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SUPPLEMENTARY MATERIAL TO

Spectral, thermal, optical and biological studies on (*E*)-4-[(2-hydroxyphenyl)imino]pentan-2-one and its complexes

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PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR THE LIGAND AND ITS METAL COMPLEXES

*(*E*)-4-[(2-Hydroxyphenyl)imino]pentan-2-one (H_2L)*. M.p.: 175–177 °C; Anal. Calcd. for $C_{11}H_{13}NO_2$ (FW: 191.23): C, 69.08; H, 6.79; N, 7.32 %. Found: C, 69.1; H, 6.8; N, 7.3 %; FTIR (KBr, cm^{-1}): 3435 (O–H), 3380 (O–H), 1598 (C=N) 1546 (C=CH), 1315 (C–O), 1238 (C–N), 1033 (δ(OH)); ^{1}H-NMR (400 MHz, DMSO-d_6) δ / ppm): 2.3 (3H, *s*, CH_3–C=N), 2.5 (3H, *s*, CH_3–C=C), 6.7––7.1 (4H, *m*, Ar-H), 5.2 (1H, *s*, HC=C), 9.93 (1H, *s*, Ar-OH); 12.15 (1H, *s*, **H**O–CH=C).

[Cu(HL)(AcO)]·3/2H_2O. M.p.: >300 °C; Anal. Calcd. for $C_{13}H_{18}CuNO_{5.5}$ ((FW: 339.54): C, 45.9; H, 5.3; N, 4.1 %). Found: C, 46.0; H, 4.7; N, 5.0 %; FTIR (KBr, cm^{-1}): 3469 (O–H), 1615 (C=N), 1601 (C=CH), 1281 (C–O), 1250 (C–N), 1032 (δ(OH)), 538 (Cu–O), 420 (Cu–N).

[Ni(HL)(AcO)]·H_2O·1/2EtOH. M.p.: >300 °C; Anal. Calcd. for $C_{14}H_{20}NNiO_{5.5}$ ((FW: 348.69): C, 48.2; H: 5.70; N, 4.0 %). Found: C, 48.30; H, 4.70; N, 4.80 %; FTIR (KBr, cm^{-1}): 3444 (O–H), 1611 (C=N), 1563 (C=CH), 1275 (C–O), 1220 (C–N), 1035 (δ(OH)), 532 (Ni–O), 426 (Ni–N).

[Co(HL)(OAc·H_2O)]·0.5EtOH. M.p.: >300 °C; Anal. Calcd. for $C_{14}H_{20}NNiO_{5.5}$ ((FW: 348.93): C, 48.1; H: 5.7; N, 4.0 %). Found: C, 47.8; H, 5.3; N, 4.5 %; FTIR (KBr, cm^{-1}): 3440 (O–H), 1610 (C=N), 1566 (C=CH), 1276 (C–O), 1221 (C–N), 1050 (δ(OH)), 530 (Co–O), 434 (Co–N).

[Zn(L)(H_2O)]. M.p.: >300 °C; Anal. Calcd. for $C_{11}H_{13}NO_3Zn$ (FW: 272.61): C, 48.46; H, 4.77; N, 5.13 %. Found: C, 48.30; H, 4.70; N, 5.19 %; ^{1}H-NMR

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(400 MHz, DMSO-d_6, δ / ppm): 2.2 (3H, *s*, CH_3–C=N), 2.4 (3H, *s*, CH_3–C=C), 7.0–7.5 (4H, *m*, Ar-H), 7.6 (1H, *s*, HC=C).

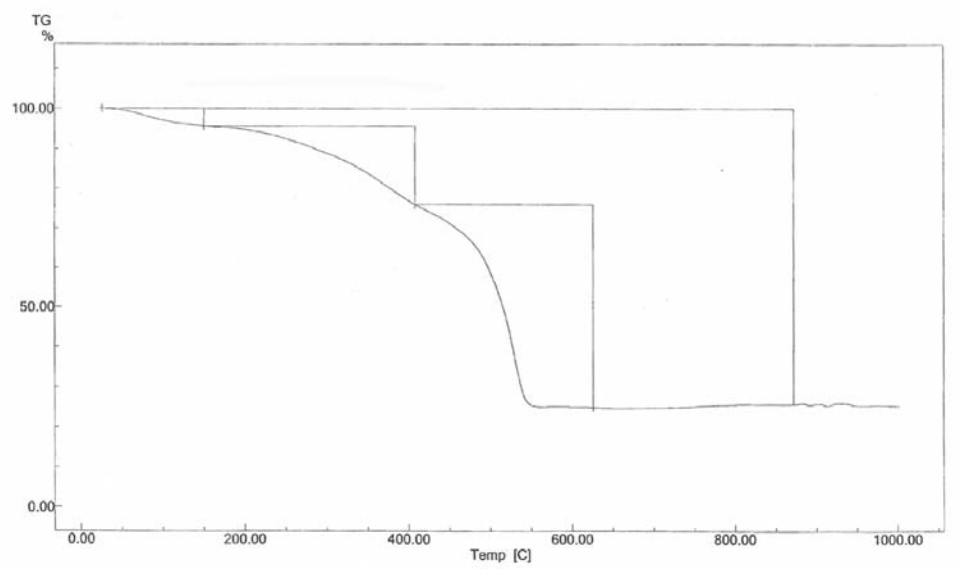


Fig. S-1. TG curve for the Zn complex.

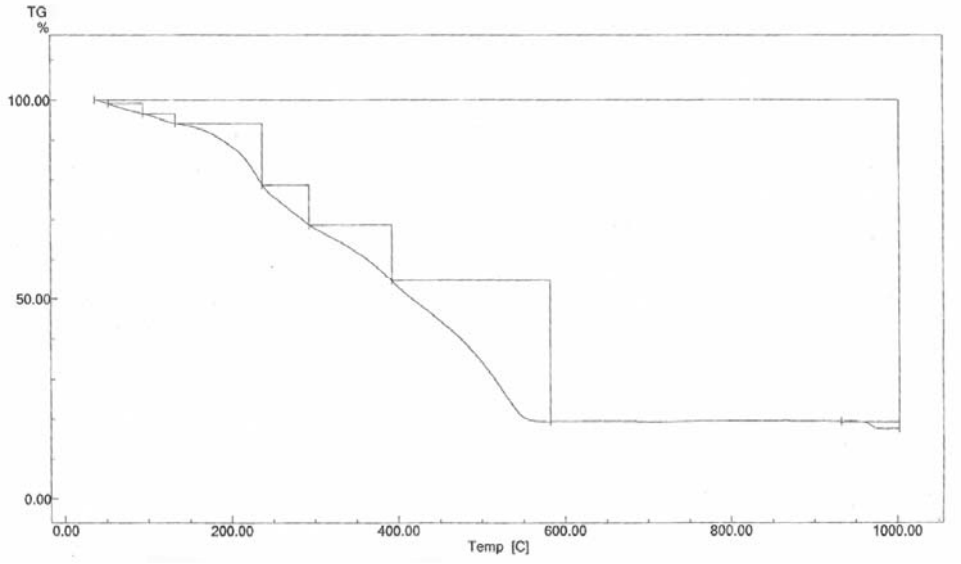


Fig. S-2. TG curve for the Cu complex.

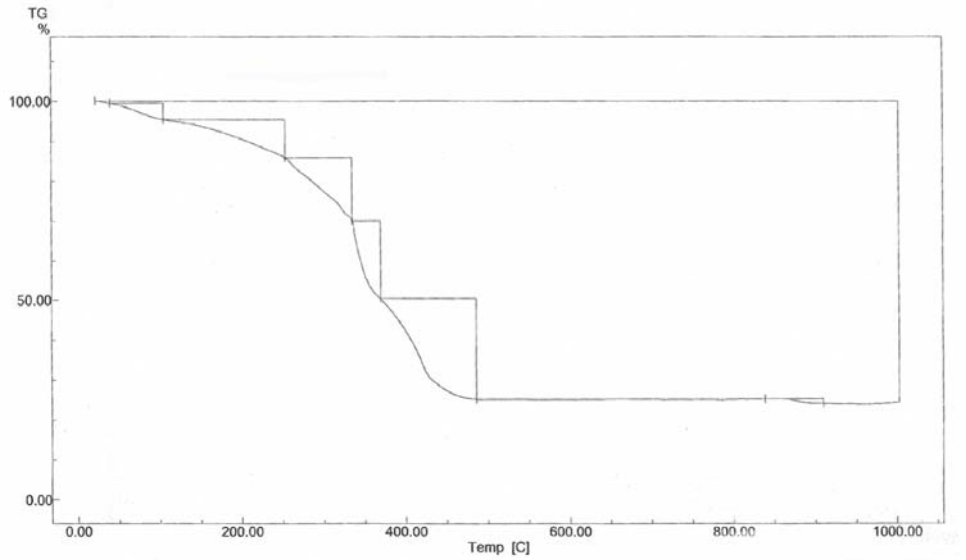


Fig. S-3. TG curve for the Ni complex.

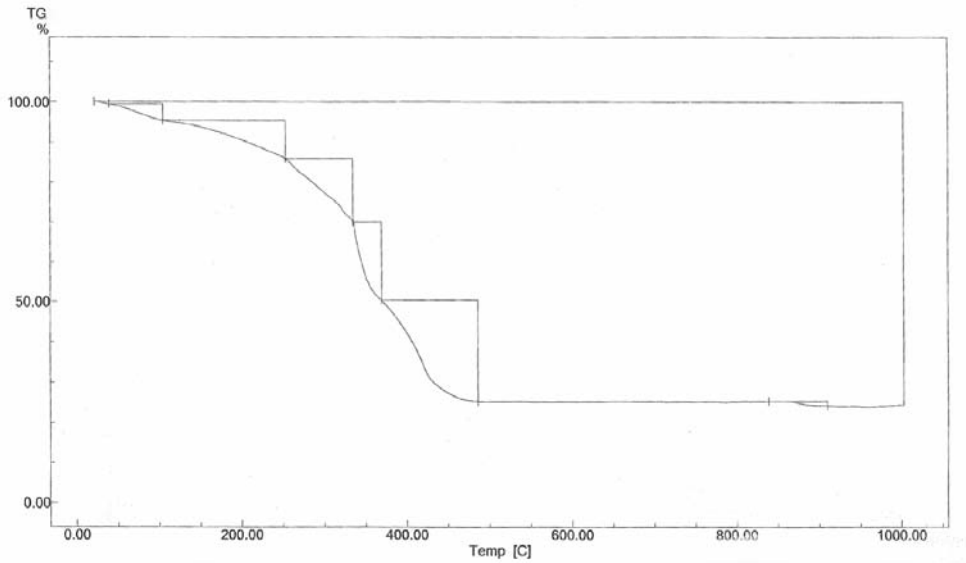
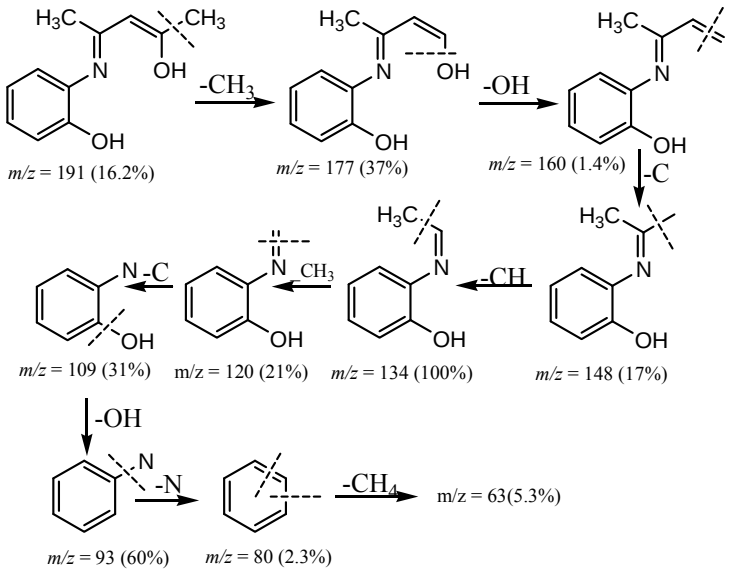
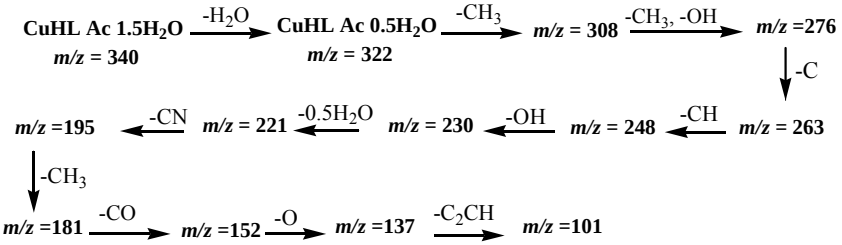


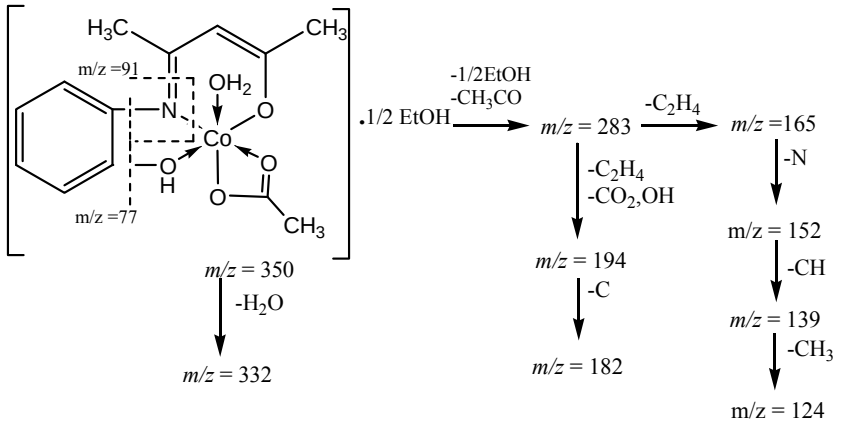
Fig. S-4. TG curve for the Co complex.



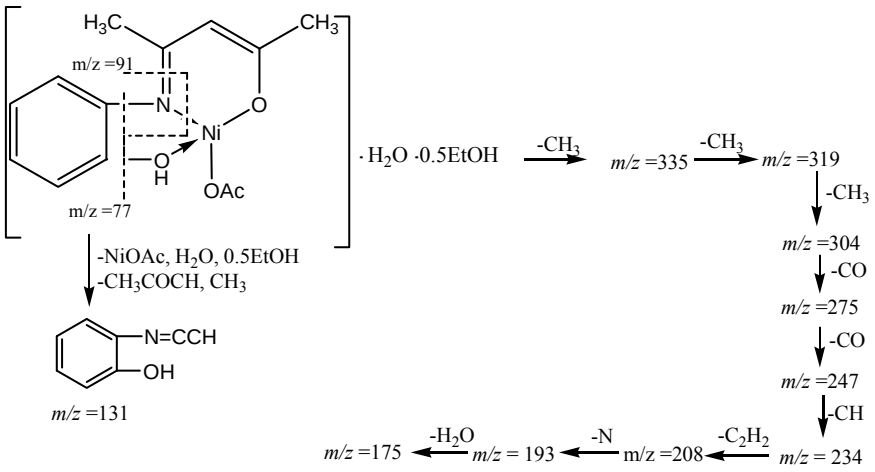
Scheme S-1. Fragmentation pattern of the ligand (H_2L).



Scheme S-2. Fragmentation pattern of the Cu(II) complex.



Scheme S-3. Fragmentation pattern of the Co(II) complex.



Scheme S-4. Fragmentation pattern of the Ni(II) complex.

TABLE S-I. Thermogravimetric results (TG) for the Co(II), Ni(II), Cu(II) and Zn(II) complexes.

Precursor	*T* range °C	Mass loss Estim. (Calcd.), %	Assignment of fragment lost
[Co(HL)OAc·H_2O]·0.5EtOH	22–104	4.7 (6.5)	1/2EtOH
	104–235	9.5 (9.4)	
	235–335	15.8 (16.8)	
	335–369	19.8 (19.4)	
	369–486	25.0 (25.7)	
	486–800	45.0 (47.4)	Residue Co_2O_3
[Ni(HL)OAc]·H_2O·0.5EtOH	54–150	10.5 (11.7)	2H_2O + 1/2EtOH
	150–276	11.3 (12.2)	
	276–534	53.4 (54.3)	
	534–800	19.8 (21.1)	Residue NiO
[Cu(HL)OAc]·3/2H_2O	26–133	5.9 (7.9)	1.5 H_2O
	133–237	15.5 (12.6)	
	237–293	12.0 (11.7)	
	293–392	12.0 (12.0)	
	392–582	35.1 (32.0)	Residue CuO
[[Zn(L)H_2O]	56–200	5.6 (6.5)	H_2O coordinated
	200–407	18.3 (20.5)	
	407–625	51.1 (48.7)	
	625–800	28.0 (29.6)	Residue ZnO

TABLE S-II. Magnetic moments, electronic bands and ligand field parameters of the Cu(II), Co(II) and Ni(II) complexes

Compound	Bands position, cm^{-1}	B	β	$10Dq$	μ_{eff} μ_B
$[Cu(HL)OAc]\cdot 1.5H_2O$	25773, 14005	–	–	–	2.1
$[Co(HL)OAc\cdot H_2O]\cdot 0.5EtOH$	19379, 15948	878	0.90	8340	5.2
$[Ni(HL)OAc]\ H_2O\cdot 0.5EtOH$	25000, 23201, 17605	–	–	–	3.9

TABLE S-III. The experimental and calculated, optimized using the PM3 method, electronic spectra of the complexes

Complex	Experimental, nm	Calculated, nm
$[Cu(HL)OAc]\cdot 1.5H_2O$	388	363
	–	383
	–	512
	714	754
$[Co(HL)OAc\cdot H_2O]\cdot 0.5EtOH$	450	479
	516	555
	627	574
		868
$[Ni(HL)OAc]\cdot H_2O\cdot 0.5EtOH$	400	360
	431	444
	568	579
	–	613
	–	651
	–	948

TABLE S-IV. Selected bond lengths (Å) and angles (°) for the optimized ligand and its metal complexes

Bond	Ligand	Complex with:			
		Co(II)	Ni(II)	Cu(II)	Zn(II)
C=C ring	1.344	1.400	1.394	1.417	1.395
C=N	1.344	1.273	1.266	1.265	1.268
C=C enolic	1.343	1.341	1.350	1.350	1.352
C–O phenolic	1.352	1.359	1.378	1.378	1.373
C–O enolic	1.357	1.354	1.364	1.363	1.365
M–O phenolic	–	1.838	1.799	1.818	1.855
M–O enolic	–	1.787	1.755	1.775	1.853
M–N	–	1.865	1.801	1.818	1.905
N–M–O phenolic	–	86.21	101.66	92.22	87.77
N–M–O enolic	–	93.67	102.59	102.40	99.4
O–M–O	–	126.4	122.1	122.3	124.7
CCNC	–0.0001	–	–	–	–