PRESS RELEASE

Resolving transformations of molecules and their chirality in the submolecular scale

Prague, November 22, 2016 **-- Scientists from the Institute of Physics and the Institute of Organic Chemistry and Biochemistry of Czech Academy of Sciences observed a chemical transformation of individual molecules on silver surface and demonstrated chirality transfer during the reaction. They employed the latest advances of scanning probe microscopy, which allows scientists to determine the chemical bond between individual atoms within molecules and thus determine their molecular structure and the chirality. The results were published in the prestigious journal Nature Chemistry.**

Chirality is a geometrical property an object (usually a molecule or ion) that cannot be matched with its mirror image. Chirality plays a key role in nature and can be demonstrated for example on the relationship of right and left hand, which are not identical in terms of symmetry. The phenomenon of chirality is important in many areas e.g. stereoselective reactions, self-assembly of molecules, biological processes (where proteins, nucleic acids or polysacharides are involved), the polarization of light or electron spin. Control of chirality in chemical reactions in solutions represents one of the greatest achievements of organic chemistry in the last fifty years.

Molecules that are not chiral in solution or gas phase (i.e. prochiral), may become chiral under certain conditions, specifically after adsorption to a solid surface, when a so-called chiral adsorbate is formed. The breakthrough method, that allows one to create an extensive two-dimensional molecular layer of chosen chirality, was developed through the combined efforts of researchers from the Institute of Physics and the Institute of Organic Chemistry and Biochemistry (IOCB Prague) of Czech Academy of Sciences, led by Dr. Pavel Jelinek and Dr. Ivo Starý. This achievement represents the first practical demonstration of the possibility that prochiral molecules at solid surfaces occupy either right or left-handed orientation on purpose.

Namely, the Czech scientists achieved that the adsorbed molecules adopted a single chirality in their whole monolayer, by using a thermally controlled chemical transformation of chiral helical molecules, so-called Helicenes to planar polyaromatic molecules (see Fig. 1). The transformation was made on a surface of a silver crystal. Moreover, the scientists could accurately determine a sequence of multi-step chemical transformations of the molecules using atomic force microscope that operates at temperatures close to the absolute zero and under conditions of ultra-high vacuum. They managed to identify both intermediates and final products of the cascade of chemical reactions, employing the unique submolecular resolution that allowed the direct deduction of the molecular structures of the relevant molecules (see Fig. 2).

This work represents a revolutionary approach enabling in-depth studies of chemical reactions on solid state surfaces and a precise determination of the chemical structure of molecules, with the possibility to track conversions of their chirality. The original method opens up new possibilities for the preparation of well-defined chiral surfaces that have significant potential for use in the field of heterogeneous catalysis, sensors of chirality, molecular electronics, spintronics, photonics and biochemistry.

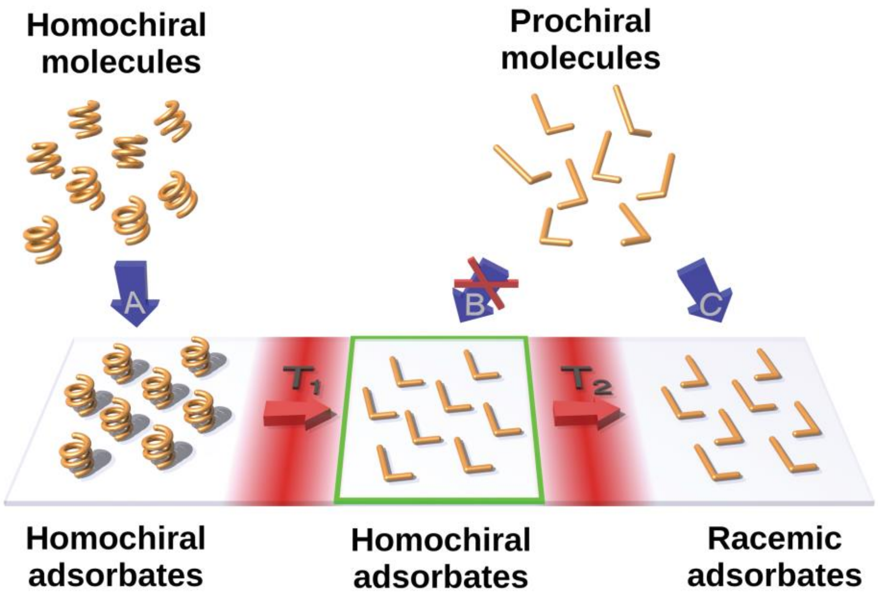

Fig.1. Schematic view of the chirality-preserving transformation of molecules deposited on a solid surface (A) using a temperature-controlled chemical reaction (T1). This reaction allows to get the same chirality of adsorbed

molecules across the whole monolayer (green frame). Importantly, this chiral arrangement cannot be reached by simple deposition of the prochiral molecules onto the surface (B and C).

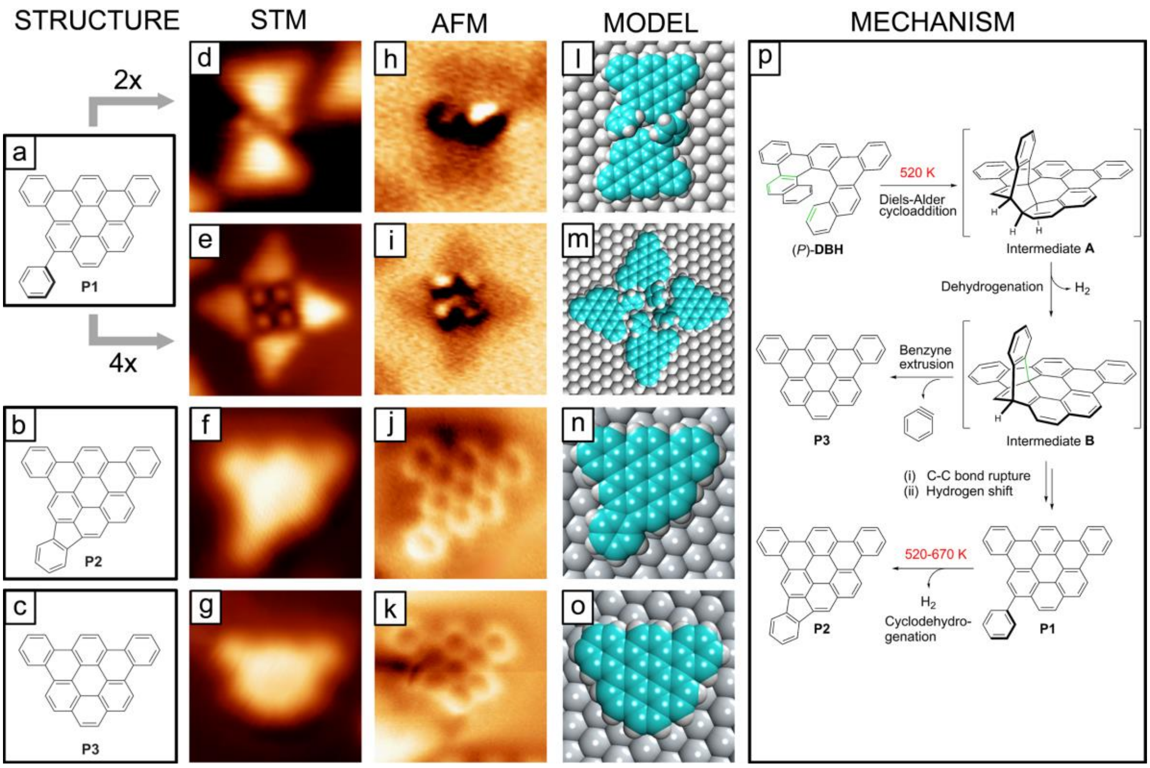

Fig.2. Molecular structures of polyaromatic molecules obtained during different stages of the chemical transformation on a crystalline silver surface (a-c). The accurate determination of the chemical structure of the individual products was carried out using scanning probe microscopes with high spatial resolution (d-k,l-o). The cascade of chemical reactions transforming the initial helicene molecules (DBH) into various intermediates and final products is schematically illustrated in (p).

From helical to planar chirality by on-surface chemistry
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Nature Chemistry
DOI: 10.1038/nchem.2662

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Institute of Physics of the Czech Academy of Sciences (FZÚ) is a public research institute, oriented on the fundamental and applied research in physics. FZÚ is the largest institute of the Czech Academy of Sciences and its present research program comprises six branches of physics: particle physics, the physics of condensed matter, solid state physics, optics, plasma and laser physics. These research branches also define how the institute is structured into six major research divisions.

The Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences (IOCB Prague) is a leading scientific institution in the Czech Republic, recognized internationally. Its primary mission is basic research in the fields of chemical biology and medicinal chemistry, organic and material oriented chemistry, chemistry of natural compounds, biochemistry and molecular biology, physical chemistry, theoretical chemistry, and analytical chemistry. The Institute's emphasis on interaction between chemistry and other sciences leads frequently to medicinal, pharmaceutical and other applications. An integral part of the mission of the Institute is to transfer the scientific results into assets which help people to live better lives.