

Applying Computational Quantum Chemistry to Devise a Reaction Mechanism for Use of Morpholine, a Surrogate Biofuel

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One of the useful compounds for studying biofuel chemistry is morpholine (cyclohexane-1,3-dimethyl-2-aminomethyl-4-oxane), which resembles cyclohexane but containing ether and amine linkages in para positions in the ring. However, the literature contains few data on thermochemistry or kinetics. We have applied computational quantum chemistry to devise a combustion mechanism for morpholine, predicting concentration profiles in a premixed flat flame with a laminar convection-diffusion model. Although this type of flame is commonly used for observing combustion kinetics qualitatively, we were able to collect unusually detailed quantitative data by applying our photoionization molecular-beam mass spectrometry apparatus at the Advanced Light Source at Lawrence Berkeley National Laboratory. These data showed we had been able to predict the kinetics and thermochemistry with remarkable accuracy. By complementing the morpholine elementary-reaction model with models we have developed for esters and aldehydes, we are moving rapidly toward predicting performance characteristics of a wide range of biofuels.