

A Comprehensive Strategy Towards Structure Elucidation of Hydroformylation Bottoms

C. Loeschel, R. Fels-Brendel, K.-H. Gunzelmann, R. Doetzer
BASF

Abstract

While the desired product in hydroformylation chemistry is often well defined and isolated with high specificity and yield, the byproducts formed in the oxo-process still contains a large amount of functionalized hydrocarbons with a variety of uses. These include applications as solvents in leather and textile processing, in metal processing, in industrial water treatment, and as surface tension modifiers. Due to the high complexity of these mixtures, full characterization, which is a significant hurdle for regulatory approval of such streams, presents a challenge; this challenge results in many potentially useful streams to be incinerated rather than being utilized as a product.

Herein, we present a comprehensive analytical approach to characterization of the hydroformylation bottoms of 1-octene. At its core stands the grouping of isomeric compounds into peak clusters using a combination of mass spectrometry approaches, particularly by means of combination of a soft (FI) and hard (EI) ionization technique. Separation of isomers is further achieved by comprehensive GC separations and ion mobility techniques. We also highlight the utility of field ionization over chemical ionization in the characterization of UVCB substances.