Predicting the composition of astronomical ices with machine learning

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Current observations taken by James Webb Space Telescope (JWST) allow to observe the absorption features of icy mantles that cover interstellar dust grains, which are mainly composed of H_2O, CO and CO_2, together with other minor species [1, 2]. Thanks to its sensitivity and spectral resolution, JWST has the potential to observe ice features towards hundreds of sources at different stages along the process of star formation. However, identifying the spectral features of the different species and quantifying the ice composition is not trivial and requires complex spectroscopic analysis [1, 2, 3].

We present AICE (*Automatic Ice Composition Estimator*), a new Python tool based on artificial neural networks. Given the infrared ice absorption spectrum between 2.5 and 10 μm, AICE predicts the ice fractional composition in terms of H_2O, CO, CO_2, CH_3OH, NH_3 and CH_4. To train the model, we used hundreds of laboratory experiments of ice mixtures from different databases like LIDA [4], which were reprocessed with baseline subtraction and normalisation.

Once trained, AICE takes less than 1 s in a conventional computer to predict the ice composition associated with the observed infrared absorption spectrum, with typical errors of ~3 % in the species fraction. We tested the performance of AICE in two spectra reported towards the NIR38 and J110621 background stars observed within the JWST Ice Age program [1], showing a good agreement with previous estimations of the ice composition. The fast and accurate performance of AICE enables the systematic analysis of hundreds of different ice spectra with a modest investment of time. In addition, this model can be enhanced and re-trained with more laboratory data, improving the precision of the predictions and enlarging the list of predicted species.

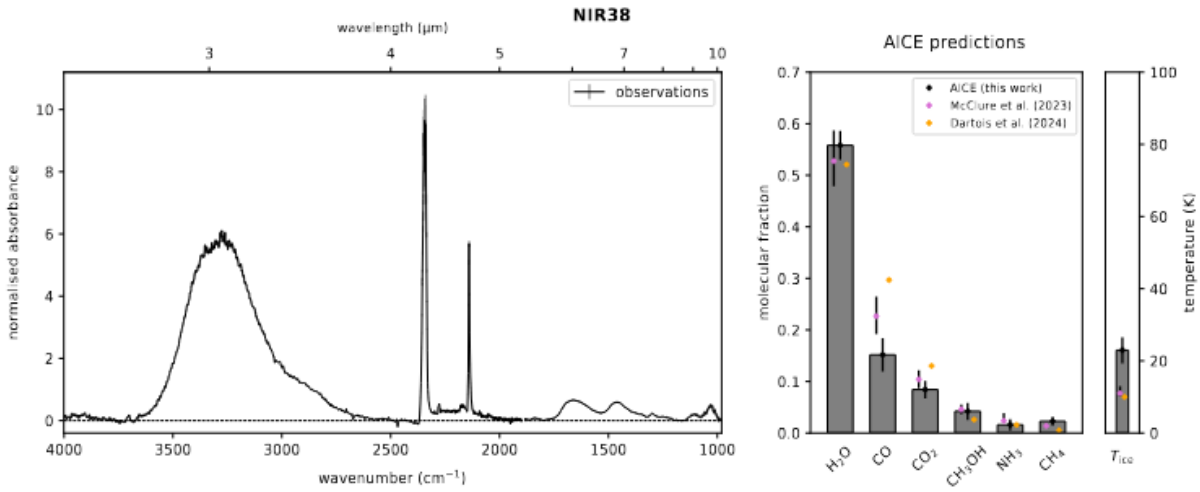

Figure 1: Absorption spectrum taken by JWST [1] and predictions of the ice composition by AICE.

References

[1] M. McClure et al., 2023, Nat. Astron. 7, 431.
[2] Z. L. Smith et al., 2025, Nat. Astron. 9, 883.
[3] E. Dartois et al., 2024, Nat. Astron. 8, 359.
[4] W. R. M. Rocha et al., 2022, A&A 668, A63.