Insights into olefin oligomerization products based on GC×GC-PI-TOFMS

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Catalyzed olefin oligomerization has been widely used to produce fuels and chemicals in the petrochemical industry [1]. The feedstock light olefins, namely ethylene, propene, butene, and pentene, are catalyzed over acidic catalysts or metal-based catalysts under typical oligomerization conditions [1]. In this study, we investigated the composition of dodecene products catalyzed by acidic catalysts, solid phosphoric acid (SPA) and zeolite, from various feedstocks, propene, propene + butene, butene, propene + nonene during oligomerization reaction.

The instrument applied in this study is two-dimensional gas chromatography (GC × GC) coupled photoionization (PI) - time of flight mass spectrometry (TOFMS). The distributions of olefin congeners, dodecene structural subgroups, and dodecene isomers were obtained by the developed method [2]. Various data sets enabled the multimodal characterization of the dodecene products from different production pathways.

By using the data set of dodecene structural subgroup distribution, the SPA and zeolite catalyzed products can be distinguished by principal component analysis (PCA) and hierarchical clustering analysis (HCA). In general, zeolite produced more linear dodecene isomers, and SPA produced more branched isomers. The T-test and partial least squares-discriminant analysis (PLS-DA) identified a few important features / dodecene isomers which could be used as catalyst indicator. Based on the data set of dodecene isomer distribution, the dodecene products from different feedstocks can also be distinguished except for propene and propene + nonene groups, which indicated the product composition from these two feedstocks did not have significant differences. Two samples with unknown feedstock composition were cumulated close to the groups of propene and propene + nonene in PCA scores. This suggested that butene was not contained in their feedstocks.

References

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