P24: ILIMITED PROJECT: UNDERSTANDING THE WATER LIQUID SORBENTS FOR HIGH TEMPERATURE APPLICATIONS

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The ILIMITED project aims to intensify CO_2 hydrogenation to methanol through the in-situ removal of methanol and water, thereby shifting the reaction equilibrium and targeting yields above 80%. Since operating temperatures may reach 513 K, this concept requires liquid sorbents combining product affinity with negligible volatility and high thermal and chemical stability.

Temperature-programmed thermogravimetric analysis was used to screen phosphonium- and ammonium-based ionic liquids with different cations, anions, and functional groups. Molecular sieve 3A, TEGDME (tetraethylene glycole dimethyl ether), Santovac 5 (polyphenyl ether), and a UiO 66-containing composite were included as benchmarks.

The $LiNTf_2$–$[P_{1444}][NTf_2]$ reference showed pronounced low-temperature sorption and high stability, whereas neat $[P_{1444}][NTf_2]$ showed no detectable sorption. $[P_{66614}]Br$ retained relatively high sorption but was slightly less stable. Other $[NTf_2]^-$-based ionic liquids exhibited comparable stability, while dicyanamide and dimethyl phosphate substantially reduced it. Ether functionalization did increased sorption midly, while UiO-66 additive did not improved it. A solid sorbent molecular sieve 3A provided greater high-temperature uptake but was solid, TEGDME was highly volatile, and Santovac 5 was less stable than $[P_{1444}][NTf_2]$.

The results identify thermally stable $[NTf_2]^-$ ionic liquids as a promising platform while highlighting the remaining challenge of achieving strong sorption at ILIMITED operating temperatures.

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