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Production of jet and diesel fuel blend stocks from dienes via catalysis

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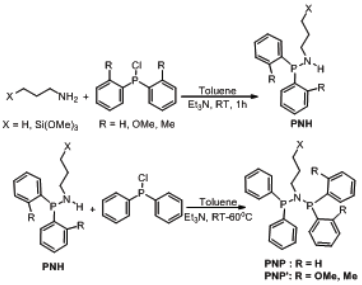
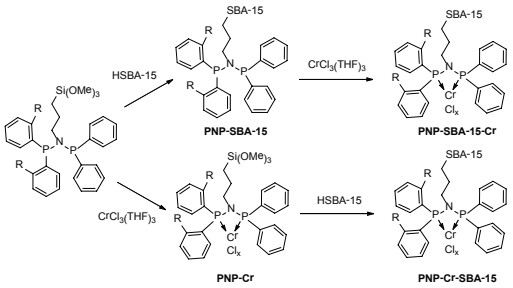
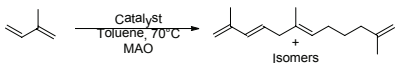
The objective of this work is to develop catalysts (homogeneous and heterogeneous) for the controlled oligomerization of dienes as a route to jet and diesel range hydrocarbon fuel blendstocks. Chromium-based catalysts with homogeneous PNP-type ligands demonstrate excellent reactivity with very high selectivity. Ligand structure plays a key role in controlling selectivity towards trimerized products. These ligands offer the ability to widely vary the electronic and steric environment at the metal center to control product selectivity. Heterogeneous catalysts are preferred in industrial use where product separation and catalyst recovery are of prime importance. We developed an active heterogeneous Cr-based catalyst for selective oligomerization of dienes. We first prepared the homogeneous ligands (Scheme 1) and validated the diene oligomerization (Scheme 2), subsequently synthesized PNP-SBA-15-Cr/PNP-Cr-SBA-15 heterogeneous ligand and tested the oligomerization of dienes. The symmetric ligand Ar2PNRPAr2 -SBA-15 and unsymmetric ligand Ar2PNRPAr2'-SBA-15 are of interest in our work because of the range of active site structures available. The symmetrical PNP ligand, where Ar is phenyl, and the asymmetrical PNP' ligand, where Ar' is o-methoxyphenyl/o-methylphenyl, were synthesized using propyl amine and chloro diarylphosphine (Scheme 2). The PNP-SBA-15-Cr/PNP-Cr-SBA-15 hetereogeneous ligands were used for the controlled oligomerization of isoprene in the presence of methylaluminoxane (MAO) at 70 °C (Scheme 3) in toluene.

Ligand Synthesis



HeterogeneousCatalyst Synthesis





Scheme 3. Trimerisation of isoprene

Biography

Padmaja Gunda has completed her Ph.D. in Organic Synthesis from The City University of New York. She has 8 years of research experience in catalysis (organic and organometallic). She also holds adjunct lecturer appointment in the Department of Chemistry, Washington State University-Tri cities. She is a DOE-EERE Awardee at PNNL (Pacific Northwest National Laboratory). She is one of four researchers that the DOE/Office of Bioenergy Program is sponsoring at various national laboratories. She received this sponsorship through a competitive proposal process. Her research is making great strides in the area of biobased jet and diesel range hydrocarbon fuels.

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