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RADIATIVE TRANSFER MODELS OF EMISSION AND ABSORPTION IN THE H_2O 6 MICRON VIBRATION-ROTATION BAND TOWARD ORION-BN-KL[1]

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ABSTRACT

We report the spectrum of Orion-BN/KL between 5.3 and 7.2 μm observed with the Short Wavelength Spectrometer (SWS) on board the *Infrared Space Observatory*. H_2O lines of the $\nu_2 = 1$–0 bending mode with $\lambda <$ 6.3 μm (the *R*-branch) are observed in absorption, while lines with $\lambda >$ 6.3 μm (the *P*-branch) are observed in emission. Radiative transfer models including the (0, 0, 0), (0, 1, 0), and (0, 0, 1) vibrational levels show that this effect is produced in a natural way by H_2O absorption of 6 μm continuum photons followed by spontaneous de-excitation to the ground state (resonant scattering). The intensities of the absorption lines can be explained with an H_2O column density of a few 10^{17} cm^{-2} in gas with a temperature of ∼150 K and $n(H_2) \sim 10^6$ cm^{-3}, although these parameters depend on the assumed location of the absorbing shell. Since the observed intensity of the H_2O emission lines are larger than those seen in absorption, we suggest that rovibrational excitation of H_2O by collisions in denser and hotter gas, such as found in shocks, also contribute to the *P*-branch emission of the 6 μm H_2O band.

Subject headings: infrared: ISM: lines and bands — ISM: abundances — ISM: individual (Orion-BN) — ISM: individual (Orion Kleinmann-Low) — ISM: molecules — radiative transfer

1. INTRODUCTION

The determination of the abundances and column densities of H_2O is a long standing problem in astrophysics, and despite ground-based observations (Zmuidzinas et al. 1995; Cernicharo et al. 1994; Menten & Melnick 1991 and references therein), this issue has only started to be analyzed in detail with the new data provided by the *Infrared Space Observatory* (*ISO*). Cernicharo et al. (1997a) have observed the pure rotational transitions of H_2O and some $H_2^{18}O$ lines with the FP-LWS in the direction of Sgr B2 and derived that H_2O is widespread with $x(H_2O/H_2) \simeq 10^{-5}$. Cernicharo et al. (1997b, 1998) and Harwit et al. (1998) have reported the detection of several pure rotational lines of H_2O in emission in Orion with the *ISO*/LWS spectrometer. The interpretation of these data is, however, limited by the large opacities associated with the pure rotational lines of H_2O. The rovibrational lines of the bending mode of water are much less optically thick than the pure rotational lines of the ground state and could be used to derive accurate values of the H_2O column density and abundance, and to constrain the physical conditions of the emitting/absorbing gas.

The SWS has been used to study the rovibrational transitions of the bending mode of H_2O in the direction of bright infrared sources (van Dishoeck & Helmich 1996; Helmich et al. 1996; van Dishoeck et al. 1998; Dartois et al. 1998). In the hotter sources, the water vapor abundance is similar to that derived by Cernicharo et al. (1994) in the direction of Orion IRc2. In an accompanying Letter, van Dishoeck et al. (1998) present the SWS spectrum in the direction of Orion IRc2. In this Letter we present the data for Orion-BN and explain, through detailed radiative transfer models, the observed pattern of the H_2O bending band at 6 μm.

2. OBSERVATIONS AND RESULTS

The *ISO*/SWS full-grating, full-resolution spectrum (2.4–45.2 μm) of Orion-BN ($\alpha_{2000} = 5^h35^m14\overset{s}{.}2$, $\delta_{2000} = -5°22'23\overset{''}{.}6$) was measured during revolution 696. The SWS aperture was oriented 10° in the NE direction. Data reduction has been carried out using the SWS Interactive Analysis System. The detector flux levels have been flat-fielded, taking as reference the average signal of the down-scan data. The resulting spectrum has been rebinned to a spectral resolution of 1400. Residual instrumental fringes have been removed by iterative fitting. In this Letter we analyze the 6 μm region of the spectrum of Orion-BN. The rest of the spectrum looks very similar to that of Orion-KL presented in van Dishoeck et al. (1998). The SWS spectrum from 5.5 to 7.2 μm is displayed in Figure 1. The water ice absorption feature around 6 μm, for which we estimate a peak opacity of ≈0.16, dominates this part of the spectrum. The continuum flux at 4.8 and 8.6 μm (not shown in Fig. 1) agrees within 10% with that measured with larger telescopes by Ney, Strecker, & Gehrz (1973) and Dyck & Howell (1982) toward BN, indicating that most of the *ISO* flux at 5–7 μm originates in BN with a minor contribution from the other IR sources in the region. The *ISO* flux observed towards IRc2 is a factor of ∼2 lower than towards BN.

Figure 1 shows a forest of emission and absorption lines. Apart from a few H I recombination, [Ar II] fine structure, and

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[1] Based on observations with *ISO*, an ESA project with instruments funded by ESA Member States (especially the PI countries: France, Germany, The Netherlands and the United Kingdom) and with the participation of ISAS and NASA.

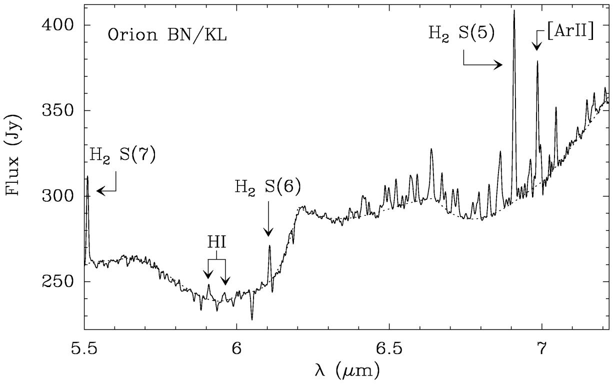

FIG. 1.—*ISO*/SWS spectrum of Orion-BN/KL between 5.5 and 7.2 μm. The dotted line is the adopted fit to the continuum emission.

H_2 rotational lines, all the other features belong to the $\nu_2 =$ 1–0 bending mode of water vapor. Surprisingly, the H_2O rovibrational lines with $\lambda < 6.3$ μm—the *R*-branch—are observed in absorption, while those with $\lambda > 6.3$ μm—the *P*-branch—are observed in emission. The lines of the *Q*-branch with $\Delta K_{-1} = +1$ are observed in absorption, while those with $\Delta K_{-1} = -1$ are in emission. The same effect is observed in the direction of IRc2. The continuum normalized spectrum is shown in Figure 2. The total flux of the emission lines is significantly higher than that of the absorption lines. It is worth noting that the depths of the absorbing lines are a factor of ∼2 more pronounced than those observed in the 6 μm spectrum of IRc2, indicating that the depths of Figure 2 are primarily determined by absorption toward BN. However, the flux of the emission lines ($\lambda > 6.3$ μm) is similar in both spectra, hence these lines arise in a more spatially extended region.

The strongest, lowest lying H_2O transitions are labeled in Figure 2. Inspection of the detected lines reveals some asymmetry between the *R*- and *P*-branch. The lines detected in absorption arise from energy levels not exceeding ≈400 K above the ground rotational state. However, some of the observed emission lines arise from levels at more than 10^3 K above the ground (e.g., the $\nu_2 = 1$–0 4_{41}–-5_{50} and the $\nu_2 = 1$–0 4_{40}–-5_{51}).

3. DISCUSSION

3.1. *General Considerations*

Excitation of the $\nu_2 = 1$ bending state of H_2O may be produced by collisions in a shocked region and by absorption of IR 6 μm continuum photons from BN (e.g., Kaufman & Neufeld 1996). In Orion-BN/KL, the foreground quiescent ridge cloud may also lead to significant absorption in the lowest lying transitions. However, excitation solely by collisions in a shocked region and absorption of photons in the foreground cloud cannot account for the observed spectrum. The reason is that there are lines with a common lower level that belong to different branches; i.e., one of them is observed in emission and the other in absorption. A representative example is the pair of lines $\nu_2 = 1 \leftarrow 04_32- - 3_21$ (in absorption) and $\nu_2 = 1 \rightarrow 02_12- - 3_21$ (in emission). Hence, although vibrational excitation by collisions cannot be neglected (see below), *pure* excitation by collisions can hardly account for the observed behavior of the H_2O lines.

Moreover, the absorption and emission lines are presumably formed in inner regions where the gas is affected by shocks, in outflows, and in general motions with typical velocities that are much higher than the velocity dispersion of the quiescent molecular cloud. In fact, Cernicharo et al. (1997b) show that the H_2O rotational lines toward Orion display line wings extended over ∼200 km s^{-1}. Consequently, the quiescent molecular cloud will only be able to absorb over a relatively small fraction of the total line widths. On the other hand, the low densities and temperatures prevailing in the ridge will be able to populate appreciably only a few rotational levels of the H_2O ground vibrational state. Hence, the contribution of this region to the absorption is expected to be small, except perhaps for lines arising in the lowest 1_{01} and 0_{00} ortho- and para-H_2O rotational levels. The circumstellar molecular gas of BN, which has been detected in the CO lines by Scoville et al. (1983), and the "plateau source," which intersects the line of sight to BN, are presumably the main components responsible for the observed absorption features.

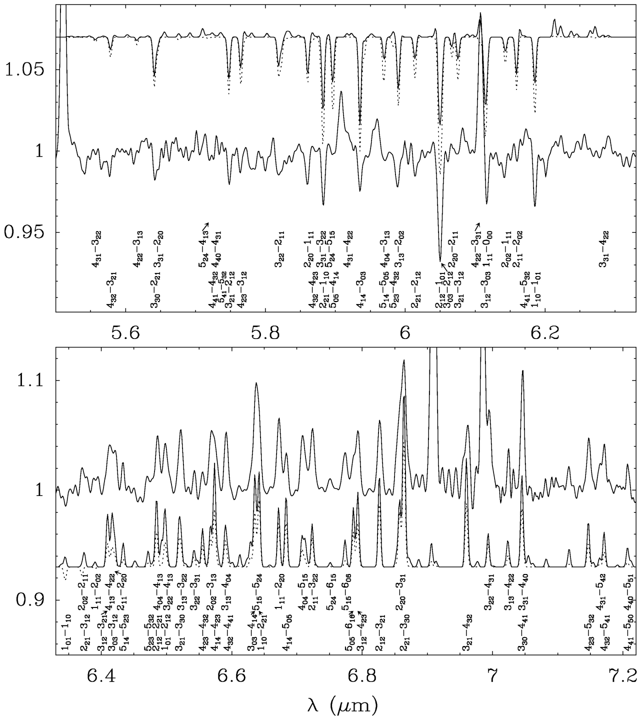

FIG. 2.—Continuum normalized spectrum of Orion-BN/KL between 5.5 and 7.2 μm. The dotted line is the result of the "radiative excitation" H_2O model described in the text. The solid line is the result of adding to the line fluxes of that model the fluxes of a collisionally excited model (see the text). The strongest lines (ortho = lower; para = upper) are labeled, the first level corresponding to the $\nu_2 = 1$ bending state and the second one belonging to the ground $\nu = 0$ state.

3.2. *Pure Radiative Model*

Absorption of continuum photons from BN in the 6 μm band followed by spontaneous decay to the ground vibrational state can readily explain the observational fact that the *P*-branch is observed in emission and the *R*-branch in absorption. González-Alfonso & Cernicharo (1998) have modeled the H_2O 6 μm excitation in O-rich evolved stars and show that this behavior is expected in the case that H_2O photons are not efficiently blanketed either by absorption by coexisting dust grains nor by the illuminating star. If so, any absorption event in the band, at any position in the envelope, will be compensated by an emission event and, *with the additional assumption of spherical symmetry*, an external observer who does not resolve the envelope spatially, will detect as many absorption events as emission events in the band. Furthermore, this statement does not depend either on the line opacities or on the excitation mechanism of the rotational levels within the ground vibrational state. The same argument can be applied to the spectrum observed in Orion-BN/KL. The bending $\nu_2 = 1$ mode is mainly excited via $\nu_2 = 1, J+1 \leftarrow \nu = 0, J$ absorption, and the subsequent de-excitation follows $\nu_2 = 1, J+1 \rightarrow \nu = 0, J+2, J+1$. In consequence, the *R*-branch lines will be observed in absorption, while those belonging to the *P*-branch will be in emission. Furthermore, diffusion of line photons may enlarge the size of the emitting region in a similar way to that discussed for HCO^+ by Cernicharo & Guélin (1987) and HCN by González-Alfonso & Cernicharo (1993).

Hence, radiative excitation of the $\nu_2 = 1$ bending mode of H_2O by IR photons from BN qualitatively explains the observed spectrum in Orion-BN/KL. Figure 2 shows the result of a model consisting of a central near-infrared source surrounded by a spherical molecular shell (*dashed line*). The near-infrared source, presumably hot dust surrounding BN, emits like a blackbody with temperature and radius of 1050 K and 1.5×10^{14} cm, respectively, matching approximately the emission at 6–7 μm of the BN "intrinsic source" fit by Lee & Draine (1985). The ortho-H_2O and para-H_2O abundances are 1.5×10^{-4} and 0.5×10^{-4}, respectively. The adopted turbulent velocity is $v_t = 20$ km s^{-1}, while the thickness of the shell, the H_2 density $n(H_2)$ and the kinetic temperature T_k are varied from model to model to obtain the better agreement with observations. The equilibrium populations are computed with the non-LTE and nonlocal radiative transfer method described in González-Alfonso & Cernicharo (1997). We include in the calculations the 40 lowest rotational levels of the ground ν state, the $\nu_2 = 1$ bending state and the $\nu_3 = 1$ stretching state of H_2O. Collisional rate coefficients for the rotational levels of the (0, 0, 0) state have been taken from Green, Maluendes, & McLean (1993). Collisional de-excitation rate coefficients for the rotational levels in the $\nu_2 = 1$ and $\nu_3 = 1$ levels are taken to be the same as those of the (0, 0, 0) level. FIR radiation emitted by dust grains was not included in the calculations of statistical equilibrium.

In the model of Figure 2, the shell has inner and outer radii, density, and temperature of 1.2×10^{15} cm, 3×10^{15} cm, 10^6 cm^{-3}, and 150 K, respectively. Similar results are also obtained if the shell is located further from the star and the density and/or the temperature increase. Although in the present model the shell is located very close to the star, further diffusion of photons away from it may give rise to the extended appearance of the emission lines. Our models are primarily sensitive to the total H_2O column density, $N(H_2O)$, in the shell. Since we assume an H_2O abundance of 2×10^{-4}, this then leads to a value of the thickness of the shell for the inferred density of 10^6 cm^{-3}. The resulting total column density through the shell of $N(H_2) = 1.8 \times 10^{21}$ cm^{-2} is comparable to that derived by Wright et al. (1998) for the warm gas from the *ISO* observations of the pure rotational H_2 lines. The "radiative excitation" H_2O model satisfactorily accounts for the observed pattern of absorption and emission lines. In the model, the moderate values of $n(H_2)$ and T_k are constrained by the lack of detected lines in absorption with levels at energies exceeding 400 K. The *P*-branch lines in emission are optically thin or have moderate opacities (<2), while the *R*-branch lines in absorption have radial opacities 1–4. The behavior of the *Q*-branch line is also well explained (preliminary results on the present calculations were presented in the review by Cernicharo 1998). However, some significant quantitative differences can be seen between the observed and model spectra. The latter overestimates the depths of the absorption lines and underestimates the fluxes of the emission lines. This discrepancy cannot be attributed to the uncertainty in the physical conditions assumed in the model. With the assumption of spherical symmetry and only the (0, 0, 0) and (0, 1, 0) levels, an external observer will detect identical emission and absorption events. In our models, radiative excitation of the $\nu_3 = 1$ state followed by the cascade (0, 0, 1)→(0, 1, 0)→(0, 0, 0) produces an enhancement of the flux of the emission lines but fails to explain quantitatively the full pattern of the ν_2 band.

Of course, the real geometry in Orion-BN/KL departs from spherical symmetry. The different physical conditions of the sources inside the SWS aperture (note that BN itself presents CO emission in the near-infrared at a velocity of 20 km s^{-1}; Scoville et al. 1983), presumably contribute to the $\nu_2 = 1$–0 H_2O emission in the *P*-branch. Diffusion of line radiation in such an extended and complex region could in principle account for the observed enhanced emissions over absorptions.

3.3. *Composite Radiative-Collisional Model*

The gas outflows centered around IRc2 have been detected in many molecular lines at millimeter wavelengths and show the presence of shocked molecular gas at high temperatures and densities (see Genzel et al. 1981; Cernicharo et al. 1994). Although excitation by collisions cannot be the dominant excitation mechanism of the $\nu_2 = 1$ H_2O bending mode, it may modify the line intensity ratio of the $\nu_2 = 1$ band. We have simulated this effect by adding to the previous model fluxes those obtained in a spherical shocked region in which H_2O vibrational excitation is uniquely caused by collisions. The source has a diameter of 10^{15} cm ($0''.15$ at 450 pc), $n(H_2) = 10^9$ cm^{-3}, $v_t = 20$ km s^{-1}, and an H_2O abundance of 10^{-4}. The kinetic temperature is that of the molecular reformation region in a dissociative *J*-shock, $T_k = 400$ K (Hollenbach & McKee 1989). These conditions resemble those of the clumps in which the strongest 22 GHz H_2O masers in Orion are thought to be formed (Elitzur, Hollenbach, & McKee 1989). No reliable information is available on the collisional rate coefficients for vibrational transitions, although the limited information on other systems suggests that they are lower by 1–2 orders of magnitude than those for rotational transitions (Flower 1990). The following crude assumption is used: For collisions between the (0, 0, 0) and (0, 1, 0) levels we assume that the collisional rate coefficient between two levels of $\nu_2 = 1$ and $\nu = 0$ is the same as that between the same rotational levels within $\nu = 0$. The vibrational excitation rates are then calculated upon detailed balance. The resulting fluxes of the composite radiative-collisional H_2O excitation model are shown with solid lines in Figure 2. The agreement with observations is excellent. Even if the vibrational collisional rates were overestimated by one order of magnitude or more, the size assumed for the shocked region is so small that a much more extended shock could be invoked without conflicting the observational millimetric data.

In conclusion, we have shown in this Letter that the combination of absorption and emission lines in the $\nu_2 = 1$–0 band of water vapor is a consequence of H_2O absorption and reemission of continuum photons proceeding preferentially from the BN source. Collisional rovibrational excitation, and the complexity of the region, could also play a role in the relatively large flux of the *P*-branch emission lines.

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