Contribution ID: **11** Contribution code: **Tu-II_1** Type: **Oral**

How we can gain structural information about individual compounds in complex energy mixtures: Theoretical calculations support high resolution data and lead to surprising results

Tuesday, August 26, 2025 11:00 AM (40 minutes)

High-resolution mass spectrometry is the method of choice for analyzing complex mixtures, as this is the only method that allows gaining detailed analytical information with high accuracy. The only problem is that mass spectrometry inherently can not provide structural information about unknown compounds per se. Liquid fuel systems are some of the most complex natural mixtures available and contain hundreds of thousands of different hydrocarbon-type compounds. Raw materials for fossil fuels are formed under geological conditions over large time frames, while biofuels are being made from a precursor source in different ways. To better understand the formation pathways it is imminent to understand how complex these mixtures are and what type of compounds are being formed under which conditions. Here, we have combined sophisticated analytical methods with different types of theoretical calculations on both the DFT- and coupled cluster level of theory to understand the structures of individual compounds in complex systems. High-resolution mass spectrometry allows the parallel detection of a vast range of different compounds, which can result in some 100,000 exactly measured signals that correspond to individual elemental compositions. Theoretical calculations allow finding the thermodynamically most stable structures of those compounds. Here, fascinating and unforeseen results from heavy fossil fuels are reported that show a surprising detection of carbon-type species. In crude oil we found naturally formed fullerenes and their building blocks, compounds that are interesting for a vast variety of applications. Fullerene synthesis happens under high-energy conditions, mostly laser ablation or high-voltage discharge is being used, while nature forms these compounds under geological conditions (ca. 150 ℃ and pressure). The results show, that nature forms a large variety of fullerenes and fullertubes, which can be detected up to C_{148}, while, additionally, electron microscopy allows a view into large multi-walled carbon nano tubes, which can also be detected. In all these findings, theoretical calculations support the results. These findings could open up a new interest in making different types of Fullerenes and functional carbon species in very different synthetic ways than before.

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Session Classification: Tuesday

Track Classification: FTMS and High Resolution Mass Spectrometry