

// SUSTAINABLE AND EFFICIENT CHLORINATION OF ALCOHOLS

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HINTERGRUND

Chlorination of alcohols is a crucial step in the production of e.g. pharmaceuticals, pesticides, dyestuffs and disinfectants.

PROBLEMSTELLUNG

Substitution reactions of hydroxy groups of alcohols with nucleophiles to give halides are a fundamental transformation of organic chemistry. In most cases direct substitution of a hydroxy function by a nucleophile is not possible, since the hydroxy group is a poor leaving group. However, most of the literature known methods to activate hydroxy functions (to e.g. chlorides) produce large waste amounts and are therefore cost-intensive. For instance the well-known Appel reaction requires the use of stoichiometric amounts of triphenylphosphane (and highly carcinogenic tetrachloromethane), which in the course of the reaction is converted into triphenylphosphane oxide as a high molecular weight waste product.

LÖSUNG

Inventors of Saarland University created a new catalytic procedure for the chlorination of alcohols with a variety of advantages. Substances produced by the new method are for example Neryl chloride [CAS 20536-36-1], 3-Methyl-3-butenyl chloride [CAS 10523-96-3], Geranyl chloride [CAS 5389-87-7] and Prenyl chloride [CAS 503-60-6].



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ENTWICKLUNGSSTAND

Machbarkeit

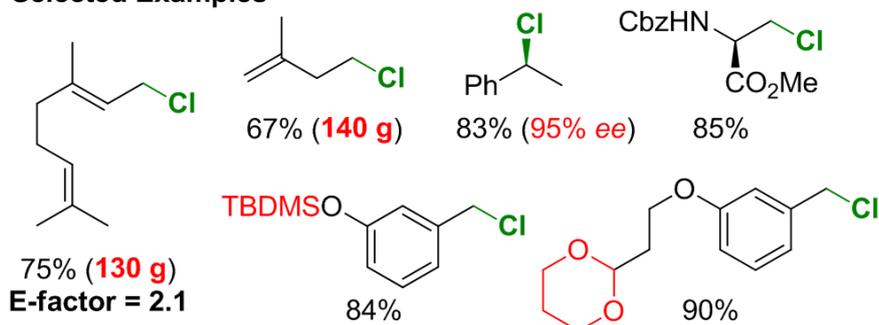
PATENTSITUATION

PCT anhängig
LU in priority year anhängig

CATEGORIES

//Neue Substanzen //Synthesen und
Verfahrenstechnik

Selected Examples



VORTEILE

- High Cost-Efficiency: Utilization of low-cost commercial available, low-molecular weight catalysts and an inexpensive commodity chemical as sole reagent.
- Good Sustainability: Chlorinations are performed in environmental-friendly solvents (e.g. MTBE, 2-MeTHF and acetone) or even under solvent-free conditions with Economy-factors being typically in the range of 1.5-6.
- Superior Scalability: Already in standard laboratory equipment chlorinations in 500-2000 mmol scales were conducted routinely.
- Excellent Stereo- and Regioselectivity: Chiral alcohols are efficiently inverted (99% ee \square \geq 95% ee); Allylic alcohols are chlorinated without isomerisation.
- Excellent Functional Group Compatibility and broad substrate scope: High Tolerance of acid-sensitive functional groups (e.g. TBDMSO-, tBuO₂C-, BocHN-); The method is applicable to primary, secondary and tertiary alcohols.

ANWENDUNGSBEREICHE

Chlorination of alcohols for production of e.g. pharmaceuticals, pesticides, dyestuffs and disinfectants.

SERVICE

We are looking for partners for further development and commercialisation of the invention.

PUBLIKATIONEN & VERWEISE

P. H. Huy, S. Motsch, S. M. Kappler, "Formamides as Lewis Base Catalysts in S_N Reactions - Efficient Transformation of Alcohols into Chlorides, Amines, and Ethers", *Angew. Chem. Int. Ed* 2016, 55, 10145-10149
