Supplementary Information

Cu(I)-containing room temperature ionic liquids as selective and reversible absorbents for propyne

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Fig. S-1 Photograph of a high pressure FT-IR cell

(a)      (b)

[DMIM][CuCl(MeHPO₃)]    \[DMIM][Cu(MeHPO₃)₂]

Fig. S-2 Optimized structures of [DMIM][CuCl(MeHPO₃)] and [DMIM][Cu(MeHPO₃)₂]: (a) [DMIM][CuCl(MeHPO₃)] ($\Delta G = -184.8$ kJ/mol), (b) [DMIM][Cu(MeHPO₃)₂] ($\Delta G = -115.4$ kJ/mol).
Fig. S-3a Computed FT-IR spectrum of 2[DMIM][MeHPO₃]. 3279, 3205 (C4-H stretching) 3074 (C2-H stretching mixed with C-H stretching), 2988 (C2-H stretching) 2241, 2229 (P-H stretching).

Fig. S-3b Computed FT-IR spectrum of Cu-RTIL prepared from CuCl and 2[DMIM][MeHPO₃]. 3262 (C4-H stretching, Cl interacting), 3238 (C4-H stretching, phosphite interacting), 3058 (C2-H interacting with phosphite coordinated to Cu), 2918 (C2-H), 2300 (P-H stretching, Cu-coordinated), 2227 (P-H stretching).
Fig. S-4a FT-IR spectra showing the interaction of [DMIM][MeHPO₃] with propylene: (a) propylene, (b) [DMIM][MeHPO₃] (c) (b)+propylene, (d) (c) after N₂ flushing.
Fig. S-4b FT-IR spectra showing the interaction of [DMIM][MeHPO₃] with propyne: (a) propyne, (b) [DMIM][MeHPO₃] (c) (b)+propyne, (d) (c) after N₂ flushing for 10 min, (e) (d) after N₂ flushing for additional 30 min.
Fig. S-4c FT-IR spectra showing the interaction of Cu-RTIL (CuCl/[DMIM][MeHPO₄] = 1/2) with propylene: (a) propylene, (b) Cu-RTIL, (c) (b)+ propylene, (d) (c) after N₂ flushing for 10 min.
Fig. S-4d FT-IR spectra showing the interaction of Cu-RTIL (CuCl/[DMIM][MeHPO₃] = 1/2) with propyne: (a) propyne, (b) Cu-RTIL (c) (b)+propyne, (d) (c) after N₂ flushing for 10 min, (e) (d) after N₂ flushing for additional 30 min.