

Discrete and polymeric Cu(II) complexes featuring substituted indazole ligands: Their synthesis and structural chemistry

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Supporting Information

Table S1: Hydrogen bonding parameters for Compounds **H₂L4**, **1**, **3** and **4****H₂L4**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O12 ¹	0.885(15)	1.947(16)	2.8154(19)	166(2)
O11	H11	O25	0.865(17)	1.811(17)	2.6688(18)	171(3)
N13	H13	O24 ²	0.899(16)	1.955(17)	2.825(2)	162(2)
O23	H23	O25 ³	0.863(17)	1.813(17)	2.6755(19)	177(3)
O25	H25A	N14 ⁴	0.867(17)	1.986(17)	2.8409(19)	168(2)
O25	H25B	N2 ¹	0.865(17)	1.959(17)	2.8073(19)	166(2)

1: '-X,-Y,1-Z'; 2: '1-X,1-Y,-Z'; 3: '-1-X,-Y,1-Z'; 4: '1+X,+Y,+Z'

Complex 1

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O44	H44A	O32 ¹	0.85	2.24	3.001(8)	149.7
O44	H44B	N41	0.85	2.12	2.913(11)	154.9
O44	H44B	O39	0.85	2.22	2.829(10)	128.4
O45	H45B	O43 ²	0.85	2.10	2.912(18)	158.7
O46	H46B	O40	0.85	2.18	2.99(2)	158.8
O46	H46B	N37	0.85	2.20	2.929(17)	143.5
O46	H46B	O36	0.85	1.51	2.353(15)	169.3

1: '-1+X,+Y,+Z'

Complex 3

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N16	H16	O30 ¹	0.88	2.39	2.940(4)	120.5
N16	H16	O35 ¹	0.88	1.90	2.751(9)	163.7
N16	H16	O36 ¹	0.88	2.24	3.033(7)	150.4
O27	H27	O35 ²	0.84(2)	1.96(3)	2.717(8)	148(5)
O27	H27	O36 ²	0.84(2)	1.94(2)	2.762(7)	166(5)
O36	H36A	O32	0.85	2.07	2.762(8)	137.8
O37	H37A	O30	0.85	2.54	3.082(7)	122.5
O37	H37A	N31	0.85	1.61	2.367(10)	145.9

1: '1+X,+Y,+Z'; 2: '1+X,1+Y,+Z'

Complex 4

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/ $^{\circ}$
O15	H15	O13	0.86(2)	2.13(4)	2.975(8)	166(14)
N3	H3	O14 ¹	0.868(19)	1.99(2)	2.817(3)	160(4)
O14	H14	O13 ²	0.841(19)	2.01(2)	2.834(3)	169(4)

1: '+X,-1+Y,+Z'; 2: '1-X,1-Y,1-Z'

Figure S1: Thermogravimetric Analysis plot for Complex 1

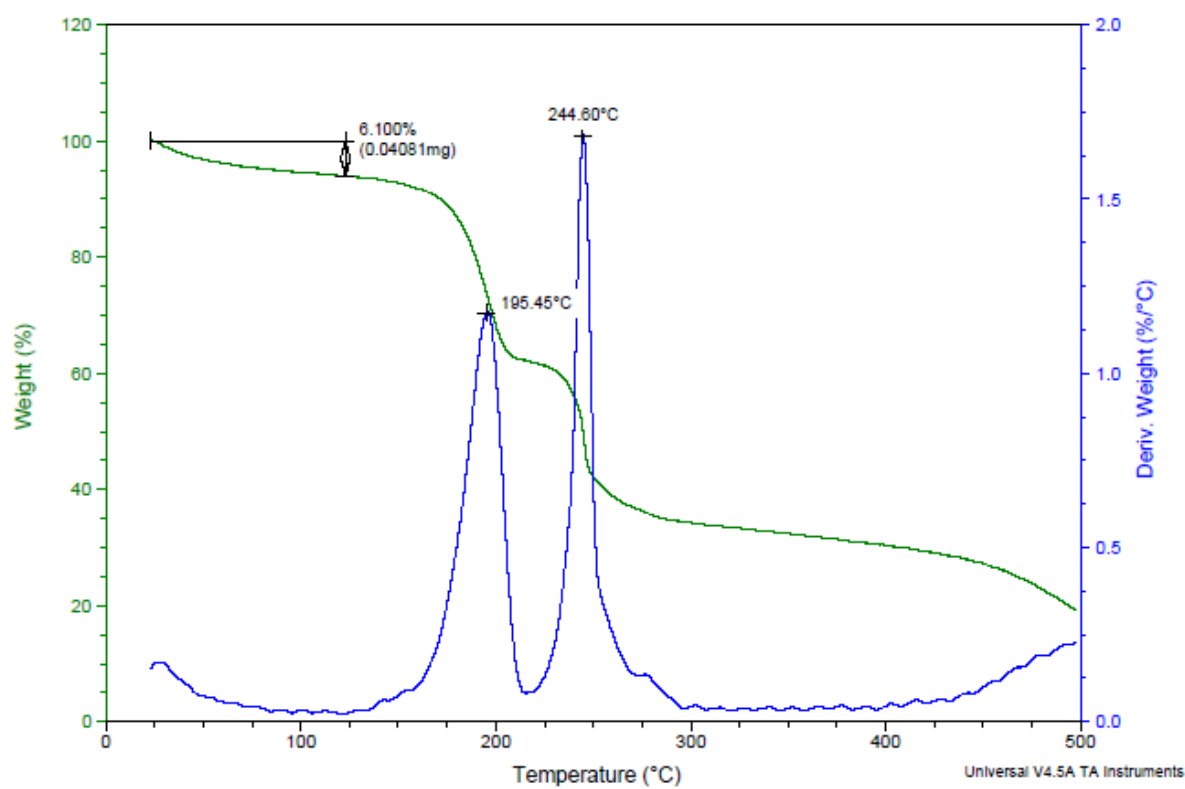


Figure S2: Thermogravimetric Analysis plot for Complex 2

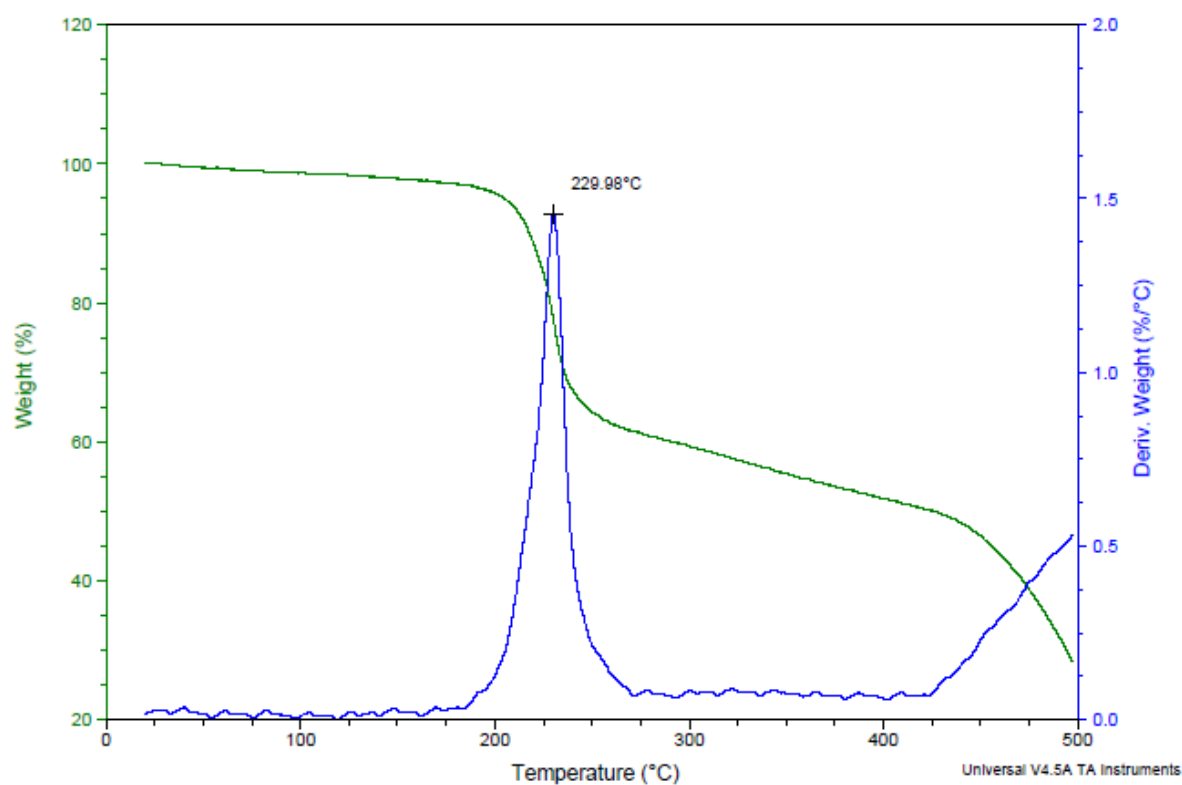


Figure S3: Thermogravimetric Analysis plot for Complex 3

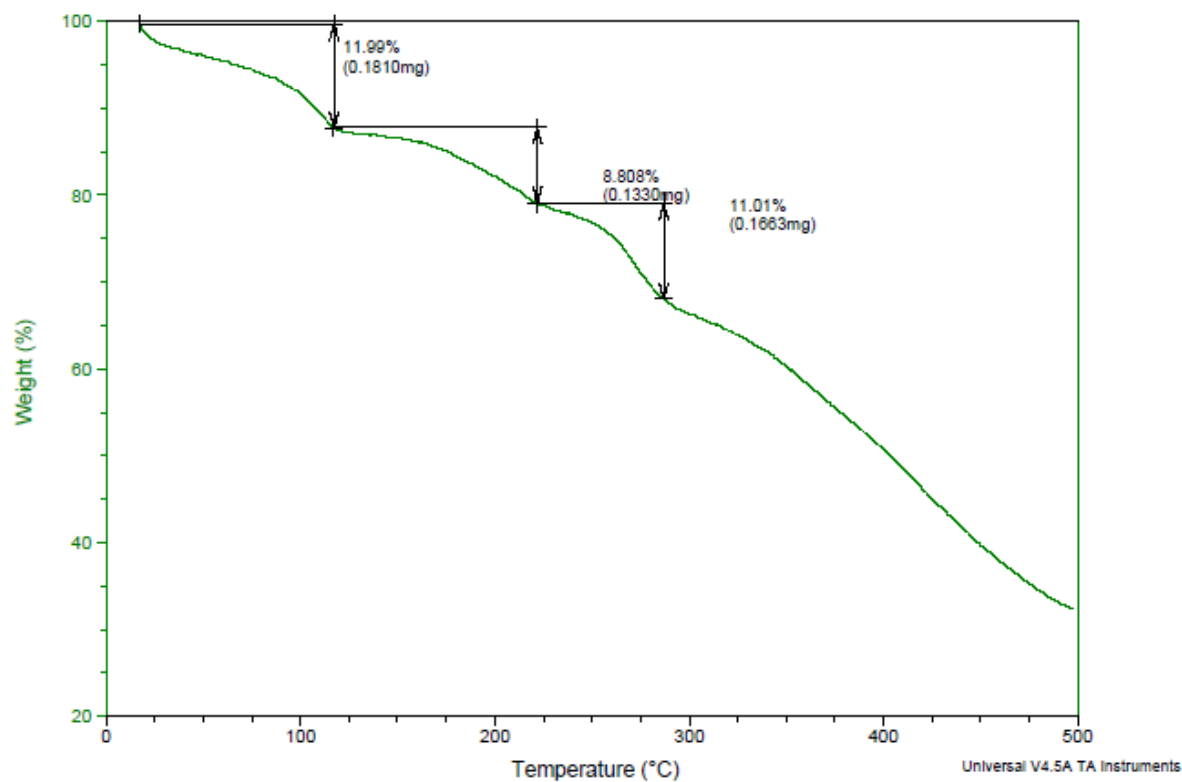


Figure S4: Thermogravimetric Analysis plot for Complex 4

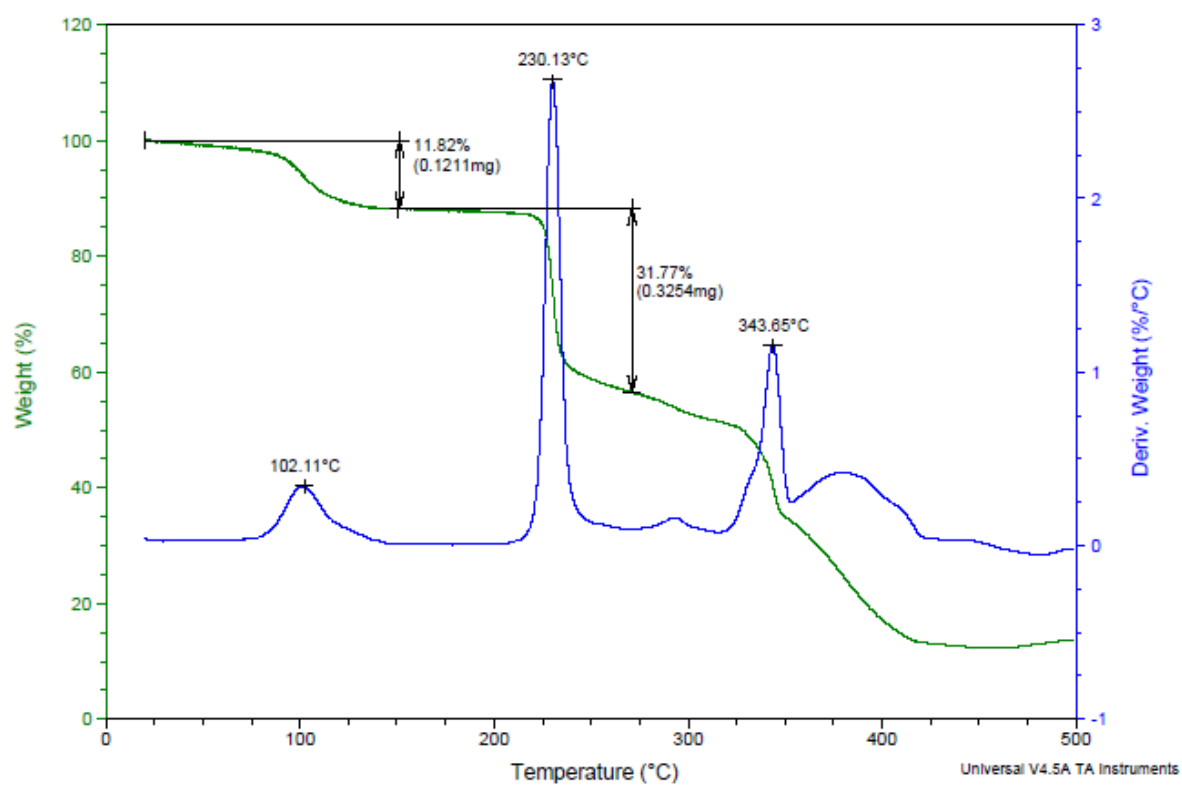


Figure S5: UV/Visible spectra of Ligands L1 and L2 (0.26mmol/L, acetonitrile)

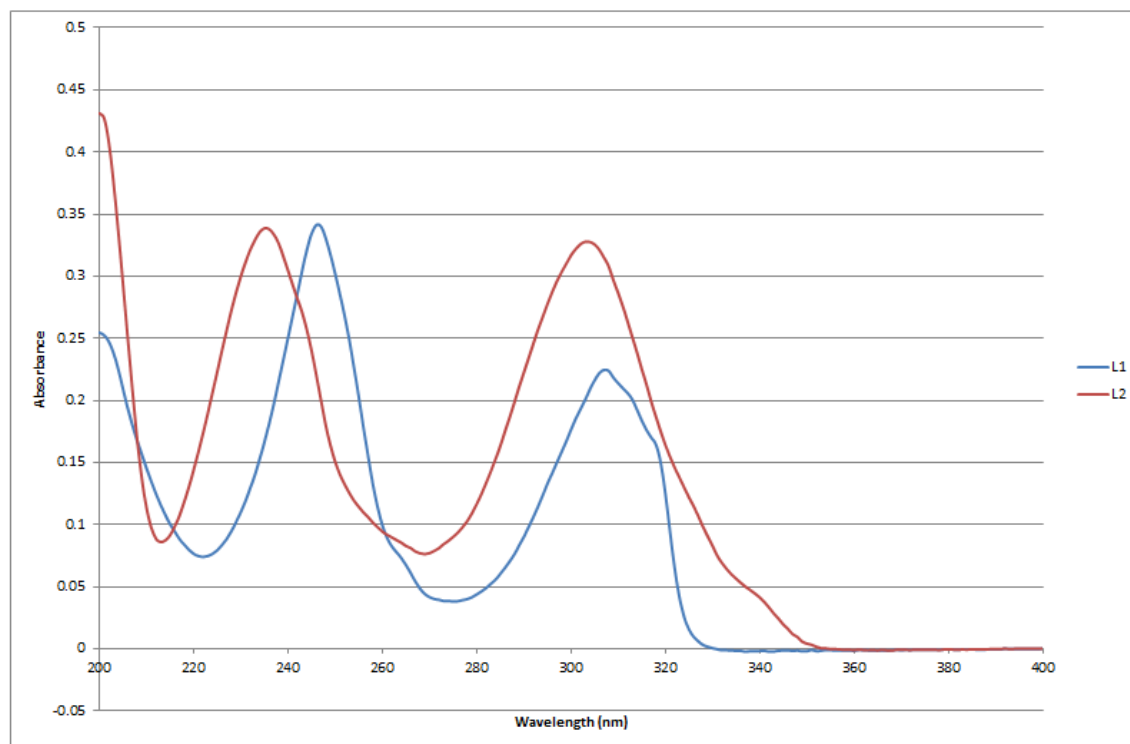


Figure S6: UV/Visible Spectra of Complexes **1** and **2** (1.0mmol/L, nitromethane)

