ORTHOTO-PARA RATIO STUDIES OF SHOCKED H₂ GAS IN THE TWO SUPERNOVA REMNANTS IC 443 AND HB 21

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ABSTRACT

We present near-infrared (2.5–5.0 μm) spectral studies of shocked H₂ gas in two supernova remnants, IC 443 and HB 21, which are well known for their interactions with nearby molecular clouds. The observations were performed with the Infrared Camera aboard the AKARI satellite. At the energy range 7000 K ≤ E(υ, J) ≤ 20,000 K, the shocked H₂ gas in IC 443 shows an ortho-to-para ratio (OPR) of 2.4±0.2, which is significantly lower than the equilibrium value 3, suggesting the existence of non-equilibrium OPR. The shocked gas in HB 21 also indicates a potential non-equilibrium OPR in the range of 1.8–2.0. The level populations are well described by the power-law thermal admixture model with a single OPR, where the temperature integration range is 1000–4000 K. We conclude that the obtained non-equilibrium OPR probably originates from the reformed H₂ gas of dissociative J-shocks, considering several factors such as the shock combination requirement, the line ratios, and the possibility that H₂ gas can form on grains with a non-equilibrium OPR. We also investigate C-shocks and partially dissociative J-shocks as the origin of the non-equilibrium OPR. However, we find that they are incompatible with the observed ionic emission lines for which dissociative J-shocks are required to explain. The difference in the collision energy of H atoms on grain surfaces would give rise to the observed difference between the OPRs of IC 443 and HB 21, if dissipative J-shocks are responsible for the H₂ emission. Our study suggests that dissociative J-shocks can produce shocked H₂ gas with a non-equilibrium OPR.

Key words: infrared: ISM – ISM: clouds – ISM: molecules – ISM: supernova remnants – shock waves

1. INTRODUCTION

Infrared H₂ line emission is a useful tool for studying shock–cloud interactions. H₂ is one of basic coolants at the postshock region (cf. Neufeld & Dalgarno 1989; Hollenbach & McKee 1989; Kaufman & Neufeld 1996), and its infrared line emission usually suffers relatively small extinction effects (cf. Draine 2003). The shock-excited H₂ line emission has been widely observed from diverse targets, such as protostellar jets and outflows, supernova remnants, and interacting galaxies (Habart et al. 2005; Omont 2007 and references therein). Ground telescopes usually observe high excitation emission lines (E(υ, J) ≥ 7000 K) in the near-infrared wave bands, while space satellites observe low excitation emission lines (E(υ, J) ≤ 3000 K) in the mid-infrared. The high excitation lines show the excitation temperature (T_ex) of a few thousand kelvin, while the low excitation lines show that of a few hundreds kelvin (e.g., Rosenthal et al. 2000; Rho et al. 2001; Giannini et al. 2006; Caratti o Garatti et al. 2008; Shinn et al. 2011).

H₂ line emission manifests one important diagnostic parameter of H₂ gas: the ortho-to-para ratio (OPR). First, we give a brief description of ortho- and para-H₂. An H₂ molecule consists of two identical proton nuclei, i.e., two identical fermions; hence, for a given nuclear spin combination, a specific rotational quantum number (space wave function) is only permitted according to the Pauli exclusion principle (cf. Field et al. 1966; Shull & Beckwith 1982). If the nuclear spins are summed to zero (I = 0, singlet), it is called para-H₂ and only even rotational quantum numbers (J) are allowed. On the other hand, if the nuclear spins sum up to one (I = 1, triplet), it is called ortho-H₂ and only odd-J is allowed. The statistical weight (g_J) for a level (υ, J) is derived by multiplying the nuclear spin degeneracy and the rotational degeneracy, g_J = (2J+1)(2J+1); i.e., g_J = 3(2J+1) for ortho-H₂ and g_J = (2J+1) for para-H₂.

The OPR is the ratio between the abundance of ortho- and para-H₂ in all (υ, J) levels. In general, lower E(υ, J) levels are much more populated than higher E(υ, J) levels (cf. Timmermann et al. 1996; Rosenthal et al. 2000). Therefore, the OPR is mainly determined by the OPR at low E(υ, J). This means that the OPR can be different from the abundance ratio of ortho- and para-H₂ in high E(υ, J). In this paper, we make a note of the energy level E(υ, J) when we mention the OPR at a specific E(υ, J) range; otherwise, the OPR means the abundance ratio of ortho- and para-H₂ summed over all (υ, J). We also note that the OPR of H₂ in local thermodynamic equilibrium (LTE) is equal to 3 at T ≥ 300 K, decreasing from 3 at T ≤ 300 K (cf. Burton et al. 1992; Sternberg & Neufeld 1999). When the OPR is different from this LTE OPR, we call it as a non-equilibrium OPR.

The OPR of H₂ is useful in estimating the thermal history of the gas (Neufeld et al. 2006). Under typical conditions of molecular clouds, the collisional interconversion between ortho- and para-H₂ is much slower than the collisional transitions between the same type of H₂ (ortho-ortho and para-para). Therefore, the OPR contains the information on how much interconversion collisions the H₂ gas experiences and what the initial OPR of the H₂ gas is. For shocked H₂ gas, the possibility of non-equilibrium OPR was briefly discussed by Chang & Martin (1991), and this question was seriously addressed later by Timmermann (1998) and Wilgenbus et al. (2000). The last two studies predicted the existence of H₂ gas with non-equilibrium OPR in C-shocks or partially dissociative J-shocks (for the types of shocks, see Draine & McKee 1993).

Observations hitherto have revealed shocked H₂ gas with non-equilibrium OPRs from mid-infrared observations, which trace low-energy levels of E(υ, J) ≤ 7000 K; e.g., Neufeld et al. 1998, 2006, 2007, 2009; Rodríguez-Fernández et al. 2000; Lefloch et al. 2003; Quanz et al. 2007; Roussel et al. 2007;
Hewitt et al. 2009; Maret et al. 2009). As far as we know, shocked H$_2$ gas with non-equilibrium OPRs has never been observed at high-energy levels of $E(\nu, J) \gtrsim 7000$ K (e.g., Gredel 1994; Smith et al. 1997; Giannini et al. 2006; Caratti o Garatti et al. 2006). Here we report on two cases that suggest shocked H$_2$ gas with non-equilibrium OPRs at such high levels, as revealed from near-infrared spectral observations with the AKARI satellite. The targets are two supernova remnants, IC 443 (G189.1+3.0) and HB 21 (G89.0+4.7), which are well known for their interactions with nearby molecular clouds (for more information about the targets, see Shinn et al. 2009, 2010, 2011). We present new near-infrared spectral observations with the AKARI satellite. The two regions, “HB 21N” and “HB 21S,” are listed in Table 1. “HB 21N” and “HB 21S” positions (“HB 21N BG” and “HB 21S BG,” Table1) were also observed in order to inspect if any background H$_2$ line emission exists.

The observations were carried out with the Infrared Camera (IRC; Onaka et al. 2007) of the AKARI satellite (Murakami et al. 2007) on 2008 June 1–3 during the post-helium phase. All the observations were performed in the observation mode IRCZ4, which is designed for general spectroscopic observations. The IRCZ4 mode acquires the spectra from multiple exposures without dithering, taking one reference image in the middle of the exposures (Onaka et al. 2009). Based on this reference image, we corrected the observed astrometric positions employing the Two Micron All Sky Survey catalog (Skrutskie et al. 2006); the resulting astrometric accuracy is smaller than 1″.4. We used the 5″ × 48″ slit and the grism, whose spectral resolution and wavelength coverage are Δλ = 0.03 μm and 2.5–5.0 μm, respectively. Figure 1 shows the slit positions over the H$_2$ $\nu = 1 \rightarrow 0$ S(1) 2.12 μm image of HB 21. The H$_2$ 2.12 μm image was acquired with the Wide-field InfraRed Camera (WIRCAM) of the Canada–France–Hawaii Telescope (CFHT) on 2007 August, and the data reduction was carried out employing the SIMPLE package (Wang et al. 2010). We first applied the reduction pipeline for the AKARI post-helium data (version 20110301; Onaka et al. 2009). The column pull-down effect was corrected and the hot pixels were masked out. No smoothing and tilt-correction were applied to the two-dimensional spectral image while running the pipeline. Then, we extracted a spectrum for each observation ID (cf. Table 1) by averaging the pixel values along the slit direction. Again, these multiple spectra for each pointing position were averaged together, and the results are presented in Figure 2. Some spectra show an alternating noise pattern along the wavelength bin, but they do not affect the measurement of the line intensity we intend. The calibration systematic error of 10% (private

![Figure 1](image_url). Observed slit positions for HB 21N (left) and HB 21S (right). The two regions correspond to “N2front” (Shinn et al. 2009) and “S1” (Shinn et al. 2010), respectively. The background images are H$_2$ $\nu = 1 \rightarrow 0$ S(1) 2.12 μm images obtained with WIRCAM of CFHT telescope. The direction to the remnant’s center is southward and northward in the left and right figures, respectively.

| Table 1: Summary of the AKARI-IRC Observations |
| --- |
| Region | Pointing Position (R.A., Decl; J2000) | Observation ID | AOT* |
| --- | --- | --- | --- |
| HB 21N | (20:47:26.891, +51:15:04.80) | 1420797.[1-4], 1420798.1 IRCZ4 |
| HB 21N BG | (20:47:32.37, +51:16:34.86) | 1420799.[1-2] IRCZ4 |
| HB 21S | (20:46:10.398, +49:58:15.20) | 1420800.[1-4], 1420801.1 IRCZ4 |
| HB 21S BG | (20:46:04.220, +49:58:13.61) | 1420802.[1-2] IRCZ4 |

Notes. The observation summary for the IC 443B data is in Shinn et al. (2011). * Astronomical Observation Template. It is a pre-defined observation sequence. See the IRC Data User Manual for Post-Helium Mission (Onaka et al. 2009).
The vertical bars indicate the location of H2 emission lines (cf. Table 2). “?” indicates the location of doubtful H2 emission line. For clarity, the error bars are omitted; the errors estimated from the pipeline are shown in Figures 3 and 4.

| Transition | Wavelength ($\mu$m) | Observed Intensity ($10^{-6}$ erg s$^{-1}$ cm$^{-2}$ sr$^{-1}$) |
|------------|---------------------|---------------------------------------------------------------|
|            |         | HB 21N | HB 21S |
| $v = 1$–$0$ O(3) | 2.80 | 9.1 ± 2.0 | 11.6 ± 2.0 |
| $v = 2$–$1$ O(3) | 2.97 | <4.1 | ... |
| $v = 1$–$0$ O(4) | 3.00 | <5.7 | ... |
| $v = 1$–$0$ O(5) | 3.23 | <6.2 | 8.3 ± 1.7 |
| $v = 1$–$0$ O(7) | 3.81 | <3.8 | ... |
| $v = 0$–$0$ S(13) | 3.85 | <4.9 | ... |
| $v = 0$–$0$ S(11) | 4.18 | 8.4 ± 1.4 | 9.0 ± 1.3 |
| $v = 0$–$0$ S(10) | 4.41 | 7.5 ± 1.4 | 8.7 ± 1.3 |
| $v = 0$–$0$ S(9) | 4.69 | 19.7 ± 2.4 | 21.6 ± 2.5 |

Notes. For those lines whose significance is lower than 3.0, the intensities are expressed with 90% upper confidence limits. The error includes both statistical and systematic components. See the text for detail.

In order to derive the level population of the shocked H2 gas, we first performed the reddening correction to the measured line intensities. We employed the extinction curve of “Milky Way, $R_V = 3.1$” (Weingartner & Draine 2001; Draine 2003), and adopted $N_H = N(H) + 2N(H_2) = 3.5 \times 10^{21}$ cm$^{-2}$ derived from the X-ray absorption toward the central region of HB 21 (Lee et al. 2001). Then, these reddening-corrected line intensities were used to derive the level population, assuming that the H2 emission is optically thin. This assumption is appropriate since the H2 emission lines become optically thick when $N(H_2) \gtrsim 10^{24}$ cm$^{-2}$, as noted in Shinn et al. (2011). If there were such a high $N(H_2) \gtrsim 10^{24}$ cm$^{-2}$ toward HB 21, the AKARI mid-infrared spectra of the background positions, “HB 21N BG” and “HB 21S BG”, hence, the background contribution of line emission is negligible. We identified that all the detected emission lines are of H2, comparing the line positions to those detected in IC 443 (Shinn et al. 2011).

The line intensities were measured by fitting a Gaussian profile plus a synthetic continuum to the emission line spectrum. The synthetic continuum was made by median-smoothing the observed spectrum with a box kernel. The kernel width is wide enough to smooth the line features out; it is about 0.19 $\mu$m. This continuum is displayed as a dashed line in Figures 3 and 4. We set the full width at half-maximum of the Gaussian profile as the spectral resolution of IRC, $\Delta \lambda = 0.03$ $\mu$m. When two lines are overlapped, we fitted both lines simultaneously. The fitting results are shown in Figures 3 and 4, and the measured line intensities are listed in Table 2.

3. ANALYSIS AND RESULTS

3.1. Line Intensity and Level Population

Figure 2 shows the AKARI spectra of HB 21. A few evident emission lines are seen from the spectra of “HB 21N” and “HB 21S.” On the other hand, no emission line is seen from the spectra of the background positions, “HB 21N BG” and “HB 21S BG”.
images (Shinn et al. 2009) should have shown absorbed features against background radiation, because the \( N(\text{H}_2) \) exceeds that of infrared dark clouds (Bergin & Tafalla 2007).

We used the following equation to derive the extinction-corrected level population of the shocked \( \text{H}_2 \) gas:

\[
N_{\text{ec}}(\nu, J) = \frac{4\pi \lambda I_{\text{ec}}(\nu, J \rightarrow \nu', J')} {hc A(\nu, J \rightarrow \nu', J')},
\]

where \( I_{\text{ec}}(\nu, J \rightarrow \nu', J') \) and \( A(\nu, J \rightarrow \nu', J') \) are the reddening-corrected line intensity and the Einstein-A radiative transition probability, respectively. \( \lambda, h, \) and \( c \) are the transition wavelength, Planck constant, and light speed, respectively. We employed the molecular physical constants tabulated in the simulation code CLOUDY (version C08.00; Ferland et al. 1998). The derived column densities are listed in Table 3. Their population diagrams are shown in Figure 5; note that the LTE population appears as a straight line in this diagram.

The populations of \((\nu, J) = (0, 11), (0, 12), (0, 13)\) show a zigzag pattern. The OPRs estimated with the single \( T_{\text{ex}} \) assumption are \( 1.8 \pm 0.4 \) and \( 1.7 \pm 0.3 \) for HB 21N and HB 21S, respectively (\( T_{\text{ex}} \sim 2000 \) K). These OPRs are non-equilibrium
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Figure 4. Fitting for the H2 emission lines observed toward HB 21S. The rest is the same as Figure 3.

Table 3
Extinction-corrected H2 Column Density

| Level | Level Energy (K) | \( \log N(H_2; \nu,J) \) (cm\(^{-2} \)) |
|-------|-----------------|----------------------------------------|
| HB 21N | HB 21S         |
| (0, 11) | 10261. | 15.10 ± 0.05 | 15.14 ± 0.05 |
| (0, 12) | 11940. | 14.50 ± 0.08 | 14.56 ± 0.07 |
| (0, 13) | 13703. | 14.39 ± 0.07 | 14.42 ± 0.06 |
| (0, 15) | 17445. | <13.90 ... |
| (1, 1) | 6149. | 14.63 ± 0.10 | 14.74 ± 0.07 |
| (1, 2) | 6471. | <14.62 ... |
| (1, 3) | 6951. | <14.82 ... |
| (1, 5) | 8365. | <14.97 ... |
| (2, 1) | 11789. | <14.13 ... |

Notes. The extinctions were corrected, using \( N_H = N(H_1) + 2N(H_2) = 3.5 \times 10^{21} \) cm\(^{-2} \) (Lee et al. 2001) and the extinction curve of “Milky Way, \( R_V = 3.1 \)” (Weingartner & Draine 2001; Draine 2003).

OPRs (cf. Section 1). Note that IC 443B also showed the zigzag pattern (Shinn et al. 2011); the OPRs are estimated to be \( 2.4 \pm 0.4 \) and \( 2.1 \pm 0.3 \) for \( (\nu, J) = (0, 11–13) \) and \( (1, 1–3) \), respectively (\( T_{\text{ex}} \sim 1000–2000 \) K). We here underline that these \( (\nu, J) \) levels all reside at high energy, \( E(\nu, J) \gtrsim 7000 \) K.

In order to ascertain whether the zigzag pattern seen from the levels \( (\nu, J) = (0, 11–13) \) reflects the intrinsic OPR < 3.0, we examined it as follows. We checked the flux calibration procedure including the data reduction pipeline, and found no indication of systematic features that can mimic the zigzag pattern. We also checked whether any blended line exists for \( \nu = 0–0 \) S(10) 4.41 \( \mu \)m, which corresponds to the level \( (\nu, J) = (0, 12) \). There are no known strong atomic or ionic lines from shocks around 4.41 \( \mu \)m (cf. Allen et al. 2008). The line blending between H2 emission lines is dealt with in Section 3.2.1.

3.2. Power-law Thermal Admixture Model of Shocked H2 Gas with a Non-equilibrium Ortho-to-para Ratio

The power-law thermal admixture model has been used to describe the level population of shocked H2 gas (Shinn et al. 2011, and references therein). We employed the same model used in Shinn et al. (2011), and slightly modified it to reproduce the non-equilibrium OPR, i.e., the zigzag pattern in the population diagram. The relative population between the ortho- and para- levels is controlled by scaling the rate coefficients for the reactive collisions with H, which mediate the ortho-to-para and para-to-ortho transitions (cf. Le Bourlot et al. 1999). The final level population is obtained by integrating the following equation,

\[
dN = aT^{-b}dT
\]

\[
a = \left( \frac{N(H_2; T > 1000 \text{ K})(b - 1)}{T_{\text{min}}^{1-b} - T_{\text{max}}^{1-b}} \right),
\]

where \( a \) and \( b \) are constants and \( T_{\text{min}} = 1000 \) K and \( T_{\text{max}} = 4000 \) K. Statistical equilibrium was assumed and the collisional
partners are H₂, He, and H. We assumed $n($He$) = 0.2 n(H₂)$, and the abundance ratio of H to H₂ was set to be a free parameter, $X_H$.

Based on the previous observations of Shinn et al. (2011), we adopted $T_{\text{min}} = 1000$ K instead of 100 K, unlike previous applications (e.g., Shinn et al. 2009, 2010). Shinn et al. (2011) found that two different densities are required to describe the level population of shocked H₂ gas in the range of $0 \text{ K} < E(\nu, J) < 25,000 \text{ K}$: one with $n($H₂$) = 10^{5.8} - 10^{8.8} \text{ cm}^{-3}$ for $E(\nu, J) < 7000 \text{ K}$ and the other with $10^{5.4} - 10^{5.8} \text{ cm}^{-3}$ for $E(\nu, J) > 7000 \text{ K}$. From these results, they recognized that only $T > 1000 \text{ K}$ gas is crucial to describe the level population of $E(\nu, J) > 7000 \text{ K}$. Therefore, we adopted $T_{\text{min}} = 1000$ K for the model calculation, since our data points are spread over $E(\nu, J) > 7000 \text{ K}$ (Figure 6).

We then applied the model to the reddening-corrected level population of shocked H₂ gas in IC 443B, HB 21N, and HB 21S. The fitting results are shown in Figure 6, and the corresponding model parameters are listed in Table 4. In the case of IC 443B, we first tried to fit the data without any fixed parameters, but failed to have inversely diverging $n($H₂$)$ and $X_H$; $n($H₂$)$ increases over $10^7 \text{ cm}^{-3}$ and $X_H$ decreases below $-3.0$. These two parameters do not seem to be well constrained by the given data and error. Since such a high $n($H₂$)$ is unreasonable, we fixed the parameter $X_H$. Two different fittings were performed with $X_H = -1.7$ and $X_H = -2.5$. $X_H = -1.7$ is chosen since it was obtained from the analysis of IC 443C (Shinn et al. 2011). $X_H = -2.5$ is chosen since IC 443B seems to be experiencing a weaker shock than IC 443C, where $X_H = -1.7$ was obtained. The intensity ratio $I(\text{CO}; J = 3–2)/I(\text{CO}; J = 2–1)$ is lower at IC 443B than IC 443C (Xu et al. 2011), and the “W-shaped” H₂ morphology of IC 443 suggests that IC 443B may be denser than IC 443C (see Figure 1 in Shinn et al. 2011). In the case of HB 21N and HB 21S, we fitted the data fixing both $n($H₂$)$ and $X_H$ because there were too few data points. We just show that the level population can be described by the power-law thermal admixture model. We adopted $n($H₂$) = 10^{5.5} \text{ cm}^{-3}$ and $X_H = -2.0$, which are thought to be typical values for the shocked H₂ gas of IC 443 (cf. Shinn et al. 2011). Figure 7 shows the $\chi^2$ contour of the model parameters for IC 443B. We did not perform the $\chi^2$ contour scan for HB 21N and HB 21S, since there were too few data points compared to the number of model parameters.

IC 443B shows $n($H₂$) = 10^{5.8} - 10^{6.5} \text{ cm}^{-3}$ somewhat higher than that of IC 443C, $n($H₂$) = 10^{5.4} \text{ cm}^{-3}$ (Shinn et al. 2011). This density difference may be related with the “W-shaped” H₂ morphology mentioned above. $N($H₂$)$ of IC 443B is $10^{18.6} - 10^{18.8} \text{ cm}^{-2}$; here, $N($H₂$)$ means $N($H₂$); T > 1000 \text{ K}$, i.e., the column density of H₂ gas whose temperature is higher than 1000 K. IC 443B shows $b = 3.9-4.5$, larger than that of IC 443C, $b = 1.6$. This difference is natural because the $b$ of IC 443C is mainly determined by the data of $E(\nu, J) < 7000 \text{ K}$, while it is not for the $b$ of IC 443B. The obtained OPRs are 2.1–2.2. Interestingly, the OPR of IC 443B shows a smaller variation than the other parameters under the different adoptions of $X_H$ (cf. Table 4). These OPRs are similar to those estimated from the levels $(\nu, J) = (0, 11–13)$ and $(1, 1–3)$ assuming a single $T_{\text{ex}}$: $2.4 \pm 0.4$ and $2.1 \pm 0.3$. The $\chi^2$ contour (Figure 7) shows that there is a weak anti-correlation between $n($H₂$)$ and $b$, but no correlation between $N($H₂$)$ and the OPR. Figure 7 definitely shows the non-equilibrium OPR even in 95% confidence level.

HB 21N and HB 21S show $N($H₂$)$ of $10^{17.4} \text{ cm}^{-2}$ and $10^{17.7} \text{ cm}^{-2}$, respectively. This is about an order of magnitude smaller than that of IC 443C, which explains the consistent difference in the line intensities (Figure 2; Shinn et al. 2011). HB 21N and HB 21S show $b$ values of 2.6 and 3.3, smaller than IC 443B; this difference is hardly meaningful because the number of HB 21 data points is just half of IC 443B. The OPRs are 1.8 and 1.6 for HB 21N and HB 21S, respectively. These values are similar to those estimated from the levels $(\nu, J) = (0, 11–13)$ assuming a single $T_{\text{ex}}$: $1.8 \pm 0.4$ and $1.7 \pm 0.3$.

### 3.2.1. Spectral Fitting to the Observed Spectrum

In order to investigate the OPR of shocked H₂ gas in IC 443B using all possible observational constraints, we additionally performed spectral fitting to the observed AKARI-IRC spectrum.
Figure 6. Model fitting results for the H\textsubscript{2} populations observed in IC 433B (top), HB 21N (bottom left), and HB 21S (bottom right). The IC 443B cases are shown for two different parameter settings: $X_{H} = -1.7$ (top left) and $X_{H} = -2.5$ (top right) (cf. Table 4). The filled-red and open-black symbols indicate the model and data points, respectively. (See the text for the model description.) The rotational quantum number ($J$) is printed near the corresponding point.

Table 4

| Region  | $\log[N(H_2)]$ (cm\textsuperscript{-2}) | $\log[n(H_2)]$ (cm\textsuperscript{-3}) | $b$ (≡ $\log[n(H_1)/n(H_2)]$) | $X_H^a$ | OPR | $\chi^2$ (≡ $\chi^2$/dof) |
|---------|---------------------------------|---------------------------------|-----------------|---------|-----|-----------------|
| IC443B  | 18.6\textsuperscript{+0.5}_{-0.2} | 5.8\textsuperscript{+0.4}_{-0.2} | 3.9\textsuperscript{+0.4}_{-0.4} | -1.7    | 2.1\textsuperscript{+0.2}_{-0.2} | 1.8 (=7.2/4.0) |
| IC443B  | 18.8\textsuperscript{+0.2}_{-0.2} | 6.5\textsuperscript{+0.3}_{-0.2} | 4.5\textsuperscript{+0.5}_{-0.5} | -2.5    | 2.5\textsuperscript{+0.2}_{-0.3} | 1.4 (=5.5/4.0) |
| HB21N   | 17.4                             | 5.5                             | 2.6             | -2.0    | 1.8             | ...             |
| HB21S   | 17.7                             | 5.5                             | 3.3             | -2.0    | 1.6             | ...             |

Notes. The confidence limits are given with a 68% significance (cf. Figure 7). $N(H_2)$ means $N(H_2; T > 1000 \text{ K})$.
See Section 3.2 for the detailed description about the parameters.

\textsuperscript{a} The parameter $X_H$ is fixed as shown. See Section 3.2 for more detail.

of IC 443B. The model spectrum is made by convolving the modeled intensity with a Gaussian kernel whose full width at half-maximum is 0.03 \textmu m. The extinction effect is included using $A_V = 13.5$ (Shinn et al. 2011) and the extinction curve of “Milky Way, $R_V = 3.1$” (Weingartner & Draine 2001; Draine 2003). We used a synthetic continuum that is made by median-smoothing the observed spectrum with a 0.29 \textmu m box kernel, and the continuum is fixed during the fitting. The calibration systematic error of 10\% (cf. Section 2) is quadratically included in the error of the spectrum. The wavelength shift is included as a free parameter, and found to be ∼+0.008 \textmu m for the best fit. The fitting results are shown in Figure 8. We fitted the spectrum
fixing $X_\text{H} = -1.7$ and $X_\text{H} = -2.5$ as in the level population fitting (Figure 6). The best-fit model parameters and the $\chi^2$ contours are shown in Table 5 and Figure 9.

The OPR is found to be $2.4^{+0.3}_{-0.2}$, which is a little higher than the ones from the level population fitting (Table 4). However, the OPR is still less than 3.0 with a 95% significance limit (Figure 9). The index $b$ also increases a little, while $N(\text{H}_2)$ and $n(\text{H}_2)$ are almost the same. The difference between the two kinds of fitting is likely induced by the constraints from the weak and blended H$_2$ emission lines, which are ignored in the level population fitting.
fitting (Figure 6). Such contributions can be seen in Table 6, for example, the three lines around 4.41 μm, \( \nu = 0-0\ S(10) \), \( \nu = 1-1\ S(11) \), and \( \nu = 2-1\ O(8) \).

For the HB 21 data, we could not get the range of OPR because there are only a few emission lines strong enough to constrain the model parameters. We estimate the OPRs of HB 21N and HB 21S with a single \( T_{ex} \) assumption using the 4.2, 4.4, 4.7 μm emission lines in Section 3.1. They are found to be 1.7–1.8. If the contribution of \( \nu = 1-1\ S(11) \) 4.42 μm to the 4.4 μm line feature and the contribution of \( \nu = 1-0\ O(8) \) 4.16 μm to the 4.2 μm line feature are, respectively, around 13% and 10% as in IC 443B (cf. Table 6), then the OPRs increase to 1.8–2.0. However, this estimation is still tentative. More near-infrared \( \text{H}_2 \) emission line data are required to assess the OPR of shocked \( \text{H}_2 \) gas in HB 21.

4. DISCUSSION

4.1. Origin of the Non-equilibrium Ortho-to-para Ratio Obtained from \( E(\nu, J) \gtrsim 7000\ K \)

We obtained results that suggest shocked \( \text{H}_2 \) gas with non-equilibrium OPRs in IC 443B (OPR = 2.4\(^{+0.5}_{-0.2} \)), HB 21N and HB 21S (OPR = 1.8–2.0; cf. Section 3.2.1). First, we examine the possibility that this non-equilibrium OPR originates from dissociative J-shocks, based on the results of Shinn et al. (2011). They studied shocked \( \text{H}_2 \) gas in IC 443 (IC 443C and IC 443G), and found that the levels we study here (7000 K \( \lesssim E(\nu, J) \lesssim 20,000\ K \)) are likely excited by dissociative J-shocks. Dissociative J-shocks mainly excite those levels at the \( \text{H}_2 \) reformation zone (cf. Flower et al. 2003) through two main excitation mechanisms: \( \text{H}_2 \) formation pumping and collisions with ambient gas (Hollenbach & McKee 1989). Therefore, the non-equilibrium OPR most likely originates from the \( \text{H}_2 \) reformation zone, if dissociative J-shocks are responsible for the level excitation of 7000 K \( \lesssim E(\nu, J) \lesssim 20,000\ K \).

When the levels of 7000 K \( \lesssim E(\nu, J) \lesssim 20,000\ K \) is dominantly populated, the temperature is a few hundred kelvin (Flower et al. 2003). This temperature is too low to render the ortho–para interconversion. For example, the number of para-to-ortho conversion is about 0.6 for the typical J-shock seen in Flower et al. (2003). We use the rate coefficient \( k_{po} \) of \( 8 \times 10^{-11} \exp(-3900/T) \) cm\(^3\) s\(^{-1}\) for H\(1\) (Schofield 1967), \( n(\text{H}) = 10^6 \) cm\(^{-3}\), \( t = 100\ yr \), and \( T = 300\ K \). Therefore, the OPR upon reformation behind dissociative J-shocks would remain unchanged until the gas cools down to as low as the preshock gas temperature. This means that the non-equilibrium OPR should be acquired when \( \text{H}_2 \) is reformed, if dissociative J-shocks are responsible for them.

\( \text{H}_2 \) reforms on grain surfaces or through the gas phase reaction (van de Hulst 1948; McDowell 1961; Field et al. 1966; Shull & Beckwith 1982, and references therein). Within the \( \text{H}_2 \) reformation zone of dissociative J-shocks, grain surface reformation is dominant because the gas phase reformation is inefficient when the ionization fraction of shocked gas is below 2% (Neufeld & Dalgarno 1989). The OPR of reformed \( \text{H}_2 \)

| Transition                  | Wavelength (μm) | Modeled Intensity \((10^{-6}\text{erg}\text{s}^{-1}\text{cm}^{-2}\text{sr}^{-1})\) |
|-----------------------------|-----------------|---------------------------------|
| \( \nu = 2-1\ Q(9) \)      | 2.72            | 1.7                             |
| \( \nu = 1-0\ Q(13) \)     | 2.73            | 0.8                             |
| \( \nu = 2-1\ Q(2) \)      | 2.79            | 2.1                             |
| \( \nu = 1-0\ O(3) \)      | 2.80            | 66.9                            |
| \( \nu = 2-1\ O(3) \)      | 2.97            | 6.9                             |
| \( \nu = 1-0\ O(4) \)      | 3.00            | 28.5                            |
| \( \nu = 2-1\ O(4) \)      | 3.19            | 3.1                             |
| \( \nu = 1-0\ O(5) \)      | 3.23            | 53.9                            |
| \( \nu = 2-1\ O(5) \)      | 3.44            | 6.2                             |
| \( \nu = 1-0\ O(6) \)      | 3.50            | 15.5                            |
| \( \nu = 2-1\ O(6) \)      | 3.72            | 1.9                             |
| \( \nu = 1-0\ O(7) \)      | 3.81            | 21.6                            |
| \( \nu = 0-0\ S(13) \)     | 3.85            | 15.2                            |
| \( \nu = 0-0\ S(12) \)     | 4.00            | 11.2                            |
| \( \nu = 2-1\ O(7) \)      | 4.05            | 2.9                             |
| \( \nu = 1-0\ O(8) \)      | 4.16            | 4.8                             |
| \( \nu = 0-0\ S(11) \)     | 4.18            | 44.6                            |
| \( \nu = 0-0\ S(10) \)     | 4.41            | 30.5                            |
| \( \nu = 1-1\ S(11) \)     | 4.42            | 4.6                             |
| \( \nu = 2-1\ O(8) \)      | 4.44            | 0.7                             |
| \( \nu = 1-0\ O(9) \)      | 4.58            | 5.4                             |
| \( \nu = 0-0\ S(9) \)      | 4.69            | 111.0                           |

Note. The best-fit models are from the spectral fitting (Figure 8) and the extinction effect is applied.
was usually assumed to be the equilibrium OPR in dissociative J-shock models (Hollenbach & McKee 1989; Flower et al. 2003), following the studies on the level population of newly formed \( \text{H}_2 \) (Black & Dalgarno 1976; Bieniek & Dalgarno 1979; Bieniek 1980; Black & van Dishoeck 1987; Flower et al. 2003). Thus, we need to scrutinize previous theoretical and experimental studies relevant to the OPR of newly formed \( \text{H}_2 \) more.

As far as we know, there are two studies that performed a quantum calculation for \( \text{H}_2 \) formation on grains and mentioned the OPR (Meijer et al. 2001; Morisset et al. 2005). Between them, the results of Morisset et al. (2005) do not exclude the possibility that the newly formed \( \text{H}_2 \) has an OPR = 1.8–2.4 (cf. Section 3.2.1). Meijer et al. (2001) and Morisset et al. (2005) respectively studied the Eley–Rideal (ER) and Langmuir–Hinshelwood (LH) formation mechanisms,\(^4\) between which the LH mechanism is more relevant to interstellar environments (Pirronello et al. 2000). The level population upon formation is biased within \( \nu \gtrsim 5 \) for the LH mechanism, while it is scattered over all the considered vibrational levels (\( \nu = 0–6 \)) for the ER mechanism. They both calculated the OPR, and it fluctuates within \( \sim 1.5–6.0 \) over the collision energy of 4–50 meV in the LH mechanism, while it is close to 3 over the initial translational energy of 0–200 meV in the ER mechanism. We think that OPR = 1.8–2.4 can be acquired through the LH formation mechanism, if the collision energy of H atoms on grain surfaces has the appropriate distribution. Note that the biased level population (\( \nu \gtrsim 5 \)) of the LH mechanism is redistributed over all levels through collisions with ambient postshock gas (i.e., ortho-to-ortho and para-to-para transitions).

We found two experimental works that studied the OPR of newly formed \( \text{H}_2 \) on grains (Perry & Price 2003; Creighan et al. 2006). However, their results do not mention whether

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\(^4\) See Tielens (2005) for the ER and LH mechanisms.
of IC 443C and IC 443G (Figure 5; Shinn et al. 2009, 2010, 2011)—the power-law thermal admixture model with two density components is required to reproduce the level population. As in IC 443, dissociative J-shocks may be needed to explain the level population of shocked H$_2$ gas in HB 21. We thus think that the non-equilibrium OPR is unlikely to originate from either C-shocks or partially dissociative J-shocks.

4.2. Ortho-to-para Ratios of Shocked H$_2$ Gas in IC 443 and HB 21

The OPR obtained from the levels of 7000 K $\lesssim E(\nu, J) \lesssim$ 20,000 K is probably in non-equilibrium for IC 443B (Section 3.2.1), while it is in equilibrium for IC 443C and IC 443G (Shinn et al. 2011). If we accept the conclusion from Section 4.1, then these OPRs are determined by the collision energy distribution of H atoms on grain surfaces. Therefore, the resulting OPRs mean that the collision energy distribution is similar to each other at IC 443C and IC 443G, while it is different for IC 443B. It is uncertain how the collision energy distribution is determined. The property of the grain surface and the environment where grains and H$_1$ gas are embedded may be included in the determining factors. We note here that IC 443B is located at the vertex of the “W-shaped” H$_2$ feature, while IC 443C and IC 443G are not (cf. Figure 1 of Shinn et al. 2011). This implies that the density at IC 443B may be higher than the others (cf. Shinn et al. 2011). The OPRs of HB 21N and HB 21S are similar to each other (Table 4). This indicates that the collision energy distribution is similar at both regions, if we accept the conclusion from Section 4.1. The OPRs of HB 21 are lower than those of IC 443, HB 21 shows a lower H$_2$ column density than IC 443 (Neufeld et al. 2007; Shinn et al. 2009, 2010, 2011). This implies a lower density for HB 21, if a similar extension of shocked H$_2$ gas along the line of sight is assumed for IC 443 and HB 21.

If our inference for the preshock density of IC 443 and HB 21 is correct, the preshock density and the obtained OPR show neither a correlation nor an anti-correlation. They are anti-correlated for IC 443B, IC 443C, and IC 443G, while they are correlated for IC 443 and HB 21. This indicates that the obtained OPRs are not simply determined by the preshock density. More information on physical parameters is required to understand how the obtained OPRs are determined at high-energy levels of 7000 K $\lesssim E(\nu, J) \lesssim$ 20,000 K.

5. CONCLUSIONS

We present the near-infrared (2.5–5.0 $\mu$m) spectral observations of shocked H$_2$ gas in two supernova remnants, IC 443 and HB 21. The observed regions are IC 443B, HB 21N, and HB 21S. At the energy range 7000 K $\lesssim E(\nu, J) \lesssim$ 20,000 K, IC 443B shows an OPR of $2.4^{+0.3}_{-0.2}$ (less than 95% confidence limit), which suggests the existence of non-equilibrium OPR. HB 21N and HB 21S also show indications of non-equilibrium OPRs in the range of 1.8–2.0. These may be the first objects observed with non-equilibrium OPR at such a high $(E(\nu, J))$ range. The level populations are well described by the power-law thermal admixture model ($1000 \lesssim T \lesssim 4000$ K) with a single OPR, where the infinitesimal column density is proportional to the inverse power of the temperature.

We conclude that the obtained non-equilibrium OPR probably originates from H$_2$ reformation through dissociative J-shocks, based on several arguments. Shinn et al. (2011) found that the H$_2$ levels of 7000 K $\lesssim E(\nu, J) \lesssim$ 20,000 K are likely

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**Table 7**

Comparison between the Expected and Observed Intensities of Br$_\alpha$

| Region    | Expected$^a$ (erg s$^{-1}$ cm$^{-2}$ sr$^{-1}$) | Observed$^b$ |
|-----------|-----------------------------------------------|-------------|
| IC443B    | (9.3e-07, 5.6e-05)                            | <1.7e-05    |
| IC443C    | (3.1e-06, 1.9e-04)                            | <1.8e-05    |
| IC443G    | (1.8e-06, 1.1e-04)                            | <2.0e-05    |
| HB21N     | (1.3e-07, 7.8e-06)                            | <4.8e-06    |
| HB21S     | (1.4e-07, 8.4e-06)                            | <4.7e-06    |

**Notes:**

$^a$ The expected intensity range of Br$_\alpha$ is calculated from the observed intensity of $\nu = 0$–0 S(11) (Shinn et al. 2011; Table 2), employing the dissociative J-shock model of Hollenbach & McKee (1989). The values are calculated for $n_0 = 10^3$ cm$^{-3}$ and $v_s = 40$–80 km s$^{-1}$.

$^b$ 99% upper confidence limit.

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the newly formed H$_2$ can have an OPR = 1.8–2.4 or not, because of experimental contaminations. They measured the level population of newly formed H$_2$ on a graphite surface, called "highly oriented pyrolytic graphite," at a base pressure of $\sim 10^{-10}$ Torr ($\sim 10^9$ cm$^{-3}$ K), which is much higher than the typical pressure of interstellar clouds, $10^2$–$10^6$ cm$^{-3}$ K (Bergin & Tafalla 2007). The obtained population is close to the LTE. However, it was known that the measured H$_2$ population had been contaminated by undissociated H$_2$ that originates from the H atom source (Islam et al. 2010).

From the above discussion, we show that non-equilibrium OPRs of 1.8–2.4 can originate from dissociative J-shocks. We note here that the dissociative J-shock interpretation is not incompatible with the observed line ratios between H$_2$ and H$_1$. We compare the intensities of Br$_\alpha$ 4.05 $\mu$m to those of $\nu = 0$–0 S(11) 4.18 $\mu$m. Table 7 shows the expected and observed intensity of Br$_\alpha$. The expected Br$_\alpha$ intensity is calculated from the observed $\nu = 0$–0 S(11) intensity (Shinn et al. 2011; Table 2), employing the dissociative J-shock model of Hollenbach & McKee (1989). We ignore the effect of extinction because the wavelengths of Br$_\alpha$ and $\nu = 0$–0 S(11) are similar. The adopted shock model parameters are $n_0 = 10^3$ cm$^{-3}$, $v_s = 40$–80 km s$^{-1}$.

Note that the dissociative J-shocks are likely propagating into interclump media of $<10^3$ cm$^{-3}$, according to Shinn et al. (2011). As seen from Table 7, the observed intensities better agree with the model expectations, when the shock velocity is slower. The intensities of $\nu = 0$–0 S(11) are also compatible with the model values, considering the possibilities of multiple shock surfaces, the shock surface viewed edge-on, the not-fully-covered shock surface because of unresolved substructures, and others.

We now examine other possibilities aside from the dissociative J-shocks. The shocked H$_2$ gas of non-equilibrium OPR can be made by C-shocks or partially dissociative J-shocks (Timmermann 1998; Wilgenbus et al. 2000). However, these shocks are incapable of producing the ionic lines observed in the shocked gas. When Shinn et al. (2011) interpreted the level population of shocked H$_2$ gas in IC 443C and IC 443G (0 K $\lesssim E(\nu, J) \lesssim$ 25,000 K), they concluded that a combination of C-shocks and dissociative J-shocks is needed. Under this interpretation, the dissociative J-shocks are mandatory to explain the observed ionic emission lines like [Ne ii] 12.8 $\mu$m and [C ii] 158 $\mu$m. Such lines were also observed at IC 443B (Noriega-Crespo et al. 2009). In HB 21, no detection of such ionic lines has been reported. However, the level population shape of shocked H$_2$ gas over 0 K $\lesssim E(\nu, J) \lesssim$ 20,000 K is similar to that of IC 443C and IC 443G (Figure 5; Shinn et al. 2009, 2010, 2011)—the power-law thermal admixture model with two density components is required to reproduce the level population.
excited by dissociative J-shocks, where H$_2$ is dissociated and then reformed. Previous quantum calculations do not exclude the possibility that the reformed H$_2$ has an OPR of 1.8–2.4, when formed with an appropriate collision energy of H atoms on grain surfaces. The observed line ratio between H$_2$ $v = 0$–$S(11)$ and Br$_\alpha$ is also compatible with the dissociative J-shock interpretation.

According to our conclusion, the difference in the obtained OPRs is caused by the different collision energies of H atoms on grain surfaces. It is uncertain how the collision energy is determined, but property of the grain surface and the environment where grains and H$_2$ gas are embedded may be included in the determining factors. We check if any simple relation holds between the obtained OPR and preshock density for IC 443 and HB 21, but it turns out to be unlikely.

More observational studies are required to confirm the non-equilibrium OPR, to validate our explanations for the obtained non-equilibrium OPR, and to grasp how a non-equilibrium OPR of shocked H$_2$ gas is determined at the energy levels of 7000 K $\lesssim E(\nu, J) \lesssim 20,000$ K. Our study suggests that dissociative J-shocks can produce shocked H$_2$ gas with a non-equilibrium OPR.

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