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**PIONEER PROJECTS**

# NEW CRADLES OF MOLECULES IN INTERSTELLAR SPACE: PLANETARY NEBULAE

**CONTRACT - BR/154/PI/MOLPLAN**

# FINAL REPORT

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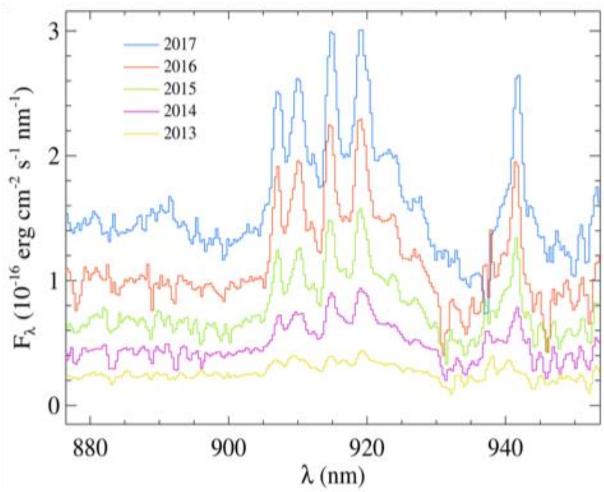
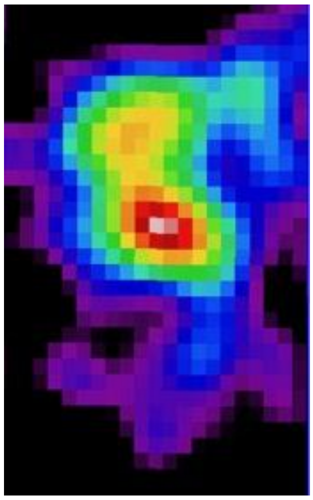
Promotor
Griet C. Van de Steene
Royal Observatory of Belgium (ROB) - Avenue Circulaire 3 Ringlaan - 1180 Brussels

Authors
Peter A.M. van Hoof (ROB)
Griet C. Van de Steene (ROB)

Royal Observatory of Belgium

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Avenue Louise 231
Louizalaan 231
B-1050 Brussels
Belgium
Tel: +32 (0)2 238 34 11 – Fax: +32 (0)2 230 59 12
http://www.belspo.be

Contact person: Georges JAMART
+32 (0)2 238 36 90



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The cover images: the left panel shows the complex of electronically excited CN lines that has been emerging since 2013 in Sakurai's object, the right panel shows the bipolar CN emission detected by ALMA.

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## SUMMARY

### Context

When low- to middleweight stars like our sun approach the end of their lives, they cast off their outer layers of gas and dust into space, creating beautiful planetary nebulae. When this mass loss happens, the stars are cool (so-called red giants) and the ejected material contains many molecules. Later the central star will start to heat up and will ionize the ejected material. This is called the planetary nebula stage. The central star will heat up to very high temperatures until finally all nuclear reactions in its interior cease and the star becomes a white dwarf. During the planetary nebula stage the white dwarf star's harsh ultraviolet radiation is expected to destroy most molecules that had previously been ejected and hamper the formation of new ones in the nebula. However, we observe that not all molecules are destroyed. Moreover, the 2014 detection of the $OH^+$ molecule with the Herschel satellite (Etxaluze et al. 2014, Aleman et al. 2014) was the first clear evidence for the formation of molecular ions in planetary nebulae. This has raised many questions regarding the survival and formation of molecules in planetary nebulae.

### Objectives

We proposed to investigate molecule formation in planetary nebulae in two different environments. The first is a new physical instability which may lead to the formation of high-density clumps in recombining ionized gas around cooling white dwarfs. It is in such clumps that molecules may survive the planetary nebula phase and new molecules may be formed. We proposed to do time-dependent theoretical modelling of recombining gas and use the spectra from the Herschel satellite to study the formation of the $OH^+$ molecule in more detail. The second environment with molecule formation is the ongoing creation of a new planetary nebula in Sakurai's object, which underwent a very late thermal pulse in the 1990's. This unique object provides a once-in-a-life time opportunity to explore molecular chemistry in real time and the chemical enrichment due to the nuclear reactions.

### Conclusions

The delayed start of the Pioneer program implied that the proprietary period of the Atacama Large Millimeter Array (ALMA) data of Sakurai's object had already nearly expired. We therefore decided to give priority to the analysis of the data on Sakurai's object. Beside the ALMA data, we also had an extensive set of data obtained with instruments at the European Southern Observatory (ESO). These data were all included in the analysis. The data reduction turned out to be fraught with problems and took much longer than expected. All this effort was well worth it though, as the combined data sets allowed us to significantly deepen our understanding of the morphology and evolution of this intriguing object. In the ALMA data we detected CO, CN, and $HC_3N$, as well as $^{13}C$ isotopologues of these molecules. The CO and $HC_3N$ emission was spatially unresolved, but surprisingly the CN emission showed a bipolar structure. We also detected the dust continuum which was also spatially unresolved. In the optical spectra we see two sets of lines. The first is a set of nebular lines (re-

combination lines of hydrogen and helium, as well as forbidden lines of heavier elements) that was first detected in 1998 (helium) and 2001 (forbidden lines). Since 2013 we see a second set of emission lines emerging. Not all lines are identified yet, but the strongest are electronically excited lines of CN. They originate much closer to the central star than the nebular lines. Chesneau et al. (2009) detected the presence of a circumstellar disk using Very Large Telescope Interferometer (VLT), and Hinkle & Joyce (2014) detected the presence of bipolar lobes using near infrared adaptive optics. Combining these old and new results leads to the following main conclusions.

Sakurai's object ejected its remaining envelope in the 1990's. Soon afterwards there was a brief but strong shock, forming the nebular lines detected from 1998 onwards. This shock likely was caused by faster ejecta hitting slower ejecta. This shocked material then started cooling. A disk (which is likely Keplerian) also formed very quickly. This disk contains all the dust and likely also the bulk of the molecules. From 2008 onwards we see the nebular lines steadily brightening. Using the data obtained with the X-Shooter instrument op de VLT, we could prove that these lines are excited in the bipolar lobes. Since 2008 there must be an increased mass loss, which could be funneled by the disk into a jet and is now hydrodynamically shaping the bipolar lobes. The nebular lines are formed in a strong J-type bow-shock at the end of the bipolar lobes. The optical CN emission is possibly formed where the molecular wind is funneled by the disk in a C-type shock, or alternatively is excited by untraviolet radiation from the central star. The CN could be formed by dissociation of HCN in the shock and then carried into the lobes. This would agree with the ALMA observations that show that the CN emission coincides with the bipolar lobes detected by Hinkle & Joyce (2014). This implies that we now have a unique and detailed data set following the very early stages of the formation of a bipolar nebula in time. Understanding this formation process has been the subject of intense study for many decades (see Balick & Frank 2002 for a review). Understanding the morphology and evolution as we do now will greatly help us in future studies of the molecular chemistry in this object and other planetary nebulae.

**Keywords**

stellar evolution – circumstellar matter – astrochemistry – nuclear synthesis

## SAMENVATTING

### Context

Wanneer sterren met lage tot gemiddelde massa zoals onze Zon het einde van hun leven naderen, stoten ze tijdens het “rode reuzen stadium” hun buitenste lagen van stof en gas af in de ruimte uit. Dit uitgestoten materiaal bevat heel veel moleculen. Nadien wordt de ster heter en ioniseert het dit materiaal om zo een prachtige “planetaire nevels” te creëren. Alle nucleaire reacties in het binnenste doven uit en de ster wordt een witte dwerg. Gedurende de planetaire nevel fase is de centrale ster een witte dwerg wiens intense UV straling in principe alle moleculen zou moeten vernietigen en de vorming van nieuwe moleculen verhinderen. We zien echter dat bijlange na niet alle moleculen vernietigd worden. De detectie in 2014 met de Herschel satelliet van $OH^+$ in de Helix nevel (Etxaluze et al. 2014, Aleman et al.2014) heeft aangetoond dat er zelfs moleculaire ionen gevormd worden. Dit geeft aanleiding tot veel nieuwe wetenschappelijke vragen over het overleven en de vorming van moleculen in planetaire nevels.

### Doelstellingen

In dit project wilden we de vorming van moleculen in planetaire nevels onderzoeken in twee verschillende omgevingen. De eerste is: of een nieuwe fysische instabiliteit aanleiding kan geven tot de vorming klonten van hoge dichtheid in het recombinerend geïoniseerd gas rond een afkoelende witte dwerg. Het is in dergelijke klonten dat moleculen de planetaire nevel fase zouden kunnen overleven en nieuwe moleculen gevormd kunnen worden. We stelden voor om een theoretisch model te ontwikkelen voor de evolutie van het recombinerend gas tijdens de planetaire nevel fase en hiervoor de spectra van de Herschel satelliet te gebruiken voor een meer gedetailleerde studie van de vorming van de $OH^+$ molecule. De tweede omgeving is de locatie waar moleculen gevormd worden bij de vorming van een nieuwe planetaire nevel, in Sakurai’s object bijvoorbeeld. Dit object onderging een heel late thermische puls begin jaren ‘90, koelde daarna snel af, werd een “herboren” rode reus, en begint nu terug heter te worden. Het zal uiteindelijk een nieuwe planetaire nevel vormen binnenin de oude. Dit geeft ons de unieke gelegenheid om de chemische verrijking veroorzaakt door nucleaire reacties in de ster en de moleculaire chemie in de nevel te onderzoeken terwijl het gebeurt.

### Besluiten

De start van het Pioneer programma werd uitgesteld en dit had als gevolg dat de periode waarin we eigendomsrechten hadden over de Sakurai’s gegevens van de Atacama Large Millimeter Array (ALMA) bijna voorbij was. Daarom besloten we voorrang te verlenen aan de analyse van de gegevens van Sakurai’s ster. Behalve de ALMA data, hadden we ook een uitgebreide set gegevens bekomen met andere instrumenten van de European Southern Observatory (ESO). Deze gegevens werden allemaal gebruikt in de analyse. Het reduceren van de gegevens ging echter met grote moeilijkheden gepaard en duurde bijgevolg veel langer dan gepland. Al die inspanningen bleken het uiteindelijk wel waard geweest te zijn, omdat de gecombineerde gegevens ons aanzienlijk meer inzicht gegeven hebben in de evolutie in morfologie van dit intrigerend object. In de ALMA data hebben we CO, CN, en $HC_3N$ gedetecteerd, en ook de $^{13}C$ isotopen van deze moleculen. De CO en $HC_3N$ emissie kwamen van een puntbron, maar de CN emissie toonde onverwacht een bipolaire structuur. We hebben ook stof continuüm gedetecteerd en dit kwam ook van een klein, centraal, niet ruimtelijk opgelost gebied. In de optische spectra hebben we twee soorten lijnen gedetecteerd. De eerste verzameling is een aantal nevellijnen (recombinatielijnen van waterstof en helium, en ook verboden lijnen van zwaardere elementen), die gedetecteerd werden in 1998 (helium) en 2001 (verboden lijnen). Sinds 2013 zien we een tweede verzameling emissielijnen opkomen en sterker worden. Niet alle lijnen zijn al geïdentificeerd, maar de sterkste zijn elektronische geëxciteerde lijnen van CN. Zij ontstaan veel dichter bij de centrale ster dan de nevellijnen. Chesneau et al. (2009) heeft met de Very Large Telescope Interferometer (VLTI) een circumstellaire schijf ontdekt, en Hinkle & Joyce (2014) de aanwezigheid van bipolaire lobben in het nabije infrarood. Als we onze nieuw resultaten met deze vorige combineren, komen we tot de volgende conclusies: Sakurai's object stootte zijn overblijvend omhulsel uit in de jaren 1990. Vlug hiernaar was er een korte maar sterke schok, waarin de nevellijnen ontstonden die we detecteerden vanaf 1998. Deze schok werd waarschijnlijk veroorzaakt doordat de uitgestoten materie sneller bewoog en zo botste met materie die trager bewoog. Dit materiaal in de schok begon dan af te koelen. Een schijf werd ook snel gevormd. Het stof en de meeste moleculen bevinden zich wellicht in deze schijf. Vanaf 2008 worden de nevellijnen steeds helderder. Met behulp van de data verkregen met het X-Shooter instrument op de VLT konden we aantonen dat deze lijnen geëxciteerd worden in de bipolaire lobben. Sinds 2008 moet het massaverlies toegenomen zijn, en dit zou via de schijf naar de bipolaire lobben kunnen worden gekanaliseerd en nu hydrodynamisch de bipolaire lobben vormgeven. De nevellijnen worden gevormd in de sterke J-type boegschok aan het einde van de bipolaire lobben. De optische CN emissie wordt mogelijk gevormd waar de moleculaire wind gekanaliseerd wordt door de schijf in een C-type schok, of een andere mogelijkheid is dat het geëxciteerd wordt door de ultraviolette (UV) straling van de centrale ster. De CN kan gevormd worden door dissociatie van de HCN in de schok en dan verspreid worden in de lobben. Dit zou overeenkomen met de ALMA waarnemingen die aantonen dat de CN emissie samenvalt met de bipolaire lobben gedetecteerd door Hinkle en Joyce (2014). Dit impliceert dat we nu een unieke gegevens hebben die in detail de heel vroege stadia van de vorming van een bipolaire nevel tonen. Het proberen begrijpen van hoe precies de vorming van bipolaire planetaire nevels gebeurt, wordt al jaren intensief bestudeerd (zie Balick & Frank 2002 voor een overzicht). Het begrijpen van de morfologie en de evolutie van dit object, zal zeker helpen bij onze toekomstige studies van de moleculaire scheikunde in dit object en andere planetaire nevels.

**Trefwoorden**

stellaire evolutie – circumstellaire materie – astrochemie – nucleaire chemie

# 1. INTRODUCTION

*Fig. 1: The planetary nebula NGC 6720*

Planetary nebulae (e.g. Fig. 1) are beautiful objects created during the final stages of a star's life whose birth mass was between 1 and 8 solar masses ($M_\odot$). Planetary nebulae consist of a nebula illuminated by a central star. The colorful nebula is actually material that was originally part of the star itself, but was cast off and is expanding outwards into interstellar space. It glows as the result of being heated and ionized by the ultraviolet radiation produced by the remnant core of the dying star, a so-called white dwarf star.

Astronomers are drawn to study these objects because the nebulae provide opportunities to analyse material that was once a part of the star. Spectra of planetary nebulae show emission lines of many heavy elements, many of which were recently synthesized by nuclear processes during the preceding phases. Studying planetary nebulae helps us to understand the physical processes that occurred within the star while nuclear fusion was active and how a star changes and evolves. In addition to the ionized component, the nebulae also contain molecules and dust, which eventually will be incorporated in the interstellar medium. In a galaxy such as our own Milky Way there are estimated to be several thousand planetary nebulae at any one time, they are regarded as important agents in the chemical enrichment of the Galaxy.

The phase before the star evolves into a planetary nebulae is called the Asymptotic Giant Branch (AGB) phase. It happens after the star has moved from the Main Sequence, through the Red Giant Phase and past the Horizontal Branch (Fig. 2). At this point the star is characterised by an inert carbon-oxygen core, surrounded by two separate nuclear burning layers surrounded by a strongly convective envelope. As the star evolves through the AGB phase it cools, expands and grows in brightness. Large pulsations and dust formation combine to drive a wind off the surface of the star with a very high mass loss rate (up to $10^{-4}$ $M_\odot$ per year), which forms a circumstellar shell that is slowly expanding with a typical velocity of 10 to 20 km/s. During this phase the star will lose most of its envelope. When the envelope mass drops to a critical value of around $10^{-3}$ $M_\odot$, the stellar mass loss will decrease by many orders of magnitude. The outer shell will become detached from the stellar core and the star will start heating up. This process is very fast and after a few thousand years the central star will become hot enough to photoionize the circumstellar shell that formed during the AGB phase. At that point a planetary nebula will have formed. During this evolution the luminosity of the central star will stay nearly constant until eventually all nuclear fuel runs out. The luminosity of the star will drop very steeply and continue to drop rapidly until eventually gravitational contraction stops and only thermal radiation is emitted by the white dwarf. The white dwarf entered the cooling track and the evolution slows down considerably. During the next billion years the white dwarf cools down. During this phase the nebula itself continues to expand and dissolves in the interstellar medium. In the end a bare white dwarf will remain.

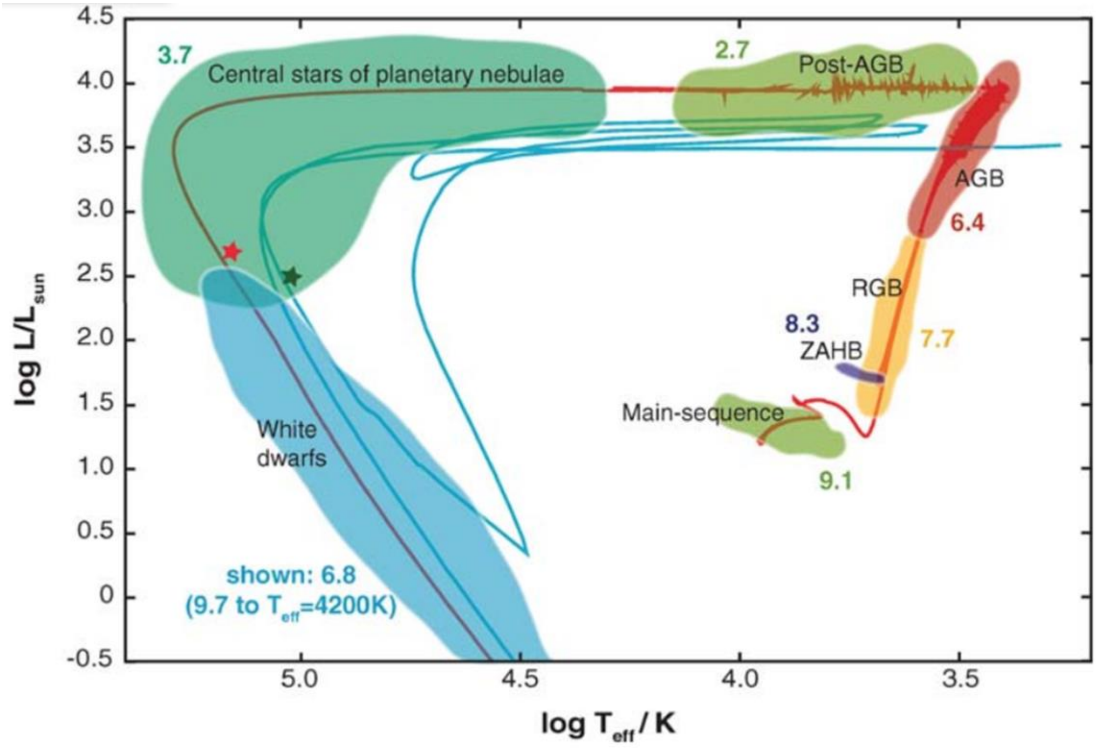


*Fig. 2: Hertzsprung-Russell diagram of a complete $2M_\odot$ evolution track for solar metallicity from the main sequence to the final white dwarf evolution stage. The blue track shows a born-again evolution (triggered by a very late thermal pulse, see Sakurai's object) of the same mass, however, shifted by approximately $\log T_{eff} = -0.2$ and $\log L/L_\odot = -0.5$ for clarity. The number labels for each evolutionary phase indicate the log of the approximate duration for a $2\ M_\odot$ case (in years). Larger or smaller mass stars would have shorter or longer evolutionary timescales, resp. (Herwig 2005).*

When a planetary nebula is formed, initially it will only be partially ionized and surrounded by the remnant AGB shell of molecular material and dust. Very young planetary nebulae like NGC 7027 and NGC 6302 are in that stage. As the evolution progresses, the central star's temperature increases while the nebula will continue to expand and its density will drop. This makes it easier for the central star to photoionize the gas and the ionization front will move outwards. What happens depends on the complex interplay of the central star's evolution, the interaction of the stellar wind with the AGB shell, and the expansion of that shell (e.g. Steffen & Schönberner 2006). A typical (simplified) scenario based on O' Dell et al. (2007) will be described here. The ionization front will continue to move outwards until eventually the entire nebula is ionized. All the molecules that formed during the AGB phase will be destroyed by the harsh ultraviolet radiation, unless they can somehow be shielded from that radiation. When the central star subsequently enters the cooling track, its luminosity will decline by a factor 10 in a few hundred years, depending on its mass (see Fig. 2). Consequently, the number of ionizing photons will decrease sharply causing the ionization front to recede and the outer regions of the nebula to start recombining and cooling (Tylenda 1986). Because the recombination timescale increases with decreasing electron density, these regions will also remain partially ionized. In this recombining partially ionized gas at low temperature non equilibrium effects are important. Due to the low temperature, the thermal pressure in the gas is low. We propose that the recombination radiation present will exert pressure on the gas, causing inhomogeneities to grow. Dust is mixed in with the gas and the instability mechanism compresses both the gas and the dust in clumps. The increase in density will speed up the recombination process and therefore more recombination radiation will be emitted, thereby causing the gas to be compressed even further and quickly start forming molecules. This is schematically depicted in Fig. 3. The shaded spheres indicate the regions of higher density. The straight arrows indicate the radiation produced by the recombining gas. This radiation is strongest in the densest regions. The wavy lines indicate the radiation pressure on the globules by the radiation from other globules. This will compress the globules further. This way many cold and dense globules will be formed.

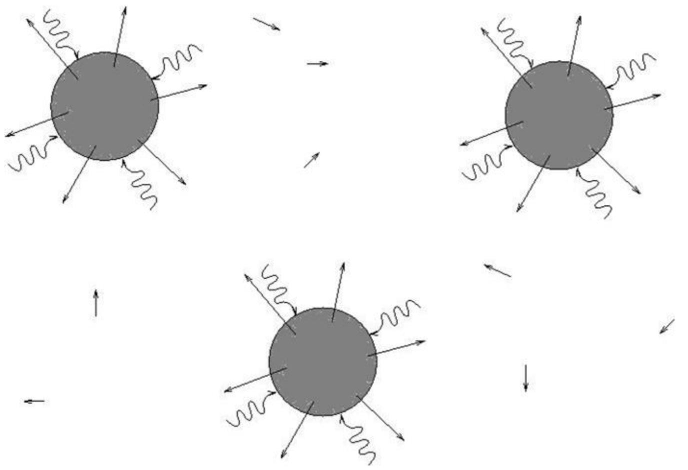

*Fig. 3: Cartoon of globule formation in recombining partially ionized gas.*


*Fig. 4: Cometary globules in the Helix nebula.*

Once the nuclear reactions have stopped completely, the decrease of the central star's luminosity will slow down drastically. Meanwhile the nebula will keep on expanding and the nebular gas density keeps on decreasing. This will cause the ionization front to move outward again and as a result the globules that formed earlier will become embedded in photoionized gas and ionizing radiation (O'Dell et al. 2007). This will cause the outer layers of the globules to heat up and be eroded away (advection flow) and to shine very brightly in molecular emission lines like $H_2$ (Henney et al. 2007). The most famous examples of a planetary nebula in this stage of evolution are the Helix nebula (NGC 7293), the Ring nebula (NGC 6720), and the Dumbbell nebulae (NGC 6853), but others are known (O'Dell et al. 2003, 2007). We show the knots in the Helix nebula in Fig. 4 (taken from O'Dell et al. 2003). The advection flows off the knots are clearly visible in this image.

The account given above should be considered controversial. Rival theories state that the knots are much older. A very different proposed origin (Dyson et al. 1989) is that these are condensations of material that existed in the extended atmosphere of the precursor AGB star. Others argue that they are the products of instabilities at the ionization front at the onset of ionization (Capriotti et al. 1973). See Matsuura et al. (2009) for a more detailed discussion. In either of these alternative scenarios the knots need to survive through the entire ionized phase of the planetary nebula evolution. In van Hoof et al. (2010) we argued that this is problematic in the case of the Ring nebula. The hydrodynamic models that we created using Cloudy to model the advection flows off the knots in the Helix nebula (Henney et al. 2007) indicate that the advected mass loss is substantial: of the order of $10^{-10}$ to $10^{-9}$ $M_{\odot}$ per year despite the very low luminosity of the central star (120 solar luminosities). Considering that the central star luminosity was much higher in the past, and the knots were much closer to the central star, survival seems problematic, though it cannot be fully excluded at this point since the advected mass loss rate is too uncertain. In order to resolve this issue we need much better constrained models of the advection flows off the knots, so that we can determine the current advected mass loss more precisely. To this end recent Herschel detections of $OH^+$ emission in the Helix nebula and other, similar, planetary nebulae would be useful (Etxaluze et al. 2014, Aleman et al. 2014). These $OH^+$ molecules must have been formed in these nebulae and their emission lines are surprisingly strong, even stronger than CO! We propose that these lines originate in the advection flows. These flows carry $H_2$ towards the ionized gas. Before the molecules are destroyed by the ultraviolet radiation, they can react with ionized oxygen: $H_2 + O^+ \rightarrow OH^+ + H$. This is the dominant formation mechanism for $OH^+$. So the advection flow creates the unique circumstances responsible for forming this molecular ion. We therefore believe that the $OH^+$ emission line spectrum will be very important to constrain the conditions in the advection flow.

*The first work package of MOLPLAN is to carry out a detailed theoretical investigation into this new instability and establish whether it could have occurred in planetary nebulae like the Helix nebula and whether it is quick enough to allow time for $H_2$ formation. We choose the Helix Nebula because it is one of the closest planetary nebulae in which these features can be studied in great detail.*

*The second work package of MOLPLAN is to use Cloudy to create a model of the advection flow by matching it to the Herschel spectrum, as well as existing ground-based $H_2$ observations. These data, combined with the known physical size of the knots, will give us both the velocity and density in the flow, and hence the mass loss rate (O'Dell et al. 2003, Henney et al. 2007, van Hoof et al. 2010). This result will then allow us to resolve the survival issue of the knots outlined above.*

Also in planetary nebulae which underwent a very late thermal pulse (VLTP) while on the cooling track, high density globules are observed (Fang et al. 2014). As a result of the VLTP event, these objects eject a significant amount of material which will quickly start to recombine as they return to the AGB and high-density globules may form that enable rap-

id molecule formation as described above. Especially in these objects molecules provide a unique test of nuclear synthesis theory, which we will discuss in more detail below.
Some central stars of planetary nebulae will undergo a VLTP while they are on the cooling track. Theory predicts that 10 – 20% of all planetary nebula central stars would undergo such a VLTP event. However, only two events have been observed directly: V605 Aql in 1918 and Sakurai's object in 1996. Sakurai's object (V4334 Sgr) is the only well observed example of a VLTP. It baffled the scientific community with its extremely fast evolution which fitted the existing evolutionary models surprisingly poorly! The star erupted between 1990 and 1995. The evolution back to the AGB took only until 1997. Around that time, dust started to form in the ejecta which now completely obscures the central star at optical wavelengths. Early VLTP models failed to account for the speed of evolution (Iben & MacDonald 1995). Herwig (2001) first reproduced the very fast evolution in stellar models by making the assumption that the star ingests the remainder of its hydrogen envelope. Detailed 3-D hydrodynamical simulations of the convection zone during a helium shell flash (Herwig et al. 2011) indicate that the remaining hydrogen from the envelope is mixed into the upper layers of the helium burning shell and ignites separately in a hydrogen ingestion flash. Under these conditions, the star will experience a double loop in the HR diagram (Lawlor & MacDonald 2006): the first loop from the hydrogen ingestion flash, with an extremely rapid return to high stellar temperatures, followed by a much slower loop caused by the helium flash (Hajduk et al. 2005, van Hoof et al. 2007). This evolution is also depicted in Fig. 2.

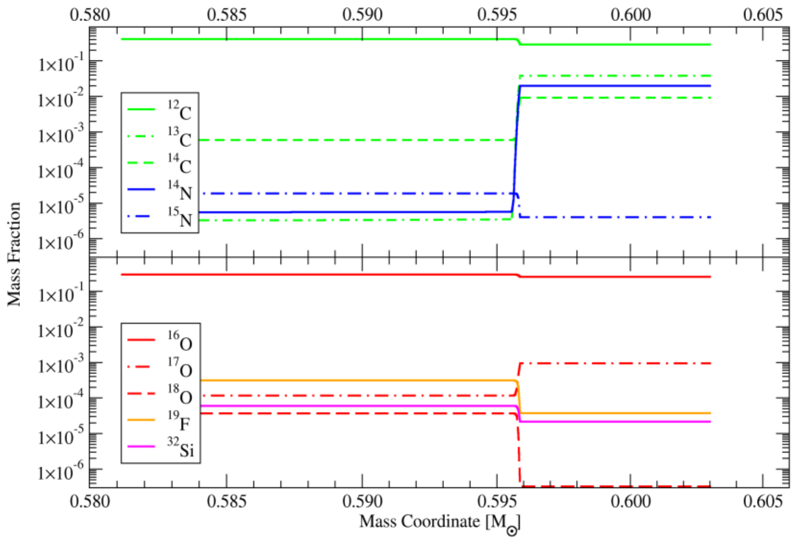


*Fig. 5: Abundance profile predictions of CNO, F, and Si isotopes according to recent simulations (Herwig et al. 2011). The hydrogen ingestion region is visible above the mass coordinate 0.596 $M_\odot$*

The hydrogen ingestion flash has wide ramifications. The mixing of proton-rich material into the $^{12}$C-rich He-shell induces exotic neutron capture nucleosynthesis. This newly proposed neutron capture mechanism is called the i-process, because it is intermediate ("i" from intermediate), between the well-known s-process (which acts in AGB stars) and r-

process (which acts in supernovae) (Bertolli et al. 2013, Herwig et al. 2014). Sakurai's object is the Rosetta stone for simulations of the i-process, because it can provide us with critically important constraints for theoretical simulations that are not available from any other source. This is important for nuclear physics, stellar physics, and even for the chemical enrichment of the early universe. Stellar evolution models of stars with very low or zero metallicity, as encountered in the first generations of stars, predict the same i-process in convective-reactive hydrogen combustion as in Sakurai's object and even pre-solar SiC grains show the signature isotopic enhancements confirming the existence of the i-process (Jadhav et al. 2013, Fujiya et al. 2013). In Sakurai's object the violent nuclear fusion processes during the hydrogen ingestion flash are predicted to produce very different burning products from the helium flash. Especially the isotopic ratios of C, N, and O provide strong constraints for the complex balance between the helium flash and the hydrogen ingestion flash. The latter yields a $^{14}N$:$^{15}N$ ratio of a few thousand, while in the helium flash region we find 1:3 (see Fig. 5)! In the hydrogen ingestion region $^{17}O$:$^{18}O$ is a few thousand whilst in the lower region $^{17}O$:$^{18}O$ = 3:1 is expected.
Current determinations of $^{13}C$ enhancement and neutron capture abundances (Asplund et al. 1999) are reproduced well in simulations by Herwig (private communication). Hence we have requested observations of isotopes using the Atacama Large Millimeter Array (ALMA), which will add key constraints on the details of the proton-capture nucleosynthesis conditions that are not available from the $^{12}C/^{13}C$ ratio and the existing heavy elemental abundances alone.

*The third work package of MOLPLAN is creating a photodissociation region model of the Atacama Large Millimeter Array spectrum using the Cloudy code (Ferland et al. 2017). The model will be used to derive the isotope ratios of C, N, and O in the ejecta of Sakurai's object. These will be used to test the i-process theory proposed by Herwig and improve the stellar structure models of Sakurai's object.*

## 2. METHODOLOGY AND RESULTS

Dr. Peter van Hoof worked on MOLPLAN from 1 March 2016 until 31 August 2017. We prioritized our efforts on reducing and analysing all available data on Sakurai’s object (work package 3). The reason for this was that the BRAIN-be Pioneer project started later than originally planned due to the secretary of state initially refusing to sign the necessary paperwork. As a result the proprietary period for the ALMA data had already nearly expired, which implied that our data would also become available to our competitors. Hence we started with the data reduction and analysis of the ALMA data that were obtained in cycle 2 in 2015. This was done in collaboration with Dr. Adam Avison, an instrument specialist from the Manchester ALMA regional center (ARC) node. Due to the fact that the instrument is very new, the data obtained with the telescope and its data reduction are not fully understood yet and it took several months to obtain satisfactory results. Different techniques needed to be tried and employed to remove the artefacts and decrease the noise. For one frequency setting (centered on a strong atmospheric band) we had to discard the data despite numerous attempts at salvaging this data cube. There was probably a problem with the instrument during the observation, or the atmospheric conditions were unfavorable. In the end 40 km/s channel images were produced for Band 6 and Band 7 observations, the latter being less qualitative. We could identify emission lines from CO, CN, and $HC_3N$ in the spectra, as well as the following $^{13}C$ isotopologues: $^{13}CO$, $^{13}CN$, $HC^{13}CCN$, and $HCC^{13}CN$ (but not $H^{13}CCCN$). Subsequently Dr. Griet Van de Steene learned to use CASA, the ALMA analysis software and wrote some scripts to analyse the data. The software package CASA has many options and a manual, which is however not very detailed. It needed some investigation to figure out exactly how and what (similar) programs were doing in the scripts and under the buttons via the interface. We made different spectral extractions, moment and position velocity maps for the identified lines. We also detected CN absorption at the blue edge of the CN emission (see Fig. 6).

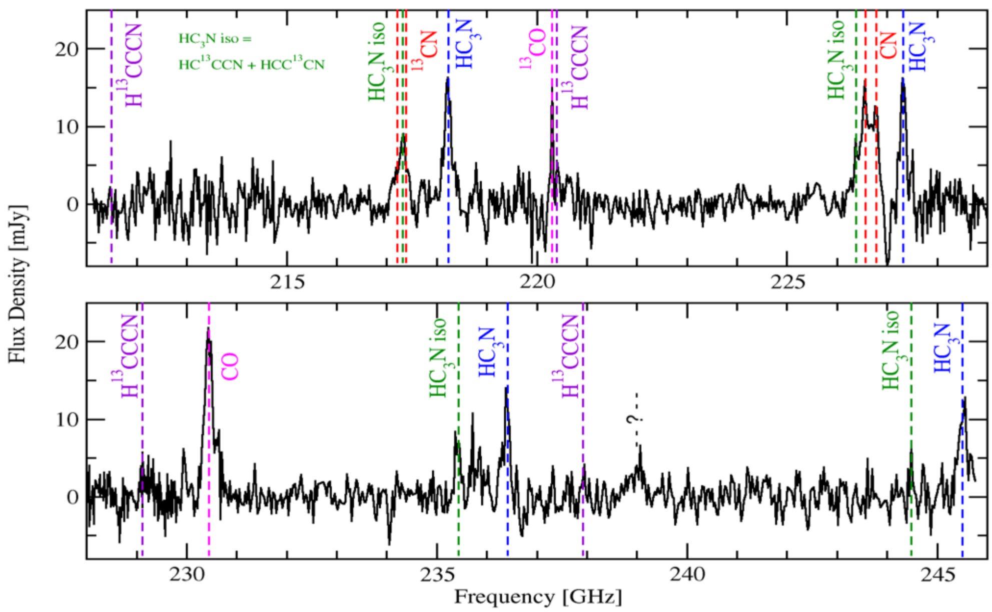


*Fig. 6: In ALMA spectra we detect the presence of CO, CN, $HC_3N$, and $^{13}C$ isotopologues.*

The data obtained in cycle 2 were incomplete. Some of the proposed observations in band 7, that quite possibly would have resulted in a detection of isotopes other than $^{13}C$, were not executed due to scheduling constraints. In cycle 3 we submitted an identical proposal, which was accepted, yet ALMA initially refused to schedule any of the missing observations. After lengthy discussions, ALMA eventually agreed to schedule them, but by then the object was no longer observable. A follow-up proposal that we submitted in cycle 4 was unfortunately not accepted, due to a negative referee report. An improved version of the proposal was accepted in cycle 5 in category C. So far no data were obtained from this proposal. To this date we have not been able to reach our goal of detecting CNO isotopes other than $^{12}C$ and $^{13}C$. The $^{12}C/^{13}C$ ratio is already well known from the time immediately after the VLTP when the central star was still directly observable (it is now heavily obscured by dust that formed in the ejecta). So no new information on isotope ratios can be derived from the existing ALMA data. The first reason for this is that our pre-ALMA models predicted line strengths about 1 dex too strong. Consequently our observations did not reach the required signal-to-noise (S/N) ratio to detect other isotopologues. This was corrected in the cycle 4 proposal (the cycle 2 data were not available yet when we submitted the cycle 3 proposal). Other reasons were adverse weather conditions due to an unusually strong El Niño event (causing a lot of potential observing time to be lost), the fact that ALMA was still under construction (leading to lots of technical downtime), and very slow bureaucracy on the ALMA side causing us to loose our observing time in cycle 3. We will continue to submit proposals until we have reached our goals, or have established that the lines are too weak to be detectable by ALMA.

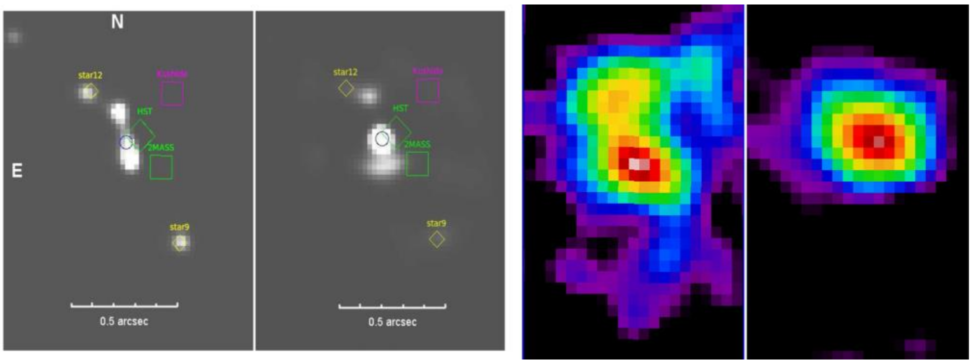


*Fig. 7: From left to right: Deconvolved Ks images taken in 2010 and 2013 from Hinkle & Joyce (2014), CN and CO emission detected by ALMA in 2015.*

Despite these difficulties, the cycle 2 data allowed us to greatly improve our understanding of the source. We found that the CN (and isotopologue) emission coincides with the bipolar structure seen by Hinkle & Joyce (2014) (see Fig. 7), while the CO and $HC_3N$ (and isotopologues) emission coincides with the central star, which means that this likely comes from the disk identified by Chesneau et al. (2009). We obtained a dust continuum image that showed that the dust emission also coincides with the central star. Our interpretation is that all the dust and nearly all the molecules reside in the disk, while the bipolar structure is free of dust. The origin of the CN is less clear. One possibility is that HCN resides in the disk (a strong HCN detection was reported by Tafoya et al. 2017) and is being ablated by the stellar wind. CN is then possibly formed by dissociation in the shocked region where the wind hits the disk.

Chilean rules require that the PI of a proposal must publish a first-author paper on the ALMA data that were obtained, otherwise he or she will not be allowed to submit any further ALMA proposals. Hence the ALMA data will be published in a refereed journal paper led by Prof. Stefan Kimeswenger (Universidad Católica del Norte, Chile). He has started writing this paper, but it was not yet finished by the end of the project.

When we realized that $HC_3N$ was observed, but not modeled in Cloudy, we started an effort to upgrade the chemical network in Cloudy. For this we chose the UDfA RATE12 network. The inclusion into the code has now been completed on a development branch of the Cloudy code called “udfa”. However, running the code with the new network revealed some unexpected instabilities, which have not been resolved at this moment. After an indepth investigation in collaboration with Dr. Robin Williams (AWE plc, UK), who is the main author of the existing chemical network in Cloudy, the root cause of the problem was found. There is an exponential runaway in the formation of long carbon-chain molecules due to the fact that destruction of these molecules is not fast enough. This leads to a situation where nearly all carbon is in the form of such carbon-chain molecules and not in the form of CO as would be expected. A solution for this problem is not yet apparent. We discussed the problem with the maintainers of the UMIST RATE12 network: Dr. Tom Millar (Queen's University Belfast, UK) and Dr. Catherine Walsh (Sterrewacht Leiden, the Netherlands). They had not seen such problems with this version of the database and could only offer general advice. The problem may be related to the fact that Cloudy calculates an equilibrium solution for the chemical abundances, while many other codes (including the code shipped with the RATE12 database) do time dependent chemistry (i.e., they integrate the rate equations up to a specified time where equilibrium may not necessarily have been reached yet). Our current idea is to reduce the size of the network by removing the longest carbon-chain molecules, thus circumventing the problems. This approach still needs to be validated. Hence further work will be needed to get this branch in a state where it can be released to the public.

Subsequently, we concentrated on the available optical and mid-infrared data of Sakurai's object, obtained using the ESO instruments FORS1/2 and X-shooter in the optical and VISIR in the mid-infrared. All the available data have been fully reduced. The data reduction of the X-shooter data was surprisingly difficult as the standard ESO pipeline yielded results of unacceptable quality. As a result the data reduction took *much* longer than anticipated. The difficulties are caused by the faintness of the source, resulting in the fact that field stars are in the slit with a strength comparable to the science target. The pipeline is not prepared for this situation. The pipeline also has other problems, e.g. producing very strong artifacts in the near-infrared data after removal of the sky lines. These are likely caused by the fact that the sky lines were overexposed when the data were taken. One of our team members, Prof. Dr. Stefan Kimeswenger (Universidad Católica del Norte, Chile), started a manual data reduction in collaboration with instrument specialists in Austria. After a considerable effort he was able to obtain a final result of publication-grade quality. Also the data reduction of the VISIR data proved difficult. The standard ESO pipeline yielded perfectly good results for the data obtained with the old detector (which was in use until 2012), but the situation was very different for data obtained with the new Aquarius detector which is in use since 2015. Several bugs in the pipeline were discovered and discussed with the ESO helpdesk (in particular Dr. Mario van den Ancker). These bugs resulted in very strong artifacts in the reduced data. ESO could not offer a full solution, but did offer workarounds for the most immediate problems. However, these could only partially resolve our problems. We had to wait for the release of a new version of the pipeline before we could obtain reduced data of acceptable quality. This delayed the data reduction by at least half a year. Unfortunately even this version still has bugs (e.g in the wavelength calibration) and we are still not entirely certain whether we can trust the pipeline results. The reason for this is that the data reduction steps implemented in the pipeline are not properly documented. As a result we do not know how the correction for telluric absorption lines is done, and hence we cannot be entirely certain if the procedure is correct for our data.

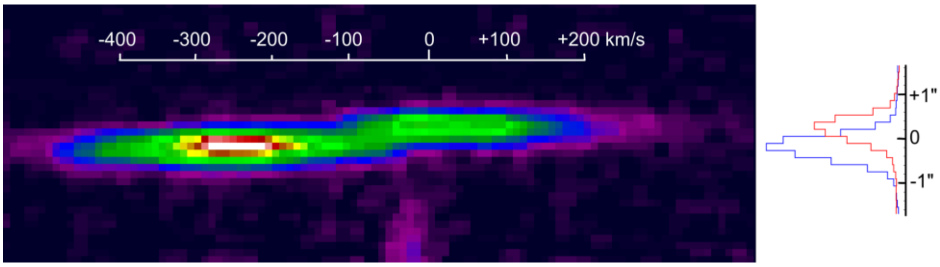


*Fig. 8: position-velocity diagram of the [N II] 658.3 nm line showing the velocity along the x-axis and spatial displacement along the y-axis. It is clear that the red-shifted emission comes from a different location than the blue-shifted emission. The spatial displacement shown in the right-hand side of the diagram agrees well with the physical dimensions of the bipolar lobes found by Hinkle & Joyce (2014).*

Proposals to continue the monitoring with FORS2 and VISIR at ESO in 2017 and 2018 were submitted, as well as a proposal for a second X-shooter spectrum to be obtained in 2018. The FORS2/VISIR proposal for 2017 as well as the X-shooter proposal for 2018 were accepted in category A, but the FORS2/VISIR proposal for 2018 was unfortunately rejected.

All the effort invested in the data reduction was well worth it though, as the combined data sets (and especially the X-shooter data) allowed us to greatly improve our understanding of the morphology of this VLTP object and better understand the hydrodynamic processes shaping the newly emerging planetary nebula. In the optical spectra we see two sets of lines that show different behavior. The first is a set of nebular lines (recombination lines of hydrogen and helium, as well as forbidden lines of heavier elements) that was first detected in 1998 (helium) and 2001 (heavier elements). When we obtained the X-shooter spectra we aligned our slit either parallel or perpendicular to the axis of the bipolar structure seen by Hinkle & Joyce (2014). This allowed us to determine that the nebular lines (e.g. [N II] 658.3 nm) are being emitted in the bipolar lobes (see Fig. 8). Most likely they are the result of a strong bow shock originating where the fast stellar wind hits ambient material. This implies that we are witnessing the very early stages of hydrodynamic shaping of a bipolar nebula!

Since 2013 we see a second set of lines emerging (see Fig. 9). Not all lines are identified yet, but the strongest are electronically excited molecular lines: the $A^2\Pi$ – $X^2\Sigma^+$ system of CN (the "red system") with some other (not yet identified) lines, possibly from other molecules. To our knowledge this is the first time optical CN emission is seen in a stellar object! It is not yet clear whether these lines are excited by the UV radiation from the central star, or by a C shock where the stellar wind is funnelled through the disk. If they are UV excited, they would be a good way to measure the evolution of the central star temperature, which would be another important test for i-process nucleosynthesis.

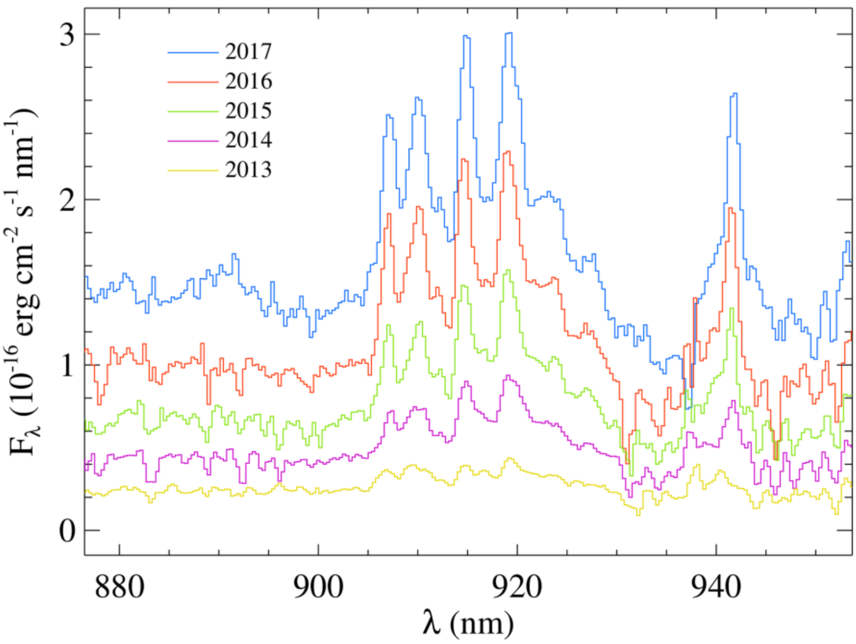


*Fig. 9: the complex of electronically excited CN lines that has been emerging since 2013 in Sakurai's object.*

Chesneau et al. (2009) detected the presence of a circumstellar disk using VLTI, and Hinkle & Joyce (2014) detected the presence of bipolar lobes using active optics. Combining these facts with the results from our analysis leads to the following conclusions. Sakurai's object ejected its remaining envelope in the 1990's. Soon afterwards there was a brief but strong shock, forming the nebular lines detected from 1998 onwards. This shock likely was caused by faster ejecta hitting slower ejecta. This shocked material then started cooling. A disk (which is likely Keplarian) also formed very quickly. This disk contains all the dust and likely also the bulk of the molecules. From 2008 onwards we see the nebular lines steadily brightening. Using the X-shooter data we could prove that these lines are excited in the bipolar lobes. Since 2008 there must be an increased mass loss, which is likely funnelled by the disk into a jet and is now hydrodynamically shaping the bipolar lobes. The nebular lines are formed in a strong J-type bow-shock at the end of the bipolar lobes. The optical CN emission is possibly formed where the molecular wind is funnelled by the disk in a C-type shock, or alternatively is excited by UV radiation from the central star. The CN could be formed by dissociation of HCN in the shock and then carried into the lobes. This would agree with the ALMA observations that show that the CN emission coincides with the bipolar lobes detected by Hinkle & Joyce (2014). This implies that we now have a unique and detailed data set following the very early stages of the formation of a bipolar nebula in time. Understanding this formation process has been the subject of intense study for many decades (see Balick & Frank 2002 for a review). Understanding the morphology and evolution as we do now will greatly help us in future studies of the molecular chemistry in this object.

Dr. Peter van Hoof started writing a refereed journal paper discussing all the optical and mid-infrared data of this object. This paper is roughly 90% written, but was not finalized by the end of the project.

Dr. Peter van Hoof attended the SKIRT days in Ghent to acquaint himself with the code via tutorials and investigate whether this code can be used to model the dust disk in Sakurai's object. SKIRT is a 3D Monte-Carlo code for dust radiative transfer. It is mainly used for modelling the interstellar matter in galaxies, but is set up as a general-purpose code capable of modelling other types of objects as well. So SKIRT should be able to model the dust disk in Sakurai's object. This will be important for the near future when the ESO MATISSE facility becomes available to do observations of this disk in unprecedented detail.

## 3. DISSEMINATION AND VALORISATION

Progress reports of our work on Sakurai's object were presented in 2016 at the Cloudy Symposium in Mexico City (by Dr. Peter van Hoof, oral presentation), in 2016 at the IAU 323 symposium on Planetary Nebulae in Beijing, China (by Dr. Griet Van de Steene, poster presentation), in 2017 at the AGB-Supernovae Mass Transition symposium in Frascati, Italy (by Dr. Peter van Hoof, poster presentation), and in 2017 the Asymmetrical Planetary Nebulae VII meeting in Hong Kong, China (by Dr. Peter van Hoof, oral presentation).

A refereed journal paper describing the optical and mid-infrared data led by Dr. Peter van Hoof is roughly 90% written and is expected to be submitted soon. A second refereed paper led by Prof. Stefan Kimeswenger that discusses the ALMA data is currently in preparation. We aim to submit this paper in 2018 as well. A third refereed paper discussing our VLA and e-Merlin radio data on Sakurai's object is led by Dr. Marcin Hajduk. He is currently (re-) reducing all radio data sets for this paper.

We have created a web page discussing MOLPLAN at http://aa.oma.be/molplan.html.

The Cloudy development branch "udfa" to implement the new chemistry network can be downloaded using a subversion client at svn://svn.nublado.org/cloudy/branches/udfa. Note that this branch is not yet in a stable state and should be considered experimental. The source code can be browsed at:

https://viewvc.nublado.org/index.cgi/branches/udfa/?root=cloudy

## 4. PERSPECTIVES

The highest priority will be to finalize the refereed journal papers discussed in Section 3. The first paper will analyze the optical and mid-infrared data and is led by Dr. Peter van Hoof. The second paper will analyze the ALMA data and is led by Dr. Stefan Kimeswenger. The third paper will analyze the VLA and e-Merlin radio data and is led by Dr. Marcin Hajduk. We will also write an article for the proceedings of APN VII meeting held in Hong Kong.

The cycle 2 data on Sakurai's object was the first ALMA data set we ever obtained. The work on this data set as part of the MOLPLAN project helped us greatly to obtain expertise using this instrument. This experience will be invaluable when analysing future data sets we plan to obtain with ALMA. We currently have an ongoing proposal targeting Sakurai's object in cycle 5. However, the category C rating of this proposal means that chances are low of actually getting data. If we are unsuccessful, we will continue to submit proposals in future calls for observing proposals in order to finalize work package 3. We may well also start using ALMA for other science projects, though there are currently no concrete plans for this.

We have been continually monitoring Sakurai's object at optical wavelengths since 2005. In 2018 we expect to obtain a second ESO X-shooter spectrum. We will continue to submit proposals to monitor the evolution of the optical spectrum using ESO FORS2 and the mid-infrared spectrum using ESO VISIR. The final goal of this monitoring program is to derive the evolution of the central star temperature as a function of time, which is another critical test of the evolutionary models of this VLTP object.

The new insights on the morphology and hydrodynamic evolution of Sakurai's object we have gained as part of the MOLPLAN project are very important in their own right, but will also be important in our future work modeling the ejecta with Cloudy and other codes such as SKIRT. This will be needed to reach our goals in work package 3 as well as our project to derive the temporal evolution of the central star temperature.

We plan to submit a proposal to use ESO MATISSE once the instrument is offered by ESO. This is a second generation VLTI instrument that enables mid-infrared interferometry using 4 telescopes (compared to 3 telescopes with the first generation instrument). This will allow us to greatly improve the observations of the dust disk done by Chesneau et al. (2009) as we will have much better UV coverage and imaging capabilities.

Dr. Peter van Hoof will continue to work on the "udfa" Cloudy branch until it is ready to be integrated into the main Cloudy release and can be made available to the wider scientific community. Cloudy is available at https://nublado.org/.

The future of work packages 1 & 2 is less clear, and is mainly dependent on funding. Dr. Griet Van de Steene en Peter van Hoof joined the ESSENcE consortium which aims to observe PNe with the JWST in order to study various hot topics. One of the goals is to study the dense, neutral clumps in evolved PNe such as the Helix nebula. This makes this collaboration a very natural continuation of the MOLPLAN proposal (and in particular work package 2). So far the consortium has not been able to secure observing time in the Director's Discretionary Early Release Science (DD ERS) call. They are now concentrating their efforts on getting targets approved for the Early Release Observations (ERO) phase of observations.

## 5. PUBLICATIONS

### Non-refereed publications

Van de Steene G.C., van Hoof P.A.M., Kimeswenger S., Zijlstra A.A., Avison A., Guzman-Ramirez L., Hajduk M., Herwig F.: The very fast evolution of Sakurai's object. Proceedings of the IAU Symp. 323: "Planetary nebulae: Multiwavelength probes of stellar and galactic evolution", eds. X.-W. Liu, L. Stanghellini and A. Karakas, 2017, IAU Symp 323, 380

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## 6. ACKNOWLEDGEMENTS

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