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CIRCUMSTELLAR MOLECULAR LINE ABSORPTION AND
EMISSION
IN THE OPTICAL SPECTRA OF POST-AGB STARS *

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Abstract. We present a list of post-AGB stars showing molecular line absorption and
emission in the optical spectrum. Two objects show CH⁺, one in emission and one in
absorption, and 10 stars show C₂ and CN in absorption. The Doppler velocities of the
C₂ lines and the rotational temperatures indicate that the line forming region is the AGB
remnant. An analysis of the post-AGB stars of which CO millimeter data is available
suggests that the C~ expansion velocity is of the same order as the CO expansion velocity.
HD 56126 has been studied in detail and we find a mass-loss rate of \( M = 2.8 \times 10^{-4} \, M_\odot \, \text{yr}^{-1} \),
\( f_{C_2} = 2.4 \times 10^{-5} \) and \( f_{CN} = 1.3 \times 10^{-5} \). The mass-loss derived from C₂ is significantly
larger than \( M = 1.2 \times 10^{-5} \, M_\odot \, \text{yr}^{-1} \) derived from CO. We find that all objects with the
21\( \mu \text{m} \) feature in emission show C₂ and CN absorption, but not all objects with C₂ and
CN detections show a 21\( \mu \text{m} \) feature.

Key words: molecules – physical conditions in AGB remnant – mass-loss history on AGB

1. Introduction

The study of molecular lines in the optical spectra of post-AGB stars started
with the paper by Waelkens et al. (1992) in which they presented a band
of narrow emission lines in the spectrum of the Red Rectangle (HD 44179).
These emission lines were identified as the (0,0) \( A^3 \Pi_u - X^1 \Sigma_g^+ \) band of
CH⁺ by Balm and Jura (1992). The presence of the Swan and Phillips bands of C₂ (Fig. 1) and red system bands of CN (Fig. 2) in the spectrum of
HD 56126 studied by Bakker (1994), showed that the outflow velocity and
the excitation conditions of C₂ suggest that these lines are formed in the
AGB remnant. This opens new possibilities to study the physical conditions
in AGB remnants. Hrivnak (1995) presents a list of post-AGB stars showing
C₂ and C₃ in absorption. Here we present the observations of post-AGB
stars that show molecular lines in the optical spectrum. For several stars

* Based on observations with the WHT/UES

Table I
Expansion velocities of the AGB remnant

<table>
<thead>
<tr>
<th>Object</th>
<th>Id*</th>
<th>$\delta V_{\text{optical}}$</th>
<th>$\delta V^+$</th>
<th>$T_{\text{rot}}$</th>
<th>$N_{10^{14}}$</th>
<th>Remark</th>
<th>$\text{[km s}^{-1}\text{]}$</th>
<th>$[\text{K}]$</th>
<th>$[\text{cm}^{-2}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRAS 04296+3429</td>
<td>C$_2$</td>
<td>-7.5</td>
<td>-12</td>
<td>138</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IRAS 05113+1347</td>
<td>C$_2$</td>
<td>-5.2</td>
<td>no</td>
<td>198</td>
<td>12</td>
<td>not observed in CO</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HD 56126</td>
<td>C$_2$</td>
<td>-8.8</td>
<td>-10.0</td>
<td>240</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IRAS 08005-2356</td>
<td>C$_2$</td>
<td>-38.1</td>
<td>-50.0</td>
<td>150</td>
<td>31</td>
<td>OH maser</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IRC +10216</td>
<td>C$_2$</td>
<td>-17.9</td>
<td>-15.7</td>
<td></td>
<td></td>
<td>AGB star</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>AFGL 2688</td>
<td>C$_2$</td>
<td>-15.0</td>
<td>-22.8</td>
<td>56</td>
<td>26</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HD 44179</td>
<td>CH$^+$</td>
<td>-4.5 em.</td>
<td>-3</td>
<td>267</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HD 213985</td>
<td>CH$^+$</td>
<td>-5.4 abs.</td>
<td>nd</td>
<td></td>
<td></td>
<td>not detected in CO</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*all stars with C$_2$ do also show CN absorption.

+ from CO millimeter emission. For IRAS 08005-2356 there is no CO data available and we used the velocities from the OH maser line.

the excitation temperature and outflow velocity have been determined. The C$_2$ absorption in HD 56126 is studied in detail by modeling the population density over the rotational quantum number (Section 3).

2. Detection of Molecules

In Table 1 we list the first results of our work. For each star the 3th and 4th column give the expansion velocity derived from respectively the optical (C$_2$,CN,CH$^+$) and the CO millimeter or OH maser line. The 5th and 6th column give the rotational temperature and column density derived from C$_2$ (3,0) or CH$^+(0,0)$ band. Negative velocities are due to outflow of material. The C$_2$ line absorption is formed closer to the star than the CO line emission, the two different molecules trace different material and hence different stages of the AGB evolution. Our data may indicate that the expansion velocity decreases as the star evolves along the AGB (Table 1). However a larger sample is needed to quantify this result. Stars showing the unidentified 21$\mu$m emission feature all exhibit C$_2$ and CN absorption, strongly suggesting that the 21$\mu$m feature is from carbon-rich material, but not all stars with C$_2$ absorption show the 21$\mu$m feature.

3. Modeling the C$_2$ absorption Bands of HD 56126

From the rotational diagram of the C$_2$ bands (Fig. 3) we find $T_{rot}$=240K and for the CN (1,0) band we find $T_{rot}$=24K with a column density of $N_{C_2} = 20 \times 10^{14}$ cm$^{-2}$ and $N_{CN} = 11 \times 10^{14}$ cm$^{-2}$. Unlike CN, C$_2$ is a homo nuclear molecule having no permanent dipole moment and the rotation
Fig. 1. Left: The Phillips (2,0) band in the spectrum of HD 56126. The C_2 absorption lines are not resolved.

Fig. 2. Right: The CN \( A^2\Pi - X^2\Sigma^+ \) (1,0) band in the spectrum of HD 56126. The computed synthetic spectrum is shifted down by 0.5.

Fig. 3. Left: Rotational Diagram of the C_2 \( A^1\Pi_u - X^1\Sigma^+ \) (1,0), (2,0), and (3,0) absorption band. The P, Q, and R branches are denoted by respectively a plus, asterisk, and a square. Only the weakest rotational band (3,0) is optically thin and gives an almost linear relation in the rotational diagram with \( T_{\text{rot}} = 240 \text{K} \) and \( N = 20 \times 10^{14} \text{ cm}^{-2} \).

Fig. 4. Right: Relative rotational diagram of the C_2 \( A^1\Pi_u - X^1\Sigma^+ \) (1,0), (2,0), and (3,0) absorption band of HD 56126 with the model fit for \( T_{\text{kin}} = 24 \text{K} \) superimposed.

Temperature is not a good indicator of the kinetic temperature because of pumping by the stellar radiation field. We use the CN rotational temperature as a measure of the kinetic temperature of the gas.

We have tried to fit the relative rotational diagram (Fig. 4) with the population density distribution derived from modeling the C_2 excitation by taking into account radiative pumping and collisional de-excitation (Van Dishoeck and Black 1982). The best fit is reached for \( n_c \sigma / I = 3.25 \times 10^{-14} \). Taking the latest \( \text{H}_2 - \text{C}_2 \) cross section of \( \sigma = 7.8 \times 10^{-16} \text{ cm}^{-2} \) (Phillips 1994) the mass-loss rate can be calculated using Eq. 1. This gives a mass-loss rate
TABLE II
Overview of derived mass-loss rates for HD 56126

<table>
<thead>
<tr>
<th>Source</th>
<th>Rate</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modeling C2 excitation</td>
<td>$2.8 \times 10^{-4} , M_{\odot} , yr^{-1}$</td>
<td>this study</td>
</tr>
<tr>
<td>Infrared excess from dust</td>
<td>$1.9 \times 10^{-4} , M_{\odot} , yr^{-1}$</td>
<td>this study; gas/dust = 100</td>
</tr>
<tr>
<td>CO millimeter emission</td>
<td>$1.2 \times 10^{-5} , M_{\odot} , yr^{-1}$</td>
<td>$^{12}$CO(2-1) Omont et al. 1993</td>
</tr>
</tbody>
</table>

of $\dot{M}_{C2} = 2.8 \times 10^{-4} \, M_{\odot} \, yr^{-1}$.

$$\dot{M} = 2.8 \times 10^{-4} \left(\frac{v_{\text{exp}}}{8.8} \cdot \frac{n_c}{1.7 \times 10^7} \cdot \frac{\sigma}{7.8 \times 10^{-16}} \cdot \frac{4.1 \times 10^5}{I}\right) \, M_{\odot} \, yr^{-1} \quad (1)$$

Fitting an optically thin dust model (Waters et al. 1988) to the spectral energy distribution of HD 56126 yields a dust inner radius of $2 \times 10^3 R_\odot$ and $M = 1.9 \times 10^{-4} \, M_{\odot} \, yr^{-1}$. Assuming that the molecular line absorption originates at this dust inner radius we find a particle abundance relative to $H_2$ of $f_{C2} = 2.4 \times 10^{-8}$ and $f_{CN} = 1.3 \times 10^{-8}$. Table 2 summarizes the mass-loss rates derived for HD 56126, where we have scaled the different mass-loss rates to $R_* = 50 R_\odot$, $T_{\text{eff}} = 6500K$ (log$L = 3.6$) and $D = 2.7 kpc$. The mass-loss rate derived from C$_2$ and from the IR excess are significantly higher than that derived from the CO millimeter emission, which might indicate that the mass loss rate increased dramatically towards the end of the AGB.

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