Supplemental Material

Cu(II)–N^6-alkyladenine Complexes: Synthesis, X-Ray Characterization and Magnetic Properties

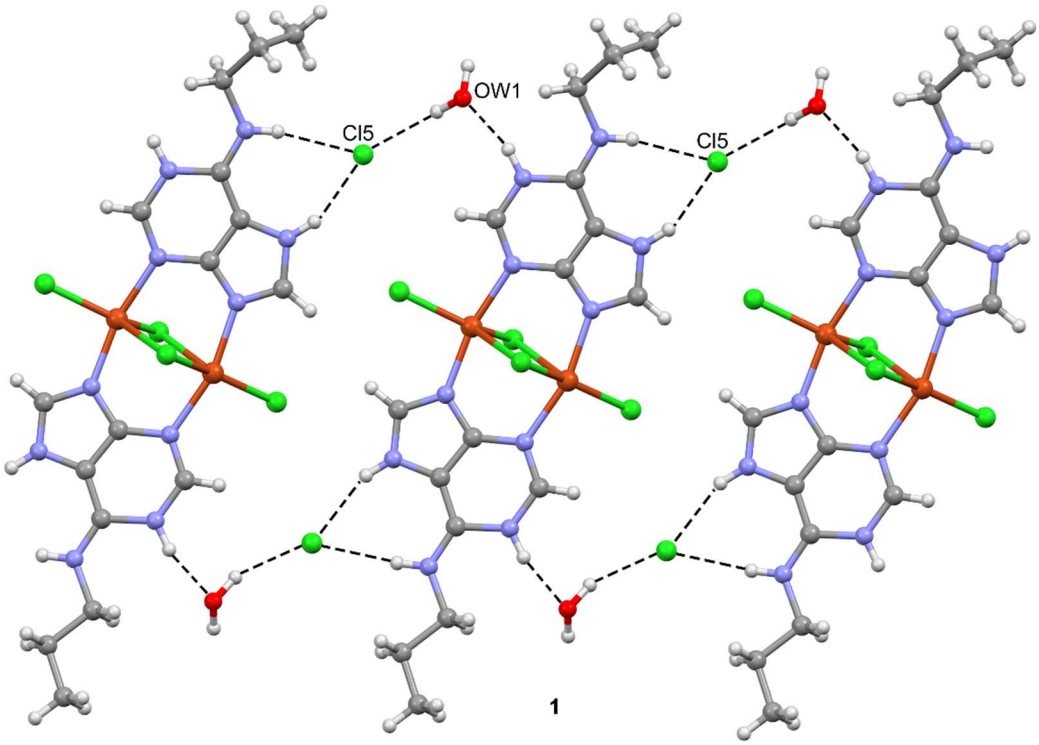

Figure S1. H-bonding network forming 2D supramolecular structures in compound **1**.

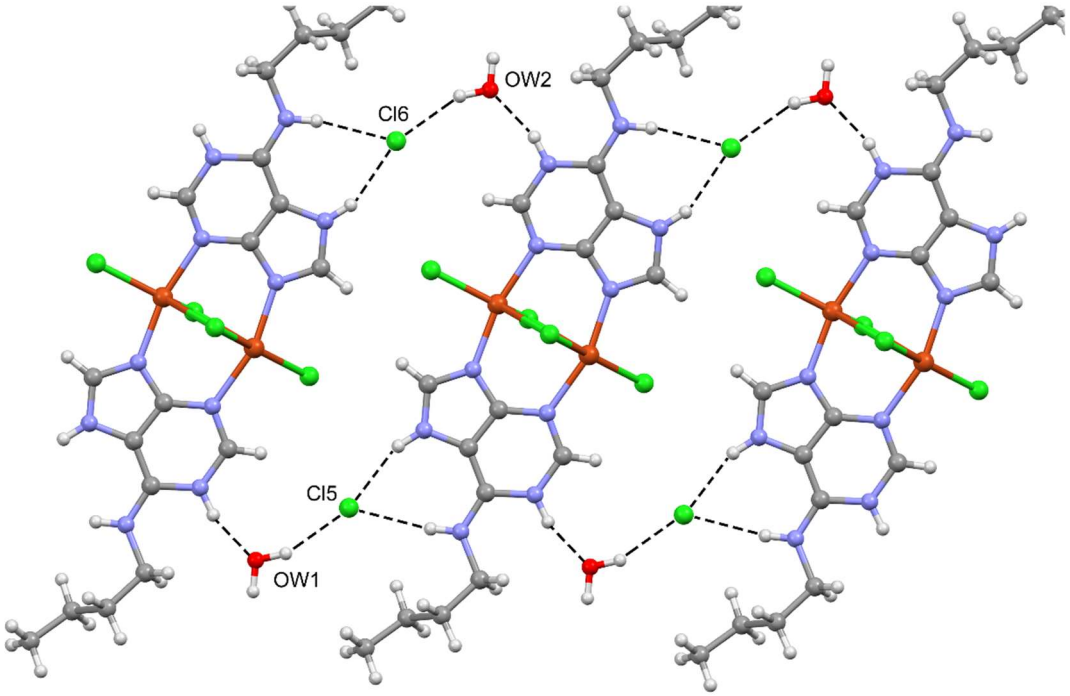

Figure S2. H-bonding network forming 2D supramolecular structures in compound **2.**

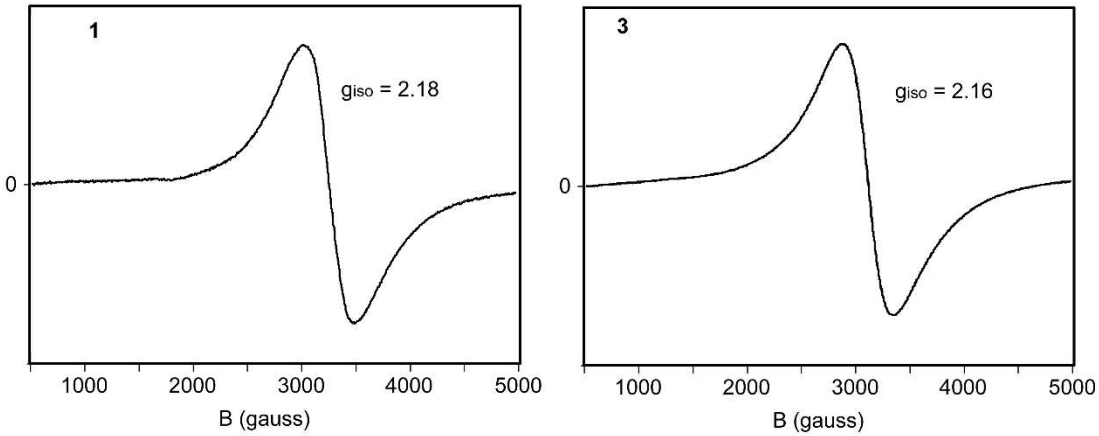

Figure S3. EPR spectra of compounds **1** and **3**.

Table S1. Coordination distances (Å) and angles (°) for compounds **1**–**3**.

Compound **1**			
Cu1-N9′ 1.993(10)	Cu1-N9 1.942(11)	N9′-Cu1-N3 163.4(4)	N9-Cu1-N3′ 164.6(4)
Cu1-N3 2.020(10)	Cu1-N3′ 2.017(10)	Cl2-Cu1-Cl1 159.17(15)	Cl4-Cu1-Cl3 137.28(16)
Cu1-Cl2 2.238(4)	Cu1-Cl4 2.247(4)	Cl2-Cu1-Cl3 94.8(1)	Cl4-Cu1-Cl1 109.67(14)
Cu1-Cl1 2.280(4)	Cu1-Cl3 2.276(4)	Cl1-Cu1-Cl3 106.0(1)	Cl3-Cu1-Cl1 113.05(14)
Cu1-Cl3 2.633(3)	Cu1-Cl1 2.701(4)	Cu1-Cu1 2.962(2)	
Compound **2**			
Cu1-N9′ 1.963(7)	Cu1-N9 1.984(7)	N9′-Cu1-N3 162.3(2)	N9-Cu1-N3′ 165.7(3)
Cu1-N3 2.039(7)	Cu1-N3′ 2.006(6)	Cl4-Cu1-Cl3 161.61(10)	Cl2-Cu1-Cl1 133.35(10)
Cu1-Cl4 2.242(2)	Cu1-Cl2 2.237(2)	Cl3-Cu1-Cl1 104.33(8)	Cl1-Cu1-Cl3 114.71(8)
Cu1-Cl3 2.291(3)	Cu1-Cl1 2.312(3)	Cl4-Cu1-Cl1 94.02(9)	Cl2-Cu1-Cl3 111.93(10)
Cu1-Cl1 2.960(2)	Cu1-Cl3 2.633(3)	Cu1-Cu1 2.9671(16)	
Compound **3**			
Cu1-N9′ 1.982(4)	Cu1-N9 1.980(4)	N9′-Cu1-N3 163.43(16)	N9-Cu1-N3′ 166.85(17)
Cu1-N3 2.042(4)	Cu1-N3′ 2.009(4)	Cl3-Cu1-Cl1 157.94(6)	Cl4-Cu1-Cl2 135.72(6)
Cu1-Cl3 2.2368(16)	Cu1-Cl4 2.2432(15)	Cl3-Cu1-Cl2 95.96(6)	Cl4-Cu1-Cl1 111.86(6)
Cu1-Cl1 2.2886(15)	Cu1-Cl2 2.2985(16)	Cl1-Cu1-Cl2 106.06(5)	Cl2-Cu1-Cl1 112.41(5)
Cu1-Cl2 2.864(2)	Cu1-Cl1 2.6660(18)	Cu1-Cu1 2.9530(14)	

Table S2. Geometric features of the hydrogen bonds in compound **1**. Distances in Å and angles in degrees.

D-H···A	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1)···O(1W)#1	1.83	2.671(15)	165.2
N(1')-H(1')···O(2W)#3	1.88	2.707(13)	160.3
N(7)-H(7)···Cl(5)#2	2.31	3.132(11)	159.0
N(7')-H(7')···Cl(6)#4	2.24	3.045(11)	156.7
N(6)-H(6)···Cl(5)#2	2.34	3.196(12)	172.0
N(6')-H(6')···Cl(6)#4	2.36	3.210(12)	168.0
O(1W)-H(1W2)···Cl(5)	2.32(15)	3.078(13)	141(20)
O(2W)-H(2W2)···N3′#5	2.84(12)	3.258(14)	110(9)
O(2W)-H(2W1)···N(1')#5	2.99(17)	3.476(16)	116(14)
O(1W)-H(1W1)···Cl2	2.34(4)	3.208(12)	161(9)
O(2W)-H(2W2)···Cl3#5	2.35(3)	3.238(11)	173(12)

Symmetry operations: #1 −x+1,−y+1,−z+1; #2 −x+2,−y+1,−z+1; #3 x+1,y−1,z; #4 x,y−1,z; #5 −x+1,−y+1,−z.

Table S3. Geometric features of the hydrogen bonds in compound **2**. Distances in Å and angles in degrees.

D-H···A	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1)···OW3$^{\#1}$	1.84	2.63(2)	150.6
N(1')-H(1')···OW2$^{\#3}$	1.85	2.683(9)	164.0
N(7)-H(7)···Cl(6)$^{\#2}$	2.26	3.080(7)	159.3
N(7')-H(7')···Cl(5)$^{\#4}$	2.24	3.048(7)	157.3
N(6)-H(6)···Cl(6)$^{\#2}$	2.44	3.262(8)	160.7
N(6')-H(6')···Cl(5)$^{\#4}$	2.33	3.180(7)	169.8

OW2-HW22···Cl(5)	2.21(4)	3.032(7)	152(7)
OW3-HW31···OW1	1.90(9)	2.69(2)	146(14)
OW3-HW32···Cl(6)	2.22(7)	3.08(2)	160(17)
OW1-HW1···Cl4$^{\#3}$	2.35(8)	3.180(8)	154(15)
OW1-HW12···Cl1$^{\#3}$	2.54(8)	3.376(9)	154(15)
OW2-HW21···Cl1	2.34(5)	3.199(7)	161(12)

Symmetry operations: #1 x−1,y,z+1; #2 x,y,z+1; #3 −x+1,−y,−z+1; #4 −x,−y,−z+1.

Table S4. Absolute energies (Hartries) and <S^2> values of low-spin and high-spin configuration in compounds **1** and **3**.

Compound	**LS (energy)**	**HS (energy)**	**LS (<S^2>)**	**HS (<S^2>)**
1	−6135.3221143	−6135.3216162	0.048	2.0060
3	−6371.0224263	−6371.0219135	0.047	2.0059