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# SEARCH OF AMINO GROUP IN THE UNIVERSE: 2-AMINOPYRIDINE

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**SUMMARY: In search for life in the Universe, scientists are interested in identification of molecules having amino (-$NH_2$) group in the interstellar space. The aminoacetonitrile ($NH_2CH_2CN$), which is precursor of the simplest amino acid glycine ($NH_2CH_2COOH$), is identified near the galactic center. The 2-Aminopyridine ($H_2NC_5H_4N$) is of interest for scientists as it has a close association with life on the earth. Based on spectroscopic studies, we have calculated intensities of 2-Aminopyridine lines due to transitions between the rotational levels up to 47 $cm^{-1}$ and have found a number of lines which may help in its identification in the interstellar medium. Frequencies of some of these transitions are found close to those detected in the envelope of IRC +10216 that are not assigned to any of the known species.**

**Key words. astrobiology; astrochemistry; ISM: molecules**

## 1. INTRODUCTION

Scientists are interested in search for life in the interstellar medium. Amino acids are responsible for the development of life on the earth where they might have been brought to either a meteorite or comet bombardment. These amino acids are supposed to be responsible for the formation of primitive building blocks of life components, e.g. proteins, which were part of primitive unicellular organisms in early stages of life on the earth, and evolved as a intelligent life system later on. Thus, the fundamental organic constituents of the life are DNA, RNA, protein, etc. which form the basis of formation of 'the cell'. More than 500 amino acids are supposed to be present in nature. Of them, only 20 amino acids are essential for human beings. These 20 major amino acids, along with hundreds of other minor amino acids, sustain our lives. For formation of more complex structures, there are different levels of interaction between the proteins, making them rigid or flexible structures to meet different functional requirements.

These 20 amino acids formed within proteins carry a huge order of chemical utility. The sequence of those amino acids of a specific protein is determined by a sequence of bases in the gene that encodes that protein. Out of 20 amino acids, 10 amino acids are produced inside the human being while the remaining 10 amino acids need to be

supplied from outside sources. Pyridines are involved in photosensitized chemistry, luminescent materials, metal complex chemistry and liquid crystals, and are used as a monomer for polymerization. Aminopyridine contains one monovalent -$NH_2$ group attached to the pyridine ring. Thus, there are three positional isomers: 2-Aminopyridine, 3-Aminopyridine, and 4-Aminopyridine. However, 2-Aminopyridine ($H_2NC_5H_4N$) has been of great interest to astronomers.

The simplest amino acid glycine ($NH_2CH_2COOH$) has been searched for in the interstellar space for a long time. At the same time, more and more complex molecules are found towards the galactic center. Though the detection of glycine has not been confirmed, its precursor aminoacetonitrile ($NH_2CH_2CN$) is identified near the galactic center (Belloche et al. 2008).

The 2-Aminopyridine molecule has been studied in laboratories and its rotational and centrifugal distortion constants are derived. Its electric dipole moment has components along $a$ and $b$ inertial axes. The lines for $b$-type transitions are significantly more intense than those for $a$-type transitions.

We have, therefore, calculated the line intensities and Einstein $A$-coefficients for $b$-type transitions between rotational levels in 2-Aminopyridine lying up to 47 cm$^{-1}$. Of these transitions, we have selected only those which may play an important role in identification of 2-Aminopyridine in the interstellar medium.

## 2. THE 2-AMINOPYRIDINE

The 2-Aminopyridine is an asymmetric top molecule having its electric dipole moment inclined with $a$ and $b$ inertial axes such that $\mu_a = 0.166$ Debye and $\mu_b = 0.86$ Debye. It has the ground $O^+$ state and the first excited $O^-$ state. We are concerned with the ground $O^+$ state. The microwave spectrum of 2-Aminopyridine was recorded by Kydd and Mills (1972). Kydd (1979) presented the room temperature vapour phase infrared spectrum of 2-Aminopyridine for the spectrum range from 100 cm$^{-1}$ to 600 cm$^{-1}$. Later on, Ye and Bettens (2004) recorded the spectrum of 2-Aminopyridine in the frequency range from 75 GHz to 110 GHz, and derived accurate rotational constants ($A$, $B$, $C$) and centrifugal distortion parameters ($D_i$), given in Table 1. Fourier transform infrared (FT-IR) and Fourier transform Raman (FT-R) spectra of 2-Aminopyridine were recorded by Jose and Mohan (2006).

**Table 1.** Parameters of 2-Aminopyridine

| Parameter | Value |
|---|---|
| $A$ (MHz) | 5780.3720 |
| $B$ (MHz) | 2733.50354 |
| $C$ (MHz) | 1857.67392 |
| $D_J$ (kHz) | 0.13653 |
| $D_{JK}$ (kHz) | 0.2029 |
| $D_K$ (kHz) | 0.9312 |
| $d_1$ (kHz) | 0.045827 |
| $d_2$ (kHz) | 0.36733 |

Since $\mu_b$ is five times larger than $\mu_a$, and the Einstein $A$-coefficient is proportional to the square of the component of electric dipole moment, the $b$-type transitions are significant and are of our interest. The $a$-type transitions are weak. Therefore, we have not included $a$-type transitions in the investigation. The levels for $b$-type transitions can be classified into two groups: (i) with $k_a + k_c =$ odd (set I) and (ii) with $k_a + k_c =$ even (set II). For the electric dipole moment along the $b$-axis of inertia, the radiative transitions between the rotational levels are governed by the selection rules:

$$\begin{aligned} J: &\quad \Delta J = 0, \pm 1 \\ k_a, k_c: &\quad \text{odd, even} \longleftrightarrow \text{even, odd} \quad \text{(set I)} \\ &\quad \text{even, even} \longleftrightarrow \text{odd, odd} \quad \text{(set II)} \end{aligned}$$

For calculation of the line-strengths and Einstein $A$-coefficients for transitions, we have employed the software ASROT (Kisiel, 2001) where the rotational and centrifugal distortion constants, given in Table 1, are used. There are 1004 set I transitions and 1001 set II transitions, and their details can be obtained from authors.

## 3. RESULTS AND DISCUSSION

For a spectral line to be a strong emission line under interstellar conditions, beside a sufficient abundance of the molecule under consideration, two further conditions need to be satisfied:

(i) The upper level of transition must be sufficiently populated. In an interstellar cloud, the basic excitation of molecules is dominated in most cases by collisions. At a given temperature, this limits the energy $E_j$ of upper level of transition; we have chosen:

$$E_j < 47 \text{ cm}^{-1}$$

which is sufficient for temperatures up to 47 K, at least.

(ii) For the transition the Einstein $A$-coefficient must be sufficiently large. Most interstellar lines are formed under non-local thermal equilibrium (NLTE) conditions implying that the occupation numbers for individual levels can only be determined by solving the statistical equilibrium equations coupled with equations of radiative transfer. For doing so, one requires the collisional rate coefficients (Sharma et al. 2014a, c, 2015). Computation of collisional rate coefficients is a cumbersome task and data are not available in literature. We therefore make the following estimate: When the Einstein $A$-value, which gives the probability for radiative transition between a pair of levels, is large compared to the probability for the collisional deexcitation between the levels, one may say that almost every excitation is followed by the emission of at least

**Table 2.** Frequency $\nu$, $A$-coefficient $A_{ji}$, line strength $S_{ji}$, energy $E_j$ of upper level for $b$-type rotational transitions in set I of 2-Aminopyridine.

| Transition | $\nu$ (GHz) | $A_{ji}$ ($s^{-1}$) | $S_{ji}$ | $E_j$ ($cm^{-1}$) | $\nu$ (GHz) (Cernicharo et al. 2000) |
|---|---|---|---|---|---|
| $10_{10,1} \rightarrow 9_{9,0}$ | 112.146 | 5.45E-06 | 9.43 | 20.042 | |
| $11_{11,0} \rightarrow 10_{10,1}$ | 123.705 | 7.39E-06 | 10.43 | 24.166 | |
| $11_{10,1} \rightarrow 10_{9,2}$ | 116.790 | 5.56E-06 | 9.33 | 21.748 | |
| $12_{11,2} \rightarrow 11_{10,1}$ | 128.350 | 7.52E-06 | 10.33 | 26.027 | |
| $12_{10,3} \rightarrow 11_{9,2}$ | 121.431 | 5.71E-06 | 9.25 | 23.612 | |
| $12_{12,1} \rightarrow 11_{11,0}$ | 135.264 | 9.74E-06 | 11.43 | 28.675 | 135.298, 135.238 |
| $13_{11,2} \rightarrow 12_{10,3}$ | 132.991 | 7.69E-06 | 10.25 | 28.045 | 132.782 |
| $13_{13,0} \rightarrow 12_{12,1}$ | 146.822 | 1.25E-05 | 12.43 | 33.569 | |
| $13_{10,3} \rightarrow 12_{9,4}$ | 126.065 | 5.87E-06 | 9.19 | 25.634 | |
| $13_{12,1} \rightarrow 12_{11,2}$ | 139.909 | 9.89E-06 | 11.33 | 30.690 | |
| $14_{11,4} \rightarrow 13_{10,3}$ | 137.628 | 7.88E-06 | 10.18 | 30.221 | 137.935 |
| $14_{13,2} \rightarrow 13_{12,1}$ | 151.467 | 1.27E-05 | 12.32 | 35.739 | |
| $14_{10,5} \rightarrow 13_{9,4}$ | 130.690 | 6.06E-06 | 9.14 | 27.815 | 130.765 |
| $14_{12,3} \rightarrow 13_{11,2}$ | 144.551 | 1.01E-05 | 11.24 | 32.863 | 144.456 |
| $14_{14,1} \rightarrow 13_{13,0}$ | 158.380 | 1.58E-05 | 13.43 | 38.848 | |
| $15_{11,4} \rightarrow 14_{10,5}$ | 142.257 | 8.10E-06 | 10.13 | 32.557 | |
| $15_{13,2} \rightarrow 14_{12,3}$ | 156.110 | 1.29E-05 | 12.24 | 38.067 | |
| $15_{15,0} \rightarrow 14_{14,1}$ | 169.938 | 1.97E-05 | 14.43 | 44.513 | 169.742 |
| $15_{10,5} \rightarrow 14_{9,6}$ | 135.301 | 6.25E-06 | 9.08 | 30.156 | 135.298, 135.238 |
| $15_{12,3} \rightarrow 14_{11,4}$ | 149.189 | 1.03E-05 | 11.18 | 35.194 | |
| $15_{14,1} \rightarrow 14_{13,2}$ | 163.025 | 1.60E-05 | 13.32 | 41.173 | 163.120, 163.179 |
| $16_{11,6} \rightarrow 15_{10,5}$ | 146.875 | 8.33E-06 | 10.07 | 35.051 | |
| $16_{13,4} \rightarrow 15_{12,3}$ | 160.750 | 1.32E-05 | 12.17 | 40.553 | |
| $16_{15,2} \rightarrow 15_{14,1}$ | 174.583 | 1.99E-05 | 14.32 | 46.993 | |
| $16_{10,7} \rightarrow 15_{9,6}$ | 139.893 | 6.45E-06 | 9.03 | 32.657 | |
| $16_{12,5} \rightarrow 15_{11,4}$ | 153.822 | 1.06E-05 | 11.12 | 37.684 | 153.783 |
| $16_{14,3} \rightarrow 15_{13,2}$ | 167.669 | 1.63E-05 | 13.24 | 43.656 | |
| $17_{9,8} \rightarrow 16_{8,9}$ | 137.367 | 5.01E-06 | 7.86 | 33.180 | |
| $17_{11,6} \rightarrow 16_{10,7}$ | 151.480 | 8.57E-06 | 10.02 | 37.707 | |
| $17_{13,4} \rightarrow 16_{12,5}$ | 165.384 | 1.35E-05 | 12.11 | 43.197 | |
| $17_{10,7} \rightarrow 16_{9,8}$ | 144.464 | 6.64E-06 | 8.96 | 35.321 | 144.456 |
| $17_{12,5} \rightarrow 16_{11,6}$ | 158.445 | 1.08E-05 | 11.06 | 40.333 | |
| $17_{14,3} \rightarrow 16_{13,4}$ | 172.309 | 1.66E-05 | 13.16 | 46.296 | |
| $18_{9,10} \rightarrow 17_{8,9}$ | 141.698 | 5.13E-06 | 7.74 | 36.020 | |
| $18_{11,8} \rightarrow 17_{10,7}$ | 156.065 | 8.81E-06 | 9.96 | 40.523 | |
| $18_{13,6} \rightarrow 17_{12,5}$ | 170.011 | 1.38E-05 | 12.05 | 46.000 | 170.025, 170.144 |
| $18_{10,9} \rightarrow 17_{9,8}$ | 148.996 | 6.84E-06 | 8.88 | 38.147 | |
| $18_{12,7} \rightarrow 17_{11,6}$ | 163.057 | 1.11E-05 | 11.01 | 43.142 | 163.120, 163.179 |
| $19_{9,10} \rightarrow 18_{8,11}$ | 146.355 | 5.25E-06 | 7.59 | 39.029 | 146.436, 146.428 |
| $19_{11,8} \rightarrow 18_{10,9}$ | 160.629 | 9.05E-06 | 9.89 | 43.501 | |
| $19_{10,9} \rightarrow 18_{9,10}$ | 153.515 | 7.02E-06 | 8.79 | 41.137 | |
| $19_{12,7} \rightarrow 18_{11,8}$ | 167.655 | 1.14E-05 | 10.95 | 46.111 | |
| $20_{9,12} \rightarrow 19_{8,11}$ | 149.958 | 5.26E-06 | 7.42 | 42.201 | |
| $20_{11,10} \rightarrow 19_{10,9}$ | 165.161 | 9.28E-06 | 9.81 | 46.642 | |
| $20_{10,11} \rightarrow 19_{9,10}$ | 157.912 | 7.17E-06 | 8.68 | 44.292 | 157.935, 157.960 |
| $21_{9,12} \rightarrow 20_{8,13}$ | 155.578 | 5.39E-06 | 7.15 | 45.557 | |

**Table 3.** Frequency $\nu$, $A$-coefficient $A_{ji}$, line strength $S_{ji}$, energy $E_j$ of upper level for $b$-type rotational transitions in set II of 2-Aminopyridine.

| Transition | $\nu$ (GHz) | $A_{ji}$ ($s^{-1}$) | $S_{ji}$ | $E_j$ ($cm^{-1}$) | $\nu$ (GHz) (Cernicharo et al. 2000) |
|---|---|---|---|---|---|
| $10_{10,0} \rightarrow 9_{9,1}$ | 112.146 | 5.45E-06 | 9.43 | 20.042 | |
| $11_{11,1} \rightarrow 10_{10,0}$ | 123.705 | 7.39E-06 | 10.43 | 24.166 | |
| $11_{10,2} \rightarrow 10_{9,1}$ | 116.790 | 5.56E-06 | 9.33 | 21.748 | |
| $12_{11,1} \rightarrow 11_{10,2}$ | 128.350 | 7.52E-06 | 10.33 | 26.027 | |
| $12_{10,2} \rightarrow 11_{9,3}$ | 121.431 | 5.71E-06 | 9.25 | 23.612 | |
| $12_{12,0} \rightarrow 11_{11,1}$ | 135.264 | 9.74E-06 | 11.43 | 28.675 | 135.298, 135.238 |
| $13_{11,3} \rightarrow 12_{10,2}$ | 132.991 | 7.69E-06 | 10.25 | 28.045 | 132.782 |
| $13_{13,1} \rightarrow 12_{12,0}$ | 146.822 | 1.25E-05 | 12.43 | 33.569 | |
| $13_{10,4} \rightarrow 12_{9,3}$ | 126.065 | 5.87E-06 | 9.19 | 25.634 | |
| $13_{12,2} \rightarrow 12_{11,1}$ | 139.909 | 9.89E-06 | 11.33 | 30.690 | |
| $14_{11,3} \rightarrow 13_{10,4}$ | 137.628 | 7.88E-06 | 10.18 | 30.221 | 137.935 |
| $14_{13,1} \rightarrow 13_{12,2}$ | 151.467 | 1.27E-05 | 12.32 | 35.739 | |
| $14_{10,4} \rightarrow 13_{9,5}$ | 130.690 | 6.06E-06 | 9.14 | 27.815 | 130.765 |
| $14_{12,2} \rightarrow 13_{11,3}$ | 144.551 | 1.01E-05 | 11.24 | 32.863 | 144.456 |
| $14_{14,0} \rightarrow 13_{13,1}$ | 158.380 | 1.58E-05 | 13.43 | 38.848 | |
| $15_{11,5} \rightarrow 14_{10,4}$ | 142.257 | 8.10E-06 | 10.13 | 32.557 | |
| $15_{13,3} \rightarrow 14_{12,2}$ | 156.110 | 1.29E-05 | 12.24 | 38.067 | |
| $15_{15,1} \rightarrow 14_{14,0}$ | 169.938 | 1.97E-05 | 14.43 | 44.513 | 169.742 |
| $15_{10,6} \rightarrow 14_{9,5}$ | 135.301 | 6.25E-06 | 9.08 | 30.156 | 135.238, 135.298 |
| $15_{12,4} \rightarrow 14_{11,3}$ | 149.189 | 1.03E-05 | 11.18 | 35.194 | |
| $15_{14,2} \rightarrow 14_{13,1}$ | 163.025 | 1.60E-05 | 13.32 | 41.173 | |
| $16_{11,5} \rightarrow 15_{10,6}$ | 146.876 | 8.33E-06 | 10.07 | 35.051 | |
| $16_{13,3} \rightarrow 15_{12,4}$ | 160.750 | 1.32E-05 | 12.17 | 40.553 | |
| $16_{15,1} \rightarrow 15_{14,2}$ | 174.583 | 1.99E-05 | 14.32 | 46.993 | |
| $16_{10,6} \rightarrow 15_{9,7}$ | 139.894 | 6.45E-06 | 9.03 | 32.657 | |
| $16_{12,4} \rightarrow 15_{11,5}$ | 153.822 | 1.06E-05 | 11.12 | 37.684 | 153.783 |
| $16_{14,2} \rightarrow 15_{13,3}$ | 167.669 | 1.63E-05 | 13.24 | 43.656 | |
| $17_{9,9} \rightarrow 16_{8,8}$ | 137.305 | 5.00E-06 | 7.86 | 33.180 | |
| $17_{11,7} \rightarrow 16_{10,6}$ | 151.480 | 8.57E-06 | 10.02 | 37.707 | |
| $17_{13,5} \rightarrow 16_{12,4}$ | 165.384 | 1.35E-05 | 12.11 | 43.197 | |
| $17_{10,8} \rightarrow 16_{9,7}$ | 144.461 | 6.64E-06 | 8.96 | 35.321 | 144.456 |
| $17_{12,6} \rightarrow 16_{11,5}$ | 158.445 | 1.08E-05 | 11.06 | 40.333 | |
| $17_{14,4} \rightarrow 16_{13,3}$ | 172.309 | 1.66E-05 | 13.16 | 46.296 | |
| $18_{9,9} \rightarrow 17_{8,10}$ | 141.863 | 5.14E-06 | 7.74 | 36.021 | |
| $18_{11,7} \rightarrow 17_{10,8}$ | 156.066 | 8.81E-06 | 9.96 | 40.523 | |
| $18_{13,5} \rightarrow 17_{12,6}$ | 170.011 | 1.38E-05 | 12.05 | 46.000 | 170.025, 170.144 |
| $18_{10,8} \rightarrow 17_{9,9}$ | 149.006 | 6.84E-06 | 8.88 | 38.147 | |
| $18_{12,6} \rightarrow 17_{11,7}$ | 163.057 | 1.11E-05 | 11.01 | 43.142 | |
| $19_{9,11} \rightarrow 18_{8,10}$ | 145.947 | 5.22E-06 | 7.60 | 39.026 | |
| $19_{11,9} \rightarrow 18_{10,8}$ | 160.628 | 9.05E-06 | 9.89 | 43.501 | |
| $19_{10,10} \rightarrow 18_{9,9}$ | 153.486 | 7.01E-06 | 8.79 | 41.137 | |
| $19_{12,8} \rightarrow 18_{11,7}$ | 167.655 | 1.14E-05 | 10.95 | 46.111 | |
| $20_{9,11} \rightarrow 19_{8,12}$ | 150.894 | 5.34E-06 | 7.40 | 42.206 | |
| $20_{11,9} \rightarrow 19_{10,10}$ | 165.166 | 9.28E-06 | 9.81 | 46.643 | |
| $20_{10,10} \rightarrow 19_{9,11}$ | 157.991 | 7.18E-06 | 8.67 | 44.293 | 157.960, 157.981 |
| $21_{9,13} \rightarrow 20_{8,12}$ | 153.572 | 5.23E-06 | 7.21 | 45.544 | |

one photon. (If a higher lying level is populated, the molecule may cascade down to the lower states by emitting a sequence of photons.) In general, the collisional rate coefficient for the transition from an upper level $j$ to a lower level $i$ is expressed as (Chang et al. 2013, Sharma et al. 2014b):

$$C_{ji} = < v\ \sigma_{ji} >$$

where $v$ is the relative velocity of collision partner, generally taken to be the most abundant molecular hydrogen $H_2$, and $\sigma_{ji}$ the collision cross section for the transition. The latter is very difficult to compute. It depends on the transition and on the collision partner. In order to obtain an estimate, we assume $\sigma_{ji} \approx 10^{-16}$ cm$^2$ and $v \approx 1$ km/s $= 10^5$ cm/s, leading to (Chang et al. 2013, Sharma et al. 2014b):

$$C_{ji} \approx 10^{-11}\ \mathrm{cm^3 s^{-1}}\,.$$

These values of collisional rate coefficient are reasonable (Sharma et al. 2014a, c, 2015). For a dense molecular cloud we have $n_{H_2} \approx 10^4 \mathrm{cm^{-3}}$ and, therefore, the product $n_{H_2} C_{ji} \approx 10^{-7} \mathrm{s^{-1}}$. According to this estimate, we included in Tables 2 and 3 the lines with

$$A_{ji} > 5 \times 10^{-6}\ \mathrm{s^{-1}} \quad \text{and} \quad E_j < 47\ \mathrm{cm^{-1}}\,.$$

Further, the line strength of the transition needs to be large. When the Einstein $A$-coefficient is larger than the collisional deexcitation rate, the probability of formation of photon is quite large. It is interesting to note that there are 46 + 46 lines having quite large value of Einstein $A$-coefficient and whose upper level is not at very high energy. These lines are quite promising for the identification of 2-Aminopyridine in the interstellar medium.

Cernicharo et al. (2000) identified a number of lines in the atmosphere of IRC+10216 which have not been assigned to any of the species. We have found that some of them, reported in the last column of Tables 2 and 3, have frequencies very close to those obtained in the present investigation.

In Tables 2 and 3, there are 14 + 11 transitions whose frequency matches with the unidentified lines of Cernicharo et al. (2000). The difference in the frequencies is less than 0.01%. This closeness of frequencies is inspiring on one hand, but also surprising. Half of these transitions have the Einstein $A$-coefficient larger than $10^{-5}$ s$^{-1}$ which is quite large and promising for identification of 2-Aminopyridine. The transitions reported in Tables 2 and 3 may play an important role for identification of 2-Aminopyridine in the interstellar space.

## 4. CONCLUSIONS

Using the derived rotational and centrifugal distortion constants of 2-Aminopyridine, energies of levels, and frequencies, line strengths and Einstein $A$-coefficients for rotational transitions are calculated. We have reported information about the potential transitions only. Frequencies of a number of lines are found very close to those observed in the spectra of IRC + 10216 and not assigned to any of the species. It is possible that some of these lines belong to 2-Aminopyridine.

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# ПОТРАГА ЗА АМИНО-ГРУПОМ У ВАСИОНИ: 2-АМИНОПИРИДИН

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УДК 524.527
*Претходно саопштење*

У потрази за животом у васиони, научници теже да у међузвезданом простору идентификују молекуле који садрже амино-групу (-$NH_2$). Аминоацетонитрил ($NH_2CH_2CN$), који је претходник просте аминокиселине глицин ($NH_2CH_2COOH$), је идентификован у близини галактичког центра. Једињење 2-аминопиридин ($H_2NC_5H_4N$) је од интереса научницима јер је у тесној вези са животом на Земљи. На основу спектроскопских студија израчунали смо интензитете линија 2-аминопиридина насталих прелазима између ротационих нивоа до 47 $cm^{-1}$ и пронашли неколико линија које би могле помоћи при његовој идентификацији у међузвезданој средини. Фреквенције неких од ових прелаза су близу фреквенцијама линија детектованим у омотачу IRC+10216 које нису приписане ни једној познатој врсти хемијских једињења.