

Electronic Supplementary Information (ESI)

Self-Assembly of a 15-Nickel Metallamacrocyclic Complex Derived from *L*-
Glutamic Acid Schiff Base Ligand

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Table S1. Selected bond lengths [Å] and bond angles [°] for **1a**.

Ni1-O3	2.035(3)	Ni6-O21	2.047(4)
Ni1-N1	2.012(5)	Ni6-O7W	2.094(3)
Ni1-O1	2.043(3)	Ni6-O8W	2.106(4)
Ni1-O17	2.035(4)	Ni7-N5	2.000(5)
Ni1-O1W	2.095(3)	Ni7-O25	2.030(3)
Ni1-O2W	2.107(3)	Ni7-O41	2.046(4)
Ni2-O1	2.001(3)	Ni7-O27	2.048(3)
Ni2-O59	2.009(4)	Ni7-O10W	2.098(3)
Ni2-O18	2.016(3)	Ni7-O9W	2.085(3)
Ni2-O7	2.018(3)	Ni8-O31	2.003(4)
Ni2-O8	2.095(4)	Ni8-O25	1.993(4)
Ni2-O2	2.089(3)	Ni8-O23	2.017(3)
Ni3-N2	1.970(5)	Ni8-O42	2.007(3)
Ni3-O7	2.036(3)	Ni8-O26	2.099(4)
Ni3-O60	2.066(4)	Ni8-O32	2.099(3)
Ni3-O9	2.073(3)	Ni9-N6	1.980(5)
Ni3-O3W	2.098(3)	Ni9-O24	2.027(4)
Ni3-O4W	2.102(3)	Ni9-O31	2.030(3)
Ni4-O13	2.007(4)	Ni9-O33	2.065(4)
Ni4-N3	1.994(5)	Ni9-O11W	2.072(3)
Ni4-O15	2.015(4)	Ni9-O12W	2.100(3)
Ni4-O29	2.048(4)	Ni10-N7	2.001(5)
Ni4-O6W	2.123(5)	Ni10-O37	1.995(4)
Ni4-O5W	2.107(4)	Ni10-O53	2.059(4)
Ni5-O11	2.005(4)	Ni10-O39	2.036(4)
Ni5-O19	2.016(4)	Ni10-O14W	2.090(4)
Ni5-O30	2.014(4)	Ni10-O13W	2.125(4)
Ni5-O13	2.029(3)	Ni11-O35	2.001(4)
Ni5-O14	2.094(4)	Ni11-O43	2.010(4)
Ni5-O20	2.072(4)	Ni11-O37	2.022(4)
Ni6-N4	2.012(4)	Ni11-O54	2.013(4)
Ni6-O12	2.024(3)	Ni11-O44	2.069(4)
Ni6-O19	2.039(4)	Ni11-O38	2.134(4)

Ni12-N8	1.948(7)	Ni14-O49	2.012(4)
Ni12-O43	2.012(5)	Ni14-O5	2.004(4)
Ni12-O45	2.051(6)	Ni14-O47	2.020(4)
Ni12-O16W	2.093(5)	Ni14-O55	2.044(4)
Ni12-O15W	2.100(4)	Ni14-O50	2.103(5)
Ni12-O36	2.086(6)	Ni14-O56	2.113(4)
Ni13-O49	2.002(5)	Ni15-N10	2.012(5)
Ni13-N9	2.001(6)	Ni15-O55	2.020(4)
Ni13-O6	2.032(4)	Ni15-O57	2.045(4)
Ni13-O51	2.042(5)	Ni15-O48	2.066(5)
Ni13-O17W	2.101(4)	Ni15-O19W	2.114(4)
Ni13-O18W	2.102(4)	Ni15-O20W	2.103(5)

O3-Ni1-N1	81.56(16)	O1-Ni2-O8	94.65(14)
O3-Ni1-O1	172.90(16)	O59-Ni2-O8	178.33(14)
N1-Ni1-O1	91.47(15)	O18-Ni2-O8	89.60(15)
O3-Ni1-O17	88.89(14)	O7-Ni2-O8	77.84(15)
N1-Ni1-O17	169.35(14)	O1-Ni2-O2	77.93(13)
O1-Ni1-O17	98.17(14)	O59-Ni2-O2	90.46(15)
O3-Ni1-O1W	93.55(14)	O18-Ni2-O2	177.34(13)
N1-Ni1-O1W	94.44(15)	O7-Ni2-O2	95.87(13)
O1-Ni1-O1W	85.62(12)	O8-Ni2-O2	89.27(15)
O17-Ni1-O1W	90.82(14)	N2-Ni3-O7	91.51(16)
O3-Ni1-O2W	90.53(14)	N2-Ni3-O60	168.79(15)
N1-Ni1-O2W	89.37(16)	O7-Ni3-O60	99.29(14)
O1-Ni1-O2W	90.73(13)	N2-Ni3-O9	81.42(17)
O17-Ni1-O2W	86.00(15)	O7-Ni3-O9	172.90(16)
O1W-Ni1-O2W	174.78(14)	O60-Ni3-O9	87.81(15)
O1-Ni2-O59	86.91(14)	N2-Ni3-O3W	92.04(15)
O1-Ni2-O18	99.77(13)	O7-Ni3-O3W	85.05(13)
O59-Ni2-O18	90.74(14)	O60-Ni3-O3W	91.89(15)
O1-Ni2-O7	170.43(14)	O9-Ni3-O3W	94.46(13)
O59-Ni2-O7	100.54(14)	N2-Ni3-O4W	90.77(15)
O18-Ni2-O7	86.24(13)	O7-Ni3-O4W	91.70(13)

O60-Ni3-O4W	85.93(15)	N4-Ni6-O19	92.0(2)
O9-Ni3-O4W	89.09(13)	O12-Ni6-O19	97.99(15)
O3W-Ni3-O4W	175.77(13)	N4-Ni6-O21	80.4(2)
O13-Ni4-N3	92.5(2)	O12-Ni6-O21	89.70(15)
O13-Ni4-O15	173.08(15)	O19-Ni6-O21	172.30(15)
N3-Ni4-O15	80.6(2)	N4-Ni6-O7W	92.25(16)
O13-Ni4-O29	99.32(15)	O12-Ni6-O7W	91.88(13)
N3-Ni4-O29	167.9(2)	O19-Ni6-O7W	85.72(15)
O15-Ni4-O29	87.60(16)	O21-Ni6-O7W	93.67(15)
O13-Ni4-O6W	88.69(18)	N4-Ni6-O8W	88.54(18)
N3-Ni4-O6W	89.08(19)	O12-Ni6-O8W	88.03(16)
O15-Ni4-O6W	91.56(19)	O19-Ni6-O8W	90.16(18)
O29-Ni4-O6W	88.39(18)	O21-Ni6-O8W	90.49(18)
O13-Ni4-O5W	86.04(15)	O7W-Ni6-O8W	175.84(18)
N3-Ni4-O5W	92.73(17)	N5-Ni7-O10W	89.47(16)
O15-Ni4-O5W	93.86(16)	O25-Ni7-O10W	91.39(13)
O29-Ni4-O5W	90.89(15)	O41-Ni7-O10W	86.86(16)
O6W-Ni4-O5W	174.50(17)	O27-Ni7-O10W	90.50(13)
O19-Ni5-O30	85.30(14)	N5-Ni7-O9W	92.69(16)
O11-Ni5-O13	85.45(14)	O25-Ni7-O9W	85.33(13)
O19-Ni5-O13	171.37(16)	O41-Ni7-O9W	91.61(15)
O30-Ni5-O13	100.21(15)	O27-Ni7-O9W	93.00(13)
O11-Ni5-O14	91.24(17)	O10W-Ni7-O9W	176.13(14)
O19-Ni5-O14	96.22(16)	N5-Ni7-O25	92.25(16)
O30-Ni5-O14	176.57(18)	N5-Ni7-O41	168.65(15)
O13-Ni5-O14	77.92(16)	O25-Ni7-O41	98.57(15)
O11-Ni5-O20	176.51(18)	N5-Ni7-O27	80.96(17)
O19-Ni5-O20	77.14(18)	O25-Ni7-O27	172.94(17)
O30-Ni5-O20	91.41(18)	O41-Ni7-O27	88.33(16)
O13-Ni5-O20	95.98(17)	O31-Ni8-O25	170.33(14)
O14-Ni5-O20	86.0(2)	O31-Ni8-O23	99.49(14)
O11-Ni5-O19	101.13(15)	O25-Ni8-O23	87.03(14)
O11-Ni5-O30	91.47(14)	O31-Ni8-O42	87.47(15)
N4-Ni6-O12	169.49(19)	O25-Ni8-O42	99.69(14)

O23-Ni8-O42	90.43(14)	O39-Ni10-O14W	90.30(18)
O31-Ni8-O26	93.36(16)	N7-Ni10-O13W	91.02(16)
O25-Ni8-O26	79.29(15)	O37-Ni10-O13W	85.75(16)
O23-Ni8-O26	91.08(15)	O53-Ni10-O13W	90.35(16)
O42-Ni8-O26	178.13(15)	O39-Ni10-O13W	93.33(16)
O31-Ni8-O32	78.65(15)	O14W-Ni10-O13W	175.37(17)
O25-Ni8-O32	94.62(15)	O35-Ni11-O43	101.15(17)
O23-Ni8-O32	177.53(14)	O35-Ni11-O37	85.38(16)
O42-Ni8-O32	91.11(14)	O43-Ni11-O37	171.67(17)
O26-Ni8-O32	87.42(16)	O35-Ni11-O54	90.55(16)
N6-Ni9-O24	168.51(15)	O43-Ni11-O54	84.86(16)
N6-Ni9-O31	91.71(16)	O37-Ni11-O54	100.37(15)
O24-Ni9-O31	98.94(15)	O35-Ni11-O44	177.63(18)
N6-Ni9-O33	80.14(17)	O43-Ni11-O44	77.72(18)
O24-Ni9-O33	89.28(16)	O37-Ni11-O44	95.56(17)
O31-Ni9-O33	171.76(17)	O54-Ni11-O44	91.41(17)
N6-Ni9-O11W	94.17(16)	O35-Ni11-O38	91.24(16)
O24-Ni9-O11W	91.01(15)	O43-Ni11-O38	96.82(17)
O31-Ni9-O11W	85.36(13)	O37-Ni11-O38	77.72(16)
O33-Ni9-O11W	94.01(15)	O54-Ni11-O38	177.26(16)
N6-Ni9-O12W	90.03(16)	O44-Ni11-O38	86.85(17)
O24-Ni9-O12W	85.52(15)	N8-Ni12-O43	94.9(3)
O31-Ni9-O12W	90.82(14)	N8-Ni12-O45	80.3(3)
O33-Ni9-O12W	90.36(14)	O43-Ni12-O45	174.9(2)
O11W-Ni9-O12W	174.39(16)	N8-Ni12-O16W	90.1(3)
N7-Ni10-O37	92.24(18)	O43-Ni12-O16W	92.4(2)
N7-Ni10-O53	169.31(19)	O45-Ni12-O16W	89.2(2)
O37-Ni10-O53	98.43(17)	N8-Ni12-O15W	91.3(2)
N7-Ni10-O39	80.74(18)	O43-Ni12-O15W	87.69(16)
O37-Ni10-O39	172.92(16)	O45-Ni12-O15W	90.8(2)
O53-Ni10-O39	88.59(17)	O16W-Ni12-O15W	178.6(2)
N7-Ni10-O14W	92.40(18)	N8-Ni12-O36	169.3(3)
O37-Ni10-O14W	91.00(17)	O43-Ni12-O36	95.50(18)
O53-Ni10-O14W	86.86(19)	O45-Ni12-O36	89.4(3)

O16W-Ni12-O36	86.8(2)	O5-Ni14-O50	175.78(18)
O15W-Ni12-O36	91.78(18)	O47-Ni14-O50	93.18(19)
O49-Ni13-N9	91.9(2)	O55-Ni14-O50	94.49(18)
O49-Ni13-O6	97.81(17)	O49-Ni14-O56	93.93(16)
N9-Ni13-O6	169.7(2)	O5-Ni14-O56	89.54(16)
O49-Ni13-O51	172.17(19)	O47-Ni14-O56	179.17(18)
N9-Ni13-O51	80.4(2)	O55-Ni14-O56	78.37(16)
O6-Ni13-O51	89.97(19)	O50-Ni14-O56	87.01(18)
O49-Ni13-O17W	86.44(16)	N10-Ni15-O55	91.05(18)
N9-Ni13-O17W	91.66(18)	N10-Ni15-O57	82.02(19)
O6-Ni13-O17W	92.23(15)	O55-Ni15-O57	173.06(17)
O51-Ni13-O17W	92.42(17)	N10-Ni15-O48	170.16(18)
O49-Ni13-O18W	90.02(19)	O55-Ni15-O48	98.59(17)
N9-Ni13-O18W	88.16(19)	O57-Ni15-O48	88.35(17)
O6-Ni13-O18W	88.54(17)	N10-Ni15-O19W	91.53(17)
O51-Ni13-O18W	91.04(19)	O55-Ni15-O19W	86.82(16)
O17W-Ni13-O18W	176.5(2)	O57-Ni15-O19W	93.09(18)
O49-Ni14-O5	98.94(17)	O48-Ni15-O19W	90.96(19)
O49-Ni14-O47	86.91(16)	N10-Ni15-O20W	91.2(2)
O5-Ni14-O47	90.30(17)	O55-Ni15-O20W	90.43(19)
O49-Ni14-O55	170.17(16)	O57-Ni15-O20W	90.0(2)
O5-Ni14-O55	87.20(16)	O48-Ni15-O20W	86.8(2)
O47-Ni14-O55	100.81(16)	O19W-Ni15-O20W	176.14(17)
O49-Ni14-O50	78.89(19)		

Table S2. Hydrogen bond parameters for **1a**.

D—H...A	d(D-H)/Å	d(H...A)/Å	d(D...A)/Å	<DHA/°
O1W—H1WA...O59	0.90(2)	1.93(3)	2.793(5)	161(3)
O2W—H2WB...O28 ^{a,b}	0.90(2)	1.96(2)	2.858(6)	175(3)
O3W—H3WA...O18	0.90(2)	2.35(3)	2.783(5)	109.4(18)
O5W—H5WA...O11	0.90(3)	1.94(3)	2.752(5)	149(3)
O10W—H10B...O4 ^{a,b}	0.90(4)	1.92(4)	2.818(6)	177(2)
O11W—H11J...O42	0.90(3)	1.94(3)	2.798(5)	159(3)
O12W—H12K...O10 ^{c,d}	0.90(3)	1.92(3)	2.818(6)	180(4)
O7W—H7WA...O30	0.900(18)	2.00(2)	2.791(5)	146(3)
O17W—H17A...O47	0.90(3)	2.02(3)	2.808(6)	145(4)
O9W—H9WB...O23	0.90(2)	2.01(3)	2.789(5)	144(3)
O19W—H19A...O5	0.90(2)	1.89(2)	2.757(6)	160(3)

Symmetry transformations used to generate equivalent atoms: a = -x,y-1/2,-z+1; b = -x,y+1/2,-z+1; c = -x+1,y-1/2,-z+1; d = -x+1,y+1/2,-z+1.

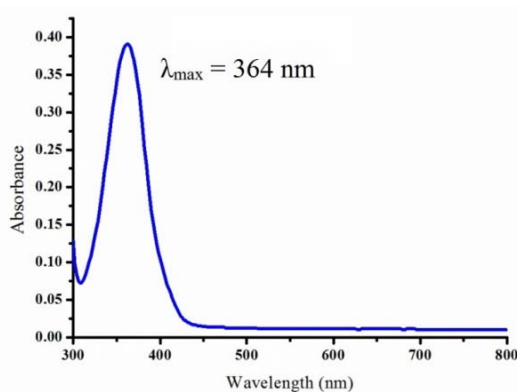


Figure S1. UV spectrum of **1** in MeOH.

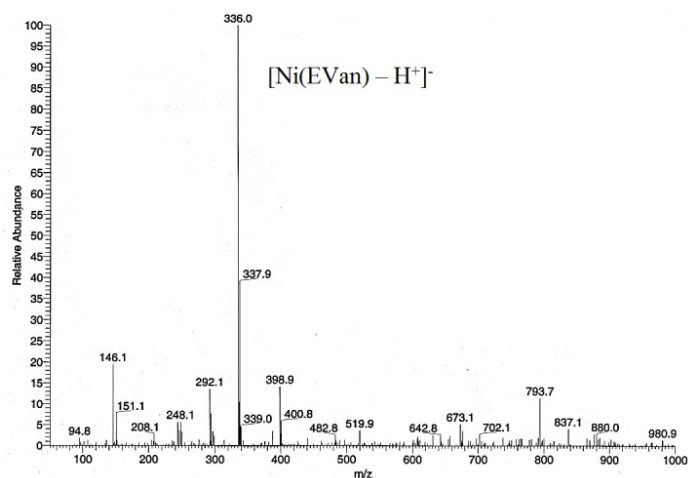


Figure S2. ESI-MS spectrum of **1**.

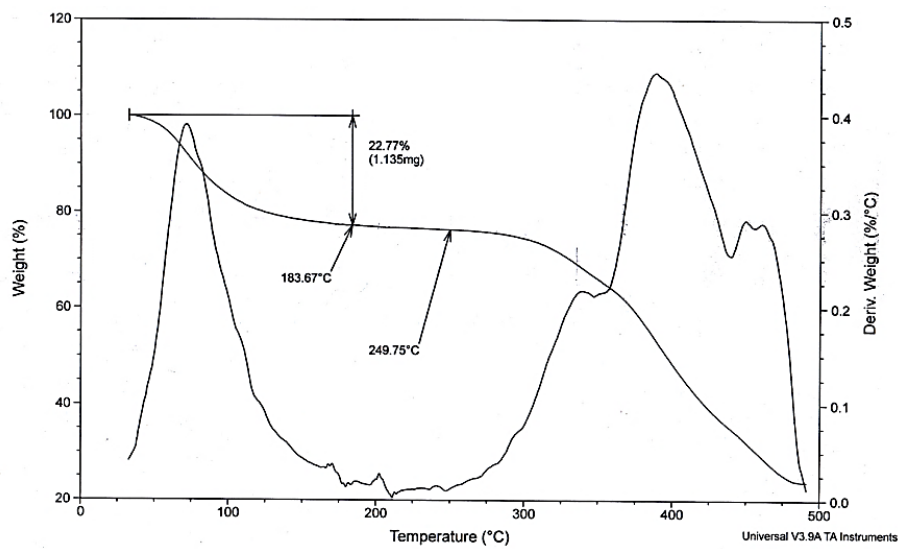


Figure S3. TGA profile of 1.