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Supplementary data

Table S1 Bond distance and bond angle of $[Cu(MeaaiEt)_2(N_3)_2]$ (**4b**)

Bond distance	(Å)	Bond angle	(º)
Cu – N1	2.011(2)	N1 – Cu –N4	68.70(8)
Cu – N4	2.661(2)	N1 – Cu –N5	91.04(10)
Cu – N5	2.011(2)	N4 – Cu –N9	99.93(9)
Cu – N8	2.693(2)	N1 – Cu –N9	89.69(10)
Cu – N9	1.960(3)	N1 – Cu – N12	170.23(11)
Cu – N12	1.972(3)	N5 – Cu – N9	170.38(11)
N3 – N4	1.262(3)	N5 –Cu –N12	87.44 (11)
N7 – N8	1.266(3)	N9 – Cu – N12	93.42 (11)
		N8 – Cu –N9	102.41(9)
		N8 –Cu –N12	101.08(10)
		N5 –Cu –N8	68.05(8)
		N4–Cu –N8	146.92(7)
		N1 – Cu –N8	87.26(8)
		N4 – Cu –N12	101.61(9)
		N4 – Cu –N5	89.27(8)

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Table S2 Bond distance and bond angle of $[Cu(HaaiMe)_2(SCN)_2]DMF$ (**5a**)

Bond distance	(Å)	Bond angle	(º)
Cu – N1	1.942(3)	N1 – Cu –N2	90.92(14)
Cu – N2	1.953(3)	N1 – Cu –N3	171.65(13)
Cu – N3	2.009(3)	N1 – Cu –N7	102.07(12)
Cu – N4	1.999(3)	N2 – Cu –N3	90.18(13)
Cu – N7	2.612(3)	N2 – Cu – N7	100.41(11)
Cu – N10	2.627(3)	N3 – Cu – N7	69.59(9)
N6 – N7	1.265(3)	N1 –Cu –N10	105.17(11)
N9 – N10	1.259(4)	N2 – Cu – N10	103.24(12)
		N1 –Cu –N4	90.22(12)
		N2 –Cu –N4	172.27(13)
		N3–Cu –N10	82.62(9)
		N4 –Cu –N10	69.10(9)
		N4 –Cu –N7	86.82(9)
		N7–Cu–N10	143.30(8)

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Table S3 UV-Vis spectra [a], I.R data, magnetic moment (RT) data (μ)

Compound	UV-Vis spectral data (λ_{max}/nm) (10^{-3} ε M^{-1} cm^{-1})	I.R. data				μ (B.M.)
		υ(N_3^-)	υ(SCN^-)	υ(C=N)	υ(N=N)	
[Cu(HaaiMe)$_2$(N_3)$_2$] (**3a**)	710(0.41), 582(0.73), 478(3.32), 385(12.43)	2045^w 2038^s		1589	1438	1.87
[Cu(HaaiEt)$_2$(N_3)$_2$] (**4a**)	712(0.43), 582(0.79), 474(2.81), 382(13.47)	2047^w 2036^s		1586	1440	1.80
[Cu(MeaaiMe)$_2$(N_3)$_2$] (**3b**)	716(0.39), 586(0.71), 474(2.69), 384(12.15)	2045^w 2035^s		1587	1440	1.83
[Cu(MeaaiEt)$_2$(N_3)$_2$] (**4b**)	718(0.39), 584(0.69), 472(3.84), 384(12.43)	2045^w 2031^s		1598	1448	1.90
[Cu(HaaiMe)$_2$(SCN)$_2$] DMF (**5a**)	700(0.51), 586(0.65), 458(2.34), 380(12.51)		2091^w 2107^s	1598	1436	1.81
[Cu(HaaiEt)$_2$(SCN)$_2$] DMF (**6a**)	702(0.56), 585(0.68), 456(2.31), 384(11.67)		2090^w 2103^s	1596	1438	1.84
[Cu(MeaaiMe)$_2$(SCN)$_2$] DMF (**5b**)	703(0.62), 580(0.75), 454(3.15), 382(10.89)		2093^w 2105^s	1597	1442	1.82
[Cu(MeaaiEt)$_2$(SCN)$_2$] DMF (**6b**)	703(0.73), 584(0.91), 452(4.85), 380(11.65)		2090^w 2098^s	1596	1436	1.86

[a] Solvent: Acetonitrile (MeCN); w = weak, s = strong

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Table S4 E.s.r and cyclic voltammetric data

Complexes	E.s.r data				Cyclic voltammetric data[b] $E_{1/2}$ (V) (ΔE_p, mV)				
	$g_{\parallel}$	$g_{\perp}$	$A_{\parallel}$	$A_{\perp}$	Cu^{II}/Cu^{I}	Cu^{I}/Cu^{0}	Ligand reduction 1st	2nd	3rd
$[Cu(HaaiMe)_2(N_3)_2]$ (**3a**)	2.245	2.043	152	16	0.42 (140)	-0.08	-0.47 (160)	-0.82 (140)	-1.05
$[Cu(MeaaiMe)_2(N_3)_2]$ (**3b**)	2.242	2.045	156	14	0.39 (130)	-0.12	-0.51 (150)	-0.88 (140)	-1.15
$[Cu(HaaiEt)_2(N_3)_2]$(**4a**)	2.248	2.042	160	13	0.44 (130)	-0.10	-0.45 (150)	-0.80 (150)	-1.08
$[Cu(MeaaiEt)_2(N_3)_2]$ (**4b**)	2.250	2.040	158	14	0.38 (140)	-0.12	-0.50 (160)	-0.91 (160)	-1.10
$[Cu(HaaiMe)_2(SCN)_2]$ DMF (**5a**)	2.257	2.062	160	14	0.38 (130)	-0.12	-0.50 (150)	-0.90 (160)	-1.14
$[Cu(MeaaiMe)_2(SCN)_2]$ DMF (**5b**)	2.249	2.051	160	13	0.34 (130)	-0.08	-0.54 (160)	-0.92 (160)	-1.16
$[Cu(HaaiEt)_2(SCN)_2]$DMF (**6a**)	2.247	2.081	160	12	0.40 (140)	-0.10	-0.55 (150)	-0.92 (140)	-1.00
$[Cu(MeaaiEt)_2(SCN)_2]$ DMF (**6b**)	2.248	2.074	158	14	0.37 (150)	-0.08	-0.50 (150)	-0.88 (140)	-1.10

[b] Solvent in MeCN, Pt-disk working electrode, supporting electrolyte, TBAP (0.01 M); solute concentration, 10^{-3} M; scan rate, 0.05 V s^{-1}; $\Delta E_p = |E_{pa} - E_{pc}|$, mV; E_{pa} = anodic peak potential, E_{pc} = cathodic peak potential, V; $E_{1/2} = 0.5(E_{pa} + E_{pc})$, V.