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Supplementary Information

Synthesis, Characterization and Magnetic studies on mono–, di–, and Trinuclear Cu(II) Complexes from a New Versatile Diazine Ligand

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Table S1: Crystal Structure Data for Complexes 1 – 4 .

	1	**2**	**3**	**4**
Formula	$C_{17}H_{26}Cl_2CuN_6O_5$	$C_{16}H_{23}Cl_3Cu_2N_6O_5$	$C_{32}H_{42}Cu_3N_{16}O_{20}$	$C_{29.50}H_{29}Cu_3N_{14}O_{11}$
FW	264.44	612.83	1161.44	946.42
Temp. (K)	150(2)	150(2)	150(2)	150(2)
Crystal system	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group	*P* -1	$P2_1/c$	*P*-1	*C*2/c
a/Å	8.350(6)	11.0539(9)	8.026(4)	24.005(17)
b/Å	12.084(9)	16.0359(14)	12.141(7)	7.518(5)
c/Å	12.264(9)	13.2399(11)	14.647(8)	21.135(15)
α/°	68.723(7)	90	68.018(6)	90
β/°	89.547(8)	103.545(2)	87.679(7)	116.849(17)
γ/°	87.922(8)	90.00	74.002(7)	90
V/Å^3	1152.3(14)	2281.6(3)	1269.2(12)	3403(4)
Z	4	4	1	4
D_c/Mg m^{-3}	1.524	1.784	1.520	1.847
μ(MoKα)/ cm^{-1}	1.220	2.257	1.331	1.943
Unique reflns	5121	5944	5587	2226
Reflns [$I>2\sigma(I)$]	4542	5158	4534	1778
R_{int}	0.032	0.038	0.0451	0.068
R_1[a], wR_2[b]	0.042, 0.099	0.034, 0.071	0.063, 0.158	0.050, 0.120
Max/min residual e^- density (eÅ^{-3})	+0.98, -0.61	+0.54, -0.43	+0.79, -1.12	+0.74, -0.61
CCDC	1520627	1520628	1520629	1520630

[a] $I > 2\sigma(I)$, [b] all data

Table S2: Selected bond lengths (Å) and angles (º) for **1**

Bond	Distance	Bond	Angle
Cu1—N2	1.953 (2)	N2—Cu1—N4	78.27 (10)
Cu1—N4	2.006 (2)	N2—Cu1—N1	79.77 (10)
Cu1—N1	2.037 (2)	N4—Cu1—N1	156.54 (9)
Cu1—Cl1	2.2027 (13)	N2—Cu1—Cl1	163.63 (7)
Cu1—Cl2	2.6250 (15)	N4—Cu1—Cl1	98.93 (8)
N4—C11	1.302 (3)	N1—Cu1—Cl1	99.81 (8)
N4—N5	1.404 (3)	N2—Cu1—Cl2	89.56 (7)
N5—C12	1.364 (3)	N4—Cu1—Cl2	97.35 (8)
C12—O1	1.217 (3)	N1—Cu1—Cl2	90.62 (9)
C12—C13	1.501 (4)	Cl1—Cu1—Cl2	106.81 (5)
C13—N6	1.270 (4)		
N6—O2	1.395 (3)		

Table S3: Selected bond lengths (Å) and angles (º) for **2**

Bond	Distance	Bond	Distance
Cu1—N2	1.9437 (18)	Cu2—Cl3	2.2754 (6)
Cu1—N4	1.9852 (18)	Cu2—O51	2.3134 (18)
Cu1—N1	2.0346 (19)	O2—N6	1.393 (2)
Cu1—Cl2	2.2125 (6)	N3—C21	1.330 (3)
Cu1—O31	2.4077 (17)	N4—C21	1.309 (3)
Cl1—Cu2	2.3087 (6)	N4—N5	1.405 (2)
O1—C22	1.236 (3)	N5—C22	1.345 (3)
Cu2—N5	1.9769 (18)	N6—C23	1.282 (3)
Cu2—N6	2.0072 (19)		
Bond	**Angle**	**Bond**	**Angle**
N2—Cu1—N4	79.49 (7)	N5—Cu2—Cl3	95.95 (5)
N2—Cu1—N1	79.79 (8)	N6—Cu2—Cl3	170.47 (6)
N4—Cu1—N1	158.23 (7)	N5—Cu2—Cl1	161.35 (6)
N2—Cu1—Cl2	170.96 (6)	N6—Cu2—Cl1	89.42 (6)
N4—Cu1—Cl2	100.06 (5)	Cl3—Cu2—Cl1	94.67 (2)
N2—Cu1—O31	89.62 (7)	N5—Cu2—O51	98.09 (7)
N4—Cu1—O31	98.61 (7)	N6—Cu2—O51	92.53 (7)
N1—Cu1—O31	87.87 (7)	Cl3—Cu2—O51	95.59 (5)
Cl2—Cu1—O31	99.36 (4)	Cl1—Cu2—O51	96.09 (5)
C11—N1—C15	118.55 (19)	C16—N2—C20	122.40 (18)
C11—N1—Cu1	126.99 (16)	C16—N2—Cu1	119.17 (15)
C15—N1—Cu1	114.41 (15)	C20—N2—Cu1	118.34 (14)
N5—Cu2—N6	77.92 (7)		

Table S4: Selected bond lengths (Å) and angles (º) for 3

Bond	Distance	Bond	Distance
Cu1—N15A	1.919 (10)	Cu2—N14A	2.078 (12)
Cu1—N15	1.960 (14)	Cu2—O41	2.430 (4)
Cu1—N11	1.984 (4)	N14—C21	1.366 (18)
Cu1—N12	1.986 (4)	N14—N15	1.421 (11)
Cu1—N16	2.047 (4)	N15—C22	1.310 (13)
Cu1—O61	2.187 (4)	N14A—C21	1.270 (12)
Cu2—O51	1.944 (3)	N14A—N15A	1.414 (10)
Cu2—N14	2.030 (11)	N15A—C22	1.315 (12)
Bond	**Angle**	**Bond**	**Angle**
N15—Cu1—N11	167.9 (7)	N15—Cu1—O61	96.4 (8)
N15—Cu1—N12	89.0 (4)	N11—Cu1—O61	94.94 (14)
N11—Cu1—N12	82.87 (15)	N12—Cu1—O61	112.52 (15)
N15—Cu1—N16	79.7 (3)	N16—Cu1—O61	90.44 (15)
N11—Cu1—N16	104.37 (15)	O51 —Cu2— O51	180.0
N12—Cu1—N16	155.49 (15)	O51— Cu2— N14	98.8(3)
O51— Cu2— $N14^{i}$	81.2(3)	O51— Cu2— N14A	81.8(3)
O51— Cu2— $N14A^{i}$	98.2(3)	N14A—Cu2 —$N14A^{i}$	180.0
O51— Cu2— O41	89.72(13)	$O51^{i}$— Cu2— O41	90.28(13)
N14— Cu2—O41	89.0(9)	N14A— Cu2 —O41	83.8(7)
$N14A^{i}$— Cu2— O41	96.2(7)	$O51^{i}$— Cu2— O41	90.28(13)
O51— Cu2 —O41	89.72(13)	$N14^{i}$— Cu2— $O41^{i}$	91.0(9)
N14A— Cu2— $O41^{i}$	96.2(7)	$N14A^{i}$— Cu2— $O41^{i}$	83.8(7)
O41— Cu2 —$O41^{i}$	180.0		

Table S5: bond lengths (Å) and angles (°) for **4**

Bond	Length	Bond	Length
Cu1—N5	1.914 (5)	C1—C2	1.392 (8)
Cu1—N6	2.049 (5)	N2—C6	1.343 (7)
Cu1—O1S	2.238 (10)	N2—C10	1.346 (7)
Cu2—N2	1.942 (5)	O1—C12	1.254 (7)
Cu2—N4	1.994 (5)	O2—N6	1.360 (5)
Cu2—N1	2.039 (5)	N4—C11	1.318 (7)
Cu2—O2	1.881 (4)	N4—N5	1.410 (6)
Cu2—O12	2.8313 (7)	N5—C12	1.336 (7)
N1—C1	1.349 (7)	C13—N6	1.298 (7)
N1—C5	1.359 (7)	O1—C12	1.254 (7)
Bond	**Angle**	**Bond**	**Angle**
N5—Cu1—N5A	173.8 (3)	N5—Cu1—O1S	84.1 (3)
N5—Cu1—N6	79.65 (18)	N5A—Cu1—O1S	101.7 (3)
N5A—Cu1—N6	97.82 (18)	N6—Cu1—O1SA	131.5 (3)
N5—Cu1—N6A	97.82 (18)	N6A—Cu1—O2S	95.0 (3)
N5A—Cu1—N6A	79.65 (18)	N6A—Cu1—O1S	131.5 (3)
N6—Cu1—N6A	132.2 (3)	N5—Cu1—O1SA	84.1 (3)
N5—Cu1—O1S	101.7 (3)	N5A—Cu1—O1SA	101.7 (3)
N5A—Cu1—O1S	84.1 (3)	N6—Cu1—O1SA	131.5 (3)
N6—Cu1—O1S	95.0 (3)	N6A—Cu1—O1Sa	95.0 (3)

Figure S1: NMR spectrum of $\mathbf{L_4H_2}$