Popular science summary

Electron paramagnetic resonance spectroscopy (EPR) is a method of studying substances containing unpaired electrons, such as: free radicals, transition metal ions, rare earth elements. The method also allows studying the electrons of conduction in metals and semiconductors. Using EPR spectroscopy, we can probe the chemical surroundings of the investigated unpaired electron, and see how it is bound to its host molecule, as well as quantify the number of unpaired electrons in a unit mass or volume of a sample.

EPR spectroscopy studies are particularly important for organic semiconductors (small-molecules or polymers, i.e.: "conjugated polymers"), since one type of charge carriers present in those substances are radicals. Their number and strength of interaction with the molecular host directly determine the conductivity of those materials. Consequently, detailed knowledge about the number and properties of radicals help understand the drastic changes in the conductivity of those substances taking place upon their oxidation and reduction. Simultaneously, the radicals present in these materials determine their magnetic properties, possibly finding application as future data carriers, storing information in the form of quantum bits.

However, in order to be able to obtain detailed information about the presence of radicals in investigated substances, it is necessary to calibrate the EPR spectrometers, making use of reference materials, enabling us to reliably determine the above-mentioned material traits. A reference material for use in EPR spectroscopy should conform to the following requirements:

- Satisfy stringent chemical purity standards, and exhibit a stable and unchanging composition even during long-term storage;
- It should be possible to determine the number of spins in the reference material using an independent analytical chemistry method;
- the EPR parameters of the reference material should be as similar to the EPR parameters of the studied sample as possible, particularly as regards their g factor, width and shape of the EPR signal, and the relaxation properties of spin populations.

Even though there are many reference materials, such as ruby crystal, vanadium (IV), copper (II) and manganese (II) salts, solid MnO/MgO i Cr_2O_3/Al_2O_3 solid solutions and a few stable neutral free organic radicals, none of them belong to the class of organic semiconductors, and particularly, to the subclass of conjugated polymers. Consequently, both qualitative and quantitative EPR spectroscopic studies are burdened with uncertainties and errors stemming from partial compatibility of the EPR standards with the investigated samples.

The main goal of the project is to resolve the above issue by developing a reference material belonging to the group of conjugated polymers. Considering several advantageous properties, doped polyaniline is being put forward as a perspective EPR standard. The project involves:

- gauging the effects of synthetic variables on the paramagnetic properties of polyaniline focused on its application as an EPR standard reference material;
- obtaining information about the properties of the spins in this synthetic material, such as: the number of component lines making up its EPR spectrum, longitudinal and transverse relaxation times of each group of spins, concentration of paramagnetic centres, g factor value and shape of each of the component lines;
- study of the changes of the above-mentioned spectral properties of polyaniline over time and during exposure to factors known to modify the paramagnetic properties of free radicals (gas atmosphere, elevated temperature, exposure to UV and visible electromagnetic radiation);

The EPR spectroscopy reference material based on polyaniline to be developed during the project will enable to reliably and precisely determine the parameters of paramagnetic centres in other conjugated polymers, due to the close similarity of the chemical nature of the centres present in the reference material and in the investigated sample.