PARENT BODY EFFECTS ON SOLUBLE ORGANIC MATTER (SOM) IN DIFFERENT LITHOLOGIES IN TAGISH LAKE J.Isa[1], F.-R. Orthous-Daunay[1], P. Beck[1], and C.D.K. Herd[2]
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Introduction: The solar system origin and especially subsequent evolution of organic matter are still not well understood. Petrological observation of inorganic chondritic components shows evidence of the geological evolution in the parent body processes including brecciation/alteration/metamorphism. Such processes in the chondrites body resulted in the variety of rock types we see today across chondrite groups. The geological environment also altered the organic compounds since the vast majority of organic compounds are subject to reactions that lead to synthesis and degradation [1]. Although the majority of organics in chondrites are large insoluble organic compounds, previous targeted/non-targeted analyses [2,3,4] have successfully identified a wide variety of soluble organic matters (SOM).

In order to comprehensively study the effect of parent body processes on SOM in meteorites, we have applied non-targeted analyses on the solvent extracts from chondrites and measured them by using the Heated Electrospray Ionization (HESI) direct-infusion with a high-resolution Orbitrap mass spectrometer. We analyzed Tagish Lake chondrites from different lithologies together with Orgueilas a comparison of aqueous alteration and relatively well-studied Murchison.

In order to eliminate the subjective point of view, this study was conducted specifically as a blind study. We conducted organic measurements and data reduction of SOMs without knowing Tagish Lake meteorite lithologies. We report the results of on-going data reduction of SOMs and we will present the results of organic analyses and associations with Tagish Lake lithologies at the conference.

Samples and Measurements: We have studied Orgueil (CI), Murchison (CM2), and Tagish Lake (C2 ungrouped) chondrites. Each meteorite was extracted by solvent, a mixture of methanol: toluene = 2:1 by volume, was used. The methanol/toluene extracted organic compounds were analyzed using the high-resolution Orbitrap mass spectrometer at the University of Grenoble Alps. The SOM together with the solvent were injected into the Orbitrap and ionized with using the HESI source. Only positive ions were analyzed for this study. After we acquired the spectra, we utilized post-processing data analysis tools, which have been developed in-house at IPAG. Attributor [1] was used for main data analyses.

Data processing: The post-processing includes mass-drift correction, peak detection, and noise rejection. From the refined mass spectra, we obtained network densities and assigned stoichiometric formulae. In order to study the data structure in the mass spectra, we analyzed *m/z* versus mass defect dimensions. The mass defect is calculated by $m/z - E(m/z+1/2)$. In this additional dimension, a repeating unit among the detected ions (e.g. -CH_2-, -NH, and isotope substitute, etc.) in the mass spectra appear as a characteristic geometric structure. These inherent geometric structures were studied by using feature extraction algorithms such as Hough transform, and graph structure were studied by treating the data points as sets of vertices and sets of edges. Overall data points often appear as a geometric point cloud in the *m/z* vs mass defect diagram (Fig. 1a and 2a). The network density within the point cloud was assessed by the deviation from a fitted Cauchy distribution among calculated slopes of all possible connections within the point cloud (Fig. 1b and 2b). After studying the graphs, we assigned a stoichiometric formula to a data point that has low *m/z* value and propagates the formulae to the rest of the data points. After the stoichiometric formulae assignment, we eliminated the impossible organic stoichiometry formula such as negative number of elements or negative values of double bond equivalent (DBE) value.

Results and Discussion: We have analyzed the Orbitrap spectra and assigned chemical formulae to Orgueil, Murchison and four Tagish Lake samples (06029d, 06030a, 06030c, and 06030d). The spectra of three another Tagish Lake samples (06029c, 06029e, and 06030b) have not been assigned. Although individual chemical formulae are not yet assigned, the geometric structures of all the spectra were studied including the last three spectra.

Stoichiometric formulae

All samples contain $C_lH_mN_nO_o$ organic compounds. The extract contains N-bearing organic compounds that are similar to and consistent with the organic compounds previously found in a methanol extract from the Murchison meteorite [2]. In our chondrite analyses, we were able to assign approximately 10% of major peaks that were detected as singly plus charged $C_lH_mN_nO_o$ compounds to within ~1 ppm of mass precision between *m/z* 150 and 750. Previously detected CH_2 homologous series and their Wesslau-like

patterns [1] were also observed in the Orgueil, Murchison and some Tagish Lake spectra. However, the Tagish Lake spectrum, 06029d, shows significant differences in regard to stoichiometric formulae and CH_2 homologous pattern. While the dominant assigned compounds have one nitrogen atom ($C_lH_mNO_o$) in most of the spectra, that is minor in the Tagish Lake spectrum, 06029d. Also, the Wesslau-like CH_2 the homologous pattern is less prominent.

Homologous series

Major homologous series were detected by searching for frequently appearing slopes in the *m/z* versus mass defect diagram. Differences between the spiked rose and blue lines indicate that there are frequently appearing slopes that would not be expected for a random set of slope distributions. These unexpectantly high occurrence of slope peaks are indicative of homologous molecular series. We note that the analyses for spectra for 06029e and 06030b exhibit significant negative slopes (Fig 1). The negative slopes below zero are suggestive of the presence of non-CHNO ions. In contrast, most of the samples (e.g. the spectrum for 06030d) consist of CHNO compounds have positive slopes in Figure 2b.

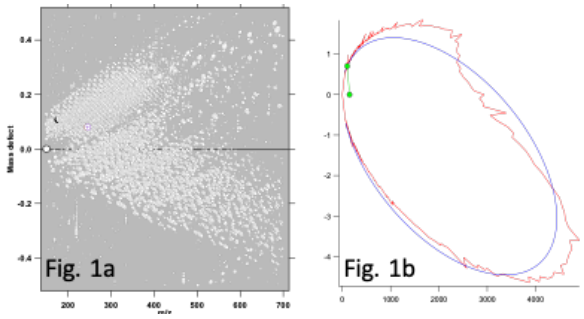

Figure 1: Data from Tagish Lake spectra 06029e. The *m/z* versus Mass defect (1a). The data points are shown by using white dots. The slope distributions were fit by using the Cauchy distribution assumption (blue line), actual slope distributions are shown by using the red line (1b). The negative mass defect values (those with values less than zero) indicate the abundance of non-CHNO compounds.

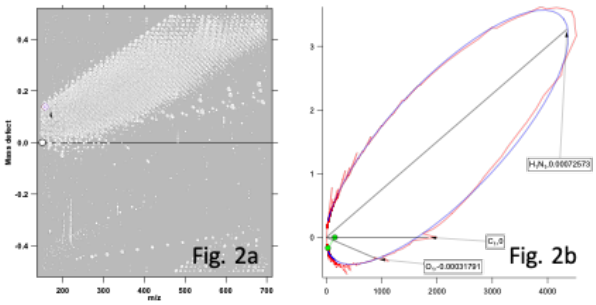

Figure 2: Data from Tagish Lake spectra 06030d. The *m/z* versus Mass defect (2a). The data points are shown by using white dots. The slope distributions were fit by using the Cauchy distribution assumption (blue line), actual slope distributions are shown by using the red line (2b). The positive mass defects indicate the points clouds are data points corresponding to CHNO compounds.

References: [1] Orthous-Daunay, F. R. et al. (2019) Geochemical Journal, 53(1), 21-32. [2] Naraoka H, et al., ACS Earth Space Chem. (2017) 1:540-550 [3] Schmitt-Kopplin, P. et al. (2010) Proceedings of the Nation-al Academy of Sciences, 107(7), 2763-2768. [4] Ruf, A. et al. (2017) Proceedings of the National Academy of Sciences, 114(11), 2819-2824. [4] Chambers, M. C. et al., (2012) Nature biotechnology, 30(10), 918.