# Catalysts for High Cetane Ethers as Diesel Fuels


## ABSTRACT

A tungstena-zirconia (WZ) catalyst has been investigated for coupling alcohols to unsymmetrical ethers and compared with earlier studied sulfated-zirconia (SZ) and Nafion-H catalysts. In all cases, the ether synthesis mechanism is a dual site $S_N2$ process involving competitive adsorption of reactants on proximal acid sites. At low reaction temperatures, methylisobutylether (MIBE) is the predominant product. However, at temperatures >135°C the WZ catalyst is very good for dehydration of isobutanol to isobutene. The surface acid sites were diagnosed by high resolution X-ray photoelectron spectroscopy (XPS) of N 1s shifts after adsorption of amines. Using pyridine, ethylenediamine, and triethylamine, it is shown that WZ has heterogeneous strong Brønsted acid sites. Theoretical study located the transition state and accounted well for XPS core-level shifts upon surface acid-base interactions. While computations have not been carried out with WZ, it is shown that the SZ catalyst is a slightly stronger acid than $CF_3SO_3H$ (a model for Nafion-H) by 1.3-1.4 kcal/mol.