Electronic Supplementary Material (ESI) for RSC Advances.

Table S1. Thermal decomposition data of the title compounds **1-4**

Complex	Stage	Weight loss process	TemperatureRange (°C)	Mass loss rate/%		Final solid products	
				Found	calcd	Found	calcd
1	I	$(H_2O)_4$	25.00~157.33	15.50	15.40	MgO	
	II	collapse	157.33~318.39	74.90	75.98	9.60	8.62
	III	collapse	318.39~581.38				
2	I	$(H_2O)_6$	25.00~179.47	20.22	20.32	MgO	
	II	collapse	179.47~376.31	72.15	72.10	7.63	7.58
	III	collapse	376.31~561.96				
3	I	$(H_2O)_5$	25.00~209.05	16.12	16.23	MgO	
	II	collapse	209.05~494.26	76.4.	76.5	7.48	7.27
	III	collapse	494.26~730.86				
4	I	$(H_2O)_4(H_2O)_2$	25.00~182.76	16.85	16.84	MgO	
	II	collapse	182.76~456.60	76.83	76.88	6.59	6.28
	III	collapse	456.60~706.18				

Table S2. Crystallographic data and structure refinement parameters for **1−4**

Compound	**1**	**2**	**3**	**4**
Empirical formula	$C_{16}H_{20}Cl_2MgO_{10}$	$C_{18}H_{28}Cl_2MgO_{12}$	$C_{16}H_{20}Cl_4MgO_{11}$	$C_{l6}H_{20}C1_6MgO_{12}$
Formula weight	467.53	531.61	554.43	641.33
Temperature (K)	298(2)	298(2)	298(2)	298(2)
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	*P*2(1)	*C*2/*c*	*P*-1	*P*2(1)/*c*
a, Å	5.1840(10)	32.25(2)	7.379(5)	6.8882(14)
b, Å	27.263(3)	7.404(4)	7.494(5)	8.7091(18)
c, Å	7.4050(10)	10.322(6)	20.56(1)	44.043(9)
α (°)	90	90.00	92.8(1)	90

β (°)	107.443(2)	101.511(8)	92.5(1)	94.482(5)
γ (°)	90	90.00	90.94(1)	90
Volume (Å ^{3})	998.4(3)	2415(2)	1134.0(2)	2634.1(9)
Z	2	4	2	4
D_c/g·cm^{-3}	1.555	1.462	1.624	1.617
μ, mm^{-1}	0.409	0.354	0.605	0.732
F (000)	484	1112	568	1304
Crystal size (mm)	0.50×0.48×0.42	0.30×0.30×0.22	0.28×0.21×0.13	0.18×0.12×0.08
	-6≤h≤6	-38≤h≤38	-8≤h≤8	-8≤h≤9
Index range	-36≤k≤27	-8≤k≤8	-9≤k≤7	-11≤k≤11
	-9≤l≤9	-12≤l≤6	-24≤l≤25	-51≤l≤58
Reflections collected	7017	6129	6149	18311
Unique reflections	3674	2252	4130	6616
R(int)	0.0365	0.0474	0.0643	0.0483
Completeness (%)	100.0	99.5	99.4	99.4
Data/restraints/ parameters	3674/1/262	2252/0/153	4130/0/291	6616/0/316
GoFon F^2	1.020	1.096	1.059	1.080
R_1,wR_2 [I>2sigma(I)]	R_1=0.0347	R_1=0.0867	R_1=0.0687	R_1=0.0557
	wR_2=0.0970	wR_2=0.2536	wR_2=0.2196	wR_2=0.1545
R_1,wR_2 (all data)	R_1=0.0359	R_1=0.1109	R_1=0.0718	R_1=0.0685

	wR_2=0.0981	wR_2=0.2662	wR_2=0.2418	wR_2=0.1666
$\Delta\rho_{max}$, $\Delta\rho_{min}$(e·Å^{-3})	0.301 and -0.368	0.616 and -0.517	0.724 and -0.666	0.340 and -0.382

Table S3. Bond lengths (Å) and angles (°) of hydrogen bond for **1−4**

D−H···A	***d(D−H)***	***d(H···A)***	***d(D···A)***	***∠DHA***
		1		
O1W−H1WB···O2	0.96	1.74	2.664(2)	161
O3W−H3WB···O5	0.96	1.90	2.712(2)	140
		2		
O1W−H1WB···O1	0.69	2.00	2.679(5)	167
O2W−H2WB···O3	0.93	2.49	3.309(6)	147
O3W−H3WA···O3	0.95	1.90	2.799(5)	156
O3W−H3WB···O2	0.92	1.67	2.569(5)	163
		3		
O2W−H2WA···Cl3	0.96	2.63	3.472(7)	147
O2W−H2WB···O4	0.96	1.90	2.860(10)	176
O3W−H3WA···O4	0.96	1.74	2.619(9)	150
O3W−H3WB···O4W	0.96	2.01	2.835(9)	143
		4		
O1W−H1WA···O2	0.96	1.81	2.732(3)	161
O1W−H1WB···O3W	0.96	1.92	2.805(3)	152
O4W−H4WB···O1	0.96	1.84	2.778(3)	166
O4W−H4WB···O1W	0.96	1.74	2.619(9)	150

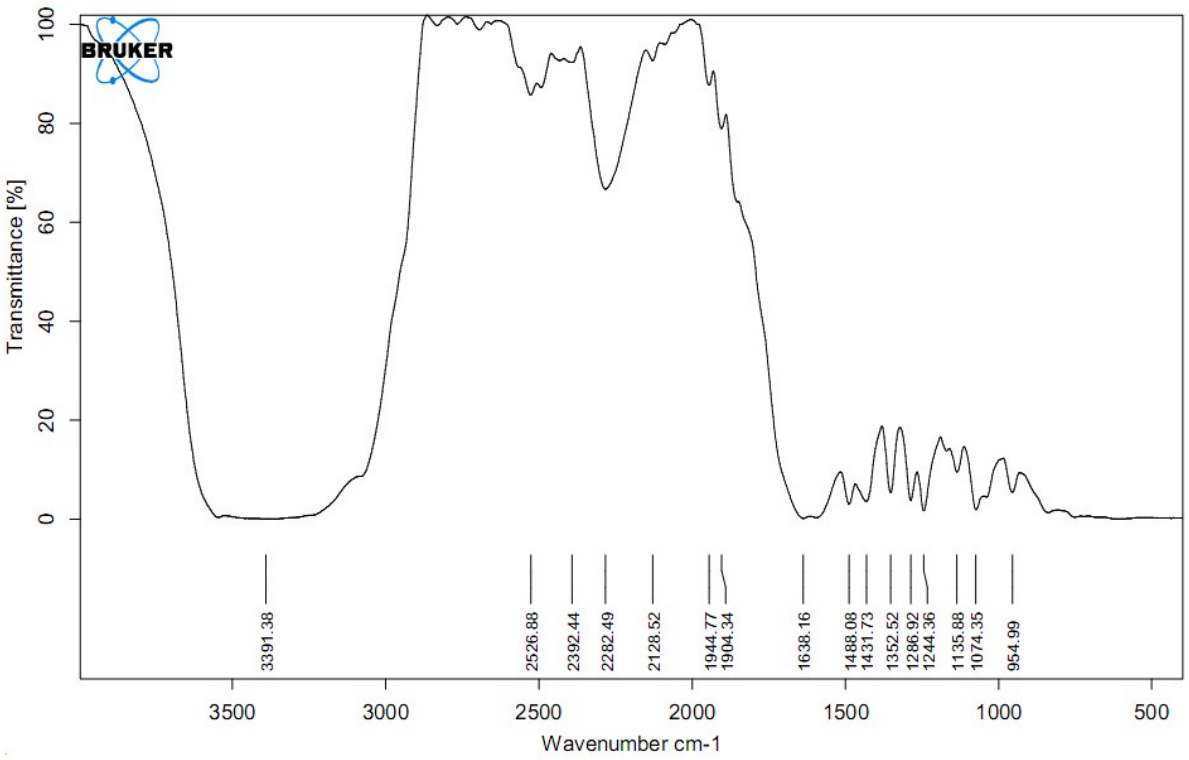
Table S4. Selected bond lengths (Å) and angles (°) for **1-4**

		1	
Mg(1)-O(1W)	2.0363(16)	Mg(1)-O(3W)	2.0400(17)
Mg(1)-O(1)	2.0701(17)	Mg(1)-O(4)	2.0804(17)
Mg(1)-O(2W)	2.0956(18)	Mg(1)-O(4W)	2.1048(18)
O(1W)-Mg(1)-O(3W)	179.44(9)	O(1W)-Mg(1)-O(1)	86.86(7)
O(3W)-Mg(1)-O(1)	92.75(7)	O(1W)-Mg(1)-O(4)	93.22(7)
O(3W)-Mg(1)-O(4)	87.16(7)	O(1)-Mg(1)-O(4)	179.84(8)
O(1W)-Mg(1)-O(2W)	90.20(7)	O(3W)-Mg(1)-O(2W)	89.39(7)
O(1)-Mg(1)-O(2W)	87.21(7)	O(4)-Mg(1)-O(2W)	92.93(7)
O(1W)-Mg(1)-O(4W)	89.37(7)	O(3W)-Mg(1)-O(4W)	91.06(7)
O(1)-Mg(1)-O(4W)	93.47(7)	O(4)-Mg(1)-O(4W)	86.39(7)
O(2W)-Mg(1)-O(4W)	179.17(8)		
		2	
Mg(1)-O(2W)A	2.031(4)	Mg(1)-O(1W)A	2.041(4)
Mg(1)-O(2W)	2.031(4)	Mg(1)-O(3W)A	2.073(3)
Mg(1)-O(1W)	2.041(4)	Mg(1)-O(3W)	2.073(3)
O(2W)A-Mg(1)-O(2W)	86.2(2)	O(1W)-Mg(1)-O(3W)A	86.06(15)
O(2W)A-Mg(1)-O(1W)	177.23(15)	O(1W)A -Mg(1)-O(3W)A	90.30(15)
O(2W)-Mg(1)-O(1W)	93.30(14)	O(2W)A -Mg(1)-O(3W)	92.43(15)
O(2W)A-Mg(1)-O(1W)A	93.30(14)	O(2W)-Mg(1)-O(3W)	91.23(15)
O(2W)-Mg(1)-O(1W)A	177.23(15)	O(1W)-Mg(1)-O(3W)	90.30(15)
O(1W)-Mg(1)-O(1W)A	87.3(2)	O(1W)A -Mg(1)-O(3W)	86.06(15)
O(2W)A -Mg(1)-O(3W)A	91.23(15)	O(3W)A -Mg(1)-O(3W)	175.0(2)
O(2W)-Mg(1)-O(3W)A	92.43(15)		
		3	
Mg(1)-O(1)	2.035(5)	Mg(1)-O(2W)	2.091(7)
Mg(1)-O(3W)	2.060(6)	Mg(1)-O(4W)	2.095(6)

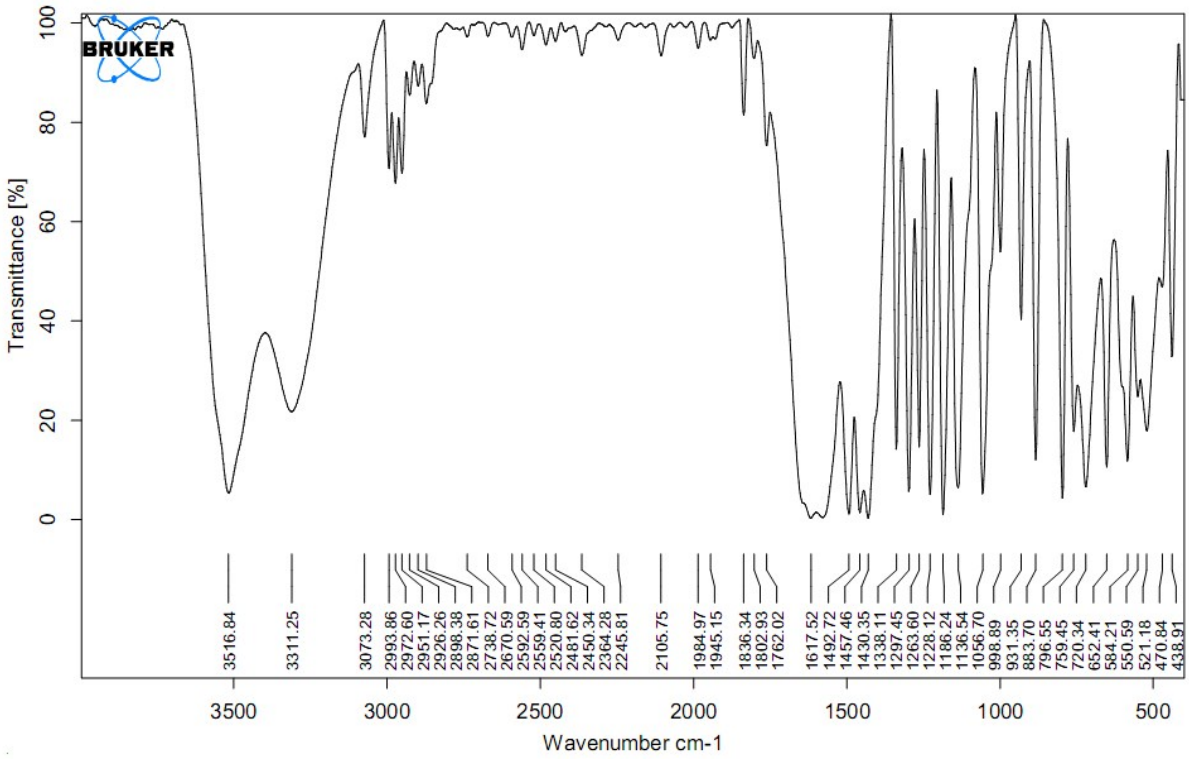
Mg(1)-O(1W)	2.063(6)	Mg(1)-O(5W)	2.098(6)
O(1)-Mg(1)-O(3W)	99.5(2)	O(1W)-Mg(1)-O(4W)	88.5(3)
O(1)-Mg(1)-O(1W)	81.9(2)	O(2W)-Mg(1)-O(4W)	174.9(3)
O(3W)-Mg(1)-O(1W)	177.0(3)	O(1)-Mg(1)-O(5W)	171.2(3)
O(1)-Mg(1)-O(2W)	93.1(3)	O(3W)-Mg(1)-O(5W)	89.1(2)
O(3W)-Mg(1)-O(2W)	86.7(3)	O(1W)-Mg(1)-O(5W)	89.4(2)
O(1W)-Mg(1)-O(2W)	95.8(3)	O(2W)-Mg(1)-O(5W)	89.0(3)
O(1)-Mg(1)-O(4W)	90.1(3)	O(4W)-Mg(1)-O(5W)	88.4(3)
O(3W)-Mg(1)-O(4W)	88.9(3)		
		4	
Mg(1)-O(4)	2.042(2)	Mg(1)-O(2W)	2.056(3)
Mg(1)-O(1)	2.046(2)	Mg(1)-O(4W)	2.098(3)
Mg(1)-O(1W)	2.054(2)	Mg(1)-O(3W)	2.157(3)
O(4)-Mg(1)-O(1)	96.23(10)	O(2W)-Mg(1)-O(4W)	83.54(10)
O(4)-Mg(1)-O(1W)	168.92(11)	O(4)-Mg(1)-O(3W)	89.26(11)
O(1)-Mg(1)-O(1W)	90.09(9)	O(1)-Mg(1)-O(3W)	83.16(11)
O(4)-Mg(1)-O(2W)	93.54(12)	O(1W)-Mg(1)-O(3W)	88.84(11)
O(1)-Mg(1)-O(2W)	88.74(11)	O(2W)-Mg(1)-O(3W)	87.90(11)
O(1W)-Mg(1)-O(2W)	95.69(12)	O(4W)-Mg(1)-O(3W)	175.68(12)
O(4)-Mg(1)-O(4W)	90.49(10)	O(1)-Mg(1)-O(4W)	173.09(10)

Symmetry transformations used to generate equivalent atoms. For **2**A –x,y,-z+1/2

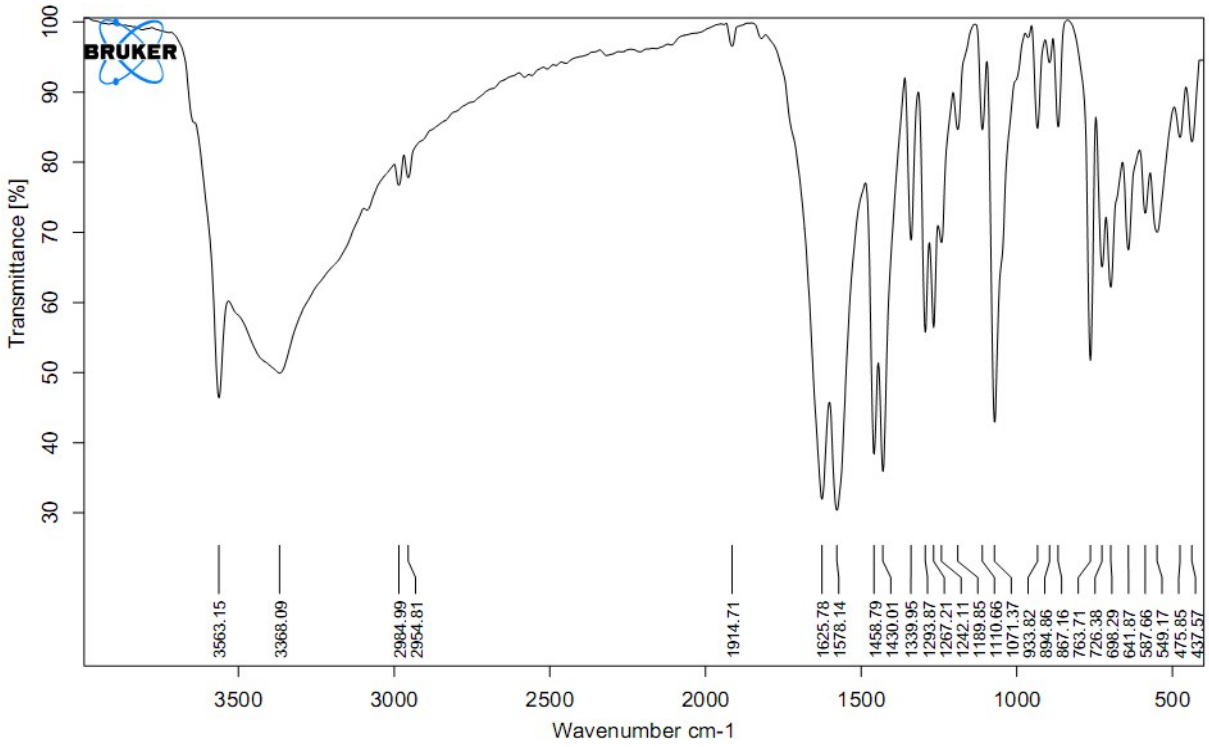
IR spectra of compound **1**



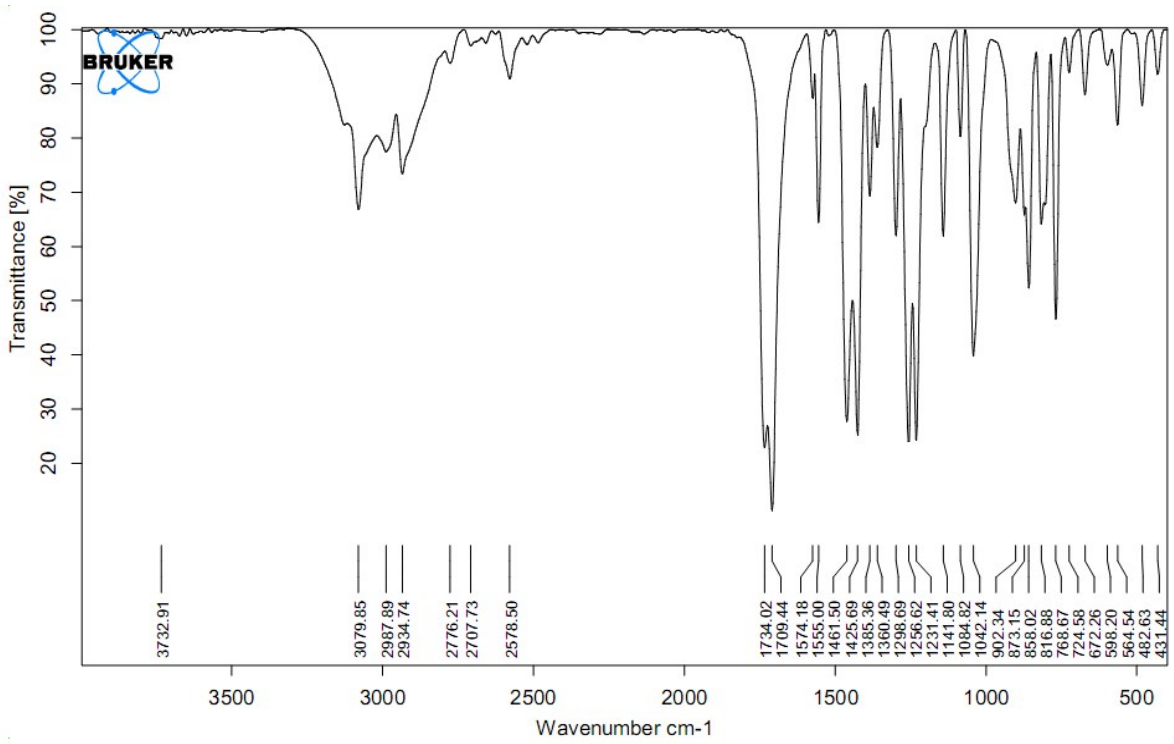
IR spectra of compound **2**



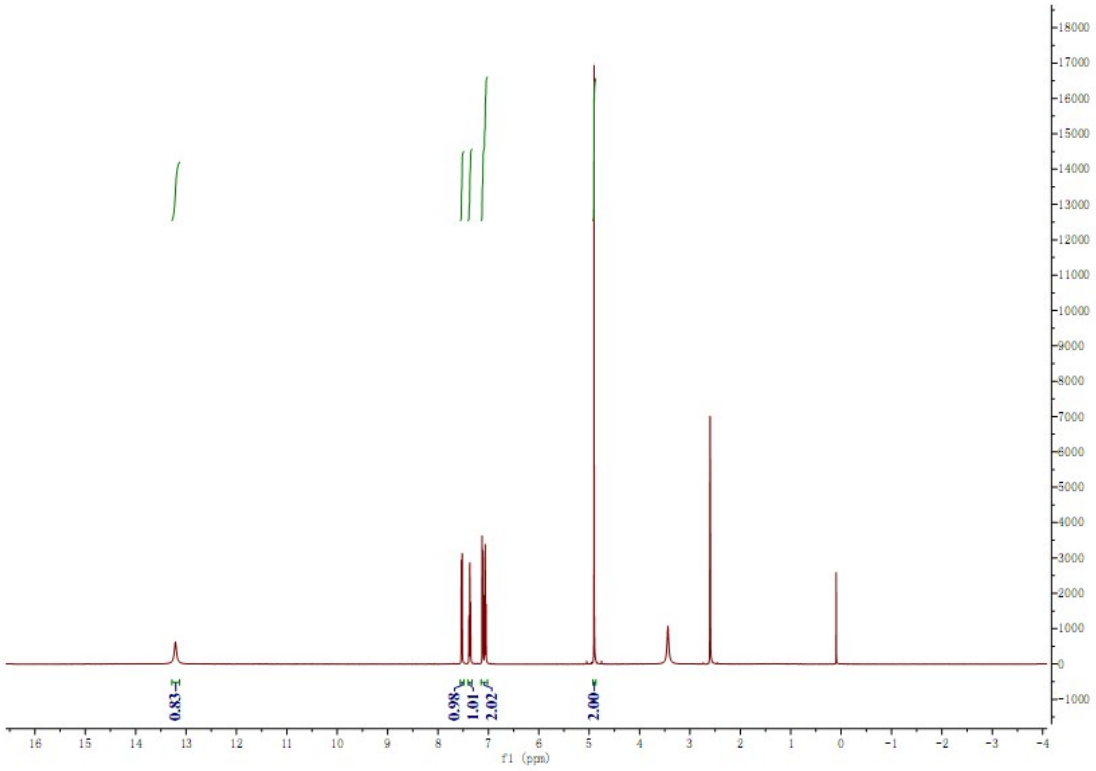
IR spectra of compound **3**



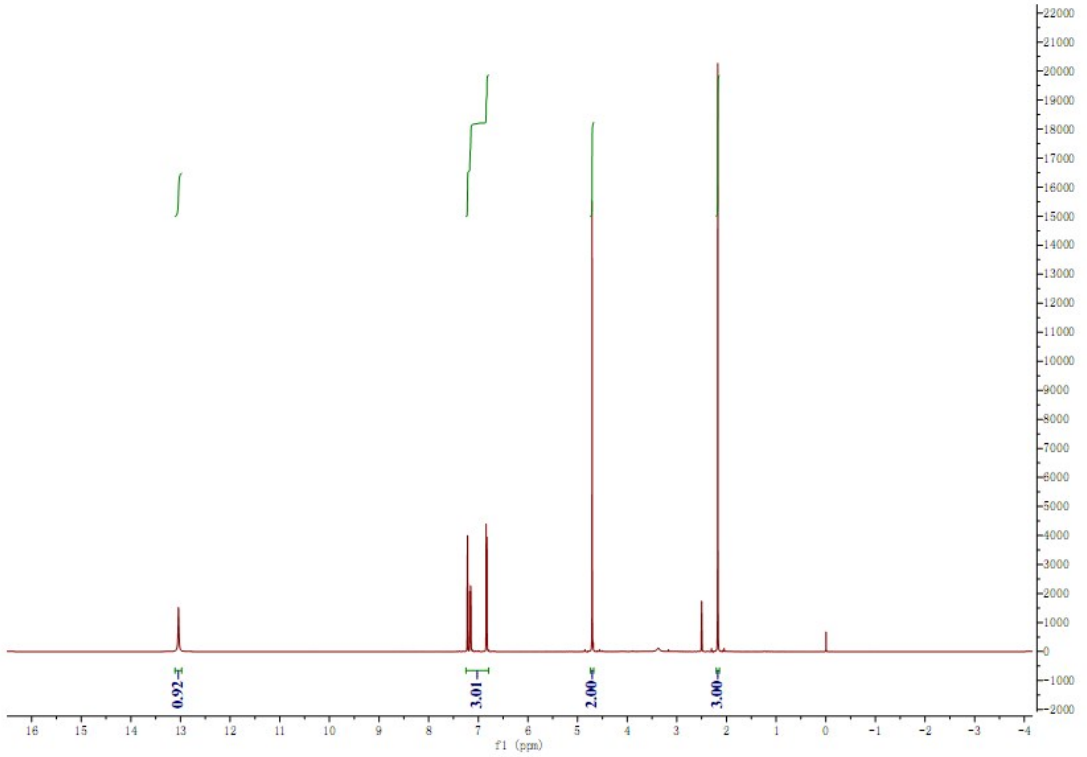
IR spectra of compound **4**



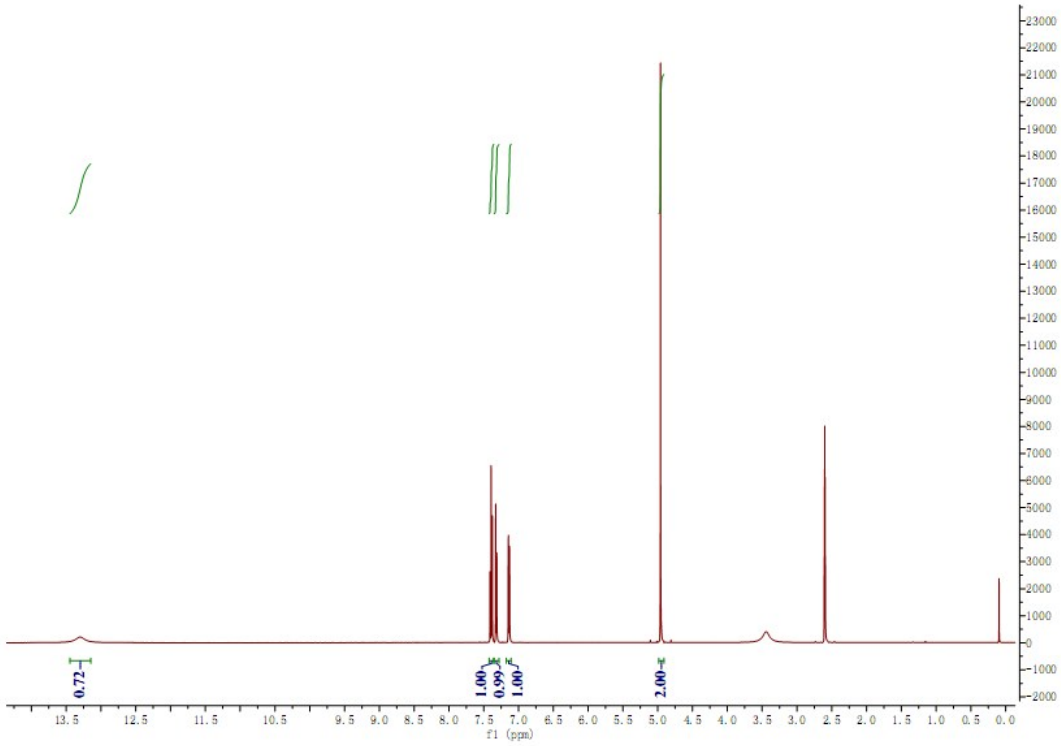
^{1}H NMR spectra of **HCPA**



^{1}H NMR spectra of **HMCPA**



^{1}H NMR spectra of **HDCPA**



^{1}H NMR spectra of **HTCPA**