

## Impact of nitrile functionalities in ILs for ethylene and ethane separation

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The solubility of ethane and ethylene was determined in a series of cyanopyridinium ILs known to form charge-transfer complexes with polyaromatics, to determine their potential to form specific interactions with the unsaturated gas. The solubility of the gases in 1-butyl-3-cyanopyridinium/1-butyl-4-cyanopyridinium/ bistrifluoromethylsulfonylimide ( $[C_3^4CNPy][NTf_2]$  and  $[C_4^4CNPy][NTf_2]$ ) was measured using an isochoric saturation method. The results show ideal ethylene separation selectivities between 1.2 and 1.4, in the same range as typical physisorbent ILs of similar MW, indicating no significant preferential IL-ethylene interactions.

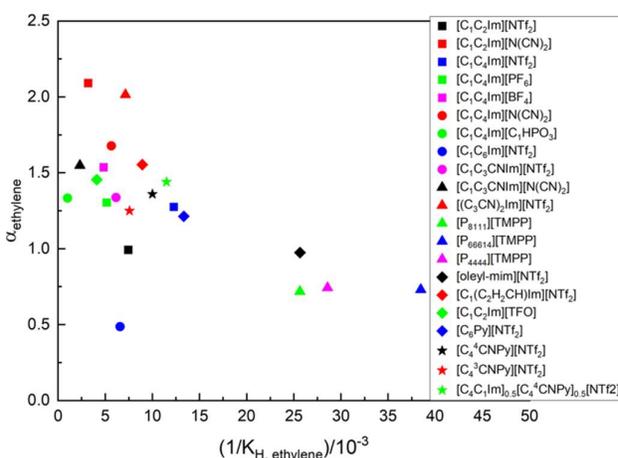


Figure 1: Ideal selectivity towards ethylene vs solubility at 313 K for reported literature data for ethylene and ethane separation in a variety of ILs.

To promote cyanopyridinium-ethylene interactions and decrease the possibility of steric constrictions to the interactions,  $[C_4C_1Im][NTf_2]$  was added as diluent to  $[C_4^4CNPy][NTf_2]$ . The mixture was found to behave almost ideally based on isothermal titration nanocalorimetry. Still, no specific gas-IL interactions were formed. MD simulations revealed that the slightly higher ethylene

solubility in  $[C_4^4CNPy][NTf_2]$  is due to a slightly stronger association with this cation.

## References

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I graduated in 2008 in MSc Chemistry (5-year) and in 2014 I completed a PhD in physical chemistry in the groups of Catherine Santini (CPE Lyon) and Margarida Costa Gomes (ICCF, Clermont-Ferrand). My thesis was awarded the 2018 European Federation of Chemical Engineering Excellence Award in Fluid Separations. After 4 years of post docs, including a MSCA Individual Fellowship in the Holbrey group in QUB, I was awarded a 5-year Royal Academy of

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