Untangling Gas, Dust, and Ice Astrochemistry with JWST Ice-Mapping

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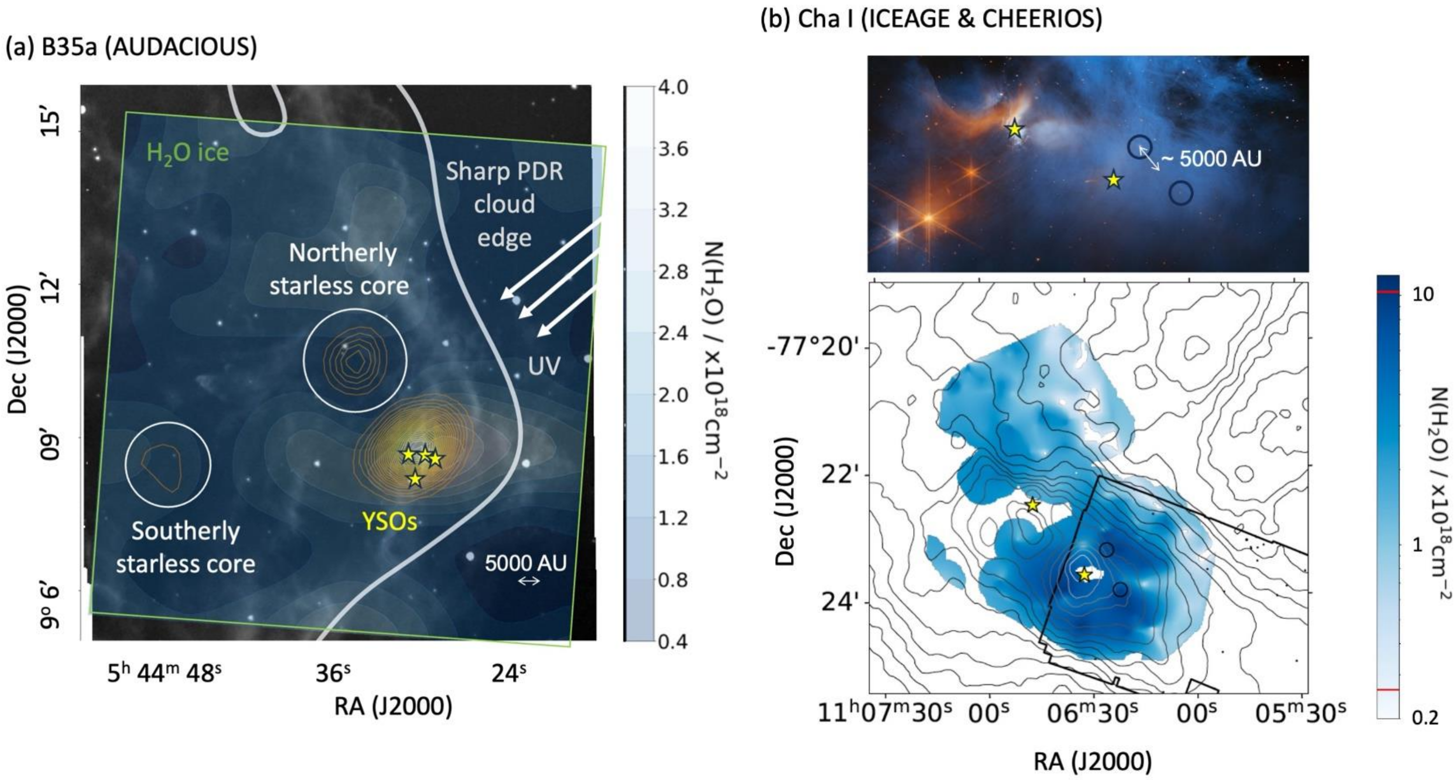

Figure: This figure shows the B35a molecular cloud (part(a)) as observed with Spitzer (grey scale) IRAM (yellow contours) and AKARI (blue shading), showing how different chemistries of a star-forming cloud, from PAH emission, cold N_2H^+ gas emission and water ice absorption, spatially overlap and help us understand the interstellar chemistry. (Part (b)) shows the Cha I molecular cloud as observed with JWST, and the much more detailed water ice map produced at the OU from these JWST data. The aim of this PhD is to generate ice-maps like that in part (b) for many other new and archival JWST datasets, and then utilise machine-learning / big-data techniques to disentangle the astrochemistry of these environments.

Project highlights:

- JWST is revolutionising Astrochemistry of star-forming regions. When JWST data are coupled with gas-phase observations on the same spatial scales, (e.g. ALMA NOEMA JCMT IRAM) or archival observations of dust and astrophysics in the same regions (e.g. Gaia Eucld Herschel Spitzer) we have the potential to disentangle the astrochemistry of these environments, and understand the chemical influences on star and planet formation
- However the problem is twofold – first we have to make equisite JWST observations, reduce the data and produce high quality ice-maps; second we have to interpret that data. This involes complex processing of high volumes of data concurrently where

there are lots of possible solutions, some more feasible than others – this is the kind of big data challenge that lends itself to moden computing analysis in the machine learning / AI sphere.

- There are three key outcomes to this PhD
    - Generate new JWST ice maps of star-forming regions
    - Interpret the astrochemistry of these regions by combining ice mapping and archival (or new) gas-phase and dust observations of the same regions
    - To develop the unique computing techniques required to jump from output 1 to output 2 above
- This PhD will be part of the DISCNET STFC DTC: as such students will join a large cohort of Phds from across 5 universities in the South East, including the OU. DICSNET runs a large training programme in big data / machine learning and AI skills with a focus to applying these to astronomy problems – you can find full information here (https://www.discnet.co.uk/). Students have a chance to undertake relevant academic and industrial placements to hone their computing skills, and present a final thesis enmbedded in Astronomy. This training and environment is augmented by the OU: basic training in presentation skills (oral and poster) writing and astrochemistry will be vital, and the student will join a vibrant research group (currently 2 academics 4 PhDs and 1 PDRA) focused on studying astrochemical cies through observations, laboratory and theoretical methods.
- This PhD is focused at the OU, but the wider JWST and ALMA observations engage key collaborators in the JWST ERS ICEAGE consortium (http://jwst-iceage.org/program/), and JWST GO and GT teams in cycles 1 ,2 and 3: in particular at Leiden Observatory, Unviersity of Hawaii, Unviersity of Arizona, Univerity of Paris, University of Marseille, University of Copenhagen, STSci and JPL.

Project description:

Ices are ubiquitious in star-forming regions. As densities increase, and temepratures fall, atoms and molecules freeze-out onto the dust grains that accumulate in molecular star-forming clouds, and through a series of surface chemical reactions, solid-state molecules, or ices, are formed. These ices are thought to be dominated by H_2O, followed by the next three dominant species, CO_2, CO and CH_3OH.

It was long an aspiration of astrochemists to be able to map the spatial distribution of solid state material in star-forming regions, in images akin to gas phase emission maps from both single beam (IRAM JCMT) and interferometric (ALMA NOEMA) sub-mm telescopes. However, ices can only be observed in the near- and mid-IR (~ 2 – 20 microns), in absorption, against a bright background source, either behind or embedded in the cloud. Until the advent of the most recent space IR telescopes, (JWST Spitzer AKARI) it was impossible to access sufficient bright background sources to undertake ice mapping: in the JWST era the equisite resolution,spectral and spatial, coupled with the sensitivity and parallel observing modes, makes JWST ice-mappng a reality. The first stage of this proposal will be for the student to engage with ice-mapping data reduction and production from the wealth of JWST data we already have access to.

This will form the huge data-set for the remainder of this PhD. To put this in context, ISO observed ice towards one background star; Spitzer ~ 10 backround stars; AKARI ~ 100. In the first JWST icemaps from the ICEAGE team consisted of many 1000's of sources that were catalogued in the field of view, 1000's of spectra extracted and many 100's of lines of sight that had ice detetcions. This is one part of one cloud! And across our JWST data in hand over the current and upcoming JWST cycles we have 4-5 more clouds or new fields of view to reduce and analyse. We have a big-data challenge.

It is impossible to apply the very manual analysis and interpretation techniques that are well described in the ice astrochemistry literature to such a large dataset. Furthermore, many of the objects against which ice is mapped are uncatalogued – we don't know what kind of star, and at what luminosity we are looking at!: what we observe is a summation of the stellar properties and the cloud properties, as well as any dust extinction in the line of sight. Then the issue is even further complicated by the fact that the ice spectra are influenced by a plethora of physical and chemical cloud conditions, right from their formation and through their evolution. So to disentangle and interpret all this data requires state-of-the art computing methods.

This PhD therefore combines astronomy expertise in astrochemistry with machine learning and image processing expertise in astronomy. We propose to address the challenge of identifying background sources by running a large grid of Phoenix models and extinction model effects, to generate a range of potential background source model SED curves and photometric spectra, convolved with extinctions. A number of our data sets also sample a rnage of background sources off-cloud from the ice features, and these (Gaia and soon Euclid) characterised sources can be used to train our analysis methods between JWST known and unknown background sources. When applied to the icemaps this is half the analysis battle.

The final stage of the project involves understanding the formation and evolution of the ice itself. This doesn't occur in isolation, but in the presence of gas and dust. So by accessing archival data, or where it is missing, proposing new observations with e.g. ALMA and NOEMA or IRAM and JCMT, we propose to combne gas emission and dust imaging with the ice maps to constrain local conditions, to disentangle the ice astrochemistry.

The project offers the successful student an opportunty to work at the forefront of JWST observations and applications in atronomy of big data handling and machine learning techniques. The project would ideally suit a student wth an interest in astrochemistry and the role of chemical processes in star- and planet formation, coupled with python programming skills. The project will involve using HPC (high performance computing) facilities with linux and bash operations, and require an enthusiasm to couple these skills with an astrochemical focus in the published outputs.

Ideally the successful will have studied a Batchelors or Masters degree in Physics, Astronomy or a closely related field, and may have undertaken a short term summer project, mini research project or research assistant role in a project involving observations IR or sub-mm astronomy, which may have included Astrochemistry. Most important is an enthusiasm to work hard, learn new skills in chemistry computing and astronomy, and an interest in the wider methods and outcomes of the project.

References:

1. McClure et al Nature Astro 2023
2. Dartois et al Nature Astro *in press* (2023) [can be updated at advert]