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New high-performance catalyst for selective hydrogenation on an industrial scale from LIKAT

Regine Rachow Press Office

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The development of new active ingredients is the basis for innovative medicines and crop protection products. Together with the Process Development Department of Bayer AG's Crop Science Division, a research group at the Leibniz Institute for Catalysis in Rostock, LIKAT, has developed a practical catalyst for one of the most important reactions in active ingredient production, the hydrogenation of so-called carbon double bonds.

The new catalyst works on the basis of a noble metal with a ligand specially optimized for this reaction, which delivers the product in a very high yield. And it proceeds in a decidedly "selective" manner, as the head of the research group Dr. Kathrin Junge from the department of Prof. Matthias Beller says.

Bayer Crop Science has now announced that the process has now been transferred to the technical pilot scale above 100 kilograms - with equally good results as in the laboratory. "It has thus reached a decisive milestone in the industrialization of the process," says Dr. Christian Beier, who heads chemical process development at Bayer Crop Science.



Presentation of a successful collaboration (from left to right): Dr. Christoph Schotes from Bayer AG and Dr. Thomas Leischner, Dr. Kathrin Junge and Prof. Matthias Beller from LIKAT. Photo: Bayer Crop Science



In many chemical reactions, biologically active molecules are formed in two variants, also known as enantiomers. These molecules have an identical structural formula, but the atoms are arranged differently, like image and mirror image or right and left hand. In nature, only one of the two molecular forms usually exhibits the desired properties. Chemists call a catalyst "selective" when it ensures, in this case, that the reaction produces only the "right-hand" variant of molecules. Says Dr. Junge: "That's exactly what our catalyst does; it's enantioselective."

At cooperation partner Bayer Crop Science, the catalyst is needed for a new, more sustainable alternative process for producing an intermediate in the production process of a new fungicide. The reaction should meet those parameters that are necessary for industrial implementation. In addition to yield and selectivity, this includes the catalyst's lifetime, measurable by the number of reaction cycles it "survives" without losing its effectiveness. "Cost-effectiveness in this case starts at more than 10,000 such cycles, and that is what we have achieved," explains Kathrin Junge.

The key step in the production of the intermediate is hydrogenation, one of the most common chemical reactions in organic chemistry. In this process, double bonds between carbon atoms, so-called unsaturated compounds, are broken by the addition of hydrogen. One example is fat hardening in margarine production.

For one and a half years, two doctoral students and one postdoctoral scientist from Dr. Kathrin Junge's team were involved in the work together with experts from Bayer. A "successful pilot", as now reported by Bayer, means that the ideas from the laboratory are transferred to "real life" and the process is ready for application. This is something that research institutes achieve comparatively rarely. LIKAT has a particular strength here and transfers such processes several times a year, says Dr. Kathrin Junge.

Scientific contact persons:

Dr. Kathrin Junge Email: Kathrin.Junge@catalysis.de Phone: +49 (0) 381 1281-138

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J. Schneekönig, W. Liu, T. Leischner, K. Junge, C. Schotes, C. Beier, M. Beller, *Org. Process Res. Dev.* **2020**, *24*, 443-447, Application of Crabtree/Pfaltz-type iridium complexes for the catalyzed asymmetric hydrogenation of an agrochemical building block.