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SUPPORTING INFORMATION

Structural, spectroscopic and magnetic properties of a novel copper(II) L-tyrosinato complex

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Table S1 Crystal data, Experimental details, and Structure Refinement Results for 1

chemical formula	$C_{18}H_{24}CuN_2O_8$
M_w	459.93
crystal system	Monoclinic
space group	$P2_1$
temperature (K)	295
a / Å	11.967(1)
b / Å	5.9986(4),
c / Å	14.936(1)
β / °	102.578(8)
V / Å^3	1046.4(2)
Z	2
Radiation type	Mo *K*α
μ / mm^{-1}	1.09
crystal size / mm	0.20 × 0.16 × 0.11
Absorption correction	Multi-scan *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.33.42. Empirical absorption correction using spherical harmonics
T_{min}, T_{max}	0.801, 0.883
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11692, 3688, 2641
R_{int}	0.052
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.610
$R[F^2 > 2\sigma(F^2)]$	0.051
$wR(F^2)$	0.134

S	0.93
no. of reflections	3688
no. of parameters	273
no. of restraints	8
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e Å^{-3}	0.68, -0.26
absolute structure	[1]
flack parameter [53]	-0.02(2)

[1] H. D. Flack, Acta Crystallogr., Sect. A: Found. Crystallogr.1983, 39, 876.

Table S2 Selected Bond (Å) Distances and Angles (deg) in complex 1

O1—C2	1.258 (7)	O3—H31	0.98 (2)
O2—C2	1.272 (7)	O4—C10	1.271 (7)
N1—C1	1.471 (8)	O5—C10	1.221 (8)
C1—C2	1.523 (8)	N2—C11	1.471 (7)
C1—C3	1.543 (8)	C10—C11	1.543 (8)
C1—H1	0.98 (2)	C11—C12	1.536 (9)
C3—C4	1.510 (8)	C12—C13	1.503 (9)
C4—C9	1.386 (11)	C13—C14	1.343 (10)
C4—C5	1.384 (8)	C13—C18	1.393 (10)
C5—C6	1.402 (9)	C14—C15	1.429 (10)
C6—C7	1.372 (10)	C15—C16	1.372 (10)

C7—O3	1.363 (8)	C16—C17	1.365 (12)
C7—C8	1.376 (9)	C16—O6	1.367 (8)
C8—C9	1.402 (10)	C17—C18	1.388 (8)
		O6—H61	0.90 (2)

N1—C1—C2	107.0 (5)	C4—C9—C8	121.2 (6)
N1—C1—C3	111.7 (4)	C7—O3—H31	113 (2)
O1—C2—O2	123.9 (5)	O5—C10—O4	123.4 (6)
O1—C2—C1	118.9 (5)	O5—C10—C11	119.9 (5)
O2—C2—C1	117.1 (6)	O4—C10—C11	116.6 (5)
C4—C3—C1	114.2 (5)	N2—C11—C12	114.2 (5)
C9—C4—C5	117.8 (5)	N2—C11—C10	108.9 (5)
C9—C4—C3	121.4 (5)	C12—C11—C10	112.2 (5)
C5—C4—C3	120.8 (5)	C12—C11—HC11	116 (5)
C4—C5—C6	121.5 (6)	C10—C11—HC11	105 (7)
C7—C6—C5	119.5 (6)	C14—C13—C18	117.0 (7)
O3—C7—C6	122.1 (6)	C14—C13—C12	122.8 (6)
O3—C7—C8	117.5 (6)	C18—C13—C12	120.3 (6)
C6—C7—C8	120.4 (6)	C13—C14—C15	123.4 (7)
C7—C8—C9	119.6 (7)	C16—C15—C14	117.1 (7)
		C17—C16—C15	121.1 (7)
		C17—C16—O6	122.2 (7)
		C15—C16—O6	116.7 (7)
		C16—C17—C18	119.7 (8)
		C17—C18—C13	121.6 (8)

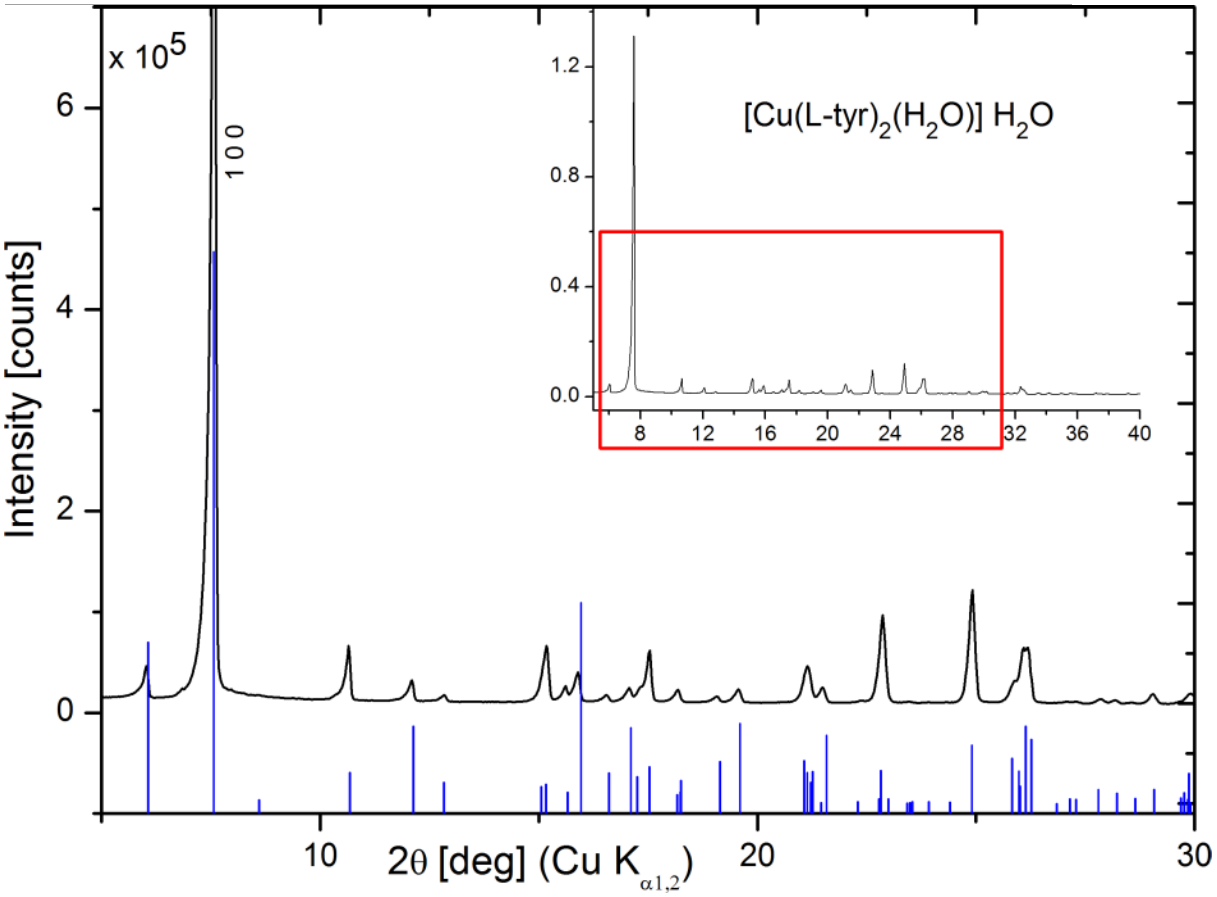

Fig. S1. XRD pattern for complex 1.

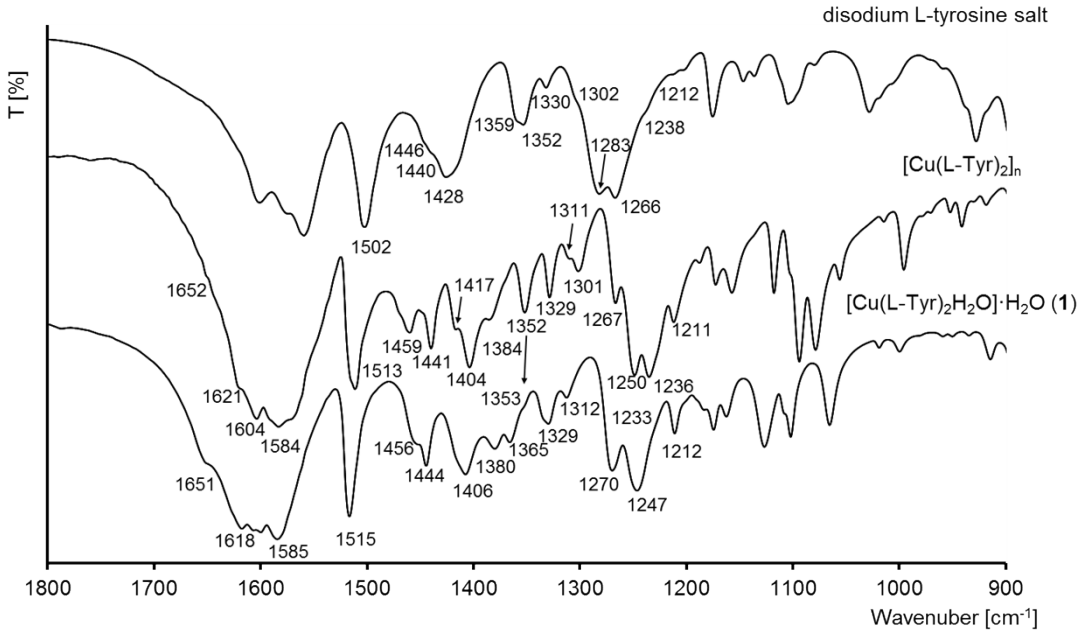

Fig. S2 Vibrational FT-IR spectra of disodium L-tyrosine salt, $[Cu(L\text{-}Tyr)_2]_n$ and complex **1**

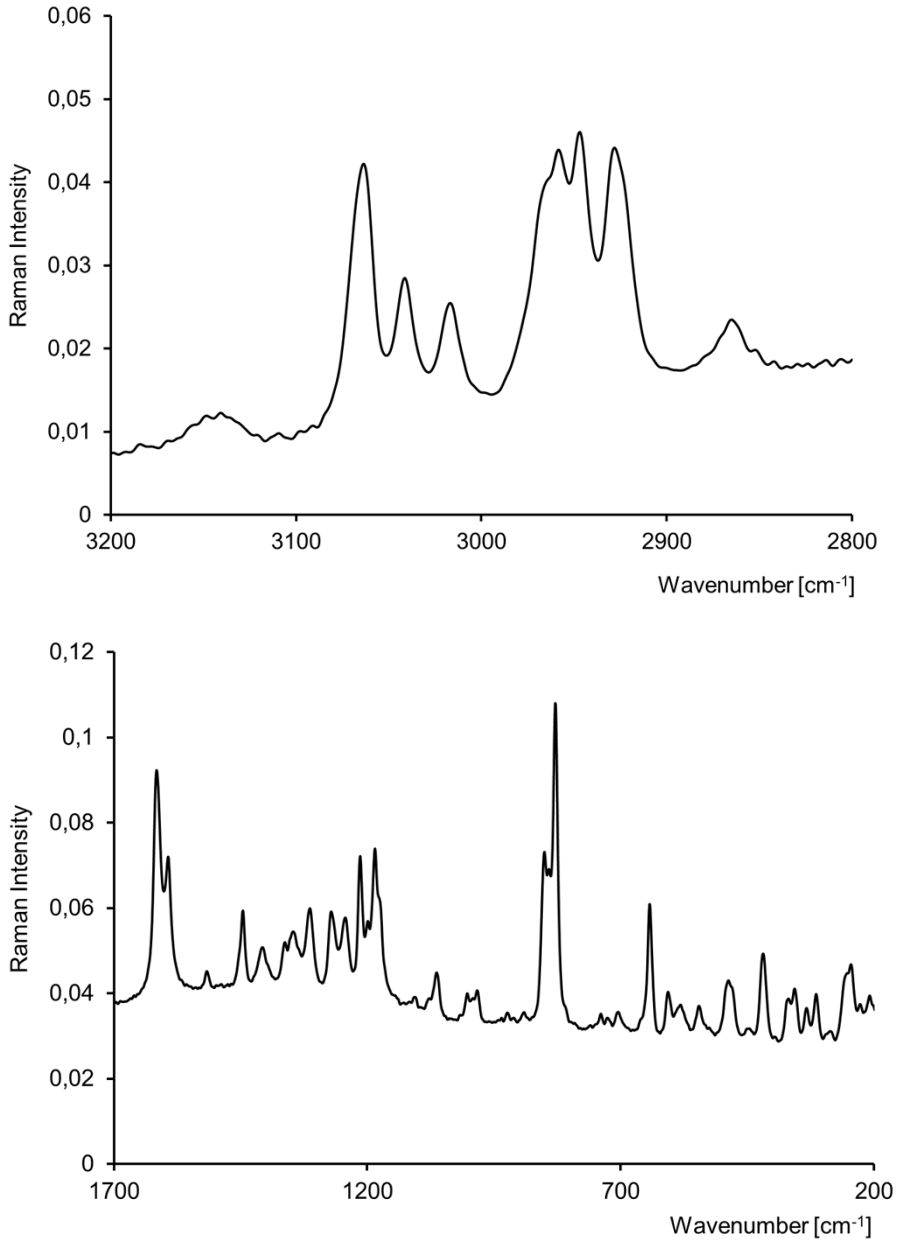

Fig. S3 Raman spectra of complex **1**

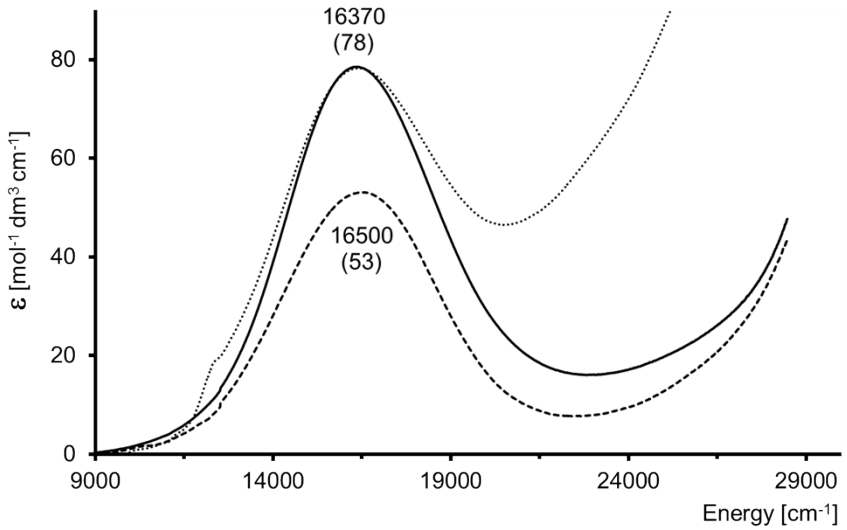

Fig. S4. Absorbance spectrum of **1** in : solid line – DMSO; broken line – MeOH, dotted line – in DMSO after 5 months.

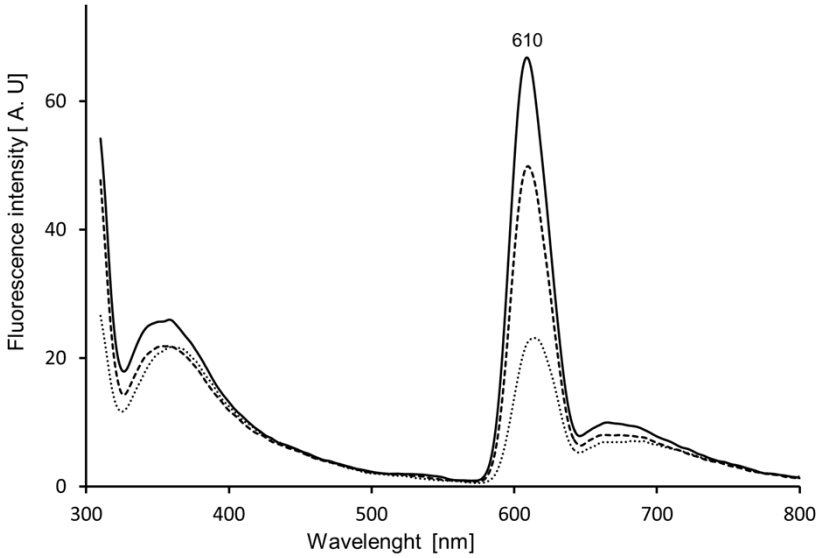

Fig. S5. Fluorescence emission spectra of **1** in DMSO (solid line – 0,125 mg/ml, broken line – 0,25 mg/mol, dotted line – 0,5 mg/ml) at λ_{ex} = 303 nm.