Electronic Supplementary Information

Ionic Liquids from Copper Complexes with Alkylimidazole-Containing Tripodal Ligands

Yusuke Funasako, Misaki Nosho and Tomoyuki Mochida*

Department of Chemistry, Graduate School of Science, Kobe University, Rokkodai, Nada, Hyogo 657-8501, Japan

Preparation of 1-alkylimidazole-2-carbaldehyde

Under a nitrogen atmosphere, 1-iodohexane (1.53 mL, 10.4 mmol) was added to a mixture of formylimidazole (1.00 g, 10.4 mmol), K₂CO₃ (1.73 g, 12.5 mmol), and DMF (20 mL). The reaction mixture was stirred for 24 h at 50 °C, and then cooled to room temperature and filtered. The precipitate was dissolved in ethyl acetate and washed repeatedly with brine. The organic layer was dried over magnesium sulfate and concentrated under reduced pressure. The residual yellow oil was dissolved in concentrated hydrochloric acid (10 mL) and washed with hexane. The aqueous phase was basified by addition of a saturated aqueous solution of NaOH, and then extracted with diethyl ether. The organic phase was dried over magnesium sulfate and concentrated under reduced pressure to give the desired product as a yellow oil (0.429 g, yield 12.3%). ¹H NMR (400 MHz, CDCl₃, TMS): $\delta = 0.88$ (m, 3H), 1.30 (m, 6H), 1.76 (m, 2H), 4.39 (t, 2H, J = 7.2 Hz), 7.15 (s, 1H), 7.29 (s, 1H), 9.81 (s, 1H).



Fig. S1 Temperature dependence of the viscosity of $[1]Tf_2N$ measured at 10–50 °C. Solid lines are the fitting curves using the VFT equation.



Fig. S2 DSC traces of (a) [1]Tf₂N, (b) [2]Tf₂N, and (c) [3]Tf₂N. The first and second cooling-heating cycles are shown in Figs. (b) and (c). I and II denote different crystal phases.



Fig. S3 ORTEP drawings of the anions in (a) $[3]Tf_2N$ and (b) $[Cu(Me_6tren)Cl]Tf_2N$.

Table S1 Absorption maxima in the UV–vis–NIR spectra of $[1]Tf_2N$ (liquid), $[2]Tf_2N$, $[3]Tf_2N$, and $[2]PF_6$ (solids).

	$\lambda_{\rm LMCT}$ / nm	λ_{d-d} / nm
[1]Tf ₂ N	302	743, 930
[2]Tf ₂ N	312	751, 944
[3]Tf ₂ N	289	735, 944
[2]PF ₆	307	734, 943