Electronic Supporting Information for

Design and synthesis of copper(II) malonates with N,N'-containing linkers

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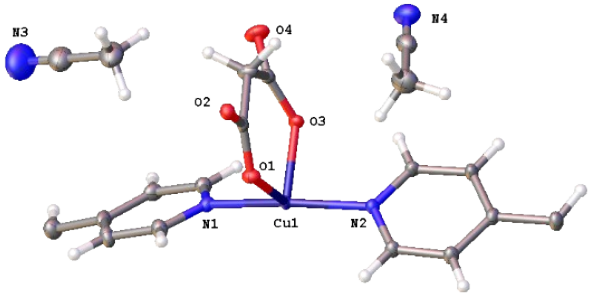
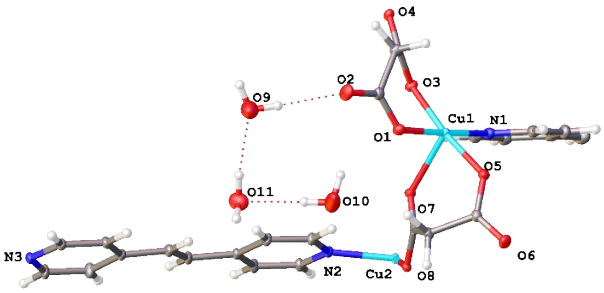
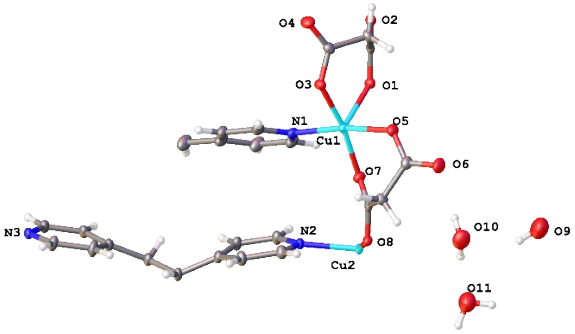


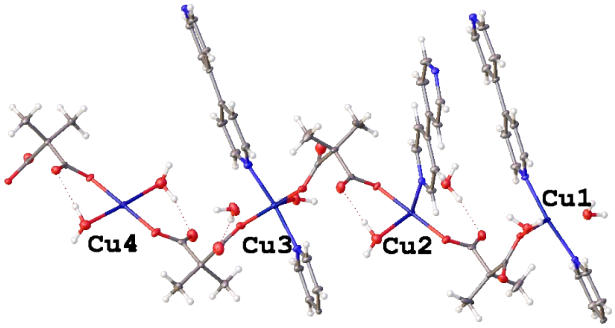
[Cu(bpe)mal] · $2CH_3CN$



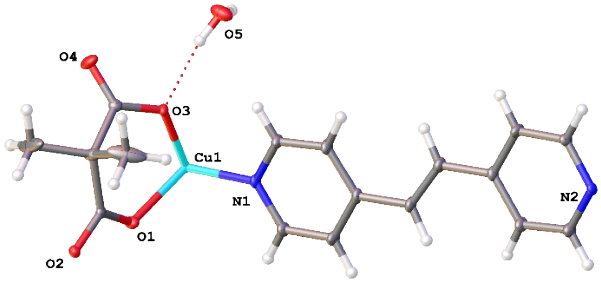
$[Cu_4(bpe)_3mal_4] \cdot 6H_2O$



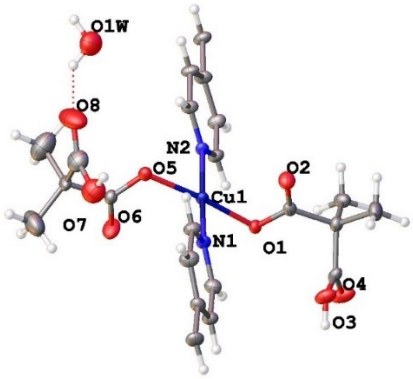
$[Cu_4(bpe)(tpcb)mal_4] \cdot 6H_2O$



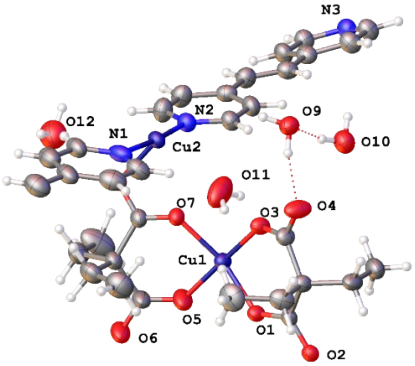
$[Cu_4(bipy)_4(Me_2mal)_4(H_2O)_5] \cdot 3H_2O$



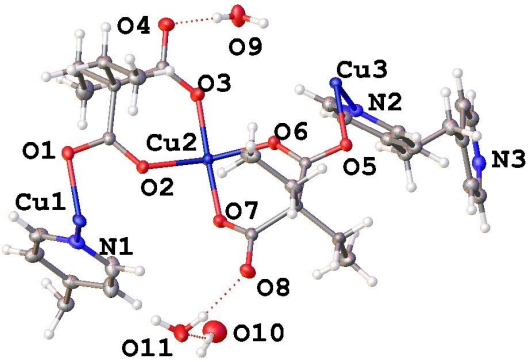
$[Cu(bpe)Me_2mal] \cdot H_2O$



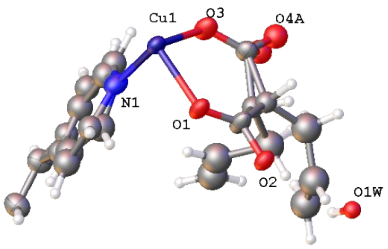
$[Cu(bpe)(HMe_2mal)_2] \cdot H_2O$



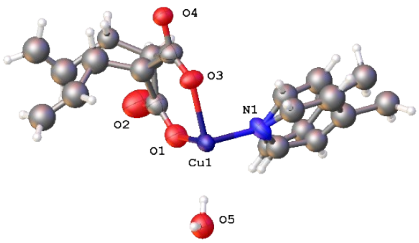
$[Cu_4(bpe)_3(Et_2mal)_4] \cdot 5H_2O$



$[Cu_4(bpa)_3(Et_2mal)_4] \cdot 5.5H_2O$

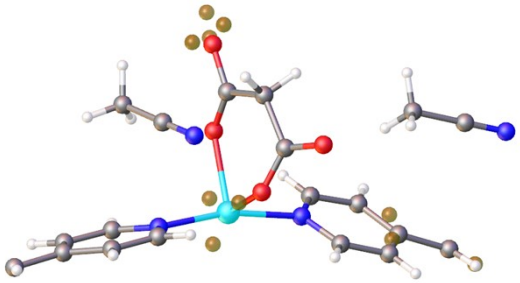


[Cu(bpe)Amal] · $0.25H_2O$

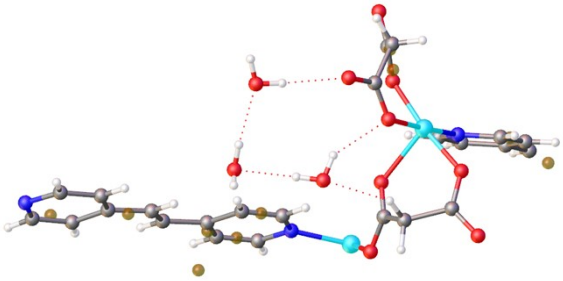


[Cu(bpa)Amal] · $0.25H_2O$

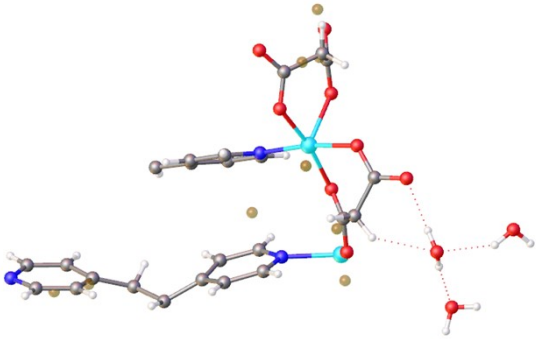
Figure S1. Asymmetric units of studied compounds.



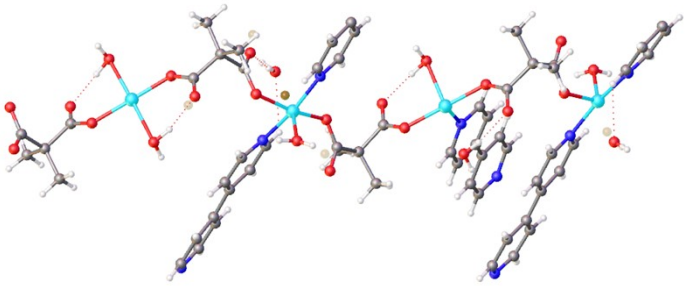
[Cu(bpe)mal] · $2CH_3CN$



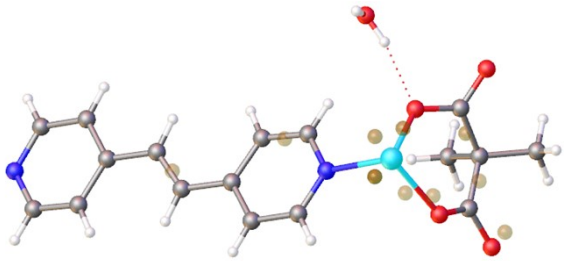
[Cu_4(bpe)$_3$$mal_4$] · $6H_2O$



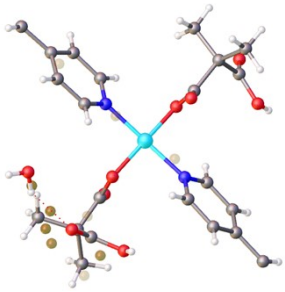
[Cu_4(bpe)(tpcb)mal_4] · $6H_2O$



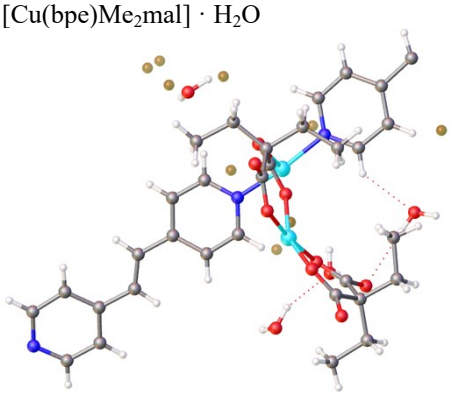
[$Cu_4(bipy)_4(Me_2mal)_4(H_2O)_5$] · $3H_2O$



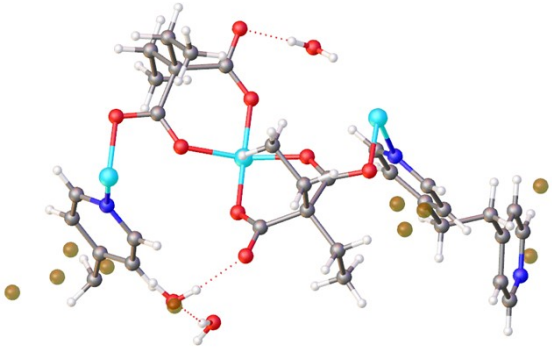
[Cu(bpe)Me_2mal] · H_2O



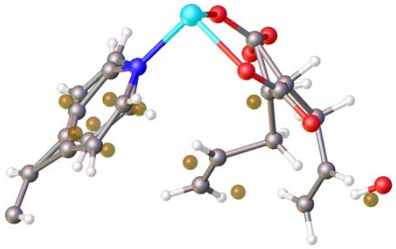
[Cu(bpe)($HMe_2mal)_2$]·H_2O



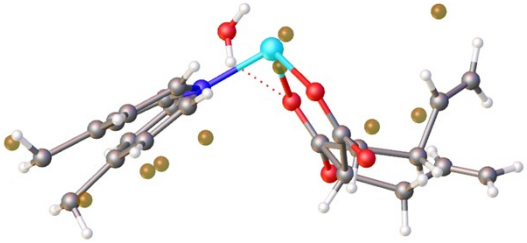
[Cu_4(bpe)$_3$($Et_2mal)_4$] · $5H_2O$



[Cu_4(bpa)$_3$($Et_2mal)_4$] · $5.5H_2O$



[Cu(bpe)Amal] · $0.25H_2O$



[Cu(bpa)Amal] · $0.25H_2O$

Figure S2. Residual density peaks Q1-Q10 (brown spheres) for compounds **1 - 10**.

Powder X-ray diffraction

The powder XRD data were collected on a Bruker D8 Advance diffractometer (Bruker, Billerica, MA, USA) with a LynxEye detector in reflection mode with the sample thinly dispersed on a zero-background Si sample holder, λ(CuKα) = 1.54060 Å, θ/θ scan with variable slits (irradiated length 20 mm), 2θ from 5° to 41°, step size 0.02°.

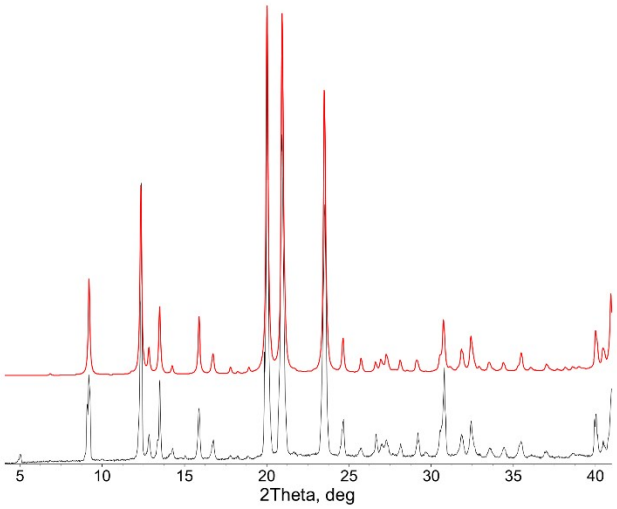


Figure S3. XRD powder patterns for compound [Cu(bpe)Me_2mal] · H_2O: experimental (black line), calculated (red line)

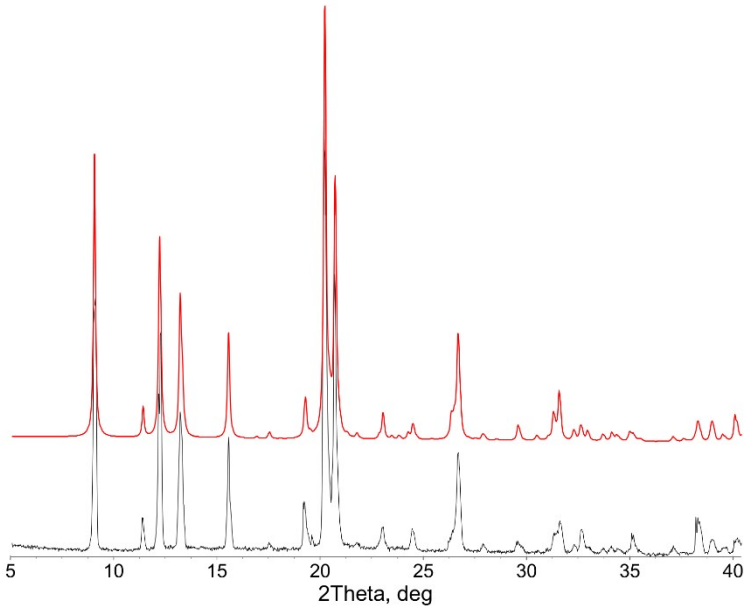


Figure S4. XRD powder patterns for compound [Cu(bpe)Amal]·0.25H_2O: experimental (black line), calculated (red line)

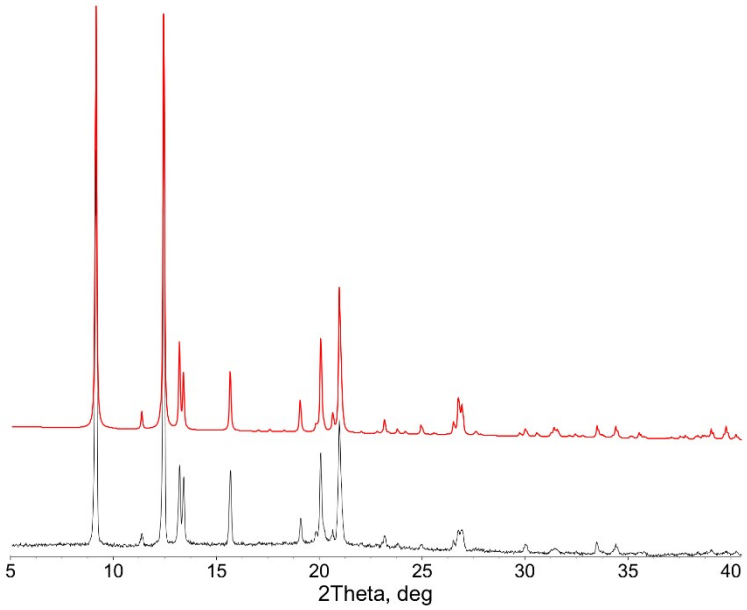


Figure S5. XRD powder patterns for compound [Cu(bpa)Amal]·0.25H_2O: experimental (black line), calculated (red line)

Table S1. Previously Reported Copper(II) Malonate Complexes with 4,4'-Bipyridine and its Analogs.

Complex	CCF	net	Refcode
$\{[Cu_2(bpe)_2(mal)_2(H_2O)_2] \cdot 2H_2O\}_n$	$A_2T^{11}{}_2B^2M^1{}_2$	**hcb**	DASVUQ
$[Cu_2(bipy)(Memal)_2(H_2O)_2]_n$	$A_2K^4{}_2B^2$	3,5T3	EDOKAK
$(H_2bpe)[Cu(mal)_2] \cdot 4H_2O$	$AB^{01}{}_2$	Isolated complex	ELOHES
$\{[Cu_4(bpe)_3(mal)_4] \cdot 6H_2O\}_n$	$A_4T^{21}{}_2T^{11}{}_2B^2{}_3$	3,3,5L29	ELOHIW
$\{[Cu_2(bipy)_4(Memal)(H_2O)(NO_3)](NO_3) \cdot H_2O\}_n$	$A_2K^{21}B^2{}_2M^1{}_2$	**pcu**	GAKTET
$\{[Cu_2(bipy)_2(Memal)_2(H_2O)] \cdot H_2O\}_n$	$A_2B^2M^1{}_3$	2C1	GAKTIX
$\{[Cu_3(bpa)_3(mal)_2(H_2O)_2](NO_3)_2 \cdot 2H_2O\}_n$	$A_3K^{21}{}_2B^2{}_3M^1{}_2$	**tfz**	HACDUL
$\{[Cu_2(bpam)_3(mal)_2(H_2O)_2] \cdot H_2O\}_n$	$A_2T^{11}{}_2B^2M^1$	**hcb**	HISTAF
$\{[Cu(bipy)(Phmal)] \cdot H_2O\}_n$	$AT^{11}B^2$	**sql**	JERLIC
$\{[Cu_2(bipy)_2(mal)_2(H_2O)_2] \cdot 2H_2O\}_n$	$A_2T^{11}{}_2B^2M^1{}_2$	**fes**	NAYJUS
$\{[Cu_2(bpam)(mal)_2(H_2O)_2] \cdot 2H_2O\}_n$	$A_2T^{11}{}_2B^2M^1{}_2$	**sql**	PASGIA
$[Cu_2(bipy)_2(cbdc)_2]_n$	$AT^{11}B^2$	**sql**	PERZOC
$[Cu(bpa)(cbdc)]_n$	$AT^{11}B^2$	**sql**	PERZUI
$\{[Cu_2(bipy)_4(mal)_2](ClO_4)_2 \cdot MeOH \cdot 4H_2O\}_n$	$A_2K^{21}{}_2B^2{}_4$	**pcu**	SEYNAM
$[Cu_2(bipy)_2(mal)_2(H_2O)_2]_n$	$A_2T^{11}{}_2B^2M^1{}_2$	**fes**	VIWQIB
$\{[Cu(dpp)(Me_2mal)] \cdot 3H_2O\}_n$	$AB^2{}_2M^1$	**sql**	VOPMAQ
$\{[Cu(dpp)_2(H_2O)_2][Cu(Et_2mal)_2] \cdot 4H_2O\}_n$	$AB^2{}_2M^1{}_2 + AB^{01}{}_2$	2C1	VOPMEU
$\{[Cu_3(dpp)_4(mal)_3] \cdot 12H_2O\}_n$	$A_3B^2{}_4B^{01}{}_2M^1{}_3$	**Sql**	VOPMIY
$\{[Cu(dpp)(mal)(H_2O)] \cdot 4H_2O\}_n$	$AB^{01}B^2M^1$	2C1	XUQBIV
$[Cu_2(bipy)_2(cbdc)_2]_n$	$AT^{11}B^2$	**sql**	YAHJUP
$\{[Cu_2(bpa)_2(cbdc)_2] \cdot MeOH\}_n$	$AT^{11}B^2$	**sql**	YAMYOD

a Etmal = ethylmalonate; Memal = methylmalonate; Me_2mal = dimethylmalonate; cbcd = cyclobutane-1,1-dicarboxylate; mal = malonate; dpp = 4,4'-propane-1,3-diyldipyridine; Phmal = phenylmalonate; bpam - 4,4'-Dipyridylamine

Table S2. Occurrences of various coordination polyhedra in 583 mixed-ligand copper(II) complexes.[a]

CN	CP	occurrence	p_{CP}, %
4	N_4	1	1
	N_3O	0	0
	N_2O_2	181	91
	NO_3	12	6
	O_4	4	2
5	N_5	0	0
	N_4O	1	0.2
	N_3O_2	6	1
	N_2O_3	195	44
	NO_4	235	53
	O_5	7	1
6	N_6	0	0
	N_5O	0	0
	N_4O_2	1	1
	N_3O_3	0	0
	N_2O_4	86	88
	NO_5	11	11
	O_6	0	0

[a] CN and CP – coordination number and coordination polyhedron of copper(II) atoms; p_{CP} is probability of occurrence of a given polyhedron.

Table S3. Crystallographic data and experimental details for malonate- and dimethylmalonate-containing compounds.

Parameter	[Cu(bpe)mal] · $2CH_3CN$ (**1**)	$[Cu_4(bpe)_3mal_4]$ · $6H_2O$ (**2**)	$[Cu_4(bipy)_4(Me_2mal)_4(H_2O)_5]$ · $3H_2O$ (**3**)	$[Cu(bpe)(HMe_2mal)_2]\cdot H_2O$ (**4**)	$[Cu(bpe)Me_2mal]\cdot H_2O$ (**5**)
CCDC	2233546	2233547	2233548	2233549	2233550
Empirical formula	$C_{19}H_{18}CuN_4O_4$	$C_{48}H_{50}Cu_4N_6O_{22}$	$C_{60}H_{72}Cu_4N_8O_{24}$	$C_{22}H_{25}CuN_2O_{8.5}$	$C_{17}H_{18}CuN_2O_5$
Formula weight	429.91	1317.10	1543.41	516.98	393.87
Color, habit	Blue, prism	Blue, plate	Blue, prism	Violet, plate	Light-Blue, prism
Crystal size (mm)	0.42×0.29×0.17	0.28×0.26×0.06	0.23×0.21×0.18	0.29×0.22×0.03	0.20×0.11×0.11
a (Å)	8.806(2)	13.4822(9)	24.8208(14)	9.193(2)	13.4355(11)
b (Å)	9.110(3)	10.2082(7)	19.2806(11)	12.176(5)	14.4906(12)
c (Å)	23.923(6)	19.4797(13)	13.1952(8)	20.620(8)	8.9824(7)
β (°)	96.827(6)	105.290(2)	95.6250(10)	98.301(18)	99.255(2)
V (Å^3)	1905.5(9)	2586.1(3)	6284.3(6)	2283.8(15)	1726.0(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group, Z	P 2_1/n, 4	P 2_1/n, 2	P 2_1/c, 4	P 2_1/c, 4	P 2_1/c, 4
D_{cal}(g cm^{-3})	1.499	1.691	1.631	1.504	1.516
μ (mm^{-1})	1.179	1.712	1.425	1.010	1.295
Reflections collected	13783	35457	57730	27039	27355
Independent reflections (R_{int})	5831 (0.037)	10607 (0.086)	18491 (0.047)	6976 (0.086)	6576 (0.051)
Obs.refl./restraints/ parameters	4602 / 0 / 255	6656 / 0 / 370	11155 / 5 / 890	4503 / 42 / 313	5187 / 0 / 231
R,[a] % [$F^2 > 2\sigma(F^2)$]	0.044	0.050	0.059	0.088	0.042
R_w,[b] % (F^2)	0.107	0.110	0.171	0.207	0.111
GOF	1.044	0.996	1.016	1.010	1.053
F(000)	884	1344	3184	1072	812

[a] $R = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$. [b] $R_w = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma(w(F_o^2))]^{1/2}$. [c] $\mathrm{GOF} = [\Sigma w(F_o^2 - F_c^2)^2/(N_{obs} - N_{param})]^{1/2}$

Table S4. Crystallographic data and experimental details for diethyl- and allylmalonate-containing complexes.

	$[Cu_4(bpe)_3(Et_2mal)_4] \cdot 5H_2O$ (**6**)	$[Cu_4(bpa)_3(Et_2mal)_4] \cdot 5.5H_2O$ (**7**)	$[Cu(bpe)Amal] \cdot 0.25H_2O$ (**8**)	$[Cu(bpa)Amal] \cdot 0.25H_2O$ (**9**)	$[Cu_4(bpe)(tpcb)mal_4] \cdot 6H_2O$ (**10**)
CCDC	2233551	2233552	2233553	2233554	2233555
Empirical formula	$C_{64}H_{80}Cu_4N_6O_{21}$	$C_{64}H_{87}Cu_4N_6O_{21.5}$	$C_{18}H_{15.5}CuN_2O_{4.25}$	$C_{18}H_{18.5}CuN_2O_{4.25}$	$C_{48}H_{50}Cu_4N_6O_{22}$
Formula weight	1523.50	1538.55	391.36	394.39	1317.10
Color, habit	Blue, plate	Blue, plate	Blue, prism	Light-blue, needle	Blue, plate
Crystal size (mm)	0.02×0.15×0.16	0.06×0.27×0.31	0.38×0.26×0.19	0.42 × 0.08 × 0.06	0.28×0.26×0.06
a (Å)	20.737(4)	16.7676(6)	9.1259(7)	9.296(6)	13.399(17)
b (Å)	8.4420(17)	13.2787(5)	13.4355(10)	13.349(8)	10.334(14)
c (Å)	40.952(8)	17.0342(6)	14.5446(11)	14.339(9)	19.28(2)
β (°)	97.09(3)	117.980(2)	90	90	103.69(3)
V (Å^3)	7114(3)	3349.4(2)	1783.3(2)	1779.4(18)	2594(6)
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic	Monoclinic
Space group, Z	C 2/c, 4	P 2_1/n, 2	P n m a, 4	P n m a, 4	P 2_1/n, 2
D_{cal}(g cm^{-3})	1.422	1.526	1.458	1.472	1.686
μ (mm^{-1})	1.653	1.333	1.250	1.253	1.707
Reflections collected	20573	45830	18649	17254	59570
Independent reflections (R_{int})	8265 (0.032)	10278 (0.028)	2845 (0.047)	2757 (0.184)	8680 (0.067)
Obs.refl./restraints/ parameters	6432 / 6 / 437	8792 / 0 / 440	2168 / 14 / 145	1082 / 10 / 113	6391 / 0 / 370
R,[a] % [$F^2 > 2\sigma(F^2)$]	0.086	0.033	0.063	0.094	0.042
R_w,[b] % (F^2)	0.223	0.093	0.140	0.226	0.109
GOF	1.039	1.067	1.059	0.997	1.034
F(000)	3160	1602	802	814	1344

[a] $R = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$. [b] $R_w = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma(w(F_o^2))]^{1/2}$. [c] $\mathrm{GOF} = [\Sigma w(F_o^2 - F_c^2)^2/(N_{obs} - N_{param})]^{1/2}$

Table S5. Selected geometry parameters of coordination polyhedra of copper(II) atoms in **1 – 10**.

Parameter	distance (Å)	Parameter	angle (°)	Parameter	angle (°)
Complex **1** coordination polyhedron $Cu(1)N_2O_3$, square pyramid					
Cu(1)–O(1)	2.1403(17)	$O(2^{i})$–Cu(1)–O(1)	97.04(6)	O(3)–Cu(1)–N(1)	89.42(7)
Cu(1)–$O(2^{i})$	1.9740(16)	$O(2^{i})$–Cu(1)–N(1)	88.83(7)	O(3)–Cu(1)–N(2)	90.02(7)
Cu(1)–O(3)	1.9319(15)	$O(2^{i})$–Cu(1)–N(2)	89.71(7)	N(1)–Cu(1)–O(1)	95.56(6)
Cu(1)–N(1)	2.0396(17)	O(3)–Cu(1)– O(1)	91.37(6)	N(1)–Cu(1)–N(2)	166.27(7)
Cu(1)–N(2)	2.0425(17)	O(3)–Cu(1)–$O(2^{i})$	171.54(6)	N(2)–Cu(1)–O(1)	98.17(6)
Complex **2** coordination polyhedron $Cu(1)NO_4$, square pyramid					
Cu(1)–O(1)	1.9903(17)	O(1)–Cu(1)–O(7)	90.95(7)	O(5)–Cu(1)–O(1)	95.23(7)
Cu(1)–O(3)	1.9809(17)	O(1)–Cu(1)–N(1)	176.27(8)	O(5)–Cu(1)–O(3)	172.888(7)
Cu(1)–O(5)	1.9624(17)	O(1)–Cu(1)–O(3)	88.16(7)	O(5)–Cu(1)–O(7)	88.16(7)
Cu(1)–O(7)	2.2598(17)	O(3)–Cu(1)–O(7)	98.06(7)	O(5)–Cu(1)–N(1)	88.48(8)
Cu(1)–N(1)	2.024(2)	O(3)–Cu(1)–N(1)	88.12(8)	N(1)–Cu(1)–O(7)	89.52(8)
Complex **2** coordination polyhedron $Cu(2)N_2O_3$, square pyramid					
Cu(2)–$O(4^{ii})$	1.9438(17)	$O(4^{ii})$–Cu(2)–O(8)	174.98(7)	O(8)– Cu(2)–N(2)	91.25(7)
Cu(2)–O(8)	1.9680(17)	$O(4^{ii})$–Cu(2)–$O(8^{iii})$	99.58(6)	O(8)–Cu(2)–$N(3^{iv})$	91.14(8)
Cu(2)–$O(8^{iii})$	2.3361(16)	$O(4^{ii})$–Cu(2)–N(2)	92.19(8)	N(2)–Cu(2)–$O(8^{iii})$	89.58(7)
Cu(2)–N(1)	2.0277(19)	$O(4^{ii})$–Cu(2)–$N(3^{iv})$	85.67(8)	N(2)–Cu(2)–$N(3^{iv})$	175.60(8)
Cu(2)–$N(3^{iv})$	2.0749(19)	O(8)–Cu(2)–$O(8^{iii})$	76.79(7)	$N(3^{iv})$–Cu(2)–$O(8^{iii})$	94.57(7)
Complex **3** coordination polyhedron $Cu(1)N_2O_3$, square pyramid					
Cu(1)–O(1)	1.948(2)	O(1)–Cu(1)–$O(15^{v})$	165.82(11)	N(1)–Cu(1)–$O(15^{v})$	88.95(11)
Cu(1)–$O(15^{v})$	1.975(2)	O(1)–Cu(1)–O(17)	111.96(10)	N(3)–Cu(1)–$O(15^{v})$	89.39(10)
Cu(1)–O(17)	2.260(3)	O(1)–Cu(1)–N(1)	87.89(10)	N(1)–Cu(1)–O(17)	93.12(11)
Cu(1)–N(1)	2.035(3)	O(1)–Cu(1)–N(3)	91.19(10)	N(3)–Cu(1)–O(17)	96.98(11)
Cu(1)–N(3)	2.031(3)	O(17)–Cu(1)–$O(15^{v})$	82.01(10)	N(1)–Cu(1)–N(3)	169.44(12)
Complex **3** coordination polyhedron $Cu(2)N_2O_3$, square pyramid					
Cu(2)–O(4)	1.962(2)	O(4)–Cu(2)–O(19)	88.61(10)	O(5)–Cu(2)–N(4)	91.92(11)
Cu(2)–O(5)	1.958(2)	O(4)–Cu(2)–N(4)	88.58(11)	O(5)–Cu(2)–$N(7^{vi})$	88.23(10)
Cu(2)–O(19)	2.389(3)	O(4)–Cu(2)–$N(7^{vi})$	91.26(10)	N(4)–Cu(2)–O(19)	88.39(11)
Cu(2)–N(4)	2.030(3)	O(5)–Cu(2)–O(4)	179.43(10)	N(4)–Cu(2)–$N(7^{vi})$	178.87(13)
Cu(2)–$N(7^{vi})$	2.031(3)	O(5)–Cu(2)–O(19)	91.68(10)	$N(7^{vi})$–Cu(2)–O(19)	92.73(11)
Complex **3** coordination polyhedron $Cu(3)N_2O_3$, square pyramid					
Cu(3)–O(7)	1.951(3)	O(7)–Cu(3)–O(9)	165.35(12)	O(9)–Cu(3)–N(6)	88.41(11)
Cu(3)–O(9)	1.973(3)	O(7)–Cu(3)–O(21)	113.17(11)	O(9)–Cu(3)–N(8)	89.74(11)
Cu(3)–O(21)	2.308(3)	O(7)–Cu(3)–N(6)	90.99(11)	N(6)–Cu(3)–O(21)	97.99(12)
Cu(3)–N(6)	2.037(3)	O(7)–Cu(3)–N(8)	88.34(11)	N(6)–Cu(3)–N(8)	170.11(14)

Cu(3)–N(8)	2.043(3)	O(9)–Cu(3)–O(21)	81.39(11)	N(8)–Cu(3)–O(21)	91.34(12)
Complex **3** coordination polyhedron $Cu(4)N_2O_4$, octahedron					
Cu(4)–O(11)	1.954(2)	O(11)–Cu(4)–O(13)	179.12(12)	O(13)–Cu(4)–N(2^{vi})	88.42(10)
Cu(4)–O(13)	1.959(2)	O(11)–Cu(4)–O(23)	90.31(11)	O(13)–Cu(4)–N(5^{ii})	91.17(10)
Cu(4)–O(23)	2.379(3)	O(11)–Cu(4)–O(24)	91.27(11)	O(23)–Cu(4)–O(24)	178.22(10)
Cu(4)–O(24)	2.434(3)	O(11)–Cu(4)–N(2^{vi})	91.99(11)	N(2^{vi})–Cu(4)–O(23)	96.68(11)
Cu(4)–N(2^{vi})	2.051(3)	O(11)–Cu(4)–N(5^{ii})	88.45(11)	N(2^{vi})–Cu(4)–O(24)	84.09(11)
Cu(4)–N(5^{ii})	2.047(3)	O(13)–Cu(4)–O(23)	88.87(11)	N(5^{ii})–Cu(4)–O(23)	85.91(11)
		O(13)–Cu(4)–O(24)	89.54(10)	N(5^{ii})–Cu(4)–N(2^{vi})	177.37(13)
Complex **4** coordination polyhedron $Cu(1)N_2O_2$, square					
Cu(1)–O(1)	1.947(3)	O(1)–Cu(1)–N(1)	91.29(16)	O(5)–Cu(1)–N(1)	88.74(16)
Cu(1)–N(1)	1.997(4)	O(1)–Cu(1)–N(2)	91.10(16)	O(5)–Cu(1)–N(2)	89.43(16)
Cu(1)–N(2)	2.001(4)	N(1)–Cu(1)–N(2)	174.20(18)		
Cu(1)–O(5)	1.944(4)	O(5)–Cu(1)–O(1)	174.03(15)		
Complex **5** coordination polyhedron $Cu(1)N_2O_3$, square pyramid					
Cu(1)–O(1)	2.160(1)	O(2^{vii})–Cu(1)–O(1)	103.76(5)	O(3)–Cu(1)–N(1)	90.23(6)
Cu(1)–O(2^{vii})	1.991(1)	O(2^{vii})–Cu(1)–N(1)	89.12(6)	O(3)–Cu(1)–N(2^{viii})	91.02(5)
Cu(1)–O(3)	1.952(1)	O(2^{vii})–Cu(1)–N(2^{viii})	88.56(6)	N(1)–Cu(1)–O(1)	97.35(6)
Cu(1)–N(1)	2.038(2)	O(3)–Cu(1)–O(1)	86.95(5)	N(1)–Cu(1)–N(2^{viii})	174.03(6)
Cu(1)–N(2^{viii})	2.052(2)	O(3)–Cu(1)–O(2^{vii})	169.26(5)	N(2^{viii})–Cu(1)–O(1)	88.54(6)
Complex **6** coordination polyhedron $Cu(1)NO_4$, square pyramid					
Cu(1)–O(1)	1.959(4)	O(1)–Cu(1)–O(7)	154.2(2)	O(3)–Cu(1)–N(3^{ix})	94.9(2)
Cu(1)–O(3)	1.918(4)	O(1)–Cu(1)– N(3^{ix})	103.3(2)	O(5)–Cu(1)–O(1)	86.5(2)
Cu(1)–O(5)	1.918(5)	O(3)–Cu(1)–O(1)	90.4(2)	O(5)–Cu(1)–O(7)	91.5(2)
Cu(1)–O(7)	1.974(4)	O(3)–Cu(1)–O(5)	171.9(2)	O(5)–Cu(1)–N(3^{ix})	93.0(2)
Cu(1)–N(3^{ix})	2.208(5)	O(3)–Cu(1)–O(7)	88.1(2)	O(7)–Cu(1)–N(3^{ix})	102.5(2)
Complex **6** coordination polyhedron $Cu(2)N_2O_3$, square pyramid					
Cu(2)–O(1^{x})	2.435(4)	O(2^{x})–Cu(2)–O(1^{x})	57.5(2)	N(1)–Cu(2)–O(8)	85.9(2)
Cu(2)–O(2^{x})	2.036(4)	O(8)–Cu(2)–O(1^{x})	127.5(2)	N(2)–Cu(2)–O(1^{x})	89.2(2)
Cu(2)–O(8)	2.007(4)	O(8)–Cu(2)–O(2^{x})	172.5(2)	N(2)–Cu(2)–O(2^{x})	93.6(2)
Cu(2)–N(1)	1.987(5)	N(1)–Cu(2)–O(1^{x})	87.2(2)	N(2)–Cu(2)–O(8)	92.1(2)
Cu(2)–N(2)	1.958(5)	N(1)–Cu(2)–O(2^{x})	89.0(2)	N(2)–Cu(2)–N(1)	173.5(2)
Complex **7** coordination polyhedron $Cu(1)N_2O_2$, square					
Cu(1)–O(1)	2.0189(13)	O(1)–Cu(1)–O(1^{xi})	180.00(7)	N(1^{xi})–Cu(1)–O(1)	88.32(6)
Cu(1)–O(1^{xi})	2.0189(13)	N(1^{xi})–Cu(1)–O(1^{xi})	91.68(6)	N(1)–Cu(1)–N(1^{xi})	180.00(10)
Cu(1)–N(1^{xi})	1.9690(14)	N(1)–Cu(1)–O(1)	91.68(6)		
Cu(1)–N(1)	1.9690(14)	N(1)–Cu(1)–O(1^{xi})	88.32(6)		
Complex **7**					

coordination polyhedron Cu(2)NO_4, square pyramid					
Cu(2)–O(2)	1.9558(12)	O(2)–Cu(2)–N(3^{ii})	107.41(5)	O(3)–Cu(2)–O(7)	169.88(6)
Cu(2)–O(3)	1.9065(13)	O(2)–Cu(2)–O(6)	155.41(6)	O(6)–Cu(2)–N(3^{ii})	97.16(5)
Cu(2)–N(3^{ii})	2.2114(15)	O(3)–Cu(2)–O(2)	90.78(5)	O(7)–Cu(2)–O(2)	88.31(5)
Cu(2)–O(6)	1.9604(12)	O(3)–Cu(2)–N(3^{ii})	93.76(6)	O(7)–Cu(2)–N(3^{ii})	96.13(6)
Cu(2)–O(7)	1.9185(13)	O(3)–Cu(2)–O(6)	86.44(5)	O(7)–Cu(2)–O(6)	90.20(5)
Complex **7** coordination polyhedron Cu(3)N_2O_2, square					
Cu(3)–N(2)	1.9722(13)	N(2)–Cu(3)–N(2^{xii})	180.00(19)	N(2)–Cu(3)–O(5^{xii})	88.58(5)
Cu(3)–N(2^{xii})	1.9722(13)	N(2)–Cu(3)–O(5)	91.42(5)	O(5^{xii})–Cu(3)–O(5)	180.00(5)
Cu(3)–O(5)	2.0138(12)	N(2^{xii})–Cu(3)–O(5^{xii})	91.42(5)		
Cu(3)–O(5^{xii})	2.0138(12)	N(2^{xii})–Cu(3)–O(5)	88.58(5)		
Complex **8** coordination polyhedron Cu(1)N_2O_3, square pyramid					
Cu(1)–O(2^{xiii})	1.974(4)	O(2^{xiii})–Cu(1)–O(1)	93.22(13)	O(3^{i})–Cu(1)–N(1^{xiv})	90.06(10)
Cu(1)–O(1)	2.144(3)	O(2^{xiii})–Cu(1)–N(1^{xiv})	89.51(10)	O(3)–Cu(1)–N(1)	90.06(10)
Cu(1)–O(3)	1.942(4)	O(2^{xiii})–Cu(1)–N(1)	89.51(10)	N(1^{xiv})–Cu(1)–O(1)	95.01(9)
Cu(1)–N(1)	2.026(3)	O(3)–Cu(1)–O(2^{xiii})	175.06(15)	N(1)–Cu(1)–O(1)	95.01(9)
Cu(1)–N(1^{xiv})	2.026(3)	O(3)–Cu(1)–O(1)	91.72(14)	N(1^{xiv})–Cu(1)–N(1)	169.97(18)
Complex **9** coordination polyhedron Cu(1)N_2O_3, square pyramid					
Cu(1)–O(1)	1.955(8)	O(1)–Cu(1)–O(3)	91.9(3)	O(4^{xv})–Cu(1)–N(1)	90.5(2)
Cu(1)–O(3)	2.142(7)	O(1)–Cu(1)–O(4^{xv})	175.0(3)	O(4)–Cu(1)–N(1^{xiv})	90.5(8)
Cu(1)–O(4^{xv})	1.969(7)	O(1)–Cu(1)–N(1^{xiv})	89.0(2)	N(1)–Cu(1)–O(3)	95.89(17)
Cu(1)–N(1)	2.025(6)	O(1)–Cu(1)–N(1)	89.0(2)	N(1^{xiv})–Cu(1)–O(3)	95.9(7)
Cu(1)–N(1^{xiv})	2.025(6)	O(4^{xv})–Cu(1)–O(3)	93.2(3)	N(1)–Cu(1)–N(1^{xiv})	168.1(8)
Complex **10** coordination polyhedron Cu(1)NO_4, square pyramid					
Cu(1)–O(1)	2.285(2)	O(3)–Cu(1)–O(1)	88.72(11)	O(5)–Cu(1)–N(1)	172.12(8)
Cu(1)–O(3)	1.955(2)	O(3)–Cu(1)–O(5)	95.86(10)	O(7)–Cu(1)–O(1)	101.03(11)
Cu(1)–O(5)	1.993(2)	O(3)–Cu(1)–O(7)	169.51(7)	O(7)–Cu(1)–O(5)	87.81(9)
Cu(1)–O(7)	1.976(3)	O(3)–Cu(1)–N(1)	88.81(10)	O(7)–Cu(1)–N(1)	86.52(9)
Cu(1)–N(1)	2.028(3)	O(5)–Cu(1)–O(1)	91.59(10)	N(1)–Cu(1)–O(1)	94.87(10)
Complex **10** coordination polyhedron Cu(2)N_2O_2, square					
Cu(2)–O(2^{xvi})	1.979(3)	O(2^{xvi})–Cu(2)–N(2)	91.14(8)	O(8)–Cu(2)–N(3^{viii})	87.13(8)
Cu(2)–O(8)	1.953(3)	O(2^{xvi})–Cu(2)–N(3^{viii})	90.60(8)	N(2)–Cu(2)–N(3^{viii})	172.13(8)
Cu(2)–N(2)	2.045(3)	O(8)–Cu(2)–O(2^{xvi})	168.98(7)		
Cu(2)–N(3^{viii})	2.073(3)	O(8)–Cu(2)–N(2)	92.54(8)		

Symmetry code to generate equivalent atoms: (i) 3/2-X,-1/2+Y,3/2-Z; (ii) 1-X,1-Y,1-Z; (iii) 1-X,-Y,1-Z; (iv) -1+X,+Y,+Z; (v) 1+X,+Y,1+Z; (vi) 1-X,-1/2+Y,1/2-Z; (vii) X, ½–Y, ½+Z; (viii)1+X,Y,Z; (ix) ½–X, –½+, ½–Z; (x) X,1+y,Z; (xi) -X,2-Y,1-Z; (xii) 1-X,2-Y,1-Z; (xiii) 1/2+X,+Y,1/2-Z; (xiv) X,1/2-Y,Z; (xv) 1/2+X,+Y,3/2-Z.