

Chemistry Theory Overview

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Overview

Method Development

Large Molecules

Applications

Alcohols

Biodiesel

Foundational Chemistry

Accuracies



Method Development

Three Complexities for Large Molecules

Accurate Energies

Size-Extensive Reduced Scaling

MRSDCI

Accurate Partition Functions

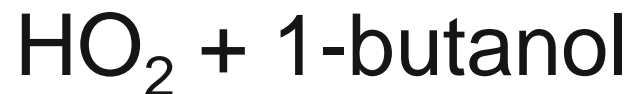
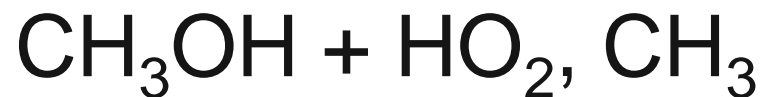
Multi-Structural Torsional Treatment

Arbitrary Molecules

Reaction Mechanism Generator



Alcohols



$\text{C}_4\text{H}_9\text{O}$ Decomposition



iso-butanol Decomposition

RMG mechanisms for all butanols



Thermochemistry

Methyl Formate for Validation

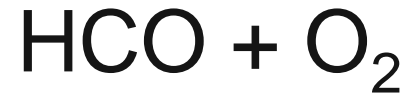
Abstractions by H, CH₃, O, OH, HO₂

Beta Scission

Calculations in progress for larger Esters



Foundational Fuel Chemistry



Uncertainties

MRSDCI - Energies

Torsional Treatments

Ab Initio Rovibrational Analysis



Future

Better coupling between specific evaluations and development of general rules

Butanol

Abstraction by OH, HO₂, CH₃, for 1-butanol, isobutanol, and buteraldehyde

Decomposition of 1-butanol, 2-butanol, and t-butanol



Future

Esters

Larger Esters

Abstractions, Beta-Fission, Decomposition

Kinetics

Foundational Fuels

$\text{HO}_2 + \text{RO}_2$

$\text{HO}_2 + \text{alkenols}$

Butyl + O_2



Questions

Prioritization of our efforts is always needed.

How accurate do our rate coefficients need to be?

Should we be focussing our efforts on generating rate coefficients or on improving our methods?

What role do we want theory to play in C0-C4 mechanism developments?

Are we aiming for the mechanism or many individual mechanisms?

Are there needs for RMG that could benefit from the input of other theoreticians on the team?

Should we all be making group rules for RMG?

Do we want to make RMG a community tool?

Shouldn't dimethyl ether really be one of our primary targets since this provides the best contact with the turbulence modeling.

