

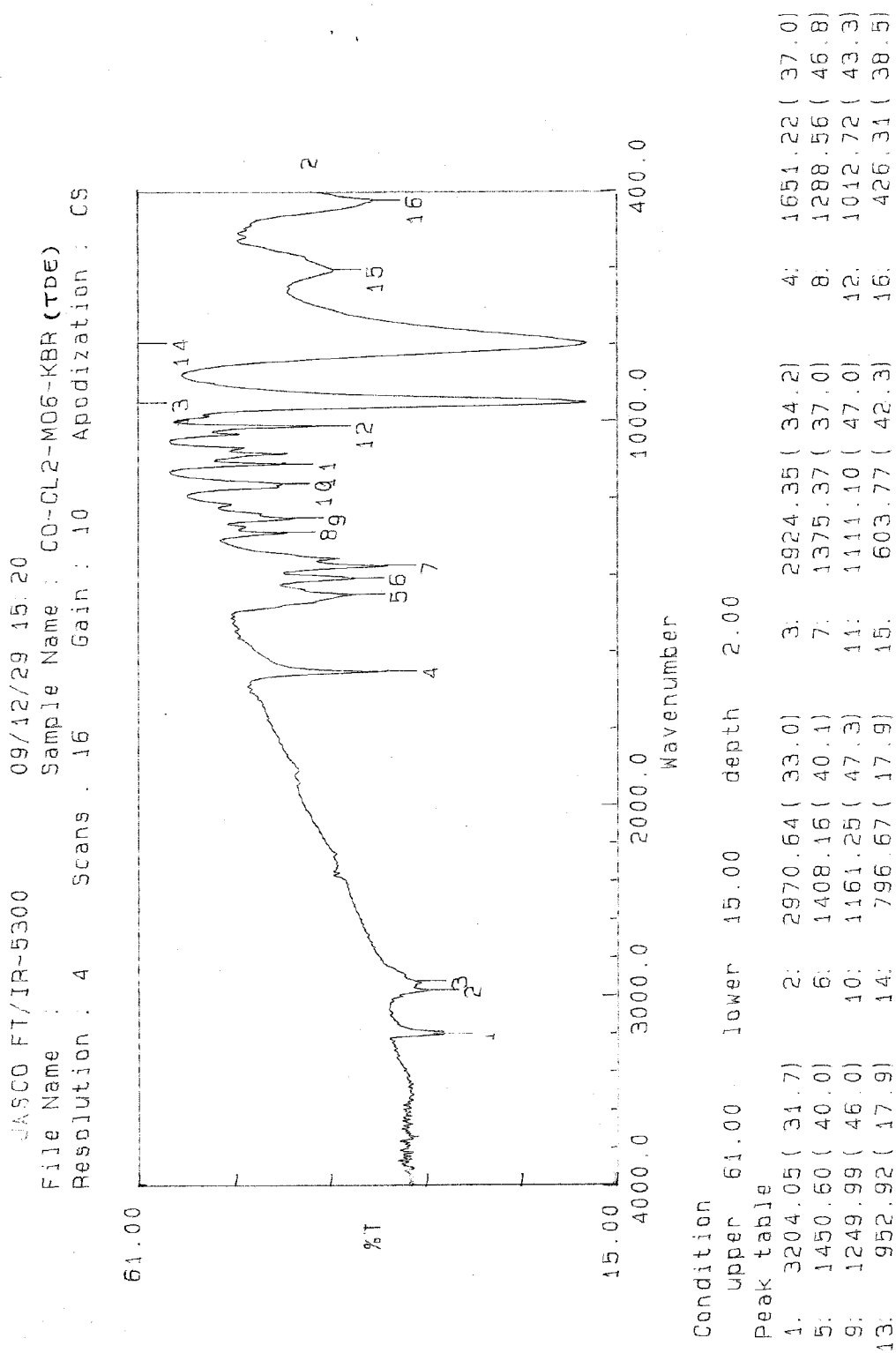
Supporting Information

**Bringing an important macrocycle into polyoxometalate matrix:
synthesis, crystal Structure, spectroscopy and electrochemistry of
[Co^{III}(transdiene)(Cl)₂]₂[Mo₆O₁₉], [Ni^{II}(transdiene)][W₆O₁₉]
·DMSO·DCM and [Zn^{II}(transdiene)(Cl)₂][W₆O₁₉]**

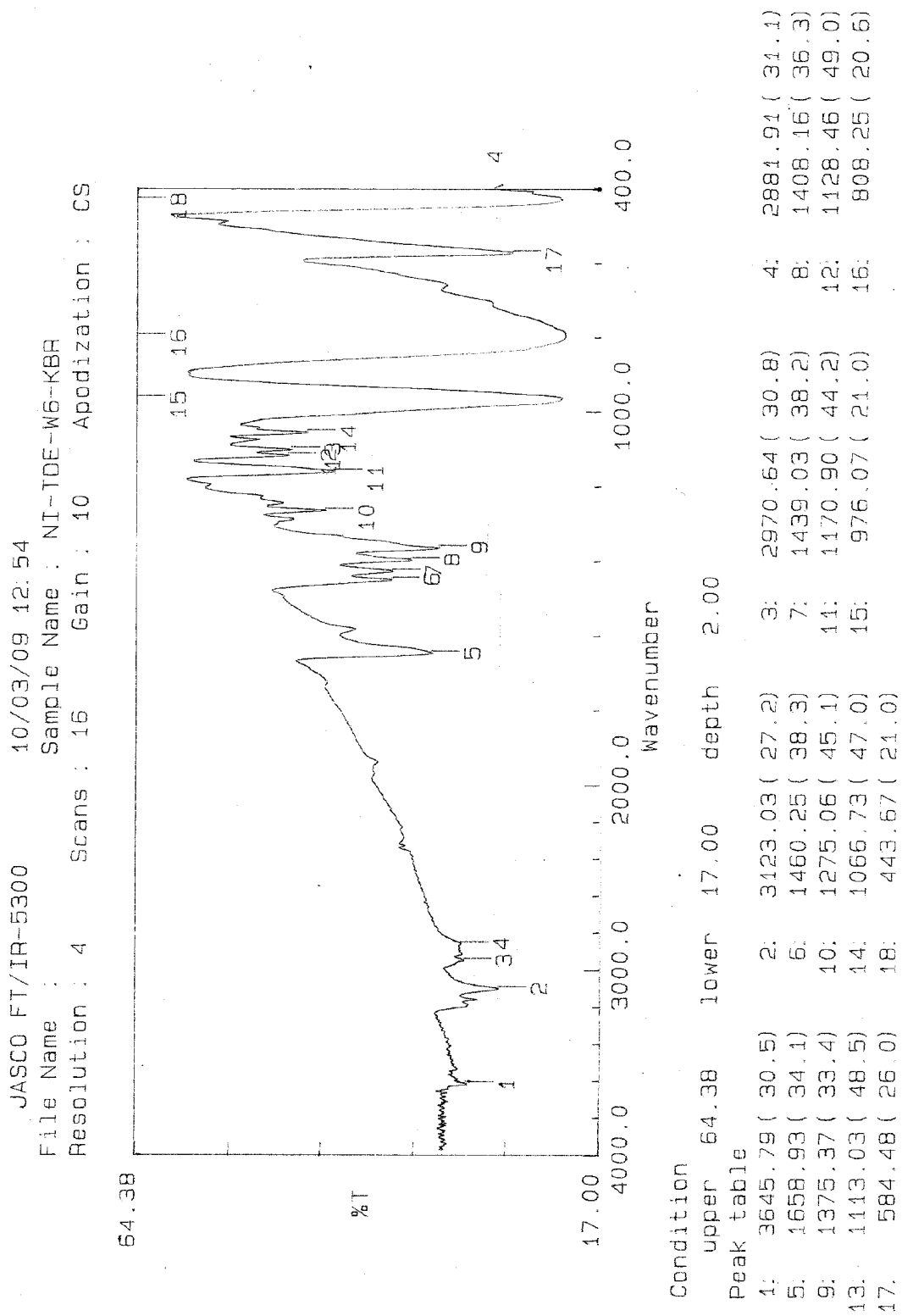
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E-mail: skdsc@uohyd.ernet.in

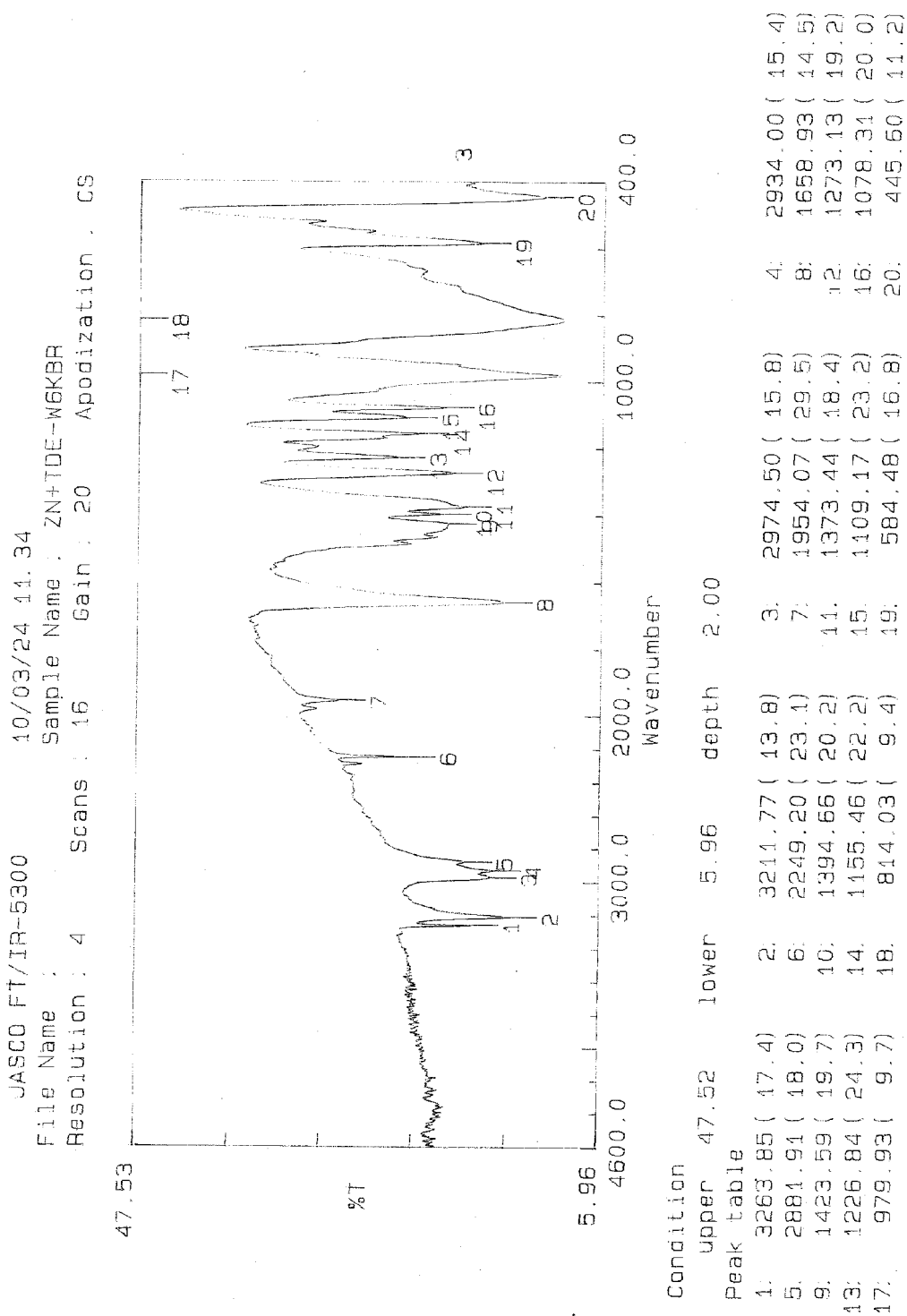
SI-Figure 1. FT-IR spectrum of compound 1 (KBr pellet, cm^{-1})



SI-Figure 2. FT-IR spectrum of compound 2 (KBr pellet, cm^{-1})

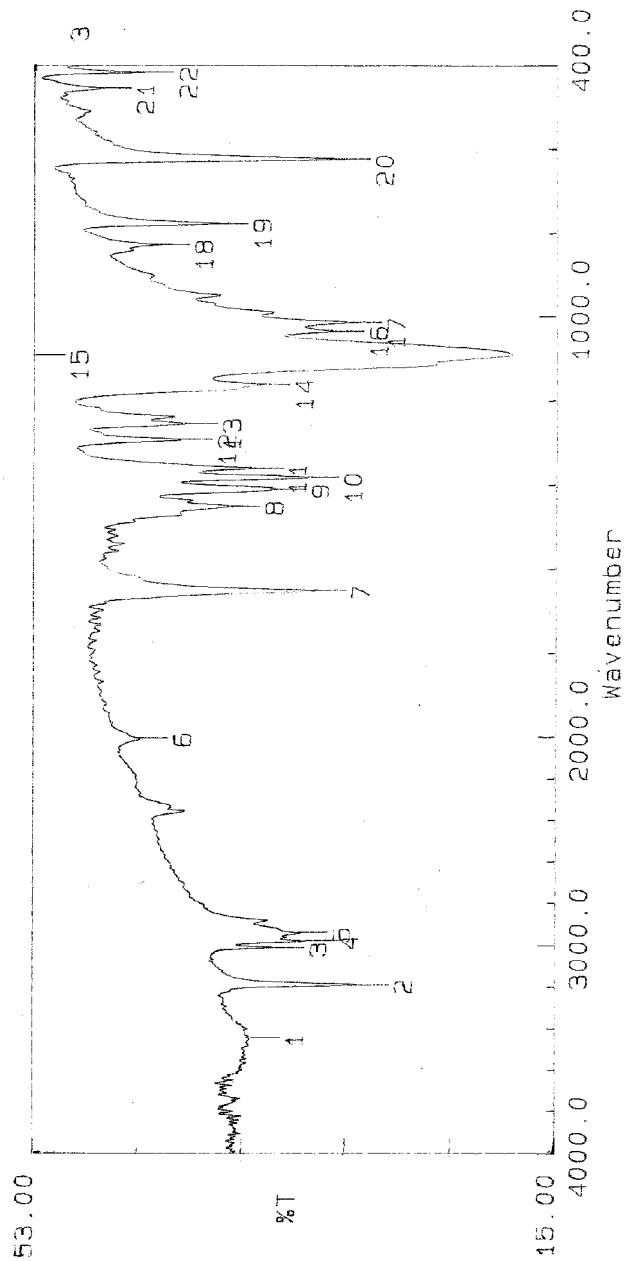


SI-Figure 4. FT-IR spectrum of compound 3 (KBr pellet, cm^{-1})



SI-Figure 5. FT-IR spectrum of compound **1a** (KBr pellet, cm^{-1})

JASCO FT/IR-5300 10/03/10 14:35
 File Name : CO-CL04-KBR
 Resolution : 4 Scans : 16 Gain : 10 Apodization : CS

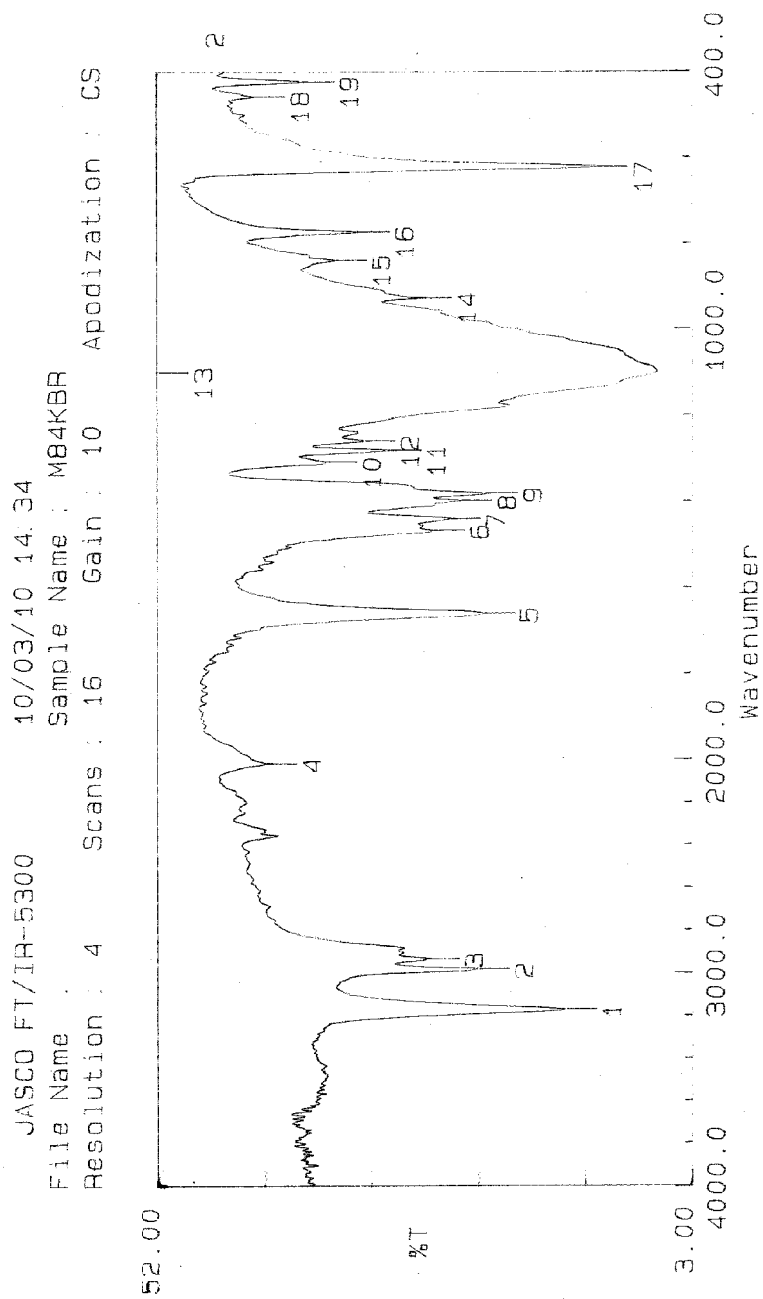


Condition upper 53.00 lower 15.00 depth 2.00

Peak table

1.	3447.10 (37.2)	2.	3190.55 (29.3)	3.	3011.15 (35.5)	4.	2980.29 (33.2)
5.	2939.78 (33.7)	6.	2008.08 (45.4)	7.	1651.22 (32.4)	8.	1450.60 (38.8)
9.	1410.09 (35.4)	10.	1381.16 (33.0)	11.	1359.94 (37.1)	12.	1290.49 (42.2)
13.	1253.84 (41.9)	14.	1161.25 (36.7)	15.	1091.81 (18.2)	16.	1035.87 (31.2)
17.	1014.65 (29.9)	18.	827.54 (44.0)	19.	777.38 (39.7)	20.	623.05 (30.8)
21.	455.24 (48.2)	22.	416.66 (45.1)				

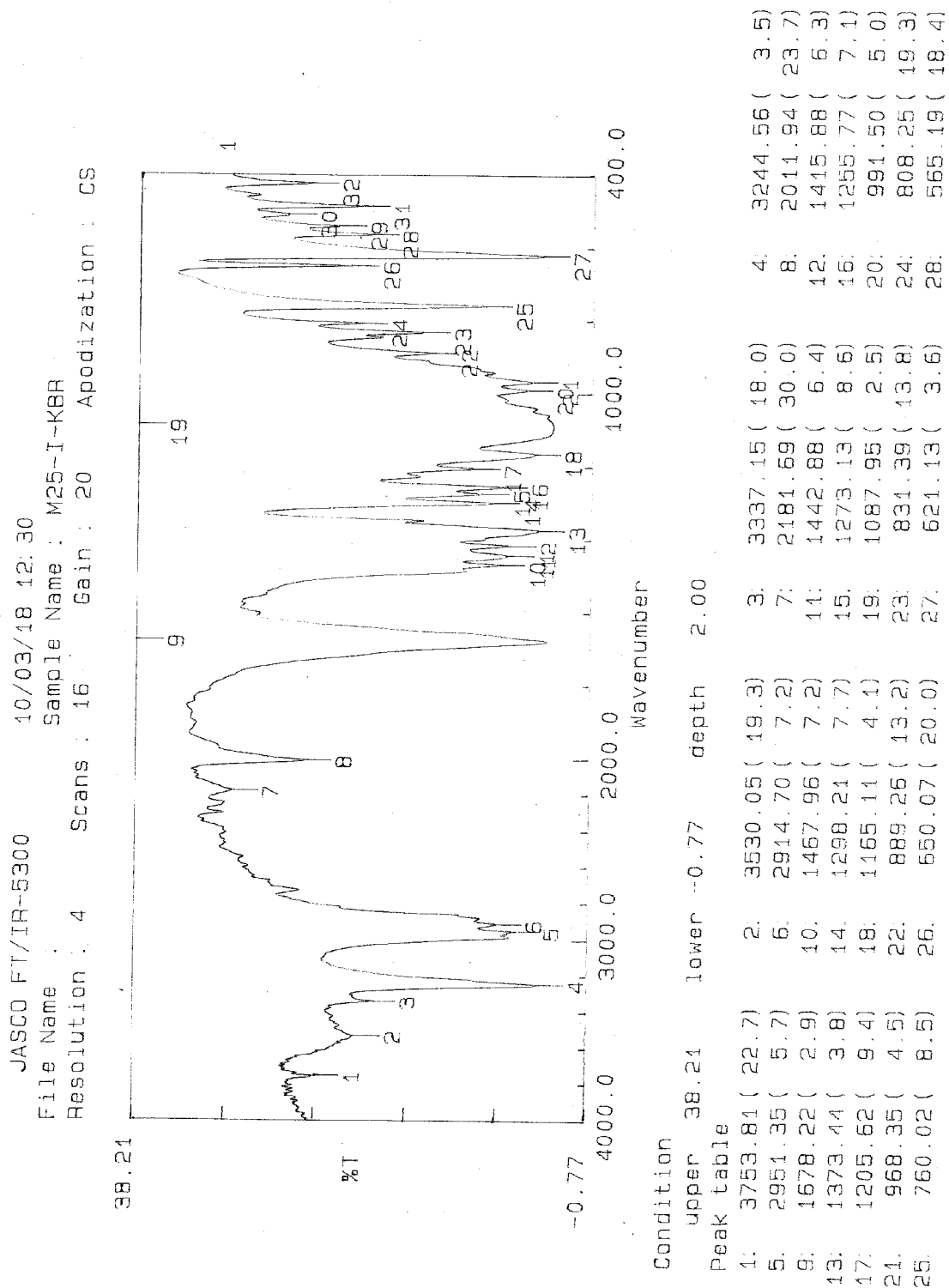
SI-Figure 6. FT-IR Spectrum of compound **2a** (KBr pellet, cm^{-1})



Condition

upper	52.00	lower	3.00	depth	2.00
Peak table					
1.	3173.19	(14.6)	2.	2982.22	(22.7)
5.	1660.86	(22.1)	6.	1467.96	(26.7)
9.	1381.16	(21.8)	10.	1307.85	(36.6)
13.	1101.45	(6.1)	14.	927.84	(27.9)
17.	623.06	(11.6)	18.	459.10	(43.1)
			3.	2934.00	(27.3)
			7.	1440.96	(25.3)
			11.	1280.85	(30.7)
			15.	839.11	(35.6)
			19.	424.38	(38.5)
			4.	2021.58	(42.1)
			8.	1398.52	(24.2)
			12.	1259.63	(33.1)
			16.	773.52	(33.5)

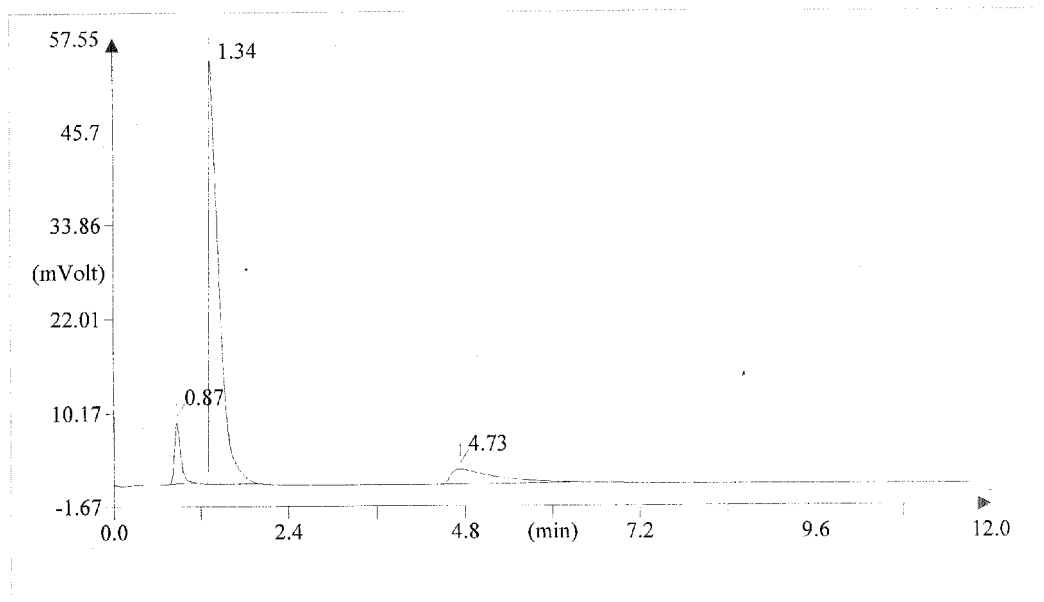
SI-Figure 7. FT-IR spectrum of compound **3a** (KBr pellet, cm^{-1})



SI-Figure 7. Elemental analysis on compound 1

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Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa
Sample ID: CO-1DE-2CL-MO6 (# 71)
Analysis type: UnkNown
Chromatogram filename: UNK-15032010-21.dat
Sample weight: 1.212



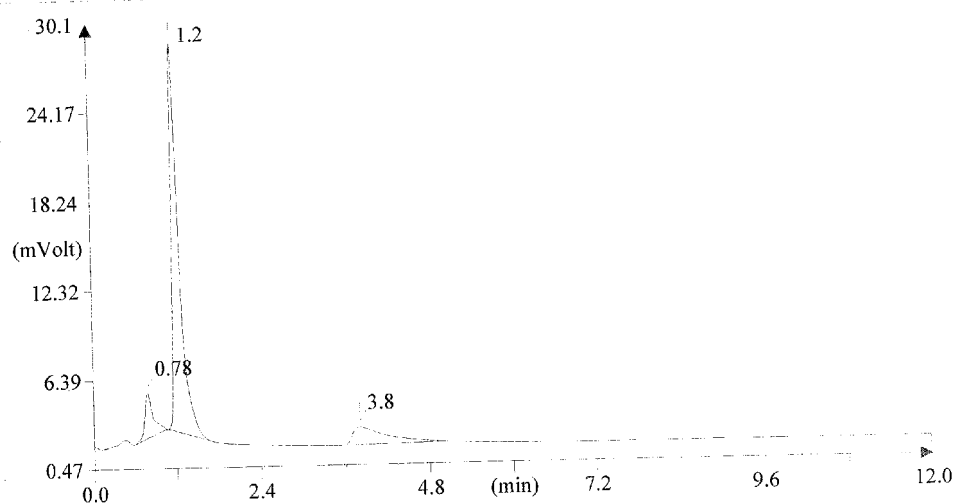
Element Name	Element %	Ret. Time
Nitrogen	6.68	0.87
Carbon	22.45	1.34
Hydrogen	3.71	4.73

Handwritten signature

SI-Figure 8. Elemental analysis on compound 2

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Method filename: E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa
Sample ID: NI-TDE-N6 (# 70)
Analysis type: UnkNown
Chromatogram filename: UNK-15032010-20.dat
Sample weight: .978



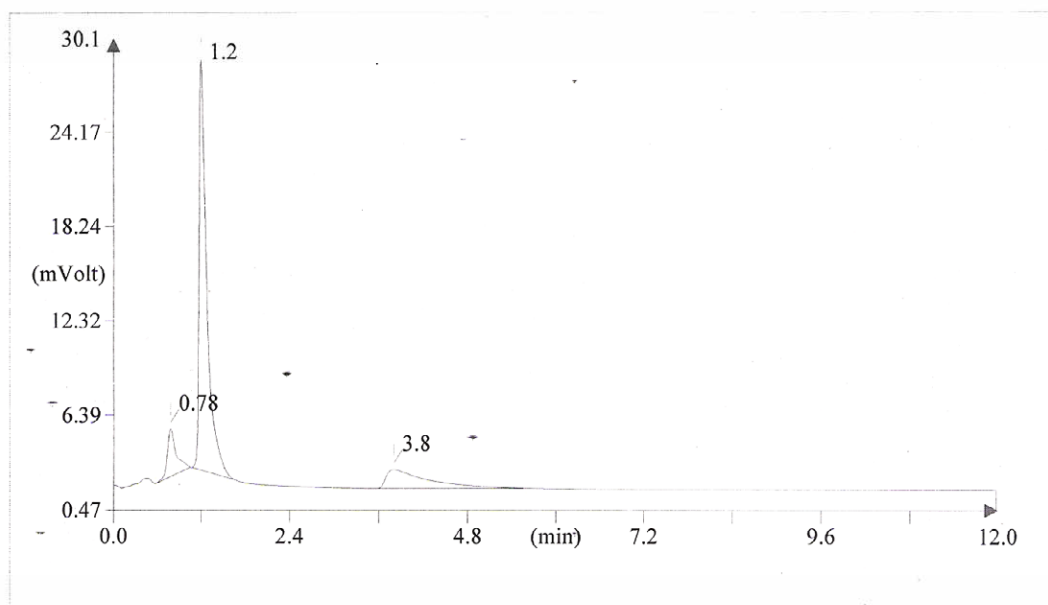
Element Name	Element %	Ret. Time
Nitrogen	2.85	0.78
Carbon	12.12	1.20
Hydrogen	2.10	3.80

Bh

SI-Figure 9. Elemental analysis on compound 3

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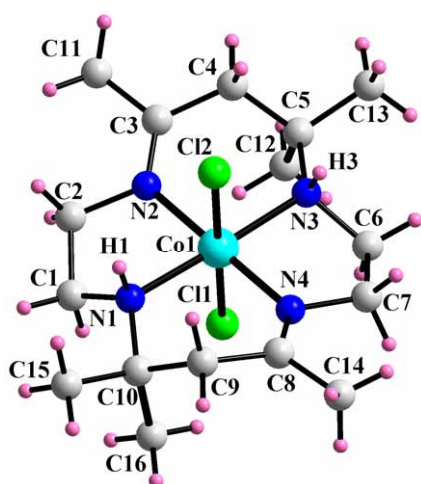
Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa
Sample ID: ZN-TDE-W6 (# 24)
Analysis type: UnkNown
Chromatogram filename: UNK-30042010-4.dat
Sample weight: 1.004



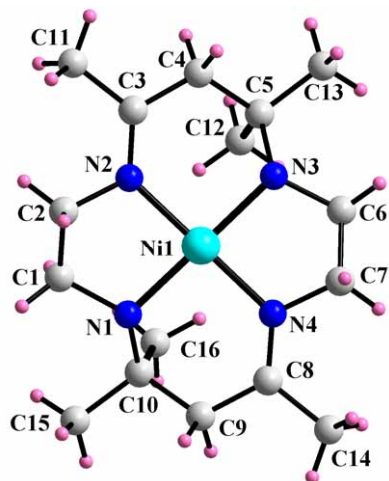
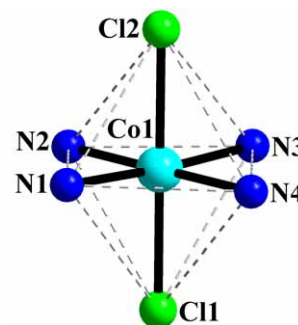
Element Name	Element %	Ret. Time
Nitrogen	5.23	0.78
Carbon	18.12	1.20
Hydrogen	2.86	3.80

CB

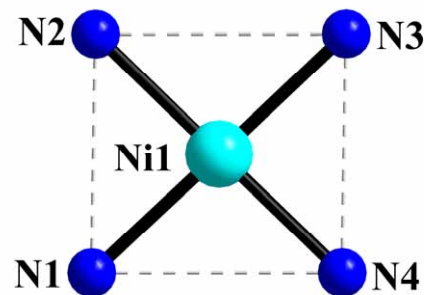
SI–Figure 10. Structure of the cations and the geometry around the concerned metal ions in the crystal structures of compounds 1–3.

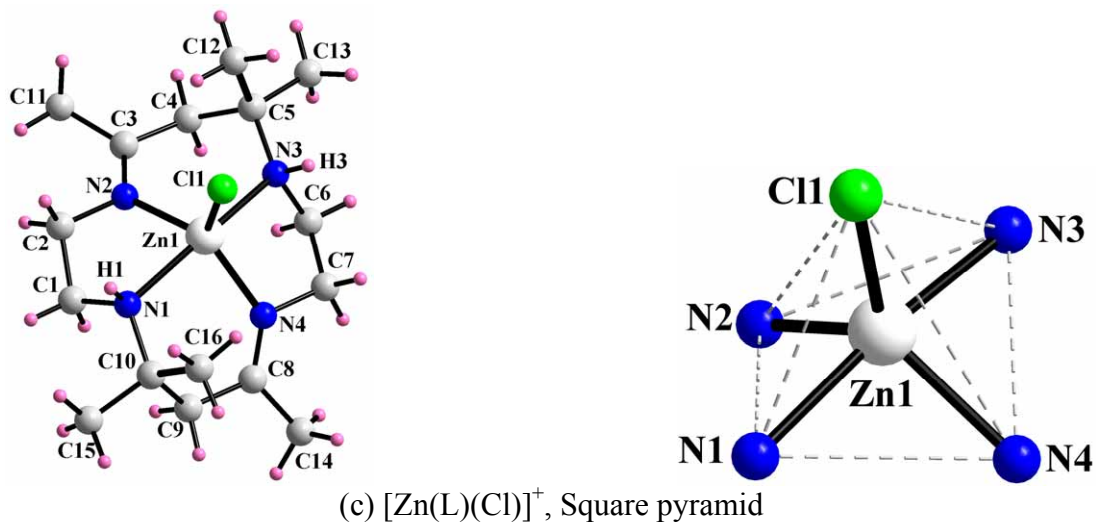


(a) $[\text{Co}(\text{L})(\text{Cl})_2]^+$, Octahedral

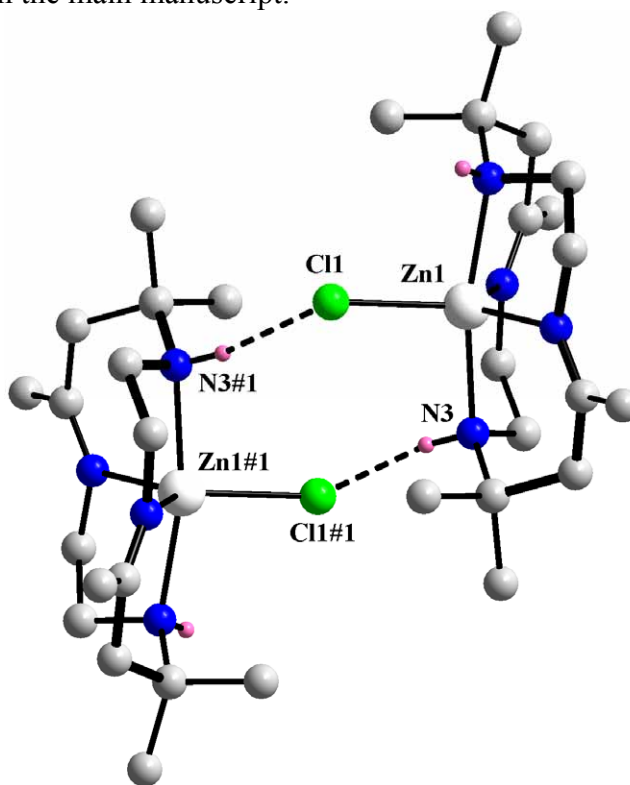


(b) $[\text{Ni}(\text{L})]^{2+}$, Square planar





SI-Figure 11. Formation of supramolecular dimer in the crystal structure of compound **3** through hydrogen bonding interactions. Atoms labelled with additional symmetry operations are in accord with that mentioned in Table 4 in the main manuscript.



SI-Table 1. Complete list of lengths and angles for the crystal structure of compound **1**

C(1)–N(1)	1.474(5)	C(1)–C(2)	1.524(6)	C(2)–N(2)	1.480(5)
C(3)–N(2)	1.277(5)	C(3)–C(4)	1.493(6)	C(3)–C(11)	1.494(5)
C(4)–C(5)	1.524(6)	C(5)–N(3)	1.509(5)	C(5)–C(12)	1.524(6)
C(5)–C(13)	1.532(6)	C(6)–N(3)	1.475(5)	C(6)–C(7)	1.512(6)
C(7)–N(4)	1.469(6)	C(8)–N(4)	1.277(5)	C(8)–C(9)	1.496(7)
C(8)–C(14)	1.498(6)	C(9)–C(10)	1.529(7)	C(10)–N(1)	1.506(5)
C(10)–C(16)	1.522(7)	C(10)–C(15)	1.526(7)	N(1)–Co(1)	1.965(3)

N(1)–H(1)	0.82(4)	N(2)–Co(1)	1.921(3)	N(3)–Co(1)	1.973(3)
N(3)–H(3)	0.82(5)	N(4)–Co(1)	1.923(3)	O(1)–Mo(1)	1.686(3)
O(2)–Mo(1)	1.899(3)	O(3)–Mo(2)	1.895(3)	O(3)–Mo(1)	1.956(3)
O(4)–Mo(2)	1.680(3)	O(5)–Mo(2)	1.871(3)	O(5)–Mo(3)	1.983(3)
O(6)–Mo(1)	2.3130(4)	O(6)–Mo(2)	2.3159(4)	O(6)–Mo(3)	2.3201(4)
O(7)–Mo(3)	1.676(3)	O(8)–Mo(3)	1.869(3)	O(9)–Mo(3)	1.893(3)
O(9)–Mo(1)	1.952(3)	O(10)–Mo(1)	1.881(3)	Cl(1)–Co(1)	2.2796(15)
Cl(2)–Co(1)	2.2762(12)				

N(1)–C(1)–C(2)	107.5(3)	N(2)–C(2)–C(1)	109.9(3)
N(2)–C(3)–C(4)	120.8(4)	N(2)–C(3)–C(11)	123.2(4)
C(4)–C(3)–C(11)	116.0(4)	C(3)–C(4)–C(5)	117.2(4)
N(3)–C(5)–C(4)	106.7(3)	N(3)–C(5)–C(12)	111.7(4)
C(4)–C(5)–C(12)	110.1(4)	N(3)–C(5)–C(13)	109.2(4)
C(4)–C(5)–C(13)	109.6(4)	C(12)–C(5)–C(13)	109.5(4)
N(3)–C(6)–C(7)	107.0(4)	N(4)–C(7)–C(6)	111.4(3)
N(4)–C(8)–C(9)	120.7(4)	N(4)–C(8)–C(14)	122.9(5)
C(9)–C(8)–C(14)	116.3(4)	C(8)–C(9)–C(10)	118.2(4)
N(1)–C(10)–C(16)	111.6(4)	N(1)–C(10)–C(15)	109.2(4)
C(16)–C(10)–C(15)	109.9(4)	N(1)–C(10)–C(9)	107.0(4)
C(16)–C(10)–C(9)	110.2(4)	C(15)–C(10)–C(9)	108.8(4)
C(1)–N(1)–C(10)	116.2(3)	C(1)–N(1)–Co(1)	107.7(2)
C(10)–N(1)–Co(1)	120.8(3)	C(3)–N(2)–C(2)	119.5(3)
C(3)–N(2)–Co(1)	126.6(3)	C(2)–N(2)–Co(1)	113.5(2)
C(6)–N(3)–C(5)	117.0(3)	C(6)–N(3)–Co(1)	108.2(3)
C(5)–N(3)–Co(1)	120.1(3)	C(8)–N(4)–C(7)	119.9(4)
C(8)–N(4)–Co(1)	126.6(3)	C(7)–N(4)–Co(1)	113.2(3)
Mo(2)–O(3)–Mo(1)	116.82(14)	Mo(2)–O(5)–Mo(3)	116.48(14)
Mo(1)–O(6)–Mo(2)	90.232(14)	Mo(1)–O(6)–Mo(3)	89.898(14)
Mo(2)–O(6)–Mo(3)	89.979(13)	Mo(3)–O(9)–Mo(1)	116.68(14)
N(2)–Co(1)–N(4)	179.70(14)	N(2)–Co(1)–N(1)	83.93(13)
N(4)–Co(1)–N(1)	96.29(14)	N(2)–Co(1)–N(3)	95.89(14)
N(4)–Co(1)–N(3)	83.88(15)	N(1)–Co(1)–N(3)	176.42(15)
N(2)–Co(1)–Cl(2)	89.66(10)	N(4)–Co(1)–Cl(2)	90.14(11)
N(1)–Co(1)–Cl(2)	87.81(11)	N(3)–Co(1)–Cl(2)	88.62(11)
N(2)–Co(1)–Cl(1)	90.64(10)	N(4)–Co(1)–Cl(1)	89.56(11)
N(1)–Co(1)–Cl(1)	92.14(11)	N(3)–Co(1)–Cl(1)	91.43(11)
Cl(2)–Co(1)–Cl(1)	179.68(5)	O(1)–Mo(1)–O(10)	104.01(15)
O(1)–Mo(1)–O(2)	104.39(16)	O(10)–Mo(1)–O(2)	89.85(13)
O(1)–Mo(1)–O(9)	101.93(16)	O(10)–Mo(1)–O(9)	87.38(13)
O(2)–Mo(1)–O(9)	153.42(13)	O(1)–Mo(1)–O(3)	102.52(15)
O(10)–Mo(1)–O(3)	153.27(12)	O(2)–Mo(1)–O(3)	86.73(13)
O(9)–Mo(1)–O(3)	84.01(12)	O(1)–Mo(1)–O(6)	177.54(13)
O(10)–Mo(1)–O(6)	77.44(9)	O(2)–Mo(1)–O(6)	77.52(9)
O(9)–Mo(1)–O(6)	76.07(9)	O(3)–Mo(1)–O(6)	75.94(9)
O(4)–Mo(2)–O(5)	104.17(14)	O(4)–Mo(2)–O(3)	104.34(16)
O(5)–Mo(2)–O(3)	90.71(13)	O(4)–Mo(2)–O(6)	177.56(13)
O(5)–Mo(2)–O(6)	77.78(9)	O(3)–Mo(2)–O(6)	76.98(9)
O(7)–Mo(3)–O(8)	104.71(14)	O(7)–Mo(3)–O(9)	103.85(16)
O(8)–Mo(3)–O(9)	90.95(13)	O(7)–Mo(3)–O(5)	102.26(14)
O(8)–Mo(3)–O(5)	152.86(12)	O(9)–Mo(3)–O(5)	85.53(13)
O(7)–Mo(3)–O(6)	177.70(11)	O(8)–Mo(3)–O(6)	77.37(8)
O(9)–Mo(3)–O(6)	76.99(9)	O(5)–Mo(3)–O(6)	75.62(8)

SI-Table 2. Complete list of lengths and angles for the crystal structure of compound **2**

C(1)–N(1)	1.494(10)	C(1)–C(2)	1.498(12)	C(2)–N(2)	1.460(11)
C(3)–N(2)	1.285(11)	C(3)–C(4)	1.485(12)	C(3)–C(11)	1.503(12)
C(4)–C(5)	1.542(12)	C(5)–N(3)	1.512(11)	C(5)–C(13)	1.513(12)
C(5)–C(12)	1.529(12)	C(6)–N(3)	1.476(11)	C(6)–C(7)	1.490(12)
C(7)–N(4)	1.470(11)	C(8)–N(4)	1.284(11)	C(8)–C(9)	1.492(12)
C(8)–C(14)	1.507(12)	C(9)–C(10)	1.518(12)	C(10)–N(1)	1.492(11)
C(10)–C(15)	1.532(13)	C(10)–C(16)	1.533(13)	C(17)–Cl(2)	1.764(10)
C(17)–Cl(1)	1.771(10)	C(18)–S(1)	1.795(9)	C(19)–S(1)	1.784(10)
N(1)–Ni(1)	1.920(7)	N(2)–Ni(1)	1.900(7)	N(3)–Ni(1)	1.930(7)
N(4)–Ni(1)	1.891(7)	O(1)–W(5)	1.707(6)	O(2)–W(5)	1.941(5)
O(2)–W(4)	1.948(5)	O(3)–W(3)	1.920(5)	O(3)–W(5)	1.926(5)
O(4)–W(3)	1.918(5)	O(4)–W(4)	1.927(6)	O(5)–W(5)	1.921(6)
O(5)–W(1)	1.927(6)	O(6)–W(4)	2.314(5)	O(6)–W(6)	2.326(5)
O(6)–W(5)	2.326(5)	O(6)–W(3)	2.326(5)	O(6)–W(1)	2.329(5)
O(6)–W(2)	2.334(5)	O(7)–W(3)	1.711(6)	O(8)–W(1)	1.920(6)
O(8)–W(3)	.925(5)	O(9)–W(2)	1.921(6)	O(9)–W(3)	1.925(5)
O(10)–W(1)	1.702(6)	O(11)–W(2)	1.919(5)	O(11)–W(1)	1.931(5)
O(12)–W(2)	1.699(6)	O(13)–W(6)	1.912(6)	O(13)–W(1)	1.934(6)
O(14)–W(4)	1.906(6)	O(14)–W(2)	1.936(5)	O(15)–W(6)	1.919(6)
O(15)–W(2)	1.923(6)	O(16)–W(6)	1.702(6)	O(17)–W(4)	1.916(5)
O(17)–W(6)	1.936(5)	O(18)–W(6)	1.933(6)	O(18)–W(5)	1.939(6)
O(19)–W(4)	1.706(6)	O(20)–S(1)	1.501(7)		

N(1)–C(1)–C(2)	107.9(7)	N(2)–C(2)–C(1)	106.2(7)
N(2)–C(3)–C(4)	122.6(8)	N(2)–C(3)–C(11)	122.8(8)
C(4)–C(3)–C(11)	114.5(7)	C(3)–C(4)–C(5)	120.0(7)
N(3)–C(5)–C(13)	110.7(7)	N(3)–C(5)–C(12)	109.6(7)
C(13)–C(5)–C(12)	110.6(8)	N(3)–C(5)–C(4)	106.0(7)
C(13)–C(5)–C(4)	108.5(7)	C(12)–C(5)–C(4)	111.3(7)
N(3)–C(6)–C(7)	108.5(7)	N(4)–C(7)–C(6)	107.9(7)
N(4)–C(8)–C(14)	122.9(8)	C(9)–C(8)–C(14)	114.6(7)
C(8)–C(9)–C(10)	119.5(7)	N(1)–C(10)–C(9)	107.1(7)
N(1)–C(10)–C(15)	110.4(7)	C(9)–C(10)–C(15)	107.7(7)
N(1)–C(10)–C(16)	111.1(7)	C(9)–C(10)–C(16)	110.8(7)
C(15)–C(10)–C(16)	109.7(8)	C(10)–N(1)–C(1)	114.7(7)
C(10)–N(1)–Ni(1)	114.4(5)	C(1)–N(1)–Ni(1)	108.1(5)
C(3)–N(2)–C(2)	120.0(7)	C(3)–N(2)–Ni(1)	129.5(6)
C(2)–N(2)–Ni(1)	110.4(5)	C(6)–N(3)–C(5)	112.9(7)
C(6)–N(3)–Ni(1)	108.6(5)	C(5)–N(3)–Ni(1)	113.6(5)
C(8)–N(4)–C(7)	120.5(7)	C(8)–N(4)–Ni(1)	129.2(6)
C(7)–N(4)–Ni(1)	109.9(5)	N(4)–Ni(1)–N(2)	173.8(3)
N(4)–Ni(1)–N(1)	92.9(3)	N(2)–Ni(1)–N(1)	87.2(3)
N(4)–Ni(1)–N(3)	87.5(3)	N(2)–Ni(1)–N(3)	92.4(3)
N(1)–Ni(1)–N(3)	179.6(3)	W(5)–O(2)–W(4)	116.4(3)
W(3)–O(3)–W(5)	117.7(3)	W(3)–O(4)–W(4)	117.2(3)
W(5)–O(5)–W(1)	117.5(3)	W(4)–O(6)–W(6)	90.21(19)
W(4)–O(6)–W(5)	90.84(19)	W(6)–O(6)–W(5)	90.13(18)
W(4)–O(6)–W(3)	90.02(18)	W(6)–O(6)–W(3)	179.7(3)
W(5)–O(6)–W(3)	90.07(19)	W(4)–O(6)–W(1)	179.2(3)
W(6)–O(6)–W(1)	89.88(18)	W(5)–O(6)–W(1)	89.91(18)
W(3)–O(6)–W(1)	89.88(19)	W(4)–O(6)–W(2)	89.57(18)
W(6)–O(6)–W(2)	89.96(19)	W(5)–O(6)–W(2)	179.6(3)
W(3)–O(6)–W(2)	89.84(18)	W(1)–O(6)–W(2)	89.68(18)
W(1)–O(8)–W(3)	117.5(3)	W(2)–O(9)–W(3)	117.7(3)

W(2)–O(11)–W(1)	117.3(3)	W(6)–O(13)–W(1)	117.5(3)
W(4)–O(14)–W(2)	116.9(3)	W(6)–O(15)–W(2)	118.1(3)
W(4)–O(17)–W(6)	117.2(3)	W(6)–O(18)–W(5)	116.6(3)
O(20)–S(1)–C(19)	104.5(5)	O(20)–S(1)–C(18)	105.5(4)
C(19)–S(1)–C(18)	97.7(5)	O(10)–W(1)–O(8)	104.8(3)
O(10)–W(1)–O(5)	103.1(3)	O(8)–W(1)–O(5)	87.1(2)
O(10)–W(1)–O(11)	104.1(3)	O(5)–W(1)–O(11)	152.7(2)
O(10)–W(1)–O(13)	102.8(3)	O(8)–W(1)–O(13)	152.4(2)
O(5)–W(1)–O(13)	85.9(2)	O(11)–W(1)–O(13)	86.8(2)
O(10)–W(1)–O(6)	178.8(3)	O(8)–W(1)–O(6)	76.3(2)
O(5)–W(1)–O(6)	76.2(2)	O(11)–W(1)–O(6)	76.5(2)
O(13)–W(1)–O(6)	76.1(2)	O(12)–W(2)–O(11)	103.4(3)
O(12)–W(2)–O(9)	103.7(3)	O(11)–W(2)–O(9)	87.1(2)
O(12)–W(2)–O(15)	104.3(3)	O(11)–W(2)–O(15)	86.9(2)
O(9)–W(2)–O(15)	152.0(2)	O(12)–W(2)–O(14)	103.8(3)
O(11)–W(2)–O(14)	152.8(2)	O(9)–W(2)–O(14)	86.4(2)
O(15)–W(2)–O(14)	86.5(2)	O(12)–W(2)–O(6)	179.9(3)
O(11)–W(2)–O(6)	76.6(2)	O(9)–W(2)–O(6)	76.2(2)
O(15)–W(2)–O(6)	75.9(2)	O(14)–W(2)–O(6)	76.2(2)
O(7)–W(3)–O(4)	103.9(3)	O(7)–W(3)–O(3)	103.4(3)
O(4)–W(3)–O(3)	86.7(2)	O(7)–W(3)–O(9)	104.1(3)
O(4)–W(3)–O(9)	86.9(2)	O(3)–W(3)–O(9)	152.5(2)
O(7)–W(3)–O(8)	103.4(3)	O(4)–W(3)–O(8)	152.6(2)
O(3)–W(3)–O(8)	86.6(2)	O(9)–W(3)–O(8)	86.9(2)
O(7)–W(3)–O(6)	179.5(2)	O(4)–W(3)–O(6)	76.3(2)
O(3)–W(3)–O(6)	76.2(2)	O(9)–W(3)–O(6)	76.3(2)
O(8)–W(3)–O(6)	76.3(2)	O(19)–W(4)–O(14)	104.6(3)
O(19)–W(4)–O(17)	104.1(3)	O(14)–W(4)–O(17)	87.6(2)
O(19)–W(4)–O(4)	102.7(3)	O(14)–W(4)–O(4)	87.2(2)
O(17)–W(4)–O(4)	153.1(2)	O(19)–W(4)–O(2)	101.6(3)
O(14)–W(4)–O(2)	153.8(2)	O(17)–W(4)–O(2)	86.6(2)
O(4)–W(4)–O(2)	86.5(2)	O(19)–W(4)–O(6)	177.9(3)
O(14)–W(4)–O(6)	77.3(2)	O(17)–W(4)–O(6)	76.6(2)
O(4)–W(4)–O(6)	76.5(2)	O(2)–W(4)–O(6)	76.5(2)
O(1)–W(5)–O(5)	104.3(3)	O(1)–W(5)–O(3)	105.0(3)
O(5)–W(5)–O(3)	87.4(2)	O(1)–W(5)–O(18)	102.3(3)
O(5)–W(5)–O(18)	86.8(2)	O(3)–W(5)–O(18)	152.7(2)
O(1)–W(5)–O(2)	103.0(3)	O(5)–W(5)–O(2)	152.7(2)
O(3)–W(5)–O(2)	86.7(2)	O(18)–W(5)–O(2)	86.3(2)
O(1)–W(5)–O(6)	178.7(3)	O(5)–W(5)–O(6)	76.4(2)
O(3)–W(5)–O(6)	76.1(2)	O(18)–W(5)–O(6)	76.6(2)
O(2)–W(5)–O(6)	76.3(2)	O(16)–W(6)–O(13)	103.7(3)
O(16)–W(6)–O(15)	103.2(3)	O(13)–W(6)–O(15)	87.5(2)
O(16)–W(6)–O(18)	103.9(3)	O(13)–W(6)–O(18)	87.1(2)
O(15)–W(6)–O(18)	152.8(2)	O(16)–W(6)–O(17)	103.7(3)
O(13)–W(6)–O(17)	152.5(2)	O(15)–W(6)–O(17)	85.9(2)
O(18)–W(6)–O(17)	86.7(2)	O(16)–W(6)–O(6)	179.3(3)
O(13)–W(6)–O(6)	76.6(2)	O(15)–W(6)–O(6)	76.1(2)
O(18)–W(6)–O(6)	76.7(2)	O(17)–W(6)–O(6)	76.0(2)

SI–Table 3. Complete list of lengths and angles for the crystal structure of compound **3**

C(1)–N(1)	1.462(9)	C(1)–C(2)	1.526(10)	C(2)–N(2)	1.474(9)
C(3)–N(2)	1.273(8)	C(3)–C(4)	1.481(11)	C(3)–C(11)	1.507(10)
C(4)–C(5)	1.546(12)	C(5)–N(3)	1.476(9)	C(5)–C(12)	1.525(11)

C(5)–C(13)	1.553(10)	C(6)–N(3)	1.485(9)	C(6)–C(7)	1.502(10)
C(7)–N(4)	1.483(9)	C(8)–N(4)	1.264(8)	C(8)–C(9)	1.497(10)
C(8)–C(14)	1.498(10)	C(9)–C(10)	1.524(10)	C(10)–N(1)	1.498(9)
C(10)–C(16)	1.541(10)	C(10)–C(15)	1.547(10)	Cl(1)–Zn(1)	2.302(2)
N(1)–Zn(1)	2.150(6)	N(1)–H(1)	0.71(5)	N(2)–Zn(1)	2.086(6)
N(3)–Zn(1)	2.151(6)	N(3)–H(3)	0.83(5)	N(4)–Zn(1)	2.070(6)
O(1)–W(1)	1.701(5)	O(2)–W(2)	1.919(5)	O(2)–W(1)	1.929(4)
O(3)–W(2)	1.704(5)	O(4)–W(2)	1.930(4)	O(5)–W(3)	1.923(5)
O(5)–W(2)	1.926(5)	O(6)–W(3)	1.917(4)	O(7)–W(3)	1.698(5)
O(8)–W(3)	1.917(5)	O(9)–W(3)	1.924(4)	O(9)–W(1)	1.929(5)
O(10)–W(1)	2.3135(4)	O(10)–W(3)	2.3257(4)	O(10)–W(2)	2.3339(4)

N(1)–C(1)–C(2)	108.8(6)	N(2)–C(2)–C(1)	109.1(6)
N(2)–C(3)–C(4)	120.8(7)	N(2)–C(3)–C(11)	123.9(7)
C(4)–C(3)–C(11)	115.3(7)	C(3)–C(4)–C(5)	120.5(7)
N(3)–C(5)–C(12)	109.0(7)	N(3)–C(5)–C(4)	109.2(7)
C(12)–C(5)–C(4)	109.2(8)	N(3)–C(5)–C(13)	111.1(7)
C(12)–C(5)–C(13)	109.4(7)	C(4)–C(5)–C(13)	108.9(7)
N(3)–C(6)–C(7)	109.9(6)	N(4)–C(7)–C(6)	110.4(6)
N(4)–C(8)–C(9)	121.4(7)	N(4)–C(8)–C(14)	123.9(7)
C(9)–C(8)–C(14)	114.7(7)	C(8)–C(9)–C(10)	123.2(6)
N(1)–C(10)–C(9)	110.2(6)	N(1)–C(10)–C(16)	107.7(6)
C(9)–C(10)–C(16)	110.0(6)	N(1)–C(10)–C(15)	110.2(6)
C(9)–C(10)–C(15)	108.5(6)	C(16)–C(10)–C(15)	110.3(6)
C(1)–N(1)–C(10)	116.3(6)	C(1)–N(1)–Zn(1)	105.6(4)
C(10)–N(1)–Zn(1)	116.5(5)	C(1)–N(1)–H(1)	99(5)
C(10)–N(1)–H(1)	111(5)	C(3)–N(2)–C(2)	120.6(6)
C(3)–N(2)–Zn(1)	129.4(5)	C(2)–N(2)–Zn(1)	108.2(4)
C(5)–N(3)–C(6)	117.4(6)	C(5)–N(3)–Zn(1)	118.9(5)
C(6)–N(3)–Zn(1)	104.5(4)	C(8)–N(4)–C(7)	121.3(6)
C(8)–N(4)–Zn(1)	130.3(5)	C(7)–N(4)–Zn(1)	108.4(4)
W(2)–O(2)–W(1)	117.2(2)	W(3)–O(5)–W(2)	117.8(2)
W(3)–O(9)–W(1)	116.6(2)	W(1)–O(10)–W(3)	89.909(12)
W(1)–O(10)–W(2)	89.951(15)	W(3)–O(10)–W(2)	90.018(16)
O(1)–W(1)–O(9)	103.0(2)	O(1)–W(1)–O(2)	104.6(2)
O(9)–W(1)–O(2)	86.77(19)	O(1)–W(1)–O(10)	178.83(17)
O(9)–W(1)–O(10)	76.85(13)	O(2)–W(1)–O(10)	76.60(13)
O(3)–W(2)–O(2)	103.4(2)	O(3)–W(2)–O(5)	104.6(2)
O(2)–W(2)–O(5)	86.82(19)	O(3)–W(2)–O(4)	104.4(2)
O(2)–W(2)–O(4)	152.15(19)	O(5)–W(2)–O(4)	86.52(19)
O(3)–W(2)–O(10)	179.3(2)	O(2)–W(2)–O(10)	76.27(13)
O(5)–W(2)–O(10)	75.98(13)	O(4)–W(2)–O(10)	75.88(13)
O(7)–W(3)–O(8)	103.9(3)	O(7)–W(3)–O(6)	102.8(2)
O(8)–W(3)–O(6)	86.4(2)	O(8)–W(3)–O(5)	152.73(19)
O(6)–W(3)–O(5)	86.8(2)	O(7)–W(3)–O(9)	104.2(2)
O(8)–W(3)–O(9)	87.1(2)	O(6)–W(3)–O(9)	152.9(2)
O(5)–W(3)–O(9)	87.03(19)	O(7)–W(3)–O(10)	179.04(19)
O(8)–W(3)–O(10)	76.50(14)	O(6)–W(3)–O(10)	76.31(14)
O(5)–W(3)–O(10)	76.23(13)	O(9)–W(3)–O(10)	76.64(13)
N(4)–Zn(1)–N(2)	120.4(2)	N(4)–Zn(1)–N(1)	91.3(2)
N(2)–Zn(1)–N(1)	83.1(2)	N(4)–Zn(1)–N(3)	84.1(2)
N(2)–Zn(1)–N(3)	89.6(2)	N(1)–Zn(1)–N(3)	168.0(2)
N(4)–Zn(1)–Cl(1)	122.47(17)	N(2)–Zn(1)–Cl(1)	117.10(17)
N(1)–Zn(1)–Cl(1)	93.44(18)	N(3)–Zn(1)–Cl(1)	98.43(18)

*****END*****

