Introduction

Molecular engineering of biofuels can be accomplished through the use of model compound studies in combination with property prediction. Model compound studies give insight to the fundamental relationships between a catalyst and a molecule that govern product selectivity. In order to provide direction towards an optimized feed, fuel properties of interest (CN, ON, solubility in water, vapor pressure, stability, cloud point, etc.) must be known for each specific reaction product. For this reason, we implement QSPR to predict fuel properties of molecules whose properties have not previously been measured. With this tool, direction is given towards the specific bonds that must be broken, etc. in order to maximize the value of a fuel. Information gained through these studies is then used to develop optimized strategies for upgrading of biofuels.

Applications to model compound studies

Model compound studies and kinetic analysis

QSPR prediction of fuel properties of potential reaction products

Results:

Maximum properties except for BP obtained with Cu at 290 °C while maximizing 2-methylfuran

Representative of compounds present in bio oil

Conclusions

A combination of QSPR with model compound studies provides direction for molecular engineering of fuels. Through these studies, catalytic strategies can be developed by optimizing fuel properties while at the same time understanding the fundamental relationships between the molecules and catalysts.

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