Supporting Information

Synthesis, characterizations and Anticancer Activities of Zn^{2+}, Cu^{2+}, Co^{2+} and Ni^{2+} Complexes Involving Chiral Amino Alcohols

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Table S1 Selected bond lengths [Å] and angles [°] for complexes (I) – (VII).

Complex (I)					
Ni1-N1	**2.071(4)**	**Ni1-O1**	**2.078(3)**	**Ni1-N2**	**2.085(4)**
Ni1-O3	2.076(3)	Ni1-N3	2.085(4)	Ni1-O2	2.130(3)
N1-Ni1-O3	91.69(16)	O3-Ni1-N3	81.43(14)	O3-Ni1-N2	97.90(14)
N1-Ni1-O1	79.95(15)	O1-Ni1-N3	97.75(15)	O1-Ni1-N2	90.69(14)
O3-Ni1-O1	171.41(13)	N1-Ni1-N2	164.77(16)	N3-Ni1-N2	94.70(15)
N1-Ni1-N3	98.42(16)	N1-Ni1-O2	88.32(15)	O3-Ni1-O2	88.48(14)
O1-Ni1-O2	93.19(15)	N3-Ni1-O2	167.99(14)	N2-Ni1-O2	80.17(14)
Complex (II)					
Co1-N1	1.931(6)	Co1-N2	1.942(6)	Co1-N3	1.943(6)
Co1-Co2	2.644(12)	Co2-O4	2.056(5)	Co2-O3	2.078(5)
Co2-O5	2.088(5)	Co2-O1	2.117(5)	Co2-O6	2.127(6)
Co2-O2	2.127(5)	Co2-Co3	2.63(13)	Co3-O4	1.897(5)
Co3-O6	1.901(6)	Co3-O5	1.908(5)	Co3-N4	1.937(7)
Co3-N5	1.940(7)	Co3-N6	1.948(6)		
O2-Co1-O1	85.8(2)	N3-Co1-Co2	121.0(2)	O3-Co2-Co1	46.11(14)
O2-Co1-O3	86.3(2)	O4-Co2-O1	177.0(2)	O5-Co2-Co1	135.72(15)
O1-Co1-O3	86.7(2)	O3-Co2-O1	77.8(2)	O1-Co2-Co1	45.88(13)
O2-Co1-N1	87.1(2)	O5-Co2-O1	105.0(2)	O4-Co3-N4	85.5(3)
O1-Co1-N1	93.3(2)	O4-Co2-O6	76.3(2)	O6-Co3-N4	171.0(3)
O3-Co1-N1	173.8(2)	O3-Co2-O6	104.5(2)	O5-Co3-N4	92.0(3)
O2-Co1-N2	86.5(2)	O5-Co2-O6	75.4(2)	O4-Co3-N5	173.7(3)
O1-Co1-N2	172.3(3)	O1-Co2-O6	105.3(2)	O6-Co3-N5	93.5(3)
O3-Co1-N2	92.6(2)	O4-Co2-O2	102.9(2)	O5-Co3-N5	87.3(3)
N1-Co1-N2	93.6(3)	O3-Co2-O2	76.95(19)	N4-Co3-N5	94.9(3)
O2-Co1-N3	172.9(3)	O5-Co2-O2	103.1(2)	O4-Co3-N6	91.6(3)
O1-Co1-N3	92.4(3)	O1-Co2-O2	75.64(19)	O6-Co3-N6	87.0(3)
O3-Co1-N3	86.7(2)	O6-Co2-O2	178.4(2)	O5-Co3-N6	172.0(3)
N1-Co1-N3	93.5(3)	O4-Co2-Co3	45.62(15)	N4-Co3-N6	95.5(3)
N2-Co1-N3	95.2(3)	O3-Co2-Co3	132.20(14)	N5-Co3-N6	94.6(3)
O2-Co1-Co2	52.76(15)	O5-Co2-Co3	45.84(14)	O4-Co3-Co2	50.79(16)
O1-Co1-Co2	52.39(15)	O1-Co2-Co3	137.23(14)	O6-Co3-Co2	52.92(16)
O3-Co1-Co2	51.22(15)	O6-Co2-Co3	45.49(15)	O5-Co3-Co2	51.70(16)
N1-Co1-Co2	124.1(18)	O2-Co2-Co3	132.99(15)	N4-Co3-Co2	119.0(2)
N2-Co1-Co2	121.8(2)	O4-Co2-Co1	131.28(15)	N5-Co3-Co2	124.2(2)
N6-Co3-Co2	121.6(2)	O6-Co2-Co1	136.05(16)	O2-Co2-Co1	45.51(14)
Complex (III)					
Cu1-O5	2.000(3)	Cu1-O3	2.020(2)	Cu1-O2	2.502(3)
Cu1-N2	2.003(3)	Cu1-O1	2.493(3)		
N1-Cu1-O5	89.41(10)	N2-Cu1-O3	88.57(11)	N1-Cu1-O2	103.47(11)
N1-Cu1-N2	177.33(16)	N1-Cu1-O1	77.88(11)	O5-Cu1-O2	90.10(9)
O5-Cu1-N2	92.97(14)	O5-Cu1-O1	91.94(9)	N2-Cu1-O2	77.74(11)
N1-Cu1-O3	89.08(14)	N2-Cu1-O1	100.83(11)	O3-Cu1-O2	89.15(9)
O5-Cu1-O3	178.11(12)	O3-Cu1-O1	88.86(9)	O1-Cu1-O2	177.57(7)
Complex (IV)					
Cu1-N1	1.987(11)	Cu1-O1S	2.770(10)	Cu2-O2A	1.967(9)
Cu1-N2	2.007(10)	Cu2-N1A	1.976(12)	Cu2-O3S	2.597(11)

Cu1-O1	1.954(9)	Cu2-N2A	1.986(14)	Cu2-O9S	2.71(3)
Cu1-O2	1.935(8)	Cu2-O1A	1.911(11)		
N1-Cu1-N2	96.3(4)	O2-Cu1-N1	173.6(4)	N1A-Cu2-O9S	96.9(8)
N1-Cu1-O1S	84.4(4)	O2-Cu1-N2	86.0(4)	N2A-Cu2-O3S	85.6(6)
N2-Cu1-O1S	81.1(4)	O2-Cu1-O1	93.3(4)	N2A-Cu2-O9S	82.9(11)
O1-Cu1-N1	85.4(4)	O2-Cu1-O1S	90.1(3)	O1A-Cu2-N1A	84.9(5)
O1-Cu1-N2	170.6(4)	N1A-Cu2-N2A	98.3(6)	O1A-Cu2-N2A	175.1(7)
O1-Cu1-O1S	108.3(3)	N1A-Cu2-O3S	88.4(5)	O1A-Cu2-O2A	91.6(5)
O1A-Cu2-O3S	98.3(4)	O1A-Cu2-O9S	93.0(10)	O2A-Cu2-N1A	173.5(5)
O2A-Cu2-N2A	85.6(5)	O2A-Cu2-O3S	86.8(4)	O2A-Cu2-O9S	88.7(8)
O3S-Cu2-O9S	167.9(8)				

Complex (V)

Zn1-O2	2.028(11)	Zn1-N2	2.085(12)	Zn2-Cl3	2.227(5)
Zn1-N1	2.047(13)	Zn1-O3	2.310(10)	Zn2-Cl1	2.283(4)
Zn1-N3	2.068(13)	Zn2-O2	1.918(11)	Zn2-Cl2	2.345(4)
O2-Zn1-N1	109.5(5)	N1-Zn1-N2	122.0(5)	N3-Zn1-O3	73.9(5)
O2-Zn1-N3	97.2(5)	N3-Zn1-N2	127.3(5)	N2-Zn1-O3	93.1(4)
N1-Zn1-N3	107.6(5)	O2-Zn1-O3	165.5(5)	O2-Zn2-Cl3	114.5(3)
O2-Zn1-N2	83.1(4)	N1-Zn1-O3	84.5(5)	O2-Zn2-Cl1	102.0(3)
Cl3-Zn2-Cl1	119.37(19)	O2-Zn2-Cl2	109.3(4)	Cl3-Zn2-Cl2	110.68(18)
Cl1-Zn2-Cl2	99.61(16)				

Complex (VI)

Co1-O3	1.883(9)	Co1-N1	1.946(12)	Co2-O3	2.095(10)
Co1-O1	1.900(10)	Co1-N3	1.958(12)	Co2-O5	2.111(9)
Co1-O2	1.920(10)	Co1-Co2	2.650(2)	Co2-O2	2.112(9)
Co1-N2	1.937(11)	Co2-O6	2.058(8)	Co2-O1	2.113(9)
Co2-O4	2.125(9)	Co2-Co3	2.649(2)	Co3-O6	1.882(9)
Co3-N6	1.902(11)	Co3-O4	1.905(9)	Co3-O5	1.945(8)
Co3-N5	1.958(10)	Co3-N4	1.988(11)		
O3-Co1-O1	86.0(4)	O3-Co1-Co2	51.7(3)	O2-Co2-O1	75.8(3)
O3-Co1-O2	86.7(4)	O1-Co1-Co2	52.2(3)	O6-Co2-O4	75.9(3)
O1-Co1-O2	85.6(4)	O2-Co1-Co2	52.1(3)	O3-Co2-O4	100.5(3)
O3-Co1-N2	173.8(5)	N2-Co1-Co2	122.6(4)	O5-Co2-O4	77.4(3)
O1-Co1-N2	91.9(5)	N1-Co1-Co2	121.5(3)	O2-Co2-O4	175.6(4)
O2-Co1-N2	87.3(4)	N3-Co1-Co2	121.1(4)	O1-Co2-O4	106.9(3)
O3-Co1-N1	91.5(4)	O6-Co2-O3	108.0(4)	O6-Co2-Co3	45.0(2)
O1-Co1-N1	86.9(4)	O6-Co2-O5	76.3(3)	O3-Co2-Co3	134.6(2)
O2-Co1-N1	172.4(5)	O3-Co2-O5	174.7(3)	O5-Co2-Co3	46.5(2)
N2-Co1-N1	94.3(5)	O6-Co2-O2	101.7(3)	O2-Co2-Co3	134.8(3)
O3-Co1-N3	88.0(4)	O3-Co2-O2	76.7(4)	O1-Co2-Co3	134.5(3)
O1-Co1-N3	173.2(4)	O5-Co2-O2	105.7(4)	O4-Co2-Co3	45.4(2)
O2-Co1-N3	90.8(5)	O6-Co2-O1	175.2(4)	O6-Co2-Co1	135.3(3)
N2-Co1-N3	93.7(5)	O3-Co2-O1	75.6(4)	O3-Co2-Co1	44.9(2)
N1-Co1-N3	96.6(5)	O5-Co2-O1	100.3(4)	O5-Co2-Co1	133.9(2)
O2-Co2-Co1	45.9(3)	O6-Co3-N6	88.6(4)	N6-Co3-O5	173.2(4)
O1-Co2-Co1	45.3(3)	O6-Co3-O4	85.6(3)	O4-Co3-O5	86.9(4)
O4-Co2-Co1	133.9(2)	N6-Co3-O4	92.5(4)	O6-Co3-N5	91.6(5)
Co3-Co2-Co1	179.29(9)	O6-Co3-O5	84.6(4)	N6-Co3-N5	92.9(5)
O4-Co3-N5	173.8(4)	O5-Co3-N5	87.3(4)	O6-Co3-N4	171.6(4)

N6-Co3-N4	93.1(5)	O4-Co3-N4	86.1(4)	O5-Co3-N4	93.6(4)
N5-Co3-N4	96.6(5)	O6-Co3-Co2	50.6(2)	N6-Co3-Co2	122.8(3)
O4-Co3-Co2	52.6(3)	O5-Co3-Co2	52.0(3)	N5-Co3-Co2	121.6(4)
N4-Co3-Co2	122.3(3)				
		Complex (VII)			
Zn1-N1	2.094(6)	Zn1-O3	2.191(6)	Zn1-O2	2.194(5)
Zn1-N3	2.101(6)	Zn1-O1	2.203(5)	Zn1-N2	2.105(6)
N1-Zn1-N3	98.6(3)	N2-Zn1-O3	94.8(2)	N1-Zn1-O1	78.7(2)
N1-Zn1-N2	100.1(2)	N1-Zn1-O2	94.5(2)	N3-Zn1-O1	94.2(2)
N3-Zn1-N2	99.3(3)	N3-Zn1-O2	166.9(3)	N2-Zn1-O1	166.5(2)
N1-Zn1-O3	165.1(2)	N2-Zn1-O2	79.4(2)	O3-Zn1-O1	86.8(2)
N3-Zn1-O3	78.8(3)	O3-Zn1-O2	88.2(2)	O2-Zn1-O1	87.2(2)

Table S2 Hydrogen bond lengths (Å) and bond angles (°) for complexes (I) - (VII).

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
		Complex (I)		
O10-H10D...O4	0.85(3)	2.19(9)	2.752(7)	123(9)
O11-H11D...O4	0.85	2.08	2.816(6)	144.7
O10-H10E...O8	0.85	2.31	3.119(6)	159.1
C12-H12...O5$^{\#1}$	0.98	2.57	3.517(7)	163.8
N3-H3B...O6$^{\#2}$	0.97	2.41	3.273(6)	147.6
N3-H3A...O7$^{\#3}$	0.97	2.32	3.258(6)	162.6
N2-H2B...O6$^{\#2}$	0.97	2.18	3.065(6)	151.8
N2-H2A...O5$^{\#1}$	0.97	2.22	3.128(6)	155.0
N1-H1B...O7	0.97	2.11	3.065(6)	168.9
N1-H1A...N5$^{\#3}$	0.97	2.70	3.657(7)	171.0
N1-H1A...O9$^{\#3}$	0.97	2.17	3.104(6)	162.1
O3-H3...O11	0.856(12)	1.80(2)	2.610(5)	158(5)
O2-H2...O8	0.870(13)	1.92(2)	2.767(5)	165(4)
O1-H1...O10$^{\#2}$	0.848(12)	1.766(17)	2.608(5)	172(6)
O1-H1...O10$^{\#2}$	0.848(12)	1.766(17)	2.608(5)	172(6)
O2-H2...O8	0.870(13)	1.92(2)	2.767(5)	165(4)
O3-H3...O11	0.856(12)	1.80(2)	2.610(5)	158(5)
N1-H1A...O9$^{\#3}$	0.97	2.17	3.104(6)	162.1
N1-H1A...N5$^{\#3}$	0.97	2.70	3.657(7)	171.0
N1-H1B...O7	0.97	2.11	3.065(6)	168.9
N2-H2A...O5$^{\#1}$	0.97	2.22	3.128(6)	155.0
N2-H2B...O6$^{\#2}$	0.97	2.18	3.065(6)	151.8
N3-H3A...O7$^{\#3}$	0.97	2.32	3.258(6)	162.6
N3-H3B...O6$^{\#2}$	0.97	2.41	3.273(6)	147.6
C12-H12...O5$^{\#1}$	0.98	2.57	3.517(7)	163.8
O10-H10E...O8	0.85	2.31	3.119(6)	159.1
O11-H11D...O4	0.85	2.08	2.816(6)	144.7
O10-H10D...O4	0.85(3)	2.19(9)	2.752(7)	123(9)
O10-H10D...O4	0.85(3)	2.19(9)	2.752(7)	123(9)

Complex (III)

N1-H1B...O1$^{\#1}$	0.85(3)	2.21(4)	3.039(4)	166(3)
N2-H2B...O2$^{\#2}$	0.83(3)	2.30(3)	3.066(4)	154(3)
N2-H2A...O5$^{\#2}$	0.87(3)	2.64(3)	3.088(5)	113(2)
C14-H14B...O6$^{\#1}$	0.98	2.43	3.374(5)	160.8
C12-H12A...O4$^{\#2}$	0.98	2.39	3.350(4)	165.8
C8-H8...O5	1.00	2.48	3.251(4)	133.5
C6-H6A...O6$^{\#3}$	0.99	2.52	3.502(4)	171.7
C2-H2C...O3	1.00	2.59	3.151(4)	115.6
O2-H2...O4	0.84	1.83	2.634(3)	159.0
O1-H1...O6	0.84	1.78	2.618(3)	174.0
N1-H1B...O1$^{\#1}$	0.85(3)	2.21(4)	3.039(4)	166(3)
N2-H2B...O2$^{\#2}$	0.83(3)	2.30(3)	3.066(4)	154(3)
N2-H2A...O5$^{\#2}$	0.87(3)	2.64(3)	3.088(5)	113(2)
C14-H14B...O6$^{\#1}$	0.98	2.43	3.374(5)	160.8
C12-H12A...O4$^{\#2}$	0.98	2.39	3.350(4)	165.8
C8-H8...O5	1.00	2.48	3.251(4)	133.5
C6-H6A...O6$^{\#3}$	0.99	2.52	3.502(4)	171.7
C2-H2C...O3	1.00	2.59	3.151(4)	115.6
O2-H2...O4	0.84	1.83	2.634(3)	159.0
O1-H1...O6	0.84	1.78	2.618(3)	174.0
O1-H1...O6	0.84	1.78	2.618(3)	174.0
O2-H2...O4	0.84	1.83	2.634(3)	159.0
C2-H2C...O3	1.00	2.59	3.151(4)	115.6
C6-H6A...O6$^{\#3}$	0.99	2.52	3.502(4)	171.7
C8-H8...O5	1.00	2.48	3.251(4)	133.5
C12-H12A...O4$^{\#2}$	0.98	2.39	3.350(4)	165.8
C14-H14B...O6$^{\#1}$	0.98	2.43	3.374(5)	160.8
N2-H2A...O5$^{\#2}$	0.87(3)	2.64(3)	3.088(5)	113(2)
N2-H2B...O2$^{\#2}$	0.83(3)	2.30(3)	3.066(4)	154(3)
N1-H1B...O1$^{\#1}$	0.85(3)	2.21(4)	3.039(4)	166(3)
O1-H1...O6	0.84	1.78	2.618(3)	174.0
O2-H2...O4	0.84	1.83	2.634(3)	159.0
C2-H2C...O3	1.00	2.59	3.151(4)	115.6
C6-H6A...O6$^{\#3}$	0.99	2.52	3.502(4)	171.7
C8-H8...O5	1.00	2.48	3.251(4)	133.5
C12-H12A...O4$^{\#2}$	0.98	2.39	3.350(4)	165.8
C14-H14B...O6$^{\#1}$	0.98	2.43	3.374(5)	160.8
N2-H2A...O5$^{\#2}$	0.87(3)	2.64(3)	3.088(5)	113(2)
N2-H2B...O2$^{\#2}$	0.83(3)	2.30(3)	3.066(4)	154(3)
N1-H1B...O1$^{\#1}$	0.85(3)	2.21(4)	3.039(4)	166(3)

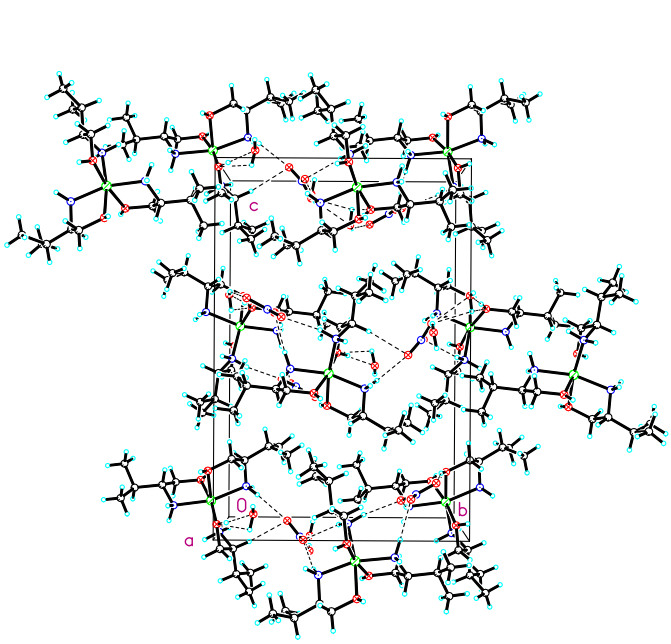
Complex (IV)

N1-H1A...O4S$^{\#1}$	0.91	2.19	3.015(15)	150.8
N1-H1B...O2$^{\#2}$	0.91	1.98	2.880(14)	169.6

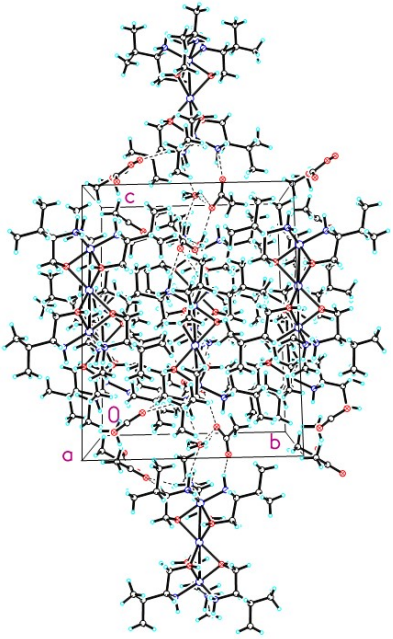
N2-H2A...O1#2	0.91	2.03	2.925(13)	166.5
N2-H2A...O1S	0.91	2.72	3.158(14)	110.6
O1-H1...O1A	0.84	1.73	2.429(14)	139.0
N1A-H1AA...O6S	0.91	2.31	3.02(3)	135.1
N2A-H2AB...O9S	0.91	2.72	3.16(4)	110.6
N2A-H2AC...O5S	0.91	2.26	3.16(3)	176.0
O2A-H2AD...O2	0.877(14)	2.05(15)	2.445(13)	106(12)
O9S-H9SB...O6S#3	0.87	2.38	3.15(4)	148.7
Complex (V)				
C24-H24B...O1#1	0.98	2.43	3.338(18)	153.4
C23-H23...Cl1#1	0.99	2.75	3.576(17)	141.9
C7-H7...Cl3#2	0.99	2.83	3.782(16)	161.8
N3-H3B...Cl2	0.98	2.77	3.567(13)	138.8
N3-H3B...Cl1	0.98	2.83	3.512(13)	127.4
N3-H3A...Cl2#3	0.98	2.43	3.338(12)	153.1
N2-H2B...Cl3#2	0.98	2.69	3.613(13)	156.2
N1-H1B...Cl1	0.98	2.46	3.295(13)	142.8
N1-H1A...Cl1#1	0.98	2.48	3.418(12)	160.4
O3-H3...Cl2#2	0.866(13)	2.49(9)	3.221(11)	142(12)
O1-H1...Cl2#1	0.83	2.53	3.281(12)	150.5
O1-H1...Cl2#1	0.83	2.53	3.281(12)	150.5
O3-H3...Cl2#2	0.866(13)	2.49(9)	3.221(11)	142(12)
N1-H1A...Cl1#1	0.98	2.48	3.418(12)	160.4
N1-H1B...Cl1	0.98	2.46	3.295(13)	142.8
N2-H2B...Cl3#2	0.98	2.69	3.613(13)	156.2
N3-H3A...Cl2#3	0.98	2.43	3.338(12)	153.1
N3-H3B...Cl1	0.98	2.83	3.512(13)	127.4
N3-H3B...Cl2	0.98	2.77	3.567(13)	138.8
C7-H7...Cl3#2	0.99	2.83	3.782(16)	161.8
C23-H23...Cl1#1	0.99	2.75	3.576(17)	141.9
C24-H24B...O1#1	0.98	2.43	3.338(18)	153.4
Complex (VII)				
N3-H3B...Cl2#1	0.97	2.63	3.456(8)	143.4
N3-H3A...Cl1#2	0.97	2.46	3.378(7)	157.3
N2-H2B...Cl2#1	0.97	2.51	3.361(7)	145.9
N2-H2A...Cl1	0.97	2.42	3.334(7)	157.2
N1-H1B...Cl2#1	0.97	2.40	3.268(7)	148.7
N1-H1A...Cl2	0.97	2.37	3.296(7)	159.9
O3-H3...Cl1	0.863(13)	2.56(8)	3.057(6)	118(7)
O2-H2...Cl2	0.867(13)	2.43(6)	3.058(6)	130(6)
O1-H1...Cl1#2	0.860(13)	2.53(7)	3.071(7)	122(7)
O1-H1...Cl1#2	0.860(13)	2.53(7)	3.071(7)	122(7)
O2-H2...Cl2	0.867(13)	2.43(6)	3.058(6)	130(6)
O3-H3...Cl1	0.863(13)	2.56(8)	3.057(6)	118(7)

N1-H1A...Cl2	0.97	2.37	3.296(7)	159.9
N1-H1B...Cl2$^{\#1}$	0.97	2.40	3.268(7)	148.7
N2-H2A...Cl1	0.97	2.42	3.334(7)	157.2
N2-H2B...Cl2$^{\#1}$	0.97	2.51	3.361(7)	145.9
N3-H3A...Cl1$^{\#2}$	0.97	2.46	3.378(7)	157.3
N3-H3B...Cl2$^{\#1}$	0.97	2.63	3.456(8)	143.4

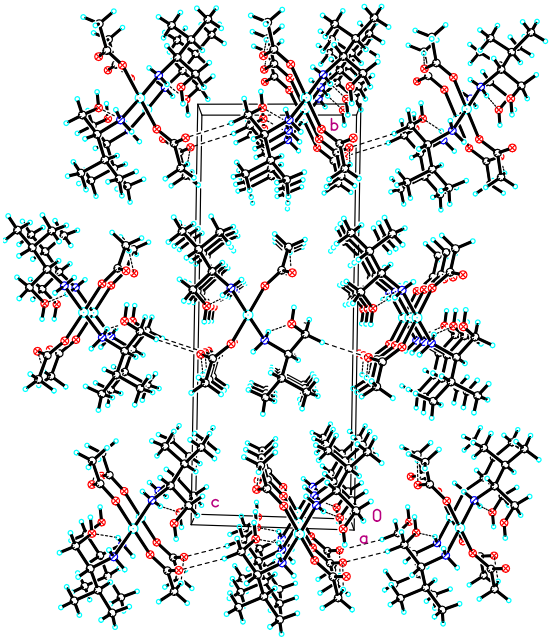
Symmetry transformations used to generate equivalent atoms: For (I), #1 = *x* + 1/2, -*y* + 3/2, - *z* + 1; #2 = *x* + 1, y, z; #3 = *x* + 1/2, - y + 1/2, - z + 1. For (III), #1 = *x* + 1, *y*, *z* ; #2 = *x* - 1, *y*, *z*; #3 = *x*, *y*, *z* - 1. For (IV), #1 = *x* + 1/2, - *y* + 3/2, - *z* + 1; #2 = *x* - 1/2, - *y* + 3/2,-*z*+1, #3 = *x* + 1, *y*, z. For (V), #1 = - *x* + 2, *y* - 1/2, - *z* + 1; #2 = *x*, *y* - 1, *z*; #3 = - *x* + 1, y - 1/2, - *z* + 1. For (VII), #1 = *x*+1/2, -*y* + 3/2, - *z* + 1; #2 = -*x* + 1, *y* + 1/2, - *z* + 1/2.



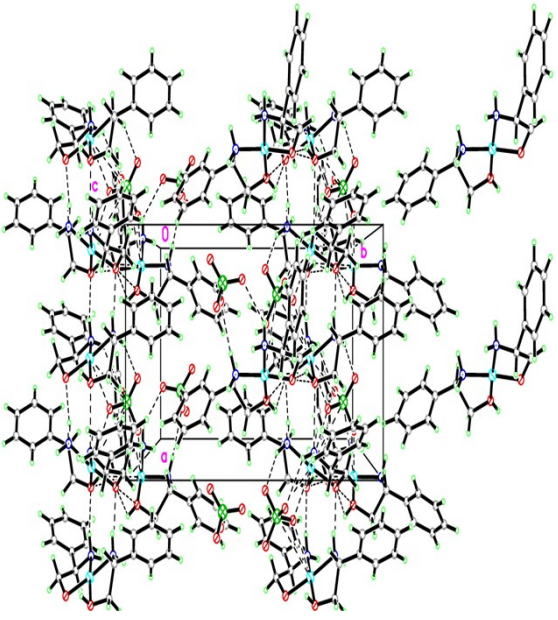
(a)



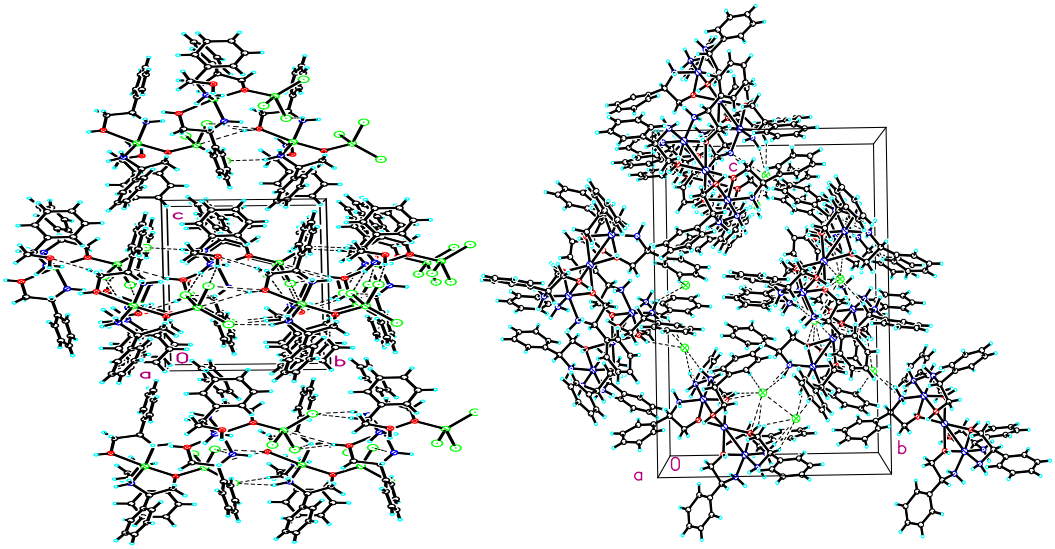
(b)



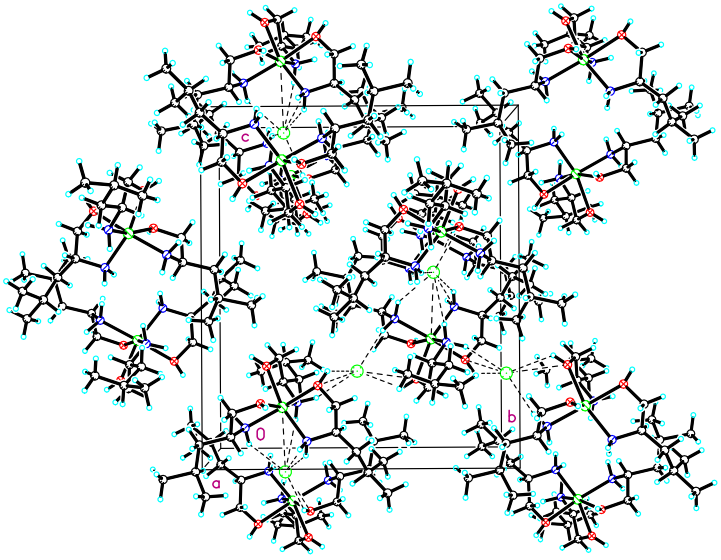
(c)



(d)



(e) (f)



(g)

Figure S1 The crystal packing of complexes (I) – (VII), showing the formation of the three-dimensional network by hydrogen bonding interactions, (a) for (I), (b) for (II), (c) for (III), (d) for (IV), (e) for (V), (f) for (VI) and (g) for (VII), respectively.

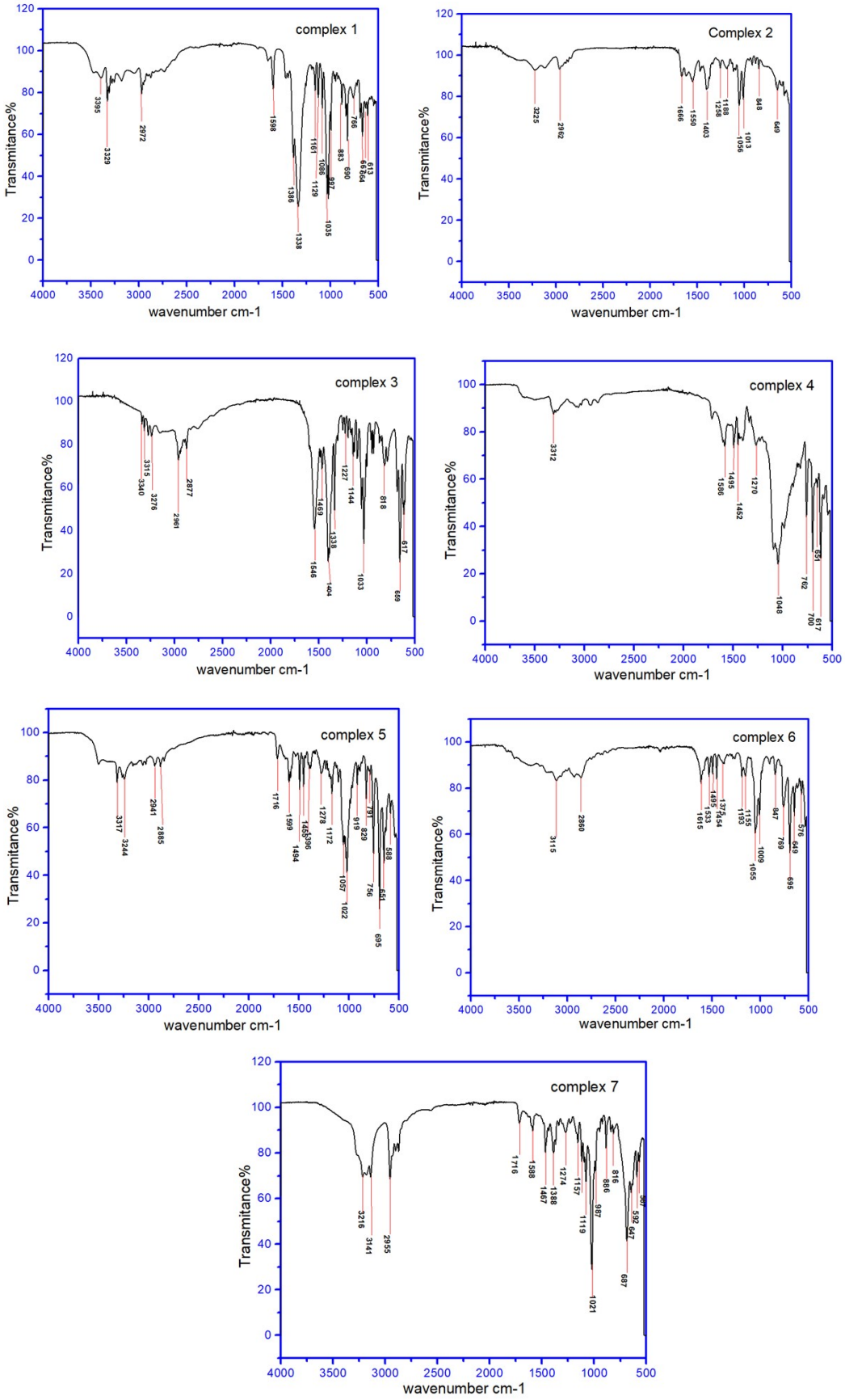


Figure S2 IR spectrums of complexes (I) - (VII).

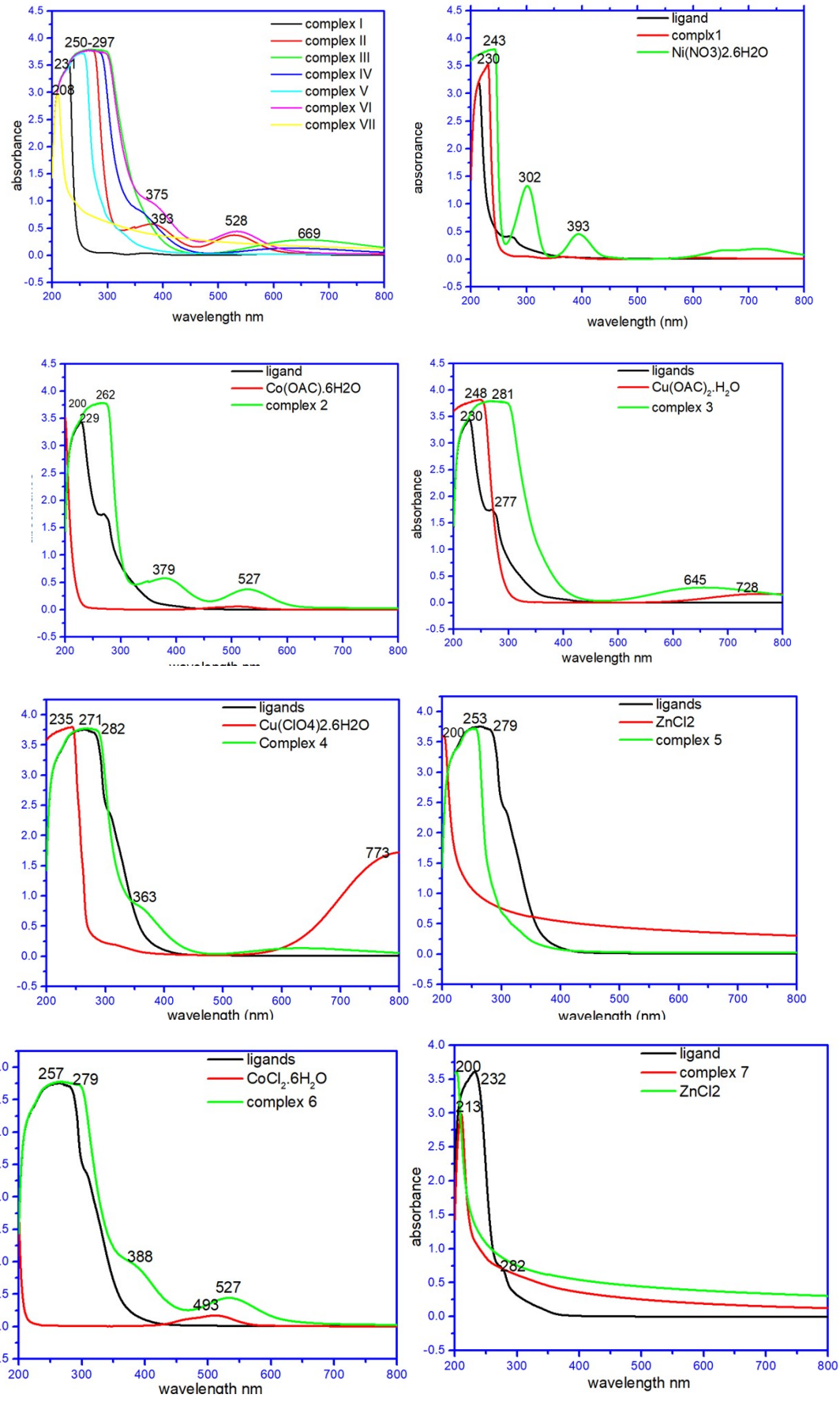


Figure S3 UV spectrum of complexes (I) - (VII).