



“Innovative Industrial Transesterification Catalysts”

Context

Transesterification is a crucial step in several industrial processes such as the production of higher acrylates or active pharmaceutical ingredients.

Typical catalysts for these reactions are alkoxides or hydroxides from alkali metals and titanium or tin-based alkoxides. For specific purposes, mineral acids, non-ionic bases and enzymes are used. Despite general use, these catalysts suffer from drawbacks if functional groups such as unsaturated bonds or amines are present in the reactant ester or alcohol.

Technical Description

This invention describes a highly active and selective transesterification catalyst for the industrial production of esters. The objective is achieved by reacting an ester and an alcohol in the presence of a catalyst consisting of a metal 1,3-dicarbonyl complex acting in combination with a salt.

The reported catalysts are prepared from readily available starting materials within the reaction medium without the need for prior isolation (in-situ preparation) and act via an innovative **dual activation** mechanism.

Benefits

These catalysts have the following **advantages**:

- *High selectivity and tolerance towards functional groups*
- *Easy preparation (mixture of two known salts)*
- *Inexpensive*
- *Easy separation*
- *Reusable*
- *Enhanced tolerance towards water (no drying required)*
- *Non-toxic Zn²⁺ or Fe³⁺*

Our Reference:

ECSPAT_002

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Transesterification, Catalysis, Mixed salt

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"Transesterification process using mixed salt acetylacetonates catalysts"

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Europe, US, Japan, China

Granting pending in:
South Korea, Mexico and Brazil

Applicant :

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Target

- (Functional) (meth)acrylates
- Multi-functionalized (heterocyclic) esters in pharmaceutical process development

Further ongoing developments

- Testing of catalyst combinations on specific substrates of customers.
- Smart throughput screening of catalysts, including benchmark catalysts.

Relevance/Opportunity

A mild and selective transesterification catalyst is presented as an alternative for $Zr(acac)_4$ which is described in over 20 catalyst patents. The mixed catalyst consists of **iron** or **zinc acetylacetonate** working in combination with a judiciously selected salt and shows similar selectivity and kinetic profiles as the Zr counterpart, but has the additional advantage of being less expensive, having an enhanced tolerance towards water and being more easily removable. Particularly, the **successful transesterification with 1,2- and 1,3-diols is unique**, as these substrates are known to deactivate metal catalyst due to their chelating properties.

*The invention has commercial relevance for chemical and pharmaceutical companies because **freedom to operate** can be offered for all substrates in transesterification reactions (the conventional catalysts are replaceable by **a novel protected species**) and the high functional group tolerance opens the door for **a one-step industrial production** of a wide range of esters, in particular **new acrylate monomers**.*

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