Supporting Information

Anion-cation interactions in a series of salts with substituted Hphen, Hbpy and H_2bpy cations and $[W(CN)_8]^{4-}$ anion: polymer with a "super-short" N-H···N hydrogen bridges containing exclusively anions and H^+

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Experimental Procedures

All chemicals, used in the syntheses, were of analytical grade (Aldrich) and were used as supplied. The cation exchange resin Amberlite IR 120 was used to synthesize the H^+ form of $K_4[W(CN)_8]\cdot 2H_2O$. Microanalyses of carbon, hydrogen and nitrogen were performed using Elementar Vario MICRO Cube elemental analyzer. IR spectra were recorded on a Nicolet iS5 FT-IR spectrophotometer. Diffuse reflectance spectra were measured in $BaSO_4$ pellets with $BaSO_4$ as a reference on Shimadzu 3600 spectrophotometer equipped with an ISR-240 integrating sphere attachment. The EPR measurements were performed at room temperature with a Bruker ELEXSYS E-500 spectrometer operating at the X band (9.8 GHz) and 100 kHz magnetic field modulation equipped with super-high-sensitivity cavity ER 4122 SHQE. The EPR parameters of the complexes were determined by X_{epr} software package. The amounts of metal cations were estimated by comparison of the sample spectrum intensity (second integral) with the standard developed in our laboratory.[1, 2] Thermogravimetric measurements were performed on a TGA/SDTA 851e Mettler Toledo Microthermogavimeter at scan speed 10 °/min in the 25 – 700 or 1000 °C range under Ar atmosphere.

Synthesis of $K_4[W(CN)_8]\cdot 2H_2O$

Sodium tungstate(VI) dihydrate (100.0 g, 0.30 mol), KCN (300.0 g, 2.6 mol) and $NaBH_4$ (20.0 g, 0.52 mol) were dissolved in 450 mL of water. To the almost transparent solution (with only traces of undissolved $NaBH_4$), vigorously stirred, 150 mL of acetic acid (80%) was added dropwise in two steps: 20 mL within a period of 1 minute and the rest within 1.5 hours, stopping addition of acid every time as the hydrogen evolution was too fast (till the end of the reaction). The reaction mixture was kept in a water bath to prevent an increase of temperature above 60 °C. Next, another portion of 150 mL of acetic acid was added within 60 minutes. The resultant orange solution (but sometimes greenish) was taken off the water bath and treated with 30% H_2O_2, which was added in 5 ml portions, until the solution color remained constantly dark orange (during this procedure the solution intensively boils). The transparent solution was left cooling in cold water, formed crystals were filtered off on Buchner filter and washed with ca. 100 mL of EtOH. The filtrate was connected with the EtOH used for washing and additional ca. 500 mL of EtOH was added till the end of product precipitation. The mixture was again filtered and the product was washed with EtOH. The crude product was combined together, dissolved in warm water, filtered warm, and precipitated again with EtOH. Yield 168 g, 95%. The purity was confirmed by elemental analysis, IR and UV-Vis spectra.

Table S1. The different synthetic conditions and yield observed for synthesis of $K_4[W(CN)_8]\cdot 2H_2O$. t_1-t_5 denotes period of time where acetic acid of volume V_1-V_5 was added.

$Na_2WO_4\cdot 2H_2O$	$NaBH_4$	KCN	water	time	CH_3COOH	time	CH_3COOH	yield	
[g]	[g]	[g]	[ml]	t_1/t_2 [min]	V_1/V_2 [ml]	$t_3/t_4/t_5$ [min]	$V_3/V_4/V_5$ [ml]	[g]	[%]
50.23	9.58	87.83	150	30	50	60	100	32.70	36.75
50.01	12.28	94.87	150	60	50	20	100	37.50	42.33
50.00	10.04	89.91	150	46	75	34	75	53.20	60.07
50.03	10.04	90.18	150	60	75	30	75	53.20	60.03
49.98	10.48	90.98	150	60	75	30	75	61.28	69.22
49.99	10.05	91.03	150	75	75	20	75	45.80	51.72

100.03	20.38	181.30	300	65	150	90	150	83.58	47.17
100.16	20.05	181.27	300	45/60	75/75	30	150	81.01	45.66
50.01	10.12	92.12	150	60	60	30	45	32.50	36.69
50.03	10.08	91.02	150	60	75	35	45	46.30	52.24
49.77	10.01	92.02	150	60	60	30	60	43.78	49.66
50.03	10.11	91.25	300	60	60	30	60	35.62	40.19
50.21	10.23	150.41	300	60	60	30	90	67.90	76.34
50.12	10.21	150.80	200	60	60	30	90	66.07	74.42
50.12	10.11	150.20	225	60	50	30	100	45.00	50.69
50.17	10.11	163.02	220	60	50	30	100	99.00	111.40
51.01	10.18	132.00	220	60	50	30	100	53.25	58.93
51.03	10.30	153.41	250	60	50	30	100	25.90	28.65
50.07	9.98	154.23	300	60	60	30	90	69.00	77.80
50.18	10.00	151.37	250	60	60	30	90	69.50	78.19
100.02	20.18	301.24	500	60	150	30	150	119.61	67.51
100.01	20.03	301.49	500	90	150	45	150	131.13	74.02
100.00	20.12	303.02	450	30	50	90/15	100/150	139.08	78.51
100.04	19.97	302.67	450	1/100	20/130	60	150	167.72	94.64
100.49	20.10	300.10	450	130	100	50	100	150.74	84.68
100.06	20.04	201.07	450	50	30	50/30/30	15/75/125	129.51	73.07
100.13	20.22	301.38	450	50	70	30/60	8/150	90.48	51.01
100.04	20.01	300.57	450	1/100	20/130	60	150	166.81	94.13
99.98	19.99	299.98	450	1/100	20/130	60	150	168.25	95.00
100.02	20.05	300.01	450	1/100	20/130	60	150	169.01	95.39

Preparation of the salts 1-9

The $K_4[W(CN)_8]\cdot 2H_2O$ (0.2 g, 0.34 mmol) was dissolved in water (ca. 5 mL) and passed through Amberlite IR 120 ion exchange resin in the H^+ form. To the resulting solution respective cation (1.4 mmol) and 2 drops of 2M HCl were added and the mixture was left for crystallization. The products were filtrated, washed with acetone (Me_2CO), and dried in the air. The yield was almost quantitative, in all cases was ca. 95±2%. The formulas of the cations are presented in Fig. S1.

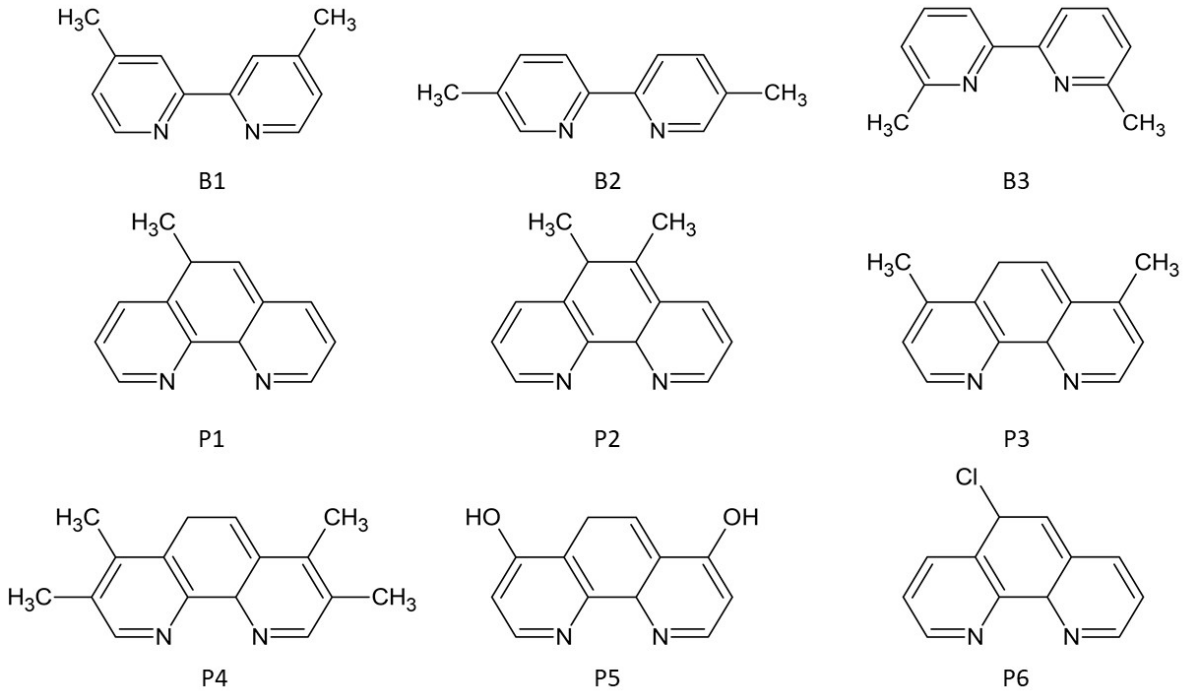

Fig. S1. The formulas of B1-P6 cations used in syntheses.

Crystallographic data collection and structure refinement

Diffraction intensity data for a single crystal of **1**, **3a** and **3b** were collected at 100(2), 130(2) and 99.98(13) K respectively on the SuperNova (Rigaku) diffractometer with mirror-monochromated Cu Kα radiation (λ = 1.54184 Å) for **1** and Mo Kα radiation (λ = 0.71073 Å) for **3a** and **3b**. Cell refinement and data reduction were performed using CrysAlisPro firmware.[3-5] Positions of all of non-hydrogen atoms were determined by direct methods using SHELXL-2017/1.[6, 7] All non-hydrogen atoms were refined anisotropically using weighted full-matrix least-squares on F^2. Refinement and further calculations were carried out using SHELXL-2017/1.[6, 7] All hydrogen atoms joined to carbon atoms were positioned with idealized geometries and refined using a riding model with U_{iso}(H) fixed at 1.2 U_{eq} (C_{arom}). Due to the dynamic disorder of the O4 water molecule in structure **3a**, it was not possible to determine the positions of the hydrogen atoms for this molecule from the differential Fourier map. The figures were made using Diamond ver. 4.6.1 software.[8] CCDC 2075584, 2084630 and 2075764 contain the supplementary crystallographic data for **1**, **3a** and **3b** respectively. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Results and Discussion

Table S2. Crystal data and structure refinement for **1**, **3a** and **3b**.

		1	**3a**	**3b**
Empirical formula		$C_{44}H_{44}N_{14}O_2W$	$C_{44}H_{45}N_{14}O_4W$	$C_{20}H_{20}N_{10}O_2W$
Formula weight		984.78	1017.79	616.31
Temperature [K]		100(2)	130(2)	99.98(13)
Wavelength [Å]		1.54184	0.71073	0.71073
Crystal system		Monoclinic	Monoclinic	Orthorhombic
Space group		P 21/n	P 21/n	P bca
Unit cell dimensions	**a [Å]**	17.3221(1)	17.4930(1)	15.3579(1)
	b [Å]	10.9893(1)	12.5476(1)	14.2995(1)
	c [Å]	22.6042(1)	21.7724(2)	20.5069(2)
	α [°]	90	90	90
	β [°]	90.158(1)	109.047(1)	90
	γ [°]	90	90	90
Volume [Å^3]		4302.87	4517.29(7)	4503.53(6)
Z		4	4	8
Density (calculated) [Mg/m^3]		1.520	1.497	1.818
Absorption coefficient [mm^{-1}]		5.421	2.616	5.170
F(000)		1984	2052	2400
Crystal size [mm^3]		1.00 × 0.10 × 0.10	0.10 × 0.10 × 0.10	0.20 × 0.10 × 0.10
Theta range for data collection [°]		3.210 to 77.064	2.545 to 30.556	1.986 to 33.460
Index ranges		-21 ≤ h ≤ 21 -13 ≤ k ≤ 13 -28 ≤ l ≤ 28	-24 ≤ h ≤ 24 -17 ≤ k ≤ 17 -30 ≤ l ≤ 30	-23 ≤ h ≤ 22 -22 ≤ k ≤ 21 -31 ≤ l ≤ 31
Reflections collected		128751	74967	271737
Independent reflections		9045 [R_{int} = 0.0851]	13157 [R_{int} = 0.0345]	8480 [R_{int} = 0.0745]
Completeness to theta [%]		100.0	99.7	99.9
Refinement method		Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Semi-empirical from equivalents
Data / restraints / parameters		9045/0/580	13157/0/574	8480/0/324
Goodness-of-fit on F2		1.083	1.105	1.028
Final R indices [I>2σ(I)]		R_1 = 0.0289 wR_2 = 0.0757	R_1 = 0.0290 wR_2 = 0.0635	R_1 = 0.0187 wR_2 = 0.0394
R indices (all data)		R_1 = 0.0293 wR_2 = 0.0760	R_1 = 0.0382 wR_2 = 0.0678	R_1 = 0.0242 wR_2 = 0.0406
Largest diff. peak and hole [e/Å^3]		0.832 and -2.456	1.676 and -0.914	0.914 and -1.240

Table S3. The selected bond lengths and angles for **1**, **3a** and **3b** [Å and °].

1		**3a**		**3b**	
bond lengths [Å]					
W(1)-C(19)	2.160(2)	W(1)-C(1)	2.165(3)	W(1)-C(5)	2.1682(15)
W(1)-C(49)	2.177(2)	W(1)-C(2)	2.174(3)	W(1)-C(21)	2.1440(15)
W(1)-C(51)	2.163(2)	W(1)-C(3)	2.172(3)	W(1)-C(23)	2.1631(15)
W(1)-C(53)	2.158(2)	W(1)-C(4)	2.161(3)	W(1)-C(25)	2.1620(15)
W(1)-C(55)	2.168(2)	W(1)-C(5)	2.165(3)	W(1)-C(27)	2.1652(15)
W(1)-C(57)	2.162(2)	W(1)-C(6)	2.164(3)	W(1)-C(29)	2.1569(15)
W(1)-C(59)	2.159(2)	W(1)-C(7)	2.168(3)	W(1)-C(31)	2.1585(15)
W(1)-C(61)	2.177(2)	W(1)-C(8)	2.165(3)	W(1)-C(33)	2.1605(15)
N(18)-C(19)	1.156(3)	N(1)-C(1)	1.142(4)	N(4)-C(5)	1.154(2)
N(48)-C(49)	1.154(3)	N(2)-C(2)	1.149(4)	N(20)-C(21)	1.150(2)
N(50)-C(51)	1.154(3)	N(3)-C(3)	1.150(4)	N(22)-C(23)	1.152(2)
N(52)-C(53)	1.158(4)	N(4)-C(4)	1.143(4)	N(24)-C(25)	1.155(2)
N(54)-C(55)	1.145(3)	N(5)-C(5)	1.147(4)	N(26)-C(27)	1.160(2)
N(56)-C(57)	1.149(3)	N(6)-C(6)	1.152(4)	N(28)-C(29)	1.1547(19)
N(58)-C(59)	1.155(3)	N(7)-C(7)	1.150(4)	N(30)-C(31)	1.1547(19)
N(60)-C(61)	1.153(3)	N(8)-C(8)	1.146(4)	N(32)-C(33)	1.156(2)
angles [°]					
N(18)-C(19)-W(1)	177.1(2)	N(1)-C(1)-W(1)	179.0(3)	N(4)-C(5)-W(1)	178.69(13)
N(48)-C(49)-W(1)	174.4(2)	N(2)-C(2)-W(1)	178.1(2)	N(20)-C(21)-W(1)	178.29(14)
N(50)-C(51)-W(1)	178.7(2)	N(3)-C(3)-W(1)	179.4(3)	N(22)-C(23)-W(1)	178.46(14)
N(52)-C(53)-W(1)	176.2(2)	N(4)-C(4)-W(1)	176.1(3)	N(24)-C(25)-W(1)	173.12(13)
N(54)-C(55)-W(1)	178.7(2)	N(5)-C(5)-W(1)	178.0(3)	N(26)-C(27)-W(1)	175.12(13)
N(56)-C(57)-W(1)	178.2(2)	N(6)-C(6)-W(1)	177.7(3)	N(28)-C(29)-W(1)	173.60(14)
N(58)-C(59)-W(1)	175.8(2)	N(7)-C(7)-W(1)	177.6(3)	N(30)-C(31)-W(1)	177.74(13)
N(60)-C(61)-W(1)	175.7(2)	N(8)-C(8)-W(1)	178.3(3)	N(32)-C(33)-W(1)	177.10(13)

Table S4. The hydrogen bonds for **1**, **3a** and **3b** [Å and °].

D-H...A	**d(D-H)**	**d(H...A)**	**d(D...A)**	**<(DHA)**
1				
N(9)-H(9N)...N(58)	0.88	2.16	2.898(3)	140.5
N(25)-H(25N)...N(48)	0.88	2.22	2.976(3)	143.2
C(27)-H(27)...N(50)#1	0.95	2.64	3.590(3)	176.7
C(21)-H(21)...N(50)#1	0.95	2.44	3.391(3)	174.7
C(41)-H(41)...N(18)#2	0.95	2.54	3.444(3)	160.0
C(36)-H(36)...N(18)#2	0.95	2.41	3.331(3)	162.4
C(8)-H(8)...N(60)	0.95	2.67	3.505(4)	146.4
C(13)-H(13)...N(60)#3	0.95	2.61	3.340(4)	133.7
C(24)-H(24)...N(52)	0.95	2.46	3.267(3)	143.2
O(2)-H(2B)...N(50)#4	0.87(4)	2.07(4)	2.933(3)	172(3)
O(2)-H(2A)...N(48)	0.78(6)	2.32(6)	3.094(3)	174(5)
N(34)-H(34N)...N(58)#5	0.82(3)	2.03(3)	2.738(3)	145(3)
O(1)-H(1A)...N(54)	0.92(6)	1.66(6)	2.565(3)	165(5)
O(1)-H(1B)...N(52)#6	0.86(6)	1.80(6)	2.648(3)	170(6)
O(1)-H(1C)...N(56)#7	0.96(4)	1.58(4)	2.543(3)	173(3)
3a				
N(10)-H(10N)...O(2)#1	0.90	1.89	2.765(3)	164.8
C(12)-H(12)...O(3)#2	0.95	2.61	3.535(4)	164.1
C(15)-H(15A)...O(2)#1	0.98	2.46	3.076(4)	120.1
C(16)-H(16)...O(1)#3	0.95	2.52	3.438(4)	162.8
N(12)-H(123)...N(11)	0.78	2.25	2.630(4)	110.1
N(12)-H(123)...O(4)	0.78	2.22	2.904(4)	145.6
C(24)-H(24)...O(1)	0.95	2.58	3.505(4)	163.1
C(26)-H(26)...O(3)#4	0.95	2.61	3.512(4)	159.5
N(13)-H(13N)...N(1)#4	0.88	2.03	2.871(3)	161.1
C(38)-H(38)...N(4)#5	0.95	2.48	3.360(4)	154.6
C(39)-H(39C)...N(5)#4	0.98	2.69	3.562(4)	148.4

C(40)-H(40)...N(4)#5	0.95	2.61	3.452(4)	147.8
C(42)-H(42)...N(6)#6	0.95	2.44	3.309(4)	152.0
O(1)-H(1AO)...N(5)#4	0.79	2.09	2.871(3)	169.7
O(1)-H(1BO)...N(3)	0.81	2.06	2.858(3)	170.7
O(2)-H(2AO)...N(8)#7	0.77	2.12	2.877(3)	171.8
O(2)-H(2BO)...O(1)	0.84	1.95	2.779(3)	166.8
O(3)-H(3BO)...N(2)#6	0.82	2.11	2.928(3)	169.2
O(3)-H(3AO)...N(7)#4	0.84	2.09	2.929(4)	176.1
3b				
N(6)-H(6)...N(24)#1	0.88	2.02	2.8938(18)	176.4
N(17)-H(17)...O(1)	0.88	1.80	2.6718(18)	173.4
C(13)-H(13)...N(24)#1	0.95	2.68	3.158(2)	111.9
C(8)-H(8)...O(1)	0.95	2.56	3.103(2)	116.5
C(18)-H(18A)...N(22)	0.98	2.63	3.471(2)	144.1
C(10)-H(10)...N(22)#2	0.95	2.53	3.372(2)	147.9
O(2)-H(2A)...N(28)	0.93(3)	1.66(3)	2.5870(17)	176(3)
O(2)-H(2C)...N(4)#3	0.85(3)	1.79(3)	2.6303(18)	169(3)
O(1)-H(1B)...N(22)#4	0.82(3)	2.09(3)	2.902(2)	168(2)
O(1)-H(1A)...N(32)	0.88(3)	1.95(3)	2.8122(19)	169(3)
O(2)-H(2B)...N(30)#5	0.91(3)	1.69(3)	2.5924(17)	176(3)
N(20)-H(20N)...N(26)#6	0.97(4)	1.68(4)	2.6510(19)	174(3)

Table S5. The π…π interactions for compounds **1** and **3a** [Å].

compound	**π…π**	**d(π…π)**	**shift**	**description**
1	Cg1···Cg2 Cg2···Cg1 Cg2···Cg2 [1-x,1-y,-z] Cg3···Cg3 [1-x,y,1-z] Cg3···Cg4 [1-x,-y,1-z] Cg4···Cg3 [1-x,-y,1-z]	3.4926(1) 3.4926(1) 3.6465(1) 3.9633(1) 3.9991(1) 3.9991(1)	0.591 0.819 1.625 2.176 2.396 2.200	Cg1: N(15)-C(10)-C(11)-C(12)-C(13)-C(14) Cg2: N(25)-C(20)-C(21)-C(22)-C(23)-C(24) Cg3: N(34)-C(35)-C(36)-C(37)-C(38-C(39) Cg4: N(45)-C(40)-C(41)-C(42)-C(43)-C(44)
3a	Cg1···Cg2 [1-x,-y,1-z] Cg1···Cg6 [1/2+x,1/2-y,1/2+z] Cg2···Cg1 [1-x,-y,1-z] Cg2···Cg5 [1/2+x,1/2-y,1/2+z] Cg3···Cg4 [-x,1-y,1-z] Cg3···Cg5 [1/2-x,1/2+y,1/2-z] Cg4···Cg3 [-x,1-y,1-z] Cg5···Cg3 [1/2-x,-1/2+y,1/2-z] Cg6···Cg1 [-1/2+x,1/2-y,-1/2+z]	3.5777(1) 3.6975(1) 3.5777(1) 4.0528(1) 3.6241(1) 3.7944(1) 3.6241(1) 3.7944(1) 3.6975(1)	-0.961 1.528 0.878 1.742 1.581 1.505 1.173 1.330 1.189	Cg1: N9-C9-C16-C17-C18-C19 Cg2: N10-C10-C14-C13-C12-C11 Cg3: N11-C21-C28-C29-C30-C31 Cg4: N12-C22-C26-C25-C24-C23 Cg5: N13-C33-C40-C41-C42-C43 Cg6: N14-C34-C38-C37-C36-C35

Table S6. The C-H…π interactions for compound **1** and **3a** [Å and °].

compound	**C-H…π**	**H···Cg**	**X···Cg**	**X-H···Cg**
1	C(14)-H(14)···Cg3 [3/2-x,1/2+y,1/2-z] C(16)-H(16A)···Cg5 [3/2-x,1/2+y,1/2-z] C(17)-H(17B)···Cg1 [3/2-x,-1/2+y,1/2-z]	2.81 2.98 2.90	3.5882(1) 3.8415(1) 3.3942(1)	139 148 112
3a	C27-H27A···Cg6 [1/2-x,1/2+y,1/2-z]	2.96	3.6458(1)	128

Cg5: N(9)-C(4)-C(5)-C(6)-C(7)-C(8)

Thermogravimetric measurements

Table S7. The TG data for complexes **1**-**9**. Scan speed 10° /min.

Complex	m [mg]	T_{max} [°C]	Δm_{exp} [%]	Δm_{calc} [%]	Attributed to
1	18.8767				
	17.8825	100	5.21	5.29	$3H_2O$
	14.1452	218	24.94	25.19	$4H_2O$ + bpy
	8.5922	462	54.56	54.22	$4H_2O$ + 2.6bpy
	7.0944	723	62.50	61.48	$4H_2O$ + 3bpy
2	15.9067				
	15.2634	125	4.04	4.25	$2.5H_2O$
	7.8724	253	50.51	50.53	$5H_2O$ + 2.3bpy
	4.2678	700	73.17	72.75	$5H_2O$ + 3bpy + $2C_2N_2$
3a	34.1866				
	32.4744	115	5.16	5.29	$3H_2O$
	25.5762	206	25.79	25.22	$4H_2O$ + bpy
	13.0268	364	61.90	61.54	$4H_2O$ + 3bpy
	7.5587	995	77.69	76.84	$4H_2O$ + 3bpy + $3C_2N_2$
3b	7.4814				
	7.0498	149	5.75	5.84	$2H_2O$
	4.8058	255	35.92	35.92	$2H_2O$ + bpy
	3.8939	452	48.08	48.66	$2H_2O$ + bpy + $2.5C_2N_2$
	3.2656	745	56.60	56.31	$2H_2O$ + bpy + $4C_2N_2$
4	19.0593				
	17.7650	164	6.79	6.89	Me_2CO
	15.9528	235	16.30	16.16	Me_2CO + 0.4phen
	11.6858	420	38.69	39.35	Me_2CO + 1.4phen
	9.990	770	47.61	48.62	Me_2CO + 1.8phen
5	15.3992				
	14.8765	84	3.39	3.29	$2H_2O$
	14.6628	156	4.78	4.94	$3H_2O$
	11.5927	301	24.72	24.17	$3H_2O$ + phen
	8.8362	505	42.62	43.41	$3H_2O$ + 2phen
	7.4197	800	51.82	53.02	$3H_2O$ + 2.5phen
6	10.6536				
	9.5491	156	10.37	10.75	$4H_2O$ + Me_2CO
	8.0928	261	24.04	24.24	$4H_2O$ + $2Me_2CO$ + 0.5phen
	6.2251	343	41.57	41.63	$4H_2O$ + $2Me_2CO$ + 1.5phen
	4.8099	430	54.85	54.79	$4H_2O$ + $2Me_2CO$ + 2phen + C_2N_2
	1.9037	996	82.13	81.11	$4H_2O$ + $2Me_2CO$ + 3phen + $3C_2N_2$
7	18.2263				
	16.9756	137	6.86	6.56	$7H_2O$
	15.0459	260	17.44	17.81	$19H_2O$
	6.3697	430	65.05	67.05	$19H_2O$ + 4phen
	4.9935	803	72.60	73.82	$19H_2O$ + 5phen
8	28.3737				
	26.6914	183	5.93	6.08	$6H_2O$
	24.7867	275	12.64	12.05	$6H_2O$ + 0.5phen
	21.1798	440	25.35	23.99	$6H_2O$ + 1.5phen
	16.6955	802	41.16	41.90	$6H_2O$ + 3phen
9	17.9729				
	16.8120	112	6.46	6.73	$4.5H_2O$
	15.6637	190	12.85	13.48	$9H_2O$
	14.0059	248	22.07	22.45	$9H_2O$ + 0.5phen
	10.8893	437	39.41	40.40	$9H_2O$ + 1.5phen
	7.9341	773	55.85	56.55	$9H_2O$ + 2.4phen

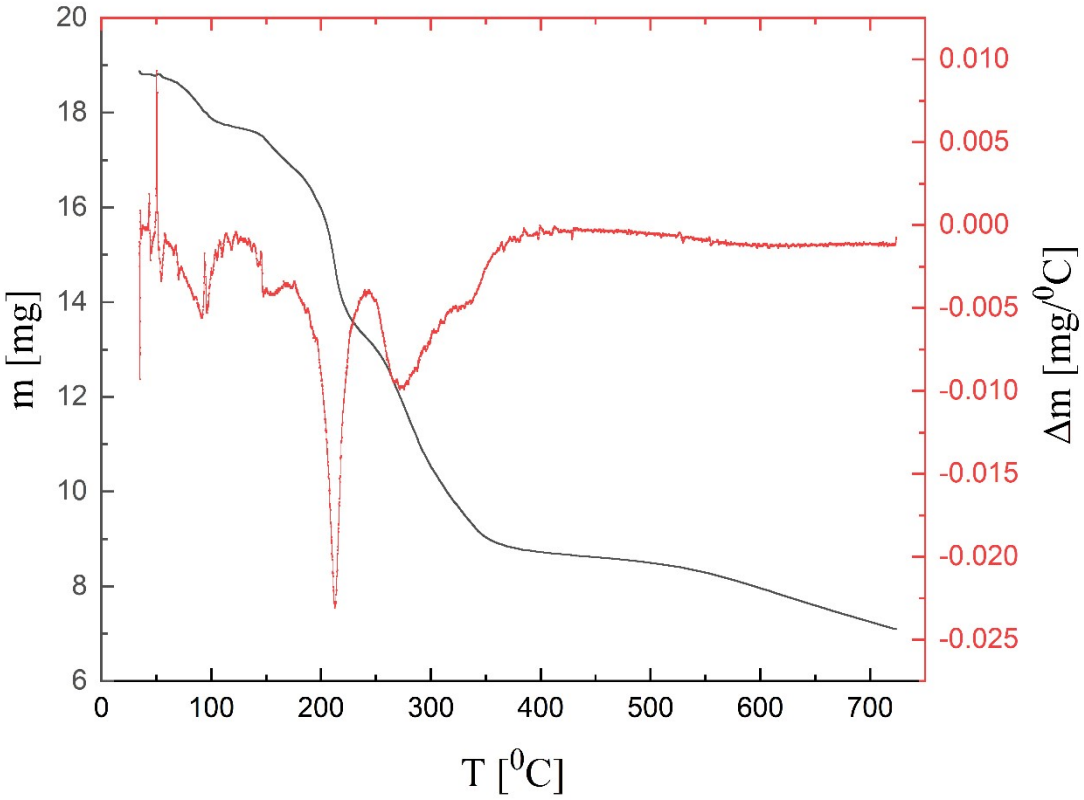

Fig S2. The TG and DTG curves for **1**.

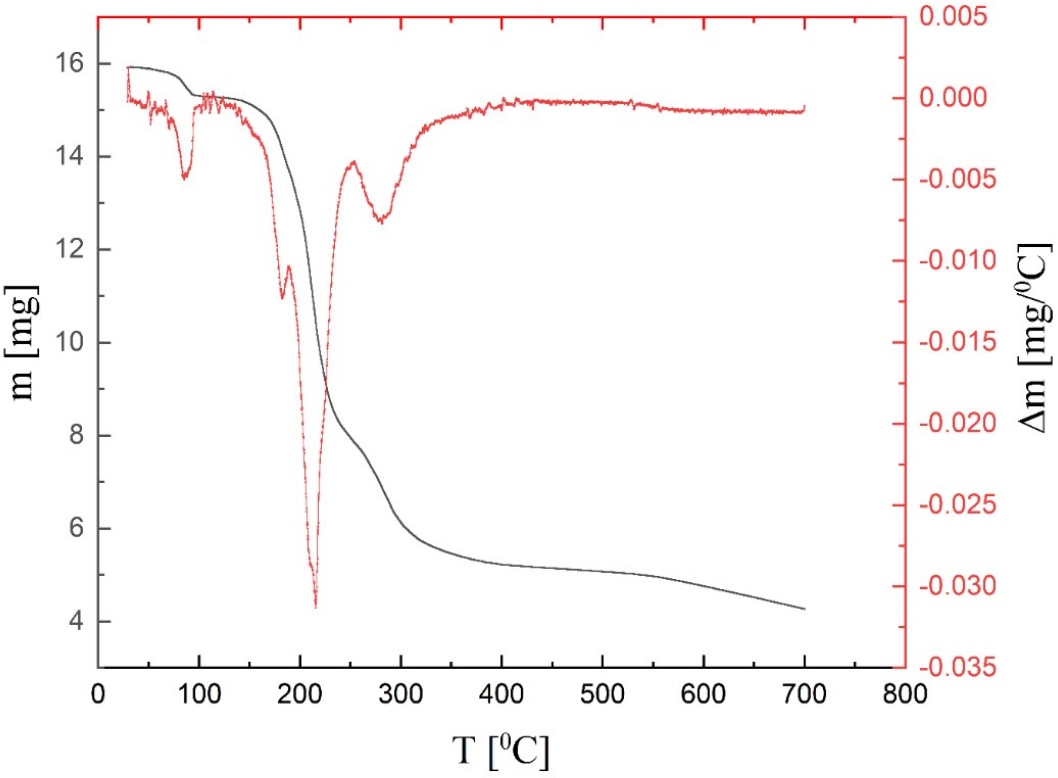

Fig S3. The TG and DTG curves for **2**.

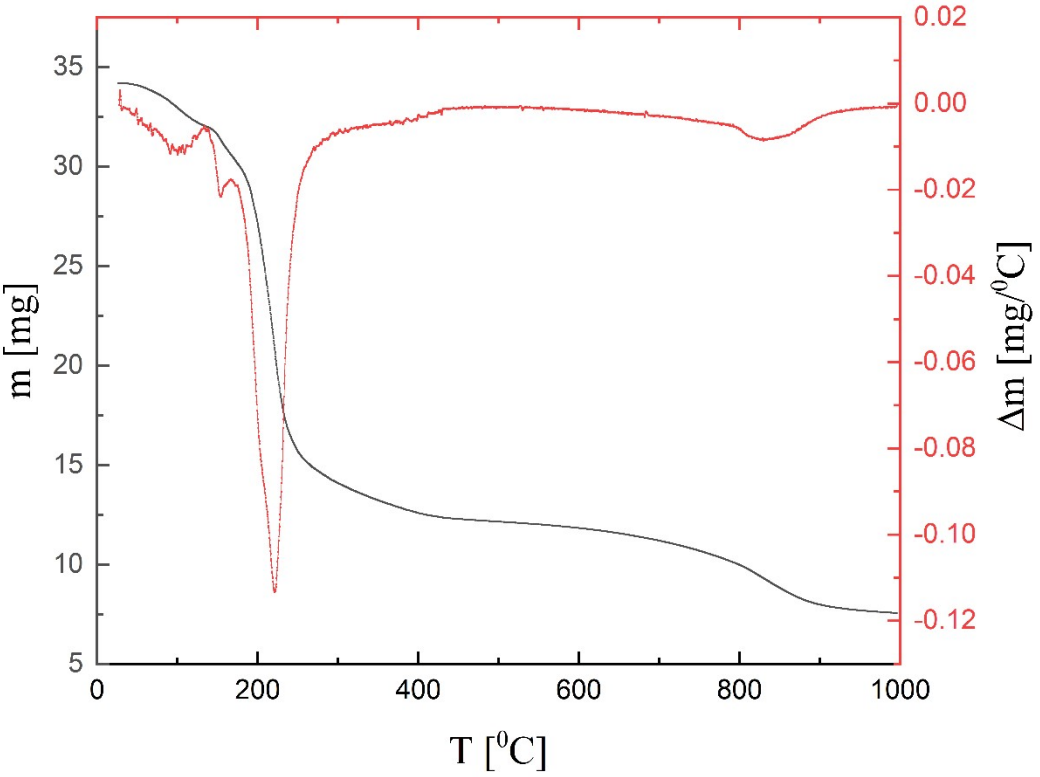

Fig S4. The TG and DTG curves for **3a**.

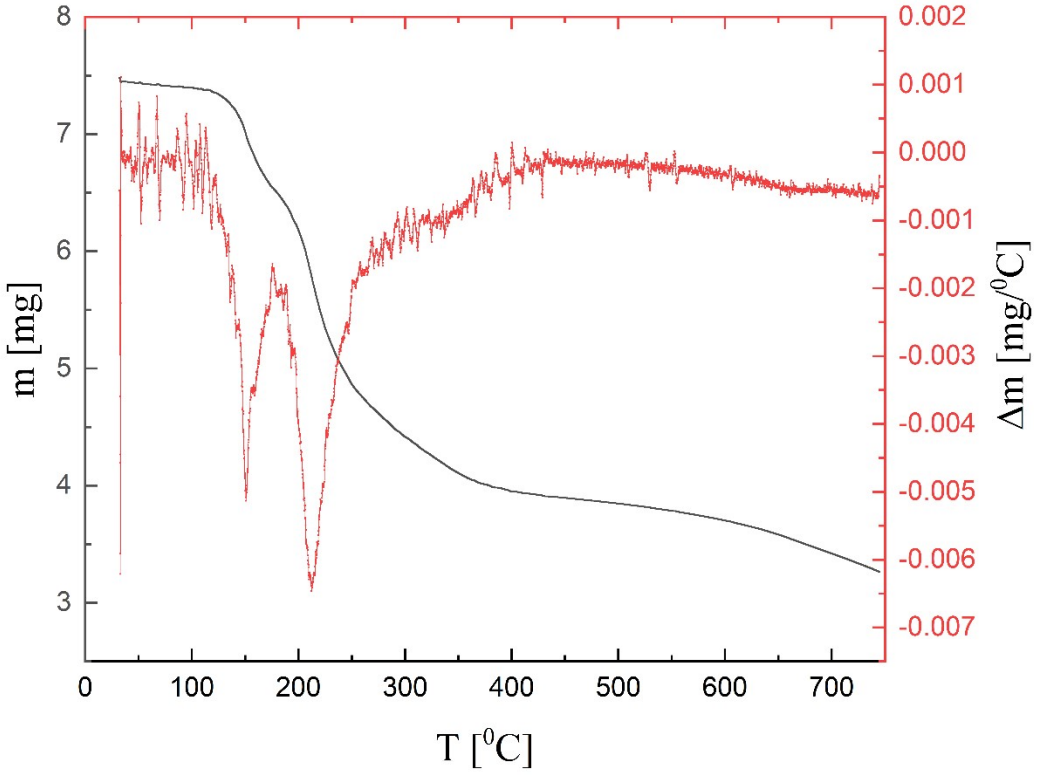

Fig S5. The TG and DTG curves for **3b**.

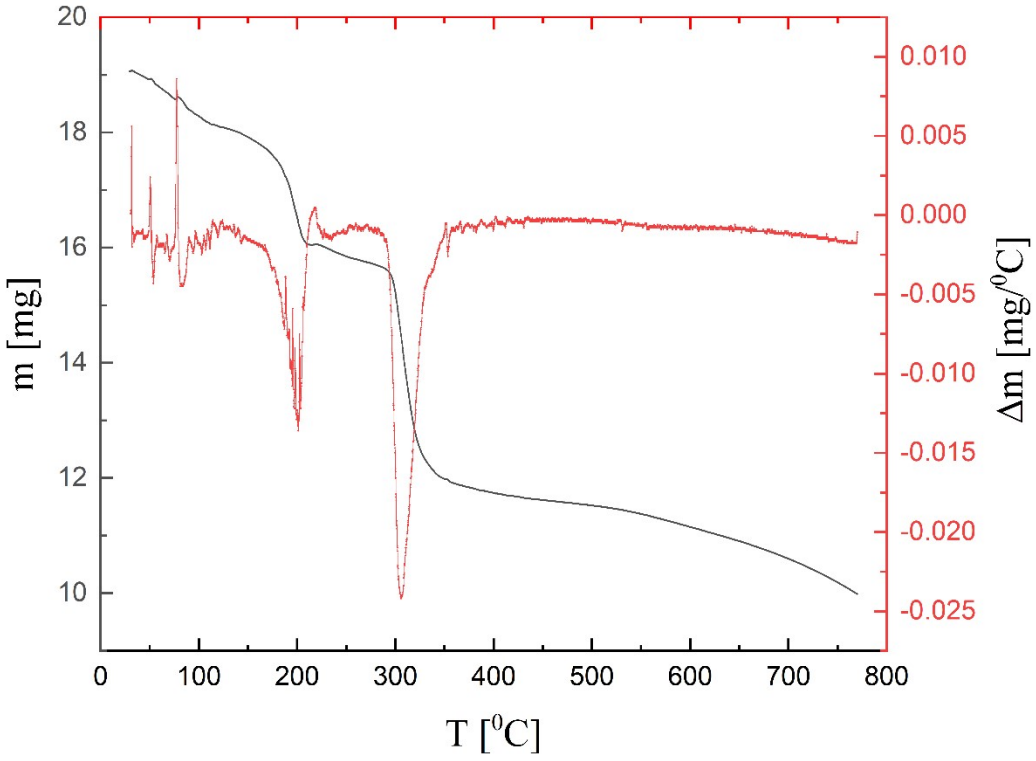

Fig S6. The TG and DTG curves for **4**.

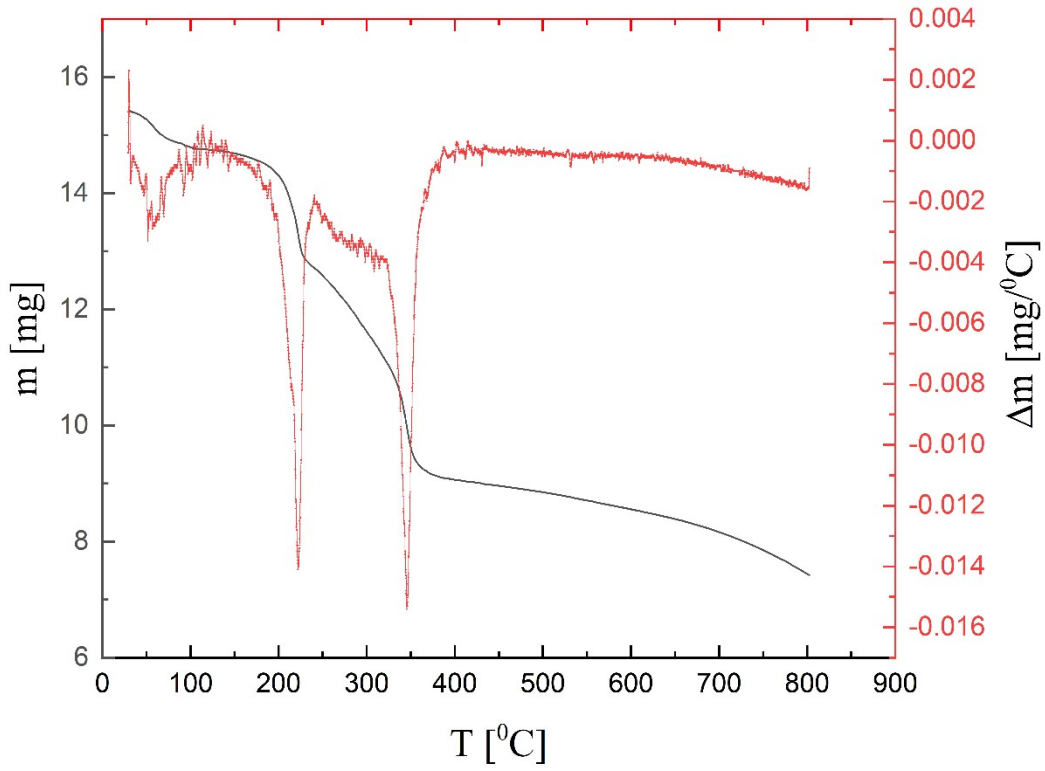

Fig S7. The TG and DTG curves for **5**.

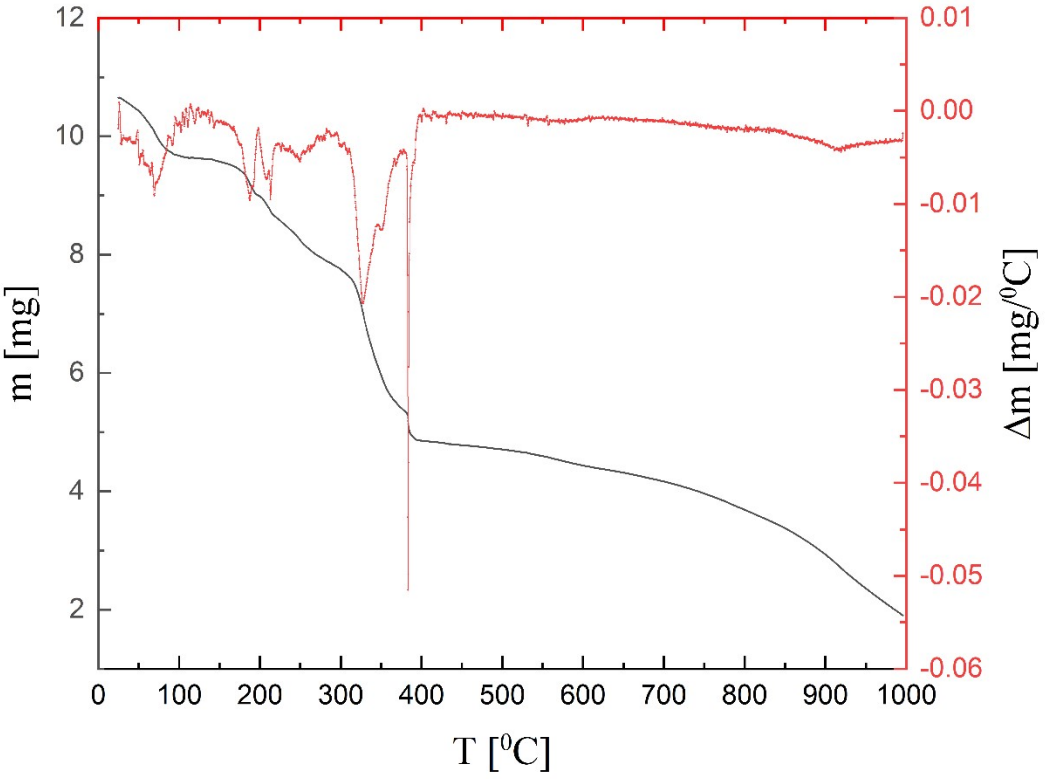

Fig S8. The TG and DTG curves for **6**.

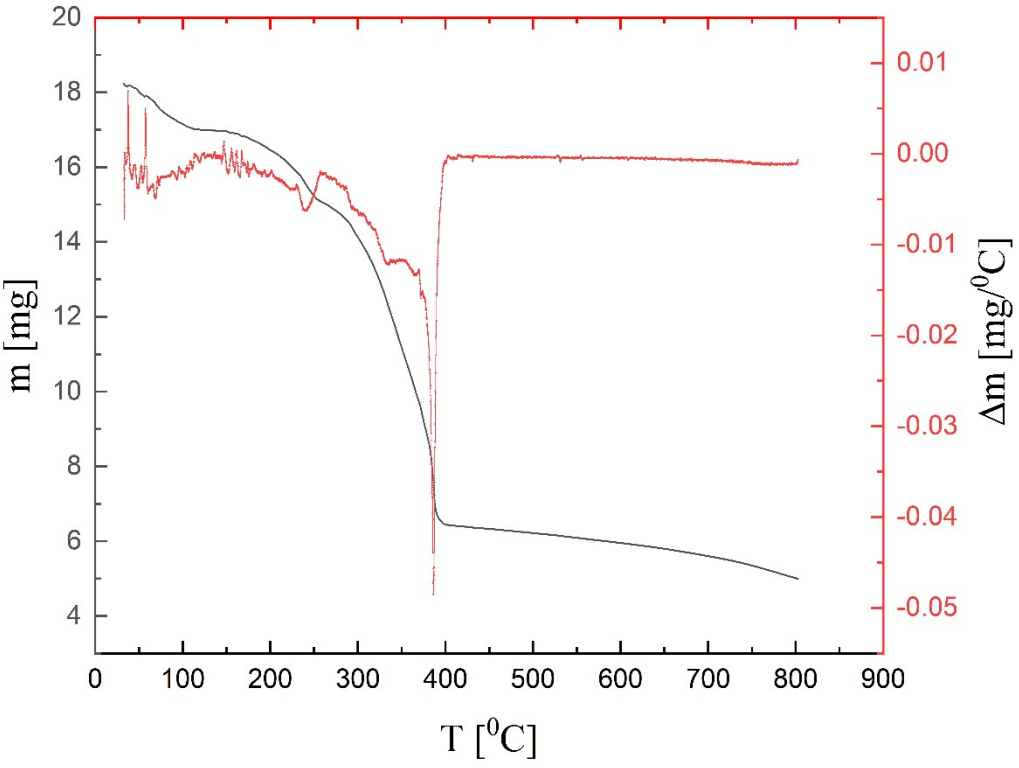

Fig S9. The TG and DTG curves for **7**.

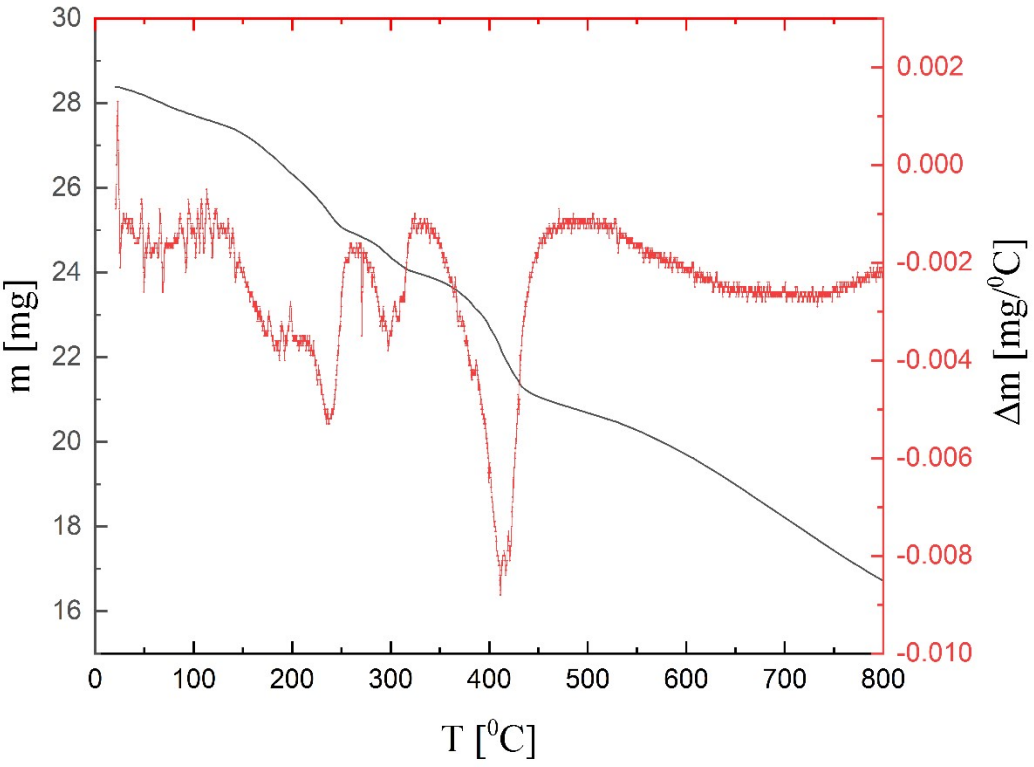

Fig S10. The TG and DTG curves for **8**.

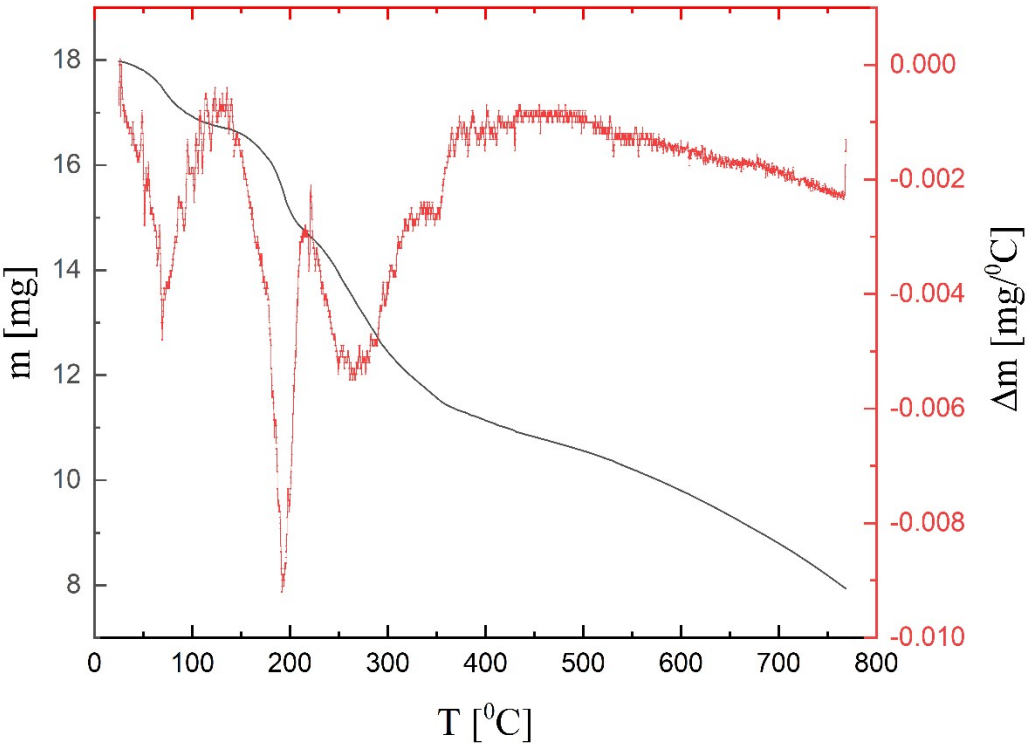

Fig S11. The TG and DTG curves for **9**.

IR spectra

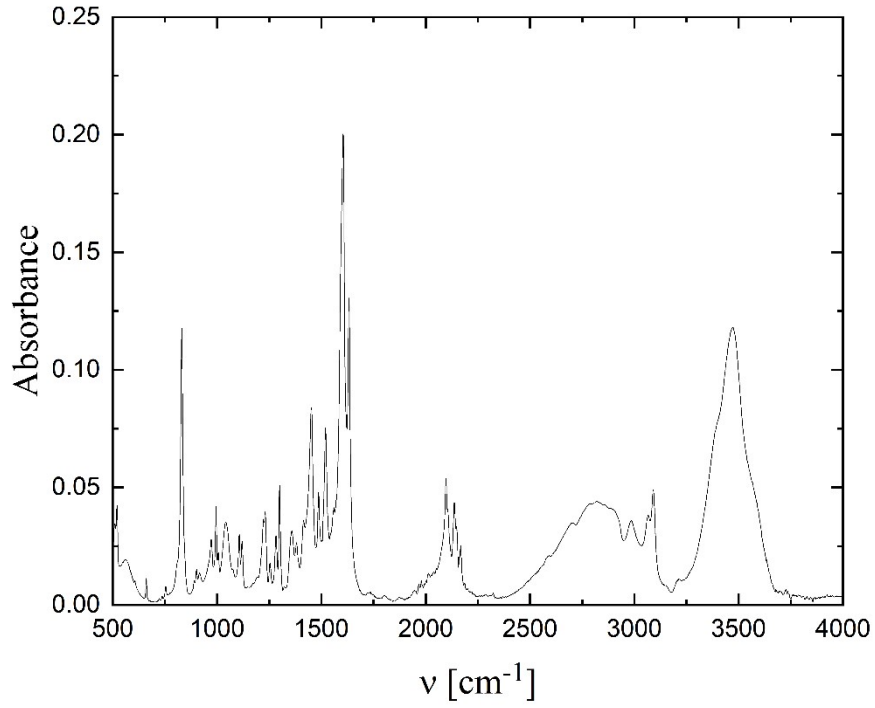

Fig S12. IR spectrum of **1**.

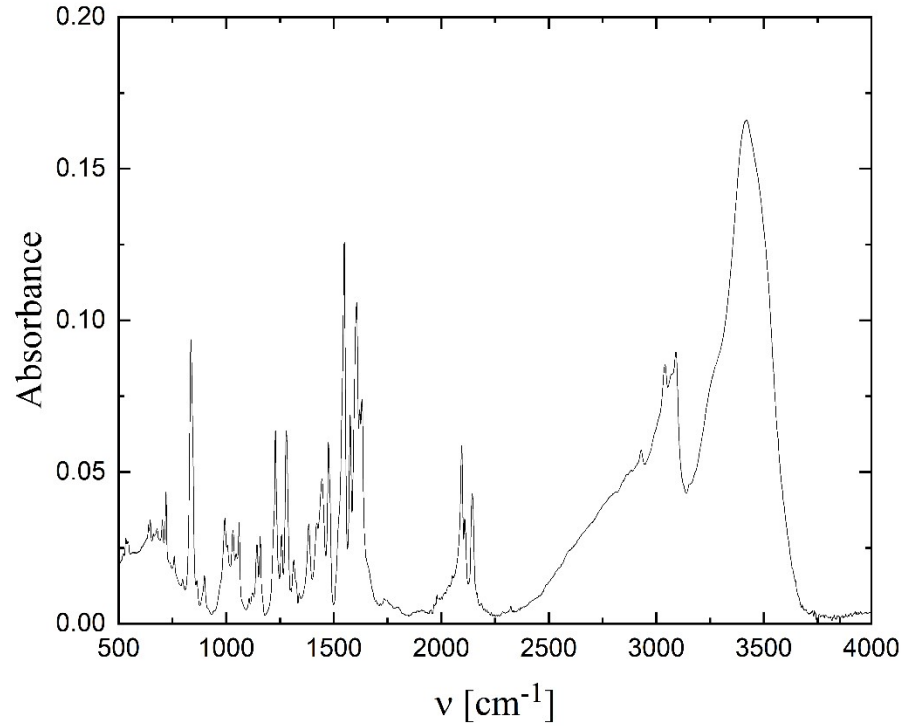

Fig S13. IR spectrum of **2**.

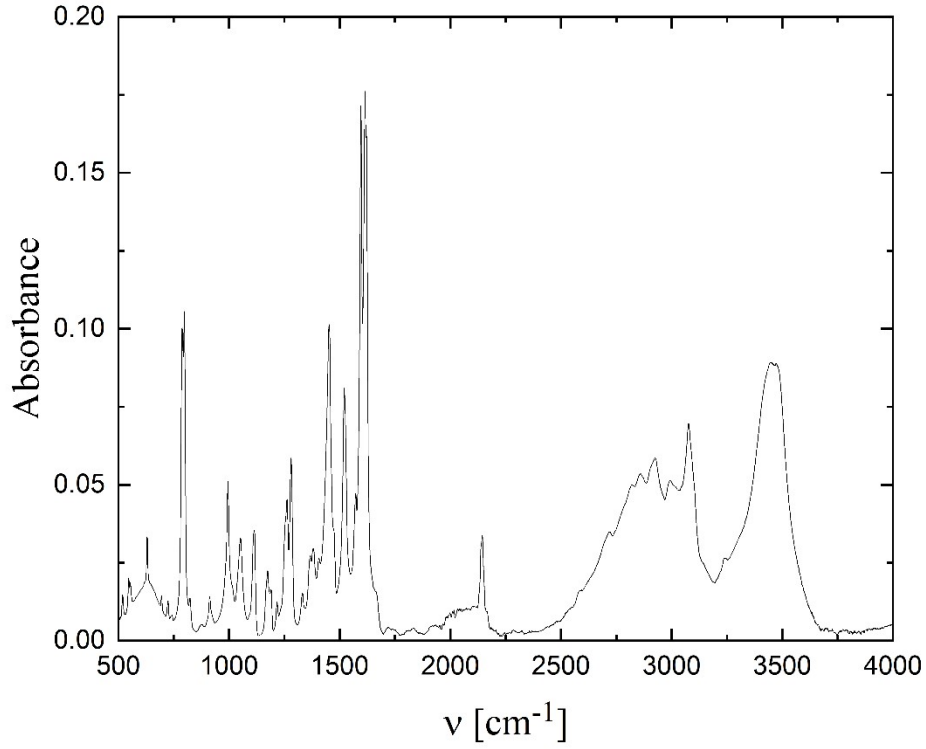

Fig S14. IR spectrum of **3a**.

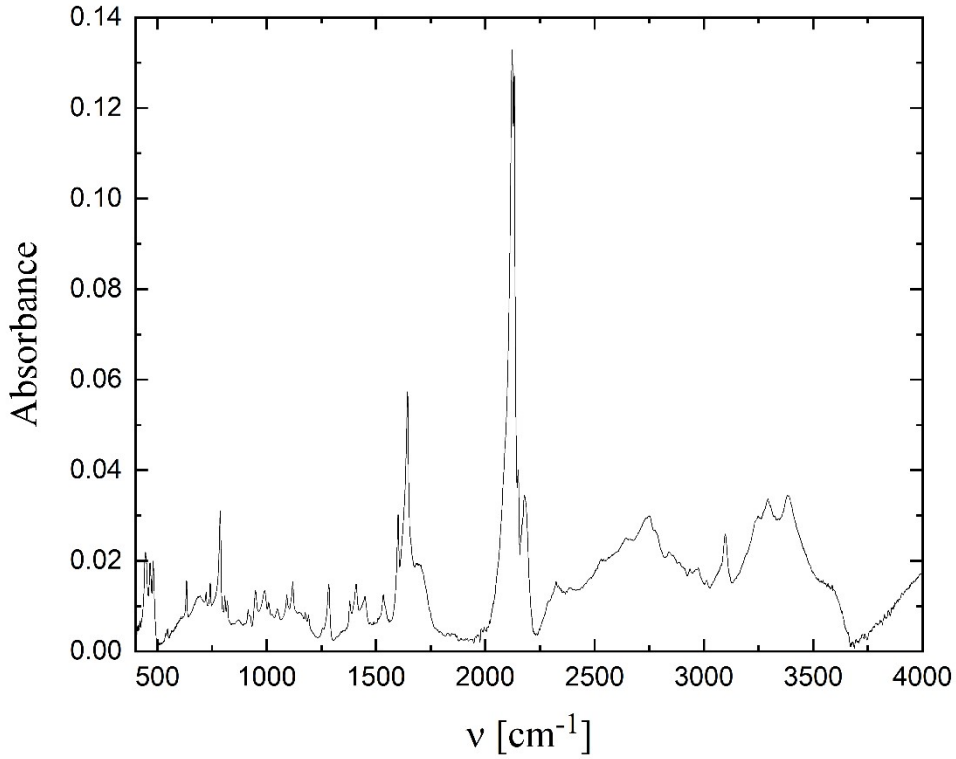

Fig S15. IR spectrum of **3b**.

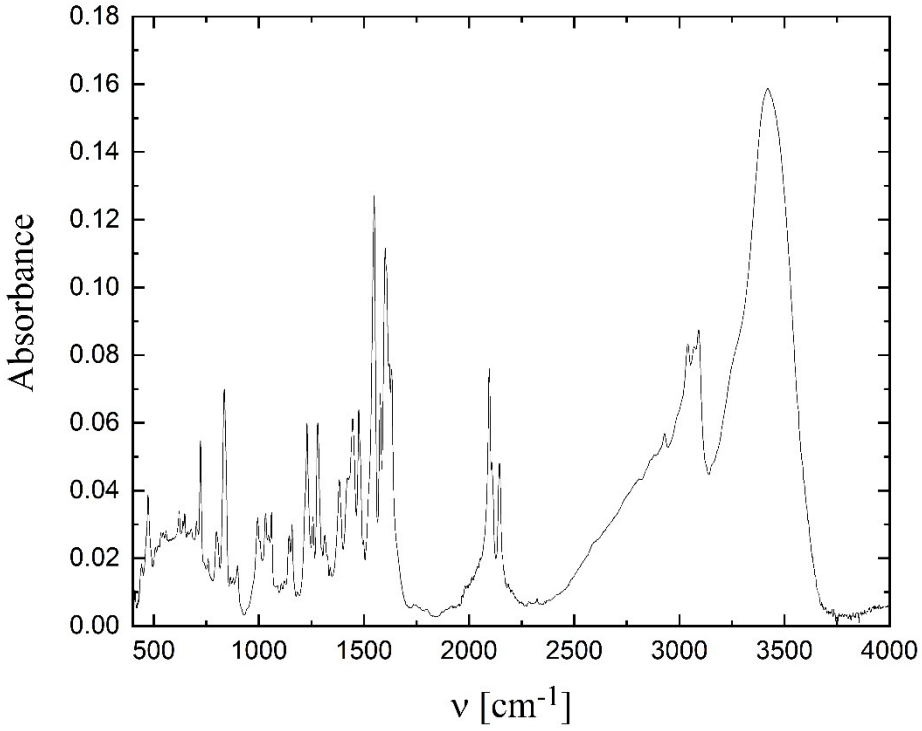

Fig S16. IR spectrum of **4**.

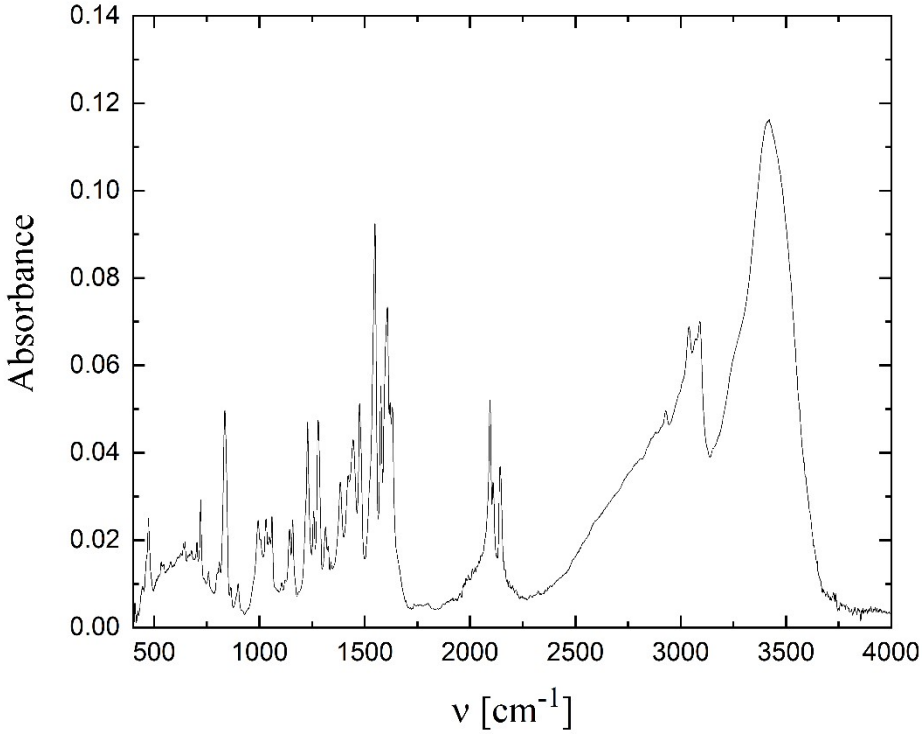

Fig S17. IR spectrum of **5**.

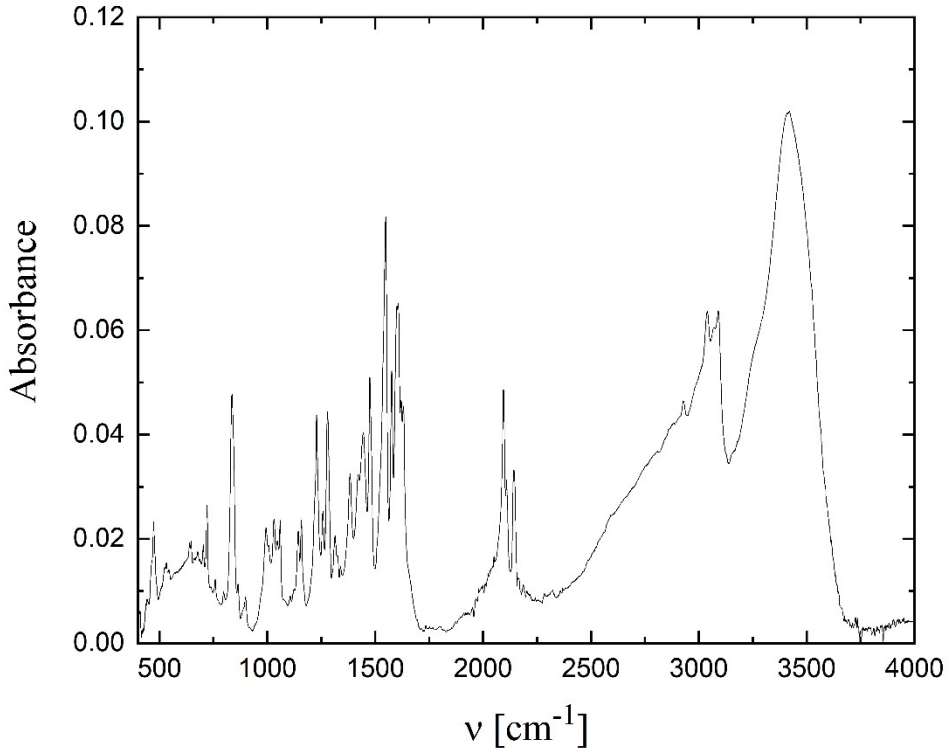

Fig S18. IR spectrum of **6**.

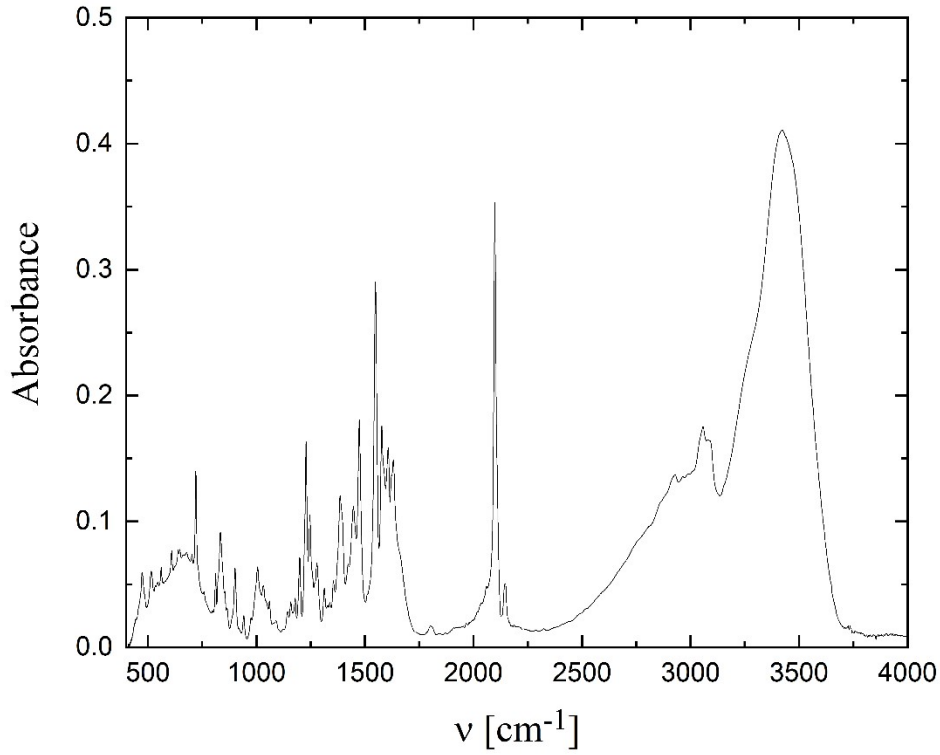

Fig S19. IR spectrum of **7**.

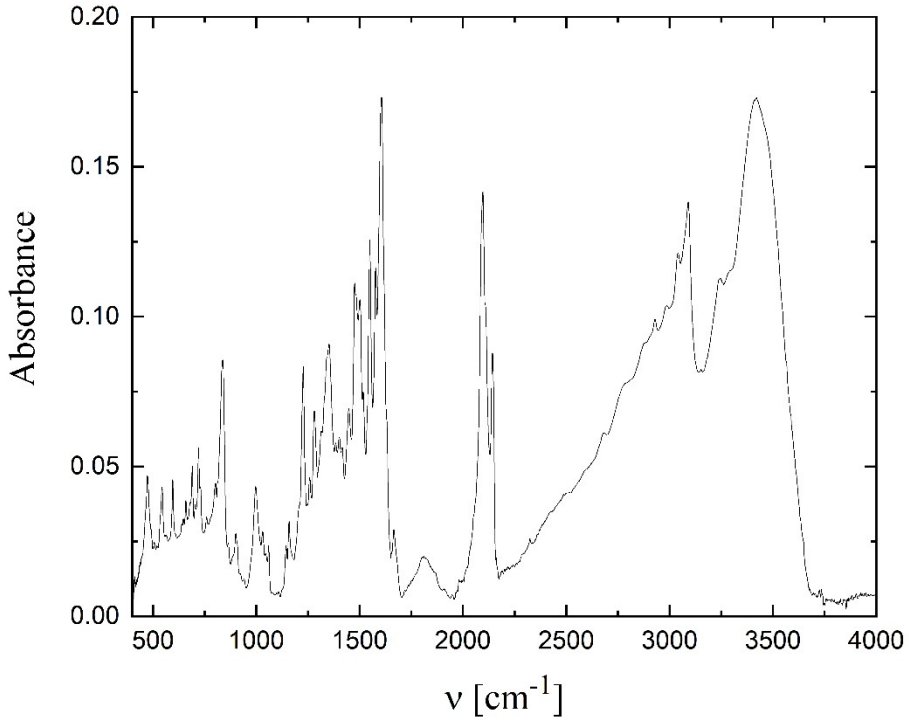

Fig S20. IR spectrum of **8**.

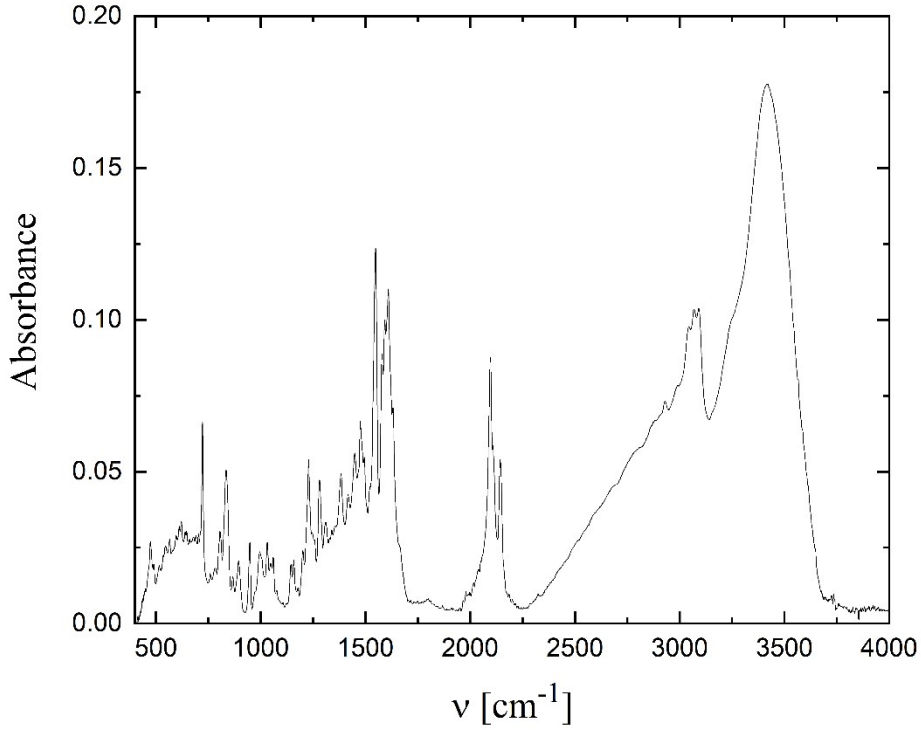

Fig S21. IR spectrum of **9**.

EPR measurements

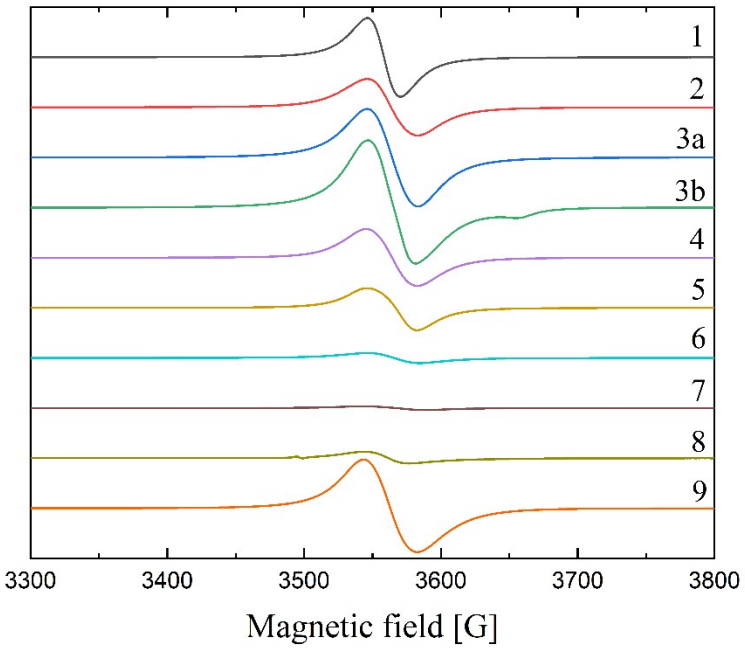

Fig S22. X-band EPR spectra of **1**-**9** registered at room temperature.

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