An evolutionary algorithm approach to PAH stability

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The dissociation of large polycyclic aromatic hydrocarbons (PAHs) results in many small fragments. In experiments, these fragments are captured by infrared (IR) spectrum and mass spectrum (MS)[1]. IR spectrum is often used to identify functional groups instead of exact molecular structures. MS can represent total mass of each fragment, but cannot tell why there are specific mass loss during dissociations of PAHs. It's significant to achieve joint interpretation of infrared and mass spectrum[2] to get more information (e.g. PAH stability, distribution of fragments) during PAH fragmentations.

Our approach to this joint interpretation is illustrated by Figure 1 which is based on an example of $C_{16}H_{17}$. At first, we can get chemical formula from each peak of a given MS. Then possible candidates for a specific chemical formula are generated by running evolutionary algorithm which is a global optimization method. Then we use hierarchical clustering to get representative candidates from all possible candidates and calculate IR spectrum of each representative candidate. Finally, these calculated IR spectrums are matched with experimental spectrum to find the most possible candidate for each fragment.

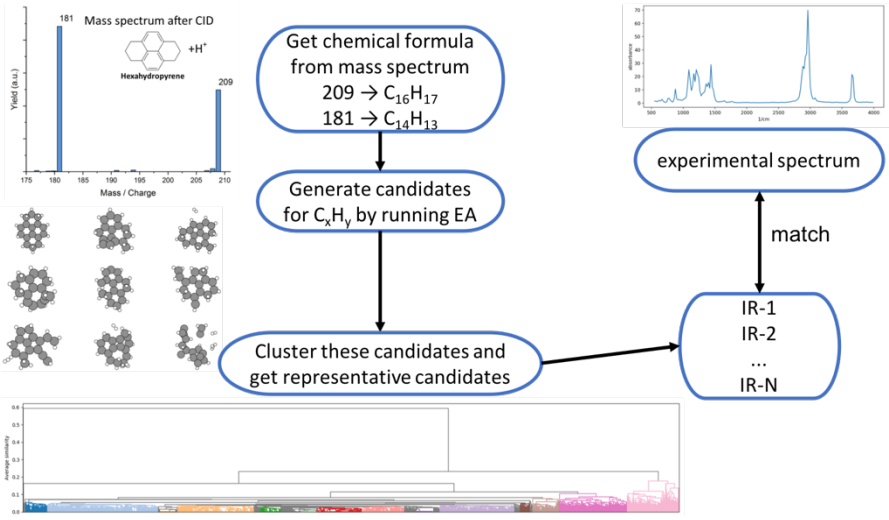

Figure 1: The joint interpretation of infrared and mass spectrum for $C_{16}H_{17}$.

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References

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