Electronic Supplementary Material (ESI) for CrystEngComm.

Phenoxido mediated antiferromagnetic and azide mediated ferromagnetic coupling in two dinuclear ferromagnetic nickel(II) complexes with isomeric Schiff bases: A theoretical insight on the pathway of magnetic interaction

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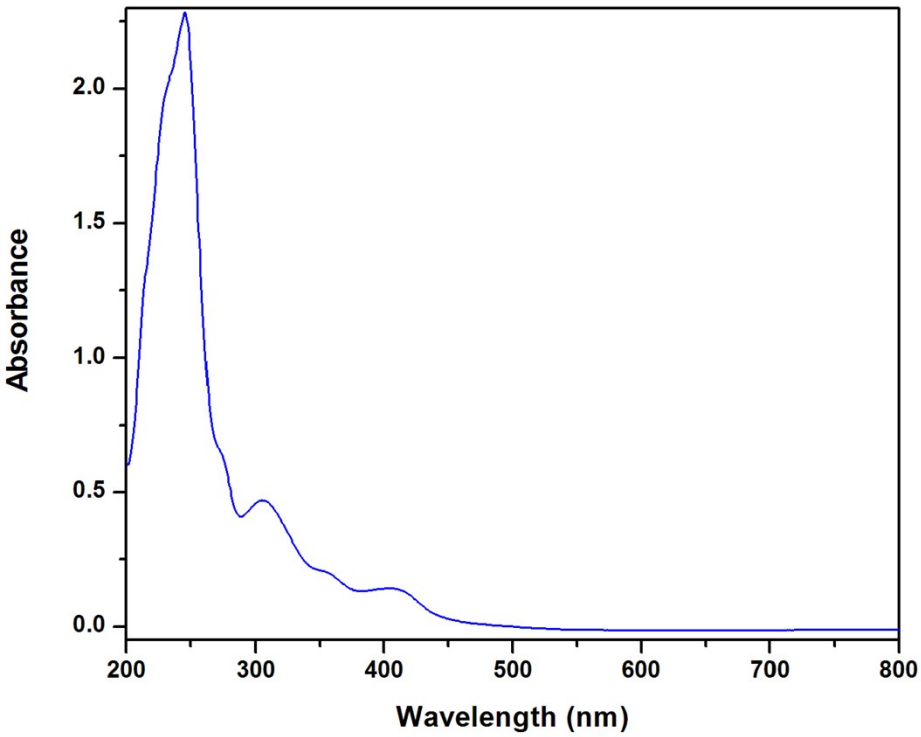

Fig. S1: Electronic spectrum of complex **1**.

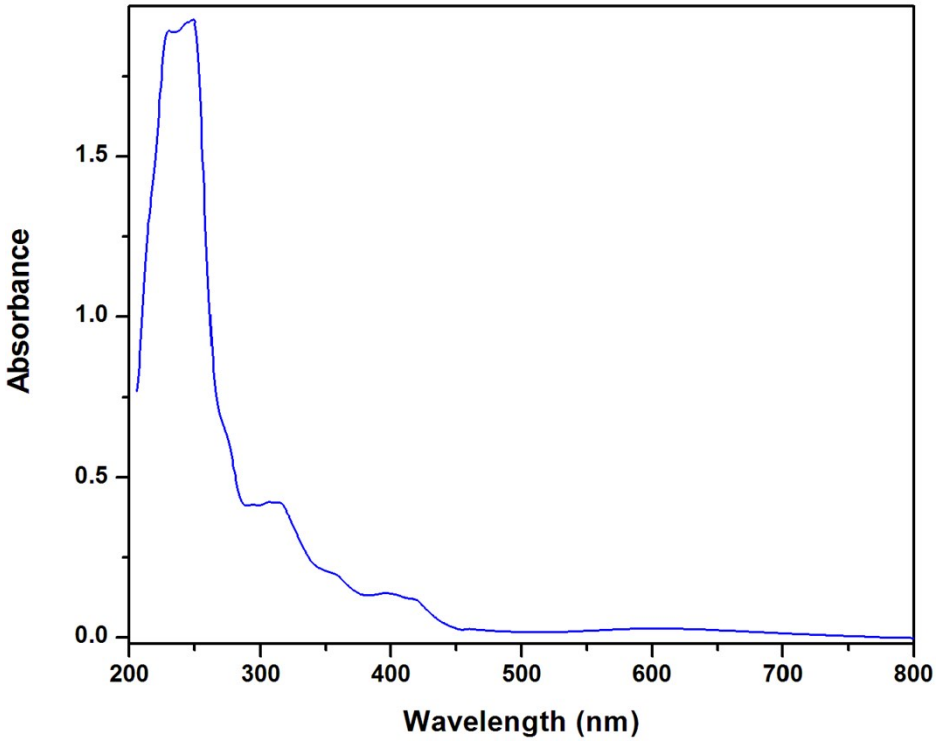

Fig. S2: Electronic spectrum of complex **2**.

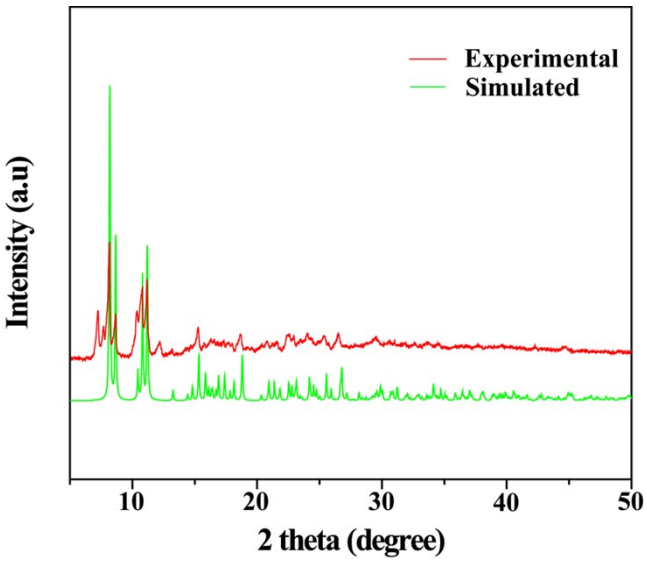

Fig. S3: Experimental and simulated powder XRD patterns of complex **1** confirming the purity of the bulk material.

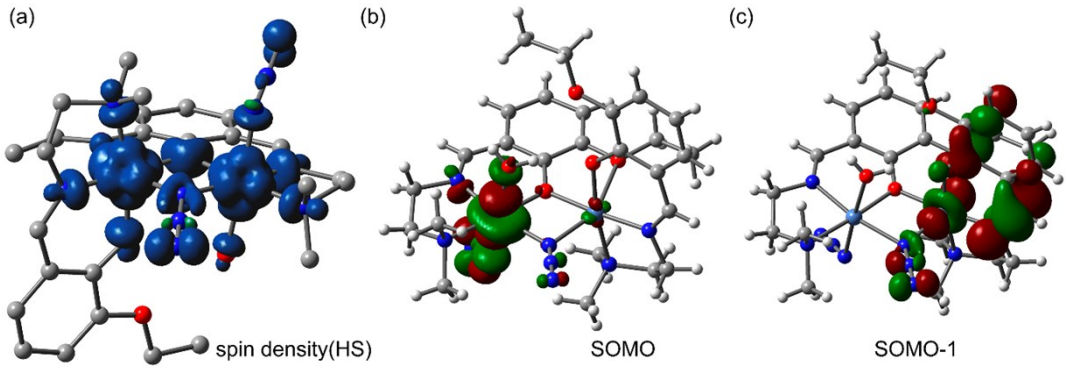

Fig. S4: (a) Graphical representation of spin density (contour 0.004 a.u.) at the ground state (high spin) configuration. (b,c) Pictorial representation of the SOMO involving the d_z2 and $d_x2_{-y}2$ orbitals of nickel(II) for the high spin state of complex **2**.

Table S1: Crystal data and refinement details of complexes **1** and **2**.

Complex	**1**	**2**
Formula	$C_{26}H_{40}Ni_2N_{10}O_5$	$C_{26}H_{40}N_{10}Ni_2O_5$, CH_4O
Formula Weight	690.06	722.10
Temperature (K)	150	296
Crystal System	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$P2_1$/n
a (Å)	11.5492(4)	11.7035(3)
b (Å)	12.4240(3)	11.3841(3)
c (Å)	21.6851(6)	25.2520(7)
β (˚)	(90)	94.194(1)

Z	4	4
d_{cal} (g cm^{-3})	1.473	1.429
μ(mm^{-1})	1.263	1.176
F(000)	1448	1520.0
Flack Parameter	0.062(13)	n/a-
Total reflection	10054	25134
Unique Reflections	5144	5786
Observe data[I>2σ(I)]	4990	4626
R(int)	0.026	0.051
R1, *w*R2 (all data)	0.0276, 0.0560	0.0522, 0.1102
R1, *w*R2 [I>2σ(I)]	0.0261, 0.0555	0.0407, 0.1053
Residual electron density e/Å^3	0.319, -0.375	0.715, -0.851

Table S2: Selected bond lengths (Å) for complexes **1** and **2**.

	1	**2**
Ni(1)-O(1)	2.094(2)	2.178(2)
Ni(1)-O(11)	2.037(2)	2.003(2)
Ni(1)-N(1)	2.185(3)	2.105(2)
Ni(1)-N(19)	2.026(3)	1.989(2)
Ni(1)-N(22)	2.113(3)	2.117(3)
Ni(1)-N(4)	2.084(3)	2.106(3)

Ni(2)-O(11)	2.005(2)	1.984(2)
Ni(2)-O(31)	2.016(3)	1.994(2)
Ni(2)-O(131)	2.238(2)	2.472(2)
Ni(2)-N(1)	2.113(3)	2.109(3)
Ni(2)-N(39)	1.995(3)	1.986(2)
Ni(2)-N(42)	2.109(3)	2.160(2)

Table S3: Selected bond angles (^{0}) for complexes **1** and **2**.

	1	**2**
N(4)-Ni(1)-O(1)	175.02(11)	177.03(10)
N(4)-Ni(1)-O(11)	91.35(10)	89.93(10)
N(4)-Ni(1)-N(1)	91.82(11)	94.63(11)
N(4)-Ni(1)-N(19)	94.62(12)	89.93(11)
N(4)-Ni(1)-N(22)	90.11(12)	89.51(11)
O(1)-Ni(1)-O(11)	90.14(10)	87.37(8)
O(1)-Ni(1)-N(1)	83.82(11)	83.68(9)
O(1)-Ni(1)-N(4)	175.02(11)	177.03(10)
O(1)-Ni(1)-N(19)	90.17(12)	91.34(9)

O(1)-Ni(1)-N(22)	89.15(12)	93.28(10)
O(11)-Ni(1)-N(1)	78.60(9)	79.93(9)
O(11)-Ni(1)-N(19)	88.22(10)	90.79(9)
O(11)-Ni(1)-N(22)	171.14(10)	175.65(9)
N(1)-Ni(1)-N(19)	165.47(10)	169.63(10)
N(1)-Ni(1)-N(22)	110.09(11)	104.42(9)
N(19)-Ni(1)-N(22)	82.95(11)	84.90(10)
O(11)-Ni(2)-O(31)	90.48(10)	88.71(8)
O(11)-Ni(2)-O(131)	75.23(9)	71.28(7)
O(11)-Ni(2)-N(1)	81.03(10)	80.25(9)
O(11)-Ni(2)-N(39)	176.97(10)	175.42(9)
O(11)-Ni(2)-N(42)	97.40(11)	97.61(9)
O(31)-Ni(2)-O(131)	85.31(9)	84.23(8)
O(31)-Ni(2)-N(1)	95.16(11)	93.12(9)
O(31)-Ni(2)-N(39)	88.15(12)	90.28(9)
O(31)-Ni(2)-N(42)	169.91(11)	171.20(9)
O(131)-Ni(2)-N(1)	156.26(10)	151.44(8)
O(131)-Ni(2)-N(39)	101.96(10)	104.18(9)
O(131)-Ni(2)-N(42)	90.60(9)	91.98(8)
N(1)-Ni(2)-N(39)	101.77(11)	104.26(10)
N(1)-Ni(2)-N(42)	92.29(11)	93.97(10)
N(39)-Ni(2)-N(42)	83.68(12)	82.93(9)

Table S4: Geometric parameters for H-bonding interaction for complexes **1** and **2**.

Complex	**D–H···A**	**D–H (Å)**	**H···A (Å)**	**D···A (Å)**	**∠D–H···A (°)**
1	O(1)–H(1)···O(31)	0.84(2)	1.80(2)	2.623(3)	163(4)
	O(1)–H(2)···N(4)[a]	0.87(2)	1.92(2)	2.771(4)	166(4)
	N(22)–H(22)···O(331)[b]	0.89(2)	2.29(3)	3.114(4)	155(3)

	N(42)–H(42)···N(6)	0.83(2)	2.55(3)	3.263(5)	145(3)
2					
	O(1)–H(1)···N(3)[c]	0.83(4)	2.34(4)	3.105(5)	155(4)
	O(1)–H(2)···O(31)	0.85(4)	1.91(4)	2.720(3)	160(4)

D, donor; H, hydrogen; A, acceptor. Symmetry transformation [a]= -1/2+x,3/2-y,-z; [b]= 1/2+x,3/2-y,-z; [c] = 1/2-x,-1/2+y,1/2-z.