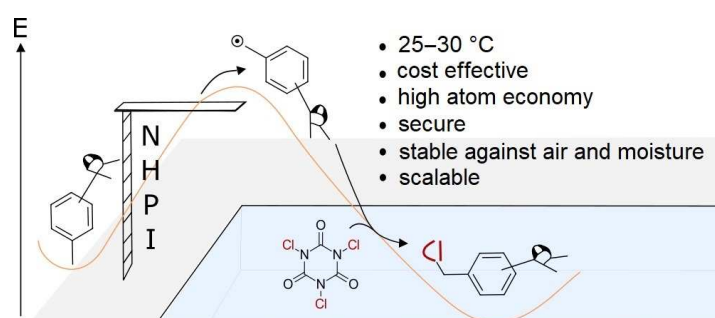


Mild and cost-effective halogenation of alkanes and alkyl groups

Halogenation of alkyl-, cycloalkyl- and benzyl-derivatives, TCCA, DIH, chemistry, synthesis

DESCRIPTION OF TECHNOLOGY / PRODUCT

Alkyl-halides and especially benzyl-halides are important intermediates within chemical production. They are manufactured and processed on a multi-ton-scale. Usually they are produced by use of elemental halides (chlorine, bromine) or by use of highly reactive and also harmful and very corrosive compounds like, e.g., sulfuryl chloride, thionyl chloride etc. Also, these conventional processes often require high reaction-temperatures and use CCl_4 as solvent, which in the meantime is forbidden in many countries due to its cancerogenity and ozone-depletion-potential.



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The new halogenation process presented here allows for a considerable increase in the efficiency of the manufacturing of halogenated alkanes, halogenated cycloalkanes and especially of benzyl halogenides. It is based upon the usage of cost-efficient and non-hazardous halogenating agents, e.g. trichloroisocyanuric acid (TCCA), *N*-iodosuccinimide (NIS), 1,3-diiodo-5,5-dimethylhydantoin (DIH) and other halogenating agents in combination with *N*-hydroxyphthalimide (NHPI) as radical initiator. Especially TCCA provides enormous cost- and security-advantages for chlorination, because it is already produced and utilized on a multi-ton scale, e.g. for disinfection of swimming pools. Thus, its hazard-free handling is already established.

AT A GLANCE ...

TECHNOLOGY FIELD / SCOPE OF APPLICATION

Organic synthesis
 Halogenation
 Manufacturing of alkyl-, cycloalkyl- and benzyl halides

MARKET / BRANCH

- Chemical industry
 - Base chemicals
 - Specialty chemicals / Custom synthesis

USP

- Selective halogenation by use of non-hazardous halogenating agents
- Cost-effective process
- Energy-efficient procedure at room-temperature

DEVELOPMENT STATUS

- ✓ The practicability is proven by way of laboratory experiments
- Next steps: Educt-screening regarding further suitable educts and scale-up

PATENT PORTFOLIO

Priority application (EP) was filed in November 2016, pending.

REFERENCE NO.: **TM 930**

The halogenating methods presented herein using NHPI as radical initiator are performed at room temperature which additionally offers enormous energetic advantages against other methods.

SCOPE OF APPLICATION

The new halogenating method can be favourably applied in the area of industrial organic synthesis. After appropriate upscaling (already done on lab-scale) into production-scale it can be applied at manufacturing of base chemicals, e.g. benzyl chloride, benzyl bromide, benzyl iodide. Besides being interesting for large scale industry the method is also of great interest for specialty chemicals manufacturers who perform customer synthesis on laboratory scale.

ADVANTAGES COMPARED TO STATE OF THE ART

Within the new halogenating method less risky halogenating agents can be applied (especially TCCA for chlorinations) and the reaction takes place at distinctly lower temperatures. It is therefore much more energy- and atom-economic than other methods (three active chlorine atoms in TCCA). On the whole the method thus offers an enormous potential for cost reduction for the producing chemical industry.

DEVELOPMENT STATUS

The basic principles of the process have been proven on lab scale by several experimental series, applying gc/ms- and nmr-technologies as well as elementary analysis upon the isolated and pure products.

MARKET POTENTIAL

Halogenated hydrocarbons are very important base chemicals which are widely used within chemical industry. The method offers an enormous potential for cost-reduction and is of great relevance for huge companies as well as for smaller manufacturers of specialty chemicals.

OFFER

On behalf of its shareholder Justus-Liebig-Universität Giessen, TransMIT GmbH is looking for cooperation partners or licensees for further development or usage of the technology in Germany, Europe, US, and Asia.

A TECHNOLOGY OF



REFERENCE NO.: **TM 930**

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