ROSKILDE UNIVERSITY
Department of Science, Systems and Models

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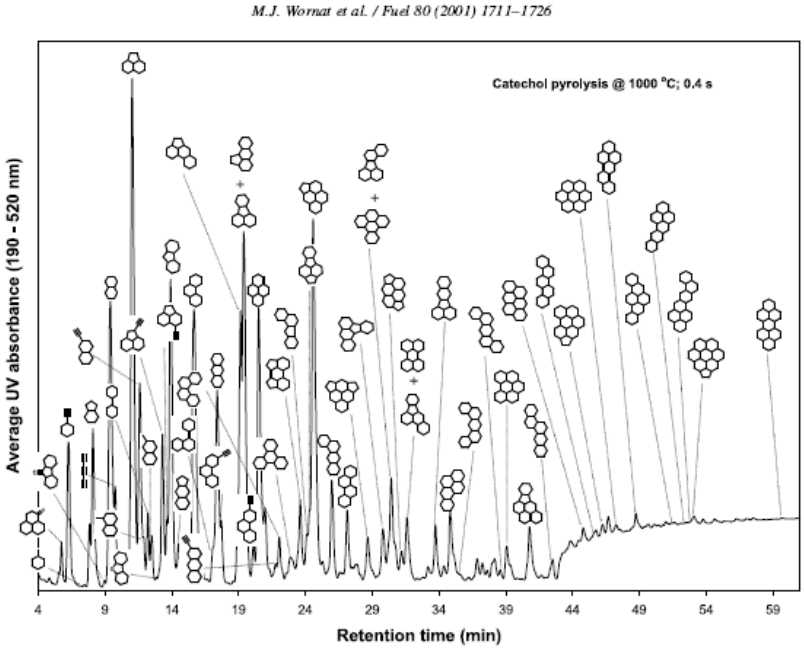
Project suggestion:

Theoretical analysis of the electronic transitions of PAHs

Polycyclic Aromatic Hydrocarbons (PAHs) are a large class of conjugated π-electron systems of fundamental importance in many research areas of chemistry as well as in astrophysics and materials science. They are produced by the combustion of organic matter and are of great importance in environmental chemistry due to their carcinogenicity. The Figure below shows the results of a HPLC analysis of the PAHs produced by a model combustion process [1]. The individual PAHs are generally identified by their characteristic UV-Vis absorption spectra, and an understanding of their electronic transitions is thus of high interest.

At our Department, a quantum chemical procedure has been developed with particular emphasis on the prediction of absorbance data for PAHs. This is the so-called LCOAO procedure [2-4] which has shown excellent results for a variety of compounds [2,3]. The computer program has recently been expanded to deal with very large PAHs (100 atoms) [4], and it is now of interest to test the procedure on a series of key compounds, including some very large species. One objective of this project would be to establish a database with data for environmentally important PAHs.



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[3] C. Johannessen, A. Gorski, J. Waluk, J. Spanget-Larsen, *Polycycl. Arom. Compds.* **25**, 23-45 (2005)
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