DETECTION OF FAR-INFRARED WATER VAPOR, HYDROXYL, AND CARBON MONOXIDE EMISSIONS FROM THE SUPERNOVA REMNANT 3C 391

William T. Reach
Infrared Processing and Analysis Center, California Institute of Technology, Pasadena, CA 91125

and

Jeonghee Rho
Service d’Astrophysique, CEA, DSM, DAPNIA, Centre d’Etudes de Saclay, F-91191 Gif-sur-Yvette Cedex, France

Received 1998 July 9; accepted 1998 August 28; published 1998 September 11

ABSTRACT

We report the detection of shock-excited far-infrared emission of H2O, OH, and CO from the supernova remnant 3C 391, using the Infrared Space Observatory Long-Wavelength Spectrometer. This is the first detection of thermal H2O and OH emission from a supernova remnant. For two other remnants, W28 and W44, CO emission was detected, but OH was detected only in absorption. The observed H2O and OH emission lines arise from levels within ~400 K of the ground state, consistent with collisional excitation in warm, dense gas created after the passage of the shock front through the dense clumps in the preshock cloud. The postshock gas we observe has a density ~2 × 10^3 cm^-3 and temperature 100–1000 K, and the relative abundances of CO:OH:H2O in the emitting region are 100:1:15 for a temperature of 200 K. The presence of a significant column of warm H2O suggests that the chemistry has been changed significantly by the shock. The existence of significant column densities of both OH and H2O, which is at odds with models for nondissociative shocks into dense gas, could be due to photodissociation of H2O or a mix of fast and slow shocks through regions with different preshock density.

Subject headings: infrared: ISM: lines and bands — ISM: individual (3C 391) — ISM: molecules — supernova remnants

1. INTRODUCTION

Long suspected to be an important component of the interstellar medium, water has proved difficult to observe because of the dominating absorption by water vapor in the Earth’s atmosphere. Water masers at radio frequencies are bright enough to penetrate the atmosphere, but they are rare and their physical conditions may be exceptional. Now that we have flown a sensitive infrared spectrometer in space, aboard the Infrared Space Observatory (ISO) (Kessler et al. 1996), transitions among energy levels ~100–1000 K above the ground state of H2O are observable. Early results from ISO indicate that H2O is a significant constituent in a cloud near the Galactic center (Cernicharo et al. 1997) and that H2O is as abundant as CO in shocked regions in Orion (Harwit et al. 1998).

The observations reported here are part of a study of the infrared emission from supernova remnants interacting with molecular clouds. Our targets were selected from a sample of supernova remnants with previous evidence for interaction with nearby molecular clouds based on X-ray and radio morphology (Rho & Petre 1998), millimeter-wave molecular line observations (Wilner, Reynolds, & Moffett 1998; Wootten 1977; Wootten 1981; Reach & Rho 1998), and OH 1720 MHz observations (Frail et al. 1996; Green et al. 1997). The presence of 1720 MHz maser emission without bright main-line OH maser emission suggests that they are collisionally excited (Elitzur 1976), and their location in bright radio remnants indicates that they are produced in the dense regions just behind molecular shocks. The first results of our ISO observations showed that the [O i] 63 μm line, which is expected to be one of the brightest cooling lines for postshock gas for a wide range of gas densities and shock velocities, is very bright at the locations of the OH masers (Reach & Rho 1996, hereafter Paper I). In a parallel observational project, we also found shock-accelerated CS, CO, and HCO+ molecules in 3C 391 (Reach & Rho 1998). In this paper, we present follow-up spectral observations to see which additional infrared lines are bright from molecular supernova shocks. These observations are the first detection of far-infrared H2O, OH, and CO lines from supernova remnants. We report here far-infrared spectral observations of a single position in each of three supernova remnants: 3C 391, W44, and W28.

2. OBSERVATIONS

All observations reported here were performed with the ISO Long-Wavelength Spectrometer (Clegg et al. 1996). We used the medium-resolution grating to fully sample the wavelength range from 42.2 to 188.6 μm. The coordinates are based on bright OH 1720 MHz masers (Frail et al. 1996) in each remnant (for W44: 18°56′28.4", +01°29′59", for W28: 18°01′52.3", −23°19′25", B1950); for 3C 391 we shifted closer to the peak of shocked CS and CO broad molecular line emission, 3C 391:BML (18°46′47.1", −01°00′51") (Reach & Rho 1998). The LWS beam size is 80", and the spectra are severely affected by fringes, because of constructive and destructive interference (inside the spectrometer) of wave fronts from our structured, extended sources. We removed the fringes using...
the ISO Spectral Analysis Package, assuming that the emitting region is extended at all wavelengths.

An important portion of the spectrum of 3C 391:BML, including the low-lying transition of ortho-H$_2$O at 179.5 μm, is shown in Figure 1. The continuum is the result of dust from the supernova remnant (some 30% of the total) and unrelated interstellar material along the line of sight (see Paper I). In addition to the H$_2$O and CO lines indicated, there are some remaining ripples in the spectrum that do not fall at the wavelength of predicted lines, nor do they have the shape expected for an unresolved spectral line. A second spectral observation toward 3C 391:BML was performed in order to confirm some of the spectral lines and to search for lines of H$_2$O and OH from energy levels higher than we had already detected. The result for the OH($^2\Pi_{3/2-3/2}$, $J = 1/2-3/2$) line is shown in Figure 2.

3. RESULTS

Very bright lines from atomic and ionic C, N, and O and weaker molecular lines were detected from all three supernova remnants. We will compile and present the complete line lists in a future paper. Of the three sources that we observed, only 3C 391:BML had a rich spectrum of molecular emission. A list of H$_2$O, OH, and CO lines detected or limited toward 3C 391:BML is shown in Table 1. For W28, the CO (16–15) and CO (15–14) emission lines were detected, and for W44 only the CO (16–15) line was detected; the CO lines are a factor

4 The ISO Spectral Analysis Package (ISAP) is a joint development by the LWS and SWS Instrument Teams and Data Centres. Contributing institutes are CESR, IAS, IPAC, MPE, RAL, and SRON.
Fig. 3.—Energy-level diagrams for ortho-H$_2$O (left) and para-H$_2$O (right). All levels within 500 K of the ground state are shown. The fastest radiative de-excitations of each level are indicated with arrows, if the wavelength of the transition is within the range of our ISO spectrum. The arrows were drawn with the following characteristics: detected lines have a filled arrow head, possible detections have an open arrow head, and nondetections have dashed arrow.

of 2 and 4 fainter for W 28 and W 44 compared with 3C 391: BML. The 95% confidence upper limit on the H$_2$O (2$_{12}$–1$_{11}$) 179.5 $\mu$m line for W 44 and W 28 is half the brightness of the line detected toward 3C 391:BML. Considering that 3C 391 also had the brightest [O i] 63 $\mu$m line and dust continuum, it is possible that both W 28 and W 44 could have similar shock-excited spectra, with the H$_2$O lines unfortunately just below our detection limit. While no OH emission was detected for W 28 and W 44, the 119 $\mu$m transition from the ground state was detected in absorption, presumably due to foreground gas.

One source of uncertainty is the identification of the lines. Although the resolving power of these observations was less than 300, such that wavelengths cannot be measured sufficiently accurately for conclusive identifications, our main conclusion—namely, that H$_2$O, OH, and CO were detected from shock-excited gas in supernova remnants—is strong. In the time-honored tradition of spectroscopy, we have detected multiple lines from each species.

All the lines we believe we have detected are from the lowest accessible energy levels of each species. For CO, the highest level we detected was $J = 16$, which lies 750 K above the ground state. The energy-level diagrams of H$_2$O and OH are shown in Figures 3 and 4. In both cases, we indicate the fast transitions whose wavelengths that fall within the range of our ISO spectrum. Including marginal detections, we see evidence for almost all the fast transitions of both ortho- and para-H$_2$O among energy levels within 320 K of the ground state. The H$_2$O (4$_{13}$–3$_{12}$) transition is masked by a bright [O i] line nearby, but there is a hint of the principal line from the next highest energy level (3$_{23}$–2$_{22}$). No transitions involving levels more than 400 K above ground are seen.

of 2 and 4 fainter for W 28 and W 44 compared with 3C 391: BML. The 95% confidence upper limit on the H$_2$O (2$_{12}$–1$_{11}$) 179.5 $\mu$m line for W 44 and W 28 is half the brightness of the line detected toward 3C 391:BML. Considering that 3C 391 also had the brightest [O i] 63 $\mu$m line and dust continuum, it is possible that both W 28 and W 44 could have similar shock-excited spectra, with the H$_2$O lines unfortunately just below our detection limit. While no OH emission was detected for W 28 and W 44, the 119 $\mu$m transition from the ground state was detected in absorption, presumably due to foreground gas.

One source of uncertainty is the identification of the lines. Although the resolving power of these observations was less than 300, such that wavelengths cannot be measured sufficiently accurately for conclusive identifications, our main conclusion—namely, that H$_2$O, OH, and CO were detected from shock-excited gas in supernova remnants—is strong. In the time-honored tradition of spectroscopy, we have detected multiple lines from each species.

All the lines we believe we have detected are from the lowest accessible energy levels of each species. For CO, the highest level we detected was $J = 16$, which lies 750 K above the ground state. The energy-level diagrams of H$_2$O and OH are shown in Figures 3 and 4. In both cases, we indicate the fast transitions whose wavelengths that fall within the range of our ISO spectrum. Including marginal detections, we see evidence for almost all the fast transitions of both ortho- and para-H$_2$O among energy levels within 320 K of the ground state. The H$_2$O (4$_{13}$–3$_{12}$) transition is masked by a bright [O i] line nearby, but there is a hint of the principal line from the next highest energy level (3$_{23}$–2$_{22}$). No transitions involving levels more than 400 K above ground are seen.

The most important emission line that is expected to be bright but is not detected is the 119 $\mu$m line of OH. But this line connects directly to the ground state, and our models (below) predict significant foreground absorption; therefore, we suspect that the 119 $\mu$m line is extinguished by foreground gas. Indeed, our spectra of W 44 and W 28, which have comparable sightlines through the Galactic disk, show absorption features at 119 $\mu$m (with an optical depth of order 0.1) due to foreground OH absorbing the dust continuum from the supernova remnants.

4. DISCUSSION

4.1. Excitation and Abundance of H$_2$O, OH, and CO

In order to determine the physical conditions that can produce the observed suite of spectral lines, and to measure the abundances of the observed species, we compared the line brightnesses with a simple model that balances collisional and radiative transitions within a uniform emitting region. We modeled the emission spectra of regions with a range of H$_2$ volume density and kinetic temperature, and the absorption spectrum of a cold slab of foreground gas with nominal molecular abundances (from Irvine, Goldsmith, & Hjalmarsøn 1987) and an H$_2$ column density of $10^{22}$ cm$^{-2}$. We solved iteratively for the excitation, modifying radiative rates by the escape probability for a line profile with a width of 30 km s$^{-1}$, as was found from the millimeter-wave CS and CO observations (Reach & Rho 1998). Collision rates were taken from Offer, van Hemert, & van Dishoeck (1994) for OH and Green, Maluendes, & McLean (1993) for H$_2$O, and the radiative transition rates were taken from Pickett et al. (1996).

The observed brightness ratio of 79 $\mu$m to 84 $\mu$m lines of
OH is sensitive to the gas density, suggesting \( n(H_2) \approx (1-6) \times 10^4 \) cm\(^{-3}\). The ratios of the \( 5 \rightarrow 4, 3 \rightarrow 2, \) and \( 2 \rightarrow 1 \) millimeter lines of CS are also sensitive to the gas density, suggesting \( n(H_2) = (3-4) \times 10^3 \) cm\(^{-3}\), and the millimeter CS and CO lines somewhat constrain the temperature, \( T > 50 \) K (Reach & Rho 1998). For the abundance calculations, we will assume \( n(H_2) = 2 \times 10^3 \) cm\(^{-3}\) and \( 100 < T < 1000 \) K, which is consistent with the presence and lack of other OH and H\(_2\)O lines in the observed wavelength range.

We determine the abundances of the various molecules assuming all lines arise from the same physical region, with constant temperature and density. The column density of OH is \( \sim 2 \times 10^{15} \) cm\(^{-2}\), and the optical depth of the 79 \( \mu\)m line is of order unity. The CO excitation is much more sensitive to temperature; to match the brightness of the well-detected \( 15 \rightarrow 14 \) line, the CO column density \( \sim 2 \times 10^{19} (T/200)^{-5} \) cm\(^{-2}\). The H\(_2\)O lines are estimated to be optically thick: if we associate the line observed at 180.69 \( \mu\)m with H\(_2\)O (\( 2_{12}-1_{11} \)), then the isotope ratio implies an optical depth \( \sim 400 \) for the brightest H\(_2\)O line. However, in the low-density limit, \( n(H_2) < 10^3 \) cm\(^{-3}\), spontaneous decay is still faster than collisional de-excitation, and the line brightness still measures the H\(_2\)O abundance (Irvine et al. 1987). The column density of H\(_2\)O from the excitation model is \( \sim 3 \times 10^{17} \) cm\(^{-2}\). To determine the absolute abundance of each species, we require a measure of the H\(_2\) column density. If we assume the emitting region is a uniform sphere with diameter equal to the observed angular size of shock-excited molecular gas (\( \sim 30'' \) from Reach & Rho 1998), and we take from the excitation model \( n(H_2) = 2 \times 10^4 \) cm\(^{-3}\), we find \( N(H_2) \sim 8 \times 10^9 \) cm\(^{-3}\). This value of \( N(H_2) \) agrees with the observed brightness (from our ISO SWAS observations, in preparation) of the S(3) line of H\(_2\), if \( T \approx 200 \). In summary, we estimate the relative abundances of CO:OH:H\(_2\)O to be 100:1:15, and the abundance of water in the shocked cloud is \([H_2/O/H_2] \sim 4 \times 10^{-2}\).

### 4.2. Chemistry of H\(_2\)O and OH

The warm H\(_2\)O in 3C 391:BML is likely due to shock-enhanced chemistry. In relatively hot gas, OH is rapidly converted into H\(_2\)O by the reaction \( OH + H_2 \rightarrow H_2O + H \), so that all the available O that is not already locked in CO would be converted into H\(_2\)O (Draine, Roberge, & Dalgarno 1983; McKee & Hollenbach 1979). Models for the oxygen chemistry predict very efficient conversion of OH into H\(_2\)O for nondissociative shocks into high-density \( (n_0 = 10^5 \) cm\(^{-3}\) clouds but comparable OH and H\(_2\)O column densities for shocks into intermediate-density \( (n_0 = 10^3 \) cm\(^{-3}\) clouds, while CO and H\(_2\)O are comparably abundant (Graff & Dalgarno 1987). Behind a fully dissociative shock, the molecules re-form in a much cooler \( (~100-500 \) K) region (Hollenbach & McKee 1989). In cooler gas, the 1420 K barrier (Wagner & Graff 1987) for the OH formation \( OH + H_2 \rightarrow H_2O + H \) reaction cannot be overcome, and OH is more abundant than H\(_2\)O (McKee & Hollenbach 1979; van Dishoeck & Black 1986), except deep inside dense molecular cores (Sternberg & Dalgarno 1995). The chemistry in cooler gas depends on photodissociation; OH is much more abundant than H\(_2\)O (van Dishoeck & Black 1986), except deep inside very dark cores, where the photodissociation rate is very low (Bergin, Langer, & Goldsmith 1995).

The relative strengths of the H\(_2\)O lines that we observe were calculated by Kaufman & Neufeld (1996), and our observations are generally consistent with the models for preshock density \( n_0 = 10^4-10^5 \) cm\(^{-3}\). However, these models predict a very low OH abundance: the H\(_2\)O 179.5 \( \mu\)m line is predicted to be 2 orders of magnitude brighter than the OH 84.5 \( \mu\)m doublet, while we observe comparable brightnesses. The relatively low excitation we observe for the H\(_2\)O and OH molecules \( (T_{\text{upper}} < 400 \) K) suggests that the gas we are observing is not presently hot enough for the rapid H\(_2\)O production. But this does not preclude the H\(_2\)O having formed in a short-lived, high-temperature region, and we observe only the cooling region. We observe more H\(_2\)O than OH, suggesting that high-temperature chemistry was operative long enough to leave a lasting effect on the chemistry of this gas.

The detection of OH, with an abundance only 15 times less than that of H\(_2\)O, disagrees with theoretical models of C shocks, which predict nearly complete conversion of OH into H\(_2\)O. This suggests that either (1) the H\(_2\)O abundance is underestimated as a result of beam dilution, (2) we are observing OH and H\(_2\)O from different types of shocks in regions with a range of preshock densities, or (3) the models are not appropriate for the molecular shocks in 3C 391. We detected bright ionic lines (including [O iii] and [N iii]) that are only expected from dissociative shocks, so we know that a range of shocks is present within our beam. However, the infrared OH line ratios are consistent with coming from a region with the same physical conditions as inferred from the infrared H\(_2\)O, millimeter-wave CS, and radio-wave OH maser lines. The disagreement between observations and predictions is at least partially due to the fact that the models are for nondissociative shocks (Kaufman & Neufeld 1996). Including the effects of photodissociation of H\(_2\)O by the interstellar radiation field—as well as radiation local to the remnant—could produce OH in the abundance we observe (Lockett, Gauthier, & Elitzur 1998).

The water abundance we derive for 3C 391:BML is significantly lower than that observed from molecular shocks in HH 54 (Liseau et al. 1996) or Orion (Harwit et al. 1998). In particular, in the Orion BN-KL region, the H\(_2\)O abundance is \([H_2/O/H_2] = 5 \times 10^{-4}\) (Harwit et al. 1998), incorporating nearly all of the oxygen in the gas. The difference between the Orion BN-KL shock and the 3C 391:BML shock could be due to limited angular resolution: 3C 391 is about 20 times farther away than Orion, while the angular resolution of our observations is the same as that of Harwit et al. (1998). The difference could also be due to details of the interaction between the energetic events (a steady stellar wind in Orion versus impulsive supernova shock in 3C 391) and the interstellar medium (a molecular cloud and H ii region in 3C 391 versus a giant molecular cloud with no H ii region in 3C 391).

### 5. Conclusions

For the first time, thermal emission from the lower energy levels of H\(_2\)O and OH were detected from a supernova remnant. The emission arises from gas cooling behind a shock front that is impinging on a particularly dense clump in the parent molecular cloud; this site is called 3C 391:BML (broad molecular line). Our spectra of interaction sites in W44 and W28 did not reveal OH or H\(_2\)O emission, although CO emission and OH (foreground) absorption were detected. 3C 391 is not a unique case of a supernova remnant–molecular cloud interaction, but the infrared molecular lines imply the presence of higher density clumps than near W44 and W28, similar to IC 443. Together with outflows from young stars, supernova remnants are energetic events capable of altering
cloud chemistry and producing substantial columns of H$_2$O and OH. Supernova–molecular cloud interactions are probably common, and they have been suggested as an explanation for a new class of mixed-morphology X-ray and radio supernova remnants (Rho & Petre 1998). We can expect substantial advances in understanding shock-induced chemistry in supernova–molecular cloud interactions by using future observatories capable of higher angular and spectral resolution in the far-infrared, such as planned for SOFIA (Erickson 1995) and FIRST (Poglitsch 1998), where we will better resolve the fast and slow shocks into gas of varying preshock density and we will better resolve a larger number of spectral lines from each molecule.

The observations that we describe in this paper are part of the ISO open time granted to US astronomers thanks to cooperation between the ESA and NASA. The research described in this paper was carried out in part by the California Institute of Technology, under a contract with the National Aeronautics and Space Administration.

REFERENCES

Bergin, E. A., Langer, W. D., & Goldsmith, P. F. 1995, ApJ, 442, 222
Cernicharo, J., et al. 1997, A&A, 323, L25
Clegg, P. E., et al. 1996, A&A, 315, L38
Draine, B. T., Robberge, W. G., & Dalgarno, A. 1983, ApJ, 264, 485
Elitzur, M. 1976, ApJ, 203, 124
Erickson, E. F. 1995, Space Sci. Rev., 74, 91
Frail, D. A., Goss, W. M., Reynoso, E. M., Giacani, E. B., Green, A. J., Otrupcek, R. 1996, AJ, 111, 1651
Graff, M. M., & Dalgarno, A. 1987, ApJ, 317, 432
Green, A. J., Frail, D. A., Goss, W. M., & Otrupcek, R. 1997, AJ, 114, 2058
Green, S., Maluendes, S., & McLean, A. D. 1993, ApJS, 85, 181
Harwit, M., Neufeld, D. A., Melnick, G. J., & Kaufman, M. J. 1998, ApJ, 497, L105
Hollenbach, D. J., & McKee, C. F. 1989, ApJ, 355, 197
Irvine, W. M., Goldsmith, P. F., & Hjalmarson, Å. 1987, in Interstellar Processes, ed. D. J. Hollenbach & H. A. Thronson, Jr. (Dordrecht: Reidel), 561
Kaufman, M. J., & Neufeld, D. A. 1996, ApJ, 456, 611
Kissler, M. F., et al. 1996, A&A, 315, L27
Liseau, R., et al. 1996, A&A, 315, L181
Lockett, P. Gauthier, E., & Elitzur, M. 1998, ApJ, in press
McKee, C. F., & Hollenbach, D. J. 1979, ApJS, 41, 555
Neufeld, D. A., & Melnick, G. J. 1991, ApJ, 368, 215
Offer, A. R., van Hemert, M. C., & van Dishoeck, E. F. 1994, J. Chem. Phys, 100, 362
Pickett, H. M., Cohen, E. A., Delitsky, M. L., Pearson, J. C., & Müller, H. S. P. 1996, Submillimeter, Millimeter, and Microwave Spectral Line Catalog: Revision 4 (JPL Publ. 80-23) (Pasadena: JPL)
Poglitsch, A. 1998, in The Far-Infrared and Submillimeter Universe (ESA SP-401), ed. G. Pilbratt, S. Volonte, & A. Wilson (ESA: Noordwijk), in press
Reach, W. T., & Rho, J.-H. 1996, A&A, 315, L27 (Paper I)
———. 1998, ApJ, submitted
Rho, J.-H., & Petre, R. 1998, ApJ, 503, L167
Sternberg, A., & Dalgarno, A. 1995, ApJS, 99, 565
van Dishoeck, E. F., & Black, J. H. 1986, ApJS, 62, 109
Wagner, A. F., & Graff, M. M. 1987, ApJ, 317, 423
Wilner, D. J., Reynolds, S. P., Moffett, D. A. 1998, AJ, 115, 247
Wootten, A. 1977, ApJ, 216, 440
———. 1981, ApJ, 245, 105