Supplementary Material (ESI) for *PCCP*

Supplementary Information

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

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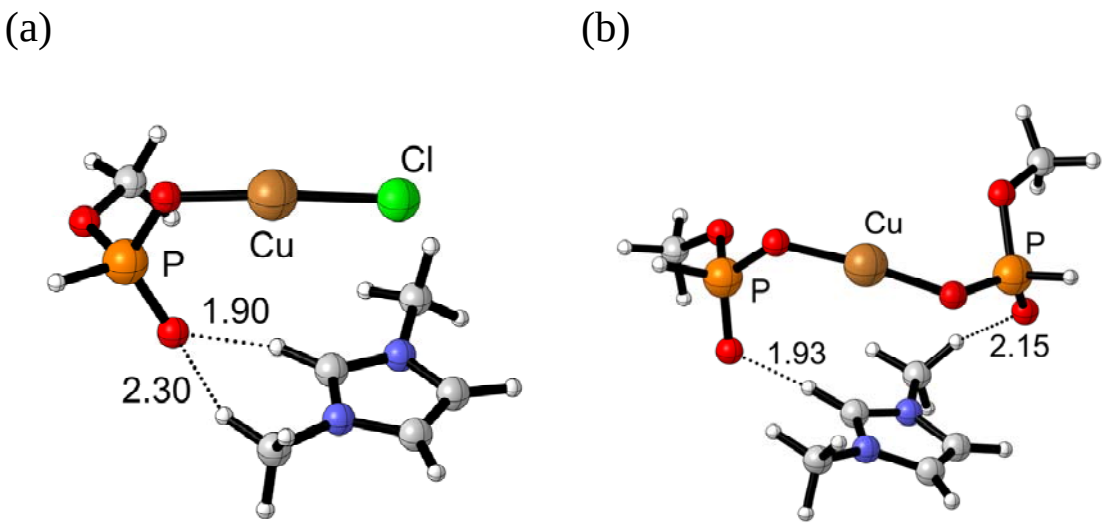
Fig. S-1 Photograph of a high perssure FT-IR cell



[DMIM][CuCl($MeHPO_3$)] [DMIM][Cu($MeHPO_3$)$_2$]

Fig. S-2 Optimized structures of [DMIM][CuCl($MeHPO_3$)] and [DMIM][Cu($MeHPO_3$)$_2$]: (a) [DMIM][CuCl($MeHPO_3$)] (ΔG = -184.8 kJ/mol), (b) [DMIM][Cu($MeHPO_3$)$_2$] (ΔG = -115.4kJ/mol).

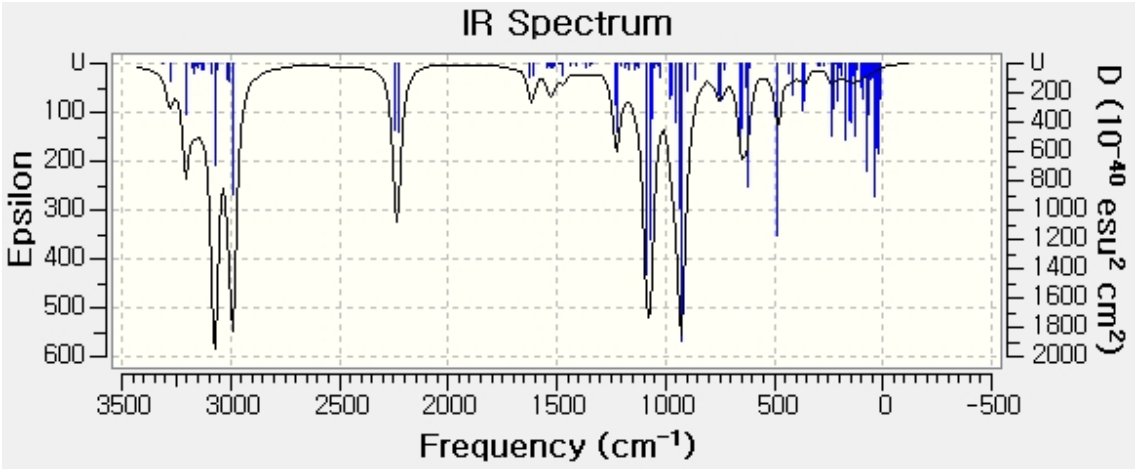


Fig. S-3a Computed FT-IR spectrum of 2[DMIM][$MeHPO_3$]. 3279, 3205 (C4-H stretching) 3074 (C2-H stretching mixed with C-H stretching), 2988 (C2-H stretching) 2241, 2229 (P-H stretching).

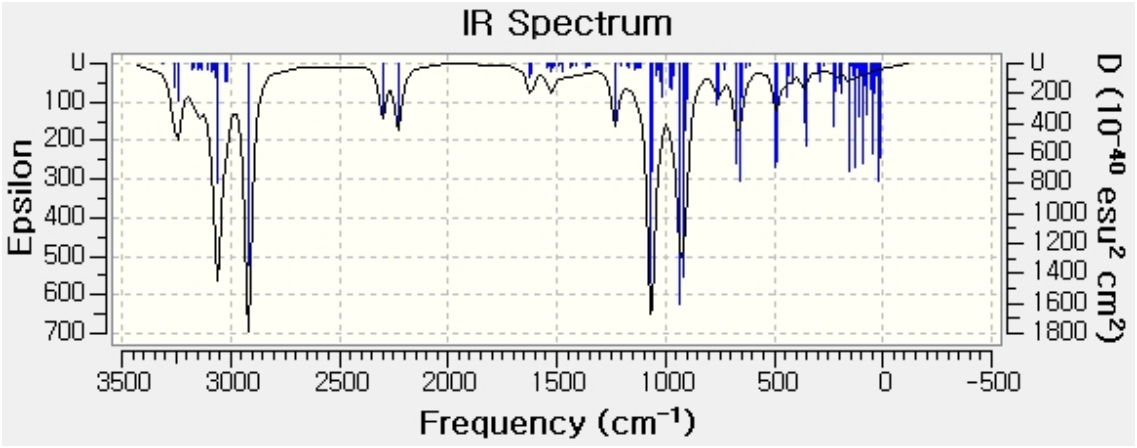


Fig. S-3b Computed FT-IR spectrum of Cu-RTIL prepared from CuCl and 2[DMIM][$MeHPO_3$]. 3262 (C4-H stretching, Cl interacting), 3238 (C4-H stretching, phosphite interacting), 3058 (C2-H interacting with phosphite coordinated to Cu), 2918 (C2-H), 2300 (P-H stretching, Cu-coordinated), 2227 (P-H stretching).

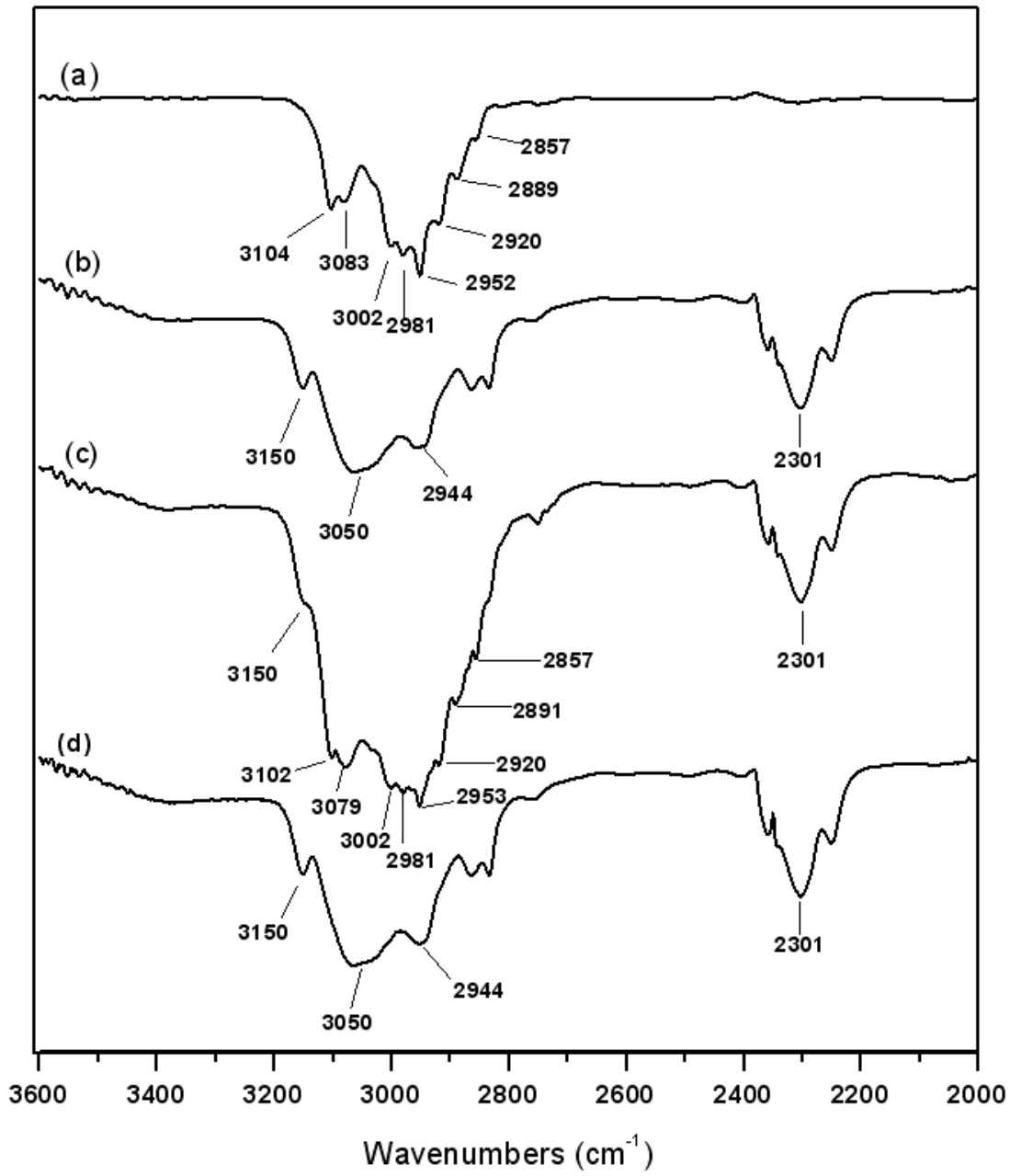


Fig. S-4a FT-IR spectra showing the interaction of [DMIM][$MeHPO_3$] with propylene: (a) propylene, (b) [DMIM][$MeHPO_3$] (c) (b)+propylene, (d) (c) after N_2 flushing.

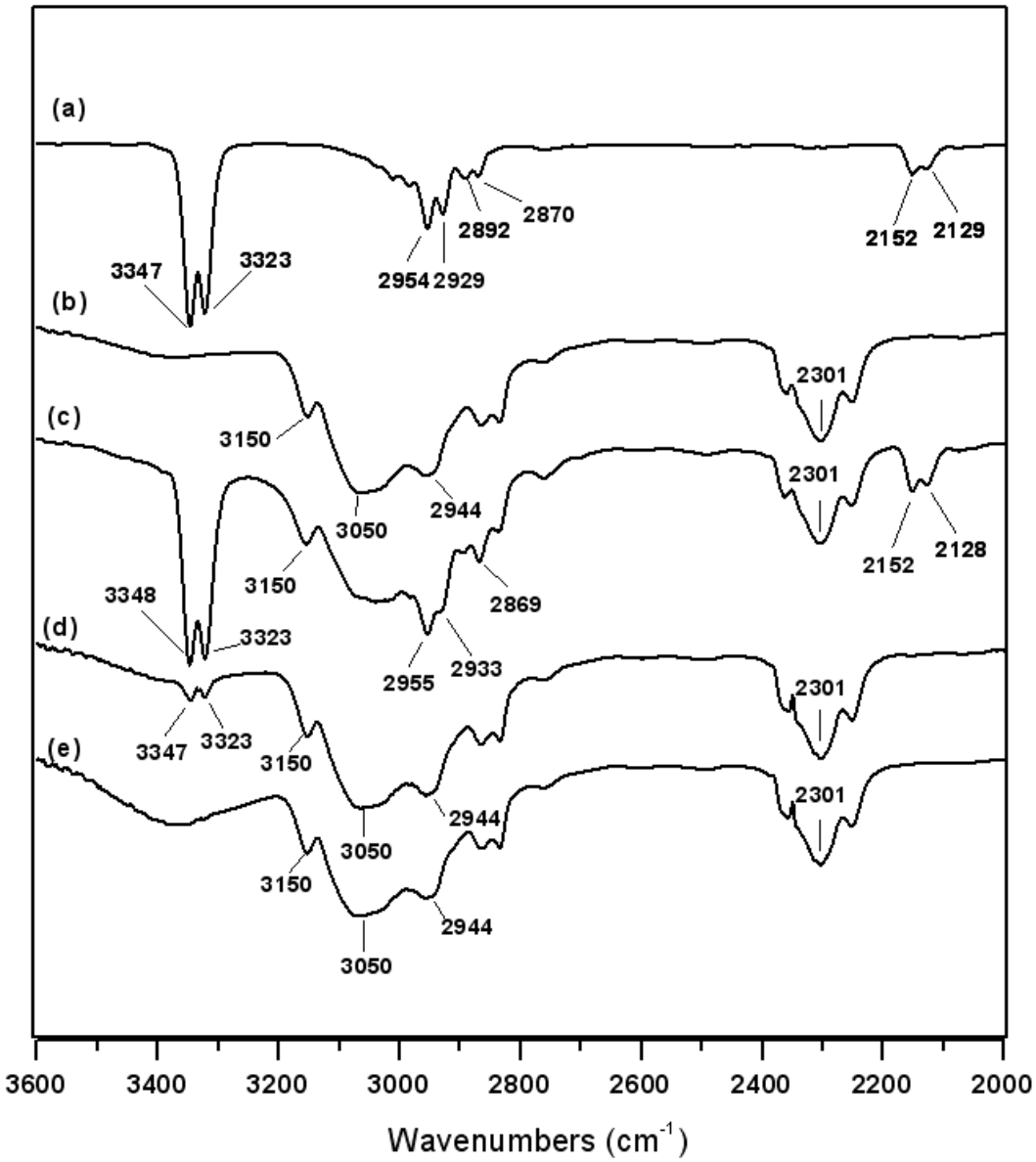


Fig. S-4b FT-IR spectra showing the interaction of [DMIM][$MeHPO_3$] with propyne: (a) propyne, (b) [DMIM][$MeHPO_3$] (c) (b)+propyne, (d) (c) after N_2 flushing for 10 min, (e) (d) after N_2 flushing for additional 30 min.

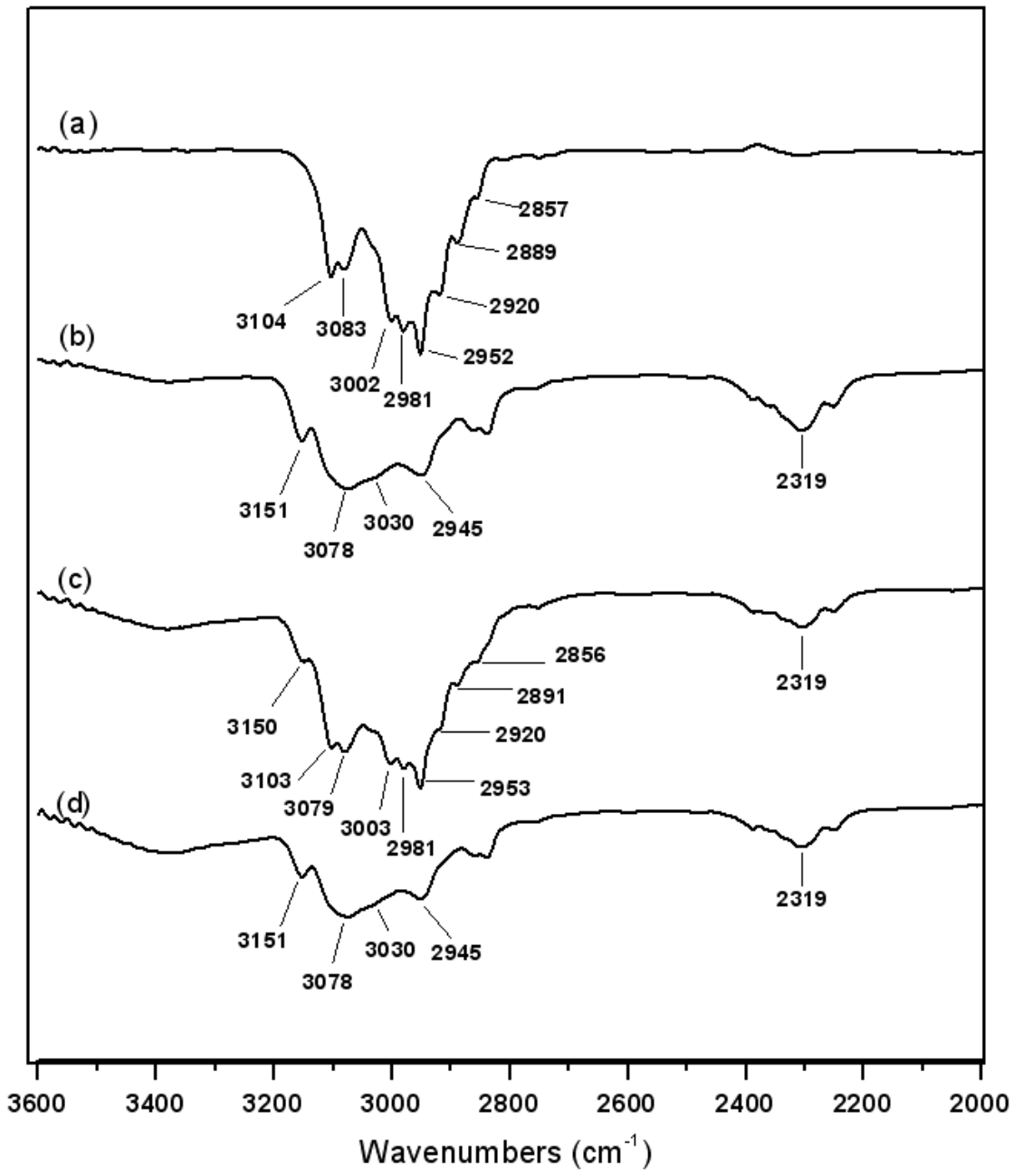


Fig. S-4c FT-IR spectra showing the interaction of Cu-RTIL (CuCl/[DMIM][$MeHPO_3$] = 1/2) with propylene: (a) propylene, (b) Cu-RTIL, (c) (b)+ propylene, (d) (c) after N_2 flushing for 10 min.

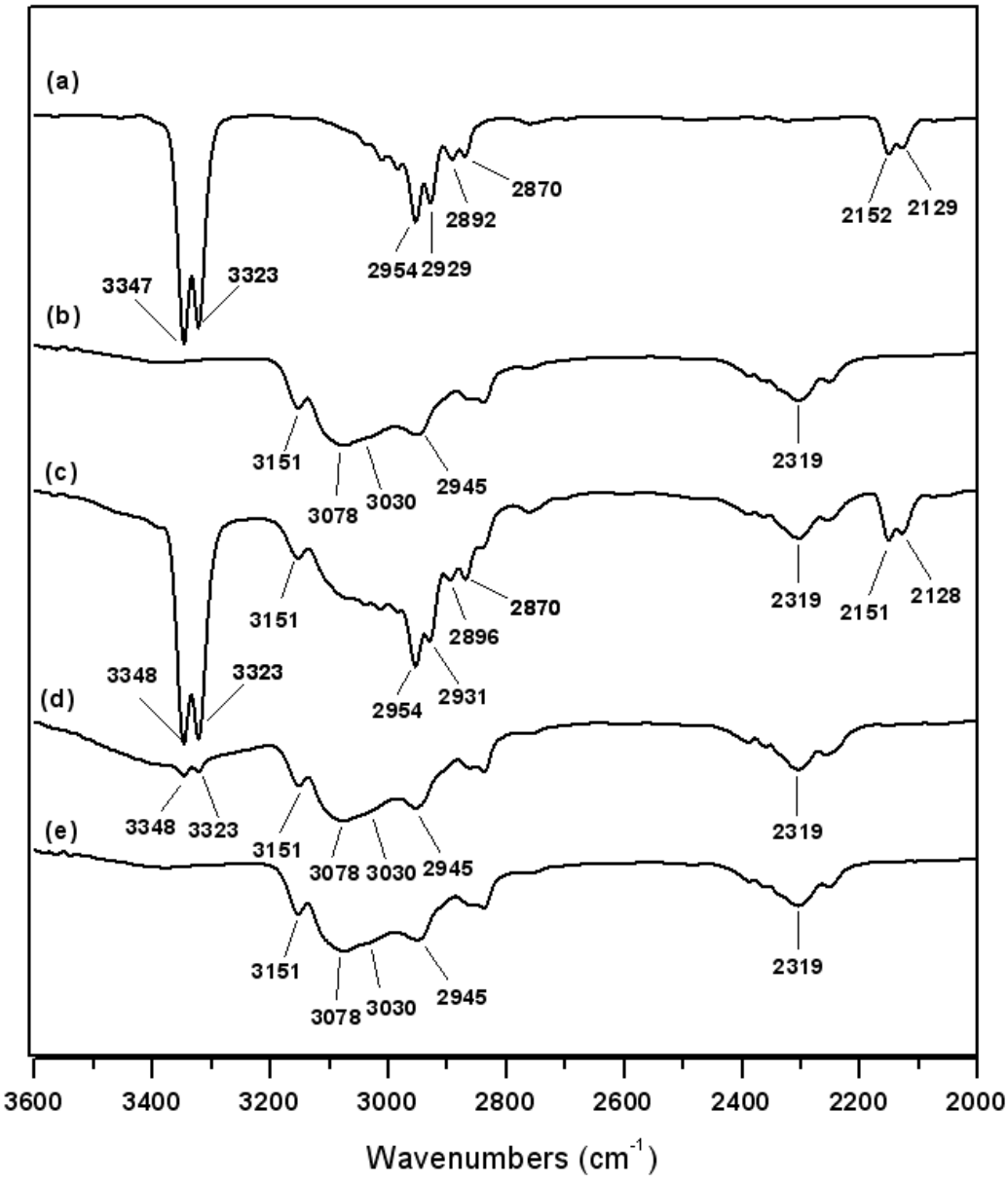


Fig. S-4d FT-IR spectra showing the interaction of Cu-RTIL (CuCl/[DMIM][$MeHPO_3$] = 1/2) with propyne: (a) propyne, (b) Cu-RTIL (c) (b)+propyne, (d) (c) after N_2 flushing for 10 min, (e) (d) after N_2 flushing for additional 30 min.