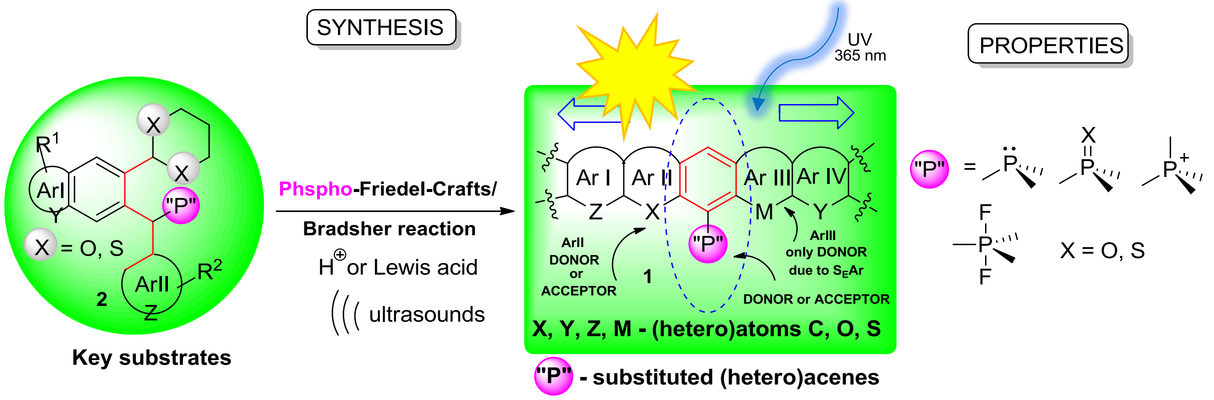
DESCRIPTION FOR THE GENERAL PUBLIC

The project goal: The project has two goals connected with the synthetic part and the measurement part. The aim of the synthetic part is elaboration of the novel phospho-Friedel-Crafts/Bradsher (F-C/B) reaction for the synthesis of P-(hetero)acenes **1** having a structural characteristic which has not been known, so far. Why it is important? Because through these structure modifications, we can influence properties of the obtained P-(hetero)acenes. Therefore, the aim of the measurement part is showing selected properties of **1**, as proofs justifying a desirability of the project. We want to show that these properties due to the presence of phosphorus atom in the molecule are better than in other analogs.



Description: The synthesis of **1** will rely on cyclization of substrates **2** under acidic conditions. The synthesis will be assisted by ultrasounds in order to accelerate it. In this type of reactions, proceeding through the common mechanism of electrophilic aromatic substitution, acceleration exceeding 7500 times may be achieved. These properties determine an applicability of a potential material under ambient conditions. The main threat for unsaturated molecules is heat, oxygen and UV light. Hence, this part of research involves measurements of photochemical and thermal stabilities and some basic photophysical properties connected with the intrinsic characteristic of P-(hetero)acenes **1** as fluorophores (absorption and emission range at various temperatures, quantum yield, fluorescence lifetime, optical gap). The photochemical stability will involve photostability and photooxidation stability at 254 nm and 365 nm under aerobic and anaerobic conditions.

Reasons for attempting a particular research topic: Astonishing effects of high thermal stability and super photostability and photoxidation stability under inert and oxygen atmosphere at 254 and 365 nm of the thio-analogs of **1,** encouraged us to investigate phosphorus substituted acenes. Why phosphorus? It would be difficult to find another heteroatom in the periodic table, a neighbor of sulfur, that would bring as many different benefits at the same time as phosphorus atom. Let's enumerate them: 1) a varied coordination number in P^{III-V} compounds, 2) an ability to change the degree of coordination from lower to higher and *vice versa*, by conversions of P^{III} to $^{IV}P{=}X$, $^{IV}P^+$ and $^{V}P\text{-}F$ compounds, and reduction of the latter back to P^{III} compounds, 3) an ability to form neutral (P^{III}, $^{IV}P{=}X$, ^{V}P) and ionic ($^{IV}P^+$) compounds, 4) an ability of ^{III}P and ^{IV}P phosphonic acids to form complexes and salts with lanthanides that are vital for applications in OLEDs and organic lasers, 5) a possibility to introduce onto (hetero)aromatic moiety both electron-acceptor $\mathbf{A_{Ar}}$ and electron-donor $\mathbf{D_{Ar}}$ groups which operate together with P-containing groups of the gradually increasing $\mathbf{A_P}$ character: $^{III}P(\mathbf{D_P}) > {}^{IV}P{=}X$ ($\mathbf{A_P}$) (X = O, S)$> {}^{V}PR_3F_2$ ($\mathbf{A_P}$)$> {}^{IV}P^+$ ($\mathbf{A_P}$) and which influence properties.

Substantial results expected: The project results will have a significant impact on development of synthetic methods and methodologies in the field of **organic, heteroatom, sono- and material chemistry**, giving an access to a new reaction in the family of hetero-F-C/B reactions and new classes of P-substituted (hetero)acenes **1**. The positive verification of the project hypotheses may bring: a) potential organic materials of high thermal stability, super photostability and photooxidation stability, b) potential optical materials of high quantum yields and other beneficial photophysical properties, c) a strong impact on sonochemistry by showing that homogenous and ionic reactions (S_EAr), which one thought could not be accelerated by ultrasounds, in fact may be significantly accelerated due to formation of naked carbocations after the shock wave.