The kinetic isotope effect in the interaction of H with PAHs

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I will present experimental data on the hydrogenation/deuteration and H₂/HD formation processes on gas-phase polycyclic aromatic hydrocarbon (PAH) cations [1]. Hydrogenation process was studied by exposing coronene radical cations, confined in a radio-frequency ion trap, to gas phase H atoms. Sequential attachment of up to 23 hydrogen atoms has been observed [2]. Exposure to atomic D instead of H allows one to distinguish attachment from competing abstraction reactions, as the latter now leave a unique fingerprint in the measured mass spectra. This is shown in Fig. 1, where H atoms are represented in blue and D atoms in red.

Modeling of the experimental results using realistic cross sections and barriers for attachment and abstraction yield a 1:2 ratio of abstraction to attachment cross sections. The strong contribution of abstraction indicates that H₂ formation on interstellar PAH cations is an order of magnitude more relevant than previously thought.

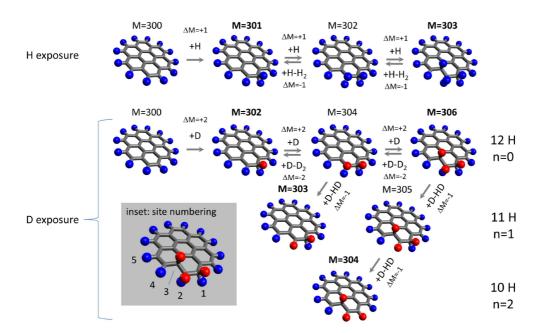


Figure 1: Schematic representation of the reaction sequences for subsequent H (top row) or D (bottom row network) interactions with a coronene cation. H atoms are marked in blue and D atoms in red. Only a selection of possible attachment (+H, +D) and abstraction (+H-H2, +D-D2, +D-HD) processes are indicated.

References

- [1] Foley, N., Cazaux, S., Egorov, D., et al. 2018, MNRAS 479, 649
- [2] Cazaux S., et al., 2016, Scientific Reports, 6, 19835