Molecular growth in extraterrestrial samples and its characteristic mass spectrometry

FRANÇOIS-RÉGIS ORTHOUS-DAUNAY¹, VÉRONIQUE VUITTON² AND LAURÈNE FLANDINET²

¹Université Grenoble Alpes CNRS/IPAG ²Université Grenoble Alpes, IPAG, Grenoble, France Presenting Author: frod@univ-grenoble-alpes.fr

High Resolution mass spectrometry, as it's the only way to achieve the equivalence between one signal and one stoichiometric formula, has brought valuable insight into natural sample compositions[1], [2].

The unparalleled analytical advantage is it provides this information for the whole mixture compounds in a single measurement.

With this type of data rises an emergent characteristic out of the relative abundances of each single molecule with regard to each other's. This requires developing new tools to describe, quantify and compare sample to another[3].

First objects to take into account the sample complexity are stoichiometric networks, that organize every compound one to another by their atomic difference. They are graphs that describe the redundancy of the numerous formulas found in a sample. In a hypothetical example of industrial polymerization process, all the products can only be a whole number of monomers bound together, the complexity would there be limited and completely described by the variability of said whole number[4], [5].

With respect to the chemical variability of a natural sample, there could be a very high complexity almost impossible to describe or on contrary highly correlated formula occurrence, nicely depending on the number of atoms and interpreted with a limited number of parameters.

Such molecular growth patterns have been measured in extraterrestrial mixtures found on meteorites, where unmatched diversity comes with high redundancy. We show there is a good chance it constrains the actual synthesis environment and how does it compare to any biological mixtures and derived products such as crude oil and petroleum. Going through an overview of the automatization tool we developed, one may find application of a universal method to identify synthesis processes patterns based on final products.

[1] Schmitt-Kopplin, P. et al. Feb. 2010.Proc. Natl. Acad. Sci.vol. 107, no. 7.pp. 2763–2768[2] Orthous-Daunay, F.-R.Thissen, R.and Vuitton, V. Apr. 2019.Proc. Int. Astron. Union.vol. 15, no. S350.pp. 193–199[3] Isa, J.Orthous-Daunay, F.-R.Beck, P.Herd, C. D. K.Vuitton, V.and Flandinet, L. Oct. 2021.Astrophys. J. Lett.vol. 920, no. 2.p. L39[4] Weßlau, V. H. 1956.Die Makromol. Chemie.vol. 20, no. 1.pp. 111–142[5] Orthous-Daunay, F.-R. et al. 2019.Geochem. J.vol. 53, no. 1.pp. 21–32