NIRSpec and MIRI view on molecular emission in irradiated environments. The case of hydrides in the Orion Bar.

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Hydrides, such as CH^+ and OH, are key molecules to study physico-chemical processes in irradiated environments. Their formation and excitation are indeed highly sensitive to the local conditions of the gas (temperature, density, UV flux). JWST, with its unique sensitivity and spatial resolution is about to revolutionize the field by mapping the emission of faint and excited molecular lines, in particular those of hydrides. Today, observations of the JWST-ERS program "PDR4ALL" (Berné et al. 2022) provides us with a unique view on the Orion Bar, a strongly irradiated PDR, and on externally irradiated disks.

In this contribution, I will present the first NIRSpec and MIRI detections of excited hydrides in this region (CH^+ and OH), and our modeling efforts to interpret these observations. OH is only detected in the disk where temperature is key to overcome the activation barrier to the formation of OH. I will then present the detection of rotational and ro-vibrational lines of OH up to an energy of 45,000 K. The series of rotationally excited lines of OH detected by MIRI-MRS are in striking agreement with the results of quantum dynamical calculations that predicted the production of rotationally excited OH following water photodissociation in its second B electronic state. The rovibrational lines of OH, which are also detected by JWST/NIRSpec, is attributed to chemical pumping by the reaction H_2+O forming OH. The remarkable agreement between observations and quantum calculations allows us to put strong constrains on physical conditions and formation rates.

CH^+ is detected in very different environments throughout both the Orion Bar PDR and the proto-planetary disk d203-506. The spatial correlation between the ro-vibrational lines of CH^+ and H_2 confirms that CH^+ is also formed and chemically pumped by the reaction $C^+ + H_2^* \rightarrow CH^+ + H$. Interestingly, the CH^+/H_2 line ratio varies by more than an order of magnitude, between the dense disk and the more diffuse PDR, unveiling a strong dependency on density of CH^+.

These observational results will be compared with state-of-the-art PDR models to investigate how density and temperature control the abundance and excitation of small hydrides to be routinely detected in other environments by JWST (disks, irradiated shocks, massive protostars). I will also highlight the pivotal role of molecular physicists and the need for new quantum calculations to build state-to-state astrochemical models in the JWST era.

O. Berné, et al., 134, 054301 (2022)