The aim of the project is to evaluate the applicability of the latest quantum crystallography methods (multipolar model and X-ray Wavefunction Refinement) to description of selected heavy elements (Au, Bi, Hg) present in model metalorganic compounds based on X-ray diffraction experiments.

The heavy-element chemistry is strongly focused on the description of relativistic effects and their influence on chemical and physical properties of atoms. In a very big simplification, an atom could be considered as a solar system model. The sun – nucleus is located in the centre, the closest planets – electrons, would have to orbit around it with a velocity of half speed of light to avoid "falling into" the nucleus. This increases the electron's mass by about 20%, and it is called the relativistic effect. The most popular examples of unexpected chemical properties of compounds resulting from the relativist effects are yellow colour of gold and liquid state of mercury. Relativity also plays a key role in a multi-billion-dollar growth industry centred around the GPS. It has been also found that ~80% of the voltage of a car battery (lead-acid) relies on the relativistic effect in the lead atom. In the old-fashioned TVs special relativity keeps the screen picture clear. More examples could be found in the literature. Relativistic effects are usually very well described from the purely theoretical and spectroscopy points of view and less from X-ray crystallography one.

In 1895, professor Wilhelm Röntgen discovered the X-ray radiation. Since then, it is broadly applicable in radiology, as well in science including X-ray crystallography. The current state of knowledge shows that it is possible to "see" relativistic effect like a doctor sees our bones – with X-rays.

The description of heavy element atoms requires high-resolution and high-quality experimental X-ray diffraction data and a suitable model of electron density of investigated compound.

Currently, the most popular and standard method in crystallography for structure solution and refinement is Independent Atoms Model (IAM). It assumes a spherical and symmetrical distribution of electron density centred on atomic nuclei. However, due to the aspherical distribution of electron density in crystal (electron density located within: chemical bonds, free electron pairs or heavy atoms) this model is insufficient. So far, alternative methods for the description of an aspherical distribution of electron density are: the Hansen-Coppens multipole model and the Hirshfeld Atom Refinement (HAR). Recent literature reports suggest that the multipole model is still insufficient for description of organo-metal compounds, while the latest HAR requires evaluation in this field.

The first stage of this project will be comprising a series of X-ray diffraction experiments using different sources of X-ray radiation (*Mo*, *Ag* and synchrotron radiation) to minimize the influence of absorption or anomalous dispersion effects on the final electron density obtained. For this reason, the high-quality data sets for crystals of six selected model compounds (Figure 1) will be used during the refinement procedures. Another purpose of the project is to find an answer how important are – and how influential are – some additional, both theoretical and experimental effects in the treatment of heavy elements.

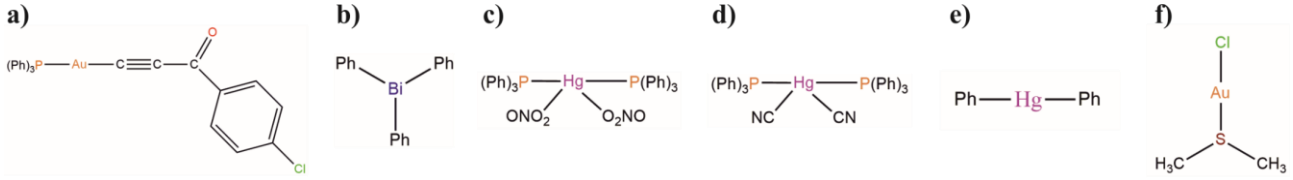

Figure 1. Investigated compounds.

The second step of the project assumes a series of refinements of aspherical electron density based on two widely used methods: Hansen-Coppens model of electron density and X-ray Wavefunction Refinement (XWR) which includes HAR method.

The research will assess whether the available methods of modern Quantum Crystallography are sufficiently good for the description of heavy elements based on refinement of high-quality experimental diffraction data. Despite the fact, that the X-ray Wavefunction Refinement is not broadly used in the description of heavy elements, current scientific publications show a large potential of this method in the description of aspherical charge distribution. Regarding all these facts, the project has a very innovative character.