

Spectral Assignment of Formaldehyde

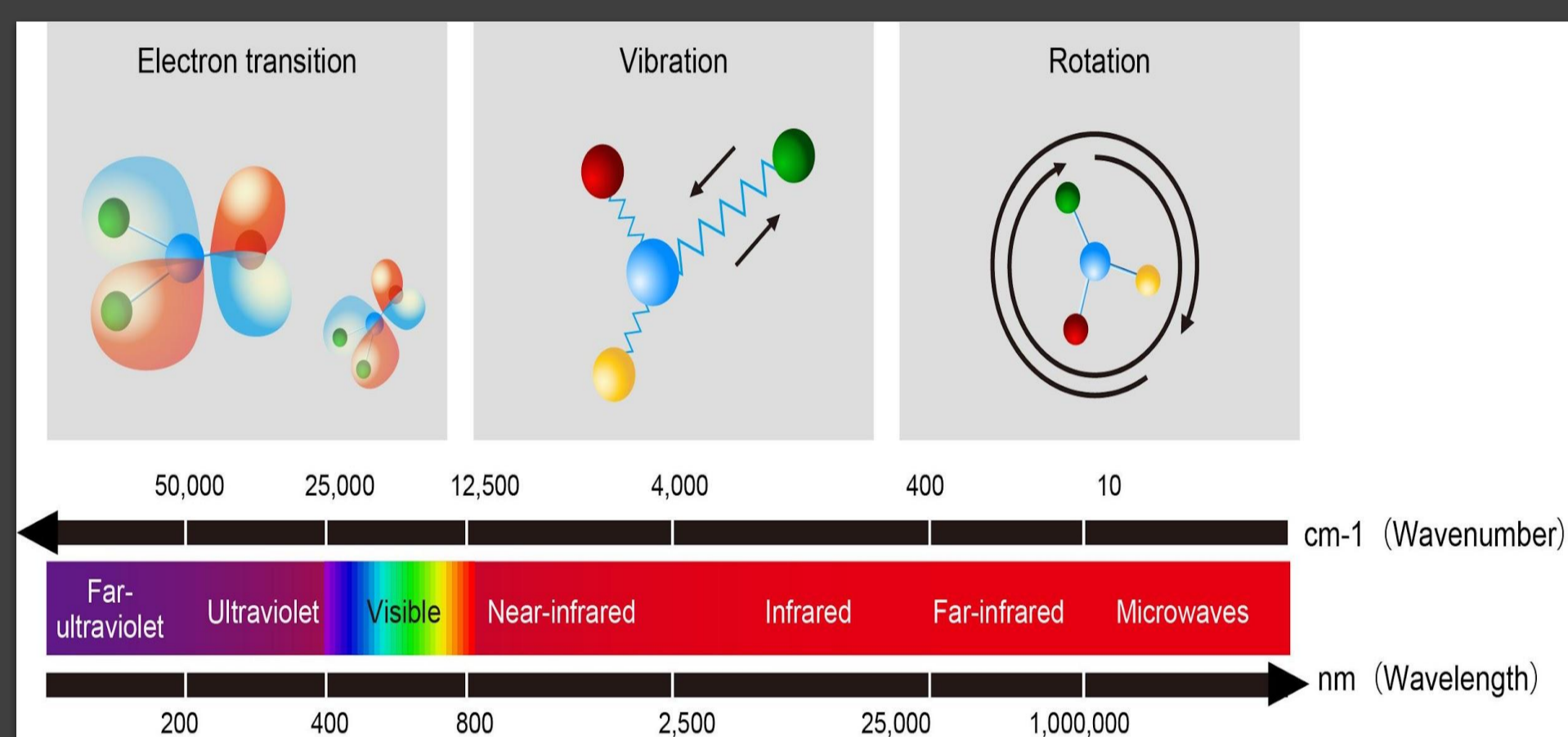
Joel Barak, Aidan Chan, Marisa Dudhia, Harry Emes, Krishna Atulkumar Gohil, Kavya Mehta, Sri Vivek Anand Muvva, Grace O'Neill, Abi Pearce, Matthieu Perrault, Lana Winter, Aarushi Yadav

We aimed to assign an experimental spectrum of Formaldehyde (CH_2O) in a region that was previously unobserved. We achieved this by first fitting voigt profiles to get positions and line profile parameters, and then assigning quantum numbers to the experimental lines through comparison with a theoretical model. Several combinations of different tests were used to confirm the line assignments.

Altogether, we assigned 38 lines in the spectral region between 6720 cm^{-1} and 6810 cm^{-1} . This assignment is useful in environmental chemistry since CH_2O is carcinogenic and can be traced within the Earth's atmosphere. It is also useful within industry, as its spectrum can be used to monitor combustion engines. CH_2O also has astrophysical importance, as it is found within protoplanetary disks which will help us to understand planetary formation processes.

TRANSITIONAL ENERGIES

The figure shows different molecular transitions and the wavenumbers/lengths at which they occur. The different transitions cause the emission or absorption of different amounts of energy, occurring at different intensities.



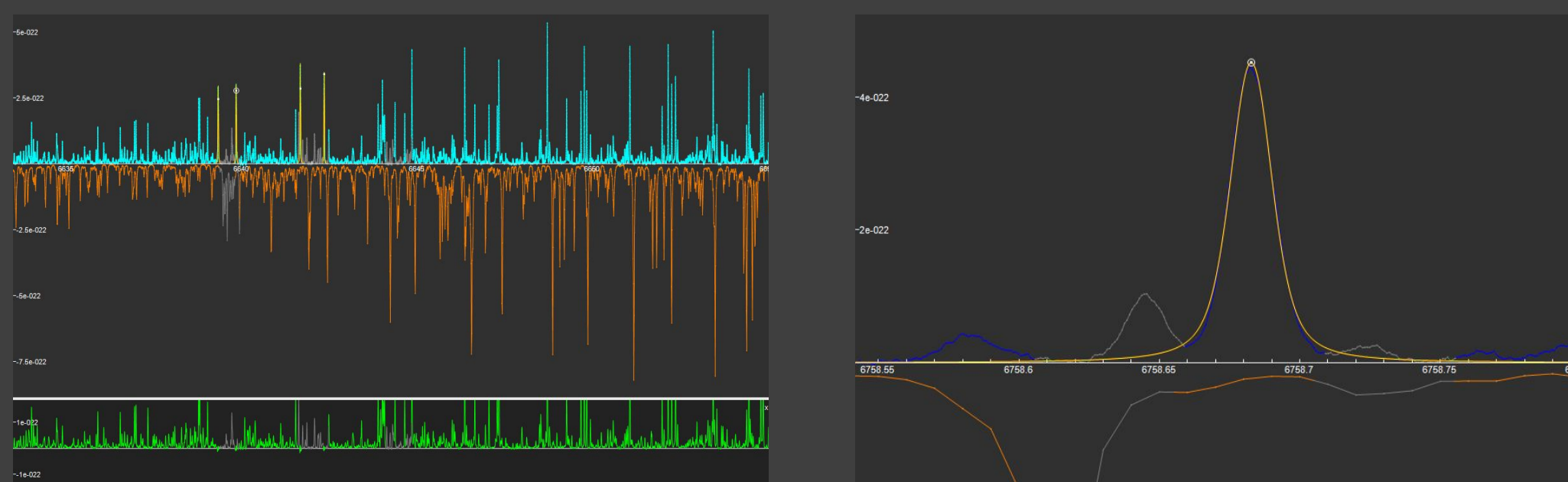
FITYK

We used Fityk to fit voigt curves to the experimental data. From these approximations, we obtained data for their centres, area and height.

In fig.1 and fig.2, the blue graph illustrates the experimental data and the orange represents the theoretical model.

This is the process we followed:

1. Find a pair (like the yellow ones highlighted in fig.1).
2. Deselect the areas around the curve so they aren't included in the fitting.
3. Draw a rough voigt curve over the one chosen and run the fitting program.
4. This will give a very accurate approximation of the actual curve, from which you can record data to update the theoretical graph.



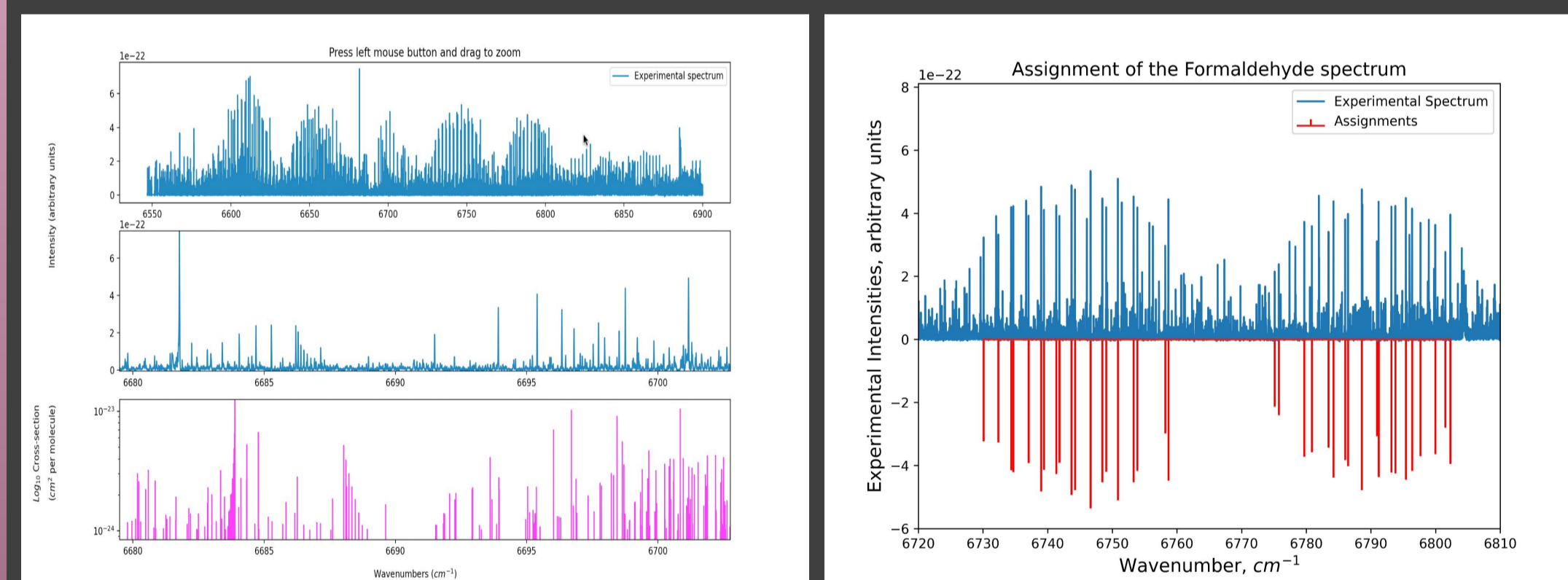
SPECTRAL ASSIGNMENT

Using python code to compare model data (pink) and experimental data (blue) and refine model data.

Zooming into the experimental spectrum and finding the corresponding lines on the model spectrum.

Model data contains quantum numbers (provides energy levels) and experimental data contains accurate wave number positioning for spectral lines.

New line assignments from jupyter (quantum number assignments) used with voigt curves fitted from fityk (line positions and profile parameters - area, height, maximum) for spectral assignment.



CONCLUSION

Overall, we provided 38 assigned lines confirmed via combination difference tests in a high-energy region of formaldehyde's spectrum that were un-assigned and not explored before. These assignments also include line profile parameters such as the FWHM and area which are useful in various studies. Using these lines, the theoretical model can be refined.

These lines and the model can be used in environmental chemistry as formaldehyde is a carcinogen found in the Earth's atmosphere and to monitor the efficiency of combustion engines (where this part of the spectrum will be particularly useful as the energy of these engines is high).