

Thermal Stability and CO₂ Uptake of Dicationic Ionic Liquids Containing 2-Cyanopyrrolide Anions

Junwon Park^{1, S}, Louise M. Cañada¹ and Joan F. Brennecke^{1, C}

¹*McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX, U.S.A.
jfb@che.utexas.edu*

Aprotic-heterocyclic anion (AHA) ionic liquids (ILs) have a potential as capture and reaction medium for carbon capture and utilization (CCU) processes. IL thermal stability is important if ILs are to withstand the extreme reaction conditions required for thermocatalytic conversion of CO₂. ILs paired with non-coordinating anions, such as bis(trifluoromethylsulfonyl)imide ([Tf₂N]⁻), have shown improvements in thermal stability when the cations were modified to have 2⁺ charge, so called dicationic ILs. However, to our knowledge, no study has paired dications with AHAs. To determine whether dicationic AHA ILs would have improved thermal stability and carbon dioxide (CO₂) reactivity compared to analogous monocationic AHA ILs, dicationic AHA ILs with 2-cyanopyrrolide anions and different chain lengths for the dication linkers were synthesized and characterized. Dicationic AHA ILs do show improvement in thermal stability compared to monocationic AHA ILs. Moreover, a CO₂ uptake experiment shows that AHA ILs uptake capacity is primarily affected by the chain length on the cation, which may affect the entropy of the reaction with CO₂. Air purging isothermal long-term thermal stress tests on phosphonium based dicationic AHA ILs show that these ILs are sensitive to the presence of oxygen due to decomposition to form phosphine oxides. This study provides new design options for AHA ILs to improve thermal stability.