Detection of Phosphorus Nitride in the Lynds 1157 B1 Shocked Region

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Abstract

We have observed the \( J = 2–1 \) rotational emission line of PN toward the low-mass star forming region L 1157 with the Nobeyama 45 m telescope. The PN line has been detected toward the two shocked regions (B1 and B2) caused by the interaction between the blue lobe of the outflow from the protostar IRAS 20386+6751 and the ambient gas, whereas it has not been detected toward the protostar position. The fractional abundances of PN relative to \( H_2 \) are evaluated to be \((2–6) \times 10^{-10}\) and \((3–7) \times 10^{-10}\) toward B1 and B2, respectively. Detection of PN in the B1 and B2 positions indicates that the formation of PN can be triggered by shocks. It seems most likely that PN is formed in the gas phase from \( \text{PH}_3 \) evaporated from grain mantles, as suggested by the existing chemical model.

Key words: ISM: individual (Lynds 1157) — ISM: molecules

1. Introduction

Phosphorus is a relatively abundant element, whose cosmic abundance relative to \( H \) is \( 4 \times 10^{-7} \). Although it is lower by two orders of magnitude in abundance than those of the other third-row elements like Si and S, six phosphorus-containing molecules have been identified in space. They are PN (phosphorus nitride: Turner & Bally 1987; Ziurys 1987; Turner et al. 1990), CP (Guélin et al. 1990), PO (Tenenbaum et al. 2007), HCP (Agúndez et al. 2007), CCP (Halfen et al. 2008), and \( \text{PH}_3 \) (Agúndez et al. 2008; Tenenbaum & Ziurys 2008), where the detection of \( \text{PH}_3 \) is tentative. Among them, PN is an only phosphorus-containing molecule found in molecular clouds, while all of them are detected toward the envelopes of evolved stars like IRC +10216. So far, PN has been detected toward high-mass star forming regions such as Orion KL, W 51, and Sgr B2, whereas it has not been found in cold starless cores (Turner & Bally 1987; Ziurys 1987; Turner et al. 1990). Hence, high temperature chemistry is thought to be important for its production (Turner & Bally 1987; Ziurys 1987).

A theoretical model for the gas-phase phosphorus chemistry in molecular clouds was first discussed by Thorne et al. (1984) on the basis of the laboratory experiment of the reaction rates for phosphorus-containing molecules. Later, Millar, Bennett, and Herbst (1987) and Millar (1991) presented the chemical model simulations including phosphorus-containing molecules, and indicated that PN is the most stable phosphorus-containing molecule in the gas phase of molecular clouds. Charnley and Millar (1994) considered the phosphorus chemistry in hot cores, and proposed that PN is formed from \( \text{PH}_3 \) evaporated from grain mantles. However, this scheme has not been confirmed because of limited observations, and hence, the phosphorus chemistry is still poorly understood.

L 1157 B1 is a famous shocked region in the L 1157 molecular cloud, which is formed by the interaction between the ambient gas and the blue lobe of the outflow from the low-mass protostar IRAS 20386+6751 (e.g., Umemoto et al. 1992; Mikami et al. 1992; Bachiller & Pérez Gutiérrez 1997). The shock in this region is unambiguously established by the bright radio emission of SiO as well as the infrared H2 emission (e.g., Mikami et al. 1992; Davis & Eisloeffel 1995). This shocked region is well apart from the protostar by \( 63^\circ \), and hence, we can study the ‘pure’ shock chemistry by using a single dish telescope without being contaminated by possible complex structures in the vicinity of the protostar. With this in mind, we have been conducting an unbiased spectral line survey toward L 1157 B1 in the 3 mm wavelength region with the Nobeyama 45 m radio telescope (Sugimura et al. 2011; T. Yamaguchi et al. in preparation).

In the course of the line survey, we have fortuitously detected the \( J = 2–1 \) line of PN toward L 1157 B1. In this paper, we present the detection of PN with some follow-up observations, and discuss the phosphorus chemistry in the shocked region.

2. Observations

Observations were conducted with the 45 m radio telescope at Nobeyama Radio Observatory from 2010 February to May. Frequencies and line strengths of the PN (\( J = 2–1 \)) line and the other shock tracer lines (SiO and CH3OH) are listed in table 1. The 2SB SIS receiver, T100 H/V, was used in the observations, whose system temperature ranged from 150 to 250 K (Nakajima et al. 2008). The image rejection ratio is typically
higher than 13 dB. The main-beam efficiency ($\eta_{mb}$) is 0.45, and the half power beam width (HPBW) of the telescope is 18". We used autocorrelation spectrometers (ACSs) and acousto-optical radio spectrometers (AOS-Hs) as the backend, whose velocity resolutions are 1.6 km s$^{-1}$ and 0.118 km s$^{-1}$, respectively, at 94 GHz. We checked the telescope pointing by observing the nearby SiO maser source (T Cep) every hour, and maintained the pointing accuracy to be better than 8". We observed the spectral lines listed in table 1 toward the B1 and B2 positions (Bachiller & Pérez Gutiérrez 1997), as well as toward the protostar position of IRAS 20386+6751. The observed positions in L 1157 are given in table 2. The offsets of the B1 and B2 positions from the protostar position are (20$^\circ$.39, 12.4$^\prime$), (20$^\circ$.02, 15.9$^\prime$), respectively. The position-switching mode was employed for all the observations, where the off position was near a SiO maser source (T Cep) every hour, and maintained the pointing accuracy to be better than 8".

### Table 2. Observed positions.

<table>
<thead>
<tr>
<th>Source</th>
<th>$\alpha$(J2000)</th>
<th>$\delta$(J2000)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L 1157 B1</td>
<td>20 39 09.8</td>
<td>+68 01 15.9</td>
</tr>
<tr>
<td>L 1157 B2</td>
<td>20 39 12.4</td>
<td>+68 00 40.9</td>
</tr>
<tr>
<td>L 1157 mm (IRAS)</td>
<td>20 39 06.2</td>
<td>+68 02 15.9</td>
</tr>
</tbody>
</table>

### 3. Results

#### 3.1. Detection of PN

We detected the $J = 2$–1 line of PN toward the position B1 in the course of the spectral line survey. The line profile is shown in figure 1, where AC is used as the backend. The systemic velocity of the quiescent gas is 2.7 km s$^{-1}$, whereas the molecular lines observed toward B1 show a slightly blueshifted feature. The $V_{lsr}$ value for the PN ($J = 2$–1) line is $-0.66$ km s$^{-1}$, which is reasonable for the line at the B1 position. Here we employ the rest frequency of the PN ($J = 2$–1) line without the hyperfine structure (93979.7695 MHz) taken from CDMS. We carefully checked the available molecular line databases (CDMS and JPL), and found no accidentally overlapping lines of molecules known toward this source both in the signal and image bands. In fact, we find no line emission in the corresponding image frequency according to our line survey observation. Furthermore, no coincidence of other molecular transitions with PN ($J = 2$–1) was reported in the Orion KL spectrum by Turner and Bally (1987). Based upon these results, we conclude that the detected line is the $J = 2$–1 line of PN.

The $J = 2$–1 line of PN splits into the hyperfine components due to the nuclear quadrupole interaction of the N nucleus ($I = 1$), as shown in table 1. The $F = 3$–2 and 2–1 components have the frequencies which are close to the above frequency without the hyperfine structure, whereas the $F = 1$–0 and $F = 2$–2 components appear at the slightly redshifted velocity by 4.9 km s$^{-1}$ (table 1). The $F = 1$–0/2–2 components were not detected clearly in this study, because of its weak intrinsic intensity (0.27 times of the $F = 3$–2/2–1 components), although a little marginal hump at the high velocity side in the AC spectrum may be a sign of the $F = 1$–0/2–2 components.

After the detection of PN toward B1, we conducted observations toward the B2 and protostar positions as well as the B1 position with the higher spectral resolution by using AOS-H. The B2 position is located downstream from B1, where the outflow is decelerated and the velocity widths of various molecules become narrower than those in the B1 position (e.g., Bachiller & Pérez Gutiérrez 1997). Toward the B2 position, we also detected the PN ($J = 2$–1) line (figure 1). The $V_{lsr}$ value for the PN line is 1.7 km s$^{-1}$ toward B2, which is close to the systemic velocity of the L 1157 cloud. On the other hand, we did not detect the PN line toward the protostar position (figure 1). These results likely suggest that the distribution of PN is localized in the shocked region.

#### 3.2. Line Profiles

Here we compare the line profiles of PN ($J = 2$–1) with those of the shock tracer lines, CH$_3$OH ($J_K = 2K – 1K$) and SiO ($J = 2$–1) (figure 1). The line widths of PN are 3.8 km s$^{-1}$ and 3.7 km s$^{-1}$ toward B1 and B2, respectively, which are narrower than those of SiO, 7.9 km s$^{-1}$ and 5.2 km s$^{-1}$, respectively (table 3). On the other hand, they are rather close to the line widths of CH$_3$OH, 6.6 km s$^{-1}$ and 4.2 km s$^{-1}$ toward B1 and B2, respectively (table 3), although toward B1, the line width of PN is still narrower than that of CH$_3$OH. The CH$_3$OH molecule in the gas phase originates from the evaporation of the grain mantle caused by shock (Avery & Chiao 1996), whereas SiO is supplied mainly by disruption of the silicate grains (Mikami et al. 1992). The requirement for the grain disruption under stronger shock conditions is evidenced by the broader SiO line profiles as compared to those of the CH$_3$OH lines. Hence, it seems that the formation of PN is related to the grain mantle evaporation rather than the disruption of the grains.

#### 3.3. Column Densities

We calculate the column density of PN, assuming the local thermodynamic equilibrium (LTE) and optically thin conditions, as summarized in table 4. The excitation temperature is uncertain for PN, and hence, we calculate the column density for three excitation temperatures, $T_{ex} = 12$ K, 30 K, and 50 K, referring the other molecules observed in this region (Sugimura et al. 2011; Arce et al. 2008; Bachiller et al. 1995). The column
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Fig. 1. Observed spectral line profiles of PN, CH$_3$OH, and SiO. Vertical lines represent the systemic velocity of the L 1157 cloud. As for the AOS-H spectrum of PN, 16 channels are summed up to improve the signal to noise ratio. The resultant velocity resolution is 1.9 km s$^{-1}$. The $V_{\text{lsr}}$ velocity for PN refers to the rest frequency without the hyperfine splitting, and that for CH$_3$OH refers to the rest frequency of the $2_0;2_{0} - 1_0;1_{0} \alpha^+$ line.

Table 3. Line parameters.$^*$

<table>
<thead>
<tr>
<th>Molecules/Sources</th>
<th>$\Delta v$ (km s$^{-1}$)</th>
<th>$T_{\text{MB}}$ (K)</th>
<th>$\int T_{\text{MB}}dV$ (K km s$^{-1}$)</th>
<th>$V_{\text{lsr}}$ (km s$^{-1}$)</th>
<th>rms (mK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PN B1</td>
<td>3.8 ± 0.4</td>
<td>0.035 ± 0.011</td>
<td>0.19 ± 0.03</td>
<td>−0.64 ± 0.17$^\dagger$</td>
<td>11</td>
</tr>
<tr>
<td>PN B2</td>
<td>3.7 ± 0.5</td>
<td>0.054 ± 0.012</td>
<td>0.24 ± 0.03</td>
<td>1.7 ± 0.2$^\dagger$</td>
<td>12</td>
</tr>
<tr>
<td>CH$_3$OH B1</td>
<td>6.6 ± 0.3$^\dagger$</td>
<td>6.2 ± 0.2$^\dagger$</td>
<td>—</td>
<td>0.9 ± 0.1$^\dagger$</td>
<td>169</td>
</tr>
<tr>
<td>CH$_3$OH B2</td>
<td>4.2 ± 0.2$^\dagger$</td>
<td>7.8 ± 0.2$^\dagger$</td>
<td>—</td>
<td>1.8 ± 0.1$^\dagger$</td>
<td>185</td>
</tr>
<tr>
<td>CH$_3$OH IRAS</td>
<td>4.5 ± 0.4$^\dagger$</td>
<td>2.0 ± 0.1$^\dagger$</td>
<td>—</td>
<td>1.6 ± 0.2$^\dagger$</td>
<td>128</td>
</tr>
<tr>
<td>SiO B1</td>
<td>7.9 ± 0.2</td>
<td>3.6 ± 0.2</td>
<td>31.4 ± 0.4</td>
<td>−1.3 ± 0.1</td>
<td>159</td>
</tr>
<tr>
<td>SiO B2</td>
<td>5.2 ± 0.1</td>
<td>4.4 ± 0.2</td>
<td>21.9 ± 0.3</td>
<td>1.55 ± 0.05</td>
<td>155</td>
</tr>
</tbody>
</table>

$^*$ Based on the AOS-H data. $\Delta v$, $T_{\text{MB}}$, and $V_{\text{lsr}}$ are obtained by a single Gaussian fit. The blue wing ($V_{\text{lsr}} < −10$ km s$^{-1}$) of the SiO emission toward B1 is ignored in the fit.

$^\dagger$ Obtained only for the $2_{0,2} - 1_{0,1}$ $\alpha^+$ transition. The overlapping of the other lines is not taken into account.

$^\ddagger$ Calculated on the basis of the rest frequency without the hyperfine splitting. This is close to those of the $F = 3–2$ and $F = 2–1$ components.

Table 4. Column densities of PN.

<table>
<thead>
<tr>
<th>Sources</th>
<th>$N$ ($T_{\text{rot}} = 12$ K) (cm$^{-2}$)</th>
<th>$N$ ($T_{\text{rot}} = 30$ K) (cm$^{-2}$)</th>
<th>$N$ ($T_{\text{rot}} = 50$ K) (cm$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>$(4.2 ± 0.9) \times 10^{11}$</td>
<td>$(7.4 ± 1.7) \times 10^{11}$</td>
<td>$(1.1 ± 0.3) \times 10^{12}$</td>
</tr>
<tr>
<td>B2</td>
<td>$(5.3 ± 1.1) \times 10^{11}$</td>
<td>$(9.4 ± 2.0) \times 10^{11}$</td>
<td>$(1.4 ± 0.3) \times 10^{12}$</td>
</tr>
<tr>
<td>IRAS*</td>
<td>$\leq 2.9 \times 10^{10}$</td>
<td>$\leq 5.2 \times 10^{10}$</td>
<td>$\leq 7.9 \times 10^{10}$</td>
</tr>
</tbody>
</table>

$^*$ Line width is assumed to be 1 km s$^{-1}$. 
density toward the B2 position is almost comparable to that toward the B1 position. These values are lower by one or two orders of magnitude than those reported for Ori KL, W 51, and Sgr B2 (Turner & Bally 1987), as shown in table 5. The fractional abundances of PN relative to H$_2$ are also evaluated. Here the N(H$_2$) value of $2 \times 10^{21}$ cm$^{-2}$ based on the C$^{18}$O observation is used for the B1 and B2 positions, whereas $5 \times 10^{21}$ cm$^{-2}$ is used for the protostar position (Bachiller & Pérez Gutiérrez 1997). The fractional abundance of PN in the protostar position is lower than those in the B1 and B2 positions by more than one order of magnitude. The fractional abundances of PN in the B1 and B2 positions are found to be comparable to or higher than those found in the high-mass star forming regions.

### 4. Discussion

Since the P$^+$ ion does not react with H$_2$, the ion–molecule reaction scheme starting from P$^+$ is ineffective (Thorne et al. 1984). Therefore, the phosphorus ions and atoms would tend to be depleted onto dust grains before reacting with the gas phase species. According to Charnley and Millar (1994), the most abundant phosphorus-bearing molecule on grain mantles is PH$_3$, which is formed through hydrogenation of the P atom on grain mantles. This molecule is evaporated in the shocked region, which triggers the gas-phase phosphorus chemistry. First, PH$_3$ reacts with the H atoms to produce PH$_2$ and PH by abstraction reactions such as

$$H + PH_3 \rightarrow PH_2 + H_2,$$

(1)

$$H + PH_2 \rightarrow PH + H_2.$$  

(2)

Although these reactions have the activation-energy barriers, they can proceed in warm conditions with the gas temperature greater than 100 K. Then, PH reacts with the oxygen atom to form PO, which further reacts with the nitrogen atom to produce PN as,

$$N + PO \rightarrow PN + O,$$

(3)

or PH directly reacts with the nitrogen atom to form PN.

With the gas kinetic temperature of 100 K and the initial PH$_3$ fractional abundance of $1.2 \times 10^{-3}$, PN can be formed on a time scale of $\geq 10^4$ yr after mantle evaporation, and can reach an abundance of a few $\times 10^{-9}$ (Charnley & Millar 1994). This is higher by one order of magnitude than the observed values for L 1157 B1 and B2. As Charnley and Millar (1994) pointed out, the PN abundance directly scales with the adopted PH$_3$ abundance, which is arbitrarily assumed to be $1.2 \times 10^{-8}$ in their calculation. Even if the PH$_3$ abundance is lower by one order of magnitude than the above assumption, our observational result for L 1157 B1 and B2 can be explained.

The model requires the high temperature conditions ($T \geq 100$ K) in order to overcome the activation barriers of the abstraction reactions (1)–(2). Indeed, such a high temperature condition is fulfilled in some parts of L 1157 B1 and B2, according to the NH$_3$ observation (Umemoto et al. 1999). The reaction time scale for these initial reactions is estimated to be less than 1000 yr according to the abundance curve of PH$_3$ in the simulation (figure 1 of Charnley & Millar 1994).

Since the cooling time of the shocked region is from a few hundred to thousand years, a substantial part of PH$_3$ will be converted to PH. The subsequent reactions to form PN are all exothermic without reaction barriers, and hence, they can proceed even after the temperature becomes below 100 K. The model requires the time scale of $10^4$ yr for the PN production. Since the timescale of the outflow is reported to be 1.8 $\times 10^4$ yr (Umemoto et al. 1992), PN can certainly be formed in the shocked region. However, the model by Charnley and Millar (1994) is targeted at hot cores, and hence, more detailed simulations including the shock structure would be necessary.

In the above scheme, PH$_3$ is first released into the gas phase by the evaporation of grain mantles, and it is then converted to PN through gas-phase reactions. Thus, the gas-phase phosphorus chemistry and the formation of PN can be triggered by relatively mild shocks, as opposed to the case of SiO, which requires the disruption of the silicate grains due to strong shocks. The narrower line widths observed for PN as compared to that of SiO supports this picture.

For further validating the above formation scenario, it would be very important to search for other phosphorus-bearing molecules which the model predicts to be abundant, such as PH$_3$ and PO. They are expected to be abundant in the relatively short time scales ($< 10^3$ yr and $< 10^4$ yr, respectively) after the mantle evaporation, according to the model by Charnley and Millar (1994). L 1157 B1 will provide us with the best opportunity to detect these molecules, because it would contain the PH$_3$ and PO abundant stage. Abundances of these molecules will further constrain the phosphorus chemistry occurring in the shocked region.

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References