \([\text{Fe} \ ii] \), \([\text{Si} \ i] \), and \([\text{Si} \ ii] \) fine-structure emissions emerge from fast shock.

Our observations of HH 54 indicate a similar offset (\( \sim 10'' \), corresponding to a projected distance of \( \sim 3 \times 10^{16} \) cm for a source distance of 200 pc) between the fine-structure and molecular hydrogen emissions. As in HH 7, the centroid of the fine-structure emissions lies closer to the presumed source of the outflow than the \( \text{H}_2 \) emissions, consistent with the two-shock picture in which the fine-structure emissions trace a fast shock that decelerates the collimated outflow.

We have compared the observed fine-structure line intensities listed in Table 2 with predictions of the fast-shock model of Hollenbach & McKee (1989, hereafter HM89). Because the beam filling factor of shocked material is not known, line ratios provide a more valuable diagnostic than absolute intensities. Although the
Fig. 6.—Fine-structure emission-line intensities observed toward HH 7. Logarithmic contours are shown, in steps of 0.1 dex, with the lowest contours corresponding to line intensities of $1 \times 10^{-5}$, $5 \times 10^{-6}$, and $2 \times 10^{-7}$ ergs cm$^{-2}$ s$^{-1}$ sr$^{-1}$, respectively, for the [Fe II] $26 \mu$m, [S I] $25 \mu$m and [Si I] $35 \mu$m transitions. The straight lines demark the regions within which each transition was mapped. The horizontal and vertical axes show the right ascension ($\Delta\alpha \cos \delta$) and declination ($\Delta\delta$) offsets in arcseconds relative to $\alpha = 3^h 29^m 37.4$, $\delta = +31^\circ 16' 04.0$ (J2000.0).

Fig. 7.—Comparison between the distribution of $H_2$ and fine-structure emission lines. The green contours are for the $H_2$ $S(3)$ line; the red contours are for the [Ne II] $12.8 \mu$m line (HH 54) or [Si II] $35 \mu$m line (HH 7). Logarithmic contours are shown, in steps of 0.1 dex, with the lowest contours corresponding to line intensities of $2 \times 10^{-6}$, $2 \times 10^{-7}$ and $3 \times 10^{-8}$ ergs cm$^{-2}$ s$^{-1}$ sr$^{-1}$, respectively, for the $H_2$ $S(3)$, [Ne II], and [Si II] transitions. The dashed circles indicate the apertures for which average spectra are shown in Fig. 8: these are denoted HH 54E+K, HH 54FS, HH 54C (left panel, from south to north), and HH 7 (right panel).
predictions of the HM89 shock models are undoubtedly somewhat uncertain—given substantial uncertainties in the collisional excitation rates for the various transitions and in the gas-phase abundances of the various elements—the predicted \([\text{Ne} \, \text{ii}]_{12.8}/C_{22} \mu\text{m} / [\text{Fe} \, \text{ii}]_{26.0}/C_{22} \mu\text{m}\) line ratio is a strongly increasing function of the shock velocity, values \(\gtrsim 60 \text{ km s}^{-1}\) being needed to ionize Ne significantly. The \([\text{Ne} \, \text{ii}]_{12.8}/C_{22} \mu\text{m} / [\text{Fe} \, \text{ii}]_{26.0}/C_{22} \mu\text{m}\) line ratio of \(\sim 0.6\) observed in HH 54 requires a shock velocity \(\sim 80 \text{ km s}^{-1}\). In HH 7, by contrast, the absence of detectable \([\text{Ne} \, \text{ii}]_{12.8}/C_{22} \mu\text{m}\) emission places an upper limit \(v_{s} < 70 \text{ km s}^{-1}\).

TABLE 2

| Transition | WAVELENGTH (\(\mu\text{m}\)) | INTENSITY \((10^{-5} \text{ ergs cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1})\) |
|------------|---------------------------|----------------------------------|
|            | HH 54FS | HH 54C | HH 54+K | HH 7 |
| \(H_{2} \, S(0) \ J = 2–0\) | 28.2188 | 0.52 | 0.44 | 0.47 | 0.78 |
| \(H_{2} \, S(1) \ J = 3–1\) | 17.0348 | 3.68 | 3.18 | 3.99 | 3.07 |
| \(H_{2} \, S(2) \ J = 4–2\) | 12.2786 | 24.7 | 20.7 | 29.5 | 20.6 |
| \(H_{2} \, S(3) \ J = 5–3\) | 9.6649 | 24.5 | 28.9 | 22.9 | 25.6 |
| \(H_{2} \, S(4) \ J = 6–4\) | 8.0251 | 33.0 | 24.4 | 32.9 | 29.0 |
| \(H_{2} \, S(5) \ J = 7–5\) | 6.9095 | 17.0 | 14.0 | 14.3 | 12.0 |
| \(H_{2} \, S(6) \ J = 8–6\) | 6.1086 | 15.6 | 12.7 | 17.2 | 16.0 |
| \(N_{e}^{+} \, P_{5/2}^{3/2} \ P_{5/2}^{1/2}\) | 12.8149 | 1.68 | 1.03 | 0.82 | <0.36 (3 \(\sigma\)) |
| \(S^{2}P_{1/2}^{1/2} \ P_{1/2}^{1/2}\) | 25.2490 | 1.75 | 0.75 | 0.75 | 1.73 |
| \(S^{2}P_{1/2}^{1/2} \ P_{1/2}^{1/2}\) | 34.8141 | 6.07 | 2.95 | 3.43 | 4.18 |
| \(F_{6}^{4} \, D_{6}^{3/2} \ D_{6}^{3/2}\) | 5.3403 | 8.6 ± 0.8 | 6.9 ± 0.8 | 2.6 ± 1.0 | 5.6 ± 0.3 |
| \(F_{6}^{4} \, D_{6}^{3/2} \ D_{6}^{3/2}\) | 17.9363 | 0.88 ± 0.18 | 0.55 ± 0.08 | <0.5 (3 \(\sigma\)) | <0.4 (3 \(\sigma\)) |
| \(F_{6}^{4} \, D_{6}^{3/2} \ D_{6}^{3/2}\) | 24.5186 | 0.23 ± 0.04 | 0.16 ± 0.02 | 0.19 ± 0.03 | <0.12 (3 \(\sigma\)) |
| \(F_{6}^{6} \, D_{6}^{3/2} \ D_{6}^{3/2}\) | 25.9882 | 3.33 | 1.69 | 1.38 | 1.69 |
| \(F_{6}^{6} \, D_{6}^{3/2} \ D_{6}^{3/2}\) | 35.3491 | 0.92 ± 0.17 | 0.45 ± 0.11 | 0.56 ± 0.08 | 0.57 ± 0.06 |

\(^{a}\) Error bars, where given, are 1 \(\sigma\) statistical errors. When error bars are not given, the uncertainty is dominated by systematic errors, which we estimate to be \(\leq 25\%\) (see Appendix A).
while our measurement of the [Fe ii] 17.9 \( \mu \)m transition requires a shock velocity\(^5\) of at least 35 km s\(^{-1}\).

The HMS9 shock models predict that the [Fe ii] and [Si ii] line intensities show a very similar dependence on the shock velocity, while the [S i]/[Fe ii] and [S i]/[Si ii] line ratios are a decreasing function of shock velocity. This prediction provides a natural explanation for the fact that the [Si ii] map is most similar to the [Fe ii] map: insofar as the fine-structure emissions may arise from a superposition of shocks at varying velocities, the [Si i] emissions would be expected to show a spatial distribution that is somewhat different from [Si ii] and [Fe ii].

An independent check of the two-shock picture is provided by our detection of multiple [Fe ii] lines. The minimum temperature derived from the [Fe ii] line ratios (~5000 K) is larger than the maximum temperature at which \( \text{H}_2 \) can survive for any appreciable time period—and is a factor \( \sim 5 \) larger than that inferred from the \( \text{H}_2 \) line ratios (see § 4.2 below)—lending strong support to the theory that both dissociative and nondissociative shocks are present in the source.

4.2. The Temperature and Column Density of Shocked Molecular Hydrogen

The \( \text{H}_2 \) S(0)–S(7) emissions provide a valuable probe of the temperature distribution in the shocked gas in which \( \text{H}_2 \) is the dominant constituent. The observed line intensities for these \( \text{H}_2 \) quadrupole transitions provide a direct measurement of the column density, \( N(J) \) in each upper state, \( J \), because all the lines involved are optically thin. As in NMH98, we applied extinction corrections based on the interstellar extinction curves of Weingartner & Draine (2001; “Milky Way, \( R_V = 3.1 \)”). For \( \text{HH} \) 54, we adopted Gredel’s (1994) estimate of 0.3 for \( E(J - K) \), obtained from observations of the [Fe ii] 1.257 and 1.644 \( \mu \)m transitions toward \( \text{HH} \) 54E+K, while for \( \text{HH} \) 7 we adopted the estimate \( E(J - K) = 0.7 \) obtained by Gredel (1996) for the nearby source \( \text{HH} \) 8.

In Figure 11, based on the line intensities tabulated in Table 2, we present rotational diagrams for each of the four circular regions for which we computed an average spectrum (§ 3.2). Two features are common to all observed positions. First, as discussed further in § 4.4 below, the rotational diagrams all show the “zigzag” patterns characteristic of nonequilibrium ortho-to-para ratios, in which a fit to the para (even-\( J \)) states lies above that for the ortho (odd-\( J \)) states. Second, the rotational diagrams all exhibit a degree of curvature, with the slope of the rotational diagram decreasing with increasing \( J \). This curvature indicates that each beam is sampling material at a range of temperatures. Furthermore, the absence of any turnover in the curvature at high \( J \) suggests that the rotational level populations are close to local thermodynamic equilibrium (LTE) even for \( J \) as high as 9.

For each circular region in Table 2, we determined an excitation temperature, \( T_{XY} \), from the ratio of the \( J = X \) and \( J = Y \) column densities and defined according to

\[
T_{XY} = \frac{E_Y - E_X}{k \ln \left[ N_X g_Y / N_Y g_X \right]},
\]

where \( E_J \) and \( g_J \) are the energy and degeneracy of state \( J \). Because the ortho-para ratio shows departures from equilibrium, the quantity \( T_{XY} \) is most useful when \( X \) and \( Y \) are either both odd or both even. The excitation temperatures \( T_{42}, T_{53}, T_{64}, T_{75}, T_{86} \),

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\(^5\) Considerably smaller shock velocities would be obtained in a comparison with the model predictions of Hartigan et al. (1989), which apply to shocks in low-density clouds that are assumed to be ionized prior to the passage of the shock.
and $T_{97}$ are given in Table 3; the inequalities $T_{42} < T_{64} < T_{86}$ and $T_{53} < T_{75} < T_{97}$ observed in every case are a simple manifestation of the curvature apparent in the rotational diagrams.

We have obtained two-component fits to the rotational diagrams, in which a least-squares fit was obtained for a combination of warm and hot gas components, assumed to be in LTE except with non-LTE ortho-to-para ratios, with temperatures $T_w$ and $T_h$ (typically found to be ~400 and ~1000 K, respectively). The solid lines in Figure 11 show the two-component fits to the rotational diagrams, while the points indicate the measured values. The two-component fits provide an excellent fit to the data, although the solution is clearly nonunique. Indeed, there is no specific evidence for a bimodal temperature distribution, and the data could be fit equally well by models that invoke a continuous distribution of warm and hot gas components, assumed to be in LTE (typically found to be ~600 K, respectively).

The best-fit temperatures, computed under the assumption of LTE, together with the beam-averaged column densities ($N_h$ and $N_w$) and the H$_2$ ortho-to-para ratios (OPR$_h$ and OPR$_w$), are listed in Table 3. Table 3 also shows the sum of the N(4)–N(9) column densities, $N_{w-9}$, all of which are derived directly from observations with the Short-Low module; not surprisingly, $N_{w-9}$ falls a factor of several below ($N_h + N_w$) because it only includes states with $J \geq 4$. The estimated gas temperatures, $T_w$ and $T_h$, are characteristic of low-velocity nondissociative shocks (which are of “C,” or “continuous,” type in the designation of Draine 1980; see also Appendix B). By means of a simple analytic treatment of energy conservation in such shocks (Appendix B), constrained by the results of the detailed shock models of Kaufman & Neufeld (1996, hereafter KN96), we find the characteristic gas temperature within such shocks to be given by

$$T_s = 375 b^{-0.36} v_{ls}^{1.35} \text{ K},$$

(eq. [B8]), where 10$v_{ls}$ km s$^{-1}$ is the shock velocity and $b(n_0/cm^3)^{1/2}$ µG is the assumed preshock magnetic field for a shock propagating in material of preshock H$_2$ density $n_0$. Given our standard assumption about the magnetic field, $b = 1$, the warm and hot gas components typically correspond to shock velocities of ~10 and ~20 km s$^{-1}$, respectively. The H$_2$ rotational diagrams predicted by KN96 and other theoretical shock models (e.g., Wilgenbus et al. 2000) all exhibit less curvature than our observed rotational diagrams, implying the presence of a range of shock velocities within each of the circular apertures demarked in Figure 7.
The preshock H$_2$ density, $n_0$, is less well constrained by the H$_2$ line fluxes. The best estimates for the density of the warm shocked gas have been obtained by observations of high-lying rotational lines of CO, for which non-LTE line ratios provide a valuable probe. Based on ISO observations of such transitions toward HH 54, Liseau et al. (1996) estimated the H$_2$ density in the warm shocked gas as 1–4 $\times 10^4$ cm$^{-3}$. Since most of the high-J CO emission occurs before the compression of the neutral species becomes large, the corresponding preshock density is only a factor $\sim$1.5 smaller (Appendix B, eq. [B6]): $n_0$ = (6–25) $\times 10^3$ cm$^{-3}$. Similar values were obtained for HH 7–11, based on measurements of CO line ratios (Molinari et al. 2000), although measurements of the CO/H$_2$ line ratios argued for smaller values ($n_0 \sim 10^3$ cm$^{-3}$) toward HH 7.

The observed column density of shocked H$_2$ is predicted to be

$$N_s = 4 \times 10^{20} \beta n_0^{0.5} v_{\theta}^{0.75} \Phi_\ell,$$

(Appendix B, eq. [B7]), where $\Phi_\ell$ is a geometric factor defined to be the ratio of the projected beam size to the surface area of the shock. In principle, the quantity $\Phi_\ell$ can be either larger or smaller than unity. For a planar shock with a beam covering factor of unity that is viewed at angle $\theta$ to the shock normal, the observed value of $\Phi_\ell$ is $\leq 1$. On the other hand, $\Phi_\ell$ can be smaller than unity when the beam is incompletely covered by shocked material. For our two component fits to the circular apertures presented in Table 3, the values of $\Phi_\ell$ required for the warm and hot components are typically 0.2$n_0^{-0.5}$ and 0.05$n_0^{-0.5}$, respectively, implying that the shocked material has a covering factor considerably smaller than unity and possesses substruc- ture that is not resolved by these observations. In HH 7, the subarcsecond resolution maps of near-IR H$_2$ vibrational emissions presented by Noriega-Crespo et al. (2002) clearly indicate that $\Phi_\ell \ll 1$ for observations with the IRS instrument.

The spectral line maps obtained for HH 54 and HH 7 also permit us to obtain a rotational diagram at each spatial position, and thereby to derive detailed maps of the gas temperature, ortho-to-para ratio, and column density of the shocked gas. While the average spectra presented in Figure 8 are of sufficient S/N to permit the two-component fits described above, the lower S/N obtained in a single spectrum does not warrant a two-component fit to the rotational diagram. Accordingly, in constructing maps of the gas temperature, we obtained a least-squares fit to the $N(4)$ through $N(7)$ column densities (all measured with the SL module) for a single gas component with a temperature and H$_2$ ortho-to-para ratio, maps of which are presented in Figure 12 (middle and bottom panels, respectively). Here the white contours show the H$_2$ $S(3)$ line intensity, and regions of low S/N have been masked and appear in black. The top panel in Figure 12 shows the sum of the $N(4)$–$N(9)$ column densities, $N_{4-9}$. Figure 12 shows that the fitted gas temperature is remarkably constant over the mapped region, lying generally within the range 900 ± 200 K, and indicating that a similar admixture of shock velocities is present along each line of sight. The ortho-to-para ratio, however, shows substantial variations—as noted previously by Wilgenbus et al. (2001)—and is discussed further in § 4.4.

4.3. Upper Limits on the H$_2$O Abundance

The increase in temperature and density behind a shock front can alter significantly the composition of the gas in its wake. Specifically, chemical reactions not favored at temperatures characteristic of the preshock quiescent material (i.e., $T \leq 50$ K) can proceed rapidly in the warm postshocked gas. One such example are the reactions that lead to the production of gas-phase H$_2$O. In the cold preshock gas, cosmic-ray–driven ion-neutral reactions are capable of converting O and H into water yielding a peak water abundance relative to H$_2$, $x(H_2O) = n(H_2O)/n(H_2)$ of $\sim 10^{-8}$ in approximately 10$^4$ yr (Bergin et al. 1998). When the gas temperature exceeds $\sim$100 K, a series of neutral-neutral reactions, H$_2$ + O $\rightarrow$ OH + H and H$_2$ + OH $\rightarrow$ H$_2$O + H, dominate and chemical models (e.g., Elitzur & de Jong 1978; Neufeld et al. 1995) predict that most of the gas-phase oxygen not bound as CO will be processed into water vapor. These reactions are rapid in warm gas, producing $x(H_2O) \sim (2 \times 10)^{-4}$ in less than a few hundred years (Bergin et al. 1998), but are negligibly slow at low temperatures because they possess significant activation barriers.

Observations of both HH 54 and HH 7 have been conducted using ESA’s ISO. ISO’s Long Wavelength Spectrometer (LWS) was used in its grating mode to acquire low-resolution ($\Delta\nu/\Delta\nu \sim$ 200) spectra between 43 and 197 $\mu$m within an 80$''$ diameter beam. Toward HH 54, Liseau et al. (1996) detected a number of low-lying (i.e., $E/k \approx 300$ K above the ground state) H$_2$O and OH lines, along with CO emission lines from the rotational upper level $J = 14$ to 19. These data are best fit by a model that assumes collisional excitation behind a 10–15 km s$^{-1}$ nondissociative C-type shock and $x(H_2O) = 10^{-5}$.

Toward HH 7, Molinari et al. (2000) find evidence for the presence of both fast dissociative J-type and slower C-type shocks. In particular, Molinari et al. find that a 15–20 km s$^{-1}$ C-type shock accounts well for the observed strengths of the CO $J = 14$–13 to $J = 17$–16 transitions plus the H$_2$ $0(0-0)$ $S(0)$–$S(5)$ transitions, which were measured with the ISO Short Wavelength Spectrometer. Assuming that the ISO-detected H$_2$O 179.5 $\mu$m $2_{12}$–$1_{01}$ and 174.6 $\mu$m $3_{03}$–$2_{12}$ lines arise predominantly from behind the same C-type shock, Molinari et al. derive $x(H_2O) \approx 6 \times 10^{-6}$. Molinari et al. suggest that the lower-than-expected postshock H$_2$O abundance is due to the rapid condensation of water onto dust grains in the postshocked gas. A similar effect is observed toward IC 443, in which a low water abundance ($2 \times 10^{-8} < x(H_2O) < 3 \times 10^{-7}$) is inferred in the presence of both C- and J-type shocks (Snell et al. 2005). Snell et al. ascribe the low water abundance to a combination of two effects. First, more than half of the preshock oxygen not in CO remains trapped as water ice on grain surfaces despite the passage of a weak C-type shock, suppressing the production of gas-phase H$_2$O in the postshocked gas. Second, ultraviolet radiation generated by the nearby fast J (or “jump”) type shock photodissociates much of the gas-phase water produced behind the C-type shock.

Eight H$_2$O transitions with upper state energies $E_u/k < 10000$ K lie within the wavelength range accessible to Spitzer IRS. Prior to the measurements reported here, none of these transitions had been observationally investigated toward either HH 54 or HH 7. To assess the extent to which the upper limits to the H$_2$O line strengths set here constrain the water abundance, the equilibrium level populations of all ortho and para rotational levels of the ground H$_2$ $^16$O vibrational state with energies $E/k$ up to 7700 K have been calculated using an escape probability method described by Neufeld & Melnick (1991). Only two updates have been made in the calculations undertaken here: (1) for collisionally induced transitions among the lowest 45 levels of ortho- and

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6 Liseau et al. significantly overestimated the compression of the neutral material, thereby obtaining a significant underestimate of the preshock density required to match the CO line ratios.

7 Snell et al. expressed their findings in terms of the ratio $n(o-H_2O)/n(CO)$. Here we make the assumption that $n(CO)/n(H_2) = 10^{-4}$. 
para-H$_2$O, the rate coefficients calculated by Green et al. (1993) for He-H$_2$O collisions were used (multiplied by 1.348 to account for the different reduced mass when H$_2$ is the collision partner), and (2) the expression for the photon escape probability used by Neufeld & Kaufman (1993) was adopted.

We obtain level populations for a plane-parallel emitting region in which the limit of large velocity gradient applies. A two-temperature-component model is used, consistent with the results of our H$_2$ measurements (which are summarized in Table 3). In addition, preshock densities of 10$^4$ and 10$^5$ cm$^{-3}$ are considered. The H$_2$ column densities and velocity gradients are assumed to be those consistent with the simple shock model presented in Appendix B, i.e.,

$$N(H_2) = 7.9 \times 10^{20} \left[ \frac{n(H_2)}{10^5} \right]^{0.5} \left( \frac{T_{\text{gas}}}{1000} \right)^{-0.555} \text{cm}^{-2},$$

and

$$\frac{dv}{dz} = 1.6 \times 10^4 \left[ \frac{n(H_2)}{10^5} \right]^{0.5} \left( \frac{T_{\text{gas}}}{1000} \right)^{1.30} \text{km} \text{s}^{-1} \text{pc}^{-1},$$

FIG. 12.—Maps of the H$_2$ column density (top panels), H$_2$ rotational temperature (middle panels), and H$_2$ ortho-to-para ratio (bottom panels) derived from a least-squares fit to the $J = 4, 5, 6,$ and 7 column densities. Superposed white contours (middle panels) show the H$_2$ S(3) line intensity (contours at 3.0, 4.5, 6.0, 7.5 $\times$ 10$^{-5}$ ergs cm$^{-2}$ s$^{-1}$ sr$^{-1}$ for HH 54 and 2.5, 3.5, 4.5, and 5.5 $\times$ 10$^{-5}$ ergs cm$^{-2}$ s$^{-1}$ sr$^{-1}$ for HH 7.) Regions where the S/N is inadequate to yield a fit to the H$_2$ rotational diagram appear in black.
where \( n(H_2) \) is the preshock gas density and \( T_{\text{gas}} \) is the gas temperature. Finally, we assume that the fraction of the beam filled by the warm and hot \( H_2O \) is given by the ratio of the measured values of \( N(H_2) \) (given in Table 3) to those derived above. For these conditions, the strongest water lines within the Spitzer IRS wavelength range are predicted to be the 29.837 \( \mu \)m \( 7_25-6_{16} \) and 30.899 \( \mu \)m \( 6_{34}-5_{25} \) ortho-\( H_2O \) transitions. Table 4 lists the Spitzer-measured 3 \sigma upper limits to the line intensities for each transition along with the derived upper limits to the gas-phase water abundance.

Several things are apparent. First, the upper limits to the \( H_2O \) abundance given in Table 4 are higher than, but nonetheless consistent with, the water abundances derived previously from the ISO data. In particular, for a preshock density of \( 10^5 \) cm\(^{-3}\), favored by the \( H_2 \) data toward HH 54 (Liseau et al. 1996)—the inferred abundance limits are less than would be expected from the full conversion of elemental oxygen not locked in \( CO \) into \( H_2O \). Unfortunately, the present 29.837 and 30.899 \( \mu \)m line flux limits are insufficient to allow us to comment further on the previous HH 54 models. Second, the \( H_2O \) 174 and 179 \( \mu \)m line fluxes measured by Liseau et al. provide an additional constraint on \( \chi(H_2O) \) within the warm and hot components discussed here. In particular, the ISO-measured flux in the \( H_2O \) 174 \( \mu \)m line, \( \sim 3 \times 10^{-20} \) W cm\(^{-2}\), requires that \( \chi(H_2O) < 2 \times 10^{-5} \) in the warm and hot \( H_2O \) components or these components will produce a 174 \( \mu \)m line flux in excess of that measured. This result is in agreement with the water abundance determined by Liseau et al. of \( 10^{-5} \) and suggests that the size of the \( H_2O \) 174 and 179 \( \mu \)m emitting region is larger than that inferred for the Spitzer-measured \( H_2 \) emission (or that assumed for the mid-infrared \( H_2O \) emission). This is plausible since the 174 and 179 \( \mu \)m lines probe cooler gas than either the \( H_2 \) or mid-infrared \( H_2O \) lines.

Toward HH 7, Molinari et al. estimate the preshock density to be \( \sim 10^4 \) cm\(^{-3}\). For this density, rather high \( H_2O \) abundances are required to reproduce the 29.837 and 30.899 \( \mu \)m line intensity limits. However, the strength of the \( H_2O \) 179 \( \mu \)m line observed by Molinari et al. does set a more stringent upper limit of \( \chi(H_2O) < 6 \times 10^{-4} \) within the warm and hot components measured here. Unfortunately, this limit remains significantly greater than the water abundance inferred from the ISO measurements and, thus, does not permit a test of their model.

4.4. The \( H_2 \) Ortho-to-Para Ratio

The \( H_2 \) ortho-to-para ratios (Table 3) derived for the two-component fits, \( \text{OPR}_{h} \), and \( \text{OPR}_{p} \), are uniformly less than the local thermodynamic ratio, \( \text{OPR}_{\text{LTE}} \sim 3 \) at the temperatures of relevance. This nonequilibrium behavior, first observed in the atmospheres of giant planets (e.g., Conrath & Gierasch 1983), was noted in ISO observations of HH 54 (NMH98; Wilgenbus et al. 2001) and subsequently observed in several other interstellar regions (e.g., Fuente et al. 1999; Rodríguez-Fernández et al. 2000). As discussed in NMH98, the \( H_2 \) ortho-to-para ratio equilibrates very slowly, exhibiting “memory effects” in which the OPR can reflect the temperature of a previous epoch in its thermal history. Thus NMH98 argued that the OPR of 1.0 \( \pm \) 0.4 observed toward HH 54 indicated that the warm \( (T \sim 650 \text{ K}) \) shocked \( H_2 \) that they observed in HH 54 must have previously acquired an OPR characteristic of equilibrium at a temperature \(< 90 \text{ K} \) and (2) that the observed gas has not been warm long enough for a high-temperature OPR to have been established.

The equilibration of ortho- and para-\( H_2 \) has been considered in the detailed shock models of Timmernagel (1998) and Wilgenbus et al. (2000). Both studies concluded that reactive collisions with atomic hydrogen are the dominant para-to-ortho conversion process in nondissociative molecular shocks:

\[
\text{para} - H_2 + H \rightarrow H + \text{ortho} - H_2.
\]

Because reaction (1) has a substantial activation energy barrier \((\Delta E_a/k \sim 3900 \text{ K})\), the efficiency of para-to-ortho conversion is a strong function of temperature (and, consequently, shock velocity). This strong temperature dependence is entirely consistent with the results in Table 3, which show that for each region the hot gas component has a much higher OPR than the warm gas component. This behavior is also apparent in the \( H_2 \) rotational diagrams (Fig. 11), in which the departures from LTE (i.e., the degree of zigzag) are plainly larger for small \( J \) than for large \( J \).

In Figure 13, the ortho-to-para ratios, \( \text{OPR}_{h} \), and \( \text{OPR}_{p} \), for the two-component fits in Table 3, are plotted as a function of the fitted gas temperatures, \( T_w \), and \( T_b \) (open triangles). We have also obtained two-component fits to the gas temperature and OPR elsewhere in the mapped regions. Averaging the observed spectra in a set of \( 5' \times 5' \) subregions to attain adequate S/N to yield meaningful two-component fits, we determined \( \text{OPR}_{w} \), \( \text{OPR}_{h} \), \( T_w \), and \( T_b \) estimates for each such subregion. Green and red squares in Figure 13 indicate, respectively, the \( (T_w, \text{OPR}_{w}) \) and

\footnote{Such effects are a well-known problem in the industrial production and storage of liquid hydrogen (LH2). The rapid refrigeration of molecular hydrogen leads to the production of LH2 with an ortho-to-para ratio \( <3 \), reflecting the “frozen-in” equilibrium value at room temperature, and greatly exceeding the value of 0.02 obtained at equilibrium at 21 K, the boiling point of LH2. Equilibration occurs over a timescale of 6.5 days, resulting in the eventual release of a total heat content that exceeds the latent heat of vaporization of LH2: without continued refrigeration, the LH2 simply boils away! The solution to this problem involves the introduction of a paramagnetic catalyst to facilitate ortho-to-para conversion during the original liquefaction process and thereby prevent the room temperature OPR from being frozen-in.}
where \( n(H) \) is the atomic hydrogen density and \( k_{\text{PO}} \) is the rate coefficient for para-to-ortho conversion, estimated as \( 8 \times 10^{-11} \exp(-3900/T) \) cm\(^3\) s\(^{-1}\) by Schofield (1967), based on the laboratory experiments of Schulz & Le Roy (1965). The black curve applies to the case \( n_2(H) = 150 \) yr, where \( n_2(H) = n(H)/10^2 \) cm\(^{-3}\). If, following NMH98, we assume that H atoms are produced primarily by reaction of O with \( H_2 \) to form OH, followed by reactions of OH with \( H_2 \) to form water, we expect an \( n(H)/n(H_2) \) ratio \( \sim 10^{-3} \), corresponding to \( n_2(H) \sim 1 \) for a preshock \( H_2 \) density \( n_0 = 10^3 \) cm\(^{-3}\). The steep rise in the black curve at \( T \sim 1000 \) K is a consequence of the strong temperature-dependence of \( k_{\text{PO}} \). To within the likely errors, all the points lie between the black and orange curves in Figure 13. This behavior then implies that all the shocked gas had an initial OPR between 0.4 and 3 and has been warm for at least 150\(n_2(H)\)\(^{-1}\)yr. The foregoing analysis is premised on the assumption that the rotational temperature inferred for the hot gas component is equal to the kinetic temperature. As discussed in § 4.2, above, subthermal excitation of the \( S(7) \) transition is allowed by the data and would mean that the actual gas temperature is higher than the rotational temperature for the hot component, \( T_h \). Such effects, in turn, would decrease the required timescale for ortho-para conversion.

For a postshock atomic H abundance \( \sim 10^{-3} \), the timescale of 150\(n_2(H)\)\(^{-1}\)yr inferred above is broadly consistent with the time period for which gas temperature is elevated on passing through a nondissociative shock. For \( n_0 = 10^2 \) cm\(^{-3}\) and \( v_0 = 15 \) km s\(^{-1}\), the simple treatment of Appendix B implies a shock column density, \( N_s \sim 10^{21} b_{\text{in}} \) cm\(^{-3}\), corresponding to a timescale \( N_s/(n_0 v_0) \sim 200b_{\text{in}} \) yr. However, the OPR values plotted in Figure 13 are entirely inconsistent with a shock model with a large H abundance, as has been invoked by Smith et al. (2003), who proposed an \( n(H)/n(H_2) \) ratio of 3 for the bow shock in HH 7. Such a large H abundance would lead to very rapid para-to-ortho conversion, producing OPR values significantly in excess of those observed here.

We may also compare the results plotted in Figure 13 with the predictions of detailed theoretical models for para-to-ortho conversion in nondissociative molecular shocks. The cyan loci in Figure 13 represent the predictions of Wilgenbus et al. (2000) for a shock propagating in gas with an initial OPR of 0.01. The loci correspond to preshock \( H_2 \) densities of \( 10^2 \), \( 10^3 \), \( 10^4 \), and \( 10^5 \) cm\(^{-3}\), respectively, from left to right, and the asterisks apply to shock velocities of 30 and 40 km s\(^{-1}\) (\( 10^3 \) cm\(^{-3}\) case, from bottom left to top right); 20, 30, and 40 km s\(^{-1}\) (\( 10^4 \) and \( 10^5 \) cm\(^{-3}\) cases, from bottom left to top right); or 10, 15, 20, 25, and 30 km s\(^{-1}\) (\( 10^6 \) cm\(^{-3}\) case, again from bottom left to top right). As in the case of the toy model (black curve), the curves for \( 10^5 \) or \( 10^6 \) cm\(^{-3}\) are a reasonable approximation to the lower envelope of the observed data points. The absence of sight lines with high temperature and low OPR is consistent with shock models in which para-to-ortho conversion is driven by reactive collisions with atomic hydrogen. On the other hand, the presence of sight-lines with low temperature and high OPR suggests that some of the shocked material has a high initial OPR. Such material is clearly present for the sight lines represented by the crosses in Figure 13. These regions lie behind the “working surface” of the jet in HH 7—11; they may, perhaps, have been heated by relatively fast shocks during a previous epoch of shock activity, thereby acquiring a larger OPR, and are currently being reheated by a slower shock. The bow shock in HH 7, by contrast, appears to be propagating into fresh material in which the OPR is \( \sim 0.25 \), corresponding to equilibrium at temperature \( \sim 50 \) K.
5. SUMMARY

We have carried out spectroscopic observations toward the Herbig-Haro objects HH 7–11 and HH 54 over the 5.2–37 μm region using the Infrared Spectrograph of the Spitzer Space Telescope, and have thereby mapped the (0)–(7) pure rotational lines of molecular hydrogen, together with emissions in fine-structure transitions of Ne⁺, Si⁺, S, and Fe⁺.

The primary results of our study are as follows:

1. The H₂ rotational emissions indicate the presence of warm gas with a mixture of temperatures in the range 400–1200 K, consistent with the expected temperature behind nondissociative shocks of velocity ~10–20 km s⁻¹.

2. The fine-structure emissions are spatially offset from the H₂ emissions, lying closer to the source of the outflow that drives the shocks in these sources. They originate in faster shocks of velocity ~35–90 km s⁻¹—that are dissociative and ionizing. Such shocks likely result from the deceleration of the outflow, and are offset from a slower nondissociative bow shock that is driven into the ambient molecular medium.

3. Maps of the H₂ line ratios reveal little spatial variation in the typical admixture of gas temperatures in the mapped regions, but show that the H₂ ortho-to-para ratio is quite variable, typically falling substantially below the equilibrium value of 3 attained at the measured gas temperatures.

4. The nonequilibrium ortho-to-para ratios are characteristic of temperatures as low as ~50 K, and are a remnant of an earlier epoch, before the gas temperature was elevated by the passage of a shock. Correlations between the gas temperature and H₂ ortho-to-para ratio show that ortho-to-para ratios <0.8 are attained only at gas temperatures below ~900 K; this behavior is consistent with theoretical models in which the conversion of para- to ortho-H₂ behind the shock is driven by reactive collisions with atomic hydrogen, a process which possesses a substantial activation energy barrier (Eₐ/k ~ 4000 K) and is therefore very inefficient at low temperature.

5. The lowest observed ortho-to-para ratios of only ~0.25 suggest that the shocks in HH 54 and HH 7 are propagating into cold clouds of temperature ≤50 K in which the H₂ ortho-to-para ratio is close to equilibrium.

6. Upper limits on the 29.837 μm 7_23–6_16 and 30.899 μm 6_14–5_05 transitions of ortho-H₂O place upper limits on the H₂O abundance that are higher than—and therefore consistent with—abundances derived previously from ISO observations of transitions at longer wavelength.

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APPENDIX A

DATA REDUCTION PROCEDURES

Our data reduction procedure involved the following steps:

1. Removal of bad pixels in the basic calibrated data (BCD) files that are generated by the Spitzer Science Center for the Short-High and Long-High modes.—Bad pixels were defined as those flagged in either the SSC bmask file or in a “grand rogue mask” generated at University of Rochester from an analysis of dark fields acquired at the start of each IRS campaign. As a rogue might not appear in every campaign dark field, we assumed that any pixel identified as a rogue in any campaign would be corrected for all campaigns; thus, the grand rogue mask contains 25% more rogue pixels than a single campaign rogue mask. They were removed with the imclean routine, which interpolates between nearby good pixels.

2. Extraction of the individual species at each position along the slit.—These spectral extractions were accomplished using an augmentation to the SMART software package that has been developed at University of Rochester. This augmentation generates a spectrum for each resolution element along the slit, resulting in a series of spectra at defined positions in right ascension and declination. The spectra were trimmed to eliminate overlap between different orders of the IRS.

3. Regridding of the spectra onto a grid that is regular in right ascension and declination.—Because there are positions that are multiply observed with more than one slit position, this regridding sometimes involves the averaging of spectra obtained at nearly identical positions.

4. Application of the slit loss correction function (SLCF).—Because the SSC-provided data are flux-calibrated using point-source calibrators, a downwards correction must be provided to obtain intensities for extended sources, the correction factor (i.e., the SLCF) being the fraction of the point-source flux that falls within the slit width. We used the SLCFs kindly provided by J. D. Smith from an analysis of the instrumental point-spread function.

5. Determination of line and continuum fluxes at each spatial position within the mapped region.—Here we used a Levenberg-Marquardt (L-M) fitting routine simultaneously to fit a Gaussian line and second-order polynomial baseline at each position. Line fits were obtained for a series of spectral lines identified in the co-averaged spectra for each field. In fitting the co-averaged spectra, which are of high S/N, the line centroids and widths were treated as fixed parameters to be optimized in the L-M fit. The resultant best-fit centroids and widths were then used as fixed parameters in the L-M fits to the lower S/N spectra obtained at individual spatial positions; for these, only the line intensities and continuum parameters were optimized. This procedure is justified by the fact that the expected Doppler shifts associated with gas motions in the source are very small compared to the spectral resolution, 2Δλ being only ~60 and ~600, respectively, for the low (SL) and high (SH and LH) resolution modules.

The data reduction procedure was accomplished using the SMART software package and a set of associated IDL procedures that we have written. The contour maps presented in Figures 1–7 were also created using IDL procedures.

To verify our data reduction procedure, we have conducted several tests. These include the following:

1. Continuum mapping of SVS 13.—Figure 14 shows contour maps obtained for several continuum wavelengths for HH 7–11 field 1 (see Table 1), which contains the strong continuum source SVS 13 at its center [i.e., at position (0, 0) in Fig. 14]. The intensity maps...
shown in Figure 14 use logarithmic contours spaced by a factor $\sqrt{2}$, with the second-highest contour corresponding to an intensity one-half the maximum. To the extent that SVS 13 can be regarded as an unresolved point source at these wavelengths, these maps represent the beam profile resulting at the end of the entire data reduction procedure.

Table 5 shows the results of Gaussian fits to the spatial profiles, and indicates that the astrometric accuracy is better than $0.1''$ in the final data product. The map at 5.8 $\mu$m clearly exhibits a sixfold rotational symmetry at intensities levels less than $3\%$ of the maximum, a behavior that is also evident in Infrared Array Camera (IRAC) observations (Hora et al. 2004) and reflects the diffraction pattern produced by the telescope.

2. Spectral extraction of SVS 13 and comparison with ISO observations.—As a check of the flux calibration, we have extracted spectra of the strong continuum source SVS 13, obtaining a co-average from the entire map of HH 7–11 field 1. For comparison, we

| WAVELENGTH ($\mu$m) | CENTROID OFFSET (arcsec) | HALF-POWER BEAM WIDTH (arcsec) (circular average) |
|---------------------|--------------------------|-----------------------------------------------|
| 5.8.................. | +0.5                     | 3.0                                           |
| 9.2.................. | +0.6                     | 3.1                                           |
| 10.5..................| +0.1                     | 5.0                                           |
| 18.5..................| +0.5                     | 5.3                                           |
| 22.0..................| +0.2                     | 9.6                                           |
| 30.5..................| -0.3                     | 10.2                                          |

Fig. 14.—Continuum maps obtained for several continuum wavelengths toward HH 7–11 field 1, which contains the strong continuum source SVS 13 at its center [i.e., at position (0, 0)]. Logarithmic contours are spaced by a factor $2^{1/2}$, with the second-highest contour corresponding to an intensity one-half the maximum. To the extent that SVS 13 can be regarded as an unresolved point source at these wavelengths, these maps represent the beam profile resulting at the end of the entire data reduction procedure.
have obtained an archival spectrum of SVS 13 from the ISO Short Wavelength Spectrometer (SWS), co-averaging multiple scans and removing bad pixels with the use of the ISAP software package. Figure 15 compares the spectrum obtained with Spitzer (heavy black line) with that obtained with ISO (red, blue, green and magenta lines, different colors being used to show the different SWS orders). Overall, the agreement is very good, with the absolute fluxes typically agreeing to within $\pm 15\%$. In the spectral region longward of 27.5 $\mu$m, the fluxes obtained with ISO SWS exceed those measured by Spitzer by as much as 25%. However, a significant order mismatch at 27.5 $\mu$m (between detectors 11 and 13) in the ISO spectrum suggests that the ISO-determined flux is an overestimate longward of 27.5 $\mu$m.

**APPENDIX B**

**SIMPLE ANALYTIC TREATMENT OF NONDISSOCIATIVE C-TYPE SHOCKS**

Here we present a simple analytic treatment of nondissociative C-type shocks, which is limited in its applicability to steady state shocks with plane parallel geometry. Detailed models of planar nondissociative C-type shocks (e.g., KN96; Wilgenbus et al. 2000), predict line strengths for the $\text{H}_2$ pure rotational transitions that yield rotational diagrams with remarkably little curvature. This behavior suggests that the warm gas behind such shocks can be approximated as an isothermal, isobaric slab. In this Appendix, we show that such a description yields predictions for the emission-line spectrum of the shocked gas that are in good agreement with those of detailed models, and we derive analytic expressions for the appropriate slab thickness, density, temperature and velocity gradient as a function of the preshock $\text{H}_2$ density, $n_0 = n_0 10^5$ cm$^{-3}$, shock velocity, $v_s = 10 v_{\text{sh}}$ km s$^{-1}$, and preshock magnetic field, $B_0 = b (n_0 / \text{cm}^{-3})^{1/2} \mu$G.

Nondissociative C-type shocks have been discussed extensively in the literature (e.g., Draine & McKee 1993 and references therein) and will not be reviewed here. They were originally defined by Draine (1980), who distinguished between J-type shocks in which the fluid velocity changes suddenly and the neutral and ionized species share a common velocity, and C-type shocks in which the fluid velocity varies slowly. The basic physics of C-type shocks had been discussed previously by Mullan (1971), who recognized ion-neutral drift to be an essential feature of magnetic shocks propagating in weakly ionized media. Ions entering the shock, being strongly coupled to the magnetic field, are decelerated fairly rapidly and quickly reach their maximum compression. Neutral species entering the shock, by contrast, are uncoupled to the magnetic field and are slowly decelerated in collisions with the ions through which they drift. Thus the maximum heating rate within the shocked material occurs where the compression of the ions is large and that of the neutral species is small. Accordingly, we make the following simplifying approximations:

1. The neutral fluid is at a constant compression, $C_n = n(\text{H}_2)/n_0$, which is slightly greater than unity; the exact value is an adjustable parameter to be determined below by a comparison with the line flux predictions of the KN96 shock models.
   
2. The ionized fluid is at a constant compression equal to the maximum that is attained behind the shock
   
   \[ C_i = n_i/n_{i0} = 2 \, M_{\lambda}^{1/2} = 7.7 v_{\text{sh}}/b, \]  

   \[ (\text{B1}) \]
where \( M_A = \frac{v_{Alf}}{(0.184b)} \) is the Alfvén Mach number and \( n_{i0} \) is the preshock ion density. Additional ionization within the shock ("self-ionization") is neglected.

3. The thickness of the emitting slab is given by

\[
t = k_1 L_{in}(n_0, \nu_d)/C_i,
\]

where \( L_{in}(n[H_2], \nu_d) \) is the ion-neutral coupling length (KN96) for \( H_2 \) density \( n(H_2) \) and ion-neutral drift velocity \( \nu_d \), and \( k_1 \) is a dimensionless constant of order unity, the exact value of which is an adjustable parameter to be determined below by a comparison with the line flux predictions of the KN96 shock models.
4. The slab is at constant temperature, $T$, determined such that the radiative output is equal to the mechanical luminosity, implying

$$n_0^2 C_n t \Lambda(T, n_0 C_n) = \frac{1}{2} \mu n_0 v_{\text{s}}^3 [1 - (2 M_A)^{-2}] \sim \frac{1}{2} \mu n_0 v_{\text{s}}^3,$$

(B3)

where $\Lambda(T, n[H_2])$ is the cooling rate coefficient for temperature, $T = 10^3 T_3 \text{K}$, and H$_2$ density, $n(H_2) = 10^5 n_5 \text{ cm}^{-3}$.

5. The velocity gradient is $dv_z/dz = k_2 v_{\text{s}}/t$, where $k_2$ is a dimensionless constant of order unity, the exact value of which is an adjustable parameter to be determined below by a comparison with the line flux predictions of the KN96 shock models.

6. We adopt as our standard assumptions an ion-neutral coupling length

$$L_{\text{in}}^0 = 3.5 \times 10^{16} n_5^{0.5} v_{\text{s6}}^{0.25} \text{ cm},$$

(B4)

based on a fit to results of KN96 (obtained for the case where polycylic aromatic hydrocarbons (PAHs) are assumed to be present), and a cooling rate coefficient,

$$\Lambda^0(T, n[H_2]) = 1.4 \times 10^{-26} n_5^{-0.5} T_3^{0.8} \text{ ergs cm}^{-3} \text{ s}^{-1},$$

(B5)

based on a fit to the results of Neufeld et al. (1995). The superscripts on $L_{\text{in}}^0$ and $\Lambda^0$ are used to denote the “standard values” adopted for our treatment.

Assumptions 1–6 above define the required properties of the isothermal, isobaric slab, once the three parameters $C_n$, $k_1$, and $k_2$ have been specified. In determining the best-fit values for these parameters, we have compared the emission predicted for the slab model with the detailed predictions of KN96. Here we assumed fixed CO and H$_2$O abundances, corresponding to the assumption that CO and H$_2$O account for all the O and C nuclei in the gas-phase. Because the O and C abundances assumed by KN96 were somewhat larger than those adopted by Neufeld et al. (1995) in computing the cooling rate coefficient, $\Lambda^0(T, n[H_2])$, we adopted $\Lambda^0(T, n[H_2]) = 1.5 \Lambda^0(T, n[H_2])$ for the purposes of this comparison. The optimum fit to the KN96-predicted emission-line spectrum is obtained for $C_n = 1.5$, $k_1 = 2$, and $k_2 = 2$.

Combining the expressions given above, we find that the slab H$_2$ density is fit best by

$$n(H_2) = 1.5 \times 10^5 \ n_05 \ \text{ cm}^{-3},$$

(B6)

the H$_2$ column density by

$$N(H_2) = 1.37 \times 10^{21} n_05^{0.5} v_{\text{s6}}^{-0.75} b (L_{\text{in}}/L_{\text{in}}^0) \ \text{ cm}^{-2},$$

(B7)

the gas temperature by

$$T = 375 v_{\text{s6}}^{1.15} b^{-0.36} (L_{\text{in}}/L_{\text{in}}^0)^{-0.36} (\Lambda/\Lambda^0)^{-0.36} \ \text{ K},$$

(B8)

and the velocity gradient by

$$dv/dz = 4500 n_05^{0.5} v_{\text{s6}}^{1.75} b^{-1} (L_{\text{in}}/L_{\text{in}}^0)^{-1} \text{ km s}^{-1} \text{ pc}^{-1}.$$

(B9)

In Figure 16 we compare the H$_2$ S(5)/S(3) line ratio and the total H$_2$, H$_2$O and CO surface luminosities derived for the simple slab model (red) with those obtained in the detailed calculations of KN96 (blue). In general, the agreement is remarkably good. Almost invariably, either (1) the shock velocity corresponding to a given flux or flux ratio agrees to within $\sim 5$ km s$^{-1}$; and/or (2) the predicted line flux or flux ratio for a given shock velocity agrees to within a factor of 2. Often, the agreement is considerably better. The main exception is for water emissions at low shock velocity ($v_{\text{s}} \leq 15$ km s$^{-1}$), where the detailed KN96 models predict considerably less H$_2$O than the slab models. This behavior results because—for the slab models—we assumed that water vapor accounts for all gas-phase oxygen nuclei not locked in CO, whereas the treatment of oxygen chemistry in KN96 predicts considerably lower water abundances at low shock velocity.

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