

ALKALI METAL-GLUCOSE INTERACTION PROBED WITH INFRARED PRE-DISSOCIATION SPECTROSCOPY

STEVEN J. KREGEL, BRETT MARSH, JIA ZHOU, ETIENNE GARAND, *Department of Chemistry, The University of Wisconsin, Madison, WI, USA.*

The efficient extraction of cellulose from biomass and its subsequent conversion to glucose derivatives is an attractive goal in the field of energy science. However, current industrial methods require high ionic strength and harsh conditions. Ionic liquids (IL's) are a class of "green" compounds that have been shown to dissolve cellulose in concentrations of up to 25 wt%. In order to understand IL's extraordinary cellulose dissolving power, a molecular level understanding of the IL-cellulose interaction is needed. Toward that end, we have acquired infrared pre-dissociation spectra of M^+ -glucose, where $M^+ = Li^+$, Na^+ , or K^+ . Through comparisons with density functional theory calculations, we have determined the relative abundances of various M^+ -glucose binding motifs in both the thermodynamic and kinetic limits. These results provide insight on the hydrogen bonding dynamics of glucose and are a step towards a fuller understanding of cellulose interactions with ionic liquids.