Researchers synthesize bio-based Methylcyclopentadiene with 3-Methylcyclopent-2-enone

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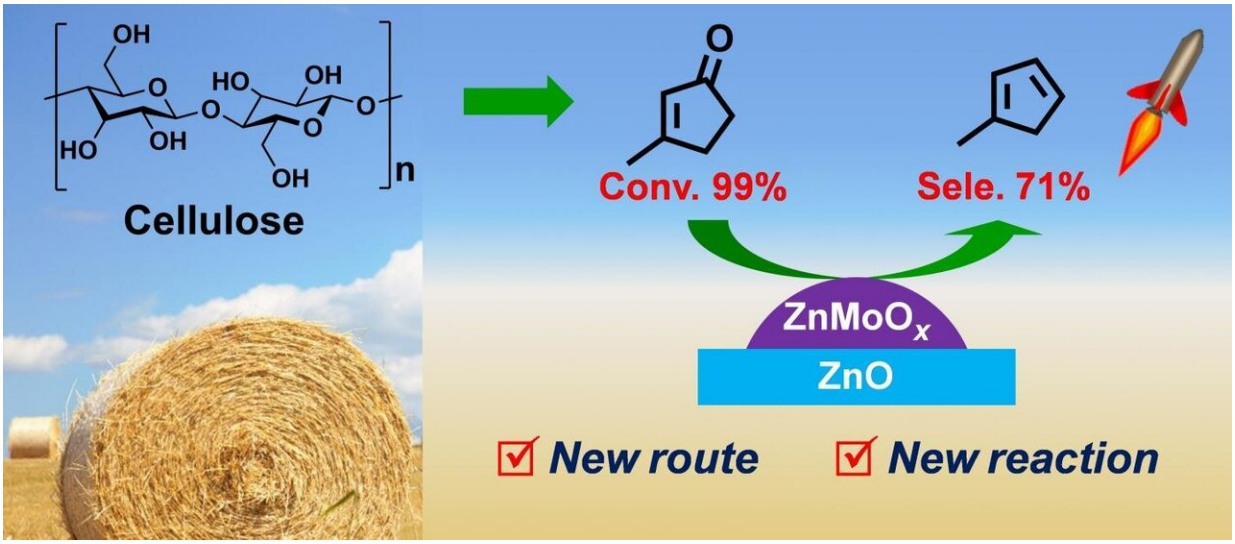

Direct hydrodeoxygenation of MCP to MCPD on the partially reduced Zn-Mo oxide catalyst. Credit: DICP

Methylcyclopentadiene (MCPD) is an important monomer in the production of RJ-4 fuel, a high-energy-density rocket fuel, and various valuable products.

Currently, MCPD is mainly obtained from the by-products of petroleum cracking tar at a very low yield of ~ 0.7 kg ton^{-1} and high price of

~10,000 USD ton^{-1}. The exploration of highly efficient processes to convert renewable biomass to MCPD is stimulated by the energy and environment problems.

Recently, a group led by Prof. Li Ning and Prof. Zhang Tao from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) synthesized bio-based MCPD via direct hydrodeoxygenation of 3-methylcyclopent-2-enone (MCP) derived from cellulose.

Their study was published in *Nature Communications* on Jan. 4.

The researchers found that selective hydrodeoxygenation of MCP to MCPD could be achieved on the partially reduced Zn-Mo oxide catalyst.

The Zn-Mo oxide catalyst formed $ZnMoO_3$ species during the reduction of $ZnMoO_4$, which might preferentially adsorb C=O bond in the presence of C=C bond in vapor phase hydrodeoxygenation of MCP led to highly selective formations of MCPD with a carbon yield of 70%.

"This is a following work of our previous report about the synthesis of 2,5-hexanedione by the direct hydrogenolysis of cellulose and the intramolecular aldol condensation of 2,5-hexanedione to MCP," said Prof. Li.

This study opens up a horizon for the production of dienes with unsaturated ketone by a direct hydrodeoxygenation process.

More information: Yanting Liu et al, Synthesis of bio-based methylcyclopentadiene via direct hydrodeoxygenation of 3-methylcyclopent-2-enone derived from cellulose, *Nature Communications* (2021). DOI: 10.1038/s41467-020-20264-3