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Supplementary information

Co(II), Ni(II) and Cu(II) complexes with phenylthiazole and thiosemicarbazone-derived ligands: synthesis, structure and cytotoxic effect

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Table S1. FAB-MS data (m/z) of the complexes **1a**– **9a, 1b**– **9b**.

compound	molecular ion	(m/z) fragment ions
1a	-	256.1 $[4a]^+$, 313.1 $[4aCo]^+$, 349.1 $[4aCoCl]^+$
2a	-	256.0 $[4a]^+$, 314.0 $[4aCo]^+$, 376.1 $[4aCoNO_3]^+$
3a	-	256.2 $[4a]^+$, 313.1 $[4aCo]^+$, 413.2 $[4aCoClO_4]^+$, 569.3 $[(4a)_2Co]^+$, 668.2 $[(4a)_2CoClO_4]^+$
5a	-	256.0 $[4a]^+$, 314.0 $[4aNi]^+$, 375.1 $[4aNiNO_3]^+$
6a	-	256.0 $[4a]^+$, 313.1 $[4aNi]^+$, 412.1 $[4aNiClO_4]^+$, 568.1 $[(4a)_2Ni]^+$, 667.1 $[(4a)_2NiClO_4]^+$
7a	-	256.1 $[4a]^+$, 318.0 $[4aCu]^+$, 353.0 $[4aCuCl]^+$
8a	-	318.2 $[4aCu]^+$, 573.3 $[(4a)_2Cu]^+$, 637.3 $[(4a)_2CuNO_3]^+$
9a	-	256.2 $[4a]^+$, 318.1 $[4aCu]^+$, 418.1 $[4aCuClO_4]^+$, 574.3 $[(4a)_2Cu]^+$
1b	-	249.0 $[5aCoCl]^+$, 404.1 $[(5a)_2CoCl]^+$
3b	-	213.0 $[5aCo]^+$, 313.0 $[5aCoClO_4]^+$, 368.0 $[(5a)_2Co]^+$, 468.0 $[(5a)_2CoClO_4]^+$
4b	-	213.0 $[5aNi]^+$, 249.0 $[5aNiCl]^+$
5b	-	213.0 $[5aNi]^+$, 275.0 $[5aNiNO_3]^+$, 369.1 $[(4a)_2Ni]^+$, 430.2 $[(5a)_2NiNO_3]^+$
6b	-	213.0 214.0 $[5aNi]^+$, 367.0 $[(4a)_2Ni]^+$, 467.0 $[(5a)_2NiClO_4]^+$
8b	-	218.0 $[5aCu]^+$, 281.1 $[5aCuNO_3]^+$, 437.2 $[(5a)_2CuNO_3]^+$
9b	-	219.0 $[5aCu]^{2+}$, 473.1 $[(5a)_2CuClO_4]^+$

Table S2. Selected bonds lengths (Å) and valence angles (º) for (**1a**), (**6a**), (**8a**) and (**5b**).

Complex	**1a**		**6a**		**8a**		**5b**	
Distances [Å]								
	Co1-N1	2.0087(19)	Ni1-O4	2.0692(17)	Cu1-N11	1.982(3)	Ni1-N11	2.033(5)
	Co1-N10	2.0782(18)	Ni1-O4^{i}	2.0692(17)	Cu1-N1	1.984(3)	Ni1-N1	2.070(6)
	Co1-Cl2	2.2064(6)	Ni1-N1^{i}	2.091(2)	Cu1-O3	1.988(3)	Ni1-O43	2.100(5)
	Co1-Cl3	2.2090(6)	Ni1-N1	2.091(2)	Cu1-N20	2.045(3)	Ni1-O42	2.212(6)
			Ni1-N10^{i}	2.1417(18)	Cu1-N10	2.275(3)	Ni1-S7	2.333(3)
			Ni1-N10	2.1417(18)	Cu2-O31	1.975(4)	Ni1-S17	2.336(2)
					Cu2-O31^{i}	1.975(4)	Ni2-N31	2.039(6)
					Cu2-O34	1.984(4)	Ni2-N21	2.058(6)
					Cu2-O34^{i}	1.984(4)	Ni2-O46	2.136(5)
							Ni2-O47	2.153(5)
							Ni2-S37	2.372(2)
							Ni2-S27	2.374(2)
Angles [º]	N1-Co1-N10	80.28(7)	O4-Ni1-O4^{i}	86.75(11)	N11-Cu1-N1	173.98(12)	N11-Ni1-N1	178.7(2)
	N1-Co1-Cl2	112.26(5)	O4-Ni1-N1^{i}	92.21(7)	N11-Cu1-O3	91.86(12)	N11-Ni1-O43	86.7(2)
	N10-Co1-Cl2	116.02(5)	O4^{i}-Ni1-N1^{i}	85.25(7)	N1-Cu1-O3	89.08(11)	N1-Ni1-O43	93.6(2)
	N1-Co1-Cl3	110.43(5)	O4-Ni1-N1	85.25(7)	N11-Cu1-N20	80.61(12)	N11-Ni1-O42	91.4(2)
	N10-Co1-Cl3	118.90(5)	O4^{i}-Ni1-N1	92.21(7)	N1-Cu1-N20	96.74(12)	N1-Ni1-O42	87.7(2)
	Cl2-Co1-Cl3	113.98(3)	N1^{i}-Ni1-N1	176.51(9)	O3-Cu1-N20	161.67(12)	O43-Ni1-O42	59.6(2)
			O4-Ni1-N10^{i}	170.11(7)	N11-Cu1-N10	108.42(12)	N11-Ni1-S7	96.46(17)
			O4^{i}-Ni1-N10^{i}	94.96(8)	N1-Cu1-N10	77.50(11)	N1-Ni1-S7	82.83(18)
			N1^{i}-Ni1-N10^{i}	78.25(7)	O3-Cu1-N10	91.34(11)	O43-Ni1-S7	163.48(18)
			N1-Ni1-N10^{i}	104.39(7)	N20-Cu1-N10	106.88(11)	O42-Ni1-S7	104.1(2)
			O4-Ni1-N10	94.96(8)	O31-Cu2-O31^{i}	92.9(2)	N11-Ni1-S17	82.44(17)
			O4^{i}-Ni1-N10	170.11(7)	O31-Cu2-O34	158.46(15)	N1-Ni1-S17	98.81(19)
			N1^{i}-Ni1-N10	104.39(7)	O31^{i} -Cu2-O34	91.53(16)	O43-Ni1-S17	93.76(17)
			N1-Ni1-N10	78.25(7)	O31-Cu2-O34^{i}	91.53(16)	O42-Ni1-S17	153.0(2)
			N10^{i}-Ni1-N10	85.03(10)	O31^{i} -Cu2-O34^{i}	158.47(15)	S7-Ni1-S17	102.71(10)
					O34-Cu2-O34^{i}	92.1(2)	N31-Ni2-N21	176.1(3)
							N31-Ni2-O46	88.4(2)
							N21-Ni2-O46	92.9(2)
							N31-Ni2-O47	92.5(2)
							N21-Ni2-O47	91.4(2)
							O46-Ni2-O47	59.7(2)
							N31-Ni2-S37	83.64(19)
							N21-Ni2-S37	92.58(19)
							O46-Ni2-S37	95.59(19)
							O47-Ni2-S37	155.2(2)
							N31-Ni2-S27	96.77(18)
							N21-Ni2-S27	83.26(18)
							O46-Ni2-S27	159.04(19)
							O47-Ni2-S27	99.68(19)
							S37-Ni2-S27	105.14(9)

(**6a**) ^{i} -x+1, y, -z+1/2; (**8a**) ^{i} -x, y, -z+1/2

Table. S3. Dihedral angles between rings in organic ligands.

parameter	(**1a**)	(**6a**)	(**8a**)		(**5b**)			
			N1 ligand	N11 ligand	N1 ligand	N11 ligand	N21 ligand	N31 ligand
$N1_p/N1_{ch}$	1.24	4.73	10.91	5.76	13.2	11.2	10.9	11.7
$N1_{ch}/S7$	0.77	12.54	14.71	13.80	----	----	----	----
S7/C91	8.59	55.67	41.3	30.8	----	----	----	----
$N1_p/S7$	1.01	14.52	17.7	14.0	----	----	----	----
$N1_p/C91$	7.89	69.67	52.6	41.3	----	----	----	----
$N1_{ch}/C91$	9.12	68.20	55.3	43.75	----	----	----	----
$Rms(N1_p)$	0.002	0.003	0.006	0.005	0.011	0.009	0.012	0.003
$Rms(N1_{ch})$	0.010	0.032	0.058	0.084	0.100	0.110	0.090	0.141
Rms(S7)	0.001	0.003	0.008	0.014	----	----	----	----
Rms(C91)	0.003	0.001	0.007	0.004	----	----	----	----

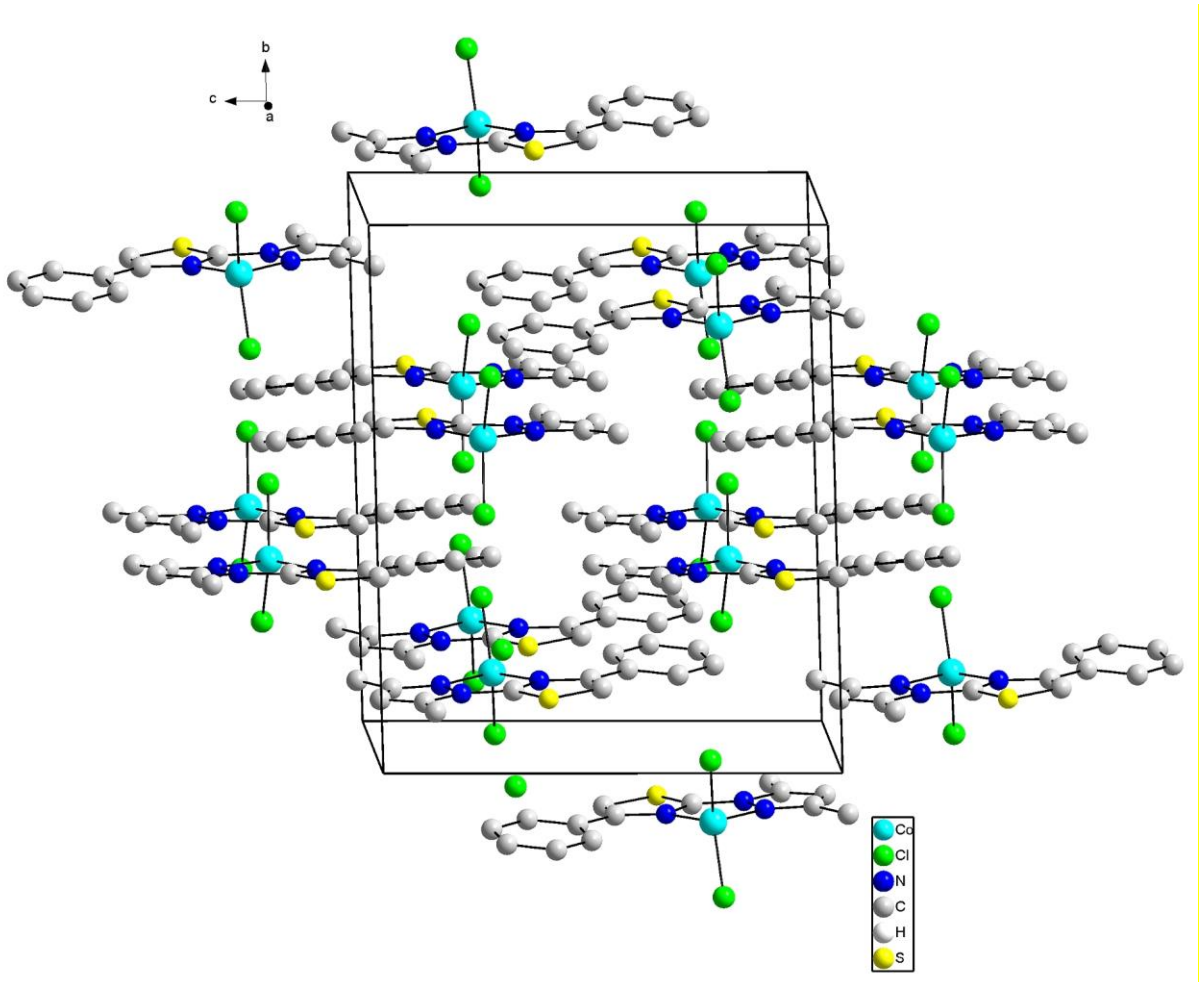

Figure S1. Crystal network of (**1a**) along *a* axis. For clarity of the figure all hydrogen atoms are omitted.

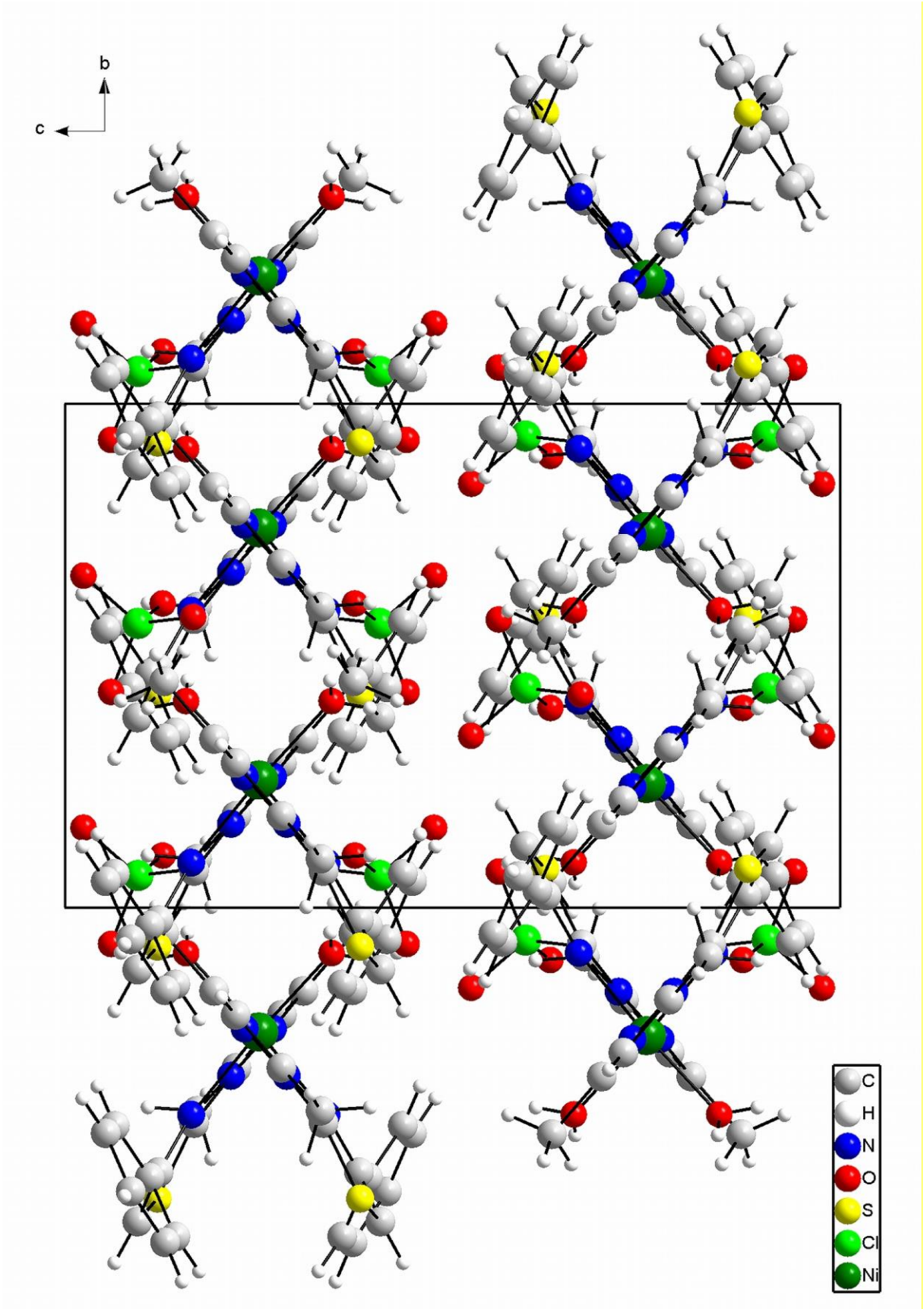

Figure S2. Crystal network of (**6a**) viewed along *a* axis.

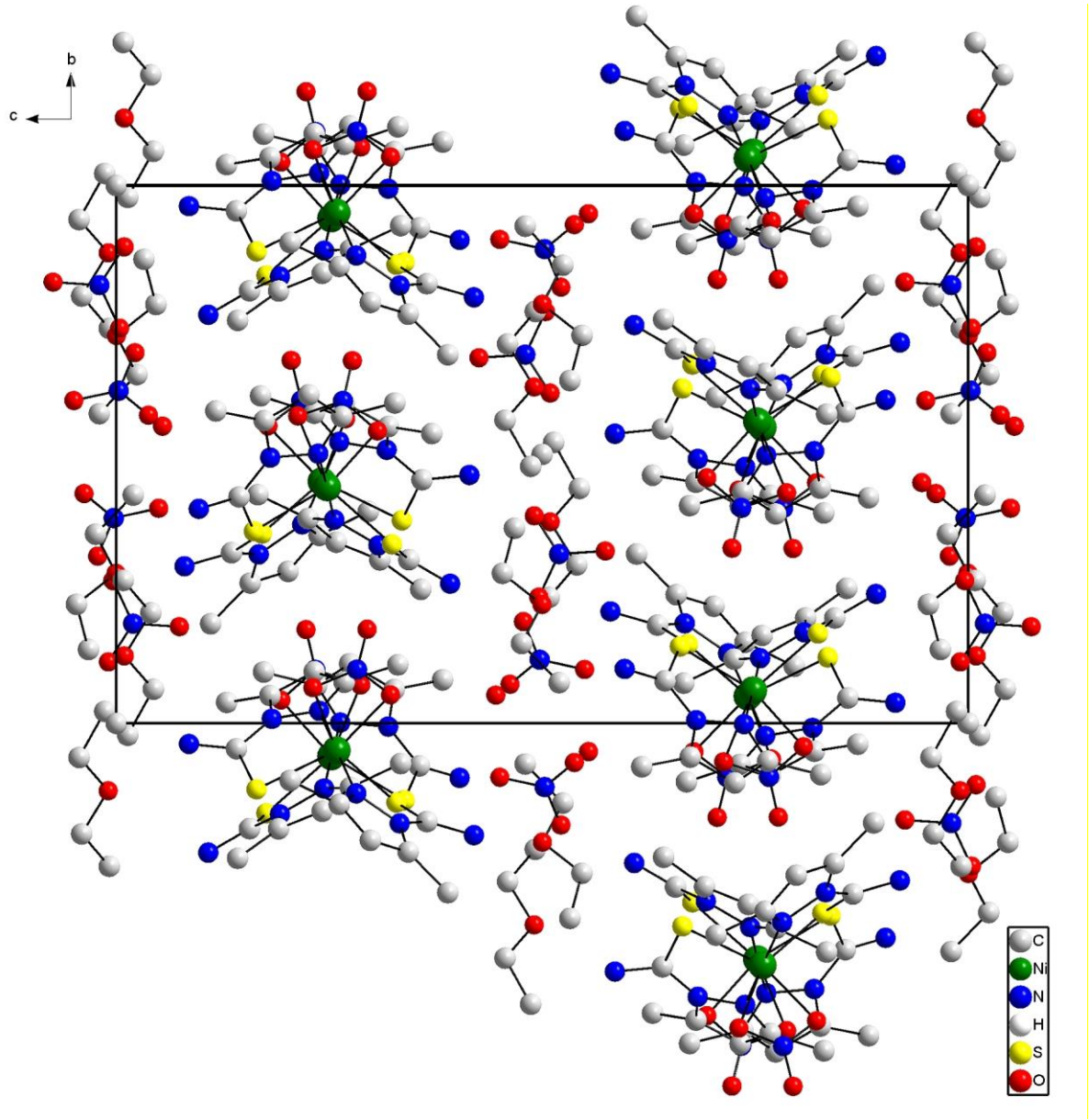

Figure S3. Crystal network of (**5b**) along *a* axis. For clarity of the figure all hydrogen atoms are omitted.