# Dust and molecules in PNe

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# Outline

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- Introduction to nebular objects
- Brief introduction to modeling nebular regions (Cloudy)
- Optimizing models of planetary nebulae
- Observations of evolved objects:

1) NGC 6720

2) NGC 7293

3) Sakurai’s Object (V4334 Sgr)

# Introduction (1)

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Photoionization is a common process in the interstellar medium (ISM) and in circumstellar material (CSM). It happens when gas is being irradiated and ionized by photons from an external source.

The ionizing source is usually a star or an ensamble of stars, but could also be an accretion disk.

Typically the distance of the ionizing source is much larger than the diameter of the source, implying that its radiation field is strongly spherically diluted when it reaches the gas.

Some classical examples of photoionized sources are:

- Regions of massive star formation
- Planetary Nebulae
- Novae / Supernovae
- Active Galactic Nuclei

# Introduction (2)

This is the star forming region N90 in the Small Magellanic Cloud. The cluster of blue massive stars that is ionizing the cloud (with $T_{eff}$ = 30–50 kK) is clearly visible in the center. The radiation pressure and the winds from these stars have blown a nearly spherical bubble in the molecular cloud from which they formed.

Image Credit: NASA, ESA and the Hubble Heritage Team (STScI/AURA)-ESA/Hubble Collaboration.

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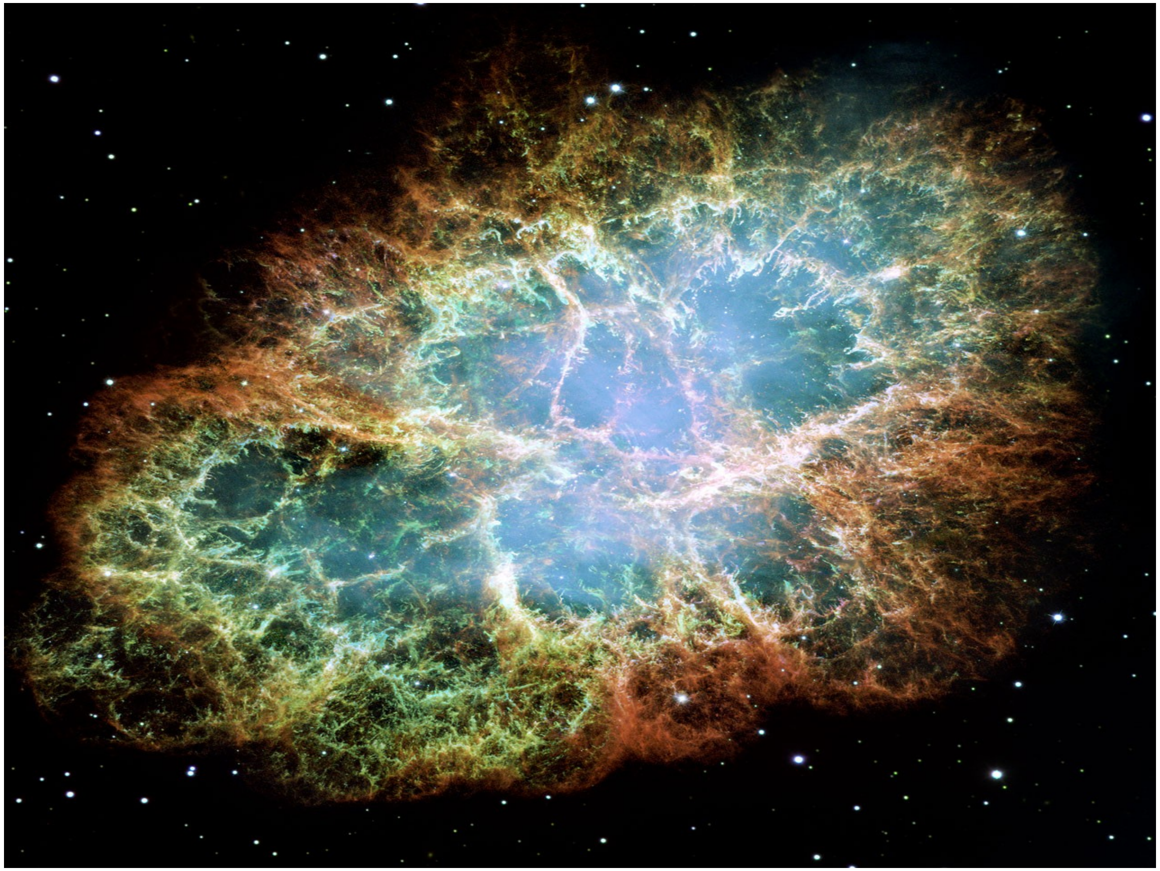
# Introduction (3)

This is the PN NGC 6302. It is very young and dense. The central star is one of the hottest known (> 200 kK) and is on its way to become a white dwarf. The current mass of the star is 0.64 Msol, but the original mass must have been much higher. Most of the stellar material has been expelled and now forms the PN. It has a bipolar (hourglass) shape with a marked equatorial density enhancement.

Image Credit: NASA, ESA and the Hubble SM4 ERO Team.

# Introduction (4)



This is the Crab Nebula (SN 1054), a supernova remnant. It is a strong X-ray and gamma-ray source. The central star is a pulsar: a neutron star with a strong magnetic field. It is obvious that the nebular material that was ejected in the supernova explosion is extremely filamentary.

Image Credit: NASA, ESA and Allison Loll/Jeff Hester (Arizona State University).

# Introduction (5)

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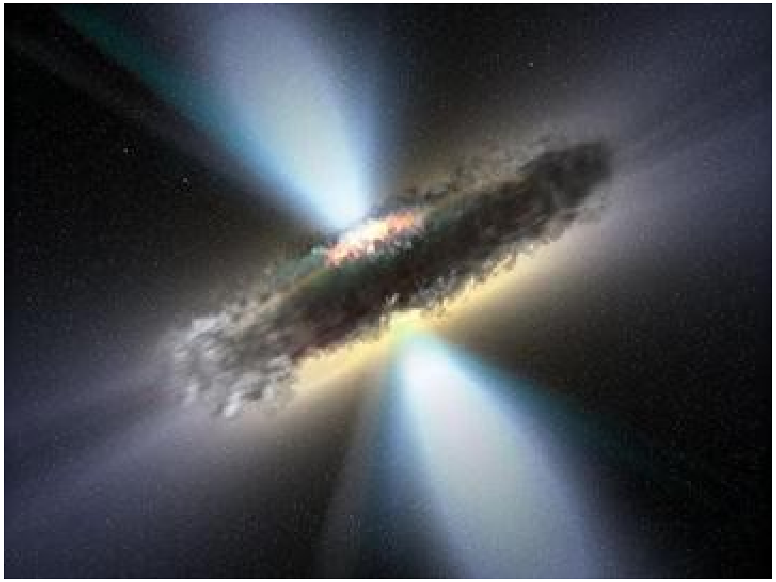

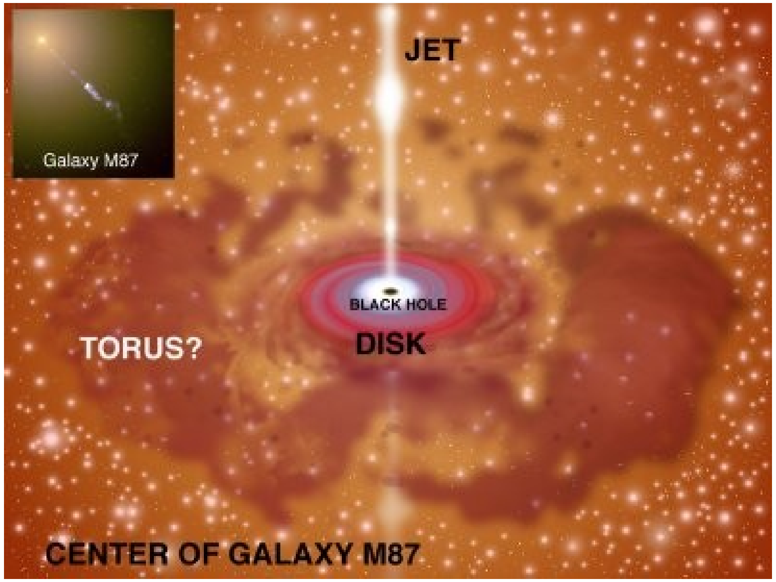


These are artists impressions of the central engine of an Active Galactic Nucleus (AGN). At the center is a supermassive black hole surrounded by an accretion disk that is heated to X-ray temperatures. These objects are also strong synchroton sources, the origin of which is not clear. Surrounding this is a fat torus of (possibly molecular) gas that is also very dusty which may obscure the central engine from certain viewing angles. The central engine often drives powerful jets that can form giant radio lobes.

Image Credit: The Gemini Observatory.

# Introduction (6)

This list of photoionized objects is certainly not exhaustive. We can draw the following conclusions:

- We have a wide variety of ionizing sources showing great differences in the level of excitation.

- The ionized gas can have very different morphologies, ranging from roughly spherical or elliptical bubbles, to bipolar shapes, tori, or even completely irregular shapes. The gas can be smooth, filamentary or clumpy.

- The gas may originate from the ionizing star, in which case it often has unusual abundance patterns (in extreme cases H- or even He-deficient), but it may also be the gas from which the ionizing source formed. In some cases the gas and ionizing source are not related at all.

- The gas may contain dust grains.

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# A typical spectrum

Shown here is a typical optical spectrum of a photoionized region, in this case the Orion nebula. What we see are strong emission lines: permitted lines from hydrogen (and also helium, but those lines are too weak to see on this scale) and a variety of forbidden lines. The continuum is difficult to detect. In the UV we see the SED from the ionizing stars.

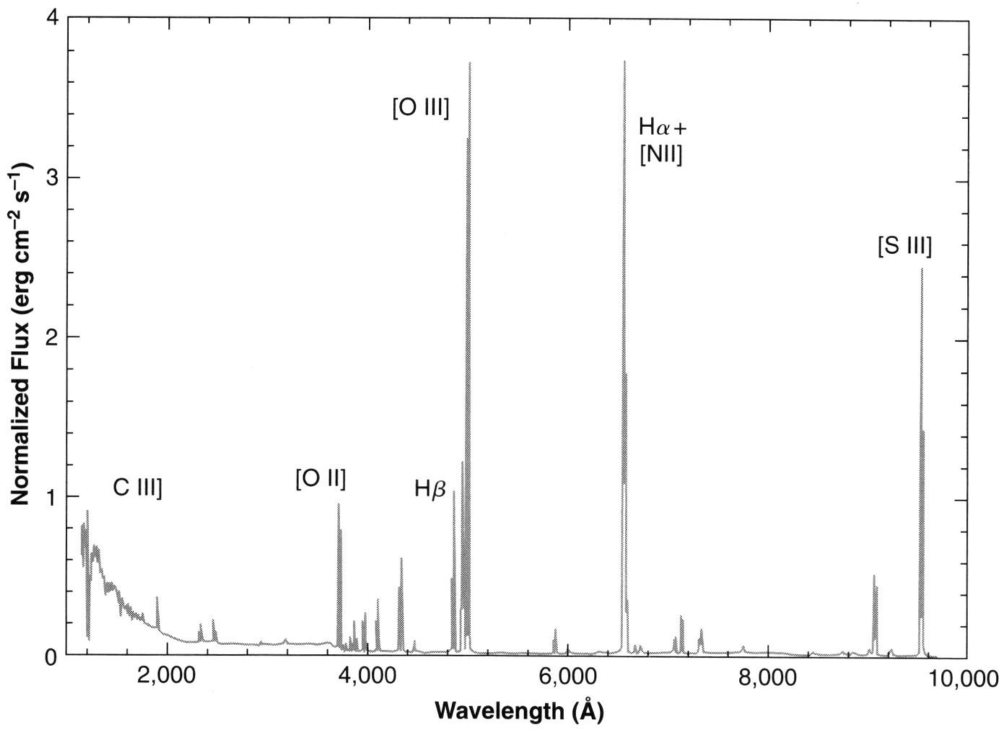


**Figure 1.1**

The ultraviolet, optical, and near infrared spectrum of inner regions of the Orion Nebula.

# Modeling a photoionized region

What we have seen in the introduction already gives us some idea of the challenges involved in understanding photoionized regions: there is a wide variety of ionizing sources, and also the morphology of the gas can be very different from one source to another. Furthermore, the gas composition may be very different from a standard solar composition. Hydrodynamic interactions, including shocks,  may complicate things further.
A sophisticated code is needed to handle all these challenges. Several codes are available, each with their own strengths and weaknesses. The most widely used code is Cloudy.

The great strength of this code is its detailed, state-of-the-art treatment of the various microphysical processes and the fact that it can produce a unified model of the ionized region and the PDR / molecular region. Most likely its biggest weakness is that it is a 1D spherically symmetric code. It also doesn't treat shocks.

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# Physical conditions (1)

The photoionized gas can be characterized by an electron temperature and the abundances of each ionization stage of every element (the ionization structure). The ionization structure implies an electron density (charge conservation). Each ion is characterized by the level populations of each of its electronic states.

Cloudy assumes that the electrons have a perfect Maxwellian distribution. Deviations do exist near strong temperature gradients (solar corona) and from secondary electrons due to cosmic ray or X-ray ionizations (molecular regions).

The dominant processes determining the ionization structure are photoionization and its inverse process, radiative recombination. Cloudy assumes that the ionization structure is in equilibrium with the radiation field (steady state). This is often a good approximation, but deviations are known (e.g., the guitar nebula, recombining PNe).

# Physical conditions (2)

The dominant processes determining the level populations of the ions are collisional (de-) excitation, spontaneous and induced radiative decay, continuum or line pumping and radiative cascades following recombination.

As was mentioned before, the radiation field is usually strongly diluted ($T_{color} >> T_{ed}$) and the gas density is usually low (typically $10^0 – 10^8$ cm$^{-3}$) so that neither the radiation field nor the collisions in the gas can establish LTE. Hence calculations of a photoionized plasma need to be done in full non-LTE.

Excitation and de-excitation processes generally are very fast, so the level populations are determined by balancing the rate equations for each of these processes (steady-state).
The electron temperature is determined by balancing heating and cooling processes. Each of these processes is a function of temperature, so we search for a temperature such that the sum of all the heating processes and all the cooling processes match exactly. Usually there is only one solution, but there can be multiple solutions, in which case the gas is bistable.

# Determining the physical conditions (1)

In a photoionization code like Cloudy, all the relevant processes need to be balanced to obtain a steady-state solution in thermal equilibrium. This is done in a nested set of solvers:

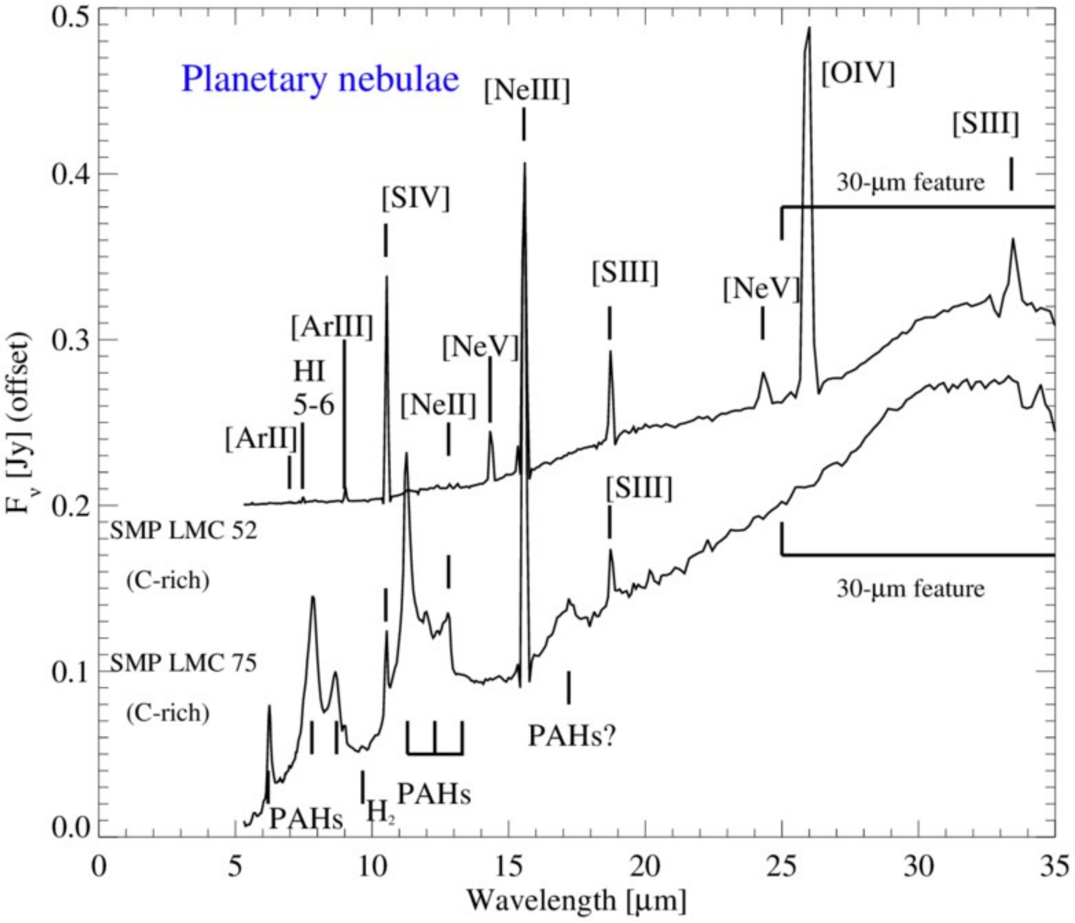
Assume gas density
- Assume electron temperature
  - Assume electron density
    - Solve the ionization structure
    - Determine the electron density from ionic abundances
  - Iterate until assumed and determined electron density match
  - Calculate the heating and the cooling
- Iterate until the heating and cooling match
- Calculate the pressure

Iterate until constant pressure is achieved

# Determining the physical conditions (2)

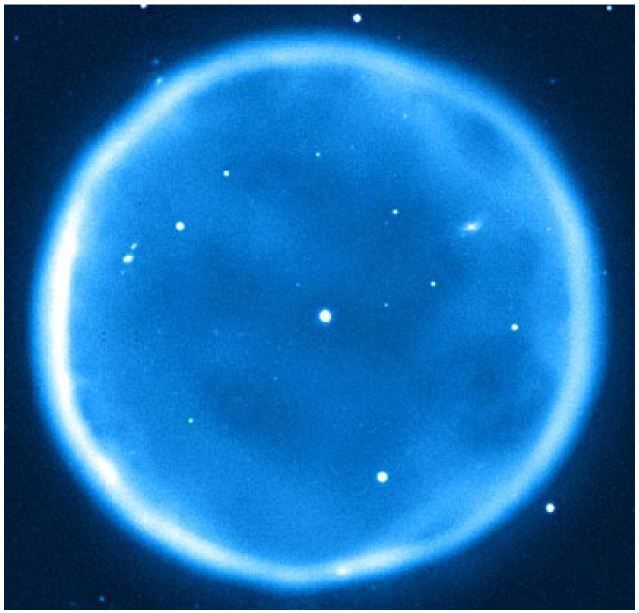
The outermost solver is only exercised in a constant pressure model. In a model with a prescribed density law, such as a constant density model, only the inner three solvers are used.
This nested iteration needs to be done for each zone. Once it has converged, it is possible the determine the opacity in that zone, e.g. photoionization cross sections of various ions and from grains.
When the opacities are known, radiative transfer can be done and the radiation field for the next zone can be determined. This will also include spherical dilution effects.
Now the solvers can be exercised again for the next zone, etc. This way the code will gradually work itself outwards until some stopping criterion is fulfilled (e.g. $T_e$ dropping below some preset value, a preset column density being reached, etc.).
Now the total line and continuum opacities are known. These are needed to calculate the escape probabilities. Normally there will be another layer of iteration to converge the line and continuum opacities.

# Optimizing models in Cloudy (1)




The problem: we have observations (typically a spectrum) and want to derive properties of the object from that. Image credit: Matsuura et al., 2014, MNRAS 439, 1472.

# Optimizing models in Cloudy (2)



- There are several ways to model the data, here we discuss optimizing the model with Cloudy.
- Images: from left to right – Abell 39, NGC 2392, NGC 6302. These nebulae show increasing levels of complexity in their morphology, yet we have to assume they all are spherical!
- Modeling bipolars can be difficult as the nebula is usually optically thick in the EDE but optically thin in the polar directions.

# Optimizing models in Cloudy (3)

Parameters:

- Central star – $T_{eff}$, $L_*$ (choose SED grid)
- Nebula – $R_{in}$, $n_H(r)$, set outer radius with stop command
- Composition – abundances, grains

# Optimizing models in Cloudy (4)

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What observables do we need?

- $T_{eff}$ – line emission from ions with different ionization potentials, <u>especially the highest stages are important</u>
- $L_*$ – absolute flux, e.g. Hβ or radio flux, angular diameter
- $R_{in}$ – hottest dust, highest ionization stages, direct observations?
- $n_H(r)$ – density sensitive line ratios, emission measure, ionization balance
- abundances – line ratios, preferably multiple ionization stages
- grains – dust continuum flux

Note the following:

- You need (many) more observables than free parameters
- Deredden the spectrum and compare to intrinsic predictions
- You need a distance, optimizing this doesn't work well
- Do multiple runs with different initial estimates
- CPU intensive → do parallel runs

# Optimizing models in Cloudy (5)

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Things to look out for:

- Errors on observables also steer the optimization since they affect $\chi^2$.
- So getting realistic errors is important, but difficult. There are many easily overseen sources that often dominate the error: flux calibration, dereddening, aperture correction, atomic data, etc. So keep a minimum of 5 – 10% on line ratios.
- Check Cloudy output for predicted lines that are strong enough to be observed, yet are absent. Use upper limits to prevent this in next run.
- Observed lines may be blended with lines that are not modeled by Cloudy, especially weak lines in very deep spectra.
- Grain properties are often poorly known (such as the size distribution) yet this is important for heating the gas.
- Check if the model makes physical sense!
- Do multiple runs with different initial estimates.

# The MESS GT key programme

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- MESS = Mass loss of Evolved StarS
- Herschel guaranteed time key programme, PI Martin Groenewegen.
- Aim 1: study the time dependence of the mass loss process via a search for shells and multiple shells.
- Aim 2: study the dust and gas chemistry as a function of progenitor mass.
- Aim 3: study the properties and asymmetries of a representative sample of evolved objects.
- Covers many phases of stellar evolution: AGB & post-AGB stars, planetary nebulae, massive stars (RSG, WR, LBV), supernovae.
- We obtain both photometry and spectroscopy using Herschel PACS and SPIRE (not all sources are done in all modes).
- I will also discuss results from the DDT Must-Do 7 (MD7) proposal led by J. Cernicharo and a follow-up OT2 proposal (P.I. P. van Hoof).

# NGC 6720: General Properties

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- NGC 6720 = M57 = Ring Nebula
- Evolved, oxygen-rich bipolar nebula seen nearly pole-on
- Ionization bounded, but optically thin in polar direction, detected in molecules ($H_2$, CO, …)
- Central star is on cooling track and outer nebula is recombining; re-ionization of the recombined material due to expansion has just started (O'Dell et al. 2007)
- $T_e = 10 – 12$ kK
- $n_e = 400 – 800$ cm$^{-3}$
- $T_{Z\text{-HeII}} = 125$ kK, $L = 200\ L_\odot$, $M_c = 0.61\text{-}0.62\ M_\odot$

# NGC 6720

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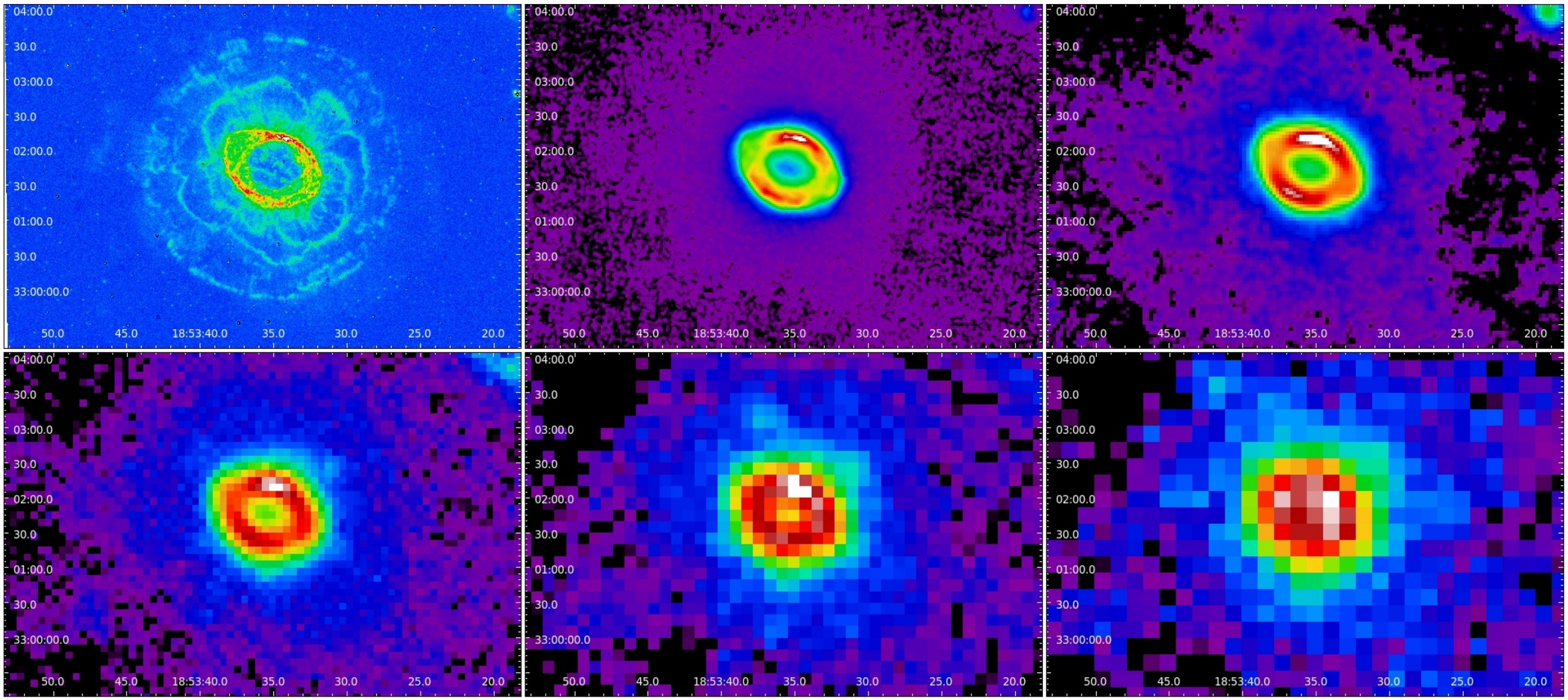


Top row – left: $H_2$ 2.12 µm (Calar Alto), middle: PACS 70 µm, right: PACS 160 µm. Bottom row – left: SPIRE 250 µm, middle: SPIRE 350 µm, right: SPIRE 500 µm image.

# NGC 6720: $H_2$ formation on dust grains

- NGC 6720 is very similar to NGC 7293 (the Helix nebula). It seems they are on the same evolutionary path.
- A static photoionization model cannot explain the $H_2$ emission in the Helix nebula, but a hydrodynamic model can (Henney et al. 2007, ApJ, 671, L137).
- This model indicates that the erosion of the knots by the radiation field of the central star is substantial: between $10^{-10}$ and $10^{-9}$ Msol/yr despite the low luminosity of the central star (120 Lsol).
- Considering the fact that the central star luminosity was much higher in the past and the knots must have been closer to the central star, survival of the knots from the AGB phase (as was e.g. proposed by Matsuura et al. 2009, ApJ, 700, 1067) to the current time seems problematic. More detailed modeling is warranted though to reach a more definitive conclusion.

# NGC 6720: $H_2$ formation on dust grains

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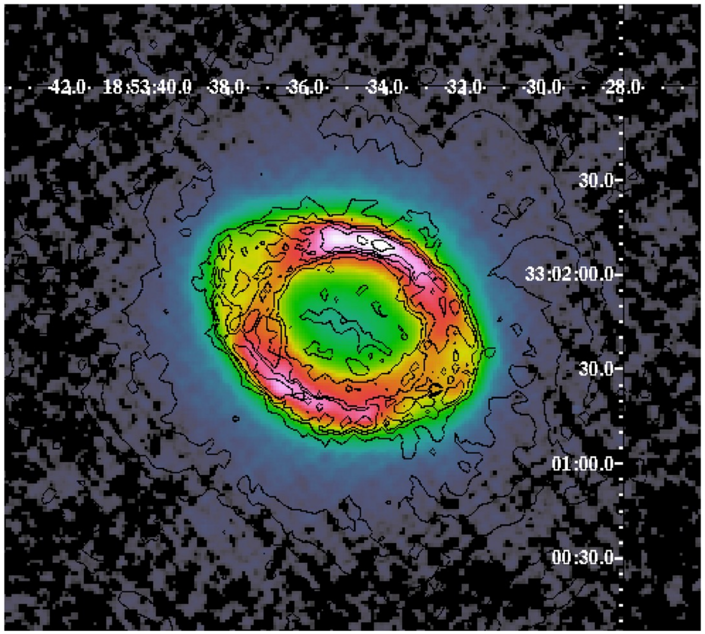
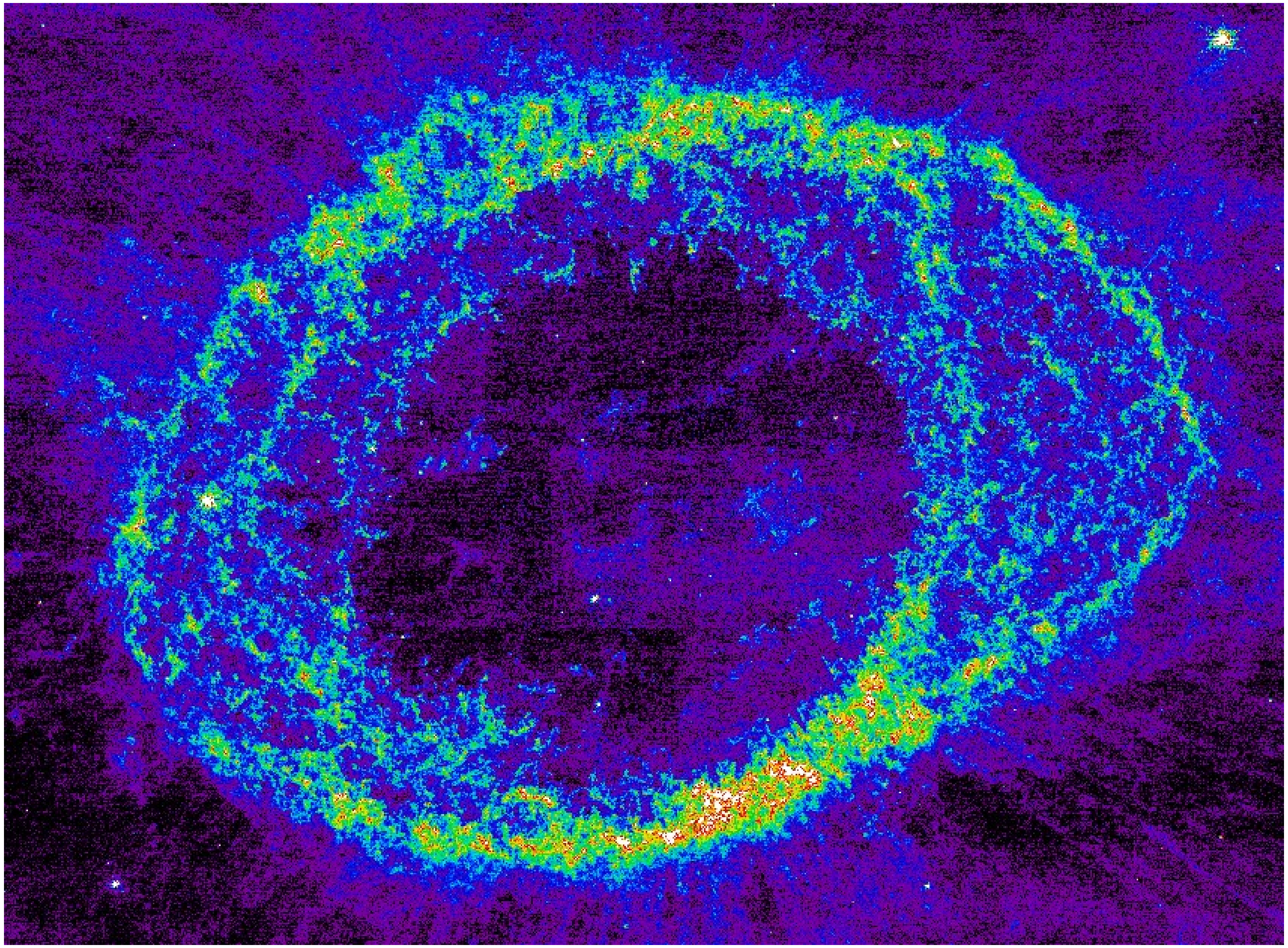


Overlay of the $H_2$ 2.12 µm emission (contours) on the PACS 70 µm image of NGC 6720 showing the dust emission.

- We have developed a photoionization model of the nebula with the Cloudy code, which we used to investigate possible formation scenarios for $H_2$.
- We conclude that the most plausible scenario is that the $H_2$ resides in high density knots which were formed after the recombination of the gas started when the central star luminosity dropped steeply around 1000-2000 years ago.
- The models show that $H_2$ formation in the knots is expected to be substantial since then, and may well still be ongoing at this moment.
- van Hoof et al. 2010, A&A, 518, L137

# JWST observations

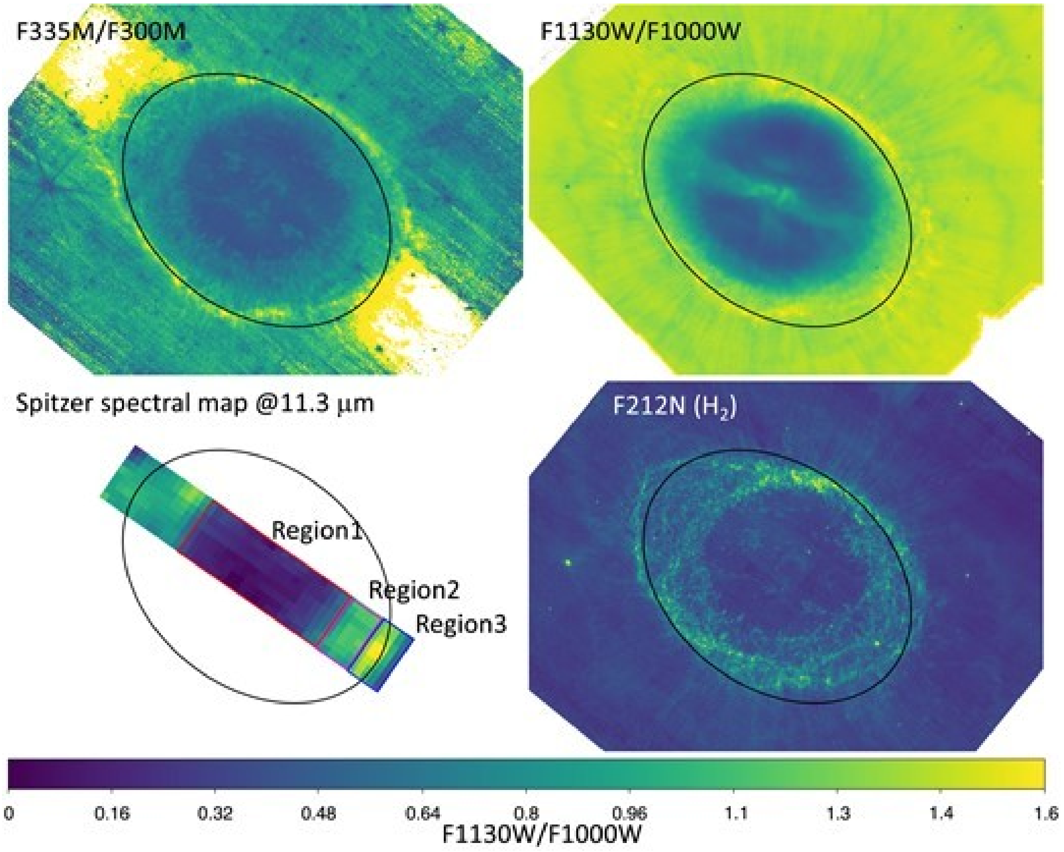
We observed NGC 6720 again with JWST NIRSpec and MIRI/MRS as well as imaging. The imaging shows the knots in unprecedented detail. Below is the $H_2$ 1-0 S(1) image.



# JWST observations

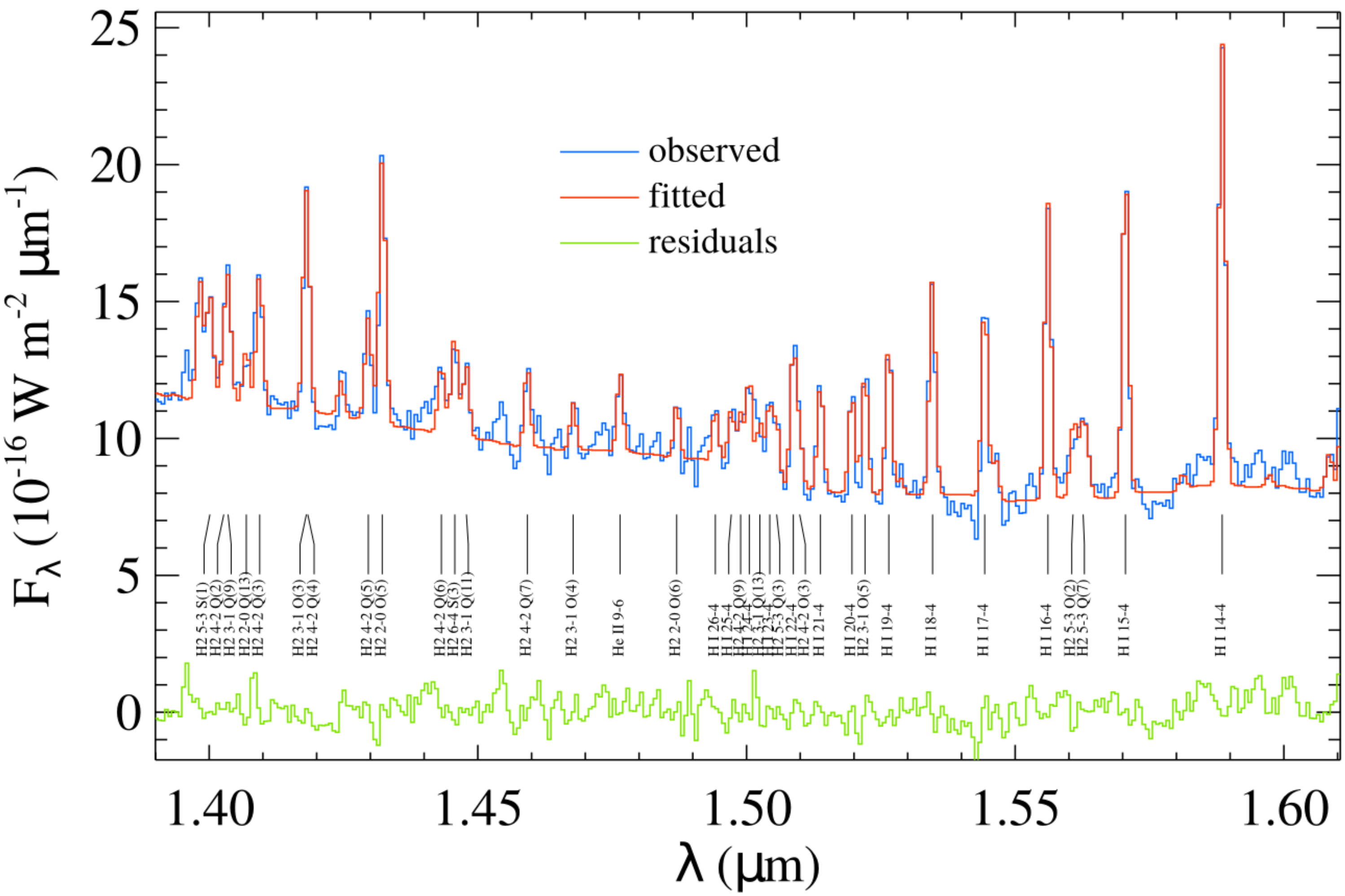
The imaging clearly shows that the $H_2$ resides in the dense globules and that the distribution is very different from the PAHs. This rules out formation of $H_2$ on PAHs as was suggested by Cox et al (2016).

Image credit: Wesson et al. (2024).



# JWST observations

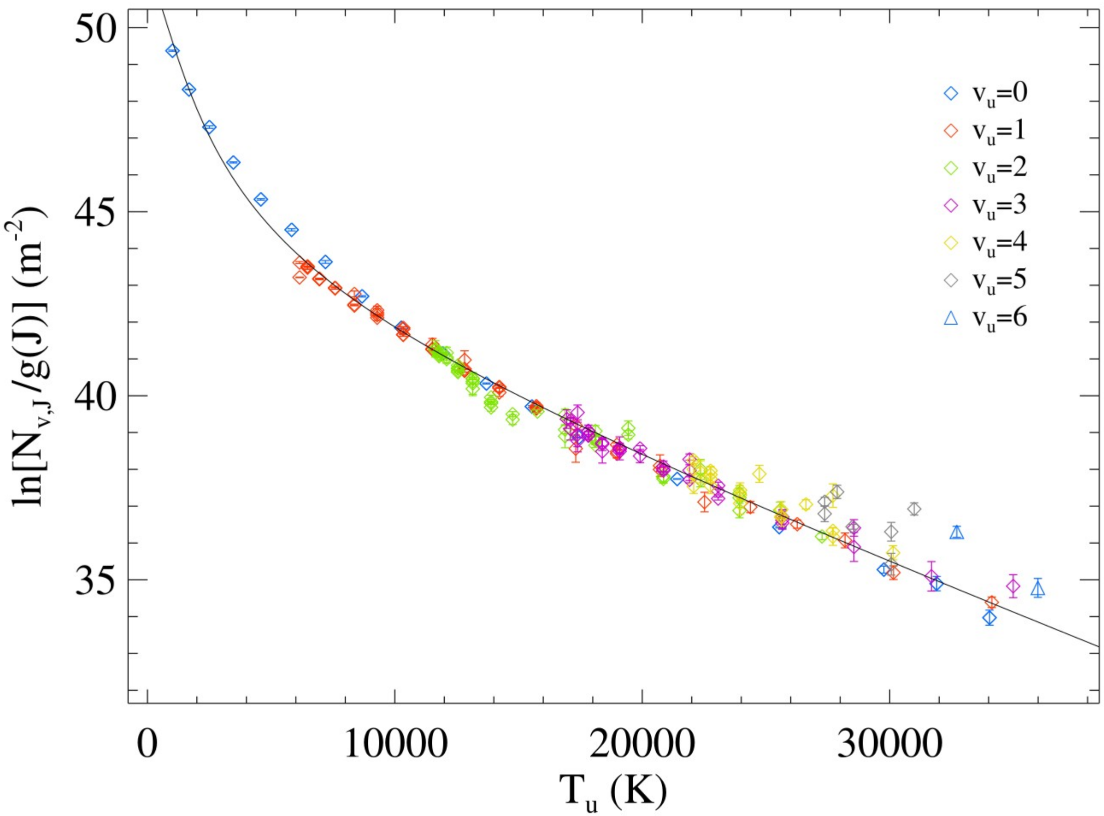
We are now studying $H_2$ using the very rich spectrum observed with JWST (almost 200 unique $H_2$ lines were detected!).



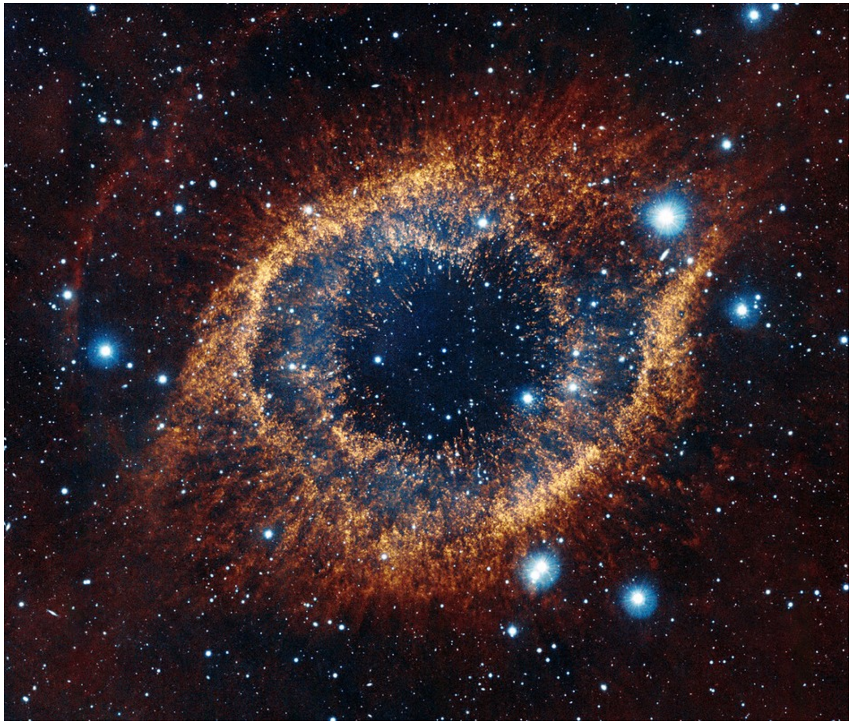
# JWST observations

Below is the excitation diagram for one of the regions we are studying. It shows that $H_2$ has a large range of temperatures.

The most likely explanation is that cold $H_2$ is being evaporated from the globules and heated to destruction as predicted by Henney at al. (2007).



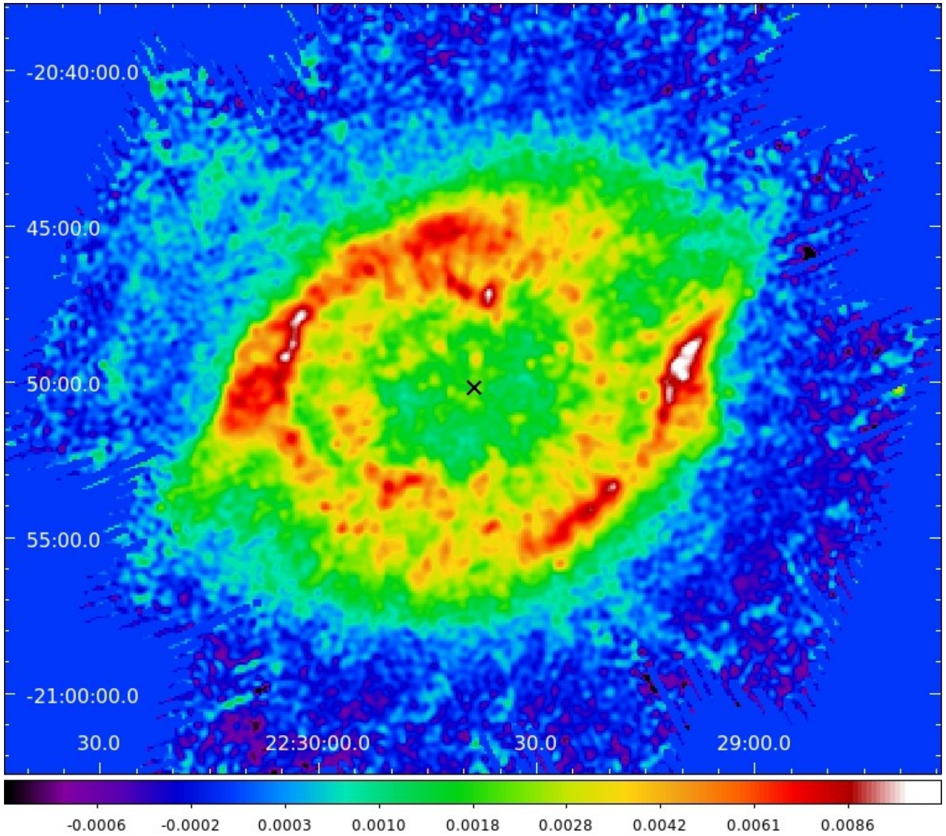
# NGC 7293



- NGC 7293 is one of the most famous planetary nebulae and also the closest to Earth (216 pc)
- It is well known for its thousands of cometary knots that are clearly seen in the HST images.
- The central star is on the cooling track ($T_{eff}$ = 120 kK, L = 76 $L_{sol}$) and is probably oxygen-rich (C/O = 0.87 ± 0.12; Henry+ 1999).

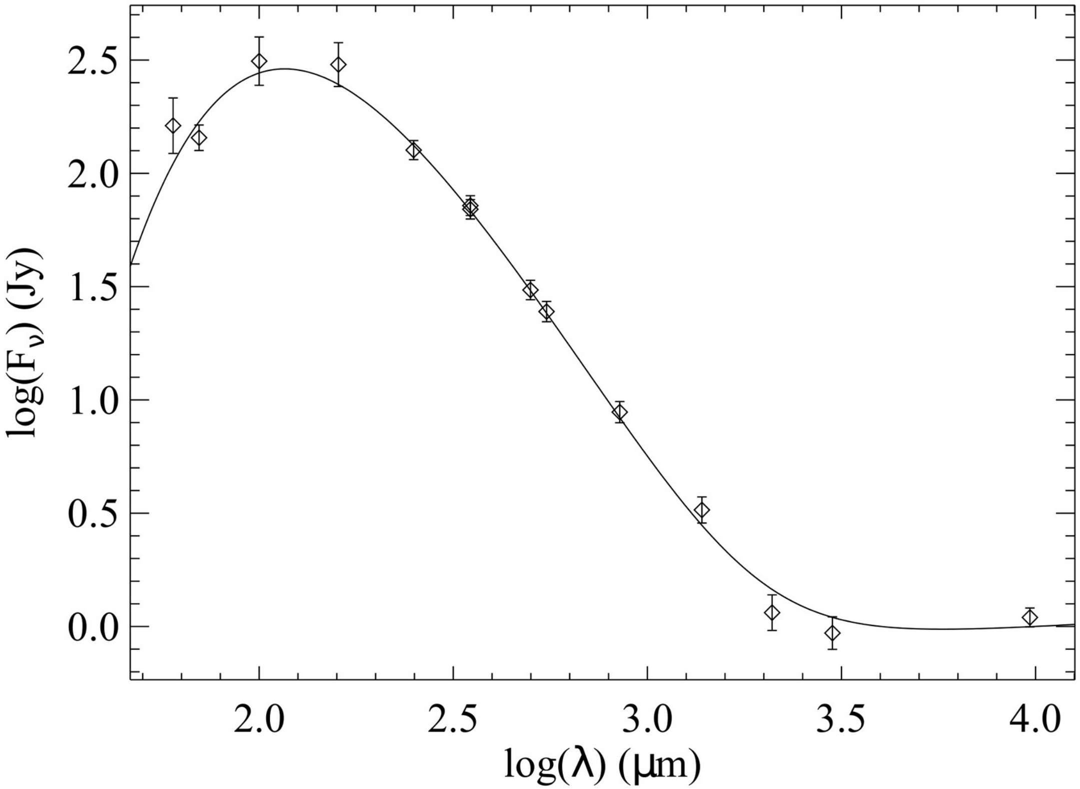
- The image above is the VISTA image of the Helix nebula in the Y, J, and K bands clearly showing the very clumpy nature of the nebular material.
- The nebula is very large (roughly 15 arcmin in diameter) making it ideal for detailed studies.
- The cometary knots are very dense (~ $10^6$ $cm^{-3}$) and contain molecules like $H_2$ and CO.

# NGC 7293



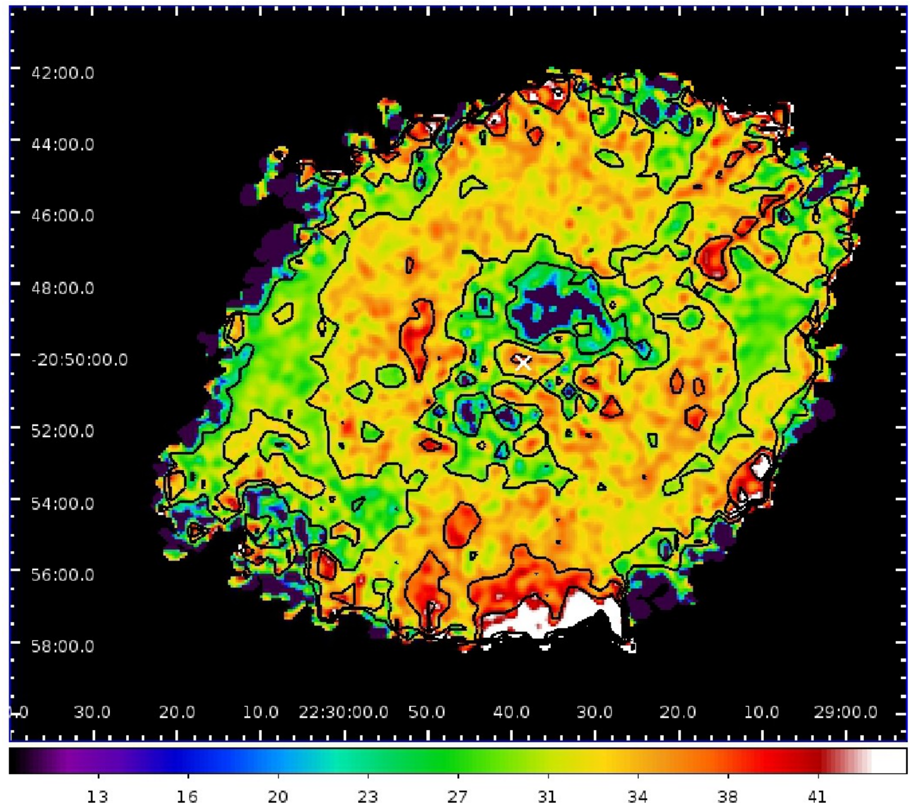

- The SPIRE 250 μm image based on the DDT MD7 data. The data clearly show the clumpy inner and outer ring, where the outer ring is much brighter. The extensions towards the NW and SE are also clearly visible and have the highest surface brightness of the whole nebula.
- Published in Van de Steene et al. (2015, A&A 574, A134).

# NGC 7293



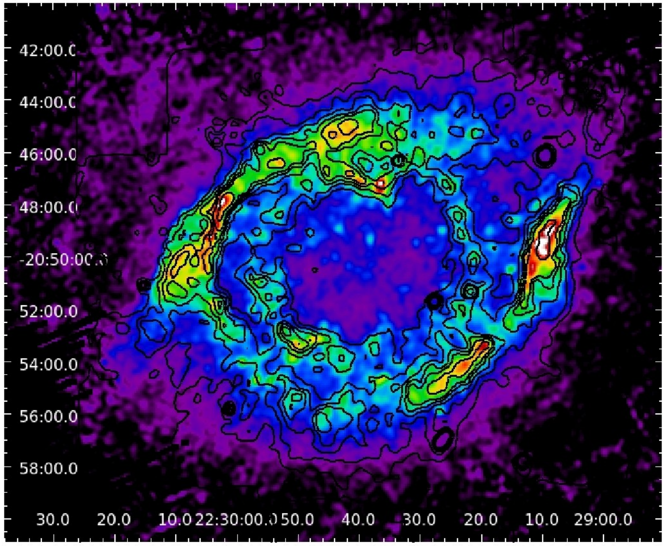

- We fitted a modified blackbody to the photometry of NGC 7293, including a component for the radio free-free emission. The data points are IRAS, PACS, SPIRE, and Planck fluxes and a 31 GHz point from Casassus+ (2004).
- The fit yielded $T_{dust}$ = 30.8 ± 1.4 K and β = 0.99 ± 0.09.
- The low β could indicate the presence of layered amorphous grains.

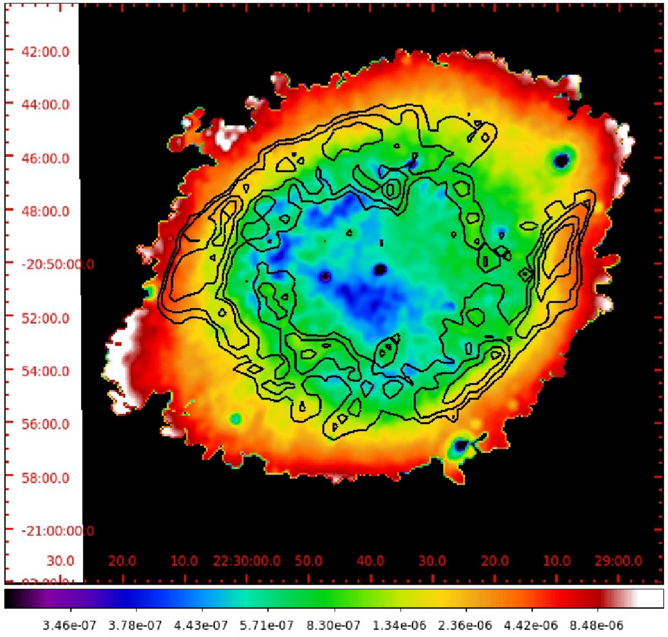
# NGC 7293




- The dust temperature map constructed from the PACS 70 μm and SPIRE 250 μm maps, assuming grains with β = 1.
- There clearly is a ring of warmer dust that encompasses both the inner and outer ring.
- The extensions towards the NW and SE are colder, likely due to a combination of greater distance and optical depth effects.

# NGC 7293




- The image on the left shows the $H_2$ emission as contours overlaid on the SPIRE 250 μm image. It emphasizes the detailed match between the $H_2$ and dust emission, as was already seen in NGC 6720.
- On the right we see the ratio of the $H_2$ and Hβ emission with the SPIRE 250 μm image overlaid as contours. The density structure has virtually disappeared and we see the rapid decrease of the ionizing radiation field outwards beyond the inner ring..

# NGC 7293

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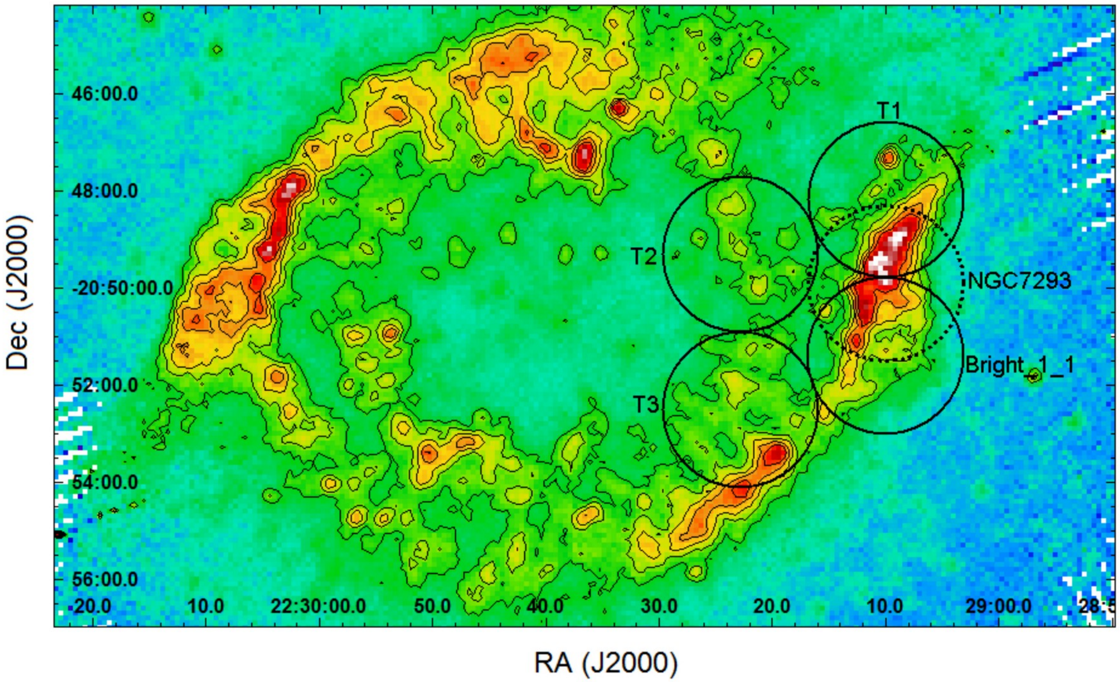
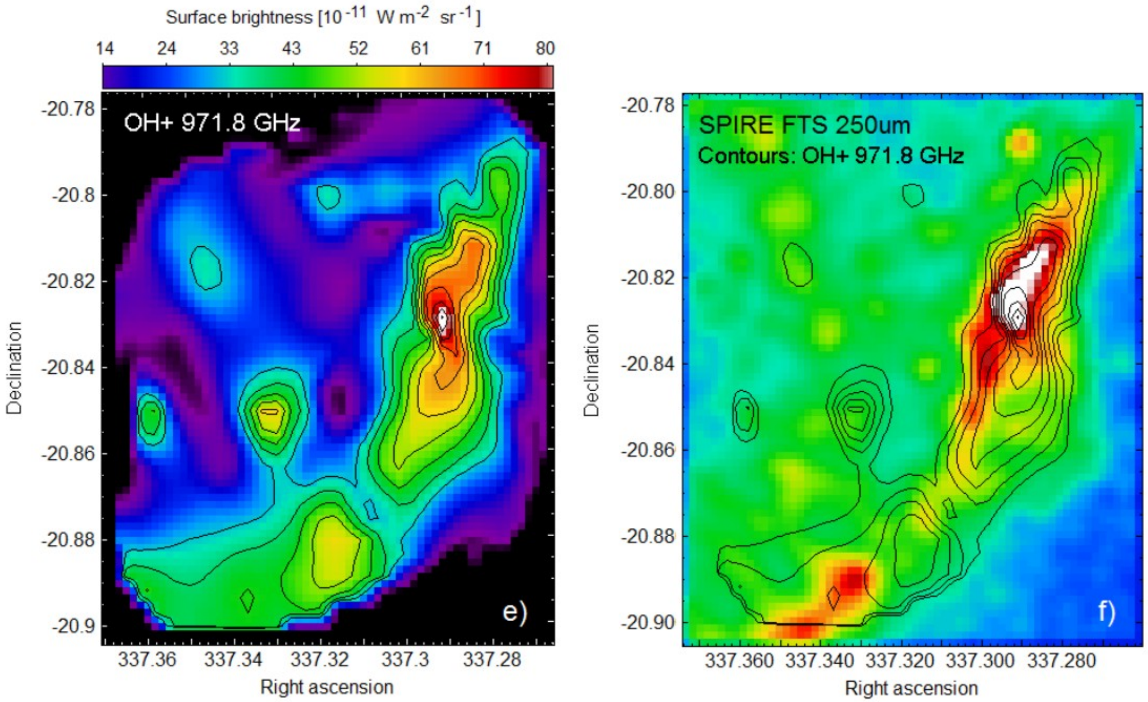



- We obtained SPIRE spectroscopy of the Helix nebula as part of the DDT MD7 proposal (solid circles) as well as a OT2 proposal (dotted circle). They cover the inner as well as the outer ring. The apertures are shown on top of the SPIRE 250 μm image.
- We have pooled these data and the following slides will show the results from the joint analysis.

# NGC 7293




- We have obtained the first detection of $OH^+$ emission in a planetary nebula!
- The left panel shows the map of the $OH^+$ 971.8 GHz emission in the western arm. The right panel shows the $OH^+$ emission as contours overlaid on the SPIRE 250 μm image. The $OH^+$ emission is mainly concentrated on the NW extension of the nebula and the outer ring.
- Shocks don't seem important to create the molecular ion. Formation mechanisms are still being discussed. A possible scenario is advection flows off the molecular knots taking $H_2$ towards the ionized gas.

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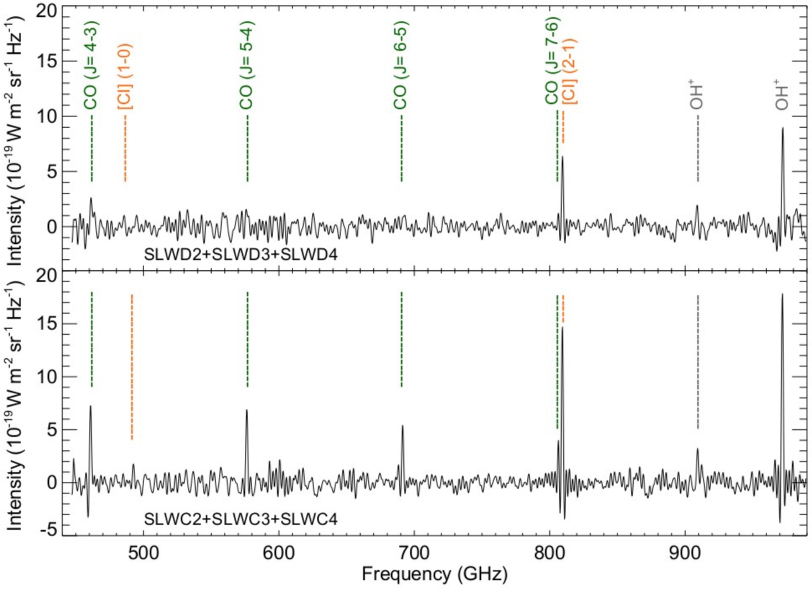
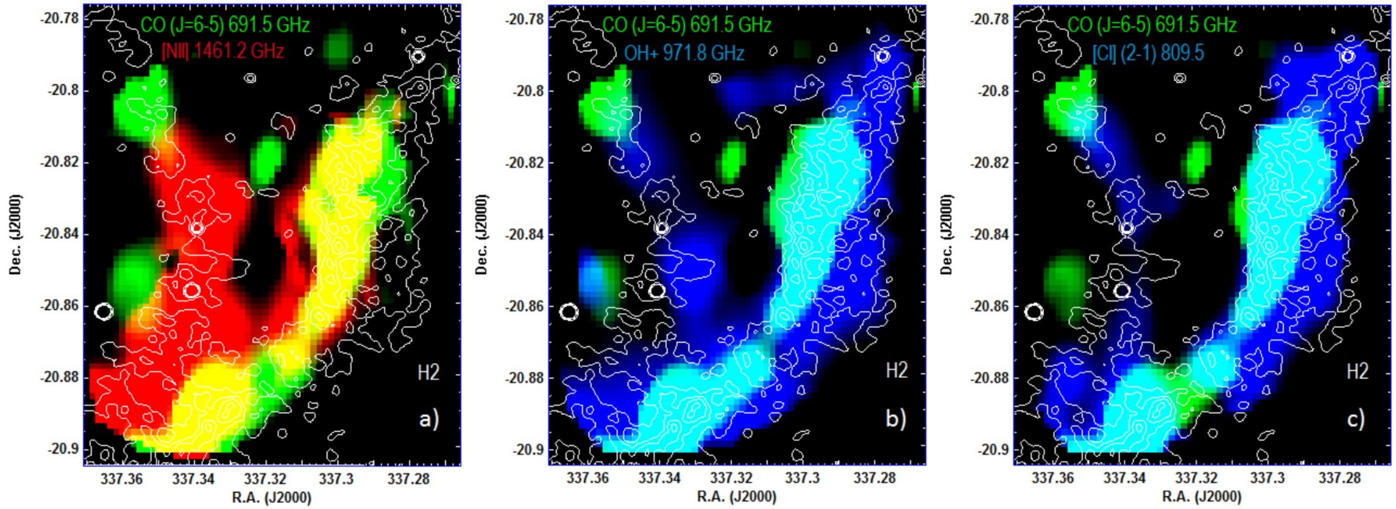
# NGC 7293




- The top and bottom panel show the co-added spectra from the inner and outer arm, respectively. The SSW spectrum is not shown.
- The $OH^+$ line at 971.8 GHz is the strongest molecular line in the spectrum, even stronger than CO! We additionally see [C I] and [N II] emission.

- We also detected $OH^+$ emission in NGC 6853, another PN from the OT2 proposal.
- The OT1 proposal HerPlaNS (P.I. T. Ueta) is a program to do photometry and spatially resolved spectroscopy of planetary nebulae. They also detected $OH^+$ emission in 3 PNe, bringing the total to 5 known PNe with $OH^+$ emission.
- Published in Etxaluze et al. (2014, A&A 566, A78) and Aleman et al. (2014, A&A 566, A79).

# NGC 7293




- Here we compare the spatial distribution of the emission in various lines.
- It is clear that the $OH^+$ and the [C I] emission have a very similar distribution. Regions that emit CO also emit $OH^+$ (with some minor differences) but the CO emission is more narrowly confined. The CO is cold (20 – 40 K).
- The [N II] emission has a very different distribution than the other lines shown. The [N II] emission is much stronger in the inner ring.

# Sakurai’s Object (1)

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V4334 Sgr (aka Sakurai's object) is the central star of an old PN that underwent a very late thermal pulse (VLTP) a few years before its discovery in 1996.

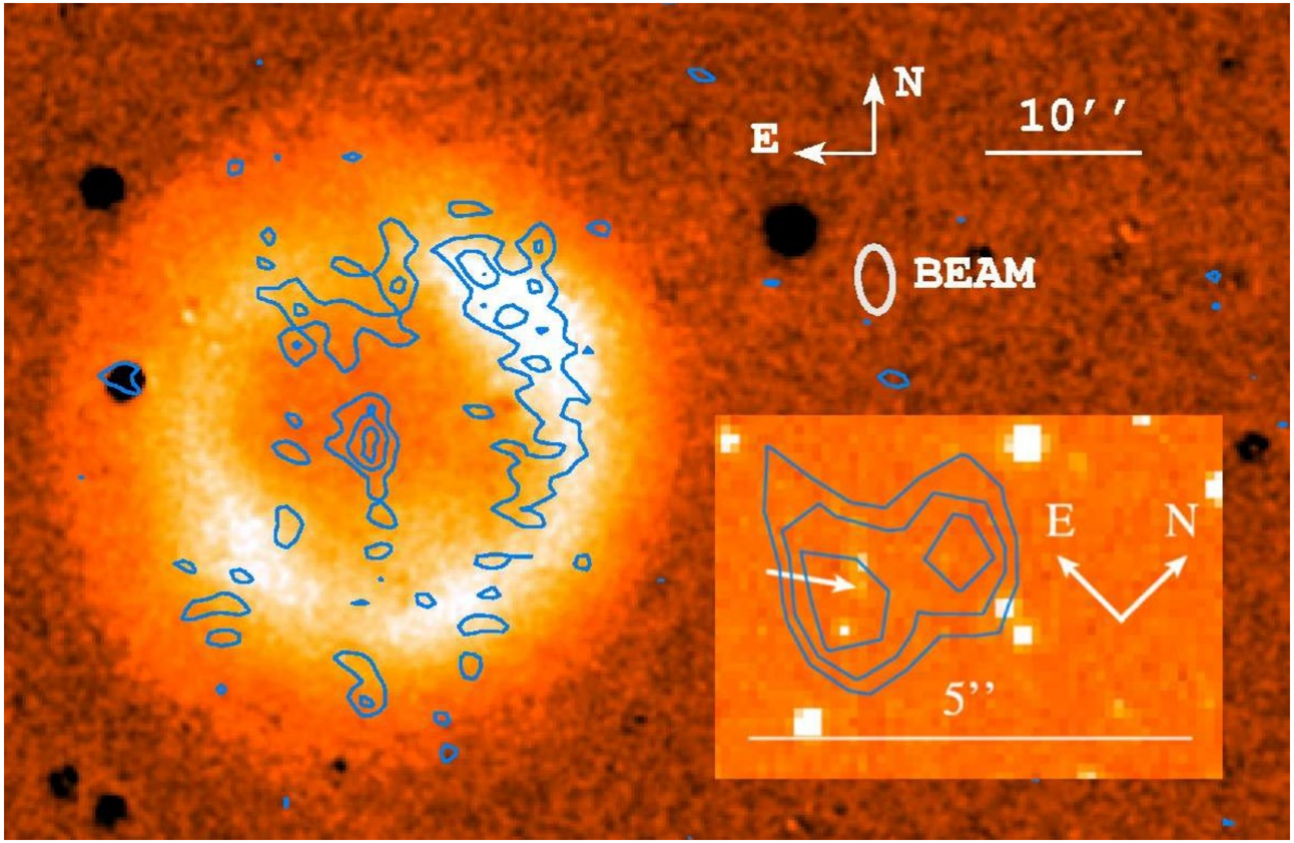
During the VLTP it ingested its remaining hydrogen-rich envelope into the helium-burning shell and ejected the processed material shortly afterwards to form a new, hydrogen-deficient nebula inside the old PN.

The star brightened considerably and become very cool (born-again AGB star) with a spectrum resembling a carbon-star.

After a few years, dust formation started in the new ejecta and the central star became highly obscured, similar to R CrB stars.

Emission lines were discovered. First He I 10830 in 1998 (Eyres+ 1999), later in 2001 also optical forbidden lines from neutral and singly ionized nitrogen, oxygen, and sulfur (Kerber+ 2002).

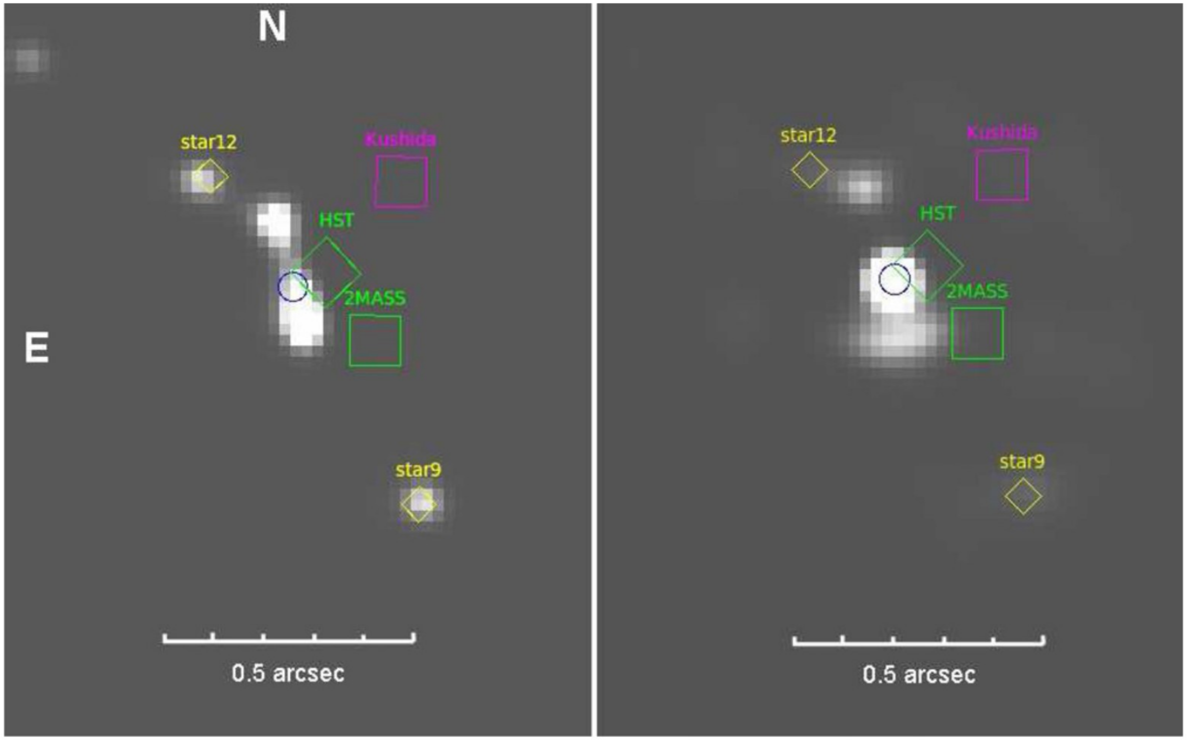
# Sakurai's Object (2)




[O III] image of the old PN with the radio contours from the 2004 VLA observations superimposed (Hajduk+ 2005).

Note that the old PN is round, while the new ejecta are bipolar!

# Ks imaging

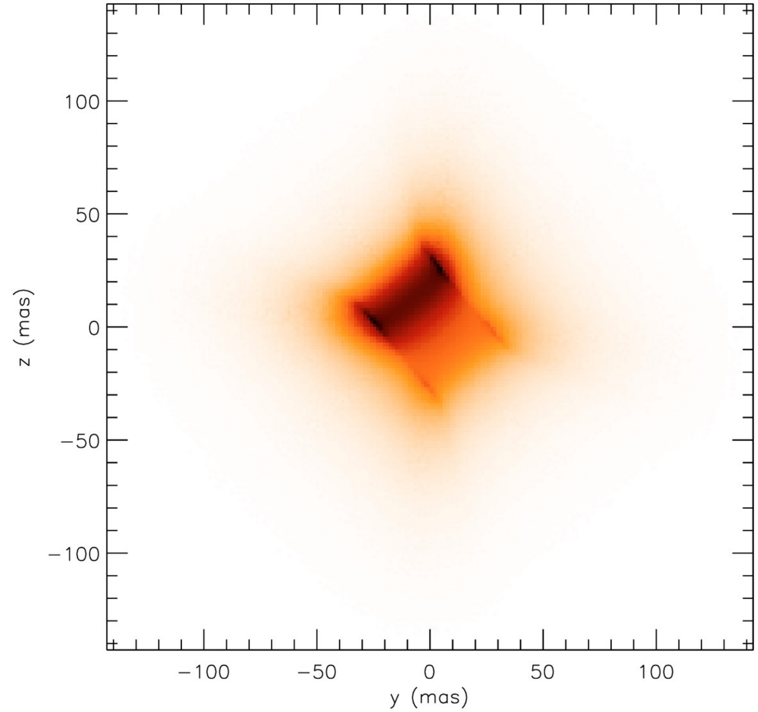



Deconvolved Ks images taken in 2010 (left) and 2013 (right) by Hinkle & Joyce (2014, hereafter HJ14).

The expansion of the bipolar structure can clearly be seen, the central star also seems to be brightening in the NIR.

Image credit: Hinkle & Joyce (2014).

# VLTI observations




Chesneau+ (2009) observed Sakurai's object using VLTI. They detected the presence of a thick and dense dust disk with dimensions 30x40 mas. This equates to 105x140 AU assuming D= 3.5 kpc. Shown above is a model at 13 μm.

Image credit: Chesneau+ (2009).

# Optical Observations

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We have been monitoring the evolution of the optical emission line spectrum since 2001. Its evolution is different from the radio flux.

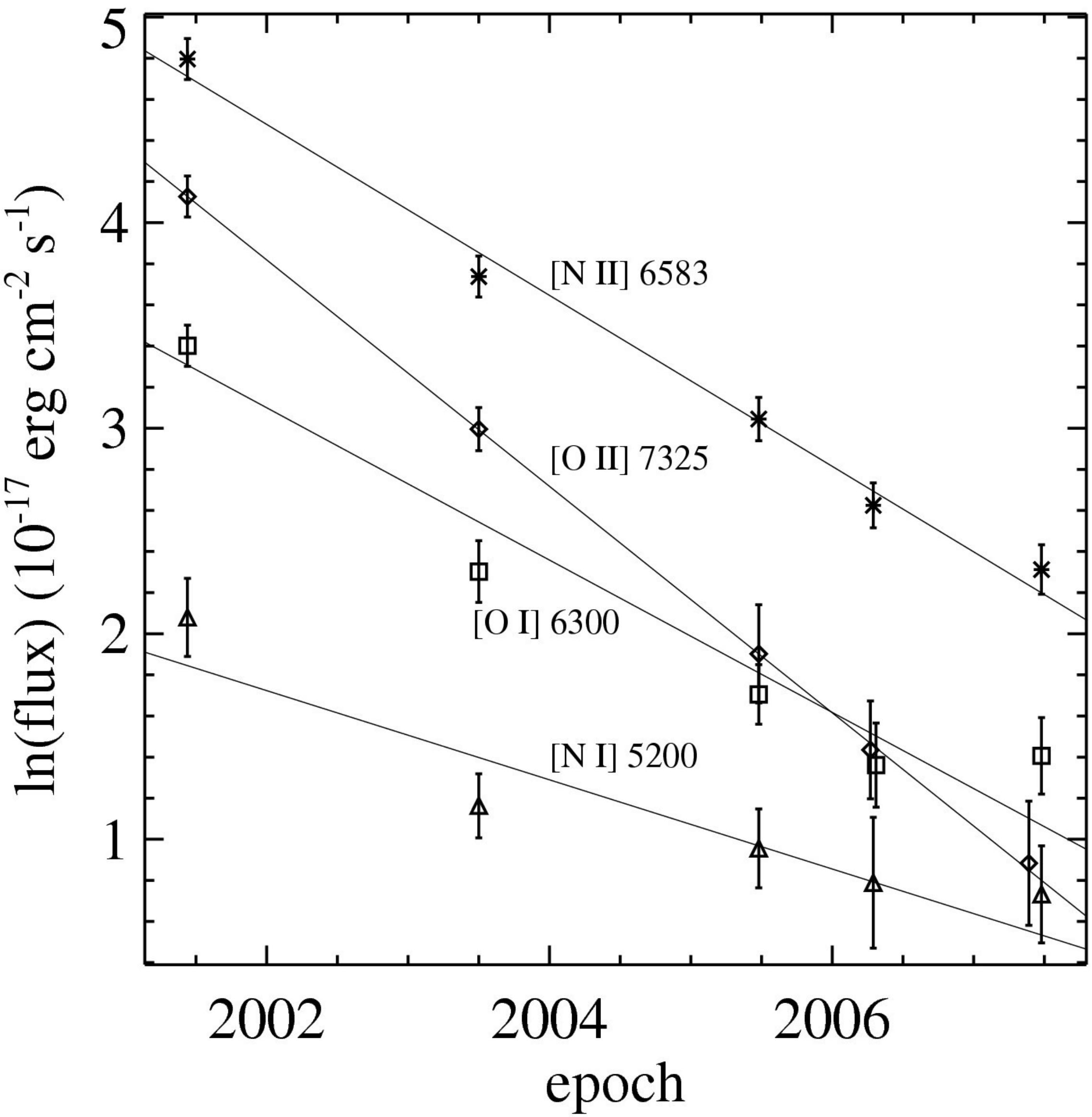
The optical lines initially showed an exponential decline in intensity, and also a decreasing level of excitation. This trend continued until 2007.

Between 2001 and 2007 the optical spectrum is consistent with a shock that occurred before 2001, and started cooling and recombining afterwards. The low $T_e$ derived from the [N II] lines in 2001 (3200 – 5500 K) and the [C I] lines in 2003  (2300 – 4300 K) is consistent with this.

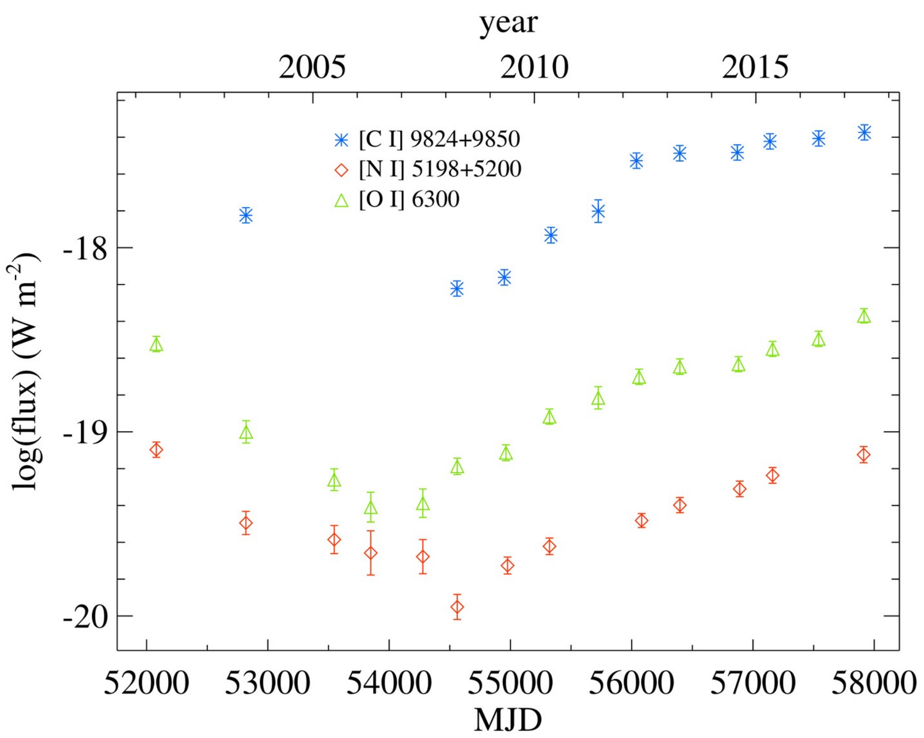
The earliest evidence for this shock is the detection of the He I 10830 recombination line in 1998 (Eyres+ 1999). This line was absent in 1997. The shock must have occurred around 1998 and must have stopped soon after, leaving cooling and recombining gas in its wake.

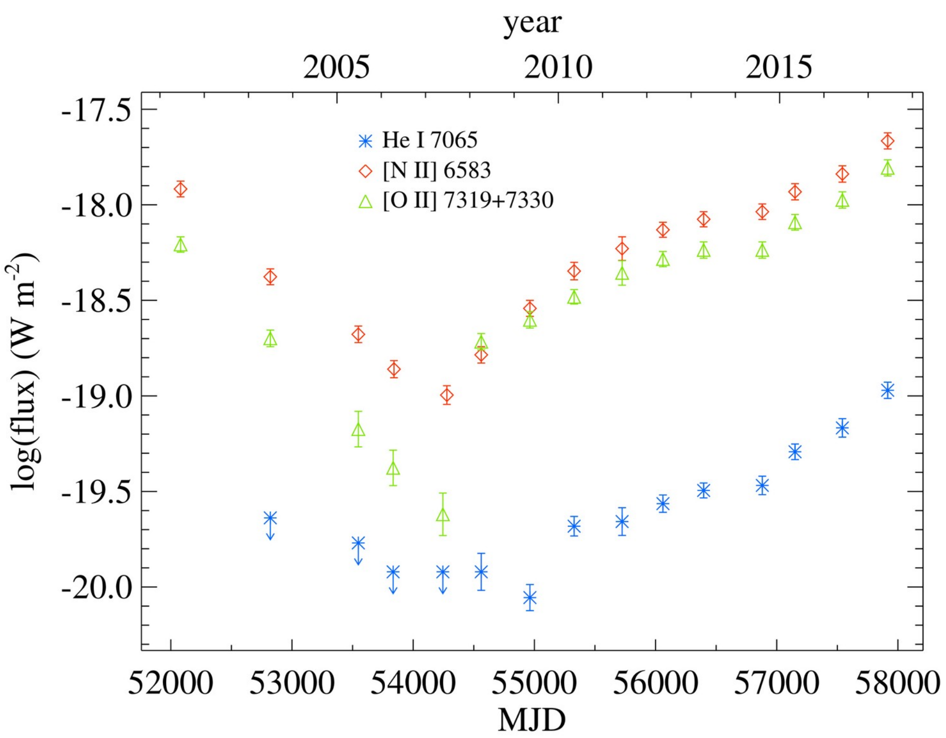
# van Hoof et al., 2007, A&A 471, L9

(figure has been extended with 2007 data)



# Line flux evolution up to 2017




Line fluxes have been monotonically increasing since 2008! This confirms the trend for [C I] 9823/50 seen by Hinkle & Joyce (2014).

Three exceptions: [O I] started increasing in 2007, [N I] dropped in 2008 and He I dropped in 2009. However, these lines are weak and some suffer from telluric contamination, so this may not be real.

There is a strong discontinuous jump in the [O II] flux in 2008!

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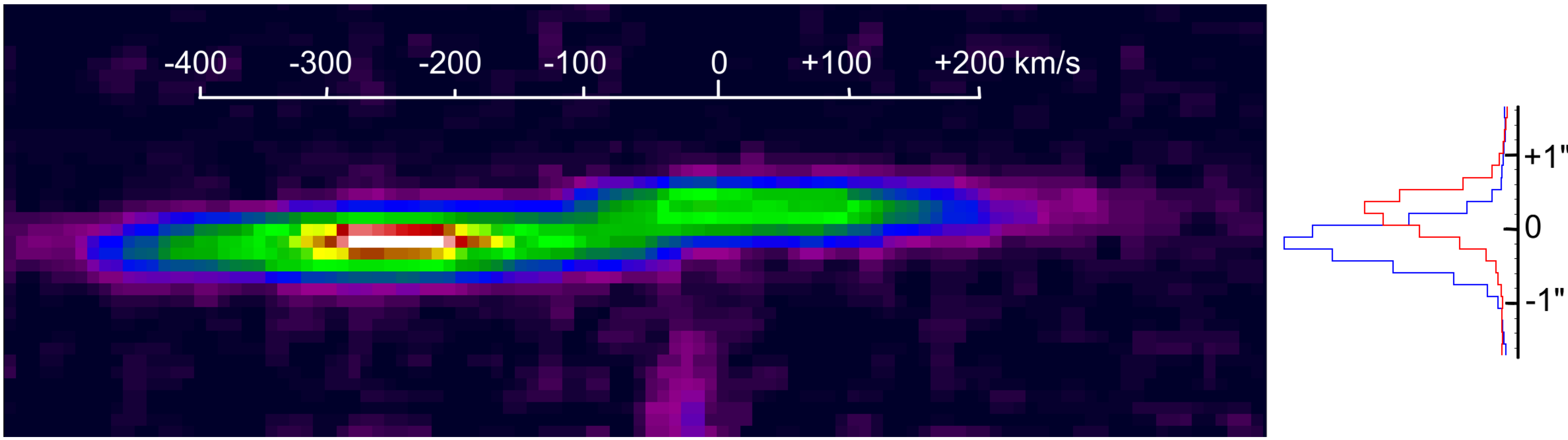
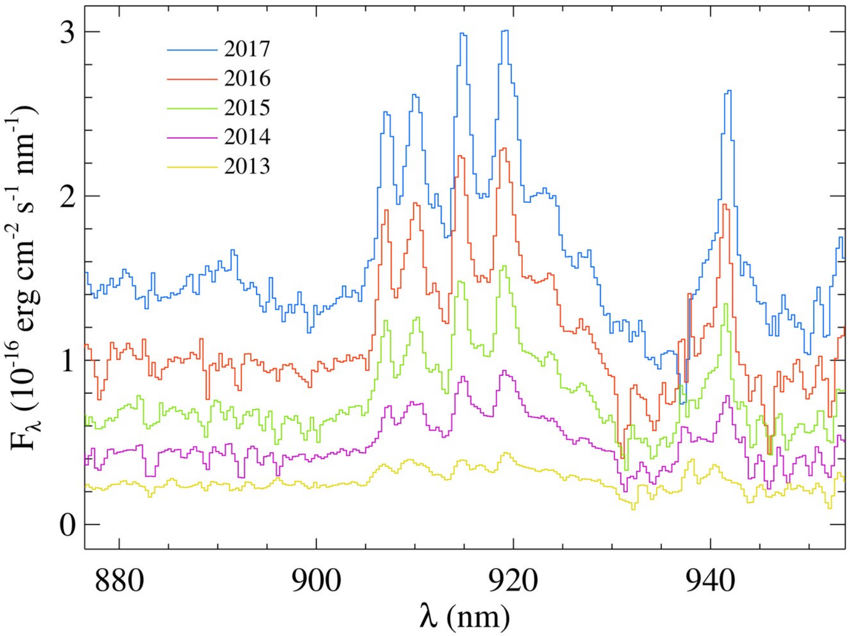
# The nebular lines




Looking at the XSHOOTER PV diagram of [N II] 6583 we can clearly see that the blue and red emission comes from different regions. The redshifted and blueshifted emission regions are +0.24” and -0.18” displaced wrt the continuum source. From this we conclude that the forbidden and recombination lines come from the bipolar lobes seen by HJ14.

# A new line complex

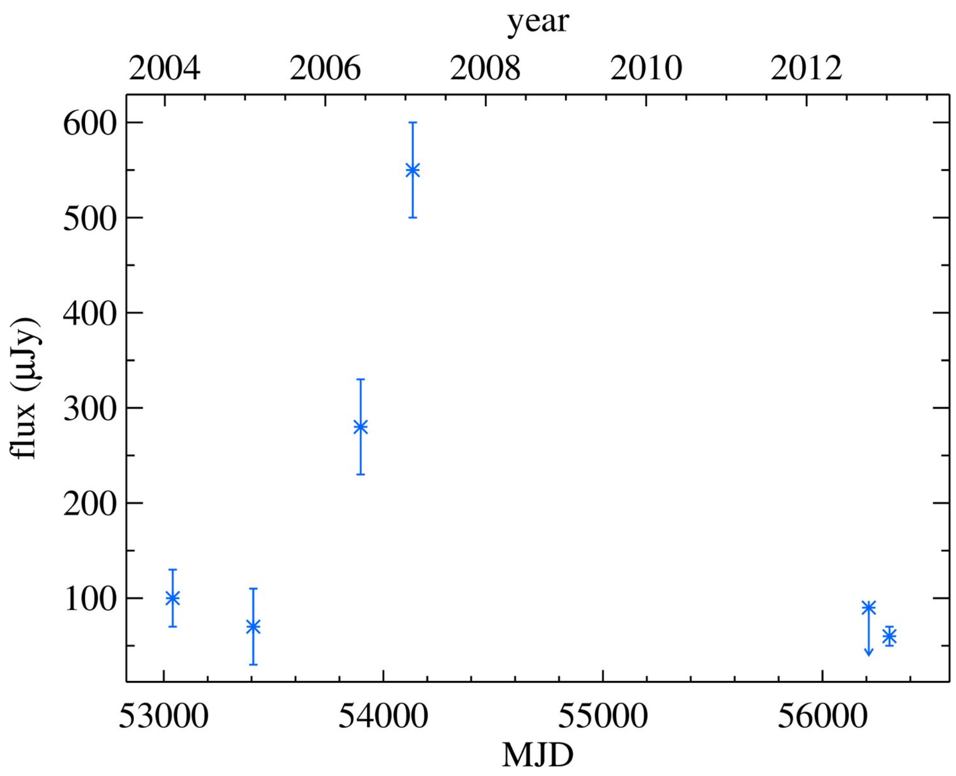



Since 2013 a complex of new lines has been emerging in the red. These are mainly carbon atomic lines.

The continuum is also rising, this was already reported by HJ14.

We interpret this as an emerging [WC9-10] spectrum. There are tentative signs that the central star is heating up!

# 8 GHz VLA Observations




Between 2004 and 2007 the radio flux was increasing.

At the time we interpreted that as evidence for the onset of photoionization.

The most recent data show that the source has faded. The only plausible explanation is that the flux rise was due to a shock.

# ALMA spectrum

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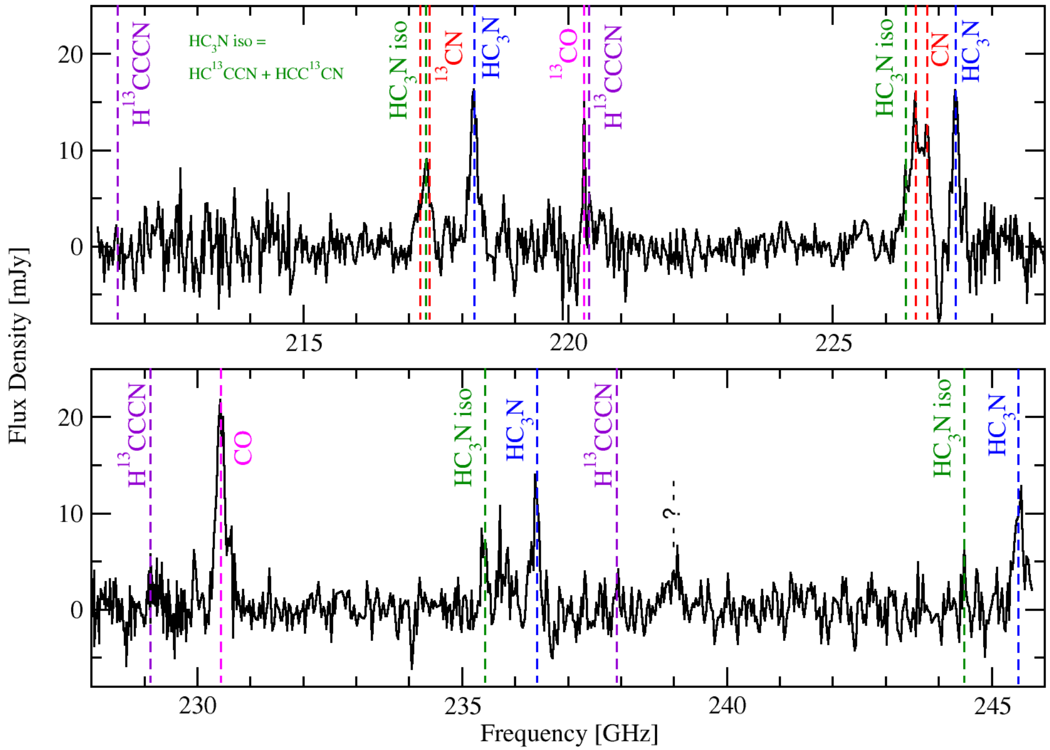
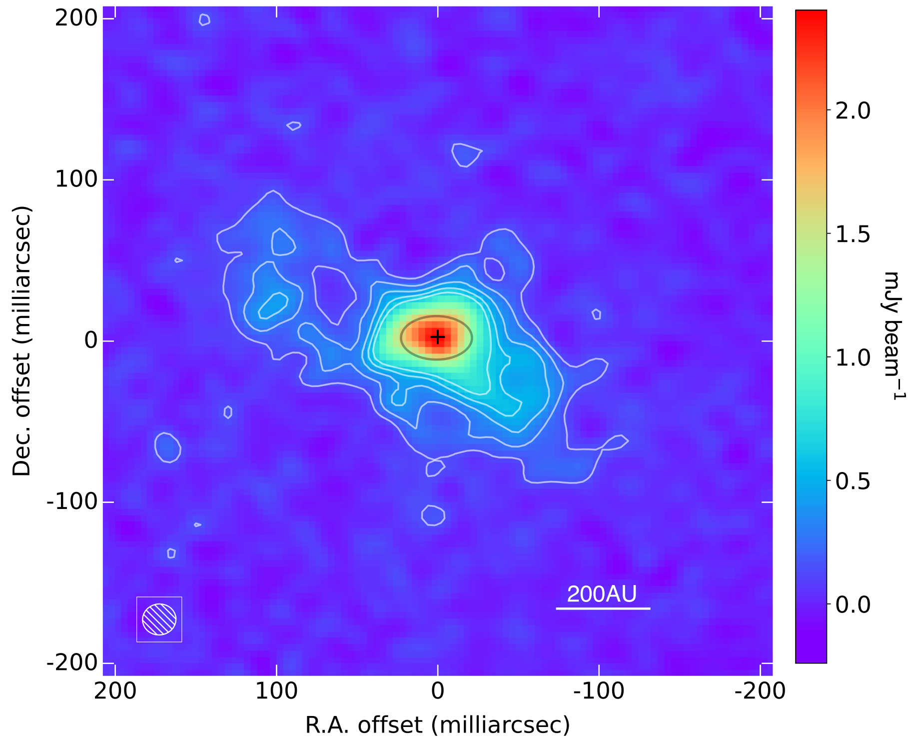



We detect lines of CO, $^{13}CO$, CN, likely $^{13}CN$ (blended), $HC_3N$, $HC_3N$ iso, and possibly $H^{13}CCCN$. The absorption on the blue side of the CN is real and associated with CN. There is also an unidentified line at 239 GHz.

# ALMA observations




We now have a much better dust continuum image obtained with ALMA. The beam is ~25 mas!

Image credit: Tafoya+ (2023).

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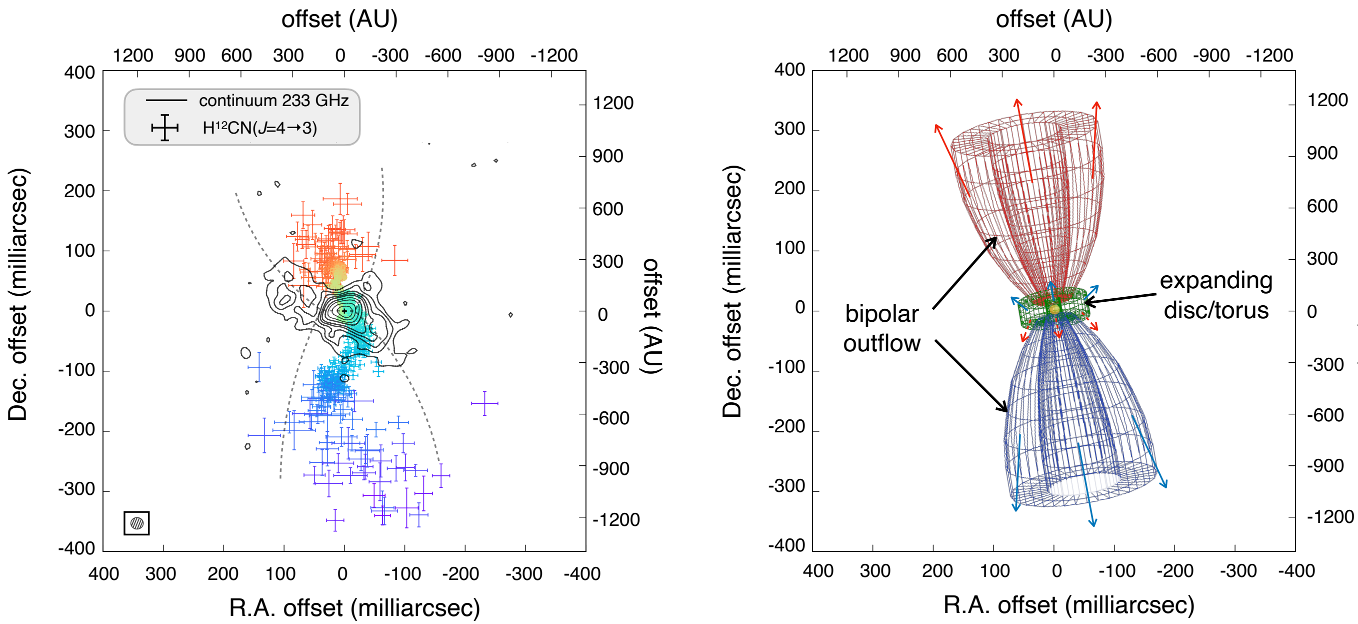
# ALMA observations




The left image shows the dust continuum image as countours, while the crosses show show the centroid of $H^{12}CN$ 4-3 emission in various velocity channels. The positions are consistent with a bipolar outflow.

Image credit: Tafoya+ (2023).

# Preliminary discussion

V4334 Sgr underwent a VLTP a few years before its discovery in 1996. It ejected a new, hydrogen-deficient nebula in the process.

The geometry of the source was clarified by Chesneau+ (2009) and later Tafoya+ (2024) who discovered the presence of a dense and thick dust disk. The disk must have formed in the VLTP event and was already in place in 1997. It may be a keplerian disk. All the dust is in the disk.

HJ14 discovered the presence of bipolar lobes in the Ks band. These appear to be expanding. The total extent of these lobes along the major axis is ~ 0.4 arcsec.

Emission lines were first discovered in 1998 (He I 10830) and 2001 (optical). The optical emission spectrum has been monitored since, showing an exponential decline in flux and the level of excitation also dropped. We see this as evidence for a brief shock that occurred around 1998.

# Preliminary discussion

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A plausible explanation is that this is the fastest material ejected in the VLTP hitting slower ejecta from the same event.

Between 2005 and 2007 the 8 GHz radio emission showed a marked increase. The radio flux has returned to pre-2005 levels since. We see no counterpart for this behavior in the optical data. A shock in an obscured region?

The optical line fluxes started to increase again since 2008. The sudden jump in the [O II] flux in 2008 could point to a second shock as the cause of the change in behavior. The shock breaks out of the obscured region?

Our working hypothesis is that the wind is now interacting with the lobes (bow shock). The nebular lines are now formed there. This is confirmed by Xshooter spectra.

# Preliminary discussion

The optical spectrum shows new lines which have been emerging since 2013. This is interpreted as an emerging [WC9-10] spectrum. There are tentative signs that reheating of the central star has started!

In ALMA spectra we detect the presence of CO, CN, $HC_3N$, HCN, HNC, $HCO^+$, and $^{13}C$ isotopologues.

The ALMA $H^{12}CN$ emission is resolved and matches the bipolar lobes.

We are witnessing the very early stages of the hydrodynamic shaping of a bipolar nebula!