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Supporting Information to

Structural, spectroscopic, magnetic behavior and DFT investigations of L-tyrosinato nickel(II) coordination polymer.

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KEYWORDS *L-tyrosine, nickel(II) complex, crystal structure, spectroscopy (FT-IR, FT-Raman, NIR-vis-UV), high-field EPR, magnetic properties, DFT calculations,*

Table S1 Crystal data and structure refinement for (1)

Empirical formula	$C_{28}H_{28}N_4NiO_6$ $4H_2O$
Formula weight *(g/mol)*	647.32
Temperature (K)	295
Wavelength	0.71073
Radiation type	Mo$K\alpha$
Crystal system, space group	Monoclinic, *P*21
a, b, c (Å)	9.6658(12), 13.5399(17), 11.4516(13)
β (°)	98.777(3)
Cell Volume (Å^3)	1481.2(3)
Z	2
D_{calc} (Mg m^{-3})	1.451
Absorption coefficient (mm^{-1})	0.72
Absorption correction	Numerical
F(000)	680
Crystal size (mm)	0.27 x 0.18 x 0.15
Colour	Grey
Index ranges h, k, l	$-13 \leq h \leq 12$, $-17 \leq k \leq 18$, $-10 \leq l \leq 15$
T_{min}, T_{max}	0.863 , 0.912
Reflection collected, independent and observed [$I > 2\sigma(I)$] reflections	17584, 7432, 3952
(R_{int})	0.084
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.694
R[$F^2 > 2\sigma(F^2)$], *w*R(F^2), S	0.085, 0.094, 1.01
Refinement	Full-matrix least-square on F^2
No. of reflections	7432
No. of parameters	430
No. of restrains	21
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Largest difference in peak and hole (e Å^{-3})	0.35, - 0.48
Absolute structure parameter	0.051(18) [Ref. S1]

Ref. S1 H. D. Flack, *ActaCryst.*, 1983, **A39**, 876-881.

Table S2 The experimental, theoretical energies and band assignments of *d-d* transition for **1**.

O_h	D_{4h}		
Ground state $^3A_{2g}$	Ground state $^3B_{1g}$	Refl. [a]	Calc. [b]
$^3T_{2g}$	^3E_g	10500	10440

	$^3B_{2g}$	11650	11700
^1E_g	$A_{1g} + B_{1g}$	13000	12908 + 12331
$^3T_{1g}(^3F)$	$^3A_{2g}$	16400	16242
	^3E_g	18400	17898
$^3T_{1g}(^3P)$	$^3A_{2g}$	27300	27644
	^3E_g	27700	27969

[a] Energies are taken from filtering the diffuse-reflectance spectrum. [b] Calculated values of energy were obtained for applying D_{4h} symmetry (Dq = 1170 cm^{-1}, Ds = 457 cm^{-1}, Dt = 130 cm^{-1}, B = 820 cm^{-1}.

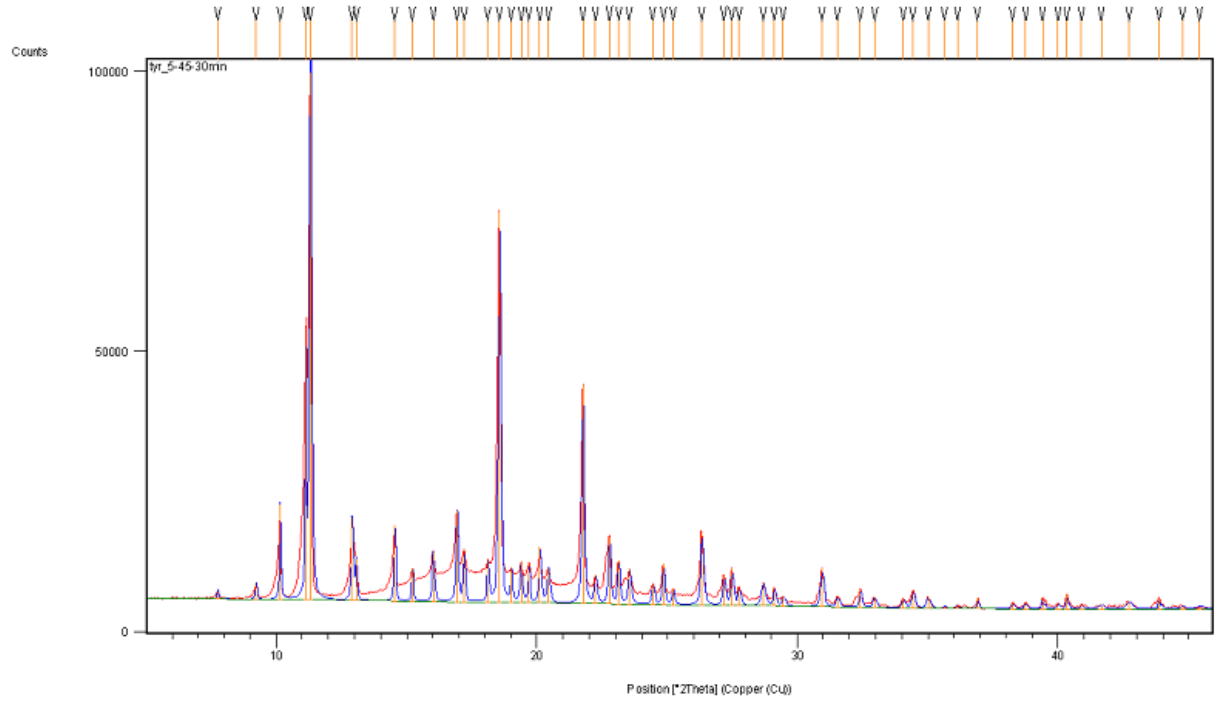


Fig. S1. XRD patterns for1.The bars at the bottom show positions and relative intensity of peaks calculated from the crystal structure model obtained from the single-crystal X-ray diffraction.

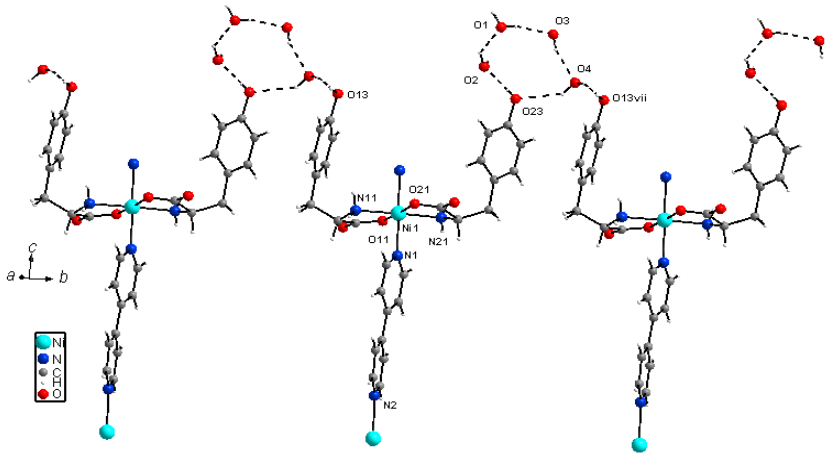


Fig. S2 The motives of five memebered rings are formed by O23—H23···O2, O2—H4*W*···O1, O1—H2*W*···O3, O3—H5*W*···O4 and O4—H8*W*···O23 hydrogen bonds as well as chain based on O4—H8*W*···O23 and O4—H7*W*···O13^{vi} bonds joining the parallel 1D polymer chains.

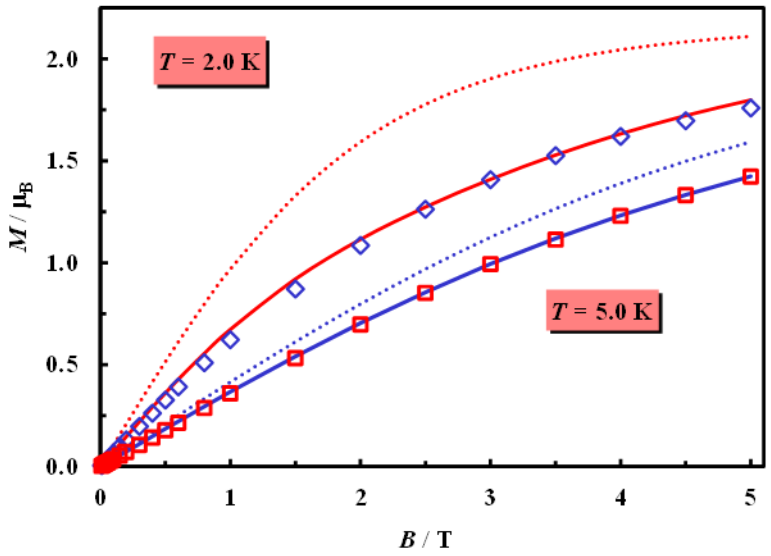


Fig. S3 Magnetization as a function of magnetic induction. The dotted lines are the Brillouin functions calculated for $S = 1$ and the average EPR $g = 2.1687$. The solid lines are calculated with the parameters obtained by least-squares fitting of the susceptibility.

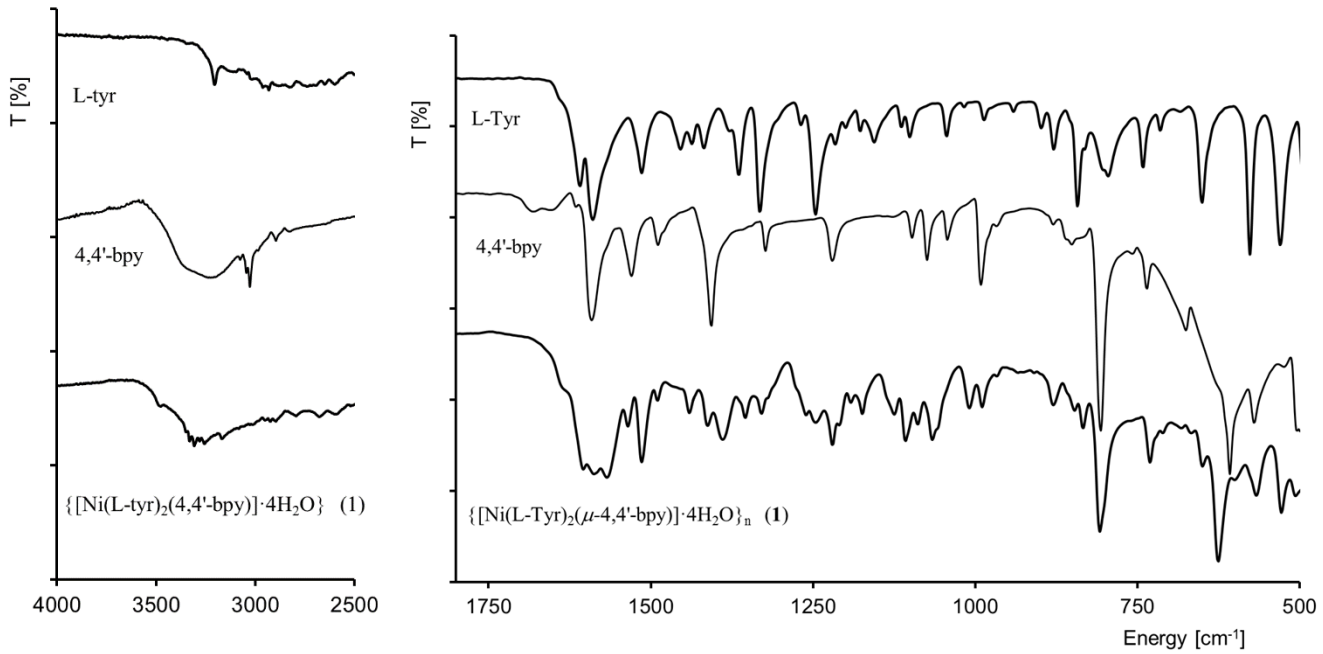


Fig. S4 FT-IR spectra of pure L-tyrosine, 4,4’-bipyridine and complex **1**.

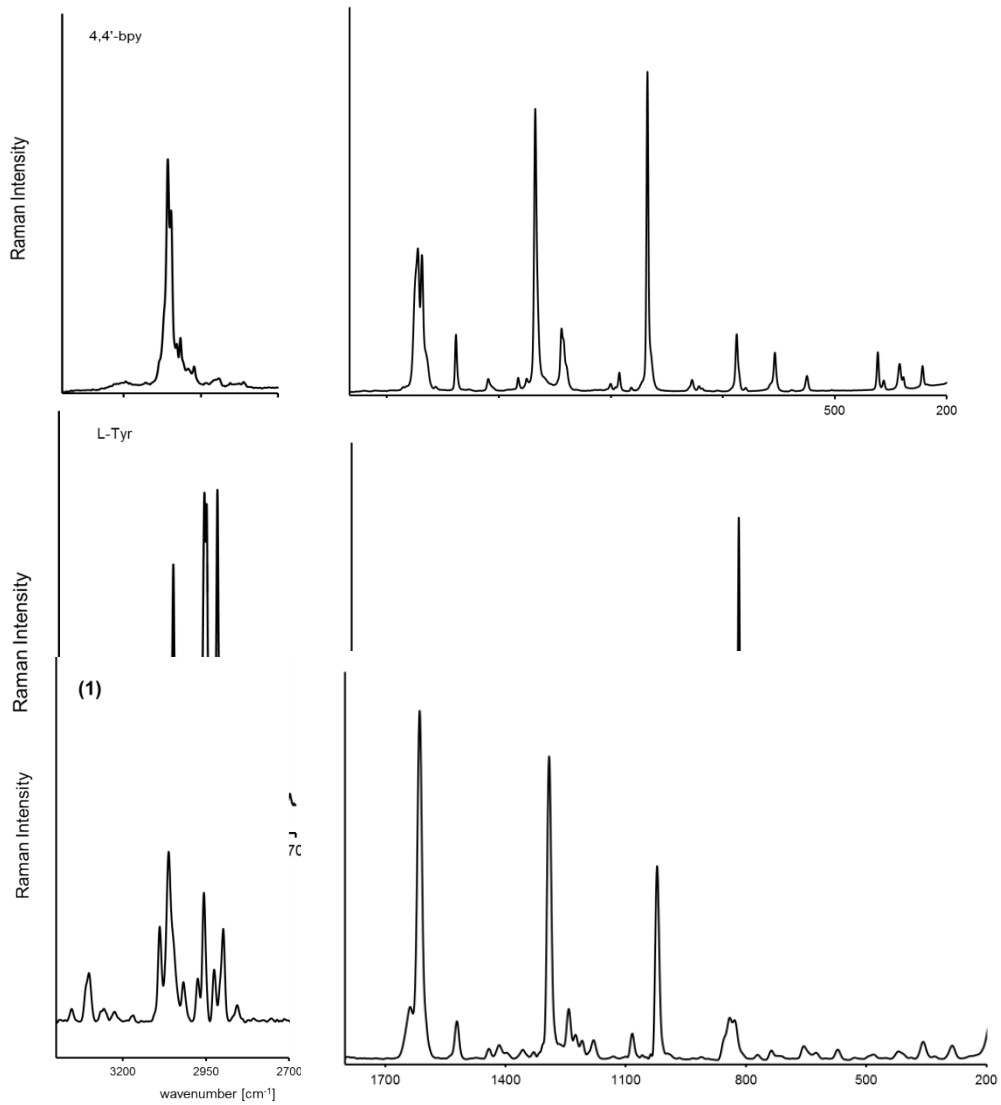
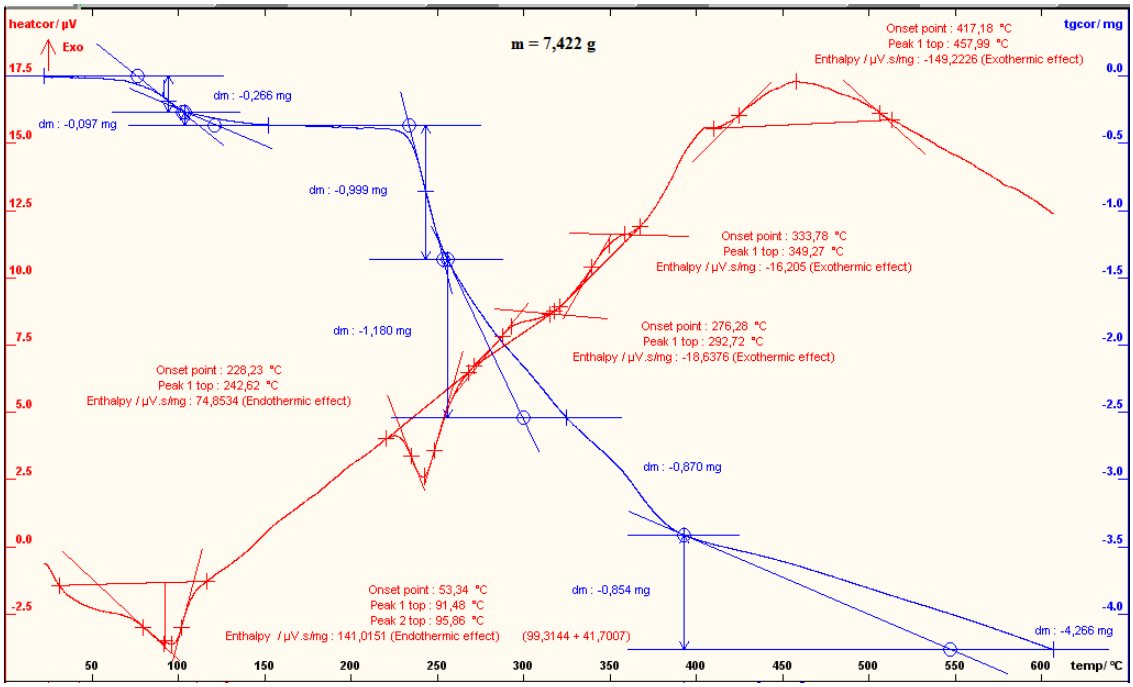


Fig. S5 The Raman of pure ligands (4,4’-bpy, L-Tyr) and complex **1**.

a)



b)

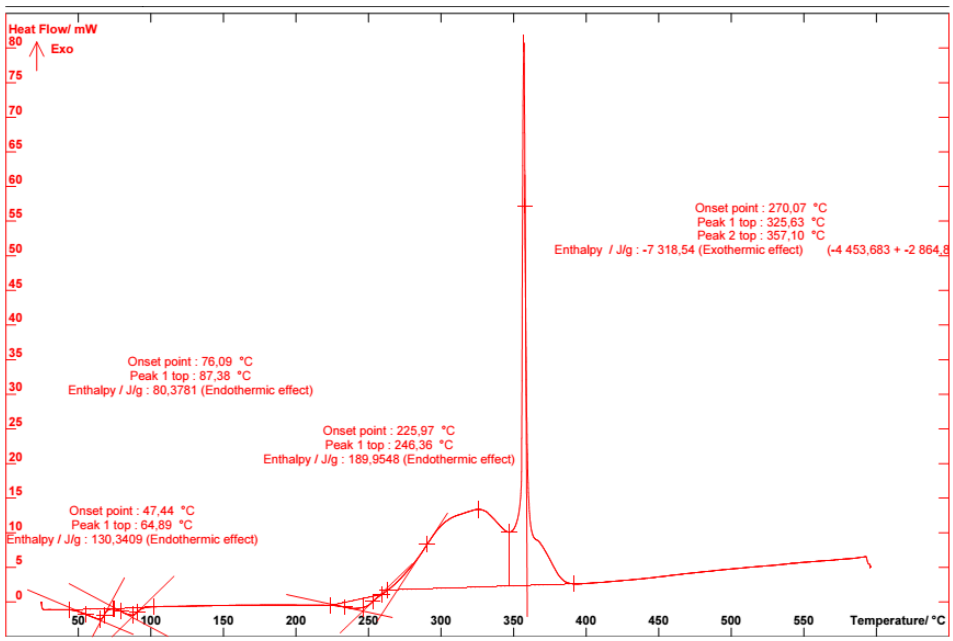


Fig. S6. a) TG-DTA and b) DSC.

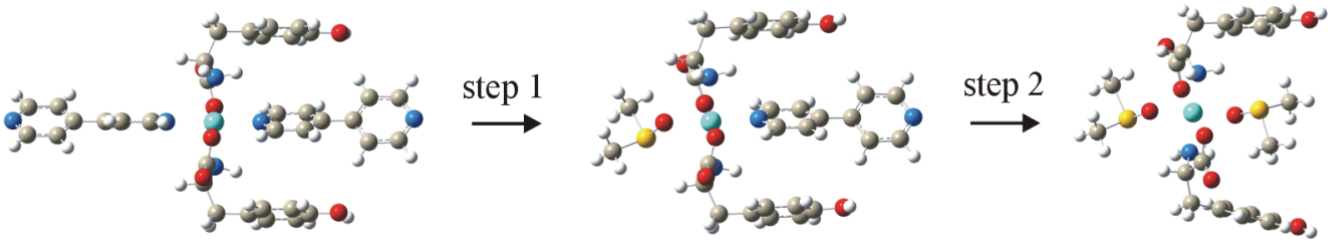


Fig. S7 Proposed simplified mechanism of the 4,4'-bipyridine replacement by the DMSO molecules in $[Ni(L\text{-}Tyr)_2(\mu\text{-}4,4'\text{-}bpy)_2]$.

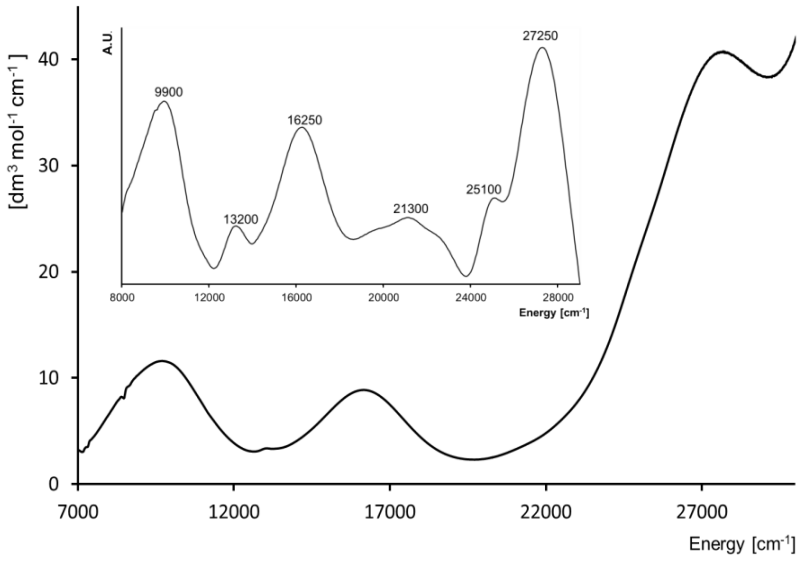


Fig. S8 The absorbance spectrum of complex **1** in DMSO and (inset) the effect of filter analysis (filter parameters : step = 50, α = 200 and N = 20).