Paramagnetic nanographenes for fundamental studies and new technologies

The proposed research project deals with unusual organic compounds, which exhibit both conductive and magnetic properties. They are flat honeycomb systems constructed with six-membered rings (Figure 1). The proposed structures, such as **A**, can be considered as part of a graphene sheet and, because of their size, are called nanographenes.

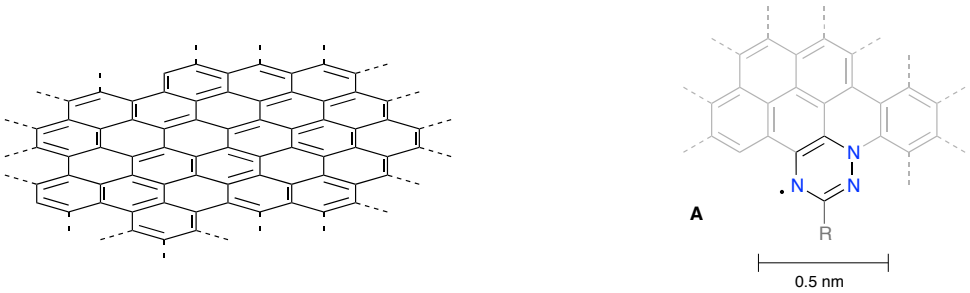

Figure 1. Fragment of a graphene sheet and general structures of the proposed paramagnetic nanographenes of type **A**.

What is a graphen? It is a large flat single-atom thick structure consisting of carbon atoms forming six-membered rings in a honeycomb pattern (Figure 1). Graphenes exhibit unique optical, electrical and mechanical properties, which are of high interest to scientist in the context of display, sensory and molecular electronic applications, including a new generation of computers. It can be added, that Poland is the first county, which started technological production of graphene.

Graphenes form large, centimeter size sheets, while nanographenes are well-defined small fragments of these sheets, smaller by 7 orders of magnitude. Exchange of some of the carbon atoms for heteroatoms, such as nitrogen, oxygen and sulfur, modifies optical and electronic properties of the nanographene, while introduction of an unpaired electron to the structure results in magnetic behavior.

In this context, the goal of the proposed research program is the development and comprehensive analysis with physical methods of a new class of rationally designed organic semiconductors containing a delocalized electron and exhibiting magnetic behavior. The proposed research will make significant contributions to basic knowledge in several areas of science, while the resulting materials will be attractive for applications in areas such as solar energy harvesting, molecular electronics and information processing. Judicious choice of type and size of the nanographene will permit the control of molecular properties and, consequently, will affect bulk behavior (e.g. magnetic, electrochemical) of the materials.

In the context of the proposed studies, new synthetic methods will be developed, unknown heterocyclic compounds and radicals will be obtained and properties, such as spectroscopic and magnetic, of the prepared materials will be investigated. Some nanographenes will be investigated also as photovoltaic and organic battery components. The planned synthesis of a large number of compounds will result in establishing of molecular structure – properties relationships, which will allow rational design of new structures with desired behavior.

The proposed program is focused on education and training of young researchers and the creation of modern interdisciplinary workforce for scientific and technological challenges of the 21st Century.