Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here].

ESI 1: Syntheses of the seven Cu^{II} complexes

Syntheses of the used ligands:

1,10-phenanthrolin-2-ol (PhenOH) was synthesized according to the literature (Qing Li et al. ***Z. Anorg. Allg. Chem.***, 2012, 639, 181).

Synthesis of 2-(1H-pyrazol-1-yl)-1,10-phenanthroline (PhenP): K_2CO_3 (4.60 g, 82 mmol) was added into a DMF solution (400 mL) containing 2-chloro-1,10-phenanthroline (4.29 g, 20 mmol) and pyrazole (6.81 g, 100 mmol) and the solution was refluxed for 24 hours. The solvent DMF was removed by vacuum distillation, and then 100 mL iced water was added into the remains and the mixture was stirred for half an hour and then a large amount of white deposition appeared. The deposition as product was separated from the solution and washed with iced water until the filtrate displayed neutral and then dried in vacuum (yield 3.92 g, 16 mmol). 1H NMR (300 MHz, CDCl3, 24°C, TMS): δ=9.19 (s, 2H), 8.38 (brs, 2H), 8.27 (s, 1H), 7.82 (brs, 3H), 7.66 (s, 1H), 6.56 ppm (s, 1H); HRMS (ESI): m/z calcd for C15H10N4+H+: 247.0978 [M+H+]; found: 247.0982.

Synthesis of 2-(1*H*-1,2,4-triazol-1-yl)-1,10-phenanthroline (PhenTA): K_2CO_3 (4.60 g, 82 mmol) was added into a DMF solution (250 mL) containing 2-chloro-1,10-phenanthroline (2.45 g, 11 mmol) and 1*H*-1,2,4-triazole (3.00 g, 43 mmol) and the solution was refluxed for 24 hours. The solvent DMF was removed by vacuum distillation, and then iced water (100 mL) was added into the remains and the mixture was stirred for half an hour and a large amount of white deposition appeared. The deposition was washed with iced water until the filtrate was neutral and then dried in vacuum (yield 2.15 g, 8.7 mmol). 1H NMR (300 MHz, CDCl3, 23°C, TMS): δ=9.83 (s, 1H), 9.20 (s, 1H), 8.47 (d, J=9 Hz, 1H), 8.31 (d, J=9 Hz, 2H), 8.18 (s, 1H), 7.86 (s, 2H), 7.69-7.73 ppm (m, 1H); HRMS (ESI): m/z calcd for C14H9N5+H+: 248.0930 [M+H+]; found: 248.0919.

Synthesis of 2-(3-methyl-pyrazol-1H-yl)-1,10-phenanthroline (PhenMP): A flask containing 2-chloro-1,10-phenanthroline (1.07 g, 5 mmol), KOH (0.56 g, 10 mmol) and 3-methyl-pyrazole (2.05 g, 25 mmol) was placed in a microwave oven and irradiated for 30 minutes under temperature 60°C. And then ethanol (50 mL) was added into the flask and stirred for a few minutes. The yellowish product (1.0 g, 3.8 mmol) was obtained after the insoluble was separated from the solution and dried in vacuum. 1H NMR (300 MHz, CDCl3, 24°C, TMS): δ=9.21 (d, J=3 Hz, 2H), 8.39-8.29 (m, 3H), 7.83-7.65 (m, 3H), 6.36 (s, 1H), 2.43 ppm (s, 3H); HRMS (ESI): m/z calcd for C16H12N4+H+: 261.1134 [M+H+]; found: 261.1140.

Synthesis of 2-(3-amine-pyrazol-1H-yl)-1,10-phenanthroline (PhenAP): KOH (2.10 g, 37 mmol) was added into a DMF solution (80 mL) of 2-chloro-1,10-phenanthroline (4.29 g, 20 mmol) and 3-amine-pyrazole (1.99 g, 24 mmol) and the mixture was stirred and refluxed for 96 hours. The deposition appeared after iced water (100 mL) was added into the solution, and then the deposition was recrystallized in a mixed solvent of ethanol and water (7:3). The yellowish powder product (3.68 g, 14 mmol) was obtained after vacuum drying of the recrystallized microcrystals. 1H NMR (300 MHz, CDCl3, 25°C, TMS): δ=9.17 (s, 1H), 8.30-8.17 (m, 4H), 7.79-7.63 (m, 4H), 3.97 ppm (s, 2H); HRMS (ESI): m/z calcd for C15H11N5+H+: 262.1087 [M+H+]; found: 262.1091.

Syntheses of the seven Cu^{II} complexes:

Synthesis of Complex C**1** [Cu(PhenOH)Cl(OH)]: the H_2O solution (10 mL) of $CuCl_2{\cdot}2H_2O$ (0.0341 g，0.200 mmol) was added into a methanol solution (10 mL) containing 2-hydroxyl-1,10-phenanthroline (0.0375 g，0.191 mmol) and the mixed solution was stirred for a few minutes. The purple single crystals were obtained after the filtrate was allowed to stand and slowly evaporate at room temperature for about two weeks. IR (cm^{-1}): 3069(s), 1625(m), 1586(m), 1559(m), 1504(s), 1483(s), 1452(s), 1422(s), 1386(s), 1141(w), 847(s), 700(s). Elemental analysis calcd (%) for $C_{12}H_9ClCuN_2O_2$: C 46.16, H 2.91, N 8.98, Cu 20.35; Found: C 46.32, H 3.21, N 8.65, Cu, 20.73.

Synthesis of Complex C**2** [Cu(PhenP)$(ONO_2)_2$]: the methanol solution of $Cu(NO_3)_3{\cdot}3H_2O$ (0.0564 g, 0.233 mmol) (10 mL) was added into a methanol solution of 2-(1H-pyrazol-1-yl)-1,10-phenanthroline (0.0525 g, 0.212 mmol) (10 mL) and the mixed solution was stirred for a few minutes. The green single crystals were obtained after the filtrate was allowed to stand and slowly evaporated at room temperature for a week. IR (cm^{-1}): 1616(w), 1597(w), 1533(m), 1508(w), 11384(s). Elemental analysis calcd (%) for $C_{15}H_{10}CuN_6O_6$: C 41.53, H 2.32, N 19.38, Cu 14.65; Found: C 41.21, H 2.50, N 19.76, Cu 14.96.

Synthesis of Complex C**3** $[Cu(PhenTA)_2]{\cdot}(ClO_4)_2CH_3CH_2OH$: the methanol solution of $Cu(ClO_4)_2{\cdot}6H_2O$ (0.0630 g, 0.170 mmol) (10 mL) was added into a methanol solution of 2-(1H-1,2,4-triazol-1-yl)-1,10-phenanthroline (0.0845 g, 0.342 mmol) (10 mL) and the mixed solution was stirred for a few minutes. The blue single crystals were obtained after the filtrate was allowed to stand and slowly evaporated at room temperature for two weeks. IR (cm^{-1}): 1595(m), 1525(s), 1432(m), 1399(s), 1296(m), 1225(m), 1085(s). Elemental analysis calcd (%) for $C_{30}H_{24}Cl_2CuN_{10}O_9$: C 44.87, H 3.01, N 17.44, Cu 7.91; Found: C 44.63, H 3.28, N 17.35, Cu 7.69.

Synthesis of Complex C**4** [Cu(PhenMP)Cl_2]: the methanol solution of $CuCl_2{\cdot}2H_2O$ (0.3440 g, 2.02 mmol) (10 mL) was added into a methanol solution containing 2-(3-methyl-pyrazol-1H-yl)-1,10-phenanthroline (0.5180 g, 1.99 mmol) (10 mL), and the mixed solution was stirred for a few minutes. The green single crystals were obtained after the filtrate was allowed to stand and slowly evaporate at room temperature for about a week. IR (cm^{-1}): 1613(m), 1593(m), 1547(m), 1509(m), 1399(s), 1354(m). Elemental analysis calcd (%) for $C_{12}H_{12}Cl_2CuN_4$: C 36.51, H 3.06, N 14.19, Cu 16.10; Found: C 36.76, H 3.25, N 14.35, Cu 16.49.

Synthesis of Complex C**5** [Cu(PhenMP)Br_2]: the blue crystal of this complex was synthesized as the similar process as complex 2 except $CuCl_2{\cdot}2H_2O$ was replaced with $CuBr_2$. IR (cm^{-1}): 1639(s), 1592(m), 1545(m), 1509(m), 1398(s), 1353(w). Elemental analysis calcd (%) for $C_{12}H_{12}Br_2CuN_4$: C 29.80, H 2.50, N 11.58, Cu 13.14; Found: C 30.01, H 2.81, N 11.83, Cu 13.49.

Synthesis of Complex C**6** $[Cu(PhenAP)(ONO_2)(HOCH_3)]{\cdot}NO_3$: the methanol solution of $Cu(NO_3)_2{\cdot}3H_2O$ (0.0507 g, 0.21 mmol) (10 mL) was added into a methanol solution containing 2-(3-amine-pyrazol-1H-yl)-1,10-phenanthroline (0.0549 g, 0.21 mmol) (10 mL) and the mixed solution was stirred for a few minutes. The green single crystals were obtained after the filtrate was allowed to stand and slowly evaporate at room temperature for four days. IR (cm^{-1}): 3426(s), 1629(m), 1591(m), 1563(m), 1522(m), 1467(m), 1426(m), 1384(s). Elemental analysis calcd (%) for $C_{16}H_{15}CuN_7O_7$: C 39.96, H 3.14, N 20.39, Cu 13.21; Found: C 40.25, H 3.31, N 20.01, Cu 13.60.

Synthesis of Complex C**7** [Cu(PhenAP)Cl_2]: the aqueous solution of $CuCl_2{\cdot}2H_2O$ (0.0341 g, 0.200 mmol) (10 mL) was added into a methanol solution of 2-(3-amine-pyrazol-1H-yl)-1,10-phenanthroline (0.0549 g, 0.21 mmol) (10 mL). The mixture was stirred for a few minutes and filtrated. The orange single crystals were obtained after the filtrate was allowed to stand and slowly evaporate at room temperature for about one weak. IR (cm^{-1}): 3393(s), 3307(s), 1613(s), 1589(m), 1561(m), 1519(s), 1468(m), 1442(w), 1422(m), 1394(w), 1339(w), 1144(w), 949(w). Elemental analysis calcd for $C_{15}H_{11}Cl_2CuN_5$: C 45.52, H 2.80, N 17.70, Cu 16.06; Found: C 45.80, H 2.98, N 18.05, Cu 16.35.

All other chemicals are analytical grade and used without further purification.

ESI 2: Selected bond lengths, associated angles and hydrogen bond for the seven Cu^{II} complexes.

ESI 2: Table 1-1: Selected bond lengths (Å) and angles (°) for **C1** Complex**.**

Cu1-Cl1	2.2227(15)	Cu1-N1	2.033(4)	Cu1-N2	1.964(4)	Cu1-O2	1.913(4)	Cu2-Cl2	2.2310(14)
Cu2-N3	2.015(4)	Cu2-N4	1.962(4)	Cu2-O4	1.941(3)	Cu3-Cl3	2.2260(15)	Cu3-N5	2.014(4)
Cu3-N6	1.986(4)	Cu3-O6	1.908(4)						
N1-Cu1-Cl1	177.01(13)	O2-Cu1-N2	169.6(2)	N2-Cu1-Cl1	94.37(13)	O2-Cu1-Cl1	91.52(14)	O2-Cu1-N1	91.22(18)
N2-Cu1-N1	83.09(17)								
O4-Cu2-N4	173.02(16)	N3-Cu2-Cl2	170.57(12)	N4-Cu2-Cl2	94.04(12)	O4-Cu2-N3	92.10(16)	O4-Cu2-Cl2	91.84(12)
N4-Cu2-N3	82.67(15)								
N5-Cu3-Cl3	177.73(12)	O6-Cu3-N6	174.30(16)	N6-Cu3-Cl3	95.08(13)	O6-Cu3-N5	92.40(15)	O6-Cu3-Cl3	89.85(12)
N6-Cu3-N5	82.66(16)								

ESI 2: Table 1-2 Hydrogen bonds for **C1** Complex.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1X)...O(2)	0.85	1.65	2.487(6)	167
O(2)-H(2X)...O(5)#1	0.85	1.87	2.652(6)	152
O(3)-H(3X)...O(4)	0.85	1.66	2.503(5)	173
O(4)-H(4X)...O(1)#2	0.85	1.92	2.715(5)	154
O(5)-H(5X)...O(6)	0.85	1.73	2.570(5)	168
O(6)-H(6X)...O(3)#3	0.85	1.99	2.780(5)	155

Symmetry transformations used to generate equivalent atoms: #1: x+1, y-1, z; #2: x, y+1, z; #3: x-1, y, z.

ESI 2: Table 2-1: Selected bond lengths (Å) and angles (°) for **C2** Complex.

Cu1 –N3	1.928(3)	Cu1-O2	1.949(3)	Cu1–N4	2.077(3)	Cu1–N2	2.077(3)	Cu1 –O5	2.258(5)
O2-Cu1-O5	107.44(17)	O2-Cu1-N2	104.48(14)	O2-Cu1-N3	160.01(14)	O2-Cu1-N4	96.34(13)	O5-Cu1-N2	90.34(16)
O5-Cu1-N3	92.38(17)	O5-Cu1-N4	90.38(15)	N2-Cu1-N3	77.32(13)	N2-Cu1-N4	157.92(13)	N3-Cu1-N4	80.60(13)

ESI 2: Table 3-1: Selected bond lengths (Å) and angles (°) for **C3** Complex.

Cu1-N9	2.343(3)	Cu1-N1	2.270(3)	Cu1-N6	2.195(3)	Cu1-N5	2.143(3)	Cu1-N7	1.963(3)
Cu1-N4	1.954(3)								
N4-Cu1-N7	174.98(11)	N5-Cu1-N1	155.12(10)	N6-Cu1-N9	152.31(10)	N7-Cu1-N1	109.57(11)	N4-Cu1-N9	105.40(11)
N4-Cu1-N6	101.79(11)	N5-Cu1-N6	97.55(11)	N7-Cu1-N5	95.08(11)	N5-Cu1-N9	92.24(11)	N1-Cu1-N9	91.22(11)
N6-Cu1-N1	90.63(11)	N4-Cu1-N5	79.90(11)	N7-Cu1-N6	78.86(11)	N4-Cu1-N1	75.43(11)	N7-Cu1-N9	74.51(11)

ESI 2: Table 3-2. Hydrogen bonds for C3 Complex.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(9)-H(9A)...N(10)#1	0.82	2.31	3.101(5)	163.0

Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+1/2,z+1/2.

ESI 2: Table 4-1: Selected bond lengths (Å) and angles (°) for **C4** Complex.

Cu1-Cl1	2.4322(10)	Cu1-Cl2	2.2086(11)	Cu1-N1	2.105(3)	Cu1-N4	2.105(3)	Cu1-N2	1.962(3)
N4-Cu1-N1	154.30(11)	N2-Cu1-Cl2	150.43(8)	Cl2-Cu1-Cl1	107.87(4)	N2-Cu1-Cl1	101.69(8)	N4-Cu1-Cl2	100.65(8)
N1-Cu1-Cl2	97.97(8)	N4-Cu1-Cl1	96.35(8)	N1-Cu1-Cl1	94.61(8)	N2-Cu1-N1	78.66(10)	N2-Cu1-N4	76.39(10)

ESI 2: Table 5-1: Selected bond lengths (Å) and angles (°) for C5 Complex.

Cu1-Br2	2.5624(7)	Cu1-Br1	2.3563(7)	Cu1-N1	2.104(3)	Cu1-N4	2.103(3)	Cu1-N3	1.966(3)
N4-Cu1-N1	154.70(12)	N3-Cu1-Br1	147.65(10)	Br1-Cu1-Br2	108.34(3)	N3-Cu1-Br2	104.00(10)	N1-Cu1-Br1	100.70(9)
N4-Cu1-Br1	97.51(9)	N1-Cu1-Br2	95.43(10)	N4-Cu1-Br2	95.33(9)	N3-Cu1-N4	78.82(13)	N3-Cu1-N1	76.39(12)

ESI 2: Table 6-1: Selected bond lengths (Å) and angles (°) for **C6** Complex.

Cu1-N2	1.923(3)	Cu1-O7	1.957(3)	Cu1-N4	2.035(4)	Cu1-N1	2.069(4)	Cu1-O1	2.206(4)
N2-Cu1-N4	77.84(15)	N2-Cu1-N1	80.16(16)	O7-Cu1-O1	92.39(15)	N4-Cu1-O1	93.54(13)	N1-Cu1-O1	93.92(15)
N2-Cu1-O1	102.59(15)	O7-Cu1-N4	103.43(15)	O7-Cu1-N1	97.10(15)	N4-Cu1-N1	157.82(13)	N2-Cu1-O7	164.90(12)

ESI 2 Table 6-2. Hydrogen bonds for **C6** Complex.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(5)-H(5A)...O(7)#1	0.86	2.54	3.138(5)	127.4
N(5)-H(5B)...O(4)#2	0.86	2.15	2.985(7)	163.8
O(1)-H(4)...O(2)	0.94	1.83	2.758(6)	170.9
O(1)-H(4)...N(7)	0.94	2.65	3.469(7)	147.0

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+1 #2 -x+2,-y+2,-z+1

ESI 2: Table 7-1: Selected bond lengths (Å) and angles (°) for **C7** Complex.

Cu1-Cl1	2.2507(11)	Cu1-Cl2	2.4448(11)	Cu1-N1	2.092(3)	Cu1-N4	2.074(3)	Cu1-N2	1.967(3)
N2-Cu1-Cl1	156.74(10)	N4-Cu1-N1	153.14(12)	Cl1-Cu1-Cl2	102.42(4)	N4-Cu1-Cl1	101.26(9)	N2-Cu1-Cl2	100.84(9)
N1-Cu1-Cl2	99.09(9)	N4-Cu1-Cl2	96.72(9)	N1-Cu1-Cl1	96.39(9)	N2-Cu1-N1	79.41(13)	N2-Cu1-N4	76.37(13)

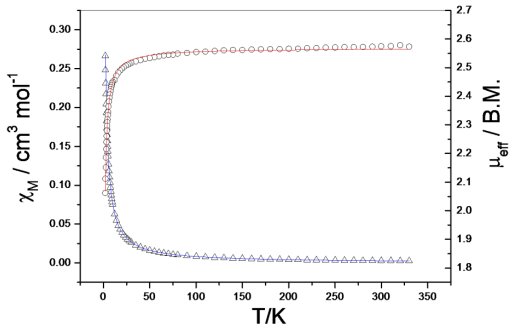
ESI 3: The information of the intermolecular magnetic coupling properties of the seven Cu^{II} complexes.

Magnetism of Complex C1. The experimental data of the variable-temperature (2.00-330 K) magnetic susceptibilities are shown in ESI 3 Fig. 1, where χ_M is the molar magnetic susceptibility per binuclear Cu^{II} unit, μ_{eff} is the magnetic moment per binuclear Cu^{II} ions. ESI 3 Fig. 1 displays that the χ_M value increases with decreasing temperature and reaches a maximum at 2.00 K. The μ_{eff} value at 300 K is 2.57 B.M., which is a little larger than isolated binuclear Cu^{II} ions (2.45 B.M. $g_{av} = 2$) at room temperature. The μ_{eff} value decreases very slowly with temperature drop until about 14 K, and then the μ_{eff} values decreases sharply with temperature drop and reaches 2.06 B.M. at 2.00 K, which suggests that there is an anti-ferromagnetic coupling between the adjacent Cu^{II} ions. The modified Bleaney-Bowers binuclear Cu^{II} fitting formulae (2) and (3) were used to fit the experimental data and the obtaining fitting parameters are g = 2.10, $2J$ = -0.82 cm^{-1}, zJ' = -0.94 cm^{-1}, $R = \Sigma(\chi_{obsd} - \chi_{calcd})^2/(\chi_{obsd})^2 = 5.0 \times 10^{-5}$. The data of the experimental magnetic susceptibility also fit Curie-Weiss formula with Weiss constant θ = -1.34 K.

$$\hat{H} = -2J\hat{S}_{Cu}\hat{S}_{Cu} \quad (1)$$

$$\chi = \frac{2Ng^2\beta^2}{\kappa T}[3 + \exp(-2J / \kappa T)]^{-1} + N_\alpha \quad (2)$$

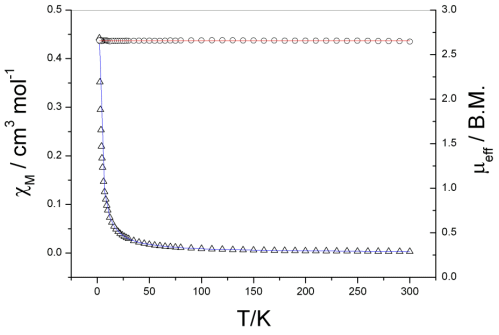
$$\chi_M = \frac{\chi}{1 - \frac{zJ'}{Ng^2\beta^2}} \quad (3)$$



ESI 3 Figure 1: Plots of χ_M (the open triangle for the experimental data) and μ_{eff} (the open circle for the experimental data) versus T for Complex C1.

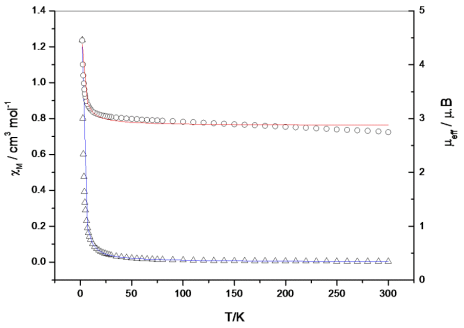
Magnetism of Complex C2. The experimental data of the variable-temperature (2.00–300 K) magnetic susceptibilities are shown in ESI 3 Fig. 2, where χ_M is the molar magnetic susceptibility per binuclear Cu^{II} unit, μ_{eff} is the magnetic moment per binuclear Cu^{II} ions. ESI 3 Figure 2 displays that the χ_M value increases with decreasing temperature, reaches a maximum at 2.00 K. The μ_{eff} value at 300 K is 2.65 B.M., which is larger than that of isolated binuclear Cu^{II} ions (2.45 B.M. for g_{av} = 2.0) at room temperature, and the μ_{eff} value fluctuates among the range of 2.65 B. M. and 2.66 B.M. in the temperature range of 300 K to 2.00 K, which suggests that there exists no magnetic interaction among the adjacent Cu^{II} ions. The fitting for the variable-temperature magnetic susceptibility data based on an Bleaney-Bowers binuclear Cu^{II} fitting equation (4) (Bleaney, B.; Bowers, K. D. Proc. R. SOC., London 1952, A214, 451.) gave the relevant fitting parameters: g = 2.17, $2J$ = 0.008 cm^{-1} and agreement factor $R = 9.85 \times 0^{-6}$.

$$\chi_m = \frac{2Ng^2\beta^2}{\kappa T}[3+\exp(-2J/\kappa T)]^{-1} \quad (4)$$



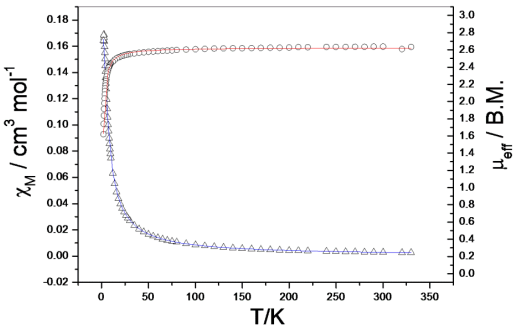
ESI 3 Figure 2: Plots of χ_M (the open triangle for the experimental data and the blue curve for the fitting values) and μ_{eff} (the open circle for the experimental data and the red curve for the fitting value) versus T for Complex C2.

Magnetism of Complex C3. The experimental data of the variable-temperature (2.00–300 K) magnetic susceptibilities are shown in ESI 3 Figure 3, where χ_M is the molar magnetic susceptibility per binuclear Cu^{II} unit, μ_{eff} is the magnetic moment per binuclear Cu^{II} ions. ESI 3 Figure 3 displays that the χ_M value increases with decreasing temperature, reaches a maximum at 2.00 K. The μ_{eff} value at 300 K is 2.75 B.M., which is larger than that of isolated binuclear Cu^{II} ions (2.45 B.M. for g_{av} = 2.0) at room temperature, and the μ_{eff} value increases very slowly with temperature drop until about 12 K, and then it increases sharply to 4.45 B. M. at 2.00 K, which suggests that there is a ferromagnetic coupling among the adjacent Cu^{II} ions. The modified Bleaney-Bowers equations (2) and (3) for exchange coupled dimer Cu^{II} ($H = -2JS_1S_2$) were used to fit the magnetic data. The equations (2) and (3) gave a good fitting for the experimental data as shown in ESI 3 Figure 3, and the obtained magnetic parameters are g = 2.34, $2J$ = 4.17 cm^{-1}, zJ' = 0.93 cm^{-1}, and agreement factor R = 3.25×10^{-3}.



ESI 3 Figure 3: Plots of χ_M (the open triangle for the experimental data and the blue curve for the fitting values) and μ_{eff} (the open circle for the experimental data and the red curve for the fitting value) versus T for Complex C3.

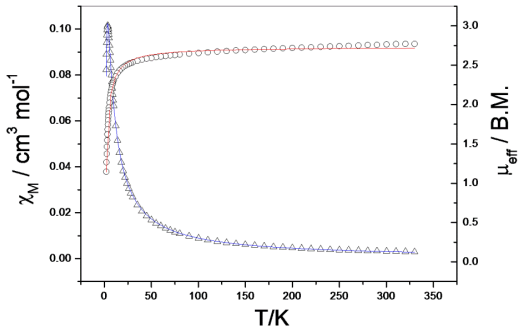
Magnetism of Complex C4. ESI 3 Figure 4 shows the experimental variable-temperature magnetic data (2.00-330 K) based on per binuclear unit and its magnetic moments change from 2.64 B. M. at 300 K to 1.62 B. M. at 2.00 K. The fitting using binuclear Cu^{II} equations as Complex C3 gave the relevant fitting magnetic parameters: g = 2.14, $2J$ = -2.63 cm^{-1}, zJ' = -0.54 cm^{-1}, and agreement factor R = 1.10×10^{-4}.



ESI 3 Figure 4: Plots of χ_M (the open triangle for the experimental data and the blue curve for the fitting values) and μ_{eff} (the open circle for the experimental data and the red curve for the fitting value) versus T for Complex C4.

Magnetism of Complex C5. ESI 3 Figure 5 displays the magnetic information of Complex C5 (2.00-330 K) based on per binuclear Cu^{II} unit and its magnetic moments range from 2.77 B. M. at 330 K to 1.15 B. M. at 2.00 K. The fitting with the identical equations as Complex C3 gave the following fitting parameters: g = 2.23, $2J$ = -3.67 cm^{-1}, zJ' = -3.31

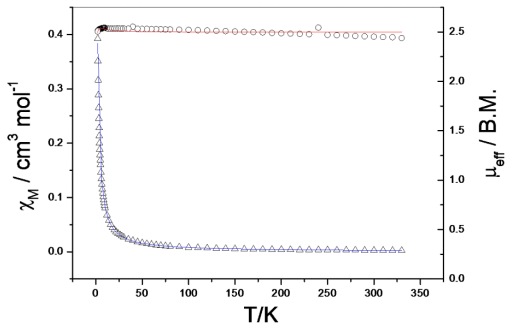
cm^{-1}, and agreement factor R = 7.30×10^{-4}, and the fitting with Curie-Weiss formula gave the Weiss constant θ = -6.52 K.



ESI 3 Figure 5: Plots of χ_M (the open triangle for the experimental data and the blue curve for the fitting values) and μ_{eff} (the open circle for the experimental data and the red curve for the fitting value) versus T for Complex C5.

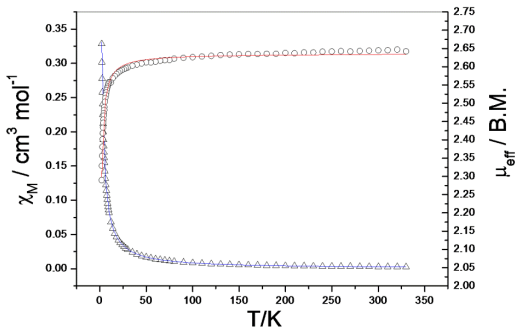
Magnetism of Complex C6. ESI 3 Figure 6 shows the data of the variable-temperature (2.00 K – 330 K) magnetic susceptibility of Complex C6, where μ_{eff} is the magnetic moment per binuclear Cu^{II} ions. The μ_{eff} value at 330 K is 2.44 B. M. and then it increases very slowly as temperature drops until 34.00 K with the maximum value 2.55 B. M., and then it deceases very slowly and reaches to 2.51 B. M. at 2.00 K, which indicates that there is a very weak magnetic interaction among the adjacent Cu^{II} ions. The fitting equation (5) gave the following fitting parameters: g = 2.04, $2J$ = 1.25 cm^{-1}, θ = -0.54 K = -0.37 cm^{-1} and R = 5.40×10^{-4}. The Weiss constant from Curie-Weiss formula is 1.65 K.

$$\chi = \frac{2Ng^2\beta^2}{\kappa(T-\theta)}[3+\exp(-2J/\kappa T)]^{-1} + N_\alpha \qquad (5)$$



ESI 3 Figure 6: Plots of χ_M (the open triangle for the experimental data and the blue curve for the fitting values) and μ_{eff} (the open circle for the experimental data and the red curve for the fitting value) versus T for Complex C6.

Magnetism of Complex C7. ESI 3 Figure 7 displays the data of the variable-temperature (2.00 – 300 K) magnetic susceptibility of this complex, where μ_{eff} is the magnetic moment per binuclear Cu^{II} ions. The value of magnetic moment is constant (2.64 B. M.) in the temperature range of 330 K to 179.92 K and then it decreases with temperature drop and reaches to 2.29 B. M. at 2.00 K. The fitting parameters, which were obtained from the equations (3) and (4), are g = 2.15, $2J$ = -0.28 cm^{-1}, zJ' = -0.72 cm^{-1} and R = 5.0×10^{-5}. The Weiss constant obtained from Curie-Weiss formula is -0.96 K.



ESI 3 Figure 7: Plots of χ_M (the open triangle for the experimental data and the blue curve for the fitting values) and μ_{eff} (the open circle for the experimental data and the red curve for the fitting value) versus T for Complex C7.

ESI 4: The spin densities on the atoms of the π-π stacking systems

ESI 4 Table 1: Spin densities for **C1** Complex.

Atom	Spin density	Atom	Spin density	Atom	Spin density	Atom	Spin density	Atom	Spin density
C1	0.012652	C13	0.007386	C25	0.011017	C1A	0.004781	C25A	0.009185
C2	0.013251	C14	0.015615	C26	0.017383	C2A	0.007552	C26A	-0.000673
C3	-0.001528	C15	0.005743	C27	-0.009968	C3A	0.001185	C27A	-0.008843
C4	-0.004709	C16	0.006492	C28	-0.004399	C4A	0.014470	C28A	0.001740
C5	0.003025	C17	-0.009551	C29	0.014502	C5A	-0.008748	C29A	0.006736
C6	-0.003672	C18	-0.007311	C30	0.006784	C6A	-0.011054	C30A	0.002808
C7	0.001436	C19	0.021592	C31	-0.002917	C7A	0.012712	C31A	0.001318
C8	0.000658	C20	-0.005492	C32	-0.003231	C8A	-0.004304	C32A	-0.005023
C9	0.009498	C21	-0.015763	C33	0.008411	C9A	0.003986	C33A	0.002448
C10	-0.012462	C22	-0.013875	C34	-0.014885	C10A	-0.007616	C34A	-0.010183
C11	-0.008879	C23	0.001628	C35	-0.007688	C11A	0.002945	C35A	0.007397
C12	-0.007334	C24	-0.011513	C36	-0.020233	C12A	-0.013159	C36A	-0.000652
Cl1	0.166397	Cl2	0.164941	Cl3	0.160243	ClA	0.177503	Cl3A	0.179552
Cu1	0.513980	Cu2	0.510910	Cu3	0.514711	Cu1A	0.494638	Cu3A	0.495643
N1	0.071101	N3	0.068593	N5	0.076780	N1A	0.070808	N5A	0.067943
N2	0.098436	N4	0.095059	N6	0.085218	N2A	0.075020	N6A	0.075002
O1	-0.016617	O3	-0.015385	O5	-0.016010	O1A	-0.009429	O5A	-0.012603
O2	0.163773	O4	0.175565	O6	0.177566	O2A	0.180400	O6A	0.184406

ESI 4 Table 2: Spin densities for **C2** Complex.

Atom	Spin density	Atom	Spin density	Atom	Spin density	Atom	Spin density
C1	-0.006621	C1A	-0.003375	C1B	-0.006835	C1C	-0.007428
C2	-0.015735	C2A	-0.014937	C2B	-0.009705	C2C	-0.005306
C3	0.004243	C3A	0.003803	C3B	0.003561	C3C	0.000920
C4	-0.009565	C4A	-0.005182	C4B	-0.007234	C4C	-0.006361
C5	0.006717	C5A	0.006096	C5B	0.005937	C5C	0.006040
C6	0.001869	C6A	0.008264	C6B	-0.005064	C6C	0.002481
C7	-0.001014	C7A	0.001115	C7B	0.000480	C7C	-0.000310
C8	0.001939	C8A	0.001448	C8B	0.002693	C8C	0.001259
C9	-0.010142	C9A	-0.004701	C9B	-0.006913	C9C	-0.005253
C10	0.003691	C10A	0.003434	C10B	0.001880	C10C	0.004630
C11	-0.007385	C11A	-0.007825	C11B	-0.009094	C11C	-0.006258
C12	0.006185	C12A	0.005529	C12B	0.007738	C12C	0.005508
C13	-0.019983	C13A	-0.010584	C13B	-0.010796	C13C	-0.014446
C14	-0.010940	C14A	-0.010318	C14B	-0.009607	C14C	-0.009040
C15	0.006938	C15A	0.003828	C15B	0.006277	C15C	0.006240
Cu1	0.622945	Cu1A	0.607783	Cu1B	0.629248	Cu1C	0.617967
N1	-0.013087	N1A	-0.010534	N1B	-0.009078	N1C	-0.007983
N2	0.093307	N2A	0.077426	N2B	0.084287	N2C	0.075716
N3	0.104672	N3A	0.090778	N3B	0.106739	N3C	0.094411
N4	0.112106	N4A	0.086260	N4B	0.094002	N4C	0.096819
N5	-0.000273	N5A	-0.005678	N5B	-0.000289	N5C	0.002540
N6	-0.004611	N6A	-0.000859	N6B	-0.004012	N6C	-0.007500
O1	0.006683	O1A	0.006358	O1B	0.006592	O1C	0.010886
O2	0.102252	O2A	0.100784	O2B	0.101660	O2C	0.120023
O3	0.015720	O3A	0.014673	O3B	0.016285	O3C	0.022554
O4	-0.000028	O4A	0.023727	O4B	0.002117	O4C	-0.000804
O5	-0.000112	O5A	0.013076	O5B	0.001769	O5C	-0.001626
O6	0.000306	O6A	0.015570	O6B	0.001665	O6C	-0.000200

ESI 4 Table 3: Spin densities for **C3** Complex.

atom	Spin density	atom	Spin density	Atom	Spin density
C1	-0.004717	C1A	-0.004586	C1B	-0.006049
C2	-0.005017	C2A	-0.005114	C2B	-0.005081
C3	-0.008354	C3A	-0.014804	C3B	-0.006942
C4	0.005372	C4A	0.009559	C4B	0.009872
C5	-0.007818	C5A	-0.006480	C5B	-0.005853
C6	-0.004727	C6A	-0.004054	C6B	0.000039
C7	0.006061	C7A	0.005676	C7B	0.006389
C8	-0.001204	C8A	-0.000364	C8B	0.001322
C9	0.000348	C9A	0.000657	C9B	0.001157
C10	0.001876	C10A	0.001884	C10B	0.000250
C11	-0.008259	C11A	-0.012798	C11B	-0.002215
C12	-0.008111	C12A	-0.005427	C12B	-0.008445
C13	-0.003632	C13A	-0.000263	C13B	-0.001510
C14	0.012371	C14A	-0.006232	C14B	-0.019378
C15	0.000845	C15A	-0.006668	C15B	-0.005219
C16	-0.009210	C16A	-0.003864	C16B	-0.005587
C17	-0.023033	C17A	-0.014439	C17B	-0.017619
C18	0.006436	C18A	0.005708	C18B	0.003853
C19	-0.004430	C19A	-0.007659	C19B	-0.004926
C20	0.009306	C20A	0.005844	C20B	0.007189
C21	0.018258	C21A	-0.001698	C21B	0.010655
C22	-0.003788	C22A	-0.001595	C22B	-0.000066
C23	0.002195	C23A	-0.000370	C23B	0.000434
C24	0.000640	C24A	0.000994	C24B	0.000473
C25	0.001742	C25A	0.001070	C25B	0.001555
C26	-0.004072	C26A	-0.005215	C26B	-0.003248
C27	-0.000362	C27A	-0.000722	C27B	-0.001248
C28	-0.008537	C28A	-0.008729	C28B	-0.008913

Cu1	0.733575	Cu1A	0.745663	Cu1B	0.724377
N1	0.024905	N1A	0.026027	N1B	0.025105
N2	-0.017325	N2A	-0.017089	N2B	-0.016753
N3	0.004664	N3A	0.004911	N3B	0.004878
N4	0.100039	N4A	0.084748	N4B	0.110930
N5	0.065500	N5A	0.045356	N5B	0.091421
N6	0.051085	N6A	0.052734	N6B	0.030739
N7	0.106027	N7A	0.119901	N7B	0.090260
N8	-0.017739	N8A	-0.010268	N8B	-0.016760
N9	0.006380	N9A	0.014915	N9B	0.004783
N10	0.001988	N10A	0.004789	N10B	0.001685

ESI 4 Table 4: Spin densities for **C4** Complex.

Atom	Spin density	Atom	Spin density	Atom	Spin density
C1	0.008984	C1A	0.003101	C1B	0.008998
C2	-0.031142	C2A	-0.010734	C2B	-0.009021
C3	0.004054	C3A	0.002244	C3B	-0.004538
C4	-0.005229	C4A	-0.007311	C4B	-0.004846
C5	-0.009630	C5A	0.003238	C5B	-0.000089
C6	0.001705	C6A	0.005697	C6B	0.006054
C7	-0.004084	C7A	-0.004382	C7B	-0.003950
C8	0.006859	C8A	0.007599	C8B	0.010778
C9	0.003145	C9A	0.002004	C9B	0.001471
C10	0.000254	C10A	-0.003584	C10B	-0.007000
C11	0.005734	C11A	0.004555	C11B	0.005953
C12	-0.000074	C12A	0.001524	C12B	0.000672
C13	-0.000045	C13A	0.001198	C13B	0.001093
C14	-0.005511	C14A	-0.008150	C14B	-0.010618
C15	0.005204	C15A	0.008289	C15B	0.007316
C16	-0.012307	C16A	-0.012917	C16B	-0.010631
Cl1	0.004559	Cl1A	0.002799	Cl1B	0.007879
Cl2	0.152753	Cl2A	0.154245	Cl2B	0.164690
Cu1	0.582206	Cu1A	0.582774	Cu1B	0.582540
N1	0.099380	N1A	0.105936	N1B	0.104741
N2	0.086695	N2A	0.082891	N2B	0.079758
N3	-0.010287	N3A	-0.010921	N3B	-0.006111
N4	0.106488	N4A	0.086797	N4B	0.075955

ESI 4 Table 5: Spin densities for **C5** Complex.

Atom	Spin density	Atom	Spin density
Br1	0.178704	Br1A	0.195366
Br2	0.013402	Br2A	0.008609
C1	0.009514	C1A	0.008174
C2	-0.021965	C2A	-0.012068
C3	0.007312	C3A	0.001801
C4	-0.010017	C4A	-0.009355
C5	-0.019636	C5A	-0.011404
C6	0.003260	C6A	0.000255
C7	-0.004036	C7A	-0.01867
C8	0.005729	C8A	0.006057
C9	0.020799	C9A	0.019693
C10	-0.007171	C10A	-0.015559
C11	0.006191	C11A	0.009895
C12	0.000987	C12A	-0.000031
C13	0.000992	C13A	-0.000565
C14	-0.009931	C14A	-0.006004
C15	0.009081	C15A	0.006177
C16	-0.013677	C16A	-0.013138
Cu1	0.563468	Cu1A	0.556919
N1	0.095853	N1A	0.082896
N2	-0.003585	N2A	-0.003277
N3	0.066571	N3A	0.066421
N4	0.104720	N4A	0.110388

ESI 4 Table 6: Spin densities for **C6** Complex.

Atom	Spin density	Atom	Spin density
C1	-0.011372	C1A	-0.011342
C2	0.007192	C2A	0.007175
C3	-0.007995	C3A	0.007977
C4	0.003734	C4A	0.003721
C5	-0.004861	C5A	-0.004842
C6	0.002356	C6A	0.002381
C7	0.000759	C7A	0.000725
C8	0.006409	C8A	0.006435
C9	0.002462	C9A	0.002429
C10	-0.007765	C10A	-0.007773
C11	0.006310	C11A	0.006314
C12	-0.017171	C12A	-0.017175
C13	-0.005013	C13A	-0.005000
C14	0.002520	C14A	0.002504
C15	-0.008498	C15A	-0.008493

C16	-0.000807	C16A	-0.000807
Cu1	0.611409	Cu1A	0.611478
N1	0.108767	N1A	0.108709
N2	0.117648	N2A	0.117609
N3	-0.016549	N3A	-0.116548
N4	0.094914	N4A	0.094895
N5	-0.004788	N5A	-0.004782
N6	-0.004607	N6A	-0.004607
O1	-0.000427	O1A	-0.000431
O5	0.004048	O5A	0.004025
O6	0.015592	O6A	0.015649
O7	0.100539	O7A	0.100539

ESI 4 Table 7: Spin densities for **C7** Complex.

Atom	Spin density	Atom	Spin density	Atom	Spin density	Atom	Spin density
C1	-0.011665	C1A	-0.012064	C1B	-0.008678	C1C	-0.012211
C2	0.006730	C2A	0.005568	C2B	0.007471	C2C	0.003464
C3	-0.007318	C3A	0.006546	C3B	-0.008977	C3C	-0.008030
C4	0.002344	C4A	0.003957	C4B	0.003078	C4C	0.007365
C5	-0.014424	C5A	-0.001286	C5B	-0.008280	C5C	-0.010016
C6	-0.002135	C6A	0.007705	C6B	-0.001364	C6C	0.019320
C7	0.008940	C7A	0.007729	C7B	0.009212	C7C	0.012645
C8	0.000069	C8A	0.000043	C8B	0.000936	C8C	0.000776
C9	0.000008	C9A	0.001563	C9B	0.001146	C9C	0.001773
C10	-0.009405	C10A	-0.004560	C10B	-0.004355	C10C	-0.004988
C11	0.002764	C11A	0.002548	C11B	0.006152	C11C	0.000735
C12	-0.017690	C12A	-0.012845	C12B	-0.001769	C12C	-0.012211
C13	-0.005356	C13A	-0.004474	C13B	-0.005377	C13C	-0.006144
C14	0.005167	C14A	0.004142	C14B	-0.004803	C14C	0.002554
C15	-0.022957	C15A	-0.010816	C15B	-0.001247	C15C	-0.006413
Cl1	0.128107	Cl1A	0.162319	Cl1B	0.159862	Cl1C	0.139082
Cl2	0.002903	Cl2A	0.007573	Cl2B	0.008439	Cl2C	0.007949
Cu1	0.587752	Cu1A	0.586790	Cu1B	0.585041	Cu1C	0.600481
N1	0.118770	N1A	0.091855	N1B	0.097115	N1C	0.104374
N2	0.114823	N2A	0.092040	N2B	0.091542	N2C	0.095266
N3	-0.012992	N3A	-0.013641	N3B	-0.005485	N3c	-0.014182
N4	0.113923	N4A	0.093598	N4B	0.078849	N4C	0.085369
N5	-0.000457	N5A	-0.004024	N5B	-0.002828	N5C	-0.003386

ESI 4 Table 8: Spin densities for radical R1.

Atom	Spin density	Atom	Spin density
Fe	-0.020182	O10	-0.010961
O20	-0.011160	N11	0.424098
N12	0.179289	N13	0.177891
N14	0.424869	N21	0.425118
N22	0.176974	N23	0.178379
N24	0.422995	C10	-0.047415
C11	0.014274	C12	0.004836
C13	0.003748	C14	0.010054
C15	-0.142185	C16	-0.043785
C17	-0.005970	C18	-0.005313
C20	-0.045806	C21	0.010285
C22	0.004025	C23	0.004214
C24	0.013540	C25	-0.137299
C26	-0.042336	C27	-0.004783
C28	-0.006511		

ESI 4 Table 9: Spin densities for radical R2.

Atom	Spin density	Atom	Spin density
S1	0.259325	S1A	0.259292
S2	0.260502	S2A	0.260525
C1	-0.080878	C1A	-0.080876
C2	-0.084607	C2A	0.-0.84597
N1	0.166733	N1A	0.166773
N2	0.164976	N2A	0.165004
N3	0.158513	N3A	0.158485
N4	0.155437	N4A	0.155393

ESI 4 Table 10: Spin densities for radical R3.

Atom	Spin density	Atom	Spin density
C1	0.026018	C1A	0.026018
C2	-0.090644	C2A	-0.090644
C3	0.283301	C3A	0.283301
C4	-0.121845	C4A	-0.121845
C5	0.303823	C5A	0.303823
C6	-0.095435	C6A	-0.095435
C7	0.292192	C7A	0.292192
C8	-0.120549	C8A	-0.120549

C9	-0.120549	C9A	-0.120549
C10	-0.120549	C10A	-0.120549
C11	0.274084	C11A	0.274084
C12	-0.124767	C12A	-0.124767
C13	0.312472	C13A	0.312472

ESI 4 Table 11: Spin densities for radical R4.

Atom	Spin density	Atom	Spin density
B	-0.017404	B1A	-0.017404
O1	0.022689	O1A	0.022689
N1	0.059027	N1A	0.059027
C1	0.106529	C1A	0.106529
C2	-0.047562	C2A	-0.047562
C3	0.104074	C3AB	0.104074
C3A	-0.036405	C3AA	-0.036405
C4	0.139232	C4A	0.139232
C5	-0.057530	C5A	-0.057530
C6	0.126461	C6AB	0.126461
C6A	-0.034504	C6AA	-0.034504
C7	0.121323	C7A	0.121323
C8	-0.051376	C8A	-0.051376
C9	0.111002	C9AB	0.111002
C9A	-0.053350	C9AA	-0.053350
C9B	0.016130	C9BA	0.016130

ESI 4 Table 12: Spin densities for radical R4*.

Atom	Spin density	Atom	Spin density
B1	-0.015141	B1A	-0.015141
O1	0.015596	O1A	0.015596
N1	0.034700	N1A	0.034700
C1	0.085759	C1A	0.085759
C2	-0.040810	C2A	-0.040810
C3	0.078412	C3AB	0.078412
C3A	-0.026801	C3AA	-0.026801
C4	0.096716	C4A	0.096716
C5	-0.039488	C5A	-0.039488
C6	0.090113	C6AB	0.090113
C6A	-0.026272	C6AA	-0.026272
C7	0.091752	C7A	0.091752
C8	-0.044882	C8A	-0.044882
C9	0.094557	C9AB	0.094557
C9A	-0.042711	C9AA	-0.042711
C9B	0.012623	C9BA	0.012623

ESI 4 Table 13: Spin densities for radical R5.

Atom	Spin density	Atom	Spin density
B1	-0.011280	B1A	-0.011280
O1	0.024784	O1A	0.024784
N1	0.059116	N1A	0.059116
C1	0.106653	C1A	0.106653
C2	-0.050432	C2A	-0.050432
C3	0.115091	C3AB	0.115091
C3A	-0.036448	C3AA	-0.036448
C4	0.141162	C4A	0.141162
C5	-0.058976	C5A	-0.058976
C6	0.137335	C6AB	0.137335
C6A	-0.038189	C6AA	-0.038189
C7	0.123582	C7A	0.123582
C8	-0.047376	C8A	-0.047376
C9	0.107798	C9AB	0.107798
C9A	-0.044711	C9AA	-0.044711
C9B	0.013000	C9BA	0.013000

ESI 4 Table 14: Spin densities for radical R6.

Atom	Spin density	Atom	Spin density
Ni2	0.093808	Ni2	0.093819
S5	0.183028	S5	0.182975
S6	0.221283	S6	0.221245
S7	0.198678	S7	0.198775
S8	0.255378	S8	0.255367
N5	0.006457	N5	0.006449
N6	0.009806	N6	0.009798
N7	0.011262	N7	0.011281
N8	0.010134	N8	0.010123
C9	0.003783	C9	0.003791
C10	0.002413	C10	0.002388
C11	0.006298	C11	0.006277
C12	-0.005764	C12	-0.005759

C13	-0.004294	C13	-0.004310
C14	0.021097	C14	0.021136
C15	-0.011760	C15	-0.011756
C16	-0.001607	C16	-0.001599

ESI 4 Table 15: Spin densities for radical R7.

Atom	Spin density	Atom	Spin density
Ni1	0.104048	Ni1	0.104011
S1	0.202953	S1	0.202858
S2	0.184108	S2	0.184010
S3	0.232722	S3	0.232857
S4	0.203038	S4	0.203121
N1	0.010350	N1	0.010338
N2	0.009115	N2	0.009100
N3	0.010562	N3	0.010588
N4	0.010680	N4	0.010700
C1	-0.000765	C1	-0.000756
C2	0.020240	C2	0.020161
C3	0.000640	C3	0.000616
C4	0.002352	C4	0.002348
C5	0.000309	C5	0.000299
C6	-0.003220	C6	-0.003188
C7	0.020760	C7	0.020817
C8	-0.007886	C8	-0.007889

ESI 4 Table 16: Spin densities for radical R8.

Atom	Spin density	atom	Spin density	Atom	Spin density
O1	-0.010027	O1A	-0.011167	O1B	-0.011459
N1	0.161995	N1A	0.191378	N1B	0.187384
N2	0.391804	N2A	0.403222	N2B	0.406143
N3	0.393547	N3A	0.407677	N3B	0.413944
N4	0.184308	N4A	0.193435	N4B	0.191612
N5	-0.031290	N5A	-0.018308	N5B	-0.016449
C1	-0.048565	C1A	-0.038609	C1B	-0.031862
C2	-0.068664	C2A	-0.182751	C2B	-0.190170
C3	0.049375	C3A	-0.015142	C3B	-0.011319
C4	0.006933	C4A	0.019272	C4B	0.013706
C5	0.027156	C5A	0.021776	C5B	0.025381
C6	-0.018475	C6A	-0.026861	C6B	-0.022644
C7	-0.008113	C7A	0.013706	C7B	0.003698
C8	-0.011086	C8A	-0.007102	C8B	-0.014166
C9	-0.017400	C9A	-0.014601	C9B	-0.014649

ESI 4 Table 17: Spin densities for radical R9.

Atom	Spin density	Atom	Spin density
B1	-0.002093	B1A	-0.001413
O1	0.017962	O1B	0.018483
C1	0.131391	C1B	0.118393
C2	-0.060401	C2B	-0.061699
C3	0.129303	C3D	0.123785
C3A	-0.060144	C3E	-0.060847
C4	0.147381	C4B	0.142410
C5	-0.059030	C5B	-0.052571
C6	0.134858	C6D	0.141914
C6A	-0.050258	C6E	-0.053161
C7	0.134801	C7B	0.143739
C8	-0.056219	C8B	-0.066650
C9	0.138356	C9F	0.155670
C9A	-0.059113	C9H	-0.056171
C9B	0.019809	C9J	0.021960
N9	0.026476	N9B	0.023197
C10	-0.009688	C10B	-0.010442
C11	-0.004240	C11B	-0.007792
C12	0.002676	C12B	-0.001192
C13	0.002104	C13B	0.004647
C14	0.000470	C14B	0.001097
C15	0.00130	C15B	0.001012
C16	0.004213	C16B	0.003247
O1A	0.018086	O1C	0.018560
C1A	0.131699	C1C	0.118573
C2A	-0.060399	C2C	-0.061689
C3B	0.129554	C3F	0.123988
C3C	-0.060145	C3H	-0.060821
C4A	0.147617	C4C	0.142487
C5A	-0.059026	C5C	-0.052498
C6B	0.135088	C6F	0.141970
C6C	-0.050296	C6H	-0.053100
C7A	0.135217	C7C	0.143905
C8A	-0.056211	C8C	-0.066581
C9C	0.138691	C9K	0.155898
C9D	-0.059121	C9L	-0.056145
C9E	0.019895	C9M	0.022002
N9A	0.026637	N9C	0.023357

C10A	-0.009695	C10C	-0.010451
C11A	-0.004255	C11C	-0.007802
C12A	0.002687	C12C	-0.001128
C13A	0.002102	C13C	0.004642
C14A	0.000471	C14C	0.001099
C15A	0.001131	C15C	0.001014
C16A	0.004227	C16C	0.003249

ESI 4 Table 18: Spin densities for radical R10.

Atom	Spin density	Atom	Spin density
Ni1	0.095381	Ni1A	0.095399
S1	0.203485	S1A	0.203427
S2	0.199839	S2A	0.199831
S3	0.208559	S3A	0.208604
S4	0.188784	S4A	0.188838
N1	0.010168	N1A	0.010167
N2	0.008698	N2A	0.008695
N3	0.011301	N3A	0.011304
N4	0.007798	N4A	0.007799
C1	-0.005396	C1A	-0.005419
C2	0.009062	C2A	0.009065
C3	0.005860	C3A	0.005819
C4	-0.000644	C4A	-0.000656
C5	-0.005223	C5A	-0.005243
C6	0.022261	C6A	0.022340
C7	0.044087	C7A	0.044080
C8	-0.004014	C8A	-0.004059