Fructose - Water - Dimethylsulfoxide Interactions by Vibrational Spectroscopy and Molecular Dynamics Simulations

Vladimiros Nikolakis,[1] *Samir H. Mushrif,*[1] *Bryon Herbert,*[2] *Karl S. Booksh,*[2] *Dionisios G. Vlachos*[1]

[1]Department of Chemical and Biomolecular Engineering, Catalysis Center for Energy Innovation, University of Delaware, 150 Academy Street, Newark, DE, 19716, USA

[2]Department of Chemistry and Biochemistry, University of Delaware, 102 Brown Laboratory, Newark, DE, 19716, USA

Supporting Information

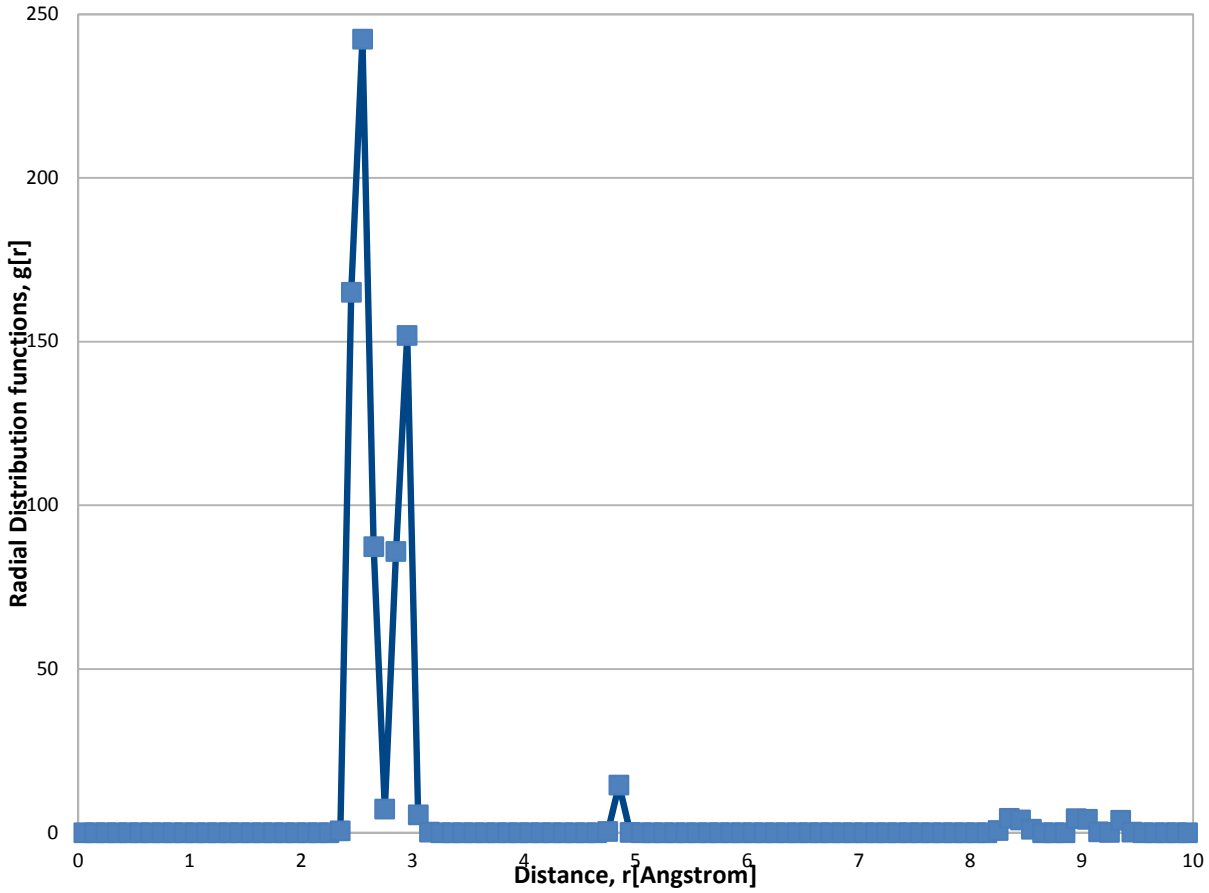

Figure SI.1: Radial distribution function of hydrogen atoms of O2 and O4, for f_{H2O}=0.

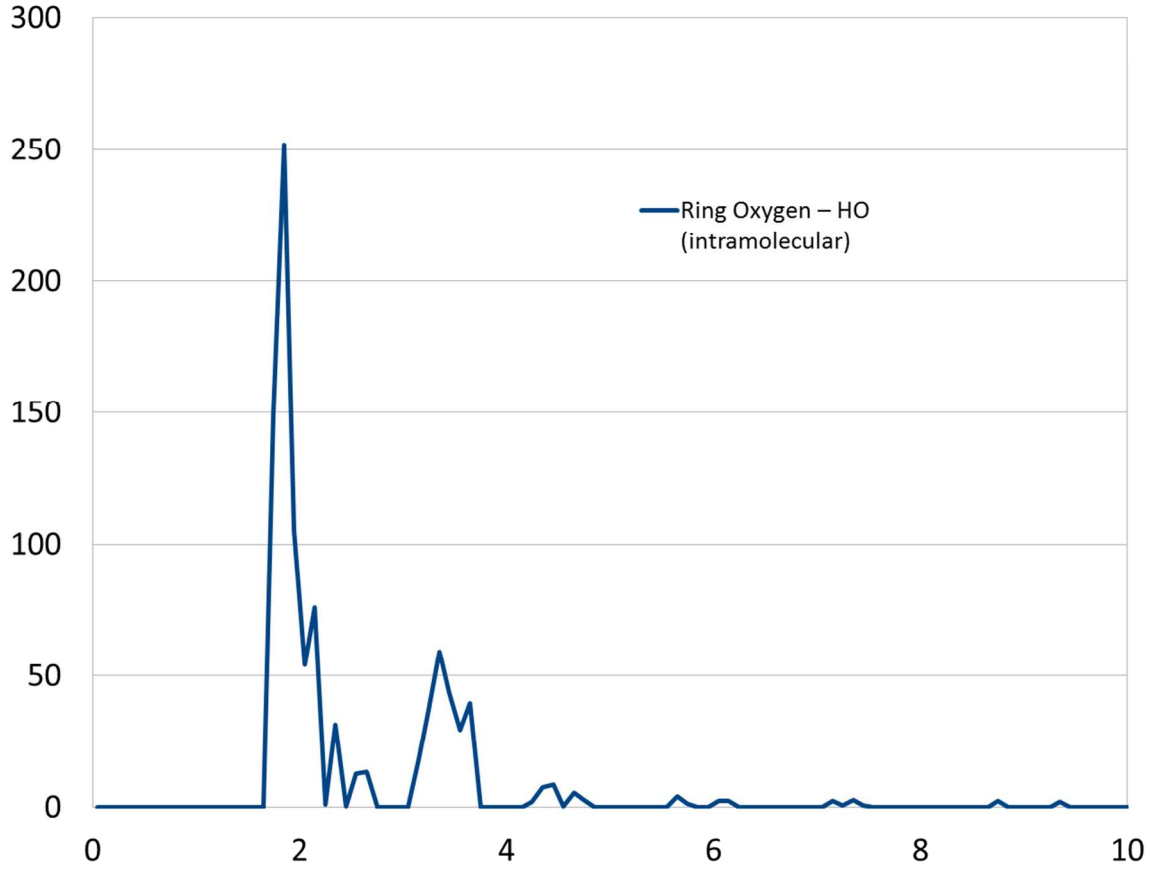

Figure SI.2: Radial distribution function of hydrogen of the furanose ring O5 and the hydrogen of O6Hfor f_{H2O}=0.

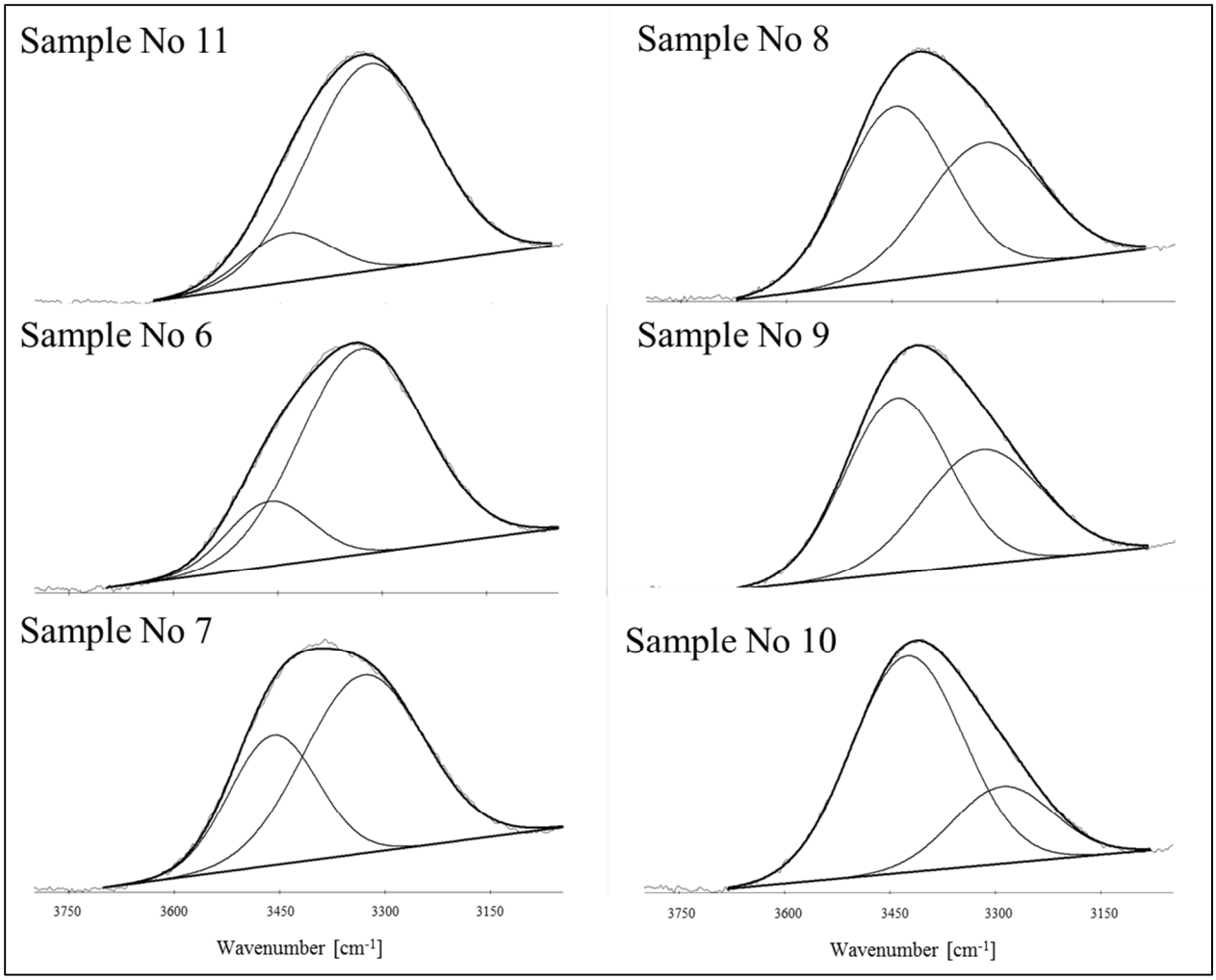

Figure SI.3: ATR/FTIR spectra of the fructose –DMSO- D_2O mixtures and corresponding curve fittings to two Gaussian-Lorentzian profiles. (The sample numbers correspond to those shown in Table 1 of the manuscript)