Lab on a Molecule – Exploring Organometallic Reactivity of Molecular Fragments under Confinement within a Carbaporphyrinoid Frame

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Very complicated chemical reactions occur continuously inside living organisms very efficiently and selectively because substrates reach movement-constraining enzymatic pockets that aligns them properly relative to the reaction center. It is a complicated machinery, thus, in my research, I decided to attach the substrate with a covalent bond in a close proximity to the reaction center, in order to reproduce and observe some of the biological processes. That forced proximity will induce new reactivity between the metal center and the attached substrate, which I want to observe.

Basic platforms that will be used in my investigations are modified porphyrins. Porphyrins are colorful macrocyclic compounds that can accommodate a metal ion in the center of the ring and held it stably inside. Porphyrins constitute some of enzyme's active centers or perform other biological functions. The examples are B12 vitamin (cobalamin), chlorophyl, heme, or factor 430. If one introduces to such a porphyrinic ring a carbocycle, carbaporphyrin will be obtain.

The project is based on insertion of the metal ion into the selected carbaporphyrin cavity with parallel reaction of the ion with a substrate of the reaction we want to investigate. The substrate attaches to the metal center and is then transferred onto a carbon fragment in the macrocycle (I Stage). Such a 'nanolaboratory' is ready for replacing the first ion, which has already fulfilled its function, for another metal ion that will induce a reaction with the attached substrate (II Stage). I will observe the transformations, determine what they depend on and try to influence them by changing various physical and chemical factors. Results from the investigations will help to better understand metal ion catalyzed processes.

