

Ammonia in circumstellar environment of V Cyg

B. Etmański, M. R. Schmidt, R. Szczerba*

Nicolaus Copernicus Astronomical Center, Polish Academy of Sciences, ul. Rabiańska 8, 87-100 Toruń, Poland

The HIFI instrument on board of the Herschel Space Observatory (HSO) has been very successful in detecting molecular lines from the circumstellar envelopes around evolved stars, like massive red supergiants, Asymptotic Giant Branch (AGB) and post-AGB stars, as well as the planetary nebulae. Among others, ammonia have been found in the circumstellar envelopes of C-rich AGB stars in amounts that significantly exceeded the theoretical predictions for C-rich stars. Few scenarios have been proposed to resolve this problem: formation of ammonia behind the shock front and photochemical processes in the inner part of the envelope partly transparent to UV background radiation due to the clumpy structure of the gas and formation of ammonia on dust grains. Careful analysis of observations may help to put the constraints on one or another mechanism of ammonia formation. Here, we present results of the non-LTE radiative transfer modeling of ammonia transitions including the crucial process of radiative pumping via the $v_2 = 1$ vibrational band (at $\sim 10 \mu\text{m}$) for V Cyg. Only the ground-based ammonia transition NH_3 $J = 1_0 - 0_0$ at 572.5 GHz has been observed by HIFI. Therefore, to determine the abundance of ammonia we estimate the photodissociation radius of NH_3 using chemical model of the envelope consistent with the dust grain properties concluded from the spectral energy distribution.

Key words: abundances; line: profile; stars: AGB, stars: carbon, individual: V Cyg

INTRODUCTION

Ammonia (NH_3) was discovered in space in 1968 [3] and its first transition was detected at 23 GHz with a radio telescope. Ammonia is mostly observed in the interstellar medium [11] and commonly in the star forming regions (see e.g. [10, 12, 26]). However, ammonia is also detected in the circumstellar envelopes of evolved stars (see, e.g. [21] for analysis of ammonia in the Asymptotic Giant Branch (AGB) star CW Leo). The Asymptotic Giant Branch stage of stellar evolution is characteristic for stars with the initial mass between $1-8 M_\odot$, that is for stars with low-to-intermediate initial mass, and is characterised by the intense mass-loss processes. The AGB stars can be divided into two main types: C-rich and O-rich ones. The C-rich AGB stars contain more carbon than oxygen atoms, i.e. $C/O > 1$. V Cyg itself belongs to this group of objects. V Cyg is Mira type variable with the period of about 417 days, C6 spectral type [27] and the distance of 420 pc [28]. The central star has the low effective temperature (2000–3000 K). The star in this phase of evolution has very weak gravitational force in the stellar atmosphere and changes periodically its radius, temperature and luminosity. Pulsations are responsible for the dust formation in the outer layers of atmosphere, and then the radiation pressure on dust can initiate the ejection of material from the atmosphere into

space. Matter ejected from the star forms Circumstellar Envelope (CSE) around the star, where new molecules, like for example ammonia, are formed. The observed abundance of NH_3 is several magnitudes larger than the models of stellar atmosphere for AGB stars predict (e.g. [13]). The formation process of ammonia is unknown. Two scenarios have been proposed for the ammonia formation in CSE. In the first scenario ammonia may be formed by the passage of shocks. In this scenario N_2 molecules have been dissociated and atoms of nitrogen are available to form the ammonia molecule [29]. Unfortunately, the last calculations have shown that this process changes the abundance of NH_3 only marginally [8]. The second mechanism is the dissociation of N_2 by the UV radiation because the CSE is inhomogeneous and the UV radiation may penetrate almost through the whole envelope [5].

In Section 2 we present description of the molecular model of ammonia. The observations and data reductions are described in Section 3. Section 4 is devoted to description of the modelling process of ammonia lines in CSE of V Cyg. At the last, in Section 5 we discuss the results of our modelling.

MODEL OF AMMONIA

Ammonia molecule exists in two species: ortho and para. These two species differ in the orienta-

*etmoon@ncac.torun.pl

tions of three hydrogen spins. Symmetry properties of the ro-vibrational (including inversion) levels are described by the symmetry group D_{3h} (C_{3v} if the inversion mode is neglected). Because of the Pauli exclusion principle, the ro-vibrational levels must belong to A' and A'' (para states) and E' and E'' (ortho states) representations of D_{3h} [2]. Ammonia oscillates in six vibrational modes, of which two pairs are degenerate, and which are described by four quantum vibrational numbers (ν_1 , ν_2 , $\nu_3^{l_3}$, $\nu_4^{l_4}$) and two vibrational angular momenta l_3 and l_4 .

Ammonia molecule has the inversional nature. It is because the potential energy surface has the double minimum corresponding to two positions of the nitrogen atom on opposite sides of the plane defined by the hydrogen atoms. The molecule may change rapidly its geometry, because its potential barrier between the two minima is small and equals 2009 cm^{-1} ($6.4 \cdot 10^{-14} \text{ erg}$). In this case the energy levels are not strongly separated and the wave functions mix together resulting in two kinds of levels: symmetric (s, +) and antisymmetric (a, -) [1].

For calculations of the excitation of a molecule in a circumstellar envelope one needs the input file containing the list of adopted energy levels, the list of radiative transitions between energy levels and the set of collisional rates. For a limited number of levels the input file is available in the database LAMDA¹, [6, 18]. Hereby, we followed [21], and the set of levels extracted from the theoretical EXOMOL database², [25] has been used. The advantage of using the computed database instead of the laboratory one is its completeness.

DATA

Observations of V Cyg were obtained with the Heterodyne Instrument for the Far Infrared instrument (HIFI) on board of the Herschel Space Observatory (HSO) in the point mode. The observations were part of the HIFISTARS Guaranteed Time Key Program (Proposal Id: KPGT_vbujarra_1, PI: V. Bujarrabal). Details of the available observations are presented in Table 1. For each observation we give the spectroscopic designation, the frequency of transition in GHz, band of the HIFI instrument, energy of the upper level in K, the observational identification, the date of observation, the phase of observation, the half power beam width (HPBW) of the HIFI instrument and the main beam efficiency

(η_{mb})³. The observational phase of variability was determined relative to the reference data of maximum, selected from the visual variability curve (see below) ($\phi = 0$ for Julian Date 2450330), and assuming the variability period of 417 days [20]). Only the ground rotational transition of ortho-NH₃ was recorded in two instrumental settings observed at the same time. The reduction of data was conducted using the HIPE v.15.0.1 software⁴. The reduction process was limited to extraction of the data from level 2, tracing continuum and removing baseline, averaging of two H and V polarisations and final averaging of two settings. For comparison with theoretical models, the antenna temperature was converted to the main beam temperature using the main beam coefficients. The final profile of the 1_0-0_0 ortho-ammonia line is shown in Figure 1 on the Doppler velocity scale relative to the Local Standard of Rest V_{LSR} . The root mean square (r.m.s.) in the continuum amounts to 3 mK. The uncertainty of the flux is expected to be less than 10 percent [15].

For the analysis of variability we used the data available in the AAVSO database⁵. The AAVSO database provides a very long sequence of photometric observations in visual band covering both HIFI and ISO periods of observations. Sequence of the data covering the ISO observations is shown in Figure 2.

The main source of data for the Spectral Energy Distribution (SED) modelling is the atlas of Infrared Space Observatory (ISO) observations available on the web page⁶ ([14, 23]). This catalogue includes 1239 full-scan AOT1 spectra from the Short Wavelength Spectrometer (SWS). These spectra contain the photometric scan between about 2.4 to $45.4 \mu\text{m}$ for each object. All spectra were reduced and ready to use for modelling [23]. In the collection of spectra we found six spectral scans of our object (Table 2). One spectral scan was observed at the variability phase close to that of the HIFI observations (ID = 69500110) and was used for modelling of the SED (Fig. 3). Photometry was updated with photometrical measurements of the V^7 , J , H and K bands [4] (date of the observation: 2000-05-04, JD date: 2451668.9397, phase: $\phi = 0.2$)⁸ and with the IRAS measurements for 12, 25, 60 and $100 \mu\text{m}$ ⁹ (in this case the flux reported in the catalogue is the average value of the IRAS observations in each band, and the phase is unknown¹⁰).

¹<https://home.strw.leidenuniv.nl/~moldata>

²<http://exomol.com>

³http://hertwiki.esac.esa.int/twiki/pub/Public/HifiCalibrationWeb/HifiBeamReleaseNote_Sep2014.pdf

⁴<https://www.cosmos.esa.int/web/herschel/hipe-download>

⁵<https://www.aavso.org/>

⁶<https://users.physics.unc.edu/~gcsloan/library/swsatlas/aot1.html>

⁷<http://simbad.u-strasbg.fr/simbad/sim-ref?querymethod=bib&simbo=on&submit=submit+bibcode&bibcode=2002yCat.2237....0D>

⁸<http://vizier.u-strasbg.fr/viz-bin/VizieR?-source=II/246>

⁹<http://vizier.u-strasbg.fr/viz-bin/VizieR-5?-out.add=&-source=II/125/main,II/126/sources&IRAS==20396%2b4757%2a>

¹⁰<https://lambda.gsfc.nasa.gov/product/iras/colorcorr.cfm>

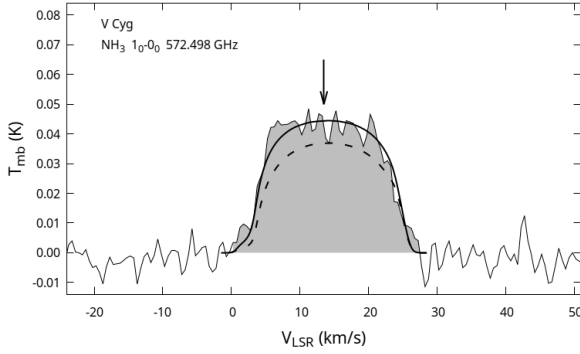


Fig. 1: The averaged line profile of NH_3 obtained from the HIFI/Herschel observations. The black solid line shows the brightness for the model of ammonia in maximum phase of variability of V Cyg, the black dashed line — in minimum phase of variability. The vertical arrow indicates the LSR velocity of the source [16].

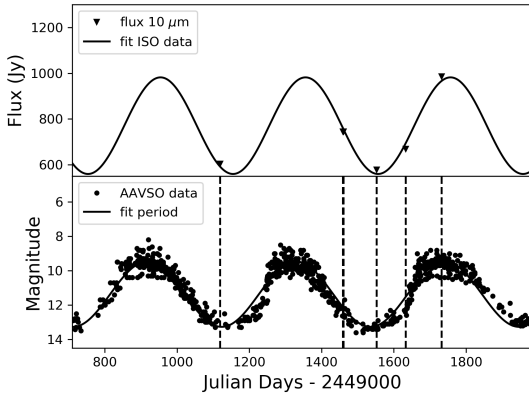


Fig. 2: Variability of V Cyg. The upper diagram shows the measurements of flux at $10\ \mu\text{m}$ from the ISO observations (triangle points) and the fit of sine function to show how the flux changes with the period of variability. The bottom diagram presents the AAVSO data (circle points, visual observations, AAVSO) and the determinations of period (solid line). The broken vertical line presents the positions of the ISO observations for V Cyg. The shift between the maxima of these two sets of data equals about 0.07.

MODELLING

The first step in modelling was preparation of the model of the dusty envelope of V Cyg. For that purpose, we used the MRT code for a dust radiative transfer [24].

In SED modelling we assumed that the amplitude of luminosity variation is about 40% relative to the average value deduced from the period-luminosity re-

lation [28] of $6600\ L_{\odot}$. Such an amplitude was deduced for the similar case for the best examined C-rich star — CW Leo [17]. Hence, in the phase of maximum the obtained luminosity equals $9200\ L_{\odot}$. The optimal model of the dusty envelope reproduces well the observed SED for V Cyg both in the maximum phase (presented in Figure 1) and in the minimum phase. The adopted parameters of the central source and of the dust are presented in Table 3.

The optical properties of the dust obtained from the SED modelling were used to calculate the photodissociation radius of ammonia. For that purpose, we used the CSENV (CircumStellar ENvelopes) code for the calculations of chemistry in expanding envelope [7]. The chemical content of the input was restricted to ammonia and products of its photodissociation. The photodissociation radius R_{ph} is defined as the radius at which the initial abundance of ammonia drops twice. In our calculations we have used the latest cross-section rates of the ammonia molecules [9]. In case of V Cyg we obtained the value of $3.5 \cdot 10^{15}\ \text{cm}$ (for the mass loss rate $\dot{M} = 1.7 \cdot 10^{-6}\ M_{\odot}\ \text{yr}^{-1}$ and the expansion velocity $V_{exp} = 11.5\ \text{km s}^{-1}$). Applying the same approach to the analysed earlier CW Leo [21], we found the theoretical $R_{ph} = 1.8 \cdot 10^{16}\ \text{cm}$, close to the obtained observationally value of $2.8 \cdot 10^{16}\ \text{cm}$ for the rotational transitions of ortho- NH_3 or $2.0 \cdot 10^{16}\ \text{cm}$ suggested by the inversional transitions. We estimate that the uncertainty of the theoretical value may be a factor of about 2.

For modelling of the ammonia lines we used the radiative transfer code MOLEXCSE (Molecular Line EXcitation in CircumStellar Envelope). This code solves the non-LTE radiative transfer in molecular lines in presence of the continuum. The code reproduces well the flux in continuum for the absorption, scattering and emissivity provided by the MRT code. The density structure of the gas envelope is determined by the assumed mass loss rate and the constant expansion velocity. The gas kinetic temperature distribution in the envelope of V Cyg was determined by finding the best fit to the CO emission lines including the radio, millimeter and sub-millimeter HIFI transitions [19].

The model of ortho-ammonia molecule includes 172 levels (all the ground vibrational and the first excited bending mode $\nu_2 = 1$ levels with $J \leq 15$), 1579 radiative transitions and the collisional excitation by H_2 . For the details of treatment of the collisional rates see [21]. Inclusion of the ro-vibrational transitions (about $10\ \mu\text{m}$) is of key importance for the proper modelling of excitation of ammonia in the circumstellar envelope (see e.g. [21]).

Table 1: Characteristics of the HIFI/Herschel observations.

Transition	Frequency (GHz)	Band	E_u , (K)	Herschel OBSID	Obs. date	Phase	HPBW	η_{mb}
$1_0(s)-0_0(a)$	572.498	1b	29	1342199153	2010-23-06	0.1	37.5''	0.62
				1342199154	2010-23-06	0.1	37.5''	0.62

Table 2: Parameters of the ISO SWS for V Cyg.

Source name	ID	Date	Time of observation (s)	Phase
V Cyg	08001855	1996-05-02	1044	0.49
	42100111	1997-10-01	1912	0.31
	42300307	1997-12-01	1913	0.31
	51401308	1997-13-04	1912	0.53
	59501909	1997-03-07	1912	0.73
	69500110	1997-10-10	1912	0.99

RESULT AND CONCLUSION

For the adopted parameters the abundance of ortho-NH₃ molecules in V Cyg star in maximum phase, which best reproduces at best the observed line profile amounts to $2.4 \cdot 10^{-6}$ relative to the molecular hydrogen. The resulting theoretical profile is shown in Figure 3 by the black solid line. The computed profile seems to reproduce very well almost flat top shape of the observed transition.

To illustrate the expected variability in the line profile, we computed the theoretical profile of 1_0-0_0 transition also for the minimum phase, using the abundance determination in the maximum phase. The resulting profile is presented in Figure 3 by means of the black dashed line. In that case we used the ISO data in the minimum phase (ID: 08001855, phase: $\phi = 0.49$). For the model of SED in the phase of minimum we adopted the central star luminosity to be equal $4000L_\odot$ and the temperature to be 2000 K. The brightness of the 572.498 GHz line is then reduced by 40% relative to its maximum.

No observations of para-ammonia are available for V Cyg. If the ortho-to-para ratio corresponds to the equilibrium conditions at higher temperatures, i.e. it is equal to one, then the total amount of ammonia in the envelope of V Cyg is $4.8 \cdot 10^{-6}$. The abundance of ammonia in the archetypical C-rich AGB star IRC+10216 amounts $6 \cdot 10^{-8}$ [21] for the adopted there mass loss rate of $3.25 \cdot 10^{-5} M_\odot \text{ yr}^{-1}$. Thus, within the uncertainties one may conclude that the mass production rate of ammonia in envelopes of both objects is significantly different and larger for smaller mass loss rate. If the photochemical reactions would be responsible for the production of ammonia in the envelopes of C-rich AGB stars, then the higher abundance of ammonia in V Cyg could be explained by the higher probability that UV photons may penetrate into the inner parts of envelope while its density is smaller. The analysis of other 6 objects

in the sample, now under consideration, will reveal if these expectations will be confirmed.

ACKNOWLEDGEMENT

This work has been supported by the grant 2016/21/B/ST09/01626 of the National Science Centre, Poland.

REFERENCES

- [1] Bernath P. F. 2005, *Spectra of atoms and molecules*, Oxford University Press, New York.
- [2] Bunker P. R. & Jensen P. 2006, National Research Council of Canada, 1, 496.
- [3] Cheung A. C., Rank D. M., Townes C. H. et al. 1968, Phys. Rev. Lett., 21, 1701.
- [4] Cutri R. M., Skrutskie M. F., van Dyk S. et al. 2003, *VizieR On-line Data Catalog: II/246*.
- [5] Decin L., Agúndez M., Barlow M. J., et al. 2010, Nature, 467, 64.
- [6] Danby G., Flower D. R., Valiron P. et al. 1988, MNRAS, 235, 229.
- [7] Glassgold A. E., Lucas R., Omont A. 1986, A&A, 157, 35.
- [8] Gobrecht D., Cherchneff I., Sarangi A., Plane J. M. C., Bromley S. T. 2016, A&A, 585, A6.
- [9] Heays A. N., Bosman A. D., van Dishoeck E. F. 2017, A&A, 602, 105.
- [10] Harju J., Walmsley C. M., Wouterloot J. G. A. 1993, A&AS, 98, 51.
- [11] Ho P. T. P. & Townes C. H. 1983, ARA&A, 21, 239.
- [12] Jijina J., Myers P. C., Adams F. C. 1999, ApJS, 125, 161.
- [13] Johnson H. R., Sauval A. J. 1982, A&A, 49, 77.
- [14] Kraemer K. E., Sloan G. C., Price S. D., Walker H., J. 2002, ApJS, 140, 389.
- [15] Roelfsema P. R., Helmich F. P., Teyssier D. et al. 2012, A&A, 537, A17.

- [16] Massalkhi S., Agúndez M., Cernicharo J., Velilla Prieto L., Goicoechea J. R. 2018, A&A, 611, A29
- [17] Men'shchikov A. B., Balega Y., Blöcker T., Osterbar R., Weigelt G. 2001, A&A, 368, 497.
- [18] Maret S., Faure A., Scifoni E. et al. 2009, MNRAS, 399, 425.
- [19] Neufeld D. A., González-Alfonso E., Melnick G. et al. 2010, A&A, 521, L5.
- [20] Samus N. N., Kazarovets E. V., Pastukhova E. N., Tsvetkova T. M., Durlevich O. V. 2009, PASP, 121, 137.
- [21] Schmidt M. R., He J. H., Szczerba R. et al. 2016, A&A, 592, A131.
- [22] Schöier F. L., Ramstedt S., Olofsson H. et al. 2013, A&A, 550, A78.
- [23] Sloan G. C., Kramear K. A., Price S. D., Shipman R. F. 2003, ApJS, 147, 379.
- [24] Szczerba R., Omont A., Volk K., Cox P., Kwok S. 1997, A&A, 317, 859.
- [25] Tennyson J., Yurchenko S. N., Al-Refaie A. F. et al. 2016, Journal of Molecular Spectroscopy, 327, 73.
- [26] Wienen M., Wyrowski F., Schuller F. et al., 2012, A&A, 544, A146.
- [27] Wallerstein G. & Knapp G. R. 1998, ARA&A, 36, 369.
- [28] Whitelock P. A., Feast M. W., Van Leeuwen F. 2008, MNRAS, 386, 313.
- [29] Willacy K., & Cherchneff I. 1998, A&A, 330, 676.

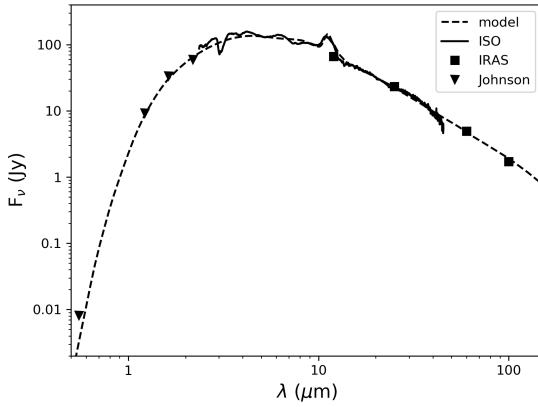


Fig. 3: SED: Triangle points show the measurements flux for V, J, H and K bands, square points – the IRAS measurements for 12, 25, 60 and 100 μm , solid line – the ISO measurements between 2.36–45.365 μm (ID: 69500110, phase: $\phi = 0.99$). Dashed line shows the model of SED.

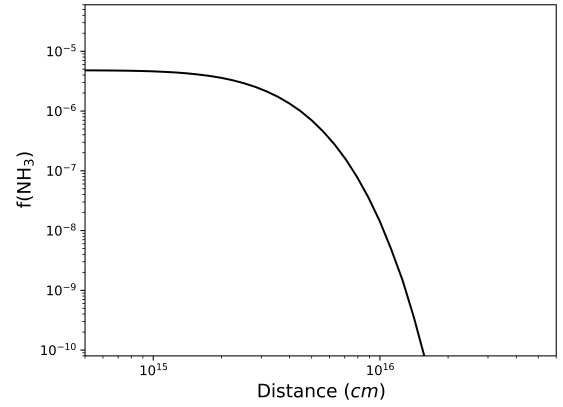


Fig. 4: Distribution of the NH_3 molecule in CSE around V Cyg. This model has been calculated by the CSENV code [7]. This distribution has been calculated for the model of dust obtained for our SED model and the latest cross-section of the ammonia molecule [9].

Table 3: Parameters for the model of V Cyg.

Name of the parameter	Value	Reference
RA (2000)	20 41 18.27	
Dec (2000)	+48 08 28.94	
Period	417 days	[20]
Distance	420 pc	[28]
V_{exp}	11.5 km s ⁻¹	Derivatives from CO lines
V_{LSR}	13.5 km s ⁻¹	[16]
R_{phot}	$3.5 \cdot 10^{15}$ cm	
M_{loss}	$1.7 \cdot 10^{-6} M_{\odot} \text{ yr}^{-1}$	[22]
Luminosity (mean)	6600 $L_{\odot}$	[28]
Luminosity (max)	9200 $L_{\odot}$	SED modelling
Luminosity (min)	4000 $L_{\odot}$	SED modelling
$T_{\text{eff,max}}$	2500 K	SED modelling
$T_{\text{eff,min}}$	2000 K	SED modelling
$f(\text{ortho-NH}_3)$	$2.4 \cdot 10^{-6}$	MOLEXCSE modelling
$f(\text{NH}_3)$	$4.8 \cdot 10^{-6}$	MOLEXCSE modelling