

Catalysts are crucial for modern civilization as they enable synthesis of thousands of materials and key compounds inevitable for humans. The examples here are polymers produced on the scale of hundreds of megatons annually, or pharmaceuticals. Because of the scale at which these materials are used, there is a continuous demand for “better” catalysts. “Better” here means cheaper, easier to handle, easy in controlling their activity and accelerating a given process with lower demand in materials and energy.

Among numerous systems examined as potential catalysts, cations in weakly basic environment deserve attention. Weakly basic environment means the surrounding in which the cation is unable to form strong bonds with adjacent molecules. It appears, that such cations show very different reactivity patterns as compared to classical systems, where these interactions are stronger. This opens the way to synthesize exotic and novel compounds but also to observe unprecedented catalytic activity of such cationic species. In order to provide such weakly basic environment, it is crucial to select both a proper solvent and anion. In that field, so called weakly coordinating anions (WCAs) have proven valuable. This is due to their large size and structure which prevents strong bonding to cations thus rendering them highly reactive.

The research project is aimed at investigation of highly promising group of novel catalysts of polymerization and cyclotrimerization based on the salts of WCA and common divalent cations, like manganese, calcium or magnesium. Both of these processes are important because of compounds and materials produced, i.e. polymers and organic compounds with 6-membered aromatic ring. As shown already by our preliminary results, some of the salts of WCA tested show extraordinary catalytic activity in abovementioned reactions – even hundreds of times higher as compared to currently used catalysts.

For that reason, the field calls for thorough investigation of the capabilities and mechanisms of a wide range of WCA-based salts of divalent cations as catalysts in reactions involving unsaturated hydrocarbons containing either double or triple C-C bond. This will be done on the basis of detailed analysis of experimental data collected for reactions with various hydrocarbons (i.e. with varying structure), physicochemical properties and structures of the resulting products and with the aid of quantum-chemical calculations. In long term perspective, which is beyond the scope of the project, these results will help to develop more efficient and more reactive catalysts for chemical processes with key role in modern economy.