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## **Supplementary Information**

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# Tryptophan moiety ligand based tri/tetra-nuclear Ni(II) complexes: syntheses, structure and magnetic properties

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#### **IR** spectral results

IR spectra of complexes **1** and **2** are shown in Figs. 1S and 2S, respectively and the most important absorption bands are briefly reported in the experimental section and in Table 1S. The v(O-H) stretching vibration broad bands appear in the region 3200-3600 cm<sup>-1</sup>.<sup>1S</sup> Stretching vibrations bands at 2920-2941 cm<sup>-1</sup> are assigned to  $C_{sp3}$ -H bonds and are seen in both the complexes. A robust and sharp band due to the asymmetric stretching bands of carboxylate appear at 1654 cm<sup>-1</sup> for complex **1**, and 1654 cm<sup>-1</sup> for complex **2**.<sup>2S</sup> Azomethane group v(C=N) stretching bands appear within the range 1560-1649 cm<sup>-1</sup>, whereas symmetric stretching band for the carboxylate is observed at 1442 cm<sup>-1</sup> for complex **1**, 1450 cm<sup>-1</sup> for **2**. Aromatic v(C=C)

stretching vibrations appear at 1384 cm<sup>-1</sup> (complex **1**) and 1374 cm<sup>-1</sup> (**2**).  $v_s(C-O)_{phenolic}$  stretching vibration appears at 1217 cm<sup>-1</sup> (complex **1**) and 1220 cm<sup>-1</sup>(**2**).<sup>3S</sup> The bands near 1070-1090 cm<sup>-1</sup> indicate the presence of (C-N)<sub>aliphatic</sub> bonds in both the complexes.

### References

- 1S K. Nakamoto, Infrared Spectra of Inorganic and Coordination Compounds, John Wiley & Sons, New York, 1997.
- 2S A. Paul, A.Figuerola, V. Bertolasi and S.C. Manna, Polyhedron, 2016, 119, 460-470
- 3S S. Mistri, E. Zangrando, E. Farnetti and S.C. Manna, Polyhedron, 2015, 89, 250-259

Vibrationmodes	1	2
v(O-H) antisymmetric and symmetric	3260 (br)	3407 (br)
stretching		
$v(C_{sp3}-H)$ stretching	2935 (br)	2928 (br)
v(C=O) antisymmetric stretching	1654 (s)	1654 (vs)
(carboxylate)		
v(C=O) antisymmetric stretching (DMF)	1667 (vs)	1654 (vs)
	(lattice DMF)	(coordinated DMF)
v( C=N) stretching	1575 (s)	1565 (vs)
v(C=O) symmetric stretching (carboxylate)	1442 (s)	1450 (s)
v(Ar C=C) stretching	1384 (vs)	1374 (vs)
v <sub>s</sub> (C-O) <sub>phenolic</sub>	1217 (vs)	1220 (vs)
v(C-N) aliphatic stretching	1083 (s)	1080 (s)

Table 1S.IR bands (cm<sup>-1</sup>) for complexes 1 and 2

s, strong; br, broad; vs, very strong; w, weak



Fig.1S IR spectrum of complex 1.



Fig. 2S IR spectrum of complex 2.

D-H	d(D-H)	d(HA)	<dha< th=""><th>d(DA)</th><th>Α</th><th>Symmetry code</th></dha<>	d(DA)	Α	Symmetry code
O1w-H1v	0.88	1.85	172	2.717(3)	017	x, y, -1+z
O1w-H1w	0.87	1.88	169	2.734(5)	O21	1-x, -1/2+y, 1-z
O2w-H2v	0.96	1.85	159	2.762(3)	O3w	intramolecular
O2w-H2w	0.87	1.88	160	2.713(3)	09	intramolecular
O2w-H2w	0.87	2.43	126	3.027(3)	012	intramolecular
O3w-H3v	0.84	2.59	100	2.859(3)	O5	intramolecular
O3w-H3v	0.84	1.93	167	2.757(3)	013	intramolecular
O3w-H3v	0.84	2.58	120	3.088(3)	016	intramolecular
O3w-H3w	0.81	1.94	171	2.742(4)	O5w	-
N2-H2n	0.88	2.04	139	2.772(5)	O7w	1-x, -1/2+y, 1-z
N4-H4n	0.88	2.36	148	3.140(5)	011	-x, 1/2+y, -z
N6-H6n	0.88	2.07	160	2.909(4)	015	-1+x, y, z
N8-H8n	0.88	2.47	129	3.097(6)	O8w	2-x, -1/2+y, 1-z
N8-H8n	0.88	2.32	142	3.065(6)	O9w	2-x, -1/2+y, 1-z
	O atoms of lattice water molecules					
O4w-H4v	0.96	1.75	178	2.704(4)	O18	-
O4w-H4w	0.82	1.97	166	2.768(3)	O17	x, y, -1+z
O5w-H5v	0.91	1.94	177	2.844(5)	O11w	-
O5w-H5w	0.88	2.08	147	2.860(6)	O10w	-
O6w-H6v	0.85	2.18	143	2.903(5)	015	-1+x, y, z
O6w-H6w	0.85	1.97	158	2.777(4)	O20	-1+x, y, z
O7w-H7v	0.94	1.84	173	2.780(5)	O11w	-
O7w-H7w	0.97	2.29	112	2.808(5)	015	-1+x, y, z
O8w-H8v	0.97	1.82	151	2.708(5)	011	1-x, 1/2+y, -z
O8w-H8w	0.93	1.94	179	2.873(5)	O20	-
O9w-H9v	0.98	2.05	152	2.954(7)	O21	x, y, -1+z
O9w-H9w	0.97	1.88	169	2.842(5)	O10	1-x, 1/2+y, -z
O10w-H10v	0.85	2.15	159	2.963(6)	015	-1+x, y, z
O11w-H11v	0.94	1.80	167	2.721(5)	O6w	-
O11w-H11w	0.94	1.78	164	2.690(4)	019	-

Table 2S. Hydrogen bond parameters (Å /°) for complex 1.



**Fig. 3S** ORTEP drawing (ellipsoid probability 50%) of complex **1** (H atoms not shown for clarity).



**Fig. 4S** ORTEP drawing (ellipsoid probability 50%) of complex **2** of C2 symmetry (H atoms not shown for clarity). The coordinated dmf molecule (O7/N7) is disordered over two positions, only that at higher occupancy (ca. 0.7) is displayed.

	$D_{6h}$	$C_{5v}$	$O_h$	D <sub>3h</sub>
	(hexagon)	(pentagonalpyramid)	(ocathedron)	(trigonalprism)
Ni1	27.63321	24.18538	1.12648	14.23716
Ni2	32.52839	26.10393	0.79398	13.53500
Ni3	33.41946	24.82109	0.97274	12.26435
Ni4	28.09930	23.35000	1.27638	13.28069

Table 3S: SHAPE analysis of the coordination geometry for complex **1**.

Table 4S: SHAPE analysis of the coordination geometry for complex **2**.

	D <sub>6h</sub>	C <sub>5v</sub>	O <sub>h</sub>	D <sub>3h</sub>
	(hexagon)	(pentagonal pyramid)	(ocathedron)	(trigonal prism)
Ni1	27.38940	27.51465	0.71995	14.84220
Ni2	32.26072	27.41360	0.42541	14.28978