Origin of 5-Hydroxymethylfurfural Stability in Water/ Dimethylsulfoxide Mixtures

Scientific Achievement

The first experimental evidence of competitive and selective solvation of the HMF carbonyl group by an aprotic solvent in the presence of water is revealed. This finding, in conjunction with the calculated effect of DMSO on the HMF LUMO energy, explain the enhanced stability of HMF toward degradation reactions when DMSO is used as an organic co-solvent.

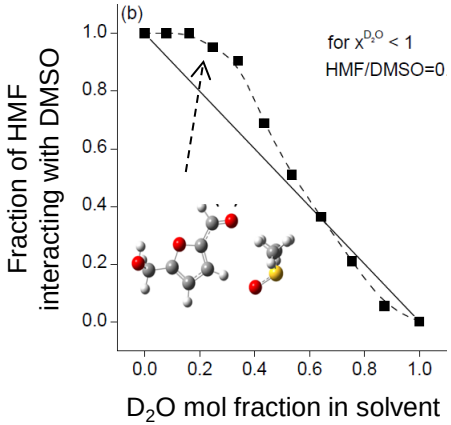
Significance and Impact

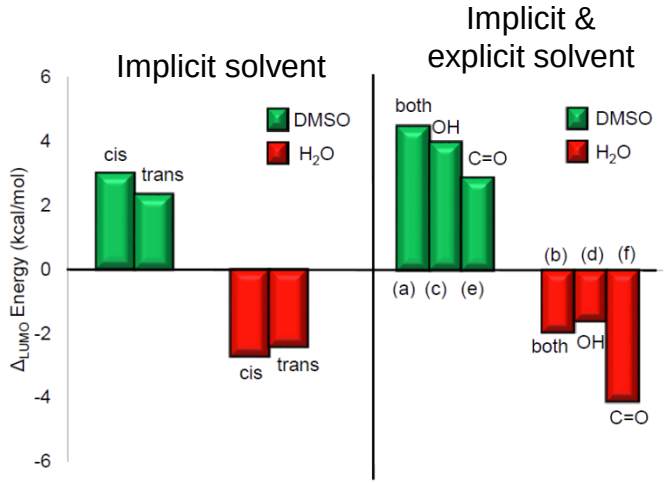
- Organic co-solvents in an aqueous reaction medium can significantly enhance HMF stability by minimizing rehydration and humin formation reactions
- The reasons behind the stability enhancement by organic co-solvents are elusive and prohibit our ability to rationally select co-solvents

Research Details

– Analysis of HMF FTIR spectra in mixed solvents reveals selective interaction of different HMF functionalities with solvent constituents

– DFT calculations in implicit and explicit solvents reveal the effect of solvent and solvent – HMF interactions on the HMF LUMO energy





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G. Tsilomelekis, T.R. Josephson, V. Nikolakis, and S. Caratzoulas, *ChemSusChem,* 2014, 7, 117 – 126
Work was performed at the University of Delaware