 DOI: 10.18727/0722-6691/5283

ATOMIUM: ALMA Tracing the Origins of Molecules In dUst forming oxygen-rich M-type stars

Leen Decin[1]
Carl Gottlieb[2]
Anita Richards[3]
Alain Baudry[4]
Taissa Danilovich[1]
Emily Cannon[1]
Thomas Ceulemans[1]
Frederik De Ceuster[1]
Alex de Koter[5]
Ileyk El Mellah[6]
Sandra Etoka[7]
Elaine Gottlieb[8]
Malcolm Gray[9]
Fabrice Herpin[4]
Ward Homan[10]
Manali Jeste[11]
Pierre Kervella[12]
Silke Maes[1]
Jolien Malfait[1]
Louise Marinho[4]
Karl Menten[11]
Tom Millar[13]
Iain McDonald[14]
Miguel Montargès[12]
Holger Müller[15]
Bannawit Pimpanuwat[7]
John Plane[16]
Ragvendra Sahai[17]
Marie Van de Sande[16]
Sofia Wallström[1]
Ka Tat Wong[18]
on behalf of the ATOMIUM Consortium[1]

1 KU Leuven, Belgium
2 Center for Astrophysics | Harvard & Smithsonian, Cambridge, USA
3 Jodrell Bank Centre for Astrophysics, Manchester, UK
4 Bordeaux University, France
5 University of Amsterdam, the Netherlands
6 Grenoble Alpes University, Grenoble, France
7 University of Manchester, UK
8 Harvard University, USA
9 NARIT, Thailand
10 ULB, Brussels, Belgium
11 Max Planck Institute for Radio Astronomy, Bonn, Germany
12 LESIA, Meudon, France
13 Queen's University Belfast, UK
14 Open University, UK
15 University of Cologne, Germany
16 University of Leeds, UK
17 Jet Propulsion Laboratory, USA
18 IRAM, Grenoble, France

The goals of the Atacama Large Millimeter/submillimeter Array (ALMA) Large Programme ATOMIUM are to obtain a quantitative understanding of the chemical and physical processes that govern the phase transition from small gaseous molecules to dust grains in the inner wind of oxygen-rich evolved stars; and to study the interplay between dynamical and chemical phenomena in the outflow of 17 asymptotic giant branch (AGB) and red supergiant (RSG) stars which span a range in (circum) stellar and wind properties — such as mass-loss rate, pulsation behaviour, and spatial structure of the wind-dominated ambient medium. The observations were made with three configurations of the ALMA array that encompass a range in angular resolution of approximately 0.02–1 arcseconds. They consist of 27-GHz-wide homogeneous spectral-line and continuum surveys in the 214–270 GHz range in each source in the sample, and provide an unambiguous comparison among sources. Equipped with these tools, we then show how the stellar winds of all the ATOMIUM sources exhibit distinct non-spherical geometries that can be explained by binary interaction and — depending on the parameters of the binary system — can produce a wide variety of morphologies as illustrated by the example of the AGB star π^1 Gru. In parallel with ATOMIUM, contemporaneous observations of all but three of the 17 sources were made in the visible with the SPHERE/ZIMPOL instrument at ESO's Very Large Telescope (VLT). The VLT/SPHERE observations provided direct images of the dust at a spatial resolution comparable to that obtained with ALMA. Novel hydrodynamical simulations of binary systems were done so as to further the interpretation of the near simultaneous observations of the gas and dust. We also present a brief overview of the 24 molecules that were identified in the survey, followed by a discussion of how the molecules inform us about the inner wind and the (super)giant outflow, and of some future possible observations with ALMA, ESO instruments, and the JWST.

ATOMIUM motivation and survey strategy

Scientific goals

Over 200 molecules and 15 dust species have been detected in the interstellar medium, stellar winds, exoplanets, supernovae, active galactic nuclei, etc. One of the most fundamental questions in astrophysics deals with the phase transition from simple molecules to larger gas-phase clusters and eventually dust grains. The outflows of evolved stars are the best laboratories in which to answer this pivotal question, given their rich chemistry and relatively simple dynamical structure. With the Atacama Large Millimeter/submillimeter Array (ALMA) Large Programme ALMA Tracing the Origins of Molecules In dUst forming oxygen-rich M-type stars (ATOMIUM[1]) we aim to establish the dominant physical and chemical processes in the winds of oxygen-rich evolved stars over a range of stellar masses, pulsation behaviours, mass-loss rates, and evolutionary phases. The goals are to unravel the phase transition from gas-phase to dust species, pinpoint the chemical pathways, map the morphological structure, and study the interplay between dynamical and chemical phenomena (Gottlieb et al., 2022). To achieve these goals, an ALMA Large Programme was submitted and accepted in Cycle 6 for a total observing time of 113.2 hours. This is still the only accepted Large Programme in the field of Stellar Evolution and the Sun.

ATOMIUM sample and observing strategy

The ATOMIUM sample consists of 17 oxygen-rich evolved stars, which span a range in (circum)stellar and wind properties, such as: mass-loss rate, pulsation behaviour, and asymptotic giant branch (AGB) versus red supergiant (RSG) stars. The sample consists of 14 AGB stars that are relatively close to Earth and three RSG stars. The selection criteria did not take into account prior evidence for possible binary companions.

A primary requirement for the ATOMIUM project was for homogeneous observations across the sample that would allow unambiguous comparison among sources. The most efficient way to achieve the science goals with ALMA was to target specific spectral frequency regions in Band 6, where we know which molecules to monitor to answer the questions about the dynamical behaviour and chemical processes in the winds of evolved stars.

To spatially resolve the dust condensation region ($r \leq 10$–$30\ R_\star$, where $R_\star$ is the stellar radius), an angular resolution (AR) of 0.025–0.050 arcseconds is needed for our targets, which all have large optical stellar angular diameters of between 0.004 and 0.020 arcseconds. The highest spatial resolution for each target was about 0.02 arcseconds. To attain the full line strength of the molecular lines, we complemented these observations with data from a medium-resolution (AR ~ 0.20 arcseconds) configuration and a low-resolution (AR ~ 1 arcsecond) configuration. In aggregate we resolve the emission on scales from the stellar radius to thousands of stellar radii.

ATOMIUM data reduction and data products

The ATOMIUM enhanced data products are being prepared for the ALMA archive. The starting point is the standard ALMA pipeline (or occasionally manual Quality Assurance 2) products. We combined the data for each star across the observed frequency range, as described by Gottlieb et al. (2022), and provide a description document and scripts for each star. These cover self-calibration (using stellar continuum), imaging and extraction of spectra. Three fully calibrated measurement sets (MS) are provided for each star, for each of the three array configurations: a continuum MS (120 channels per 1.875 GHz), a line MS (1920 channels per 1.875 GHz with about 1.2 km s^{-1} resolution) and a continuum-subtracted line MS. We also combined the data for each star for all configurations, giving one MS for the calibrated continuum visibility data (after flagging line channels) and another for the continuum-subtracted line data. The MS are a suitable starting point for re-imaging, for example to select a particular line and use different averaging or weighting to improve the sensitivity or to change the angular or spectral resolution.

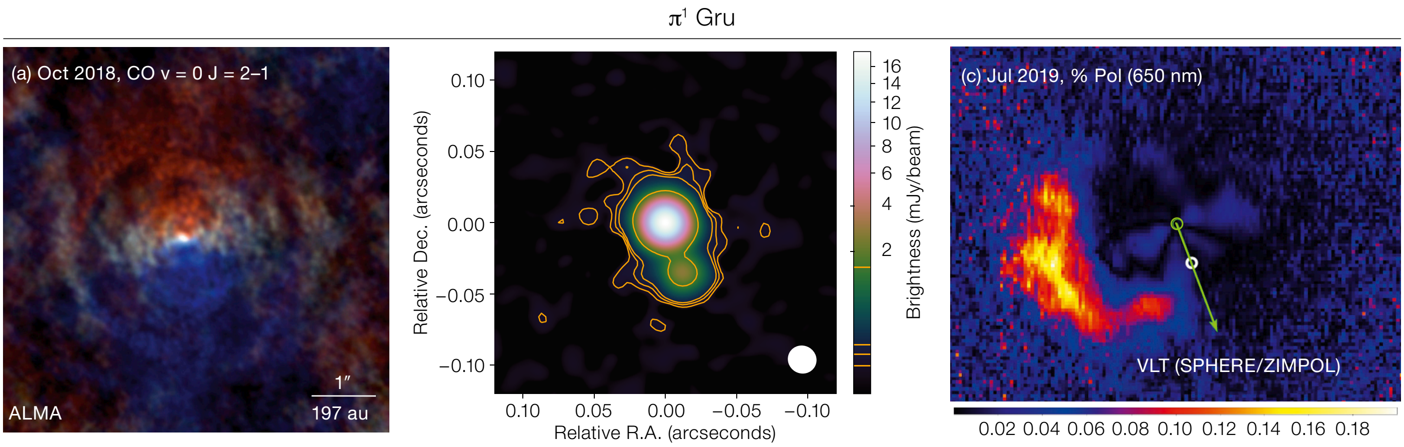
Ready-made spectral cube images are available for each spectral window and array configuration (low, medium and high spatial resolution). They provide an angular resolution of approximately 0.8, 0.2 and 0.02 arcseconds, and sensitivities of a few mJy per channel. A fourth set of cubes was made from the combined data. All cubes were made using consistent parameters, but users can also take the calibrated visibility data to make images at customised resolutions to favour lines or features of interest. We made continuum-only images for each of the three configurations and the combined data, which is dominated by stellar emission (resolved at the higher resolutions) and sometimes also reveals hot dust. For the exact frequencies covered, angular resolutions, sensitivities and other details, see the appendices of Gottlieb et al. (2022). The final set of archived products are spectra extracted from each cube, for a range of extraction aperture radii (depending on configuration) from 0.02 to 5.4 arcseconds.

Hydrodynamical behaviour of stellar winds

Companions shaping the winds of AGB and RSG stars

The new revolution in observational techniques accommodates high-spatial-resolution (reconstructed) images and provides direct evidence that the circumstellar envelopes created by the stellar winds harbour small- and large-scale inhomogeneities. Flow instabilities induced by convection result in the formation of granulation cells on the surfaces of the giant stars, and of small-scale density structures in the stellar wind, with sizes of about 1–50 au. A remarkable new thesis delivered by the ALMA telescopes is that planetary or stellar companions impact the wind morphology of almost all AGB and RSG stars with a mass-loss rate

Figure 1. ALMA and VLT SPHERE/ZIMPOL observations towards π^1 Gru. (a) ALMA ATOMIUM CO v = 0 J = 2–1 emission map of the wind structure of π^1 Gru; angular resolution of ~0.3 arcseconds. (b) ALMA 1.2-mm continuum emission towards π^1 Gru at epoch July 2019; angular resolution of 0.019 arcseconds. Contours (in orange) are plotted at 3, 6, 10 and 100 times the continuum noise value. The secondary peak (white circle) south-west of the central star is likely due to a close companion. (c) SPHERE/ZIMPOL percentage polarisation at 644.9 nm towards π^1 Gru at epoch July 2019; angular resolution of 0.024 arcseconds.



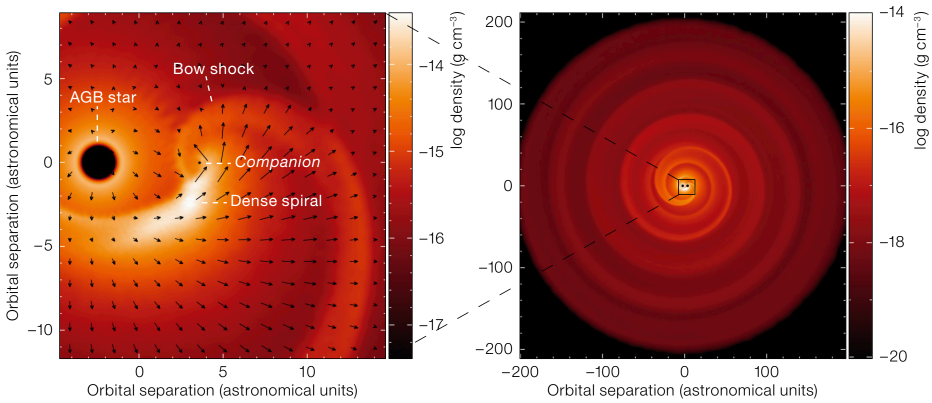


Figure 2. Density distribution in a slice through the orbital plane for the binary configuration described in the text, with the centre of mass located at the (0,0) position. The left panel shows the inner density structures formed around the primary and the companion; the right panel displays the global orbital plane morphology (Malfait et al., 2021).

$\dot{M} \geq 10^{-7} M_\odot$ yr^{-1}. In a fraction of stars, the companion induces a change in the wind's expansion velocity and mass-loss rate.

In particular, we have shown that the winds of all sources observed within the ATOMIUM programme exhibit distinct non-spherical geometries with extents greater than about 100 au, and morphologies which are similar to those of planetary nebulae (Decin et al., 2020). These morphological characteristics can be explained by binary interaction. Depending on the parameters of the binary system, a wide variety of morphologies can arise, including spiral structures, a circumbinary disc, an accretion disc around the companion, a bipolar outflow, an equatorial density enhancement. An example of such a binary-induced morphology is shown in the left panel of Figure 1, which displays the ATOMIUM CO $v = 0$ $J = 2$-1 emission map for the AGB star π^1 Gru (Decin et al., 2020). Emission that is redshifted with respect to the local standard of rest velocity is shown in red, blueshifted emission is in blue, and the gas at the rest velocity is in white. The scale bar has an angular extent of 1 arcsecond. Prior to the ATOMIUM data, it was known that π^1 Gru has a companion residing at about 440 au. However, that companion is too far away to create the structures revealed by the observations with ALMA. Remarkably, the ALMA continuum data (middle panel of Figure 1) show two maxima separated by about 6 au. An investigation of the ALMA continuum data — and the maps of the CO, SiO, and HCN emission — reveals that the second maximum could be a companion of mass $\lesssim 1.1\ M_\odot$ that creates an inclined, radially outflowing equatorial density enhancement and a spiral structure (Homan et al., 2020).

VLT SPHERE/ZIMPOL observations

The ALMA ATOMIUM data only provide minimal inference of the geometry of the dust distribution around the AGB stars. For that reason we have acquired contemporaneous observations of the ATOMIUM sources using the SPHERE/ZIMPOL instrument at ESO's Very Large Telescope (VLT). The ZIMPOL instrument provides polarimetric images in the visible at an angular resolution that is comparable to the highest spatial resolution in the ALMA data (right panel of Figure 1). The observed polarized light comes from the scattering by the dust grains and originates primarily from regions near the plane of the sky going through the centre of the target. Green and white circles mark the inferred locations of π^1 Gru and the close companion. The companion is not directly seen in the ZIMPOL images, but is inferred to lie at the head of the spiral structure created by the gravitational interaction between the AGB star (and its wind) and the companion (Montargès et al., 2022).

Hydrodynamical simulations

To further the interpretation of the ALMA and SPHERE observations, we have performed novel hydrodynamical simulations for binary systems in which the primary is a mass-losing AGB star (El Mellah et al., 2020; Maes et al., 2021; Malfait et al., 2021). Figure 2 shows the density distribution for a simulation in which the primary star is an AGB star of mass 1.5 $M_\odot$ that launches a stellar wind with initial velocity of 10 km s^{-1} and mass-loss rate of $1 \times 10^{-6}\ M_\odot$ yr^{-1}. A companion star of mass 1 $M_\odot$ orbits the AGB star in a circular orbit with orbital separation of 6 au. The wind–companion interaction creates a dense spiral flow behind the companion and a second spiral emerging from a bow shock in front of the moving companion (left panel of Figure 2). This stable bow shock shapes the global morphology into an approximate Archimedes spiral structure (right panel of Figure 2).

Chemical processes in stellar winds

Twenty-four molecules were identified in the ATOMIUM sample by means of their rotational spectra (CO, SiO, HCN, SO, SO_2, CS, SiS, H_2S, OH, H_2O, TiO, TiO_2, AlO, AlOH, PO, SiC, SiC_2, SiN, CN, HCCCN, AlCl, AlF, NaCl, KCl). The first three molecules were observed in all the stars in our sample, but some of the others were observed primarily in the denser regions of the stellar wind in only some of the stars.

Shown in Figure 3 is a small portion of the spectrum observed in the oxygen-rich Mira variable R Hya, accompanied by high-resolution maps of the integrated intensity. The spectrum contains several species believed to be precursors of the dust, including TiO in the ground and first excited vibrational level (1451 K above ground), three transitions of vibrationally excited SiO (between 1790 and 5266 K above ground), and (see Figure 4) vibrationally excited H_2O and highly excited transitions of OH (5480 K above ground). Measurements such as these provide a direct means to examine the properties of the inner wind, and serve as benchmarks for the chemical kinetic calculations.

Because our observations allow us to examine a wide variety of chemical species found throughout the stellar

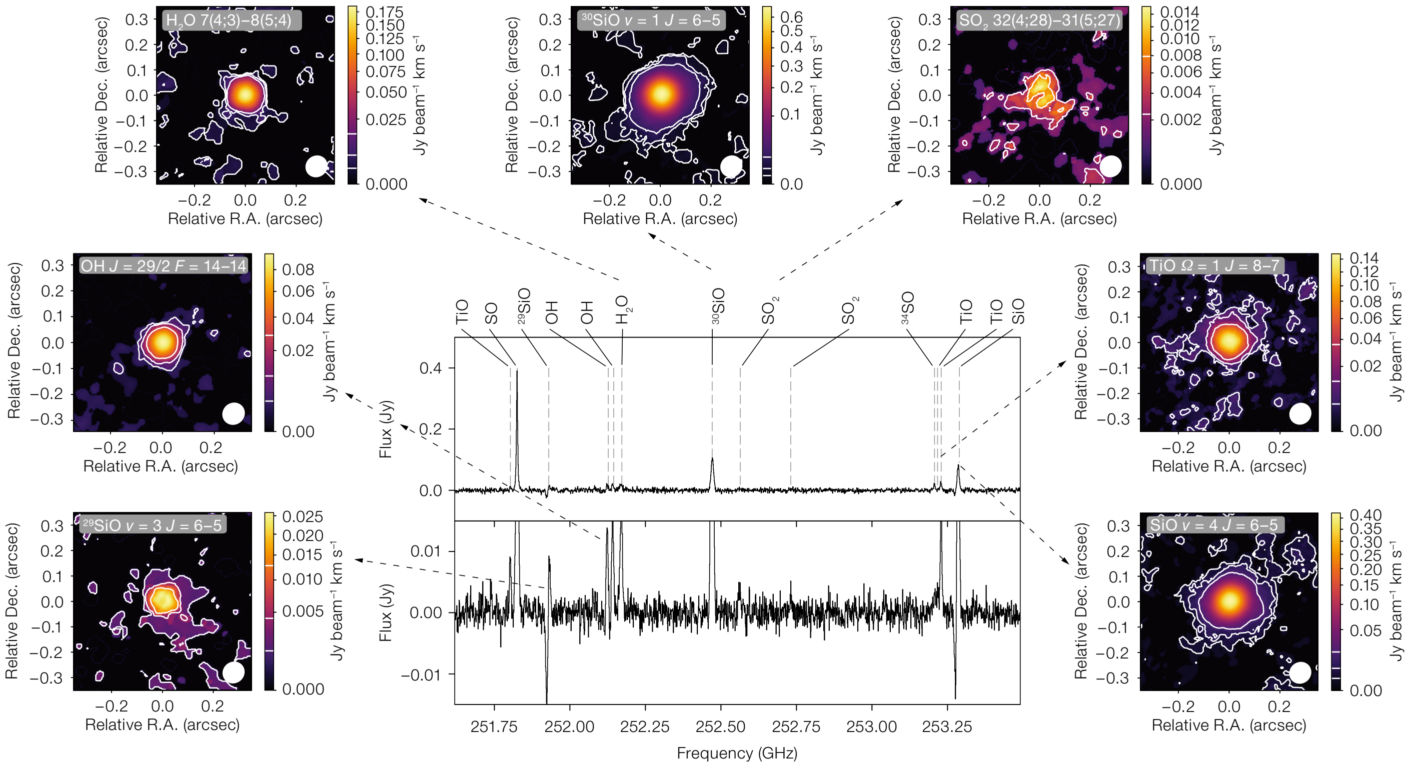


Figure 3. R Hya. Upper panel: Spectrum extracted from the medium-spatial-resolution configuration for an aperture of 0.2 arcseconds. Lower panel: Spectrum extracted from the high-spatial-resolution configuration for an aperture of 0.02 arcseconds. Images show the integrated intensity maps for some molecular lines computed from the combined dataset. White contours are at 3,10 and 30 times the noise in the integrated intensity maps. The ellipse in the bottom right corner of each image represents the beam of the combined dataset.

wind, we are able to refine the chemical kinetics codes used to predict the molecular abundances. For example, we established that the wind density plays a key role in wind chemistry, on the basis of an analysis of our recent observations of AlCl and AlF towards W Aql in close collaboration with physical chemists (Danilovich et al., 2021).

Overall, the ATOMIUM observations allow us to investigate several major astrochemical topics. These include: (i) molecules in the inner few stellar radii that are expected to be intimately involved in the formation of the initial dust grains; (ii) the interpretation of the spectra of 10 transitions in H_2O (Baudry et al., 2022, and see Figure 4) and vibrationally excited SiO which are both sensitive tracers of clumps, shocks, and complex gas motion; (iii) detailed analyses of the spectra and maps of CO and SiO (in maser and non-maser emission) that reveal the morphology and the wind dynamics in the inner wind and throughout the outflow in all the stars — supplemented with the maps and spectra of other molecules, such as HCN (Homan et al., 2020) and SO_2 (see, for example, Figure 4 of Gottlieb et al., 2022); (iv) constraining the reaction rates used in chemical kinetic codes that aim to reproduce the molecular abundances derived from the ATOMIUM observations in each stellar type, and the quantity of the dust inferred from the VLT/SPHERE-ZIMPOL observations of Montargès et al. (2022); and (v) looking for the possible influence of companions on the chemistry in the inner wind (Van de Sande & Millar, 2022).

Another important area involving the gas-dust interactions which has begun to be addressed by recent chemical kinetic codes (Van de Sande, Walsh & Danilovich, 2020), concerns the deposition of the more abundant molecules on the grains in the AGB outflows. However much remains to be done by observers, working in close collaboration with chemists. The crucial observational quantities needed are reliable estimates of the fraction by which the abundances of key molecules (for example, SiO, SiS, H_2O, HCN, CS, and SO_2) are depleted in the outflow versus the distance from the star.

Other topics addressed by ATOMIUM

Building on the core goals of the ALMA ATOMIUM Large Programme, the ATOMIUM team[2] has grown during the past few years and currently includes 48 researchers with complementary expertise. ATOMIUM team members have addressed or are currently addressing: (i) the small- and large-scale morphologies of AGB and RSG stellar winds; (ii) the cause of inhomogeneous mass-loss events in RSGs; (iii) the distribution of molecules in the winds of AGB and RSG stars; (iv) quantum-chemical calculations of the cluster geometries and reaction rates of dust-forming gaseous precursors; (v) the molecular assignment of still unidentified spectral features; (vi) maser emission, in particular SiO masers to

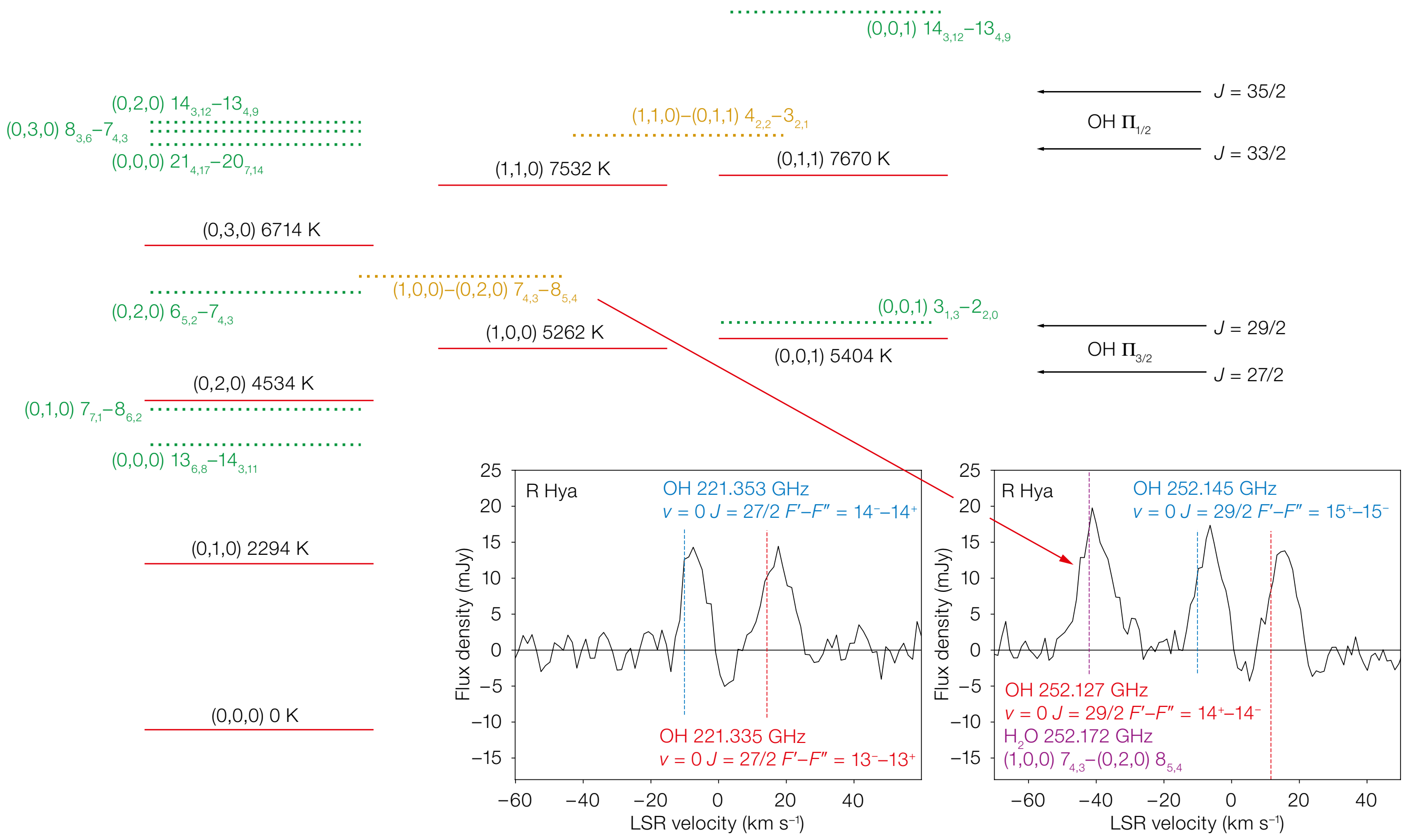


Figure 4. The lowest eight vibrational states of H_2O are displayed as horizontal red lines with their quantum numbers (v_1, v_2, v_3) and associated energy in kelvins. The horizontal dotted green and orange lines are the ten rotational transitions observed in various vibrational states of the ATOMIUM survey. The four horizontal black arrows to the right show the energy levels of the OH Λ-doublet transitions in the four rotational states observed in our survey. The two lower right panels present the J = 27/2 and 29/2 Λ-doublet spectra observed in R Hya, simultaneously with one rovibrational transition of H_2O next to the J = 29/2 OH spectrum (rightmost panel). The observed frequency is converted to velocity in the Local Standard of Rest frame by using the rest frequencies shown above and below the spectra corrected for the systemic star velocity (Baudry et al., 2022).

constrain excitation models as well as the kinematics close to the star, whilst conditions out to the wind acceleration zone are probed by water masers; (vii) the construction of chemical networks of relevance for AGB and RSG winds, and the study of their chemical predictions including that of dust nucleation; (viii) morphological studies of binary systems based on state-of-the-art hydrodynamical (HD) numerical codes; (ix) coupling of the HD codes to fast chemical network emulators and radiative transfer calculations; and (x) laboratory studies aimed at understanding dust nucleation/sublimation, and molecular collisions between water and H_2 or He, etc.

Next (observational) steps

The ATOMIUM Large Programme was designed to study oxygen-rich evolved stars via spatially resolved maps of molecular line and dust emission. From our first paper (Decin et al., 2020) it is already clear that binarity is a key parameter for understanding the chemical and morphological complexities of an evolved star's winds, although that parameter was not included in the original sample selection criteria. Aiming to understand the impact of (hidden) planetary and stellar companions, the ATOMIUM source sample should be extended to include carbon-rich evolved stars, oxygen-rich evolved stars for which we know the initial mass, and a larger variety of red supergiants. In addition, there is the need for complementary ALMA data targeted, on one hand at the same frequency bands to derive the time variability of morphological and chemical emission patterns, and on the other hand at another frequency band (i) to study the molecules via various rotational transitions spanning a range of energies, and (ii) to constrain the spectral index of the continuum in order to determine the nature of the proposed companions. On top of that, other ESO instruments such as GRAVITY and MATISSE of the Very Large Telescope Interferometer can provide crucial information about the dust location, and offer the potential for detecting the proposed companions. The ATOMIUM results will also stimulate many new radio observations of evolved stars with other interferometers or single antennas in the millimetre- and centimetre-wave domains (NOEMA, SMA, e-Merlin and large sensitive single antennas), for example to monitor masers using the Atacama Pathfinder EXperiment (APEX) (SiO) and Medicina, Pushchino and e-Merlin (22 GHz water). And although the ATOMIUM sources are bright in the infrared, the chronographic modes or off-source pointing offered by the NIRCAM and MIRI instruments on board the JWST should allow us to get high sensitivity infrared images of the stellar winds, similar to the recent Early Release Science data of the colliding wind Wolf-Rayet binary WR140 (Lau et al., 2022).

Acknowledgements

ALMA data: ADS/JAO.ALMA#2018.1.00659.L, 'ATOMIUM: ALMA tracing the origins of molecules forming dust in oxygen-rich M-type stars'. ALMA is a partnership of ESO (representing its Member States), NSF (USA) and NINS (Japan), together with NRC (Canada) and NSC and ASIAA (Taiwan), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO and NAOJ. SPHERE/ZIMPOL data: ESO programme 0103.D-0772(A).

References

Baudry, A. et al. 2022, submitted to A&A
Danilovich, T. et al. 2021, A&A, 655, A80
Decin, L. et al. 2020, Science, 369, 1497
El Mellah, I. 2020, A&A, 637, A91
Gottlieb, C. A. et al. 2022, A&A, 660, A94
Homan, W. et al. 2020, A&A, 644, A61
Lau, R. M. et al. 2022, Nature Astronomy, in press
Maes, S. et al. 2021, A&A, 653, A25
Malfait, J. et al. 2021, A&A, 652, A51
Montargès, M. et al. 2022, submitted to A&A
Van de Sande, M., Walsh, C. & Danilovich, T. 2020, MNRAS, 495, 1650
Van de Sande, M. & Millar, T. 2022, MNRAS, 510, 1204

Links

[1] The ATOMIUM project website: https://fys.kuleuven.be/ster/research-projects/aerosol/atomium
[2] ATOMIUM consortium members list: https://fys.kuleuven.be/ster/research-projects/aerosol/atomium/consortium-members

ALMA (ESO/NAOJ/NRAO)

A number of ALMA's 66 high-precision radio antennas can be seen in this image, connected by cleared pathways. The array spends its time observing the cool Universe and its phenomena — star formation, molecular clouds, stellar evolution, and the early Universe.