Supporting Information

Iodocuprate-containing Ionic Liquids as Promoters for Green Propulsion

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Materials and Methods

All reagents were obtained from commercial resources were used as received. ^{1}H and ^{13}C NMR spectra were measured on Bruker AV II-600 MHz and 400 MHz spectrometers, using DMSO-d_6 and $CDCl_3$ as solvents. Single-crystal data were collected on an Oxford Xcalibur diffractometer with a CCD detector Mo-Kα radiation (λ = 0.71073 Å) using a ω scan for CuILs **1-4** at 173 °C. The direct method and full-matrix least-squares method on F2 contained in the SHELXTL program package were used to resolve and refine the structures of CuILs **1-4**. Crystallographic data of CuILs **1-4** are shown in Table S1. Powder X-ray diffractions (PXRD) were carried out on Rigaku D/MAX-rA diffractometers using Cu-Kα radiation. FTIR (ATR) spectra were recorded on a Nicolet impact 410 FTIR spectrometer. Differential Scanning calorimeters (DSC) were performed using a Netzsch STA 449c instrument under a flow of nitrogen with a heating rate of 10 °C·min^{-1}. Density of materials was measured at RT on a gas pycnometer. Bomb calorimetry measurements (using benzoic acid as a reference standard) were conducted on Parr 6200 Bomb Calorimeter. The samples were placed on a stainless-steel pan and burned under 3.2 MPa atmosphere of pure oxygen.

^{1}H NMR and ^{13}C NMR Spectroscopy

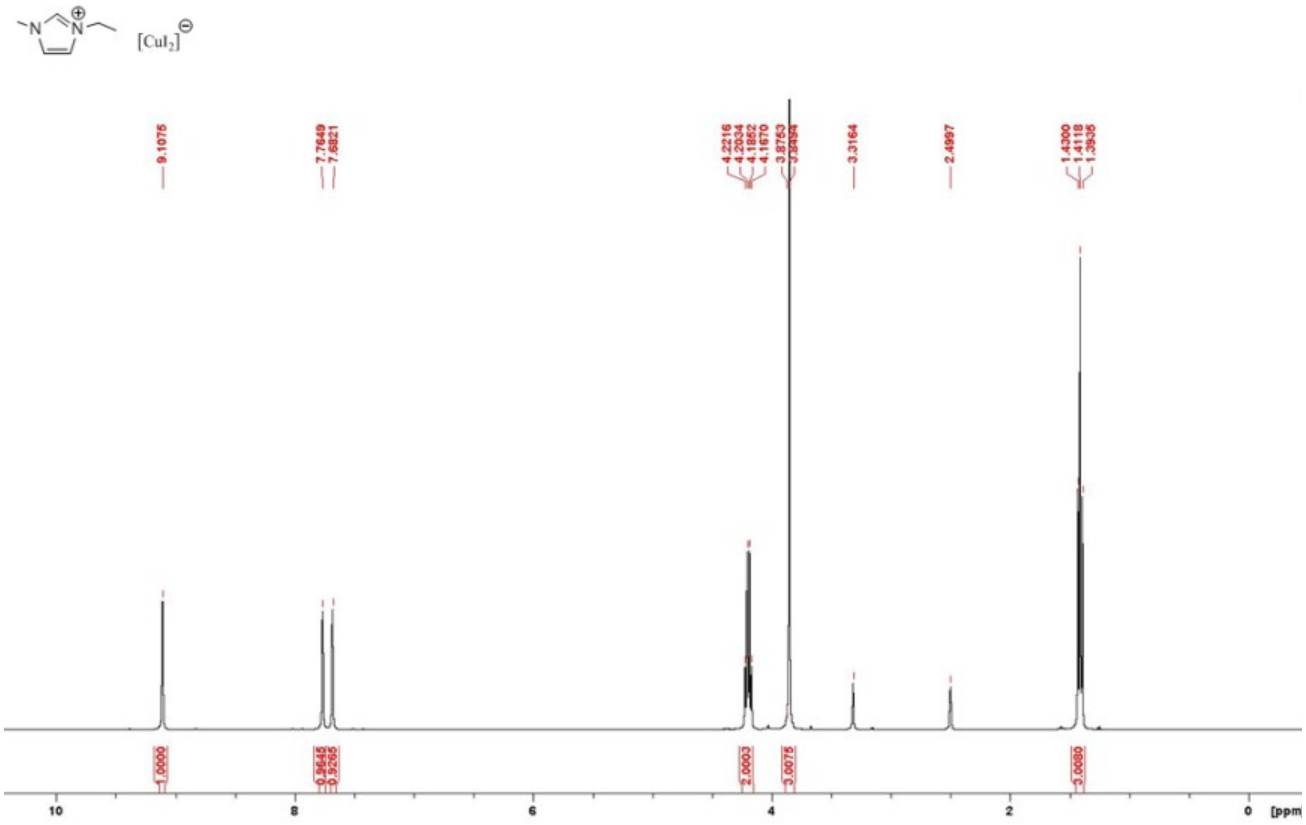


Figure S1. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **1**.

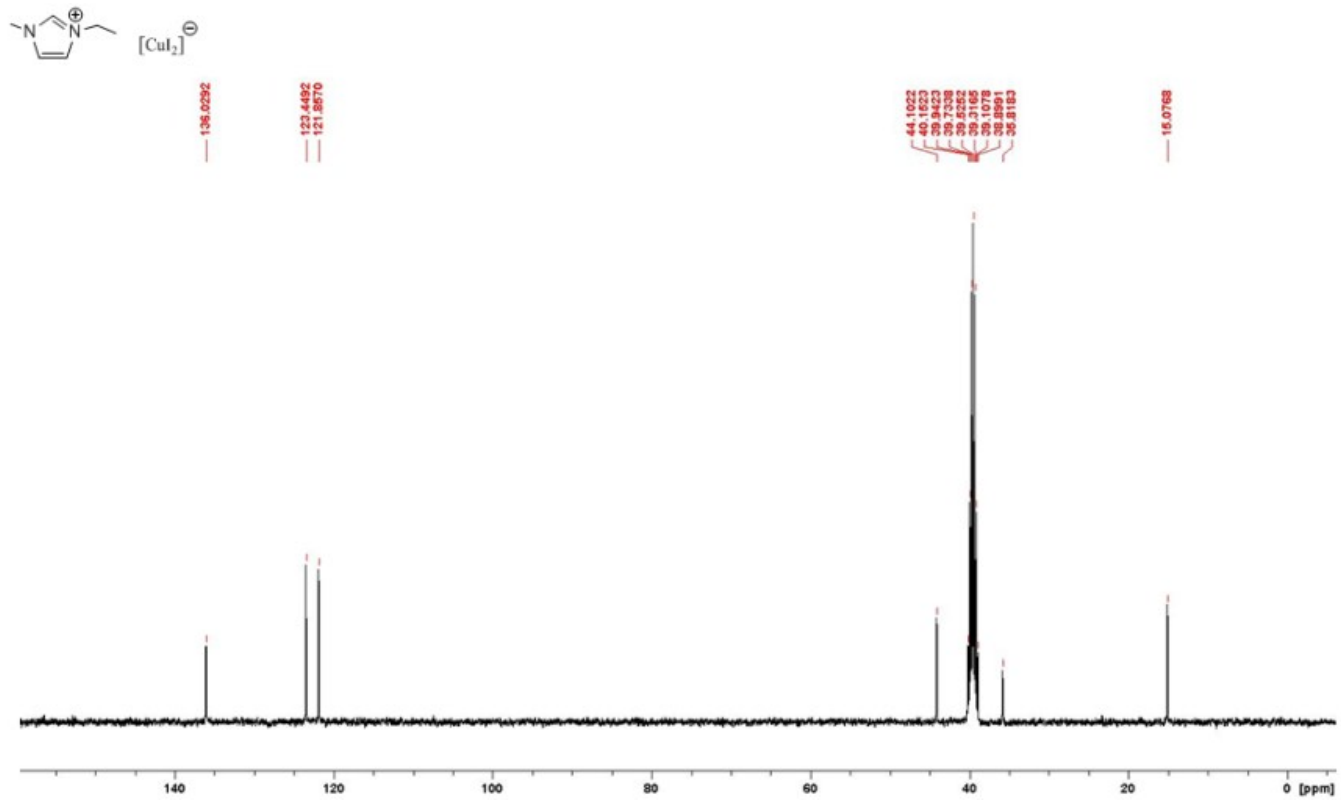


Figure S2. ^{13}C NMR (100 MHz, DMSO-d_6) of CuIL **1**.

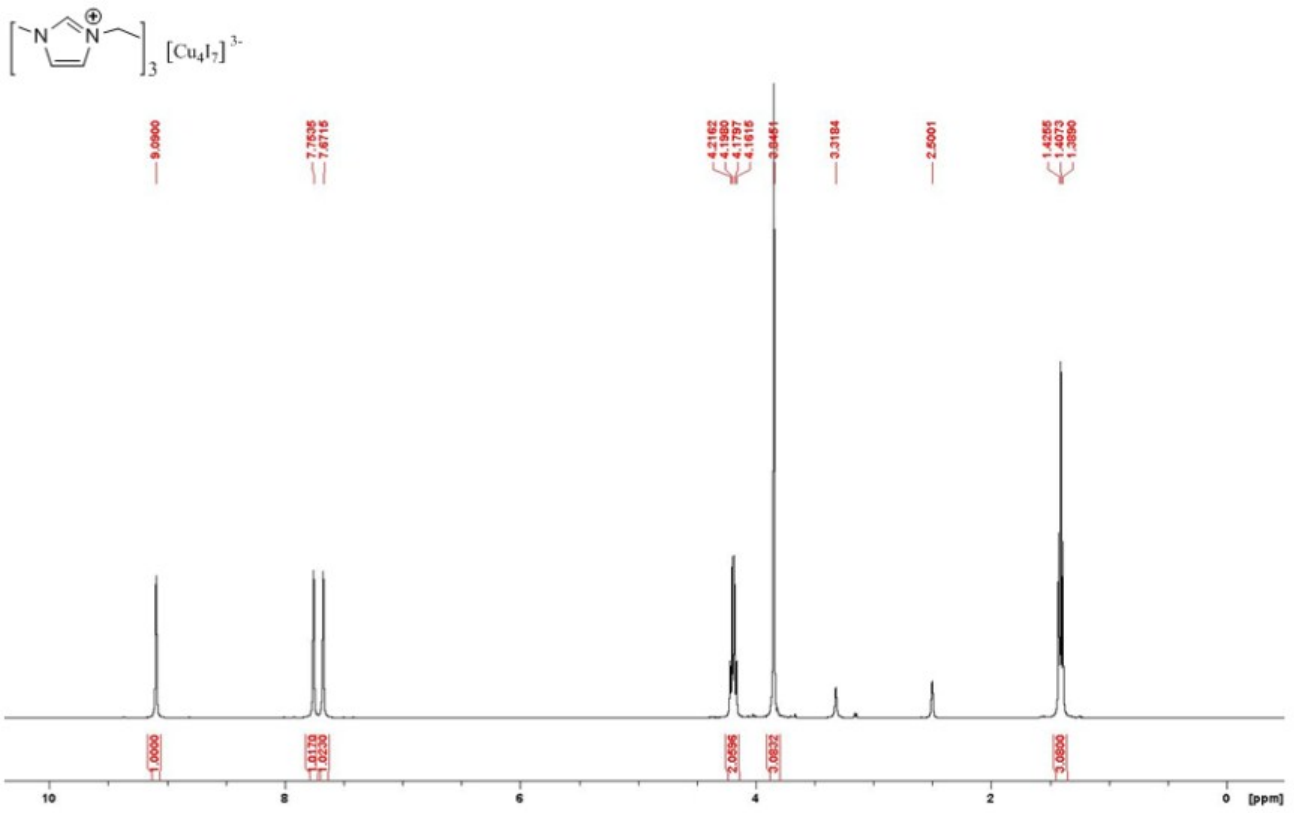


Figure S3. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **2**.

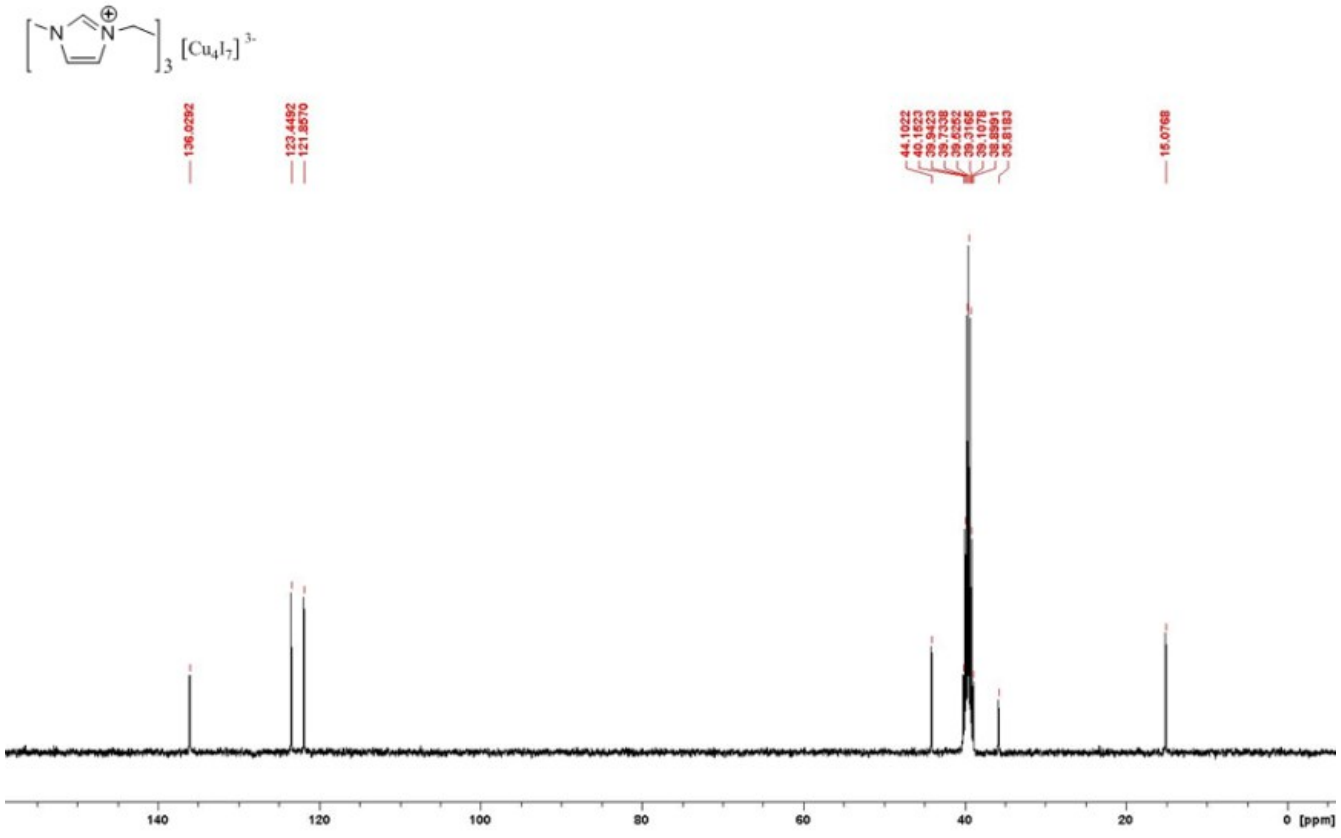


Figure S4. ^{13}C NMR ^{1}H NMR (100 MHz, DMSO-d_6) of CuIL **2**.

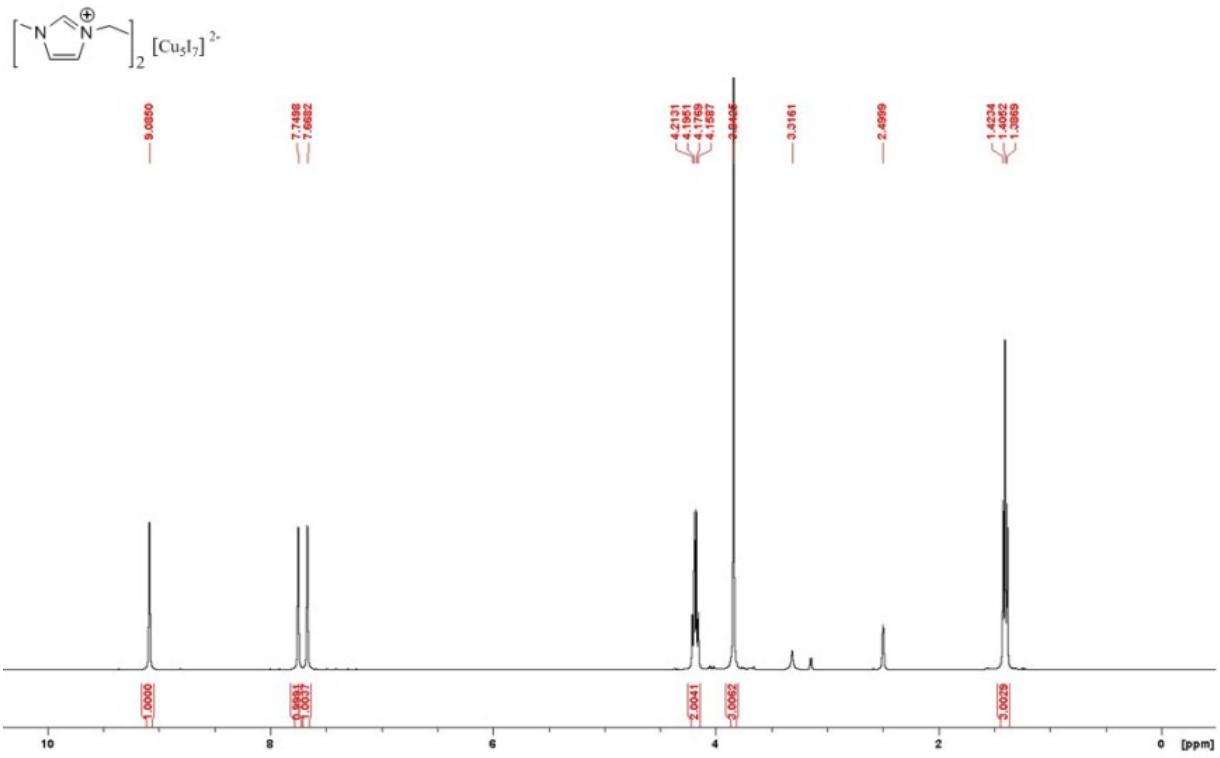


Figure S5. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **3**.

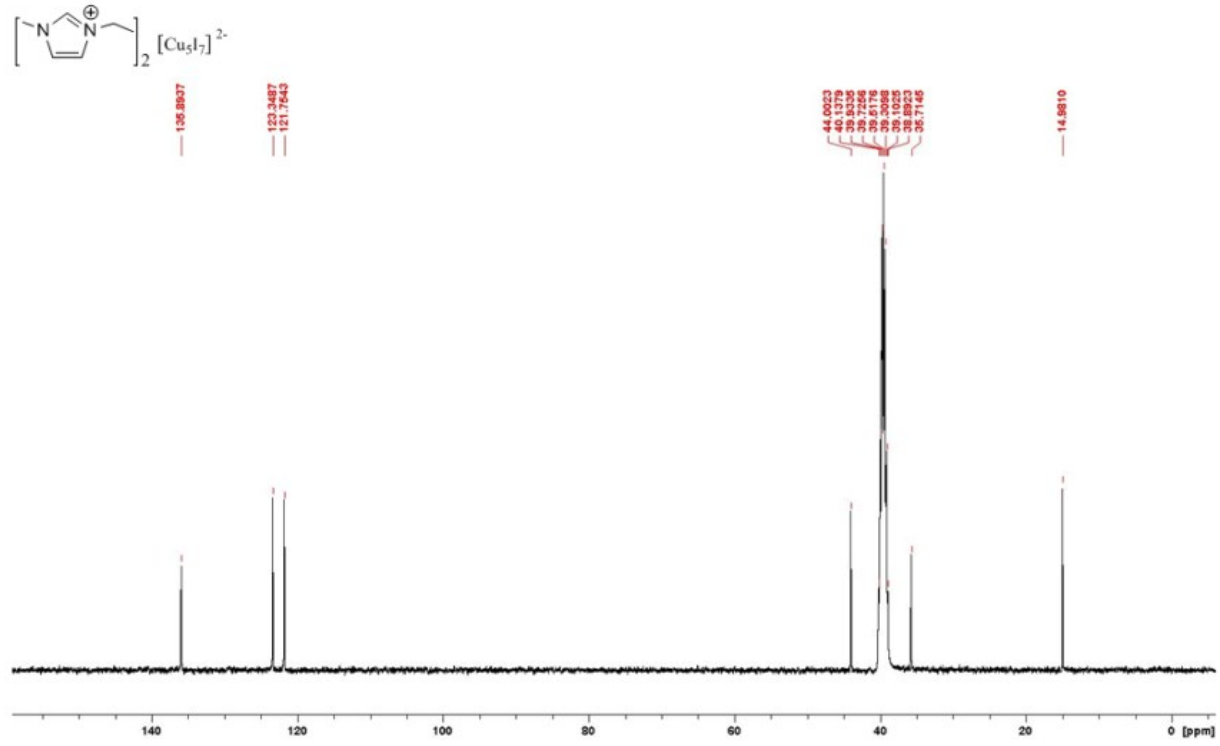


Figure S6. ^{1}C NMR (100 MHz, DMSO-d_6) of CuIL **3**.

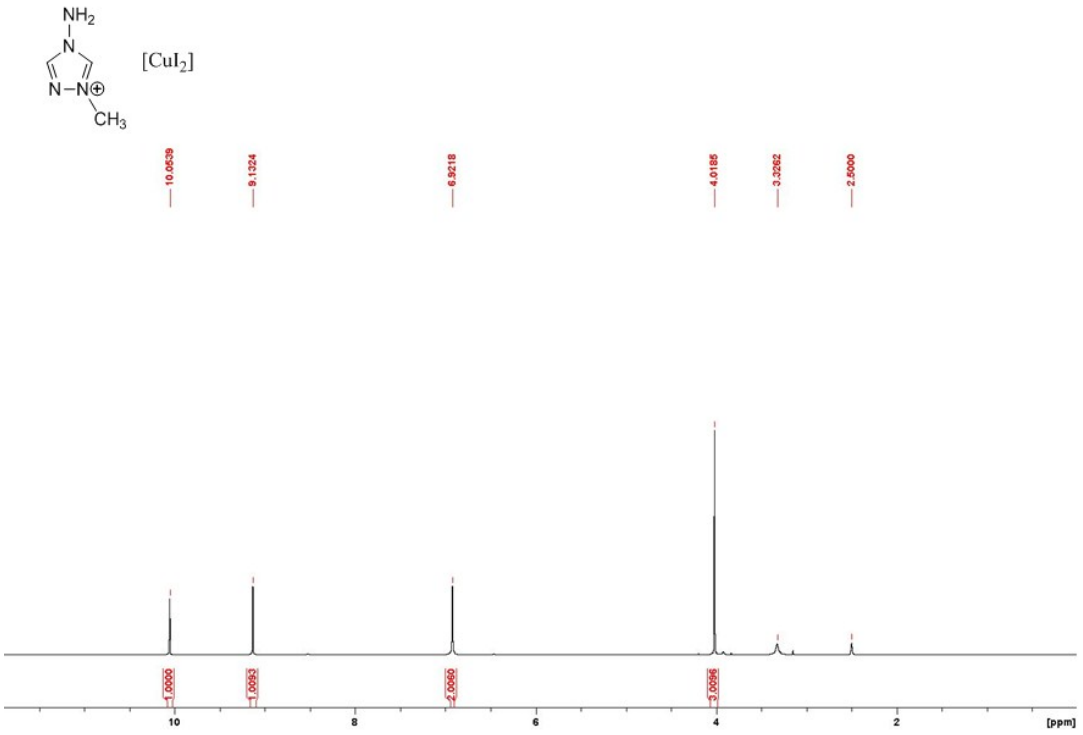


Figure S7. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **4**.

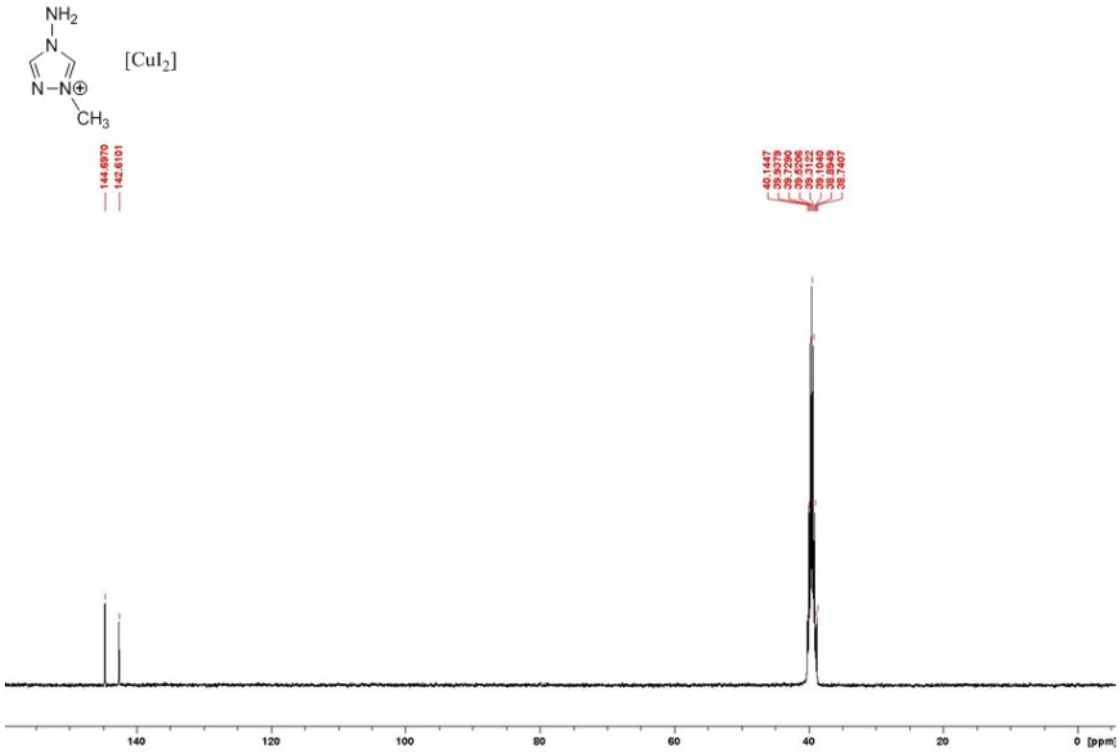


Figure S8. ^{13}C NMR (100 MHz, DMSO-d_6) of CuIL **4**.

Powder XRD of CuILs 1-4.

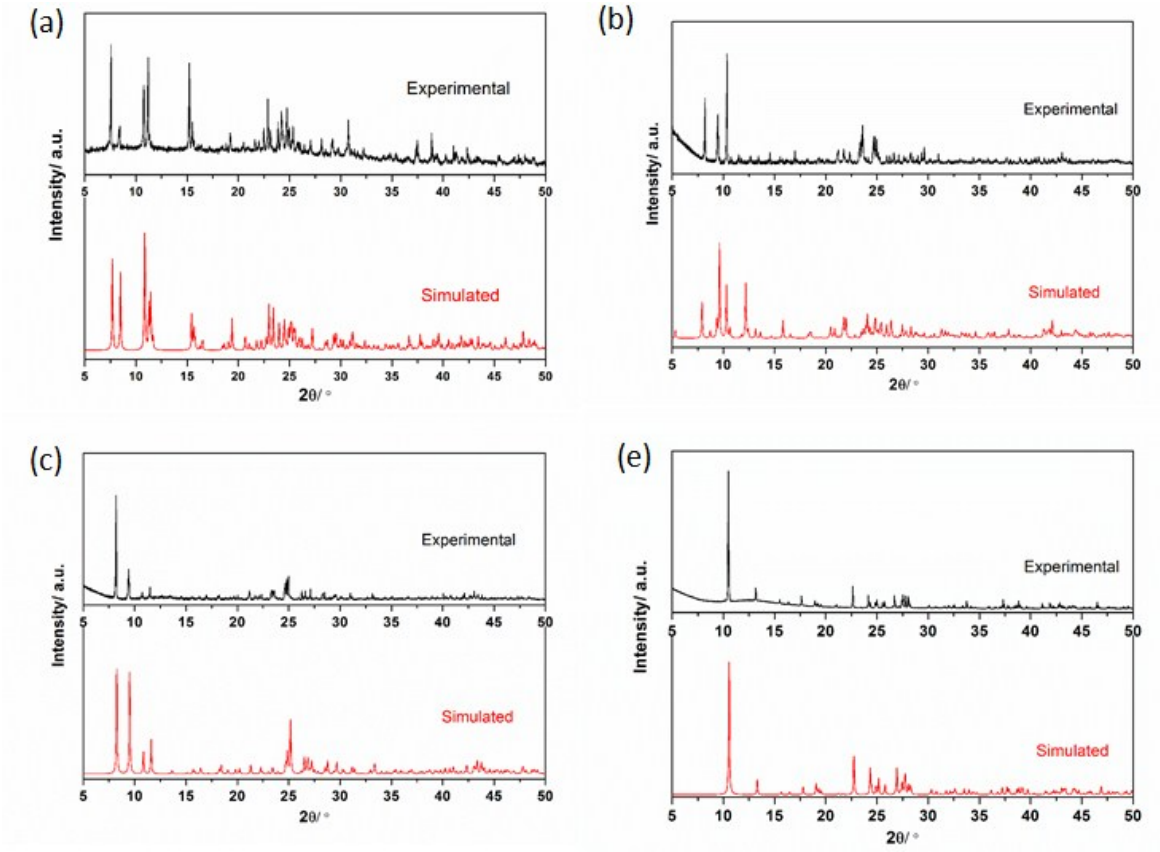


Figure S9. Simulated and experimental PXRD patterns. (a): CuIL **1**; (b): CuIL **2**; (c) CuIL **3** and (d) CuIL **4**.

SEM Images of CuILs 1-4.

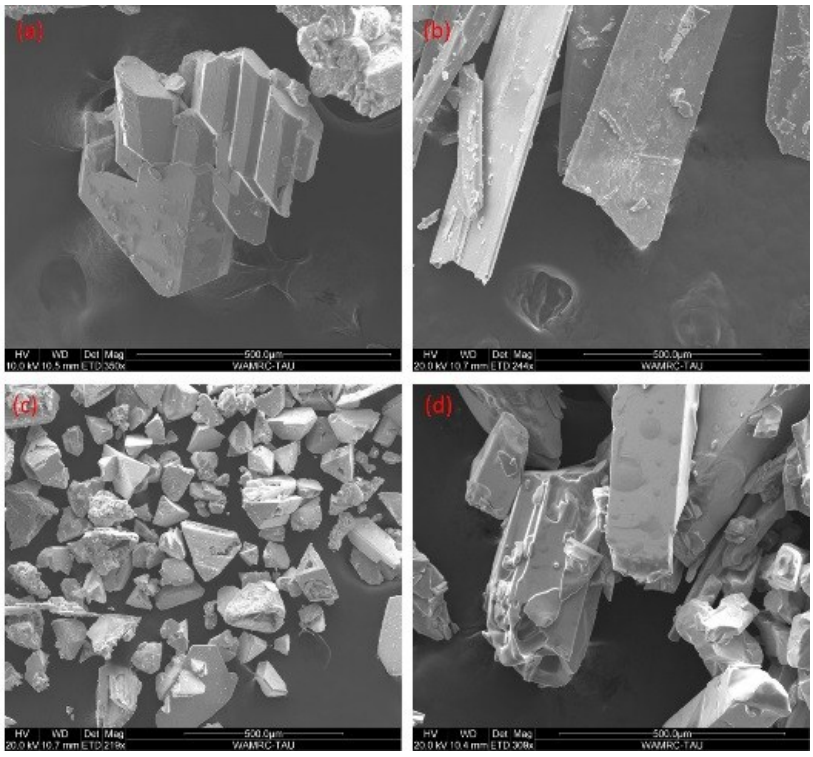


Figure S10. SEM images of crystals. (a): CuIL **1**; (b): CuIL **2**; (c) CuIL **3** and (d) CuIL **4**.

Crystallographic Data for CuILs 1-4.

Table S1. Crystal Data and Structure Refinement for CuILs **1-4.**

Compounds	**1**	**2**	**3**	**4**
Empirical formula	$C_6H_{11}N_2CuI_2$	$C_{18}H_{33}N_6Cu_4I_7$	$C_{12}H_{22}N_4Cu_5I_7$	$C_3H_7N_4CuI_2$
Formula weight	428.51	1475.96	1428.33	416.47
Temperature/K	173	173	173	173
Crystal system	triclinic	triclinic	orthorhombic	monoclinic
Space group	*P*-1	*P*-1	*Pnma*	$P2_1/n$
a/Å	9.562(2)	9.733(1)	13.266(2)	6.701(1)
b/Å	11.187(2)	11.353(2)	21.421(3)	13.303(3)
c/Å	12.146(3)	17.404(2)	10.319(2)	11.176(3)
α/°	84.86(1)	79.24(1)	90	90
β/°	70.86(1)	76.12(1)	90	105.77(2)
γ/°	68.64(1)	86.65(1)	90	90
Volume/Å^3	1142.4(4)	1834.0(3)	2932.4(6)	958.7(3)
Z	2	2	4	4
ρ_{calc} g/cm^3	2.491	2.673	3.235	2.885
μ/mm^{-1}	7.267	8.198	10.945	8.661
F(000)	784.0	1340.0	2552.0	752.0
Radiation	0.71073	0.71073	0.71073	0.71073
2θ /°	3.55-54.86	2.45-53.17	3.80-52.87	6.124-55.472
Index ranges	-12 < h < 12 -14 < k < 13 -15 < l < 15	-12 < h < 12 -14 < k < 14 -21 < l < 21	-16 < h < 15 -26 < k < 26 -12 < l < 12	-8 < h < 8 -17 < k < 17 -14 < l < 14
Reflections collected	10223	14459	20641	7481
Independent reflections	5094 [R_{int} = 0.0294, R_{sigm} = 0.0468]	7470 [R_{int} = 0.0456, R_{sigm} = 0.0747]	3092 [R_{int} = 0.0611, R_{sigm} = 0.0391]	2214 [R_{int} = 0.0426, R_{sigm} = 0.0431]
Data/restraints/ parameters	5094/0/203	7474/0/322	3092/0/135	2217/87/119
Goodness-of-fit on F^2	1.019	1.024	1.096	1.053
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0303, wR_2 = 0.0861	R_1 = 0.0428, wR_2 = 0.1126	R_1 = 0.0347, wR_2 = 0.0868	R_1 = 0.0414, wR_2 = 0.0944
Final R indexes [all data]	R_1 = 0.0366, wR_2 = 0.0903	R_1 = 0.0604, wR_2 = 0.1389	R_1 = 0.0429, wR_2 = 0.1016	R_1 = 0.0481, wR_2 = 0.0984

Selected Bond Length and Angles in CuILs 1-4.

Table S2. Bond lengths in CuIL **1.**

atom-atom	length/ Å	atom-atom	length/ Å
I1 -Cu2	2.5765(8)	N1- C2	1.341(7)
I1- Cu2[1]	2.7799(10)	N1- C5	1.380(7)
I1- Cu1[1]	2.9185(11)	N1- C3	1.469(7)
I4 -Cu2	2.6893(9)	N3 -C12	1.373(7)
I4- Cu1	2.6866(10)	N3 -C8	1.330(7)
I2 -Cu2	2.6989(8)	N3 -C7	1.470(8)
I2 -Cu1	2.7108(10)	N4 -C11	1.379(7)
I3 -Cu1	2.5174(8)	N4 -C8	1.317(7)
Cu2-I1[1]	2.7800(9)	N4 -C9	1.488(7)
Cu1- I1[1]	2.9186(11)	C6 -C5	1.370(8)
N2 -C6	1.366(7)	C12 -C11	1.341(8)
N2 -C2	1.330(7)	C3 -C4	1.516(9)
N2- C1	1.464(7)	C9 -C10	1.492(9)

[1]2-X,1-Y,1-Z

Table S3. Bond angles in CuIL **1.**

atom-atom-atom	angle/ º	atom-atom-atom	angle/ º
Cu2-I1-Cu2[1]	61.58(3)	C2-N2-C1	125.5(5)
Cu2[1]-I1-Cu1[1]	53.05(2)	C2-N1-C5	109.0(4)
Cu2-I1-Cu1[1]	114.64(3)	C2-N1-C3	125.3(5)
Cu1-I4-Cu2	56.58(2)	C5-N1-C3	125.5(5)
Cu2-I2-Cu1	56.20(2)	C12-N3-C7	125.5(5)
I1-Cu2-I1[1]	118.42(3)	C8-N3-C12	109.4(5)
I1-Cu2-I4	115.93(3)	C8-N3-C7	125.0(5)
I1-Cu2-I2	115.75(3)	C11-N4-C9	125.6(5)
I4-Cu2-I1[1]	101.06(3)	C8-N4-C11	109.5(5)
I4-Cu2-I2	102.47(3)	C8-N4-C9	124.8(5)
I2-Cu2-I1[1]	100.60(3)	N2-C6-C5	108.1(5)
I4-Cu1-I1[1]	97.67(3)	N2-C2-N1	108.6(4)
I4-Cu1-I2	102.23(3)	C6-C5-N1	105.7(5)
I2-Cu1-I1[1]	96.92(3)	C11-C12-N3	106.8(5)
I3-Cu1-I1[1]	113.93(3)	N1-C3-C4	112.0(5)
I3-Cu1-I4	121.62(3)	C12-C11-N4	106.7(5)
I3-Cu1-I2	119.75(3)	N4-C8-N3	107.6(5)
C6-N2-C1	125.9(5)	N4-C9-C10	109.2(6)
C2-N2-C6	108.6(4)		

[1]2-X,1-Y,1-Z

Table S4. Bond lengths in CuIL **2.**

atom-atom	length/ Å	atom-atom	length/ Å
I1-Cu2	2.5765(8)	N2-C1	1.464(7)
I1-Cu2[1]	2.7799(10)	N1-C2	1.341(7)
I1-Cu1[1]	2.9185(11)	N1-C5	1.380(7)
I4-Cu2	2.6893(9)	N1-C3	1.469(7)
I4-Cu1	2.6866(10)	N3-C12	1.373(7)
I2-Cu2	2.6989(8)	N3-C8	1.330(7)
I2-Cu1	2.7108(10)	N3-C7	1.470(8)
I3-Cu1	2.5174(8)	N4-C11	1.379(7)
Cu2-I1[1]	2.7800(9)	N4-C8	1.317(7)
Cu1-I1[1]	2.9186(11)	N4-C9	1.488(7)
N2-C6	1.366(7)	C6-C5	1.370(8)
N2-C2	1.330(7)	C12-C11	1.341(8)

[1]2-X,1-Y,1-Z

Table S5. Bond angles in CuIL **2.**

atom-atom-atom	**angle/ º**	**atom-atom-atom**	**angle/ º**
Cu2-I1-Cu2[1]	61.58(3)	C2-N2-C1	125.5(5)
Cu2[1]-I1-Cu1[1]	53.05(2)	C2-N1-C5	109.0(4)
Cu2-I1-Cu1[1]	114.64(3)	C2-N1-C3	125.3(5)
Cu1-I4-Cu2	56.58(2)	C5-N1-C3	125.5(5)
Cu2-I2-Cu1	56.20(2)	C12-N3-C7	125.5(5)
I1-Cu2-I1[1]	118.42(3)	C8-N3-C12	109.4(5)
I1-Cu2-I4	115.93(3)	C8-N3-C7	125.0(5)
I1-Cu2-I2	115.75(3)	C11-N4-C9	125.6(5)
I4-Cu2-I1[1]	101.06(3)	C8-N4-C11	109.5(5)
I4-Cu2-I2	102.47(3)	C8-N4-C9	124.8(5)
I2-Cu2-I1[1]	100.60(3)	N2-C6-C5	108.1(5)
I4-Cu1-I1[1]	97.67(3)	N2-C2-N1	108.6(4)
I4-Cu1-I2	102.23(3)	C6-C5-N1	105.7(5)
I2-Cu1-I1[1]	96.92(3)	C11-C12-N3	106.8(5)
I3-Cu1-I1[1]	113.93(3)	N1-C3-C4	112.0(5)
I3-Cu1-I4	121.62(3)	C12-C11-N4	106.7(5)
I3-Cu1-I2	119.75(3)	N4-C8-N3	107.6(5)
C6-N2-C1	125.9(5)	N4-C9-C10	109.2(6)
C2-N2-C6	108.6(4)		

[1]2-X,1-Y,1-Z

Table S6. Bond lengths in CuIL **3.**

atom-atom	length/ Å	atom-atom	length/ Å
I2-Cu1	2.6901(15)	I4-Cu3	2.5913(12)
I2-Cu3	2.7376(13)	I4-Cu2	2.6230(12)
I2-Cu3[1]	2.7376(13)	Cu1-I5[3]	2.7501(17)
I2-Cu2	2.9058(15)	Cu1-I1[1]	2.6007(9)
I2-Cu2[1]	2.9058(14)	Cu3-I1[2]	2.7043(12)
I5-Cu1[2]	2.7501(17)	N1-C3	1.367(10)
I5-Cu3	2.6240(12)	N1-C2	1.320(10)
I5-Cu3[1]	2.6240(12)	N1-C1	1.524(11)
I1-Cu1	2.6007(9)	N2-C4	1.379(10)
I1-Cu3[3]	2.7042(12)	N2-C2	1.300(10)
I1-Cu2	2.6948(12)	N2-C5	1.456(10)
I3-Cu2[1]	2.5749(13)	C3-C4	1.339(12)
I3-Cu2	2.5749(13)	C6-C5	1.483(13)

[1]+X,3/2-Y,+Z; [2]1/2+X,+Y,3/2-Z; [3]-1/2+X,+Y,3/2-Z; [4]-1/2+X,3/2-Y,3/2-Z

Table S7. Bond angles in CuIL **3.**

atom-atom-atom	angle/ °	atom-atom-atom	angle/ °
Cu1-I2-Cu3	126.48(4)	I4-Cu3-I2	108.01(4)
Cu1-I2-Cu3[1]	126.48(4)	I4-Cu3-I5	117.49(5)
Cu1-I2-Cu2	64.98(4)	I4-Cu3-I1[2]	107.94(4)
Cu1-I2-Cu2[1]	64.98(4)	I3-Cu2-I2	112.67(4)
Cu3-I2-Cu3[1]	65.14(5)	I3-Cu2-I1	111.50(4)
Cu3[1]-I2-Cu2	94.28(4)	I3-Cu2-I4	119.60(5)
Cu3[1]-I2-Cu2[1]	61.97(3)	I3-Cu2-Cu1	103.11(4)
Cu3-I2-Cu2[1]	94.28(4)	I3-Cu2-Cu3	108.21(5)
Cu3-I2-Cu2	61.97(3)	I3-Cu2-Cu2[1]	55.20(3)
Cu2-I2-Cu2[1]	60.75(5)	I4-Cu2-I2	102.39(4)
Cu3[1]-I5-Cu1[2]	61.58(4)	I4-Cu2-I1	108.11(4)
Cu3-I5-Cu1[2]	61.58(4)	C3-N1-C1	126.5(7)
Cu3-I5-Cu3[1]	68.34(5)	C2-N1-C3	107.5(7)
Cu1-I1-Cu3[3]	62.49(4)	C2-N1-C1	125.8(7)
Cu1-I1-Cu2	69.29(4)	C4-N2-C5	126.1(7)
Cu2-I1-Cu3[3]	128.97(4)	C2-N2-C4	107.8(7)
Cu2[1]-I3-Cu2	69.59(6)	C2-N2-C5	126.1(7)
Cu3-I4-Cu2	67.82(4)	C4-C3-N1	107.5(7)
I2-Cu1-I5[3]	94.85(5)	C3-C4-N2	106.9(7)
I5-Cu3-I2	111.87(4)	N2-C2-N1	110.3(7)
I5-Cu3-I1[2]	112.29(4)	N2-C5-C6	112.6(7)
I1[2]-Cu3-I2	97.28(4)		

[1]+X,3/2-Y,+Z; [2]1/2+X,+Y,3/2-Z; [3]-1/2+X,+Y,3/2-Z; [4]-1/2+X,3/2-Y,3/2-Z

Table S8. Bond lengths in CuIL **4.**

atom-atom	length/ Å	atom-atom	length/ Å
I2-Cu1[1]	2.6483(11)	N2-N1	1.445(16)
I2-Cu1	2.6488(10)	N2-N1A	1.406(18)
I1-Cu1	2.6609(11)	N4-N3	1.357(11)
I1-Cu1[2]	2.6542(11)	N4-C4	1.270(13)
Cu1-I2[1]	2.6483(11)	N4-C3	1.489(19)
Cu1-I1[2]	2.6542(11)	N3-C1	1.290(12)
N2-C1	1.323(10)	N3-C2	1.496(17)
N2-C4	1.290(11)		

[1]X,1-Y,1-Z; [2]1-X,1-Y,1-Z

Table S9. Bond angles in CuIL **4.**

atom-atom-atom	angle/ °	atom-atom-atom	angle/ °
Cu1[1]-I2-Cu1	77.44(3)	C4-N2-N1	138.6(11)
Cu1[2]-I1-Cu1	79.23(3)	C4-N2-N1A	107.8(13)
I2[1]-Cu1-I2	102.56(3)	N3-N4-C3	137.4(10)
I2[1]-Cu1-I1[2]	117.21(4)	C4-N4-N3	108.1(8)
I2[1]-Cu1-I1	110.40(4)	C4-N4-C3	113.4(9)
I2-Cu1-I1[2]	112.65(4)	N4-N3-C2	143.2(10)
I2-Cu1-I1	113.74(4)	C1-N3-N4	105.9(7)
I12-Cu1-I1	100.77(3)	C1-N3-C2	110.8(9)
C1-N2-N1	114.1(11)	N3-C1-N2	109.0(7)
C1-N2-N1A	144.8(13)	N4-C4-N2	109.7(8)
C4-N2-C1	107.3(7)		

[1]-X,1-Y,1-Z; [2]1-X,1-Y,1-Z

DSC Thermograms of CuILs 1-4

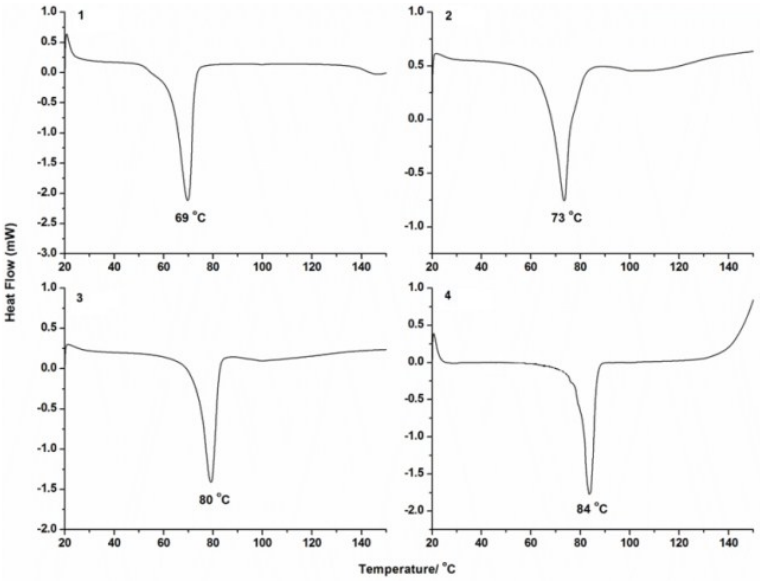


Figure S11. DSC curves of CuILs **1-4**.

Promoter-in-Fuel (10 wt.%) Stability Studies at Room Temperature ^{1}H NMR Studies

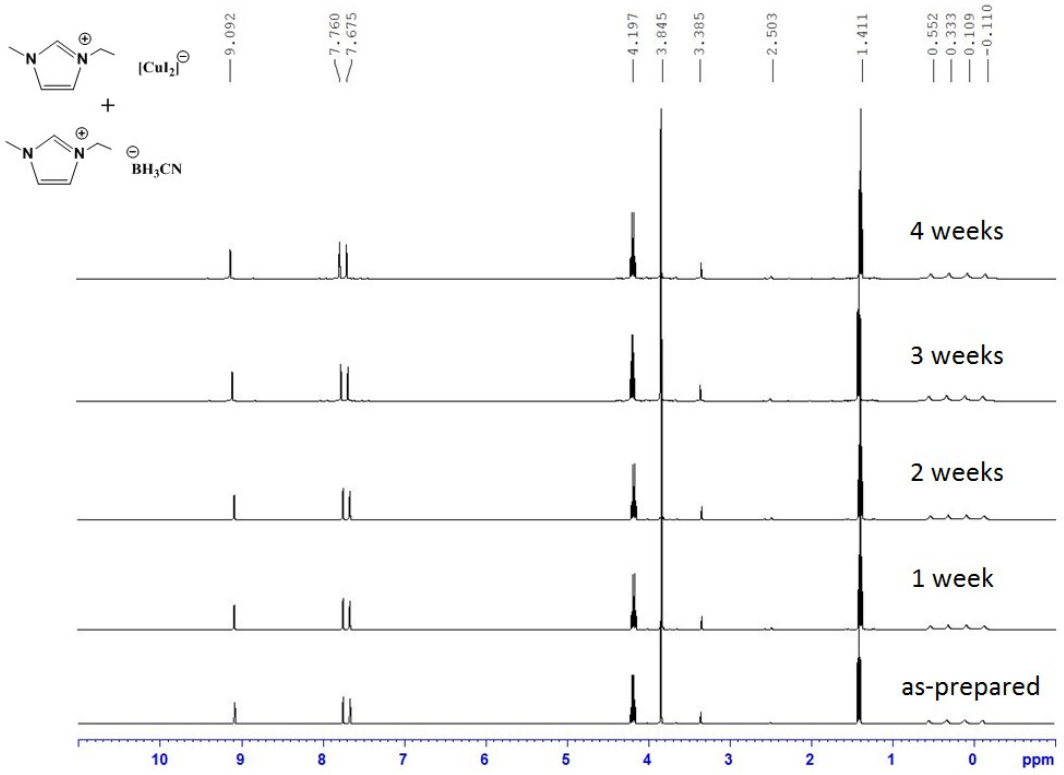


Figure S12. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **1** in [EMIM$^+$][BH_3CN^-] fuel.

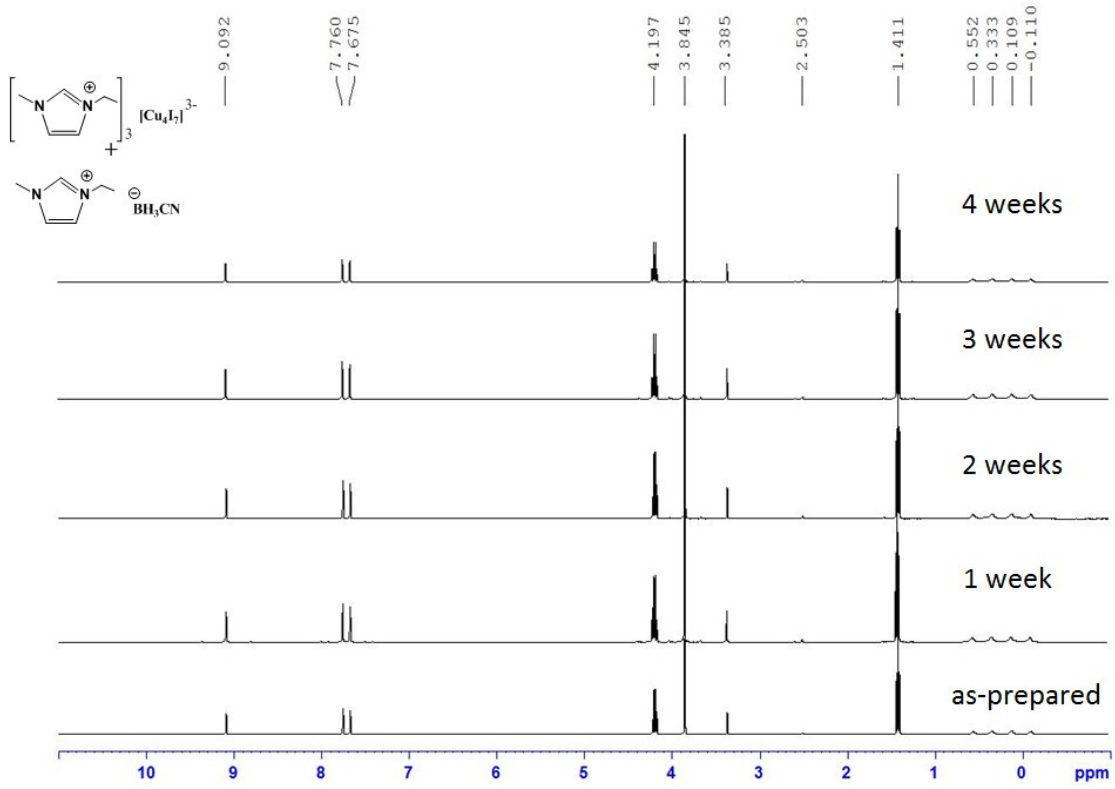


Figure S13. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **2** in [EMIM$^+$][BH_3CN^-] fuel.

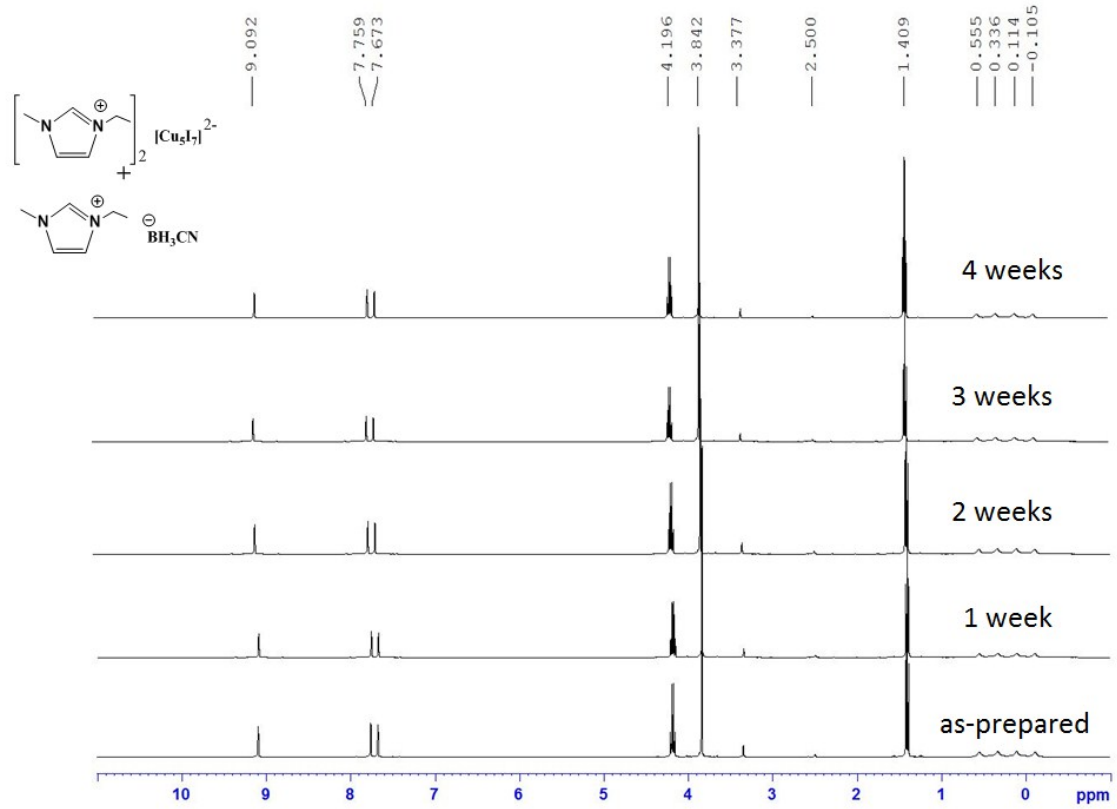


Figure S14. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **3** in [EMIM$^+$][BH_3CN^-] fuel.

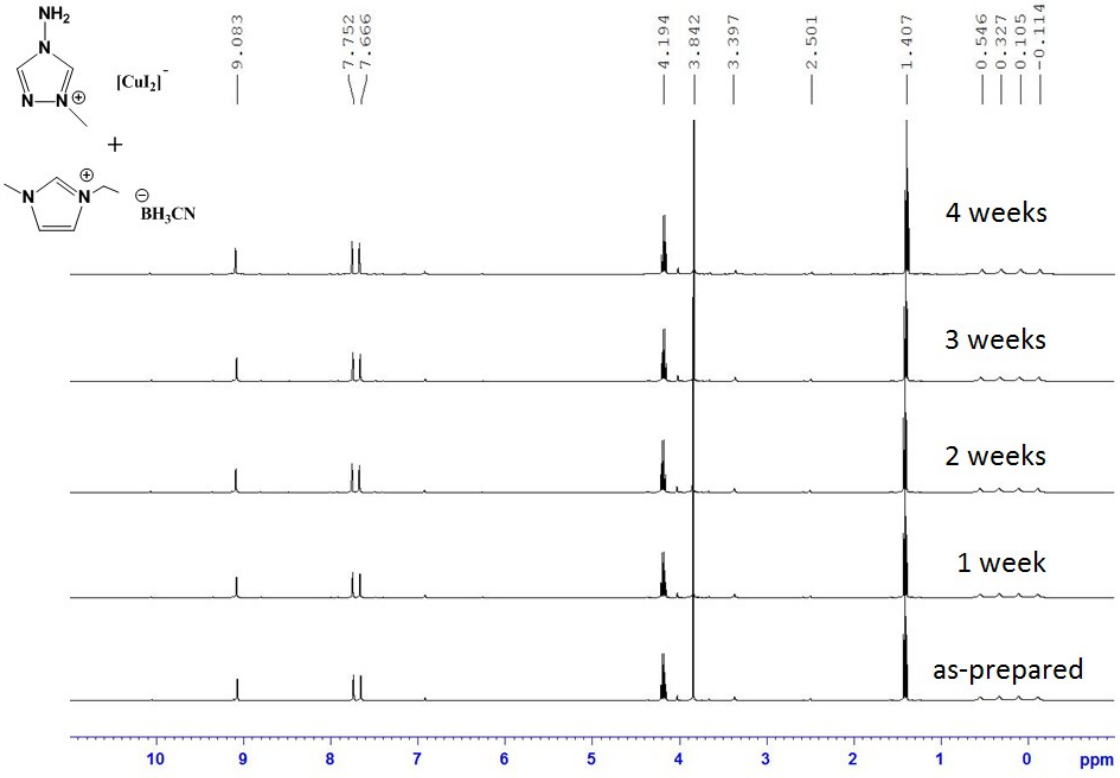


Figure S15. ^{1}H NMR (400 MHz, DMSO-d_6) of CuIL **4** in [EMIM$^+$][BH_3CN^-] fuel.

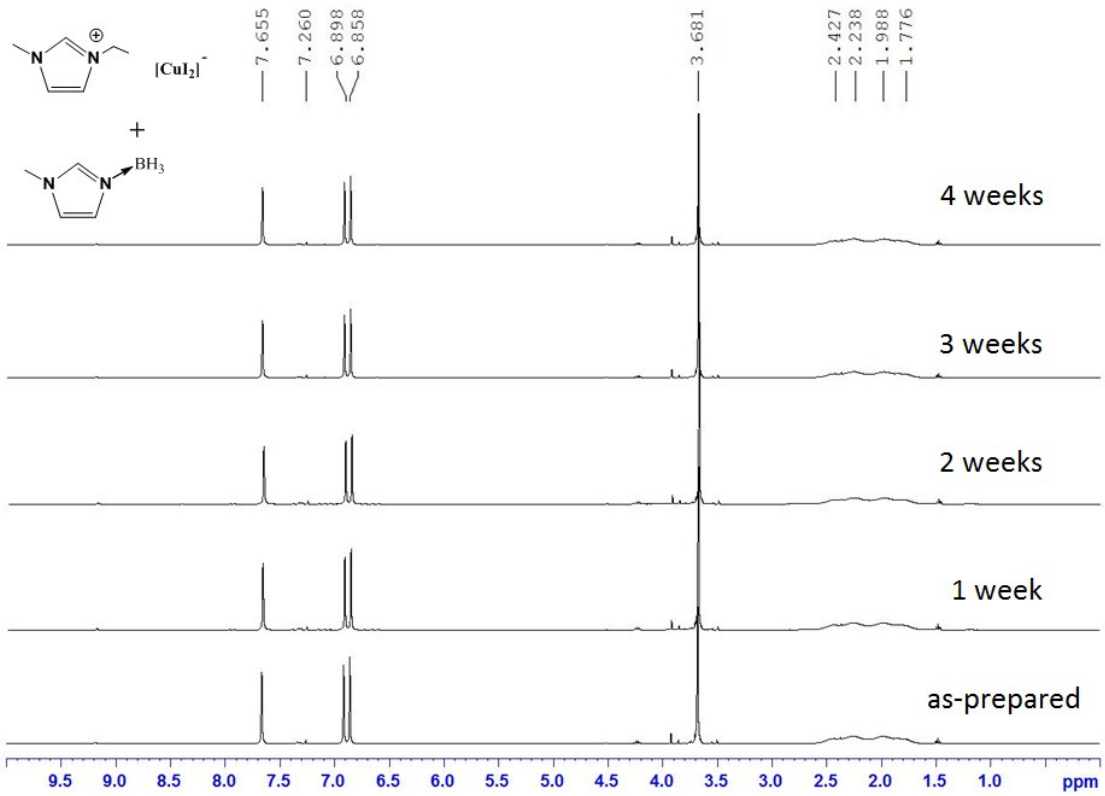


Figure S16. ^{1}H NMR (400 MHz, $CDCl_3$) of CuIL **1** in [MIM^+][BH_3^-] fuel.

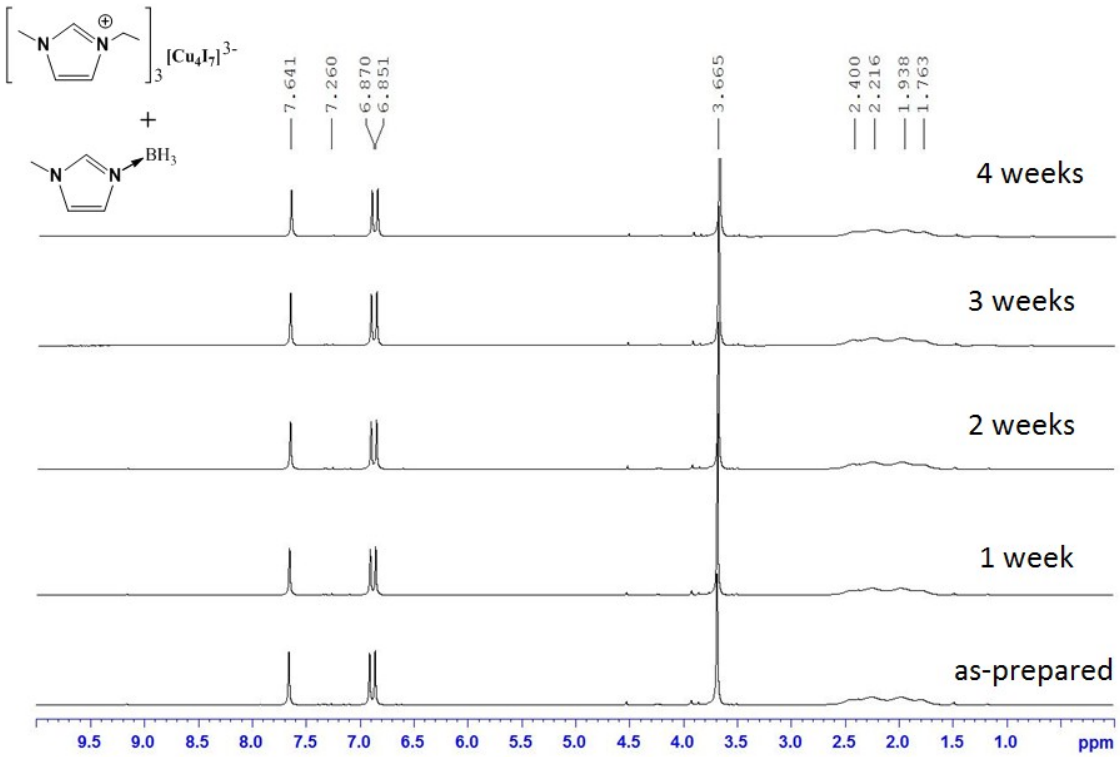


Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) of CuIL **2** in [MIM^+][BH_3^-] fuel.

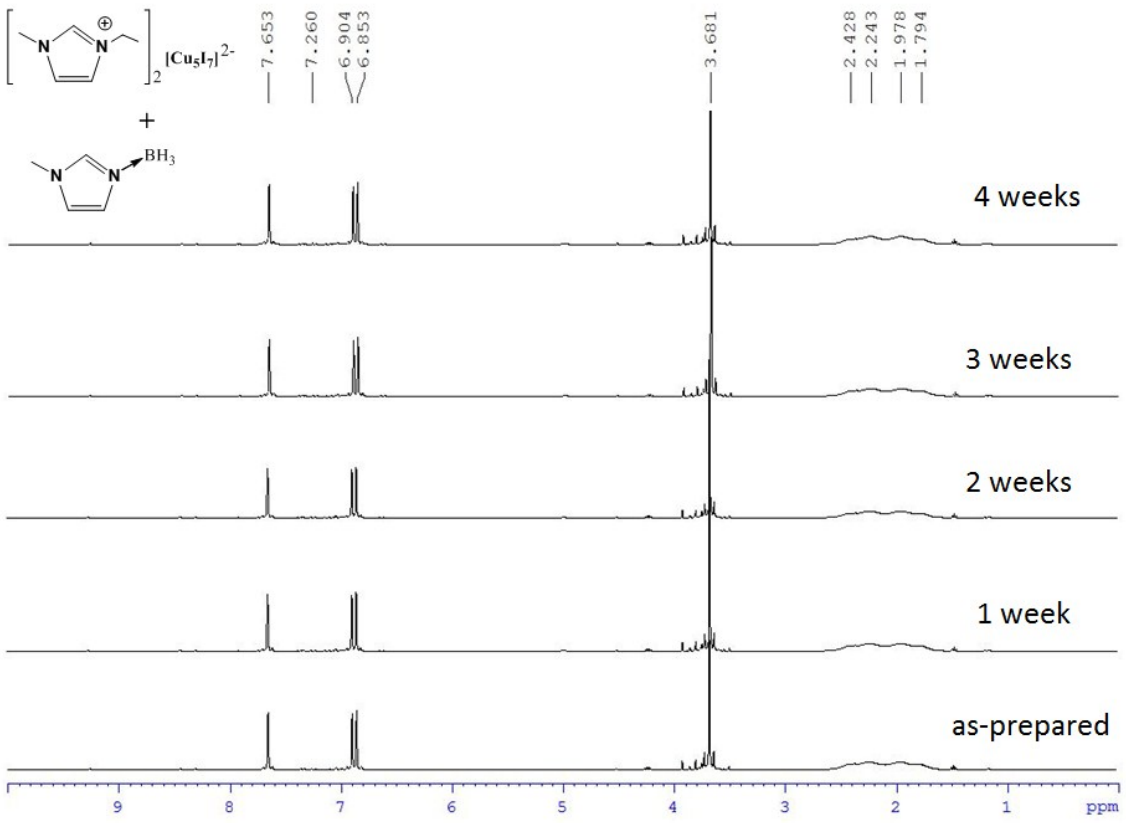


Figure S18. ^{1}H NMR (400 MHz, $CDCl_3$) of CuIL **3** in [MIM^+][BH_3^-] fuel.

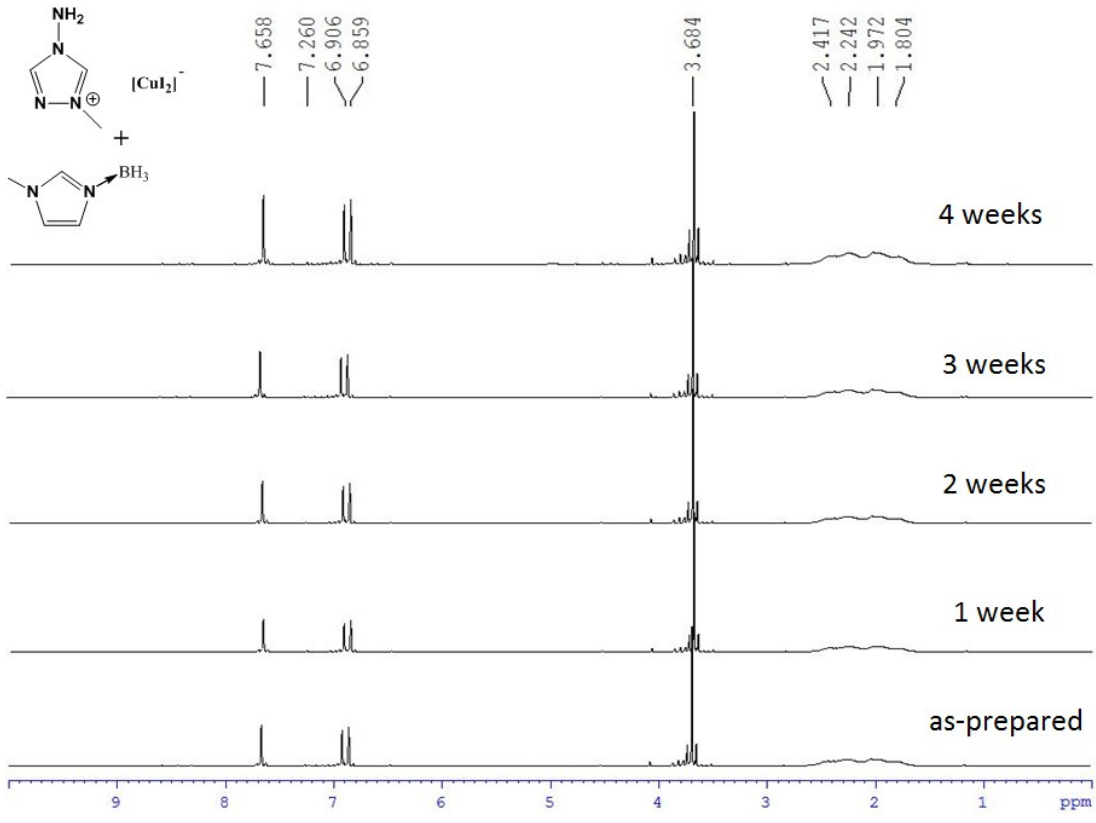


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) of CuIL **4** in [MIM^+][BH_3^-] fuel.

High-speed Camera Images of Hypergolic Ignition Experiments with H_2O_2 (95%).

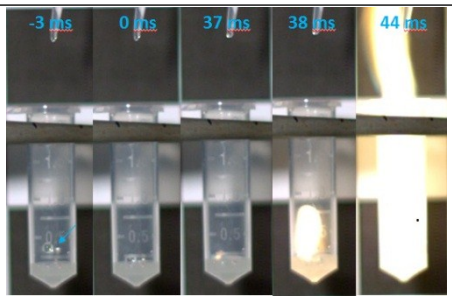


Figure S20. CuIL **1** with [EMIM$^+$][BH_3CN^-] fuel.

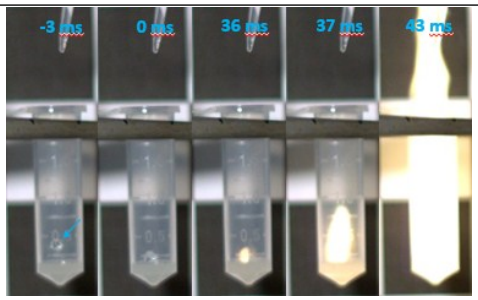


Figure S21. CuIL **2** with [EMIM$^+$][BH_3CN^-] fuel.

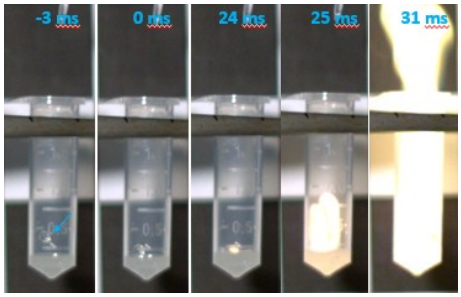


Figure S22. CuIL **3** with [EMIM$^+$][BH_3CN^-] fuel.

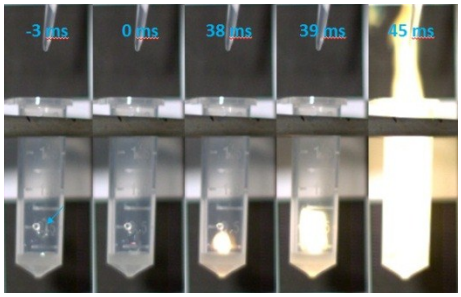


Figure S23. CuIL **4** with [EMIM$^+$][BH_3CN^-] fuel.

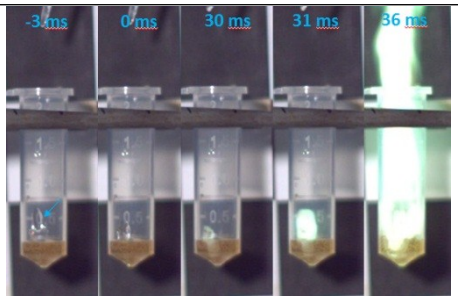


Figure S24. CuIL **1** with [MIM]·[BH_3] fuel.

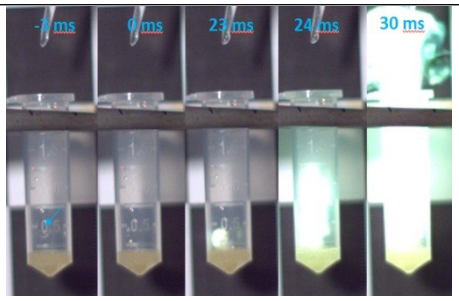


Figure S25. CuIL **2** with [MIM]·[BH_3] fuel.

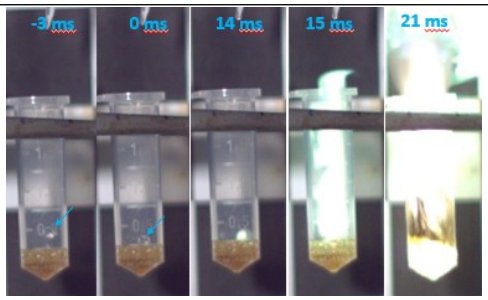


Figure S26. CuIL **3** with [MIM]·[BH_3] fuel.

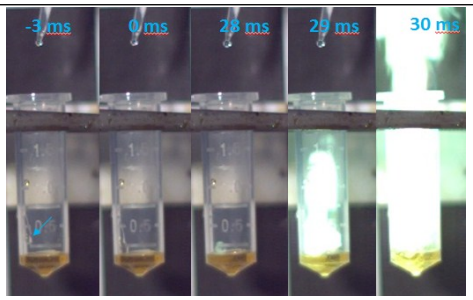


Figure S27. CuIL **4** with [MIM]·[BH_3] fuel.

Energetic Performance

Table S10. Calculated heats of formation (ΔH_f, based on bomb calorimetry measurements) and specific impulses (I_{sp}) of fuels **F1, F2** and promoters CuILs **1-4** (calculated by EXPLO5 v6.02).

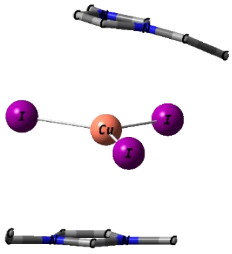
	F1	**F2**	**CuIL 1**	**CuIL 2**	**CuIL 3**	**CuIL 4**
ΔH_f (kJ·mol^{-1})	218.6	15.39	1429.23	1599.18	2042.74	810.24
I_{sp} (s)	269	266.6	226.4	192.1	217.9	201.8

Table S11. Calculated specific impulses (I_{sp}) of the examined promoter-in-fuel mixtures based on the I_{sp} of pure promoters and fuels, mixed in 1:9 promoter-to-fuel ratio.

Promoter-in-Fuel	I_{sp} (s)
CuIL 1-in-F1	264.7
CuIL 2-in-F1	261.3
CuIL 3-in-F1	263.9
CuIL 4-in-F1	262.3
CuIL 1-in-F2	262.5
CuIL 2-in-F2	259.1
CuIL 3-in-F2	261.7
CuIL 4-in-F2	260.1

DFT Calculations

DFT calculations were performed using Gaussian 09.2 Geometry optimization of all the molecules, intermediates were carried out by using the wB97XD method with Ahlrichs' def2-SVP basis set, and with the relativistic effect of iodine, which was accounted for by the Stuttgart-Dresden ECP, implemented in the Gaussian 09 software. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis of all the molecules and intermediates contained no imaginary frequency showing that these are energy minima. The transition states geometries gave one imaginary frequency at expected reaction coordinates confirming that it is a first-order saddle point.



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H	3.60204900	-0.00111200	-1.00854900
C	2.96397600	1.18608200	1.94658700
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H	4.05167300	-3.17817400	0.92775600
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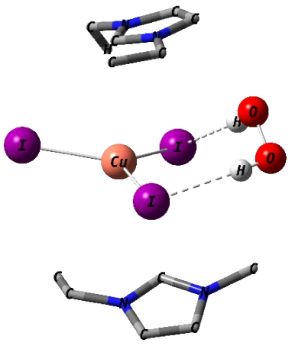

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H	-2.20447700	0.14343000	-1.81514200
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C	-3.12200800	2.34459500	-0.25408100
H	-2.36690000	2.36233200	0.54883800
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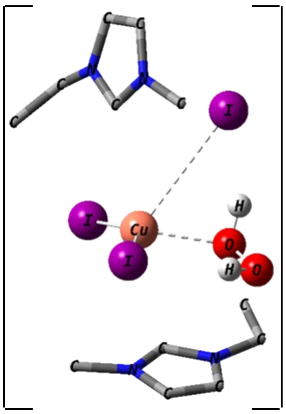

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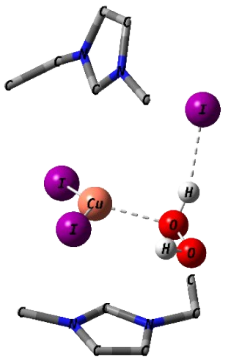

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H	2.40497800	-1.50782300	-2.43518300
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O	1.12356200	1.87752700	-1.93179600
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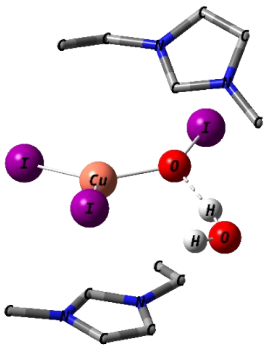

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N	-3.46270800	-1.75412700	0.66423600
N	-3.19019500	-0.74629500	-1.23423700

C	-4.66358600	-1.15319300	0.35216900
H	-5.52786700	-1.21574000	1.00574100
C	-2.59017000	-1.48702800	-0.30480600
H	-1.55694000	-1.83626800	-0.33274200
C	-4.49051800	-0.51923800	-0.83875700
H	-5.17176600	0.08857400	-1.42563400
C	-3.14461400	-2.50698300	1.87162900
H	-2.18512900	-2.15327200	2.28131700
H	-3.08750900	-3.57970400	1.64420700
H	-3.93678100	-2.33146200	2.60809100
C	-2.52135300	-0.14832400	-2.39851300
H	-1.83506400	0.62869600	-2.02618900
H	-3.30908300	0.35116000	-2.97813300
C	-1.77382100	-1.16443000	-3.24045900
H	-0.95763500	-1.63748700	-2.67424200
H	-1.30877100	-0.64407600	-4.08870500
H	-2.44809000	-1.94393800	-3.62517700
N	3.74668700	-0.26287600	0.84107800
N	2.39395000	0.74715500	2.20069600
C	3.60043000	-1.07459900	1.94214700
H	4.08202100	-2.04459200	2.01091900
C	2.99470400	0.82330900	1.01490300
H	2.87075400	1.61538700	0.27854000
C	2.75101500	-0.44009500	2.79623800
H	2.31591400	-0.75436600	3.73919700
C	4.44999000	-0.59900500	-0.38725200
H	4.02047900	-1.52494200	-0.79371800
H	4.28610100	0.20360000	-1.11610600
H	5.52210500	-0.72030200	-0.18624300
C	1.39951300	1.69108700	2.72474600
H	0.41746700	1.24222400	2.52240000
H	1.55277800	1.73431400	3.81153800
C	1.50738100	3.06262400	2.09001500
H	1.26067900	3.03149800	1.01750600
H	0.77601600	3.72850100	2.56688200
H	2.50906500	3.49972500	2.22222800
O	-0.90932600	0.27381600	0.88003800
I	-2.07972700	1.94385400	0.99762300
O	-0.26295000	-1.26845700	2.91758900
H	-0.57827900	-0.61533700	2.23937900
H	0.22209400	-1.89067300	2.35758800

Sum of electronic and zero-point Energies= -1071.691644
Sum of electronic and thermal Energies= -1071.661045
Sum of electronic and thermal Enthalpies= -1071.660101
Sum of electronic and thermal Free Energies= -1071.760528

H_2O_2:

O	0.00000000	0.70868900	-0.05434200
H	-0.81150200	0.89629300	0.43473400
O	0.00000000	-0.70868900	-0.05434200
H	0.81150200	-0.89629300	0.43473400

Sum of electronic and zero-point Energies= -151.349036
Sum of electronic and thermal Energies= -151.345788
Sum of electronic and thermal Enthalpies= -151.344844
Sum of electronic and thermal Free Energies= -151.370665

H_2O:

O	0.00000000	0.00000000	0.11911600
H	0.00000000	0.75472700	-0.47646200
H	0.00000000	-0.75472700	-0.47646200

Sum of electronic and zero-point Energies= -76.315279
Sum of electronic and thermal Energies= -76.312444
Sum of electronic and thermal Enthalpies= -76.311500
Sum of electronic and thermal Free Energies= -76.332926

O_2:

O	0.00000000	0.00000000	0.59559100
O	0.00000000	0.00000000	-0.59559100

Sum of electronic and zero-point Energies= -150.088493
Sum of electronic and thermal Energies= -150.086131
Sum of electronic and thermal Enthalpies= -150.085187
Sum of electronic and thermal Free Energies= -150.107398