MS35-P21 | FILLING THE GAPS: WHAT NEW POLIMORPHS OF ACETYLPYRENE TELL US ABOUT THE FLUORESCENCE OF PYRENE DERIVATIVES

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Policyclic Aromatic Hydrocarbons (PAHs) have been shown to feature interesting electronic and optical properties, which showcase them as one of the most potent synthons for modern material design. The compounds are easily modified by the means of chemical substitution, which allows to use them in a wide range of applications, from conducting metal-organic frameworks to luminescent bio-markers.

Partly because of the presence of large π-conjugated systems, PAHs are known to form various aggregates, whose spectroscopic properties tend to depend significantly on individual molecules' environment. Luminescence of even the simplest compound such as pyrene undergoes a significant modifications whenever a formation of π-dimers is possible, i.e. in concentrated solution or solid state. The following trend is preserved in its derivatives.

In the course of our studies, two new polymorphs of acetylpyrene (AP) have been found and their structures have been characterised. In contrast to the already known crystal form AP-Cc, which features no π-stacking and exhibits very weak luminescence in the solid state, two new-found polymorphs denoted AP-P2_1 and AP-P2_1/c feature strong aggregation of aromatic rings, which reflects in their sharp colours when exposed to ultraviolet. While the individual differences between two new forms are very small, they impact on the electronic structure of AP heavily enough so that individual crystals of these forms are easily distinguishable under UV light with a naked eye.