ISO observations of molecular hydrogen in HH 54*: measurement of a non-equilibrium ortho- to para-H$_2$ ratio

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ABSTRACT

We have detected the S(1), S(2), S(3), S(4) and S(5) pure rotational lines of molecular hydrogen toward the outflow source HH 54, using the Short Wavelength Spectrometer (SWS) on board the Infrared Space Observatory (ISO). The observed H$_2$ line ratios indicate the presence of warm molecular gas with an H$_2$ density of at least 10$^5$ cm$^{-3}$ and a temperature $\sim 650$ K in which the ortho- to para-H$_2$ ratio is only 1.2 $\pm$ 0.4, significantly smaller than the equilibrium ratio of 3 expected in gas at that temperature. These observations imply that the measured ortho- to para-H$_2$ ratio is the legacy of an earlier stage in the thermal history of the gas when the gas had reached equilibrium at a temperature $\lesssim 90$ K. Based upon the expected timescale for equilibration, we argue that the non-equilibrium ortho- to para-H$_2$ ratio observed in HH 54 serves as a chronometer that places a conservative upper limit of $\sim 5000$ yr on the period for which the emitting gas has been warm. The S(2)/S(1) and S(3)/S(1) H$_2$ line ratios measured toward HH 54 are consistent with recent theoretical models of Timmermann for the conversion of para- to ortho-H$_2$ behind slow, ‘C’-type shocks, but only if the preshock ortho- to para-H$_2$ ratio was $\lesssim 0.2$. 

1. Introduction

Molecular hydrogen is the dominant constituent of dense interstellar gas, and H$_2$ quadrupole transitions are a significant coolant of such gas over a wide range of temperatures and densities (Neufeld, Lepp & Melnick 1995). Although quadrupole vibrational transitions of H$_2$ near 2 $\mu$m have been widely observed from interstellar clouds that are strongly irradiated by ultraviolet radiation or have been heated by shock waves to temperatures $T \sim 2000$ K (e.g. Shull & Beckwith 1982; Beckwith et al. 1978; Gatley et al. 1987; Chrysostomou et al. 1993; and many others), molecular hydrogen within cooler clouds that are not UV-irradiated is only detectable by means of its pure rotational lines. With a broad spectral coverage that is uninterrupted by atmospheric absorption regions, the Short Wavelength Spectrometer (SWS; de Graauw et al. 1996) on board the Infrared Space Observatory (ISO; Kessler et al. 1996) has allowed the complete H$_2$ rotational spectrum to be observed from the interstellar medium for the first time.

Pure rotational emissions from H$_2$ have been detected by ISO toward several regions of star formation within the Galaxy – including S140 (Timmermann et al. 1996), Cepheus A West (Wright et al. 1996), the BD+40°4124 group (Wesselius et al. 1996), and Orion-IRc2 (van Dishoeck et al. 1998) – as well as towards several external galaxies (e.g. Arp 220; Sturm et al. 1996). The observed H$_2$ line ratios provide valuable constraints upon the physical conditions in the emitting gas, implying typical temperatures of 500 - 800 K for those Galactic sources that have been observed to date. These temperatures are much greater than those typical of cold quiescent clouds ($\sim 30$ K), and presumably reflect the effects of shock heating or radiative heating by a nearby star or protostar. As far as we are aware, all ISO observations of such sources (prior to those reported in this Letter) are consistent with an ortho- to para-H$_2$ ratio of three, the value expected at temperatures above $\sim 200$ K if the observed regions have been warm long enough to reach equilibrium between the ortho (odd $J$ states with total nuclear spin 1) and para states (even $J$ states with total nuclear spin zero).

In this Letter we report the results of ISO observations of molecular hydrogen in the source HH 54, a Herbig-Haro object located at the edge of the Chamaleon II dark cloud at an estimated distance $\sim 200$ pc from the Sun (Hughes & Hartigan 1992). The source of the outflow responsible

\footnote{Other earlier astronomical observations of H$_2$ also indicated ortho- to para-H$_2$ ratios consistent with the values expected in thermal equilibrium. Thus infrared absorption line observations of NGC 2024 IRS 2 (Lacy et al. 1994) implied an ortho- to para-H$_2$ ratio $< 0.8$, consistent with the value of 0.2 expected at the temperature ($\sim 45$ K) of the absorbing gas, while ultraviolet absorption line observations toward hot stars (Savage et al. 1977) using the Copernicus satellite have revealed typical ortho- to para-H$_2$ ratios $\sim 1$ in diffuse clouds, again consistent with thermal equilibrium at the temperatures $\sim 80$ K that are typical of such clouds. We note that vibrational emissions from warm photodissociation regions and planetary nebulae often exhibit ortho- to para-H$_2$ ratios in excited vibrational states that are smaller than the value of 3 expected in equilibrium at high temperature (e.g. Hasegawa et al. 1987, Ramsay et al. 1993, Chrysostomou et al. 1993, Hora & Latter 1996), with typical values in the range 1.7 - 2.1. However, Sternberg & Neufeld (1998) have argued that these ortho- to para-H$_2$ ratios measured for excited vibrational states do not require true ortho- to para-H$_2$ ratios smaller than 3 but are simply a consequence of optical depth effects in the fluorescent pumping of the observed vibrational emissions.}
for HH 54 is believed to be IRAS 12496-7650 (Hughes et al. 1989), a deeply embedded young stellar object lying approximately 4′ to the southwest. Previous observations of infrared H$_2$ vibrational lines (Gredel 1994) and optical line emissions (Schwarz & Dopita 1980) have suggested the presence of hot, shock-excited gas in HH 54.

Our observations are described in §2 below, and our results reported in §3 below. A discussion follows in §4, in which particular emphasis is placed upon the non-equilibrium ortho- to para-H$_2$ ratio $\sim 1.2$ measured in HH 54.

2. Observations and data reduction

Using the SWS of ISO in its grating mode (SWS02), we observed the S(1), S(2), S(3), S(4) and S(5) lines of H$_2$ toward the source HH 54 on 1997 November 4th. The ISO beam was centered midway between two strong sources of H$_2$ vibrational emission, positions E and K (Sandell et al. 1987), at coordinates $\alpha = 12h 55m 53.4s$, $\delta = -76^\circ 56' 20.5''$ (J2000), with the long axis of the beam oriented at position angle 118°. The total observing time on target was 6400 s, including overheads for dark current measurements and calibration. The rest wavelength, spectral resolution, and beam size are given in Table 1 for each of the five observed H$_2$ lines.

| Line | Wavelength ($\mu$m) | Velocity (km s$^{-1}$) | Beam size (arcsec) | Line Flux (W cm$^{-2}$) | Line Intensity (erg cm$^{-2}$ s$^{-1}$ sr$^{-1}$) | Upper state column density ($\text{cm}^{-2}$) |
|------|-------------------|----------------------|--------------------|-------------------------|---------------------------------------------|-----------------------------------------------|
| S(1) | 17.0348           | 160                  | 14 × 27            | 4.8 × 10$^{-20}$        | 5.4 × 10$^{-5}$                           | 1.3 × 10$^{19}$                               |
| S(2) | 12.2786           | 240                  | 14 × 27            | 2.1 × 10$^{-19}$        | 2.4 × 10$^{-4}$                           | 7.5 × 10$^{18}$                               |
| S(3) | 9.6649            | 160                  | 14 × 20            | 1.7 × 10$^{-19}$        | 2.6 × 10$^{-4}$                           | 2.2 × 10$^{18}$                               |
| S(4) | 8.0251            | 200                  | 14 × 20            | 1.6 × 10$^{-19}$        | 2.4 × 10$^{-4}$                           | 5.0 × 10$^{17}$                               |
| S(5) | 6.9095            | 240                  | 14 × 20            | 1.9 × 10$^{-19}$        | 2.9 × 10$^{-4}$                           | 2.2 × 10$^{17}$                               |

$^a$ FWHM of the instrumental profile for an extended source, from the ISO SWS Observer’s manual, Issue 3.0. For a point source, the spectral resolution is roughly a factor of two better.

$^b$ uncorrected for extinction

$^c$ beam averaged

$^d$ computed with a correction for extinction (see text)
The initial data reduction was carried out with version 6.22 of the ISO pipeline software, and the ISAP software package\textsuperscript{2} was then used to remove bad data points and to co-add the individual spectral scans.

3. Results

Figure 1 shows the SWS H$_2$ spectra observed toward HH 54 E+K. In every case, the observed line width is no broader than the instrumental response function, i.e. the lines are unresolved at the resolution of the SWS grating mode.

The measured line fluxes, beam-averaged line intensities and beam-averaged H$_2$ column densities in rotational states $J = 3$ through 7 are given in Table 1. The current SWS flux calibration is believed accurate to $\sim 30\%$. In computing the H$_2$ column densities, we used the spontaneous radiative rates of Turner, Kirby-Docken, & Dalgarno (1977; confirmed recently by the more precise calculations of Wolniewicz, Simbotin & Dalgarno 1998) for quadrupole transitions of H$_2$, which imply that the lines that we observed are all optically thin. We also applied dust extinction corrections based upon the interstellar extinction curves of Draine (1989), adopting Gredel’s (1994) estimate of 0.3 mag for $E(J - H)$ that was obtained from observations of the [FeII] lines at 1.257 and 1.644 $\mu$m toward HH 54 E+K. The assumed extinctions for the S(1), S(2), S(3), S(4) and S(5) lines were accordingly 0.10, 0.12, 0.30, 0.09 and 0.04 mag respectively\textsuperscript{3}.

Figure 2 shows a “rotational plot” for H$_2$ rotational states $J = 3$ through 7. Here the logarithm of $N_J/(g_Jg_S)$ is plotted against $E_J/k$, where $N_J$ is the beam-averaged column density, $g_J = 2J + 1$ is the rotational degeneracy, $g_S$ is the spin degeneracy (1 for even $J$ and 3 for odd $J$), and $E_J$ is the energy of the state of rotational quantum number $J$. Open squares correspond to the values tabulated in Table 1, with column densities averaged over regions of size $14'' \times 27''$ for $J = 3$ and 4 and size $14'' \times 20''$ for $J = 5$, 6, and 7. The filled squares for $J = 3$ and 4 show values that have been corrected to the smaller beam size of $14'' \times 20''$, on the assumption that the emission region is small compared to either beam. That assumption, adopted hereafter in the discussion, is appropriate if the H$_2$ S(1) and S(2) emission follows the compact distribution of the higher-excitation vibrational emission mapped by Gredel (1994).

Figure 2 shows that the points corresponding $J = 3$, 5, and 7 are colinear to within the observational uncertainties, consistent with the emission expected from gas in thermal equilibrium.

\textsuperscript{2}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.

\textsuperscript{3}The assumed extinction for the S(3) line – and to a lesser extent for the S(1), S(2) and S(4) lines – is enhanced by silicate features in the assumed extinction curve (Draine 1989), the strength of which may vary from one source to another. However, we found that the gas temperature and ortho-para-H$_2$ ratio derived below are only very weakly dependent upon the exact shape of the assumed extinction curve and are negligibly altered even if the silicate features are assumed to be entirely absent.
Fig. 1.— ISO Short Wavelength Spectrometer (SWS) spectra of pure rotational lines of H$_2$ observed toward HH 54 E+K, for a beam of size $14'' \times 27''$ [S(1) and S(2) lines] or $14'' \times 20''$ [S(3), S(4) and S(5)] centered at $\alpha = 12h 55m 53.4s$, $\delta = -76^\circ 56' 20.5''$ (J2000). The S(2), S(3), S(4) and S(5) lines are respectively offset by 10, 20, 30, and 40 Jy.
Fig. 2.— Rotational plot for $\text{H}_2$ rotational states $J = 3$ through 7. The logarithm of $N_J/(g_J g_S)$ is plotted against $E_J/k$, where $N_J$ is the beam-averaged column density, $g_J = 2J + 1$ is the rotational degeneracy, $g_S$ is the spin degeneracy (1 for even $J$ and 3 for odd $J$) and $E_J$ is the energy of the state of rotational quantum number $J$. Open squares correspond to the values tabulated in Table 1, with column densities averaged over regions of size $14'' \times 27''$ for $J = 3$ and 4 and size $14'' \times 20''$ for $J = 5$, 6, and 7. Filled squares for $J = 3$ and 4 show values that have been corrected to the smaller beam size of $14'' \times 20''$, on the assumption that the emission region is small compared to either beam. Straight lines show the fit for a gas temperature of 650 K and an ortho- to para-$\text{H}_2$ ratio of 1.2 (see text).
at a temperature $T \sim 700$ K. However, the column densities in $J = 2$ and 4 lie substantially above the best-fit line for the ortho (odd-$J$ states), implying that the ortho-para-\text{H}_2$ ratio (OPR) is smaller than the high temperature equilibrium value of 3 expected at 700 K. Our best fit to all the data points implies an OPR of $1.2 \pm 0.4$, a gas temperature of 650 K, and a total \text{H}_2$ column density of $9 \times 10^{19}$ cm$^{-2}$ (averaged over a $14'' \times 20''$ beam).

The rotational temperature derived for HH 54 E+K is larger than the temperature $\sim 330$ K derived by Liseau et al. (1996) from ISO Long Wavelength Spectrometer (LWS) observations of CO transitions towards HH 54 B, a difference that presumably results from the different pointing and larger LWS beam size used by Liseau et al. On the other hand, the \text{H}_2$ rotational temperature we derived towards HH 54 E+K is smaller than the temperature of 2100 K derived by Gredel (1994) from the observed ratio of the \text{H}_2$ $v = 1 - 0$ and $v = 2 - 1$ vibrational bands. Again, such a discrepancy is unsurprising and probably indicates that a mixture of shock velocities and gas temperatures is present within the beam, with vibrational emissions selectively probing hotter gas associated with faster shocks.

4. Discussion

Our measurement of an OPR smaller than 3 in gas of temperature $\sim 650$ K is \textit{prima facie} evidence that the gas has not been warm long enough to reach equilibrium between the ortho and para states; thus the measured OPR $\sim 1.2$ is the legacy of an earlier stage in the thermal history of the gas when the OPR had reached equilibrium at a value $\lesssim 1.2$ (corresponding to a gas temperature $\lesssim 90$ K).

We can place an upper limit on the time period, $\tau$, for which the emitting gas has been warm by estimating the timescale for conversion from para- to ortho-\text{H}_2$, $\tau_{\text{conv}}$. In media of low fractional ionization, the conversion of para- to ortho-\text{H}_2$ is dominated by reactive collisions with atomic hydrogen, for which the rate coefficient at 650 K is $1.0 \times 10^{-13}$ cm$^3$ s$^{-1}$ (Tiné et al. 1997): thus $\tau_{\text{conv}}$ is given by $3000 [100 \text{cm}^{-3} / n(\text{H})]$ yr, where $n(\text{H})$ is the density of hydrogen atoms. (Even if other interconversion mechanisms are significant, this is in any case an upper limit on $\tau_{\text{conv}}$.)

Models for the chemistry of dense molecular gas (e.g. Neufeld, Lepp & Melnick 1995) predict that once the temperature of the gas exceeds $\sim 300$ K, atomic oxygen will be rapidly converted to water, a prediction that has been supported by recent observations of water toward warm shocked regions in the Orion Molecular Cloud (Harwit et al. 1998). The production of water takes place by means of a series of two hydrogen atom abstraction reactions with \text{H}_2$ and therefore leads to the production of two hydrogen atoms for each water molecule produced; thus the atomic hydrogen density in recently-heated gas at temperature 650 K is at least twice the atomic oxygen density that was present in the gas prior to its being heated. Assuming an initial O abundance, $n(\text{O}) / n(\text{H}_2)$ of $3.5 \times 10^{-4}$ (consistent with the gas-phase oxygen and carbon abundances of Cardelli et al. 1995 and the assumption that O accounts for most of the
gas-phase oxygen not bound as CO), this places an upper limit of 5000 \( [10^5 \text{ cm}^{-3}/n(\text{H}_2)] \) yr on \( \tau_{\text{conv}} \). (This conservative upper limit still applies, of course, even if atomic hydrogen is produced by other mechanisms in addition to the reaction of O with \( \text{H}_2 \) to form water). Finally, the fact that the \( J = 7 \) state is apparently thermalized (c.f. Figure 2) implies a lower limit on the \( \text{H}_2 \) density of \( \sim 10^5 \text{ cm}^{-3} \), the critical density at which the collisional de-excitation rate for \( J = 7 \) (Tiné et al. 1997) is equal to the spontaneous radiative decay rate (Turner et al. 1977). Thus we conclude that the emitting gas that we observed in HH 54 has been warm for a period \( \tau \lesssim \tau_{\text{conv}} \lesssim 3000 \text{ [100 cm}^{-3}/n(\text{H})] \) yr \( \lesssim 5000 \text{ [10}^5 \text{ cm}^{-3}/n(\text{H}_2)] \) yr \( \lesssim 5000 \text{ yr} \).

Transient heating by shock waves – observed widely in Herbig-Haro objects – provides a natural explanation of the non-equilibrium OPR that we observed. Indeed, a non-equilibrium OPR within molecular gas heated by slow shocks has been predicted recently by Timmermann (1998), who presented a detailed theoretical treatment of ortho-para interconversion within slow ‘C’-type shocks. Timmermann obtained predictions for the \( \text{H}_2 \) rotational line strengths for shocks of velocity 10 to 30 km s\(^{-1}\) that propagate in gas of preshock \( \text{H}_2 \) density \( 5 \times 10^3, 5 \times 10^4 \) and \( 5 \times 10^5 \text{ cm}^{-3} \) and preshock ortho to para-\( \text{H}_2 \) ratio OPR\(_i\) = 1 or 3. The results show that para-to-ortho conversion is incomplete for shock velocities smaller than 20 to 25 km s\(^{-1}\) – the timescale for equilibration being longer than the shock timescale – so that slow shocks with OPR\(_i\) = 1 show a non-equilibrium OPR within the postshock region.

Figure 3 shows a quantitative comparison between the observed S(2)/S(1) and S(3)/S(1) line flux ratios and Timmermann’s predictions for a preshock \( \text{H}_2 \) density of \( 5 \times 10^5 \text{ cm}^{-3} \). In fact, none of the shock parameters actually considered by Timmermann yields a S(2)/S(1) ratio large enough (i.e. a postshock OPR small enough) to match the observations. However, we have interpolated and extrapolated Timmermann’s results to cases (dotted lines) where the initial OPR is other than 1 or 3, assuming that the line fluxes depend linearly\(^4\) upon the initial para-\( \text{H}_2 \) fraction, \( (\text{OPR}_i + 1)^{-1} \). Our extrapolation shows that a shock of velocity \( \sim 22 \text{ km s}^{-1} \) can provide a satisfactory fit to the S(2)/S(1) and S(3)/S(1) line ratios, given a sufficiently small initial ortho-para-\( \text{H}_2 \) ratio, \( \text{OPR}_i \lesssim 0.2 \).

The results of Timmermann et al. (1998) also provide an explanation for why previous studies (e.g. Smith, Davis & Lioure 1997) of vibrational emissions from protostellar outflows and Herbig-Haro objects have always revealed an OPR close to 3: vibrational emissions inevitably trace faster, hotter shocks in which the atomic hydrogen fraction is enhanced by streaming ion-neutral collisions and the rate coefficients for reactive collisions between H and \( \text{H}_2 \) are larger. Thus Timmermann’s models predict that para-to-ortho conversion is rapid enough to yield an equilibrium OPR of 3 behind any shock that is fast enough to excite significant vibrational emission.

\(^4\)A linear dependence would obtain exactly provided that the temperature structure of the shock is independent of the initial OPR. Our extrapolation method yields the expected result that the fluxes in ortho-\( \text{H}_2 \) transitions tend to zero in the limit of small initial OPR and small shock velocity.
Fig. 3.— Comparison between the observed S(2)/S(1) and S(3)/S(1) H$_2$ line flux ratios (filled square) and the predictions of Timmermann (1998) for a 'C'-type shock propagating in gas of H$_2$ density 5 × 10$^5$ cm$^{-3}$, shown as a function of the shock velocity, $v_s$, and the initial (i.e. preshock) ortho- to para-H$_2$ ratio, OPR$_i$. The observed fluxes have been corrected for extinction (see text). We have extrapolated or interpolated Timmermann’s results to cases (dotted lines) where the initial OPR is other than 1 or 3, assuming that the line fluxes depend linearly upon the initial para-H$_2$ fraction, (OPR$_i + 1)^{-1}$.
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