Supporting Information

Importance of the non-covalent interactions on the coordination geometry of Ni(II) in Ni(II)-M(II) complexes (M = Zn and Hg) with a salen type N_2O_2 Schiff base ligand and thiocyanate as coligand

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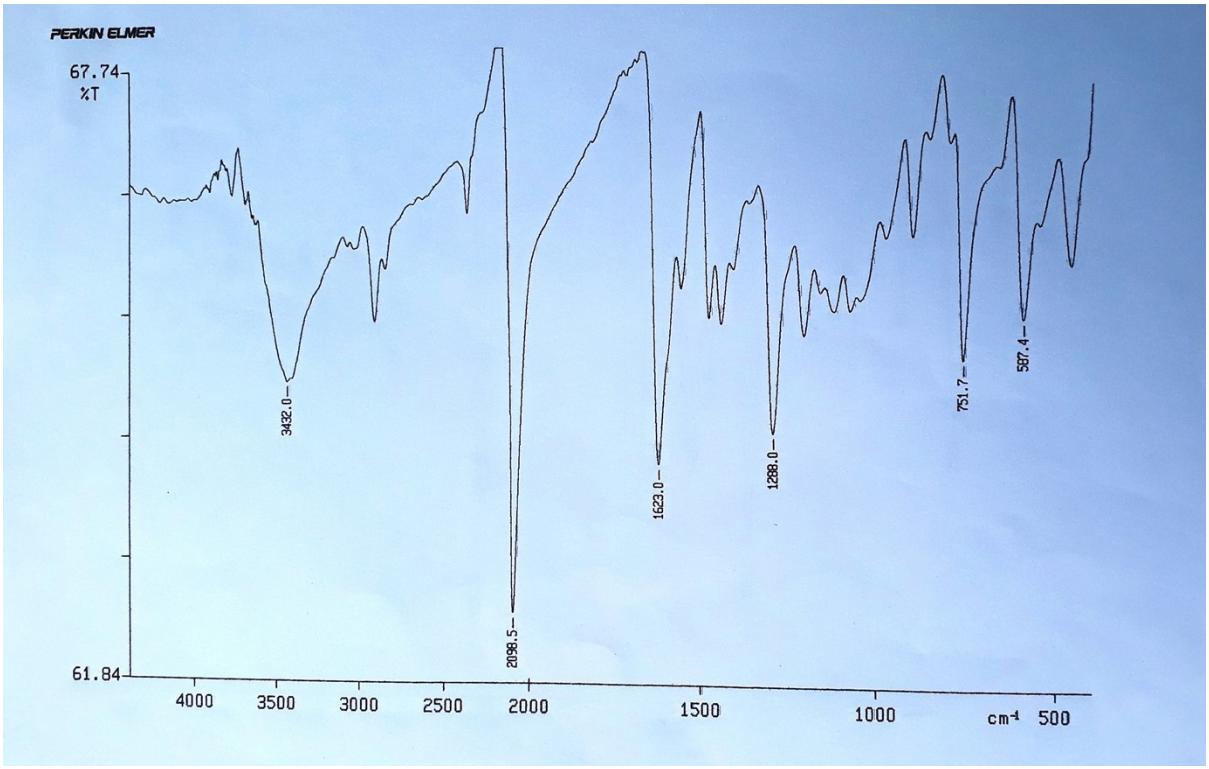

Fig. S1. IR spectrum of complex **1**.

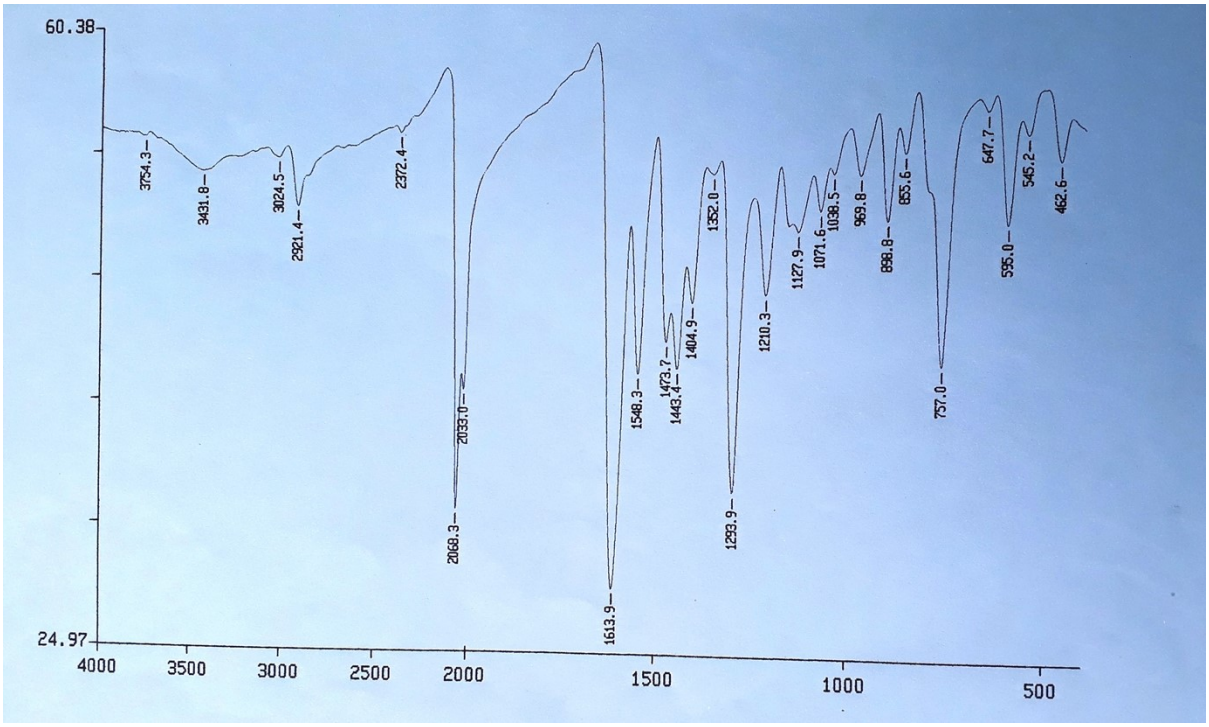

Fig. S2. IR spectrum of complex **2**.

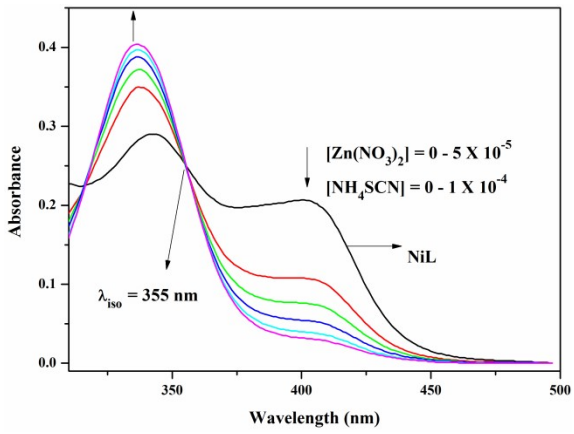

Fig. S3. Spectrophotometric titration of the metalloligand (5×10^{-5} M) by a mixture of $Zn(NO_3)_2$ (5×10^{-3} M) and NH_4SCN (1×10^{-2} M) in methanol. The range of concentration in the figure indicates their final concentration in solution.

Table S1. Bond distances (Å) and angles (°) around metal atoms for complexes **1** and **2**.

Bond distances (Å)			
1		**2**	
Zn(1)-O(1)	1.950(2)	Hg(1)-S(1)	2.383(3)
Zn (1)-O(2)	1.959(2)	Hg(1)-S(2)	2.411(3)
Zn (1)-N(3)	1.934(3)	Hg(1)-O(1)	2.410(5)
Zn (1)-N(4)	1.939(2)	Hg(1)-O(2)	2.588(4)
Ni(1)-S(1)[a]	2.557(2)	Ni(1)-O(1)	1.869(5)
Ni(1)-S(2)[b]	2.703(2)	Ni(1)-O(2)	1.844(5)
Ni(1)-O(1)	2.008(2)	Ni(1)-N(1)	1.871(6)
Ni(1)-O(2)	2.027(2)	Ni(1)-N(2)	1.868(6)
Ni(1)-N(1)	2.008(2)		
Ni(1)-N(2)	2.007(2)		
Bond angles (°)			
1		**2**	
O(1)-Zn(1)-O(2)	81.90(7)	S(1)-Hg(1)-S(2)	155.97(9)
O(1)-Zn(1)-N(3)	113.97(10)	S(1)-Hg(1)-O(1)	101.60(15)
O(1)-Zn(1)-N(4)	114.97(9)	S(1)-Hg(1)-O(2)	100.53(13)
O(2)-Zn(1)-N(3)	121.70(9)	S(2)-Hg(1)-O(1)	102.22(15)
O(2)-Zn(1)-N(4)	110.02(9)	S(2)-Hg(1)-O(2)	88.91(12)
N(3)-Zn(1)-N(4)	111.46(11)	O(1)-Hg(1)-O(2)	59.21(15)
S(1)[a]-Ni(1)-S(2)[b]	168.11(3)	O(1)-Ni(1)-O(2)	83.6(2)
S(1)[a]-Ni(1)-O(1)	89.96(6)	O(1)-Ni(1)-N(1)	91.3(2)
S(1)[a]-Ni(1)-O(2)	82.91(5)	O(1)-Ni(1)-N(2)	169.3(3)
S(1)[a]-Ni(1)-N(1)	99.08(6)	O(2)-Ni(1)-N(1)	168.7(2)
S(1)[a]-Ni(1)-N(2)	90.99(7)	O(2)-Ni(1)-N(2)	94.8(2)
S(2)[b]-Ni(1)-O(1)	89.26(6)	N(1)-Ni(1)-N(2)	92.1(3)
S(2)[b]-Ni(1)-O(2)	85.30(5)		
S(2)[b]-Ni(1)-N(1)	92.80(6)		
S(2)[b]-Ni(1)-N(2)	87.56(7)		
O(1)-Ni(1)-O(2)	78.83(7)		
O(1)-Ni(1)-N(1)	90.97(9)		
O(1)-Ni(1)-N(2)	169.00(8)		
O(2)-Ni(1)-N(1)	169.64(9)		
O(2)-Ni(1)-N(2)	90.41(8)		
N(1)-Ni(1)-N(2)	99.70(10)		

Symmetry transformation [a] = 1-x,-y,1-z and [b] = 1-x,1-y,-z for **1** and [a] = 1-x,-y,1-z for **2**