Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Imino-bridged N-rich energetic materials: $C_4H_3N_{17}$ and their derivatives assembled from the powerful combination of four tetrazoles

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Table of Contents

Experimental Procedures

Cautions! There have been no explosions when dealing with these compounds, but we strongly encourage to take strict precautions because of their high energy and mechanical sensitivity.

General methods

All reagents are purchased from Energy Chemical of analytical grade and were used strictly in accordance with regulations. ^{1}H and ^{13}C NMR were recorded on a Bruker 500 MHz nuclear magnetic resonance spectrometer operating at 500 and 126 MHz, respectively. IR spectra were recorded using KBr pellets with a Thermo Nicolet iS10 sprctrometer. Elemental analyses were carried out on a vario EL III CHNOS elemental analyzer. The melting and decomposition (onset) points were measured on a differential scanning calorimeter (Mettler Toledo DSC823e) at a scan rate of 5 K min^{-1}. Densities were confirmed at room temperature by using the Micromeritics AccuPyc 1340 gas pycnometer. Impact and friction sensitivity were obtained using a standard BAM Fallhammer and a BAM friction tester.

Computations

Computations were performed by using the Gaussian09 suite of programs.[1] The theoretical gas phase enthalpies of formation were calculated used the hybrid DFTB3LYP methods with 6-311++G** basis set[2] based on isodemic reactions (Scheme S1).

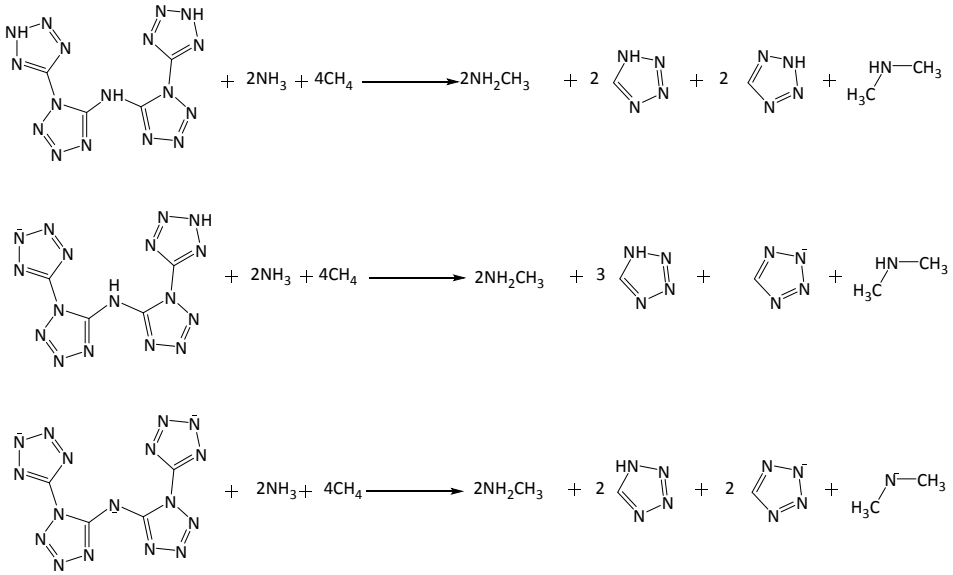

Figure S1 Isodesmic reactions for calculating heats of formation.

Table S1 Calculated total energy (E_0), zero-point energy (*ZPE*), thermal correction to enthalpy (H_T) and gas phase heats of formation (HOF)

Compound	E_0/a.u.	*ZPE*/kJ mol^{-1}	ΔH_T/kJ mol^{-1}	HOF/ kJ mol^{-1}
CH_4	-40.5339263	112.26	10.04	-74.6
NH_3	-56.5826356	86.27	10.05	-45.9
NH_2CH_3	-95.8938402	160.78	11.64	-22.5
$(CH_3)_2NH$	-135.1814215	237.51	14.29	-20.60
$(CH_3)_2N^-$	-134.5397348	189.81	13.47	86.64
tetrazolium	-257.7329825	87.02	11.26	170
tetrazole	-258.2567	123.13	11.83	333.2
2H-tetrazole	-257.7068416	124.96	11.45	318.2

For energetic salts, the solid-phase heat of formation is calculated based on a Born-Haber energy cycle (Figure S2).[3]

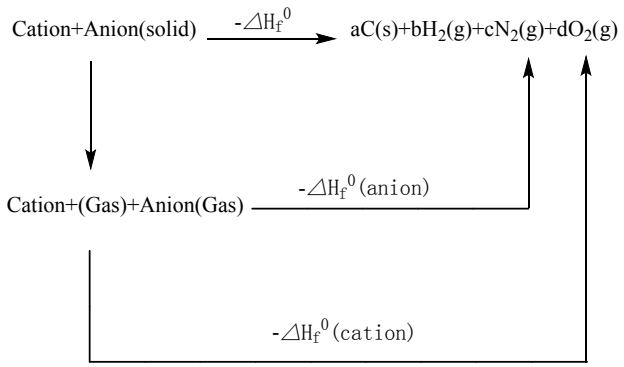

Figure S2 Born-Haber Cycle for the formation of energetic salts.

The number is simplified by equation 1:

H_f^0 (salt, 298 K) = H_f^0 (cation, 298K) + H_f^0 (anion, 298K) – H_L (1)

where H_L is the lattice energy of the salts, which could be predicted by using the formula suggested by Jenkins et al. [Eq. (2)]

$H_L = U_{POT} + [p(n_M/2 - 2) + q(n_X/2 - 2)]RT$ (2)

where n_M and n_X depend on the nature of the ions, M^{q+} and X^{p-}, and are equal to 3 for monatomic ions, 5 for linear polyatomic ions, and 6 for nonlinear polyatomic ions.

The equation for lattice potential energy U_{POT} [Eq. (3)] has the form:

U_{POT} [kJ mol^{-1}] = $\gamma(\rho_m/M_m)^{1/3} + \delta$ (3)

where ρ_m [g cm^{-3}] is the density of the salt, M_m is the chemical formula mass of the ionic material, and values for (g) and the coefficients γ (kJ mol^{-1} cm) and δ (kJ mol^{-1}) are assigned literature values.[2]

The solid-state enthalpy of formation for neutral compound can be estimated by subtracting the heat of sublimation from gas-phase heat of formation. Based on the literature,[3] the heat of sublimation can be estimated with Trouton's rule according to supplementary equation (4), where T represents either the melting point or the decomposition temperature when no melting occurs prior to decomposition:

ΔH_{sub} = 188/J mol^{-1}K^{-1} × T (4)

Table S2 Densities, calculated lattice energies, and calculated heats of formation

Compound	D[a](g cm^{-3})	H_{Lat} [b](kJ mol^{-1})	H_f[c](kJ mol $^{-1}$/KJ g^{-1})
2	1.88	2833.46	256.48/0.72
3	1.72	-	1509.08/5.22
4	2.05	2757.50	87.33/0.22
5	1.68	2734.46	497.06/1.67
6	1.63	2471.83	878.81/1.88
7	1.70	2646.38	1017.37/2.64
8	1.81	-	877.669/2.08
9	1.83	467.01	1299.046/4.17

[a] Density was measured by gas pycnometer at room temperature. [b] Calculated lattice energy. [c] Calculated heat of formation.

Results and Discussion

Table S3. Crystallographic data for **3**·2C_2H_6OS, **4**·2.25H_2O, **6**, **7**·H_2O.

Compd	**3**·2C_2H_6OS	**4**·2.25H_2O	**6**	**7**·H_2O
Empirical formula	$C_4H_3N_{17}$·2C_2H_6OS	$C_4K_3N_{17}$·2.25H_2O	$C_6H_8N_{26}$	$C_4H_{15}N_{23}$·H_2O
Formula weight	445.49	443.96	446.47	403.33
Temperature/K	296	296	296	296
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	C 2	C 2/c	P -1	P -1
a/Å	13.226	14.981	7.2340	7.4436
b/Å	10.403	12.023	10.5985	10.1464
c/Å	7.7069	16.981	13.966	11.1808
α/°	90	90	70.681	89.5300
β/°	117.138	104.519	89.167	74.8050
γ/°	90	90	71.541	86.082
Volume/ Å^3	943.7(3)	2960.8(9)	953.6(3)	812.97(6)
Z	2	2	2	2
ρ_{calc}/g cm^{-3}	1.568	1.992	1.625	1.648
F(000)	460	1780	484	420
θ range[°]	2.6-27.5	2.346-24.955	2.157-27.948	2.75-27.41
Index ranges	-16≤h≤17 -13≤k≤11 -10≤l≤8	-17≤h≤17 -14≤k≤12 -17≤l≤20	-8≤h≤9 -13≤k≤13 -18≤l≤18	-9≤h≤9 -13≤k≤13 -14≤l≤14
Data/restraints/parameters	1758/1/135	2551/0/240	4501/0/298	3699/0/254
GOF on F^2	1.081	1.096	1.030	1.031
R[$F^2 > 2\sigma(F^2)$]	0.311	0.0901	0.0971	0.0397
wR(F^2)	0.0804	0.2102	0.1047	0.0959
CCDC number	2072406	2047779	2079019	2050808

Table S4. Crystallographic data for **8**·2H_2O**,** and **9**·3CH_3OH,**10**·2.25H_2O,**11**·H_20.

Compd	**8**·2H_2O	**9**·3CH_3OH	**10**·2.25H_2O	**11**·H_20
Empirical formula	$C_4H_{15}N_{21}O_4$·2H_2O	C_4NaN_{17}·3CH_3OH	$C_4NaK_2N_{17}$·2.25H_2O	$C_4H_8NaN_{19}$·H_2O
Formula weight	457.31	407.34	432.44	363.30
Temperature/K	296	296	296	296
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	P -1	P -1	C 2/c	P -1
a/Å	7.3804	7.2417	14.9928	9.5696
b/Å	11.4595	10.6666	12.1180	9.5808
c/Å	11.8445	11.9926	16.8960	9.5851
α/°	64.029	77.757	90	81.051
β/°	81.549	85.569	105.961	81.699
γ/°	89.905	80.379	90	60.468
Volume/ Å^3	888.60	891.72(12)	2951.4(2)	752.90(15)
Z	2	2	4	2
ρ_{calc}/g cm^{-3}	1.709	1.517	1.946	1.603
F(000)	476.0	420.0	1736	372
θ range[°]	2.80-27.47	2.4-27.5	2.2-27.5	2.2-27.5

	-9≤h≤9	-9≤h≤9	-19≤h≤19	-12≤h≤12
Index ranges	-14≤k≤14	-13≤k≤13	-15≤k≤15	-12≤k≤12
	-15≤l≤15	-15≤l≤15	-21≤l≤20	-12≤l≤12
Data/restraints/parameters	4023/0/285	4061/0/255	3403/0/240	3401/0/260
GOF on F^2	1.049	1.020	1.040	1.050
$R[F^2 > 2\sigma(F^2)]$	0.0397	0.0451	0.0470	0.0443
$wR(F^2)$	0.0978	0.1137	0.1323	0.1230
CCDC number	2051823	2053784	2034088	2051824

Table S5 Bond lengths (Å) for **4·2C_2H_6OS.**

C(1)-N(2)	1.305(4)	C(4)-H(4B)	0.9600
C(1)-N(5)	1.356(3)	C(4)-H(4C)	0.9600
C(1)-N(1)	1.371(3)	N(1)-H(1)	0.78(6)
C(2)-N(6)	1.314(3)	N(2)-N(3)	1.382(3)
C(2)-N(9)	1.330(4)	N(3)-N(4)	1.275(4)
C(2)-N(5)	1.397(3)	N(4)-N(5)	1.372(3)
C(3)-S(1)	1.777(3)	N(6)-N(7)	1.322(3)
C(3)-H(3A)	0.9600	N(7)-N(8)	1.303(3)
C(3)-H(3B)	0.9600	N(7)-H(7)	0.8600
C(3)-H(3C)	0.9600	N(8)-N(9)	1.345(4)
C(4)-S(1)	1.766(3)	O(1)-S(1)	1.531(2)
C(4)-H(4A)	0.9600		

Table S6 Bond angles (°) for **3·2C_2H_6OS.**

N(2)-C(1)-N(5)	109.6(2)	C(1)#1-N(1)-C(1)	122.9(3)
N(2)-C(1)-N(1)	128.8(3)	C(1)#1-N(1)-H(1)	118.53(16)
N(5)-C(1)-N(1)	121.6(3)	C(1)-N(1)-H(1)	118.53(17)
N(6)-C(2)-N(9)	114.5(3)	C(1)-N(2)-N(3)	105.0(2)
N(6)-C(2)-N(5)	124.5(2)	N(4)-N(3)-N(2)	111.9(2)
N(9)-C(2)-N(5)	121.0(2)	N(3)-N(4)-N(5)	106.1(2)
S(1)-C(3)-H(3A)	109.5	C(1)-N(5)-N(4)	107.3(2)
S(1)-C(3)-H(3B)	109.5	C(1)-N(5)-C(2)	130.3(2)
H(3A)-C(3)-H(3B)	109.5	N(4)-N(5)-C(2)	122.3(2)
S(1)-C(3)-H(3C)	109.5	C(2)-N(6)-N(7)	100.6(2)
H(3A)-C(3)-H(3C)	109.5	N(8)-N(7)-N(6)	114.8(2)
H(3B)-C(3)-H(3C)	109.5	N(8)-N(7)-H(7)	122.6
S(1)-C(4)-H(4A)	109.5	N(6)-N(7)-H(7)	122.6

S(1)-C(4)-H(4B)	109.5	N(7)-N(8)-N(9)	105.8(2)
H(4A)-C(4)-H(4B)	109.5	C(2)-N(9)-N(8)	104.3(2)
S(1)-C(4)-H(4C)	109.5	O(1)-S(1)-C(4)	104.74(15)
H(4A)-C(4)-H(4C)	109.5	O(1)-S(1)-C(3)	103.70(15)
H(4B)-C(4)-H(4C)	109.5	C(4)-S(1)-C(3)	98.53(16)

Table S7. Hydrogen bonds in **3·2C_2H_6OS**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(7)-H(7)...S(1)#2	0.86	2.77	N3.582(3)	158.8
N(7)-H(7)...O(1)#2	0.86	1.70	2.557(3)	171.7
N(1)-H(1)...N(9)#1	0.78(6)	2.22(4)	2.806(4)	132.1(12)
N(1)-H(1)...N(9)	0.78(6)	2.22(4)	2.806(4)	132.1(12)

Table S8 Bond lengths (Å) for **4·2.25H_2O**

K(1)-N(1)	2.701(10)	K(3)-H(3B)#2	2.644(7)
K(1)-N(2)#1	2.728(9)	C(1)-N(1)	1.273(12)
K(1)-N(10)#2	2.764(7)	C(1)-N(4)	1.327(12)
K(1)-N(8)#2	2.767(8)	C(1)-N(5)	1.401(11)
K(1)-N(17)	2.770(8)	C(2)-N(9)	1.333(10)
K(1)-O(2)#3	2.929(9)	C(2)-N(8)	1.343(10)
K(1)-N(9)	3.098(7)	C(2)-N(5)	1.372(9)
K(1)-K(1)#1	4.002(4)	C(3)-N(9)	1.328(10)
K(1)-K(3)#4	4.092(3)	C(3)-N(10)	1.361(10)
K(1)-K(2)#2	4.193(3)	C(3)-N(13)	1.381(10)
K(1)-K(2)#3	4.468(3)	C(4)-N(14)	1.320(10)
K(1)-K(3)#3	4.761(3)	C(4)-N(17)	1.321(10)
K(2)-O(1)	2.779(10)	C(4)-N(13)	1.399(10)
K(2)-N(3)#5	2.867(8)	N(1)-N(2)	1.371(11)
K(2)-N(15)#4	2.913(7)	N(2)-N(3)	1.297(12)
K(2)-N(11)#6	2.970(7)	N(3)-N(4)	1.333(11)
K(2)-N(8)	3.047(8)	N(5)-N(6)	1.362(9)
K(2)-N(10)	3.050(8)	N(6)-N(7)	1.260(10)
K(2)-N(15)#7	3.183(8)	N(7)-N(8)	1.369(10)
K(2)-N(16)#7	3.285(9)	N(10)-N(11)	1.365(9)
K(2)-K(2)#8	4.504(4)	N(11)-N(12)	1.276(10)
K(3)-O(3)	2.771(2)	N(12)-N(13)	1.360(9)

K(3)-O(2)	2.818(9)	N(14)-N(15)	1.339(10)
K(3)-N(14)	2.889(8)	N(15)-N(16)	1.290(10)
K(3)-N(6)#9	2.929(7)	N(16)-N(17)	1.350(10)
K(3)-N(4)#9	2.943(8)	O(1)-H(1A)	0.8501
K(3)-N(1)#5	2.943(9)	O(1)-H(1B)	0.8500
K(3)-N(12)	3.028(7)	O(2)-H(2A)	0.8500
K(3)-N(17)#5	3.050(9)	O(2)-H(2B)	0.8500
K(3)-O(1)#6	3.211(12)	O(3)-H(3A)	0.8501
K(3)-N(9)#5	3.311(7)	O(3)-H(3B)	0.8500
K(3)-H(1B)#6	2.479(11)	O(3)-H(3A)#2	0.8501
K(3)-H(3A)#2	2.573(9)	O(3)-H(3B)#2	0.8499

Table S9 Bond angles (°) for **4·2.25H_2O**

N(1)-K(1)-N(2)#1	119.3(3)	O(3)-K(3)-K(1)#5	171.94(11)
N(1)-K(1)-N(10)#2	133.0(2)	O(2)-K(3)-K(1)#5	58.6(2)
N(2)#1-K(1)-N(10)#2	107.5(2)	N(14)-K(3)-K(1)#5	110.61(18)
N(1)-K(1)-N(8)#2	90.0(2)	N(6)#9-K(3)-K(1)#5	112.71(16)
N(2)#1-K(1)-N(8)#2	132.2(3)	N(4)#9-K(3)-K(1)#5	110.9(2)
N(10)#2-K(1)-N(8)#2	59.1(2)	N(1)#5-K(3)-K(1)#5	41.2(2)
N(1)-K(1)-N(17)	93.4(3)	N(12)-K(3)-K(1)#5	110.35(15)
N(2)#1-K(1)-N(17)	89.0(2)	N(17)#5-K(3)-K(1)#5	42.60(15)
N(10)#2-K(1)-N(17)	82.8(2)	O(1)#6-K(3)-K(1)#5	124.1(3)
N(8)#2-K(1)-N(17)	128.7(2)	N(9)#5-K(3)-K(1)#5	48.05(12)
N(1)-K(1)-O(2)#3	77.0(3)	O(3)-K(3)-K(1)#7	119.3(3)
N(2)#1-K(1)-O(2)#3	81.9(2)	O(2)-K(3)-K(1)#7	34.81(19)
N(10)#2-K(1)-O(2)#3	115.6(3)	N(14)-K(3)-K(1)#7	113.90(16)
N(8)#2-K(1)-O(2)#3	68.2(2)	N(6)#9-K(3)-K(1)#7	114.61(16)
N(17)-K(1)-O(2)#3	161.2(3)	N(4)#9-K(3)-K(1)#7	158.72(19)
N(1)-K(1)-N(9)	62.7(2)	N(1)#5-K(3)-K(1)#7	48.86(16)
N(2)#1-K(1)-N(9)	149.1(2)	N(12)-K(3)-K(1)#7	71.60(14)
N(10)#2-K(1)-N(9)	75.3(2)	N(17)#5-K(3)-K(1)#7	82.56(15)
N(8)#2-K(1)-N(9)	76.4(2)	O(1)#6-K(3)-K(1)#7	75.8(2)
N(17)-K(1)-N(9)	60.5(2)	N(9)#5-K(3)-K(1)#7	97.47(13)
O(2)#3-K(1)-N(9)	125.6(2)	K(1)#5-K(3)-K(1)#7	53.09(6)
N(1)-K(1)-K(1)#1	61.19(18)	O(3)-K(3)-H(1B)#6	41.9(3)
N(2)#1-K(1)-K(1)#1	58.98(19)	O(2)-K(3)-H(1B)#6	74.1(4)
N(10)#2-K(1)-K(1)#1	165.23(18)	N(14)-K(3)-H(1B)#6	100.9(4)
N(8)#2-K(1)-K(1)#1	124.02(18)	N(6)#9-K(3)-H(1B)#6	71.3(3)
N(17)-K(1)-K(1)#1	101.76(18)	N(4)#9-K(3)-H(1B)#6	110.2(3)

O(2)#3-K(1)-K(1)#1	59.47(18)	N(1)#5-K(3)-H(1B)#6	117.4(3)
N(9)-K(1)-K(1)#1	119.27(15)	N(12)-K(3)-H(1B)#6	59.0(3)
N(1)-K(1)-K(3)#4	45.91(18)	N(17)#5-K(3)-H(1B)#6	127.3(4)
N(2)#1-K(1)-K(3)#4	104.45(19)	O(1)#6-K(3)-H(1B)#6	8.76(9)
N(10)#2-K(1)-K(3)#4	119.82(17)	N(9)#5-K(3)-H(1B)#6	174.9(3)
N(8)#2-K(1)-K(3)#4	122.22(17)	K(1)#5-K(3)-H(1B)#6	130.0(3)
N(17)-K(1)-K(3)#4	48.18(19)	K(1)#7-K(3)-H(1B)#6	79.2(3)
O(2)#3-K(1)-K(3)#4	118.4(2)	O(3)-K(3)-H(3A)#2	17.81(2)
N(9)-K(1)-K(3)#4	52.66(13)	O(2)-K(3)-H(3A)#2	105.1(3)
K(1)#1-K(1)-K(3)#4	72.05(7)	N(14)-K(3)-H(3A)#2	89.6(5)
N(1)-K(1)-K(2)#2	132.99(19)	N(6)#9-K(3)-H(3A)#2	48.8(6)
N(2)#1-K(1)-K(2)#2	89.36(19)	N(4)#9-K(3)-H(3A)#2	67.6(4)
N(10)#2-K(1)-K(2)#2	46.62(16)	N(1)#5-K(3)-H(3A)#2	154.4(6)
N(8)#2-K(1)-K(2)#2	46.58(16)	N(12)-K(3)-H(3A)#2	82.7(6)
N(17)-K(1)-K(2)#2	125.8(2)	N(17)#5-K(3)-H(3A)#2	121.2(6)
O(2)#3-K(1)-K(2)#2	70.8(2)	O(1)#6-K(3)-H(3A)#2	45.8(3)
N(9)-K(1)-K(2)#2	111.50(14)	N(9)#5-K(3)-H(3A)#2	140.7(3)
K(1)#1-K(1)-K(2)#2	122.89(9)	K(1)#5-K(3)-H(3A)#2	159.6(5)
K(3)#4-K(1)-K(2)#2	164.05(7)	K(1)#7-K(3)-H(3A)#2	121.64(19)
N(1)-K(1)-K(2)#3	149.97(19)	H(1B)#6-K(3)-H(3A)#2	43.2
N(2)#1-K(1)-K(2)#3	54.15(19)	O(3)-K(3)-H(3B)#2	17.860(15)
N(10)#2-K(1)-K(2)#3	60.65(14)	O(2)-K(3)-H(3B)#2	103.2(2)
N(8)#2-K(1)-K(2)#3	116.03(16)	N(14)-K(3)-H(3B)#2	75.4(4)
N(17)-K(1)-K(2)#3	59.17(19)	N(6)#9-K(3)-H(3B)#2	77.2(6)
O(2)#3-K(1)-K(2)#3	125.0(2)	N(4)#9-K(3)-H(3B)#2	93.4(4)
N(9)-K(1)-K(2)#3	107.15(14)	N(1)#5-K(3)-H(3B)#2	123.6(6)
K(1)#1-K(1)-K(2)#3	109.45(8)	N(12)-K(3)-H(3B)#2	52.1(6)
K(3)#4-K(1)-K(2)#3	104.65(6)	N(17)#5-K(3)-H(3B)#2	148.4(6)
K(2)#2-K(1)-K(2)#3	76.81(6)	O(1)#6-K(3)-H(3B)#2	37.1(3)
N(1)-K(1)-K(3)#3	101.13(18)	N(9)#5-K(3)-H(3B)#2	150.7(3)
N(2)#1-K(1)-K(3)#3	49.63(18)	K(1)#5-K(3)-H(3B)#2	155.3(3)
N(10)#2-K(1)-K(3)#3	112.66(17)	K(1)#7-K(3)-H(3B)#2	102.2(3)
N(8)#2-K(1)-K(3)#3	90.68(16)	H(1B)#6-K(3)-H(3B)#2	29.2
N(17)-K(1)-K(3)#3	138.11(16)	H(3A)#2-K(3)-H(3B)#2	30.8
O(2)#3-K(1)-K(3)#3	33.31(17)	N(1)-C(1)-N(4)	114.1(8)
N(9)-K(1)-K(3)#3	158.79(14)	N(1)-C(1)-N(5)	125.3(8)
K(1)#1-K(1)-K(3)#3	54.85(6)	N(4)-C(1)-N(5)	120.5(8)
K(3)#4-K(1)-K(3)#3	126.91(6)	N(9)-C(2)-N(8)	131.9(7)
K(2)#2-K(1)-K(3)#3	68.28(5)	N(9)-C(2)-N(5)	122.6(7)

K(2)#3-K(1)-K(3)#3	93.59(5)	N(8)-C(2)-N(5)	105.5(6)
O(1)-K(2)-N(3)#5	158.1(3)	N(9)-C(3)-N(10)	131.3(7)
O(1)-K(2)-N(15)#4	87.6(3)	N(9)-C(3)-N(13)	123.8(7)
N(3)#5-K(2)-N(15)#4	85.4(3)	N(10)-C(3)-N(13)	104.8(7)
O(1)-K(2)-N(11)#6	76.9(3)	N(14)-C(4)-N(17)	113.6(7)
N(3)#5-K(2)-N(11)#6	106.5(2)	N(14)-C(4)-N(13)	121.1(7)
N(15)#4-K(2)-N(11)#6	163.1(2)	N(17)-C(4)-N(13)	125.3(7)
O(1)-K(2)-N(8)	92.0(3)	C(1)-N(1)-N(2)	104.0(8)
N(3)#5-K(2)-N(8)	105.7(2)	C(1)-N(1)-K(1)	118.7(7)
N(15)#4-K(2)-N(8)	72.5(2)	N(2)-N(1)-K(1)	114.1(7)
N(11)#6-K(2)-N(8)	114.2(2)	C(1)-N(1)-K(3)#4	117.4(6)
O(1)-K(2)-N(10)	131.6(3)	N(2)-N(1)-K(3)#4	109.9(6)
N(3)#5-K(2)-N(10)	70.3(2)	K(1)-N(1)-K(3)#4	92.9(3)
N(15)#4-K(2)-N(10)	107.8(2)	N(3)-N(2)-N(1)	108.5(8)
N(11)#6-K(2)-N(10)	87.78(19)	N(3)-N(2)-K(1)#1	130.0(6)
N(8)-K(2)-N(10)	53.16(18)	N(1)-N(2)-K(1)#1	118.5(7)
O(1)-K(2)-N(15)#7	72.1(3)	N(2)-N(3)-N(4)	109.7(7)
N(3)#5-K(2)-N(15)#7	86.6(2)	N(2)-N(3)-K(2)#4	115.7(6)
N(15)#4-K(2)-N(15)#7	84.8(2)	N(4)-N(3)-K(2)#4	133.9(6)
N(11)#6-K(2)-N(15)#7	84.0(2)	C(1)-N(4)-N(3)	103.7(8)
N(8)-K(2)-N(15)#7	152.9(2)	C(1)-N(4)-K(3)#10	120.1(6)
N(10)-K(2)-N(15)#7	152.1(2)	N(3)-N(4)-K(3)#10	131.7(6)
O(1)-K(2)-N(16)#7	93.5(3)	N(6)-N(5)-C(2)	109.0(6)
N(3)#5-K(2)-N(16)#7	66.3(2)	N(6)-N(5)-C(1)	117.3(7)
N(15)#4-K(2)-N(16)#7	93.8(2)	C(2)-N(5)-C(1)	133.6(7)
N(11)#6-K(2)-N(16)#7	80.6(2)	N(7)-N(6)-N(5)	106.9(7)
N(8)-K(2)-N(16)#7	165.0(2)	N(7)-N(6)-K(3)#10	126.7(6)
N(10)-K(2)-N(16)#7	129.27(19)	N(5)-N(6)-K(3)#10	120.8(5)
N(15)#7-K(2)-N(16)#7	22.93(18)	N(6)-N(7)-N(8)	111.6(7)
O(1)-K(2)-K(1)#2	90.4(2)	C(2)-N(8)-N(7)	106.9(7)
N(3)#5-K(2)-K(1)#2	111.39(19)	C(2)-N(8)-K(1)#2	126.4(5)
N(15)#4-K(2)-K(1)#2	113.62(17)	N(7)-N(8)-K(1)#2	113.9(5)
N(11)#6-K(2)-K(1)#2	73.74(15)	C(2)-N(8)-K(2)	101.6(5)
N(8)-K(2)-K(1)#2	41.26(14)	N(7)-N(8)-K(2)	114.1(6)
N(10)-K(2)-K(1)#2	41.20(13)	K(1)#2-N(8)-K(2)	92.2(2)
N(15)#7-K(2)-K(1)#2	154.47(15)	C(3)-N(9)-C(2)	116.5(6)
N(16)#7-K(2)-K(1)#2	152.46(15)	C(3)-N(9)-K(1)	118.2(5)
O(1)-K(2)-K(1)#7	119.1(3)	C(2)-N(9)-K(1)	113.4(5)
N(3)#5-K(2)-K(1)#7	55.5(2)	C(3)-N(9)-K(3)#4	113.1(5)

N(15)#4-K(2)-K(1)#7	134.28(17)	C(2)-N(9)-K(3)#4	110.3(5)
N(11)#6-K(2)-K(1)#7	52.44(14)	K(1)-N(9)-K(3)#4	79.29(15)
N(8)-K(2)-K(1)#7	135.44(15)	C(3)-N(10)-N(11)	106.3(7)
N(10)-K(2)-K(1)#7	82.51(13)	C(3)-N(10)-K(1)#2	125.8(5)
N(15)#7-K(2)-K(1)#7	71.38(14)	N(11)-N(10)-K(1)#2	114.3(5)
N(16)#7-K(2)-K(1)#7	51.63(14)	C(3)-N(10)-K(2)	102.2(5)
K(1)#2-K(2)-K(1)#7	103.19(6)	N(11)-N(10)-K(2)	114.8(5)
O(1)-K(2)-K(2)#8	75.9(2)	K(1)#2-N(10)-K(2)	92.2(2)
N(3)#5-K(2)-K(2)#8	84.6(2)	N(12)-N(11)-N(10)	113.1(7)
N(15)#4-K(2)-K(2)#8	44.74(16)	N(12)-N(11)-K(2)#6	120.3(5)
N(11)#6-K(2)-K(2)#8	123.05(17)	N(10)-N(11)-K(2)#6	126.4(5)
N(8)-K(2)-K(2)#8	115.77(15)	N(11)-N(12)-N(13)	105.4(6)
N(10)-K(2)-K(2)#8	145.30(15)	N(11)-N(12)-K(3)	131.9(5)
N(15)#7-K(2)-K(2)#8	40.09(13)	N(13)-N(12)-K(3)	115.4(5)
N(16)#7-K(2)-K(2)#8	52.55(14)	N(12)-N(13)-C(3)	110.4(6)
K(1)#2-K(2)-K(2)#8	153.74(9)	N(12)-N(13)-C(4)	119.4(6)
K(1)#7-K(2)-K(2)#8	103.05(7)	C(3)-N(13)-C(4)	130.2(7)
O(3)-K(3)-O(2)	113.8(3)	C(4)-N(14)-N(15)	103.1(7)
O(3)-K(3)-N(14)	74.3(4)	C(4)-N(14)-K(3)	121.2(5)
O(2)-K(3)-N(14)	148.5(2)	N(15)-N(14)-K(3)	131.6(5)
O(3)-K(3)-N(6)#9	66.6(6)	N(16)-N(15)-N(14)	110.6(7)
O(2)-K(3)-N(6)#9	80.7(2)	N(16)-N(15)-K(2)#5	113.0(5)
N(14)-K(3)-N(6)#9	128.0(2)	N(14)-N(15)-K(2)#5	134.6(6)
O(3)-K(3)-N(4)#9	75.6(4)	N(16)-N(15)-K(2)#3	83.0(5)
O(2)-K(3)-N(4)#9	127.5(2)	N(14)-N(15)-K(2)#3	101.9(5)
N(14)-K(3)-N(4)#9	83.8(2)	K(2)#5-N(15)-K(2)#3	95.2(2)
N(6)#9-K(3)-N(4)#9	54.8(2)	N(15)-N(16)-N(17)	109.4(7)
O(3)-K(3)-N(1)#5	137.9(6)	N(15)-N(16)-K(2)#3	74.1(5)
O(2)-K(3)-N(1)#5	77.9(3)	N(17)-N(16)-K(2)#3	105.3(6)
N(14)-K(3)-N(1)#5	77.2(3)	C(4)-N(17)-N(16)	103.3(7)
N(6)#9-K(3)-N(1)#5	153.1(3)	C(4)-N(17)-K(1)	124.6(6)
N(4)#9-K(3)-N(1)#5	131.1(2)	N(16)-N(17)-K(1)	114.0(5)
O(3)-K(3)-N(12)	66.7(6)	C(4)-N(17)-K(3)#4	115.3(6)
O(2)-K(3)-N(12)	98.4(2)	N(16)-N(17)-K(3)#4	110.1(6)
N(14)-K(3)-N(12)	55.31(19)	K(1)-N(17)-K(3)#4	89.2(2)
N(6)#9-K(3)-N(12)	128.0(2)	K(2)-O(1)-K(3)#6	114.6(3)
N(4)#9-K(3)-N(12)	129.7(2)	K(2)-O(1)-H(1A)	108.6
N(1)#5-K(3)-N(12)	71.7(2)	K(3)#6-O(1)-H(1A)	126.0
O(3)-K(3)-N(17)#5	138.7(6)	K(2)-O(1)-H(1B)	108.7

O(2)-K(3)-N(17)#5	63.3(2)	K(3)#6-O(1)-H(1B)	26.4
N(14)-K(3)-N(17)#5	131.6(2)	H(1A)-O(1)-H(1B)	109.5
N(6)#9-K(3)-N(17)#5	72.6(2)	K(3)-O(2)-K(1)#7	111.9(3)
N(4)#9-K(3)-N(17)#5	76.6(2)	K(3)-O(2)-H(2A)	108.8
N(1)#5-K(3)-N(17)#5	83.3(2)	K(1)#7-O(2)-H(2A)	123.8
N(12)-K(3)-N(17)#5	152.0(2)	K(3)-O(2)-H(2B)	109.4
O(3)-K(3)-O(1)#6	47.9(3)	K(1)#7-O(2)-H(2B)	91.6
O(2)-K(3)-O(1)#6	66.6(3)	H(2A)-O(2)-H(2B)	109.5
N(14)-K(3)-O(1)#6	109.7(3)	K(3)-O(3)-K(3)#2	178.7(12)
N(6)#9-K(3)-O(1)#6	66.3(2)	K(3)-O(3)-H(3A)	113.5
N(4)#9-K(3)-O(1)#6	110.5(3)	K(3)#2-O(3)-H(3A)	67.8
N(1)#5-K(3)-O(1)#6	118.3(2)	K(3)-O(3)-H(3B)	106.5
N(12)-K(3)-O(1)#6	66.0(2)	K(3)#2-O(3)-H(3B)	72.5
N(17)#5-K(3)-O(1)#6	118.6(3)	H(3A)-O(3)-H(3B)	109.5
O(3)-K(3)-N(9)#5	139.97(14)	K(3)-O(3)-H(3A)#2	67.8(6)
O(2)-K(3)-N(9)#5	105.4(2)	K(3)#2-O(3)-H(3A)#2	113.5(6)
N(14)-K(3)-N(9)#5	76.8(2)	H(3A)-O(3)-H(3A)#2	53.1
N(6)#9-K(3)-N(9)#5	113.77(19)	H(3B)-O(3)-H(3A)#2	149.7
N(4)#9-K(3)-N(9)#5	74.3(2)	K(3)-O(3)-H(3B)#2	72.5(4)
N(1)#5-K(3)-N(9)#5	57.7(2)	K(3)#2-O(3)-H(3B)#2	106.5(4)
N(12)-K(3)-N(9)#5	116.39(18)	H(3A)-O(3)-H(3B)#2	149.7
N(17)#5-K(3)-N(9)#5	55.45(18)	H(3B)-O(3)-H(3B)#2	96.0
O(1)#6-K(3)-N(9)#5	172.0(3)	H(3A)#2-O(3)-H(3B)#2	109.5

Table S10. Hydrogen bonds in **4·2.25H_2O**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...N(4)#11	0.85	2.52	3.284(13)	149.3
O(1)-H(1B)...O(3)#6	0.85	1.90	2.463(15)	122.6
O(2)-H(2A)...N(16)#5	0.85	2.18	2.893(12)	142.1
O(2)-H(2A)...N(17)#5	0.85	2.64	3.085(11)	113.8
O(2)-H(2B)...N(7)#6	0.85	2.24	2.879(11)	131.6
O(2)-H(2B)...N(8)#6	0.85	2.62	3.195(10)	126.2
O(3)-H(3A)...N(6)#12	0.85	2.30	3.13(3)	167.4
O(3)-H(3B)...N(12)#2	0.85	2.52	3.19(3)	137.5
O(3)-H(3B)...O(1)#3	0.85	1.94	2.463(15)	118.8

Table S11 Bond lengths (Å) for **6.**

C(1)-N(1)	1.3354(15)	C(5)-N(20)	1.3295(16)
C(1)-N(2)	1.3476(16)	N(18)-H(18A)	0.8600

C(1)-N(5)	1.3735(16)	N(18)-H(18B)	0.8600
C(2)-N(9)	1.3160(16)	N(19)-H(19A)	0.8600
C(2)-N(6)	1.3208(17)	N(19)-H(19B)	0.8600
C(2)-N(5)	1.4058(16)	N(20)-H(20A)	0.8600
C(3)-N(1)	1.3334(16)	N(20)-H(20B)	0.8600
C(3)-N(10)	1.3474(17)	C(6)-N(21)	1.3196(18)
C(3)-N(13)	1.3794(16)	C(6)-N(22)	1.3215(17)
C(4)-N(17)	1.3185(17)	C(6)-N(23)	1.3232(17)
C(4)-N(14)	1.3250(16)	N(21)-H(21A)	0.8600
C(4)-N(13)	1.4060(16)	N(21)-H(21B)	0.8600
N(2)-N(3)	1.3569(16)	N(22)-H(22A)	0.8600
N(3)-N(4)	1.2814(16)	N(22)-H(22B)	0.8600
N(4)-N(5)	1.3669(14)	N(23)-H(23A)	0.8600
N(6)-N(7)	1.3470(17)	N(23)-H(23B)	0.8600
N(7)-N(8)	1.2992(17)	C(7)-N(25)	1.3145(18)
N(8)-N(9)	1.3531(16)	C(7)-N(24)	1.3175(18)
N(10)-N(11)	1.3522(17)	C(7)-N(26)	1.3292(17)
N(11)-N(12)	1.2824(17)	N(24)-H(24A)	0.8600
N(12)-N(13)	1.3666(15)	N(24)-H(24B)	0.8600
N(14)-N(15)	1.3481(17)	N(25)-H(25A)	0.8600
N(15)-N(16)	1.3008(18)	N(25)-H(25B)	0.8600
N(16)-N(17)	1.3517(16)	N(26)-H(26A)	0.8600
C(5)-N(19)	1.3192(17)	N(26)-H(26B)	0.8600
C(5)-N(18)	1.3225(17)		

Table S12 Bond angles (°) for **6**.

N(4)-N(5)-C(2)	117.66(10)	C(5)-N(20)-H(20B)	120.0
C(1)-N(5)-C(2)	133.13(10)	H(20A)-N(20)-H(20B)	120.0
C(2)-N(6)-N(7)	103.60(11)	N(21)-C(6)-N(22)	120.24(12)
N(8)-N(7)-N(6)	109.48(11)	N(21)-C(6)-N(23)	120.22(13)
N(7)-N(8)-N(9)	109.91(11)	N(22)-C(6)-N(23)	119.54(13)
C(2)-N(9)-N(8)	103.18(11)	C(6)-N(21)-H(21A)	120.0
C(3)-N(10)-N(11)	106.38(11)	C(6)-N(21)-H(21B)	120.0
N(12)-N(11)-N(10)	113.06(11)	H(21A)-N(21)-H(21B)	120.0
N(11)-N(12)-N(13)	105.45(11)	C(6)-N(22)-H(22A)	120.0
N(12)-N(13)-C(3)	109.13(10)	C(6)-N(22)-H(22B)	120.0
N(12)-N(13)-C(4)	117.86(10)	H(22A)-N(22)-H(22B)	120.0
C(3)-N(13)-C(4)	132.97(11)	C(6)-N(23)-H(23A)	120.0
C(4)-N(14)-N(15)	103.54(11)	C(6)-N(23)-H(23B)	120.0

N(16)-N(15)-N(14)	109.46(11)	H(23A)-N(23)-H(23B)	120.0
N(15)-N(16)-N(17)	110.06(12)	N(25)-C(7)-N(24)	120.13(13)
C(4)-N(17)-N(16)	103.20(11)	N(25)-C(7)-N(26)	120.53(13)
N(19)-C(5)-N(18)	119.94(12)	N(24)-C(7)-N(26)	119.34(13)
N(19)-C(5)-N(20)	119.88(12)	C(7)-N(24)-H(24A)	120.0
N(18)-C(5)-N(20)	120.18(12)	C(7)-N(24)-H(24B)	120.0
C(5)-N(18)-H(18A)	120.0	H(24A)-N(24)-H(24B)	120.0
C(5)-N(18)-H(18B)	120.0	C(7)-N(25)-H(25A)	120.0
H(18A)-N(18)-H(18B)	120.0	C(7)-N(25)-H(25B)	120.0
C(5)-N(19)-H(19A)	120.0	H(25A)-N(25)-H(25B)	120.0
C(5)-N(19)-H(19B)	120.0	C(7)-N(26)-H(26A)	120.0
H(19A)-N(19)-H(19B)	120.0	C(7)-N(26)-H(26B)	120.0
C(5)-N(20)-H(20A)	120.0	H(26A)-N(26)-H(26B)	120.0

Table S13 Hydrogen bonds in **6**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(18)-H(18A)...N(9)	0.86	2.16	2.9978(17)	164.8
N(18)-H(18B)...N(14)#1	0.86	2.57	3.2838(17)	141.5
N(18)-H(18B)...N(15)#1	0.86	2.56	3.3879(18)	161.2
N(19)-H(19A)...N(8）	0.86	2.05	2.8997(17）	169.2
N(19)-H(19B)...N(3)#2	0.86	2.47	3.2019(17)	143.7
N(20)-H(20A)...N(2)#2	0.86	2.38	3.0976(17)	141.2
N(20)-H(20A)...N(26)#3	0.86	2.57	3.1461(18)	125.4
N(20)-H(20B)...N(14)#1	0.86	2.13	2.9522(17)	160.5
N(21)-H(21A)...N(4)#4	0.86	2.29	3.1153(16)	161.8
N(21)-H(21B)...N(17)	0.86	2.11	2.9521(17)	166.3
N(22)-H(22A)...N(3)#4	0.86	2.22	3.0592(17)	165.1
N(22)-H(22B)...N(2)#5	0.86	2.39	3.1420(17)	146.8
N(23)-H(23A)...N(16)	0.86	2.30	3.1347(19)	162.3
N(23)-H(23B)...N(10)#5	0.86	2.29	3.0851(18)	152.9
N(23)-H(23B)...N(11)#5	0.86	2.65	3.3240(18)	135.8
N(24)-H(24A)...N(15)	0.86	2.45	3.2125(19)	148.4
N(24)-H(24A)...N(16)	0.86	2.14	2.9886(17)	167.4
N(24)-H(24B)...N(11)#5	0.86	2.04	2.9021(18)	176.7
N(25)-H(25A)...N(15)	0.86	2.37	3.1547(17)	151.6
N(25)-H(25B)...N(6)#6	0.86	2.13	2.9465(18)	157.7
N(26)-H(26B)...N(12)#5	0.86	2.65	3.4667(18)	159.2
N(26)-H(26B)...N(20)#3	0.86	2.66	3.1461(18)	116.8

N(26)-H(26A)...N(6)#6	0.86	2.58	3.2842(18)	139.6
N(26)-H(26A)...N(7)#6	0.86	2.24	3.0860(19)	166.5

Table S14 Bond lengths (Å) for **7·H_2O.**

C(1)-N(2)	1.3372(18)	N(15)-N(16)	1.303(2)
C(1)-N(1)	1.3442(18)	N(16)-N(17)	1.3504(18)
C(1)-N(5)	1.3660(18)	N(18)-N(19)	1.4396(18)
C(2)-N(9)	1.3157(19)	N(18)-H(18A)	0.9600
C(2)-N(6)	1.3169(19)	N(18)-H(18B)	0.9601
C(2)-N(5)	1.4040(18)	N(18)-H(18C)	0.9601
C(3)-N(1)	1.3360(18)	N(19)-H(19A)	0.8491
C(3)-N(10)	1.3390(19)	N(19)-H(19B)	0.9811
C(3)-N(13)	1.3696(18)	N(20)-N(21)	1.4304(19)
C(4)-N(14)	1.3217(19)	N(20)-H(20A)	0.9600
C(4)-N(17)	1.3234(19)	N(20)-H(20B)	0.9601
C(4)-N(13)	1.3993(19)	N(20)-H(20C)	0.9600
N(2)-N(3)	1.3617(17)	N(21)-H(21A)	0.8900
N(3)-N(4)	1.2808(17)	N(21)-H(21B)	0.8900
N(4)-N(5)	1.3644(16)	N(22)-N(23)	1.4323(19)
N(6)-N(7)	1.349(2)	N(22)-H(22A)	0.8900
N(7)-N(8)	1.301(2)	N(22)-H(22B)	0.8900
N(8)-N(9)	1.3556(18)	N(23)-H(23A)	0.8900
N(10)-N(11)	1.3599(18)	N(23)-H(23B)	0.8900
N(11)-N(12)	1.2799(19)	N(23)-H(23C)	0.8900
N(12)-N(13)	1.3665(17)	O(1)-H(1B)	0.8946
N(14)-N(15)	1.3476(19)	O(1)-H(1A)	0.8797

Table S15 Bond angles (°) for **7·H_2O**.

N(2)-C(1)-N(1)	131.76(13)	N(15)-N(16)-N(17)	109.64(13)
N(2)-C(1)-N(5)	106.80(12)	C(4)-N(17)-N(16)	103.03(12)
N(1)-C(1)-N(5)	121.44(12)	N(19)-N(18)-H(18A)	109.2
N(9)-C(2)-N(6)	113.89(13)	N(19)-N(18)-H(18B)	109.6
N(9)-C(2)-N(5)	124.72(13)	H(18A)-N(18)-H(18B)	109.5
N(6)-C(2)-N(5)	121.37(13)	N(19)-N(18)-H(18C)	109.6
N(1)-C(3)-N(10)	132.23(13)	H(18A)-N(18)-H(18C)	109.5
N(1)-C(3)-N(13)	121.53(13)	H(18B)-N(18)-H(18C)	109.5
N(10)-C(3)-N(13)	106.22(12)	N(18)-N(19)-H(19A)	99.8
N(14)-C(4)-N(17)	114.26(14)	N(18)-N(19)-H(19B)	103.7
N(14)-C(4)-N(13)	120.78(13)	H(19A)-N(19)-H(19B)	101.6

N(17)-C(4)-N(13)	124.95(13)	N(21)-N(20)-H(20A)	109.6
C(3)-N(1)-C(1)	117.35(12)	N(21)-N(20)-H(20B)	109.5
C(1)-N(2)-N(3)	106.01(12)	H(20A)-N(20)-H(20B)	109.5
N(4)-N(3)-N(2)	112.52(12)	N(21)-N(20)-H(20C)	109.3
N(3)-N(4)-N(5)	105.61(11)	H(20A)-N(20)-H(20C)	109.5
N(4)-N(5)-C(1)	109.05(11)	H(20B)-N(20)-H(20C)	109.5
N(4)-N(5)-C(2)	119.23(11)	N(20)-N(21)-H(21A)	109.2
C(1)-N(5)-C(2)	131.69(12)	N(20)-N(21)-H(21B)	109.2
C(2)-N(6)-N(7)	103.53(13)	H(21A)-N(21)-H(21B)	109.5
N(8)-N(7)-N(6)	109.75(13)	N(23)-N(22)-H(22A)	109.1
N(7)-N(8)-N(9)	109.38(13)	N(23)-N(22)-H(22B)	108.9
C(2)-N(9)-N(8)	103.44(12)	H(22A)-N(22)-H(22B)	109.5
C(3)-N(10)-N(11)	106.68(12)	N(22)-N(23)-H(23A)	109.8
N(12)-N(11)-N(10)	112.15(12)	N(22)-N(23)-H(23B)	109.7
N(11)-N(12)-N(13)	105.85(12)	H(23A)-N(23)-H(23B)	109.5
N(12)-N(13)-C(3)	109.10(12)	N(22)-N(23)-H(23C)	108.9
N(12)-N(13)-C(4)	118.84(12)	H(23A)-N(23)-H(23C)	109.5
C(3)-N(13)-C(4)	132.06(12)	H(23B)-N(23)-H(23C)	109.5
C(4)-N(14)-N(15)	102.90(13)	H(1B)-O(1)-H(1A)	97.9
N(16)-N(15)-N(14)	110.17(12)		

Table S16 Hydrogen bonds in **7·H_2O**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(18)-H(18A)...N(3)#1	0.96	2.02	2.9261(18)	156.9
N(18)-H(18B)...N(9)	0.96	2.09	2.9475(19)	147.6
N(18)-H(18C)...N(4)#2	0.96	2.56	3.1308(17)	118.5
N(18)-H(18C)...N(6)#2	0.96	1.99	2.9113(19)	159.9
N(19)-H(19A)...N(22)#3	0.85	2.25	3.077(2)	165.9
N(19)-H(19B)...N(7)#4	0.98	2.65	3.174(2)	113.9
N(19)-H(19B)...N(11)#5	0.98	2.38	3.221(2)	144.0
N(20)-H(20A)...N(15)#6	0.96	1.88	2.8314(19)	169.9
N(20)-H(20B)...N(12)#7	0.96	2.57	3.2214(18)	125.1
N(20)-H(20B)...N(14)#7	0.96	2.06	2.9211(18)	148.5
N(20)-H(20C)...N(1)	0.96	2.40	3.0909(18)	128.4
N(20)-H(20C)...N(9)	0.96	2.58	3.094(2)	114.1
N(20)-H(20C)...N(17)	0.96	2.19	2.9775(19)	138.0
N(21)-H(21A)...O(1)	0.89	2.12	2.981(2)	162.0
N(21)-H(21B)...O(1)#8	0.89	2.34	3.105(2)	144.2
N(22)-H(22A)...N(7)#9	0.89	2.46	3.111(2)	130.8

N(22)-H(22B)...O(1)#10	0.89	2.49	3.369(3)	167.4
N(23)-H(23A)...N(2)	0.89	2.35	2.9305(18)	123.2
N(23)-H(23A)...N(10)	0.89	2.00	2.8174(19)	152.5
N(23)-H(23B)...N(21)#11	0.89	2.03	2.921(2)	174.5
N(23)-H(23C)...N(19)#1	0.89	2.02	2.907(2)	172.0
O(1)-H(1B)...N(16)	0.89	2.05	2.858(2)	149.0
O(1)-H(1A)...N(7)#8	0.88	2.57	3.379(3)	153.3
O(1)-H(1A)...N(8)#8	0.88	2.70	3.278(3)	124.8

Table S17 Bond lengths (Å) for **8·2H$_2$O**.

C(1)-N(1)	1.3371(19)	N(18)-O(1)	1.3996(17)
C(1)-N(2)	1.3408(19)	N(18)-H(18A)	0.8900
C(1)-N(5)	1.3740(18)	N(18)-H(18B)	0.8900
C(2)-N(6)	1.3215(19)	N(18)-H(18C)	0.8900
C(2)-N(9)	1.3241(19)	N(19)-O(2)	1.4098(16)
C(2)-N(5)	1.4016(18)	N(19)-H(19A)	0.8900
C(3)-N(10)	1.3407(19)	N(19)-H(19B)	0.8900
C(3)-N(1)	1.3422(18)	N(19)-H(19C)	0.8900
C(3)-N(13)	1.3702(18)	N(20)-O(3)	1.4024(17)
C(4)-N(17)	1.3216(19)	N(20)-H(20A)	0.8900
C(4)-N(14)	1.3275(19)	N(20)-H(20B)	0.8900
C(4)-N(13)	1.4022(19)	N(20)-H(20C)	0.8900
N(2)-N(3)	1.3632(18)	N(21)-O(4)	1.4009(19)
N(3)-N(4)	1.2787(19)	N(21)-H(21A)	0.8900
N(4)-N(5)	1.3721(17)	N(21)-H(21B)	0.8900
N(6)-N(7)	1.3484(18)	N(21)-H(21C)	0.8900
N(7)-N(8)	1.3062(19)	O(2)-H(2)	0.9446
N(8)-N(9)	1.3525(18)	O(3)-H(3)	0.8200
N(10)-N(11)	1.3614(19)	O(4)-H(4)	0.9600
N(11)-N(12)	1.2745(19)	O(5)-H(5A)	0.9186
N(12)-N(13)	1.3659(17)	O(5)-H(5B)	0.8631
N(14)-N(15)	1.3417(19)	O(6)-H(6A)	0.9084
N(15)-N(16)	1.308(2)	O(6)-H(6B)	0.9530
N(16)-N(17)	1.3523(18)		

Table S18 Bond angles (°) for **8·2H$_2$O.**

N(1)-C(1)-N(2)	131.62(13)	N(15)-N(16)-N(17)	109.82(12)
N(1)-C(1)-N(5)	122.31(12)	C(4)-N(17)-N(16)	102.85(12)

N(2)-C(1)-N(5)	106.07(12)	O(1)-N(18)-H(18A)	109.5
N(6)-C(2)-N(9)	113.76(13)	O(1)-N(18)-H(18B)	109.5
N(6)-C(2)-N(5)	121.47(13)	H(18A)-N(18)-H(18B)	109.5
N(9)-C(2)-N(5)	124.77(13)	O(1)-N(18)-H(18C)	109.5
N(10)-C(3)-N(1)	131.27(13)	H(18A)-N(18)-H(18C)	109.5
N(10)-C(3)-N(13)	106.61(12)	H(18B)-N(18)-H(18C)	109.5
N(1)-C(3)-N(13)	122.11(12)	O(2)-N(19)-H(19A)	109.5
N(17)-C(4)-N(14)	114.24(13)	O(2)-N(19)-H(19B)	109.5
N(17)-C(4)-N(13)	125.18(13)	H(19A)-N(19)-H(19B)	109.5
N(14)-C(4)-N(13)	120.58(13)	O(2)-N(19)-H(19C)	109.5
C(1)-N(1)-C(3)	116.54(12)	H(19A)-N(19)-H(19C)	109.5
C(1)-N(2)-N(3)	106.70(12)	H(19B)-N(19)-H(19C)	109.5
N(4)-N(3)-N(2)	112.39(12)	O(3)-N(20)-H(20A)	109.5
N(3)-N(4)-N(5)	105.66(12)	O(3)-N(20)-H(20B)	109.5
N(4)-N(5)-C(1)	109.17(11)	H(20A)-N(20)-H(20B)	109.5
N(4)-N(5)-C(2)	118.27(11)	O(3)-N(20)-H(20C)	109.5
C(1)-N(5)-C(2)	132.51(12)	H(20A)-N(20)-H(20C)	109.5
C(2)-N(6)-N(7)	103.88(12)	H(20B)-N(20)-H(20C)	109.5
N(8)-N(7)-N(6)	109.17(12)	O(4)-N(21)-H(21A)	109.5
N(7)-N(8)-N(9)	110.19(12)	O(4)-N(21)-H(21B)	109.5
C(2)-N(9)-N(8)	103.01(12)	H(21A)-N(21)-H(21B)	109.5
C(3)-N(10)-N(11)	106.12(12)	O(4)-N(21)-H(21C)	109.5
N(12)-N(11)-N(10)	112.47(12)	H(21A)-N(21)-H(21C)	109.5
N(11)-N(12)-N(13)	106.08(12)	H(21B)-N(21)-H(21C)	109.5
N(12)-N(13)-C(3)	108.71(11)	N(19)-O(2)-H(2)	102.0
N(12)-N(13)-C(4)	118.02(12)	N(20)-O(3)-H(3)	109.5
C(3)-N(13)-C(4)	133.15(12)	N(21)-O(4)-H(4)	109.2
C(4)-N(14)-N(15)	103.10(13)	H(5A)-O(5)-H(5B)	96.6
N(16)-N(15)-N(14)	109.99(13)	H(6A)-O(6)-H(6B)	109.2

Table S19 Hydrogen bonds in **8·2H$_2$O**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(18)-H(18A)...N(2)#1	0.89	2.39	3.1346(19)	141.1
N(18)-H(18A)...N(10)#1	0.89	2.33	3.0886(19)	143.8
N(18)-H(18B)...N(7)#2	0.89	2.33	3.138(2)	150.9
N(18)-H(18B)...O(6)#3	0.89	2.41	2.9573(18)	119.7
N(18)-H(18C)...N(11)#4	0.89	2.26	3.0222(19)	143.3
N(18)-H(18C)...O(5)#5	0.89	2.24	2.8822(17)	128.6
N(19)-H(19A)...N(6)#2	0.89	1.98	2.8504(18)	165.3

N(19)-H(19B)...N(1)	0.89	2.61	3.0671(17)	113.0
N(19)-H(19B)...N(4)#2	0.89	2.64	3.0807(18)	111.6
N(19)-H(19B)...O(2)#1	0.89	2.15	2.8583(17)	135.9
N(19)-H(19C)...N(9)	0.89	2.07	2.9042(18)	155.3
N(20)-H(20A)...N(15)#6	0.89	1.99	2.8683(19)	168.7
N(20)-H(20B)...N(1)#7	0.89	2.53	3.2149(18)	134.8
N(20)-H(20B)...N(9)#7	0.89	2.63	3.1422(19)	117.9
N(20)-H(20B)...N(17)#7	0.89	2.31	2.9696(19)	131.1
N(20)-H(20C)...N(12)	0.89	2.27	3.0921(19)	154.5
N(20)-H(20C)...N(14)	0.89	2.35	2.9884(19)	129.1
N(21)-H(21A)...N(16)#8	0.89	2.00	2.8655(19)	165.5
N(21)-H(21B)...O(3)#7	0.89	2.49	3.1539(19)	132.0
N(21)-H(21B)...O(4)#8	0.89	2.25	2.7813(19)	117.7
N(21)-H(21C)...N(8)	0.89	1.98	2.8229(19)	156.9
O(2)-H(2)...N(18)	0.94	2.49	3.3487(17)	151.4
O(2)-H(2)...O(1)	0.94	1.57	2.5069(15)	172.6
O(3)-H(3)...O(6)#2	0.82	1.80	2.5835(18)	159.7
O(4)-H(4)...N(18)	0.96	2.51	3.3456(19)	145.0
O(4)-H(4)...O(1)	0.96	1.58	2.5290(16)	169.3
O(5)-H(5A)...N(3)#9	0.92	2.00	2.8917(17)	164.4
O(5)-H(5B)...O(1)	0.86	1.84	2.6974(16)	170.7
O(6)-H(6A)...O(5)#10	0.91	1.75	2.6540(17)	171.9
O(6)-H(6B)...N(2)	0.95	2.03	2.9586(17)	163.4

Table S20 Bond lengths (Å) for **9·3CH$_3$OH**.

C(1)-N(2)	1.314(2)	N(2)-N(3)	1.373(2)
C(1)-N(5)	1.344(2)	N(2)-Na(1)	2.4301(16)
C(1)-N(1)	1.364(2)	N(3)-N(4)	1.281(2)
C(2)-N(6)	1.312(2)	N(4)-N(5)	1.3660(19)
C(2)-N(9)	1.313(2)	N(6)-N(7)	1.3541(19)
C(2)-N(5)	1.4059(19)	N(7)-N(8)	1.297(2)
C(3)-N(10)	1.319(2)	N(8)-N(9)	1.347(2)
C(3)-N(13)	1.343(2)	N(10)-N(11)	1.371(2)
C(3)-N(1)	1.359(2)	N(10)-Na(1)	2.5048(16)
C(4)-N(14)	1.307(2)	N(11)-N(12)	1.280(2)
C(4)-N(17)	1.322(2)	N(12)-N(13)	1.366(2)
C(4)-N(13)	1.406(2)	N(14)-N(15)	1.338(2)
C(5)-O(1)	1.417(3)	N(15)-N(16)	1.300(2)
C(5)-H(5A)	0.9600	N(15)-H(15)	0.9366

C(5)-H(5B)	0.9600	N(16)-N(17)	1.320(2)
C(5)-H(5C)	0.9600	Na(1)-O(2)	2.3470(15)
C(6)-O(2)	1.420(3)	Na(1)-O(1)	2.4308(15)
C(6)-H(6A)	0.9600	Na(1)-O(1)#1	2.6736(18)
C(6)-H(6B)	0.9600	Na(1)-O(2)#2	2.7381(18)
C(6)-H(6C)	0.9600	Na(1)-Na(1)#2	3.8327(16)
C(7)-O(3)	1.412(3)	Na(1)-Na(1)#1	3.8825(16)
C(7)-H(7A)	0.9600	O(1)-H(1A)	0.9726
C(7)-H(7B)	0.9600	O(2)-H(2)	0.9792
C(7)-H(7C)	0.9600	O(3)-H(3)	0.9535
N(1)-H(1)	0.8867		

Table S21 Bond angles (°) for **9·3CH$_3$OH**.

N(2)-C(1)-N(5)	108.90(14)	C(3)-N(13)-N(12)	108.61(14)
N(2)-C(1)-N(1)	128.96(15)	C(3)-N(13)-C(4)	129.43(15)
N(5)-C(1)-N(1)	122.11(14)	N(12)-N(13)-C(4)	121.95(15)
N(6)-C(2)-N(9)	114.70(14)	C(4)-N(14)-N(15)	99.30(15)
N(6)-C(2)-N(5)	124.18(14)	N(16)-N(15)-N(14)	114.73(14)
N(9)-C(2)-N(5)	121.12(15)	N(16)-N(15)-H(15)	114.6
N(10)-C(3)-N(13)	108.87(15)	N(14)-N(15)-H(15)	130.7
N(10)-C(3)-N(1)	128.03(16)	N(15)-N(16)-N(17)	105.79(14)
N(13)-C(3)-N(1)	123.10(14)	N(16)-N(17)-C(4)	104.98(15)
N(14)-C(4)-N(17)	115.20(15)	O(2)-Na(1)-N(2)	161.38(6)
N(14)-C(4)-N(13)	124.55(16)	O(2)-Na(1)-O(1)	93.02(5)
N(17)-C(4)-N(13)	120.25(15)	N(2)-Na(1)-O(1)	101.68(5)
O(1)-C(5)-H(5A)	109.5	O(2)-Na(1)-N(10)	96.48(5)
O(1)-C(5)-H(5B)	109.5	N(2)-Na(1)-N(10)	71.70(5)
H(5A)-C(5)-H(5B)	109.5	O(1)-Na(1)-N(10)	165.04(7)
O(1)-C(5)-H(5C)	109.5	O(2)-Na(1)-O(1)#1	110.49(6)
H(5A)-C(5)-H(5C)	109.5	N(2)-Na(1)-O(1)#1	83.32(5)
H(5B)-C(5)-H(5C)	109.5	O(1)-Na(1)-O(1)#1	81.07(5)
O(2)-C(6)-H(6A)	109.5	N(10)-Na(1)-O(1)#1	84.78(5)
O(2)-C(6)-H(6B)	109.5	O(2)-Na(1)-O(2)#2	82.47(5)
H(6A)-C(6)-H(6B)	109.5	N(2)-Na(1)-O(2)#2	82.68(5)
O(2)-C(6)-H(6C)	109.5	O(1)-Na(1)-O(2)#2	105.28(5)
H(6A)-C(6)-H(6C)	109.5	N(10)-Na(1)-O(2)#2	87.46(5)
H(6B)-C(6)-H(6C)	109.5	O(1)#1-Na(1)-O(2)#2	165.55(5)
O(3)-C(7)-H(7A)	109.5	O(2)-Na(1)-Na(1)#2	45.09(4)
O(3)-C(7)-H(7B)	109.5	N(2)-Na(1)-Na(1)#2	119.29(5)

H(7A)-C(7)-H(7B)	109.5	O(1)-Na(1)-Na(1)#2	102.74(5)
O(3)-C(7)-H(7C)	109.4	N(10)-Na(1)-Na(1)#2	92.15(5)
H(7A)-C(7)-H(7C)	109.5	O(1)#1-Na(1)-Na(1)#2	154.97(5)
H(7B)-C(7)-H(7C)	109.5	O(2)#2-Na(1)-Na(1)#2	37.38(3)
C(3)-N(1)-C(1)	124.16(14)	O(2)-Na(1)-Na(1)#1	105.90(5)
C(3)-N(1)-H(1)	119.7	N(2)-Na(1)-Na(1)#1	92.67(5)
C(1)-N(1)-H(1)	116.0	O(1)-Na(1)-Na(1)#1	42.86(4)
C(1)-N(2)-N(3)	105.31(14)	N(10)-Na(1)-Na(1)#1	122.83(6)
C(1)-N(2)-Na(1)	134.38(12)	O(1)#1-Na(1)-Na(1)#1	38.21(3)
N(3)-N(2)-Na(1)	120.31(10)	O(2)#2-Na(1)-Na(1)#1	146.28(5)
N(4)-N(3)-N(2)	111.71(13)	Na(1)#2-Na(1)-Na(1)#1	139.64(4)
N(3)-N(4)-N(5)	105.86(14)	C(5)-O(1)-Na(1)	118.97(13)
C(1)-N(5)-N(4)	108.23(13)	C(5)-O(1)-Na(1)#1	113.48(14)
C(1)-N(5)-C(2)	129.60(14)	Na(1)-O(1)-Na(1)#1	98.93(5)
N(4)-N(5)-C(2)	122.14(13)	C(5)-O(1)-H(1A)	109.5
C(2)-N(6)-N(7)	102.84(13)	Na(1)-O(1)-H(1A)	113.6
N(8)-N(7)-N(6)	109.58(13)	Na(1)#1-O(1)-H(1A)	100.3
N(7)-N(8)-N(9)	109.95(13)	C(6)-O(2)-Na(1)	120.60(14)
C(2)-N(9)-N(8)	102.93(13)	C(6)-O(2)-Na(1)#2	120.17(15)
C(3)-N(10)-N(11)	104.75(14)	Na(1)-O(2)-Na(1)#2	97.53(5)
C(3)-N(10)-Na(1)	132.58(12)	C(6)-O(2)-H(2)	104.2
N(11)-N(10)-Na(1)	122.39(11)	Na(1)-O(2)-H(2)	113.7
N(12)-N(11)-N(10)	112.52(15)	Na(1)#2-O(2)-H(2)	99.0
N(11)-N(12)-N(13)	105.25(15)	C(7)-O(3)-H(3)	105.2

Table S22 Hydrogen bonds in **9·3CH$_3$OH**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5C)...N(3)	0.96	2.71	3.578(3)	150.5
C(6)-H(6B)...N(16)#3	0.96	2.67	3.563(3)	154.7
C(6)-H(6C)...N(11)	0.96	2.63	3.451(3)	143.4
N(1)-H(1)...N(9)	0.89	2.11	2.7931(19)	133.0
N(1)-H(1)...N(17)	0.89	2.15	2.7863(19)	127.7
N(15)-H(15)...O(3)#4	0.94	1.71	2.619(2)	164.2
O(1)-H(1A)...N(7)#3	0.97	2.00	2.9617(19)	169.5
O(1)-H(1A)...N(8)#3	0.97	2.68	3.543(2)	148.3
O(2)-H(2)...N(8)#3	0.98	1.87	2.8445(19)	171.2
O(3)-H(3)...N(6)	0.95	1.79	2.743(2)	176.8

Table S23 Bond lengths (Å) for **10·2.25H$_2$O**

C(1)-N(1)	1.340(3)	K(2)-N(12)	3.178(2)
C(1)-N(2)	1.342(3)	K(2)-Na(1)#3	4.0129(13)
C(1)-N(5)	1.372(3)	K(2)-H(3A)	2.8016
C(2)-N(6)	1.324(3)	K(2)-H(2A)#6	2.7376
C(2)-N(9)	1.327(4)	K(2)-H(2B)#6	2.6931(10)
C(2)-N(5)	1.404(3)	N(1)-Na(1)	2.850(2)
C(3)-N(1)	1.341(3)	N(2)-N(3)	1.354(3)
C(3)-N(10)	1.350(3)	N(2)-Na(1)#6	2.633(3)
C(3)-N(13)	1.370(3)	N(3)-N(4)	1.285(3)
C(4)-N(14)	1.316(3)	N(4)-N(5)	1.367(3)
C(4)-N(17)	1.322(3)	N(6)-N(7)	1.349(4)
C(4)-N(13)	1.399(3)	N(7)-N(8)	1.302(4)
K(1)-O(1)	2.757(3)	N(8)-N(9)	1.358(3)
K(1)-N(15)	2.825(2)	N(8)-Na(1)#7	2.520(3)
K(1)-N(11)#1	2.847(2)	N(9)-Na(1)	2.457(3)
K(1)-N(7)#2	2.863(2)	N(10)-N(11)	1.359(3)
K(1)-N(10)#3	3.058(2)	N(10)-Na(1)#6	2.590(2)
K(1)-N(2)#3	3.093(2)	N(11)-N(12)	1.282(3)
K(1)-N(16)#4	3.222(3)	N(12)-N(13)	1.367(3)
K(1)-N(15)#4	3.398(3)	N(14)-N(15)	1.351(3)
K(1)-Na(1)#5	4.1207(13)	N(15)-N(16)	1.299(3)
K(1)-Na(1)#4	4.3481(11)	N(16)-N(17)	1.355(3)
K(1)-K(1)#4	4.7378(13)	N(17)-Na(1)	2.583(3)
K(1)-K(2)	5.0370(9)	O(1)-H(1A)	0.8632
K(2)-O(3)	2.714(4)	O(1)-H(1B)	0.9678
K(2)-N(14)	2.857(2)	O(2)-H(2A)	0.8500
K(2)-O(2)	2.9019(7)	O(2)-H(2B)	0.8501
K(2)-N(6)#2	2.964(3)	O(2)-H(2A)#6	0.8500
K(2)-N(4)#2	2.988(2)	O(2)-H(2B)#6	0.8501
K(2)-N(9)#3	3.099(3)	O(3)-H(3A)	0.9012
K(2)-N(1)#3	3.111(2)	O(3)-H(3B)	1.0510
K(2)-N(17)#3	3.170(3)		

Table S24 Bond angles (°) for **10·2.25H_2O.**

N(1)-C(1)-N(2)	131.1(2)	N(6)#2-K(2)-H(2A)#6	70.29(8)
N(1)-C(1)-N(5)	122.5(2)	N(4)#2-K(2)-H(2A)#6	70.58(8)

N(2)-C(1)-N(5)	106.4(2)	N(9)#3-K(2)-H(2A)#6	139.09(9)
N(6)-C(2)-N(9)	113.9(2)	N(1)#3-K(2)-H(2A)#6	129.31(4)
N(6)-C(2)-N(5)	121.5(2)	N(17)#3-K(2)-H(2A)#6	142.84(9)
N(9)-C(2)-N(5)	124.6(2)	N(12)-K(2)-H(2A)#6	67.90(8)
N(1)-C(3)-N(10)	131.9(2)	Na(1)#3-K(2)-H(2A)#6	173.50(5)
N(1)-C(3)-N(13)	121.9(2)	K(1)-K(2)-H(2A)#6	78.522(17)
N(10)-C(3)-N(13)	106.22(19)	H(3A)-K(2)-H(2A)#6	101.3
N(14)-C(4)-N(17)	113.9(2)	O(3)-K(2)-H(2B)#6	90.98(12)
N(14)-C(4)-N(13)	121.5(2)	N(14)-K(2)-H(2B)#6	92.50(8)
N(17)-C(4)-N(13)	124.6(2)	O(2)-K(2)-H(2B)#6	16.950(5)
O(1)-K(1)-N(15)	73.62(9)	N(6)#2-K(2)-H(2B)#6	78.64(7)
O(1)-K(1)-N(11)#1	86.10(9)	N(4)#2-K(2)-H(2B)#6	50.98(9)
N(15)-K(1)-N(11)#1	158.40(7)	N(9)#3-K(2)-H(2B)#6	146.01(8)
O(1)-K(1)-N(7)#2	156.66(10)	N(1)#3-K(2)-H(2B)#6	153.05(5)
N(15)-K(1)-N(7)#2	94.85(8)	N(17)#3-K(2)-H(2B)#6	125.53(8)
N(11)#1-K(1)-N(7)#2	101.32(7)	N(12)-K(2)-H(2B)#6	74.93(8)
O(1)-K(1)-N(10)#3	133.57(10)	Na(1)#3-K(2)-H(2B)#6	156.89(4)
N(15)-K(1)-N(10)#3	109.13(6)	K(1)-K(2)-H(2B)#6	104.62(2)
N(11)#1-K(1)-N(10)#3	90.13(6)	H(3A)-K(2)-H(2B)#6	75.3
N(7)#2-K(1)-N(10)#3	69.07(6)	H(2A)#6-K(2)-H(2B)#6	29.6
O(1)-K(1)-N(2)#3	87.31(9)	C(1)-N(1)-C(3)	116.8(2)
N(15)-K(1)-N(2)#3	72.07(7)	C(1)-N(1)-Na(1)	112.24(14)
N(11)#1-K(1)-N(2)#3	115.13(7)	C(3)-N(1)-Na(1)	117.23(15)
N(7)#2-K(1)-N(2)#3	108.78(6)	C(1)-N(1)-K(2)#8	110.03(15)
N(10)#3-K(1)-N(2)#3	53.07(6)	C(3)-N(1)-K(2)#8	111.36(14)
O(1)-K(1)-N(16)#4	94.33(10)	Na(1)-N(1)-K(2)#8	84.50(6)
N(15)-K(1)-N(16)#4	91.49(7)	C(1)-N(2)-N(3)	106.5(2)
N(11)#1-K(1)-N(16)#4	82.53(6)	C(1)-N(2)-Na(1)#6	123.79(16)
N(7)#2-K(1)-N(16)#4	65.20(7)	N(3)-N(2)-Na(1)#6	118.75(16)
N(10)#3-K(1)-N(16)#4	131.02(6)	C(1)-N(2)-K(1)#8	101.13(15)
N(2)#3-K(1)-N(16)#4	162.34(6)	N(3)-N(2)-K(1)#8	111.88(15)
O(1)-K(1)-N(15)#4	72.33(10)	Na(1)#6-N(2)-K(1)#8	91.68(7)
N(15)-K(1)-N(15)#4	81.25(7)	N(4)-N(3)-N(2)	112.4(2)
N(11)#1-K(1)-N(15)#4	85.63(6)	N(3)-N(4)-N(5)	105.8(2)
N(7)#2-K(1)-N(15)#4	86.07(7)	N(3)-N(4)-K(2)#9	129.26(17)
N(10)#3-K(1)-N(15)#4	153.46(6)	N(5)-N(4)-K(2)#9	119.69(16)
N(2)#3-K(1)-N(15)#4	150.20(6)	N(4)-N(5)-C(1)	108.9(2)
N(16)#4-K(1)-N(15)#4	22.43(6)	N(4)-N(5)-C(2)	118.4(2)
O(1)-K(1)-Na(1)#5	95.69(9)	C(1)-N(5)-C(2)	132.7(2)

N(15)-K(1)-Na(1)#5	111.67(6)	C(2)-N(6)-N(7)	103.2(2)
N(11)#1-K(1)-Na(1)#5	77.07(5)	C(2)-N(6)-K(2)#9	121.71(18)
N(7)#2-K(1)-Na(1)#5	107.51(6)	N(7)-N(6)-K(2)#9	134.89(17)
N(10)#3-K(1)-Na(1)#5	38.87(4)	N(8)-N(7)-N(6)	110.3(2)
N(2)#3-K(1)-Na(1)#5	39.70(5)	N(8)-N(7)-K(1)#9	126.16(18)
N(16)#4-K(1)-Na(1)#5	156.55(5)	N(6)-N(7)-K(1)#9	123.57(18)
N(15)#4-K(1)-Na(1)#5	159.70(5)	N(7)-N(8)-N(9)	109.4(2)
O(1)-K(1)-Na(1)#4	125.66(8)	N(7)-N(8)-Na(1)#7	122.32(17)
N(15)-K(1)-Na(1)#4	136.95(6)	N(9)-N(8)-Na(1)#7	127.87(19)
N(11)#1-K(1)-Na(1)#4	51.90(5)	C(2)-N(9)-N(8)	103.2(2)
N(7)#2-K(1)-Na(1)#4	51.35(6)	C(2)-N(9)-Na(1)	124.57(18)
N(10)#3-K(1)-Na(1)#4	85.02(4)	N(8)-N(9)-Na(1)	123.77(19)
N(2)#3-K(1)-Na(1)#4	137.68(5)	C(2)-N(9)-K(2)#8	100.55(16)
N(16)#4-K(1)-Na(1)#4	52.87(4)	N(8)-N(9)-K(2)#8	108.16(18)
N(15)#4-K(1)-Na(1)#4	71.78(4)	Na(1)-N(9)-K(2)#8	91.74(8)
Na(1)#5-K(1)-Na(1)#4	104.54(2)	C(3)-N(10)-N(11)	106.39(19)
O(1)-K(1)-K(1)#4	67.31(9)	C(3)-N(10)-Na(1)#6	123.29(15)
N(15)-K(1)-K(1)#4	45.14(5)	N(11)-N(10)-Na(1)#6	116.83(15)
N(11)#1-K(1)-K(1)#4	119.98(5)	C(3)-N(10)-K(1)#8	101.97(15)
N(7)#2-K(1)-K(1)#4	90.07(6)	N(11)-N(10)-K(1)#8	113.14(15)
N(10)#3-K(1)-K(1)#4	146.82(4)	Na(1)#6-N(10)-K(1)#8	93.33(7)
N(2)#3-K(1)-K(1)#4	116.03(5)	N(12)-N(11)-N(10)	112.28(19)
N(16)#4-K(1)-K(1)#4	49.65(4)	N(12)-N(11)-K(1)#10	123.28(15)
N(15)#4-K(1)-K(1)#4	36.11(4)	N(10)-N(11)-K(1)#10	124.27(15)
Na(1)#5-K(1)-K(1)#4	153.24(2)	N(11)-N(12)-N(13)	106.04(19)
Na(1)#4-K(1)-K(1)#4	102.20(2)	N(11)-N(12)-K(2)	133.22(15)
O(1)-K(1)-K(2)	122.27(8)	N(13)-N(12)-K(2)	114.42(14)
N(15)-K(1)-K(2)	49.26(5)	N(12)-N(13)-C(3)	109.06(18)
N(11)#1-K(1)-K(2)	151.63(5)	N(12)-N(13)-C(4)	118.55(19)
N(7)#2-K(1)-K(2)	53.10(6)	C(3)-N(13)-C(4)	132.26(19)
N(10)#3-K(1)-K(2)	70.36(4)	C(4)-N(14)-N(15)	103.7(2)
N(2)#3-K(1)-K(2)	69.82(4)	C(4)-N(14)-K(2)	127.54(17)
N(16)#4-K(1)-K(2)	94.73(4)	N(15)-N(14)-K(2)	128.34(16)
N(15)#4-K(1)-K(2)	102.53(4)	N(16)-N(15)-N(14)	109.5(2)
Na(1)#5-K(1)-K(2)	97.73(2)	N(16)-N(15)-K(1)	117.54(17)
Na(1)#4-K(1)-K(2)	104.44(2)	N(14)-N(15)-K(1)	132.58(17)
K(1)#4-K(1)-K(2)	76.495(16)	N(16)-N(15)-K(1)#4	71.16(16)
O(3)-K(2)-N(14)	140.85(13)	N(14)-N(15)-K(1)#4	101.78(17)
O(3)-K(2)-O(2)	101.98(12)	K(1)-N(15)-K(1)#4	98.75(7)

N(14)-K(2)-O(2)	75.81(8)	N(15)-N(16)-N(17)	109.9(2)
O(3)-K(2)-N(6)#2	128.25(13)	N(15)-N(16)-K(1)#4	86.40(17)
N(14)-K(2)-N(6)#2	90.58(7)	N(17)-N(16)-K(1)#4	96.67(16)
O(2)-K(2)-N(6)#2	82.05(7)	C(4)-N(17)-N(16)	103.1(2)
O(3)-K(2)-N(4)#2	78.89(13)	C(4)-N(17)-Na(1)	126.91(17)
N(14)-K(2)-N(4)#2	131.06(7)	N(16)-N(17)-Na(1)	123.54(17)
O(2)-K(2)-N(4)#2	66.53(8)	C(4)-N(17)-K(2)#8	101.24(16)
N(6)#2-K(2)-N(4)#2	55.20(6)	N(16)-N(17)-K(2)#8	108.40(17)
O(3)-K(2)-N(9)#3	74.91(13)	Na(1)-N(17)-K(2)#8	87.85(7)
N(14)-K(2)-N(9)#3	80.76(7)	K(1)-O(1)-H(1A)	109.8
O(2)-K(2)-N(9)#3	136.86(8)	K(1)-O(1)-H(1B)	114.8
N(6)#2-K(2)-N(9)#3	134.26(7)	H(1A)-O(1)-H(1B)	120.0
N(4)#2-K(2)-N(9)#3	148.02(7)	K(2)#6-O(2)-K(2)	176.12(14)
O(3)-K(2)-N(1)#3	111.67(13)	K(2)#6-O(2)-H(2A)	70.5
N(14)-K(2)-N(1)#3	79.23(6)	K(2)-O(2)-H(2A)	109.5
O(2)-K(2)-N(1)#3	146.30(4)	K(2)#6-O(2)-H(2B)	67.5
N(6)#2-K(2)-N(1)#3	75.87(6)	K(2)-O(2)-H(2B)	109.2
N(4)#2-K(2)-N(1)#3	117.37(6)	H(2A)-O(2)-H(2B)	109.5
N(9)#3-K(2)-N(1)#3	58.39(6)	K(2)#6-O(2)-H(2A)#6	109.472(14)
O(3)-K(2)-N(17)#3	67.20(12)	K(2)-O(2)-H(2A)#6	70.474(14)
N(14)-K(2)-N(17)#3	136.14(7)	H(2A)-O(2)-H(2A)#6	178.5
O(2)-K(2)-N(17)#3	141.88(8)	H(2B)-O(2)-H(2A)#6	69.3
N(6)#2-K(2)-N(17)#3	78.29(7)	K(2)#6-O(2)-H(2B)#6	109.23(6)
N(4)#2-K(2)-N(17)#3	75.43(6)	K(2)-O(2)-H(2B)#6	67.47(6)
N(9)#3-K(2)-N(17)#3	77.70(7)	H(2A)-O(2)-H(2B)#6	69.3
N(1)#3-K(2)-N(17)#3	56.93(6)	H(2B)-O(2)-H(2B)#6	74.7
O(3)-K(2)-N(12)	89.74(12)	H(2A)#6-O(2)-H(2B)#6	109.5
N(14)-K(2)-N(12)	53.93(6)	K(2)-O(3)-H(3A)	86.1
O(2)-K(2)-N(12)	62.64(8)	K(2)-O(3)-H(3B)	116.1
N(6)#2-K(2)-N(12)	133.70(7)	H(3A)-O(3)-H(3B)	126.3
N(4)#2-K(2)-N(12)	123.95(7)	N(9)-Na(1)-N(8)#7	104.94(9)
N(9)#3-K(2)-N(12)	74.26(6)	N(9)-Na(1)-N(17)	102.55(10)
N(1)#3-K(2)-N(12)	117.82(5)	N(8)#7-Na(1)-N(17)	87.23(8)
N(17)#3-K(2)-N(12)	147.54(6)	N(9)-Na(1)-N(10)#6	141.99(8)
O(3)-K(2)-Na(1)#3	67.21(12)	N(8)#7-Na(1)-N(10)#6	112.85(8)
N(14)-K(2)-Na(1)#3	109.13(6)	N(17)-Na(1)-N(10)#6	83.60(8)
O(2)-K(2)-Na(1)#3	168.13(3)	N(9)-Na(1)-N(2)#6	89.08(8)
N(6)#2-K(2)-Na(1)#3	108.29(6)	N(8)#7-Na(1)-N(2)#6	130.63(9)
N(4)#2-K(2)-Na(1)#3	114.13(5)	N(17)-Na(1)-N(2)#6	136.30(8)

N(9)#3-K(2)-Na(1)#3	37.74(5)	N(10)#6-Na(1)-N(2)#6	63.48(7)
N(1)#3-K(2)-Na(1)#3	44.99(4)	N(9)-Na(1)-N(1)	69.15(7)
N(17)#3-K(2)-Na(1)#3	40.02(4)	N(8)#7-Na(1)-N(1)	150.17(8)
N(12)-K(2)-Na(1)#3	110.95(5)	N(17)-Na(1)-N(1)	66.68(7)
O(3)-K(2)-K(1)	161.52(12)	N(10)#6-Na(1)-N(1)	79.67(7)
N(14)-K(2)-K(1)	49.83(5)	N(2)#6-Na(1)-N(1)	79.15(7)
O(2)-K(2)-K(1)	95.531(18)	N(9)-Na(1)-K(2)#8	50.52(6)
N(6)#2-K(2)-K(1)	48.29(5)	N(8)#7-Na(1)-K(2)#8	102.34(7)
N(4)#2-K(2)-K(1)	103.10(5)	N(17)-Na(1)-K(2)#8	52.13(6)
N(9)#3-K(2)-K(1)	96.30(5)	N(10)#6-Na(1)-K(2)#8	121.37(6)
N(1)#3-K(2)-K(1)	50.81(4)	N(2)#6-Na(1)-K(2)#8	121.82(6)
N(17)#3-K(2)-K(1)	95.27(4)	N(1)-Na(1)-K(2)#8	50.51(5)
N(12)-K(2)-K(1)	103.68(4)	N(9)-Na(1)-K(1)#11	130.39(7)
Na(1)#3-K(2)-K(1)	95.78(2)	N(8)#7-Na(1)-K(1)#11	90.56(7)
O(3)-K(2)-H(3A)	18.7	N(17)-Na(1)-K(1)#11	125.40(7)
N(14)-K(2)-H(3A)	129.8	N(10)#6-Na(1)-K(1)#11	47.81(5)
O(2)-K(2)-H(3A)	84.3	N(2)#6-Na(1)-K(1)#11	48.62(5)
N(6)#2-K(2)-H(3A)	132.0	N(1)-Na(1)-K(1)#11	115.93(5)
N(4)#2-K(2)-H(3A)	77.1	K(2)#8-Na(1)-K(1)#11	166.40(3)
N(9)#3-K(2)-H(3A)	83.6	N(9)-Na(1)-K(1)#4	152.42(7)
N(1)#3-K(2)-H(3A)	129.3	N(8)#7-Na(1)-K(1)#4	59.98(6)
N(17)#3-K(2)-H(3A)	85.0	N(17)-Na(1)-K(1)#4	56.67(6)
N(12)-K(2)-H(3A)	76.0	N(10)#6-Na(1)-K(1)#4	59.88(5)
Na(1)#3-K(2)-H(3A)	84.3	N(2)#6-Na(1)-K(1)#4	118.40(6)
K(1)-K(2)-H(3A)	179.7	N(1)-Na(1)-K(1)#4	111.43(5)
O(3)-K(2)-H(2A)#6	118.83(12)	K(2)#8-Na(1)-K(1)#4	107.14(3)
N(14)-K(2)-H(2A)#6	64.82(8)	K(1)#11-Na(1)-K(1)#4	75.46(2)
O(2)-K(2)-H(2A)#6	17.015(4)		

Table S25 Hydrogen bonds in **10·2.25H_2O.**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...N(16)	0.86	2.37	3.040(4)	134.4
O(1)-H(1B)...O(2)#4	0.97	1.90	2.858(4)	170.9
O(2)-H(2A)...O(1)#10	0.85	2.16	2.858(4)	139.2
O(2)-H(2B)...N(4)#12	0.85	2.46	3.231(4)	151.4
O(2)-H(2B)...O(1)#4	0.85	2.43	2.858(4)	111.6
O(3)-H(3B)...N(16)#3	1.05	2.38	3.120(6)	126.4

Table S26 Bond lengths (Å) for **11·H_2O.**

C(1)-N(2)	1.342(2)	N(9)-Na(1)	2.4277(17)
C(1)-N(1)	1.344(2)	N(10)-N(11)	1.364(2)
C(1)-N(5)	1.367(2)	N(10)-Na(1)#1	2.5309(17)
C(2)-N(9)	1.319(2)	N(11)-N(12)	1.283(2)
C(2)-N(6)	1.325(2)	N(12)-N(13)	1.366(2)
C(2)-N(5)	1.397(2)	N(14)-N(15)	1.349(2)
C(3)-N(1)	1.341(2)	N(15)-N(16)	1.301(2)
C(3)-N(10)	1.342(2)	N(16)-N(17)	1.356(2)
C(3)-N(13)	1.369(2)	N(17)-Na(1)	2.4386(18)
C(4)-N(17)	1.311(2)	N(18)-H(18A)	0.906(14)
C(4)-N(14)	1.321(2)	N(18)-H(18B)	0.890(14)
C(4)-N(13)	1.407(2)	N(18)-H(18C)	0.897(14)
N(1)-Na(1)	2.6592(16)	N(18)-H(18D)	0.902(14)
N(2)-N(3)	1.359(2)	N(19)-H(19A)	0.929(15)
N(2)-Na(1)#1	2.5613(17)	N(19)-H(19B)	0.935(16)
N(3)-N(4)	1.280(2)	N(19)-H(19C)	0.936(15)
N(4)-N(5)	1.3674(19)	N(19)-H(19D)	0.929(16)
N(6)-N(7)	1.347(2)	O(1A)-H(1AA)	0.8501
N(7)-N(8)	1.303(2)	O(1A)-H(1AB)	0.8500
N(8)-N(9)	1.355(2)	O(1B)-H(1BB)	0.8501
N(8)-Na(1)#2	2.4463(17)	O(1B)-H(1BA)	0.8500

Table S27 Bond angles (°) for **11·H_2O.**

N(2)-C(1)-N(1)	131.59(16)	N(12)-N(13)-C(4)	118.88(14)
N(2)-C(1)-N(5)	106.71(14)	C(3)-N(13)-C(4)	132.13(15)
N(1)-C(1)-N(5)	121.70(15)	C(4)-N(14)-N(15)	102.78(16)
N(9)-C(2)-N(6)	114.19(16)	N(16)-N(15)-N(14)	110.44(15)
N(9)-C(2)-N(5)	124.68(16)	N(15)-N(16)-N(17)	108.82(16)
N(6)-C(2)-N(5)	121.11(15)	C(4)-N(17)-N(16)	103.68(15)
N(1)-C(3)-N(10)	131.51(15)	C(4)-N(17)-Na(1)	123.02(12)
N(1)-C(3)-N(13)	122.13(16)	N(16)-N(17)-Na(1)	123.24(13)
N(10)-C(3)-N(13)	106.36(15)	H(18A)-N(18)-H(18B)	112.1(14)
N(17)-C(4)-N(14)	114.28(16)	H(18A)-N(18)-H(18C)	107.5(14)
N(17)-C(4)-N(13)	124.83(15)	H(18B)-N(18)-H(18C)	109.7(14)
N(14)-C(4)-N(13)	120.88(17)	H(18A)-N(18)-H(18D)	108.3(14)
C(3)-N(1)-C(1)	117.30(15)	H(18B)-N(18)-H(18D)	109.7(14)
C(3)-N(1)-Na(1)	115.94(10)	H(18C)-N(18)-H(18D)	109.4(14)
C(1)-N(1)-Na(1)	114.02(11)	H(19A)-N(19)-H(19B)	111.6(15)
C(1)-N(2)-N(3)	106.17(14)	H(19A)-N(19)-H(19C)	110.1(15)

C(1)-N(2)-Na(1)#1	120.45(11)	H(19B)-N(19)-H(19C)	108.6(15)
N(3)-N(2)-Na(1)#1	121.24(11)	H(19A)-N(19)-H(19D)	109.4(14)
N(4)-N(3)-N(2)	112.41(14)	H(19B)-N(19)-H(19D)	108.1(15)
N(3)-N(4)-N(5)	105.91(14)	H(19C)-N(19)-H(19D)	108.9(14)
N(4)-N(5)-C(1)	108.79(14)	N(9)-Na(1)-N(17)	105.92(7)
N(4)-N(5)-C(2)	118.49(14)	N(9)-Na(1)-N(8)#2	101.39(6)
C(1)-N(5)-C(2)	132.62(14)	N(17)-Na(1)-N(8)#2	99.40(6)
C(2)-N(6)-N(7)	102.76(14)	N(9)-Na(1)-N(10)#1	89.58(6)
N(8)-N(7)-N(6)	110.51(15)	N(17)-Na(1)-N(10)#1	144.25(6)
N(7)-N(8)-N(9)	109.20(15)	N(8)#2-Na(1)-N(10)#1	109.02(6)
N(7)-N(8)-Na(1)#2	114.68(12)	N(9)-Na(1)-N(2)#1	146.32(5)
N(9)-N(8)-Na(1)#2	130.95(12)	N(17)-Na(1)-N(2)#1	85.17(6)
C(2)-N(9)-N(8)	103.34(14)	N(8)#2-Na(1)-N(2)#1	108.12(6)
C(2)-N(9)-Na(1)	123.08(12)	N(10)#1-Na(1)-N(2)#1	65.91(5)
N(8)-N(9)-Na(1)	127.66(12)	N(9)-Na(1)-N(1)	72.36(5)
C(3)-N(10)-N(11)	106.68(14)	N(17)-Na(1)-N(1)	71.60(5)
C(3)-N(10)-Na(1)#1	120.27(11)	N(8)#2-Na(1)-N(1)	166.42(6)
N(11)-N(10)-Na(1)#1	118.24(12)	N(10)#1-Na(1)-N(1)	83.33(5)
N(12)-N(11)-N(10)	111.75(15)	N(2)#1-Na(1)-N(1)	81.74(5)
N(11)-N(12)-N(13)	106.20(14)	H(1AA)-O(1A)-H(1AB)	104.5
N(12)-N(13)-C(3)	108.98(14)	H(1BB)-O(1B)-H(1BA)	109.5

Table S28 Hydrogen bonds in **11·H_2O.**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(18)-H(18A)...N(7)#3	0.906(14)	1.953(14)	2.856(2)	174.5(18)
N(18)-H(18B)...N(3)#4	0.890(14)	2.089(15)	2.898(2)	150.6(17)
N(18)-H(18C)...N(2)#1	0.897(14)	2.592(17)	3.254(2)	131.3(15)
N(18)-H(18C)...N(10)#1	0.897(14)	2.285(16)	3.051(2)	143.1(16)
N(18)-H(18D)...N(15)#5	0.902(14)	2.000(14)	2.882(2)	165.5(18)
N(19)-H(19A)...O(1A^a)	0.929(15)	2.25(2)	3.031(9)	140.8(18)
N(19)-H(19A)...O(1B^b)	0.929(15)	1.963(15)	2.889(3)	175(2)
N(19)-H(19B)...N(12)#5	0.935(16)	2.61(2)	3.155(2)	117.7(16)
N(19)-H(19B)...N(14)#5	0.935(16)	2.087(16)	2.994(3)	163.2(19)
N(19)-H(19C)...N(1)#1	0.936(15)	2.297(17)	3.138(2)	149.4(18)
N(19)-H(19D)...N(4)#3	0.929(16)	2.315(18)	3.112(2)	143.7(18)
N(19)-H(19D)...N(6)#3	0.929(16)	2.463(19)	3.243(2)	141.6(17)
O(1A^a)-H(1AA^a)...N(19)	0.85	2.51	3.031(9)	120.4
O(1B^b)-H(1BB^b)...N(18)#6	0.85	2.62	3.222(3)	129.2
O(1B^b)-H(1BA^b)...N(11)#7	0.85	2.37	3.100(3)	144.3

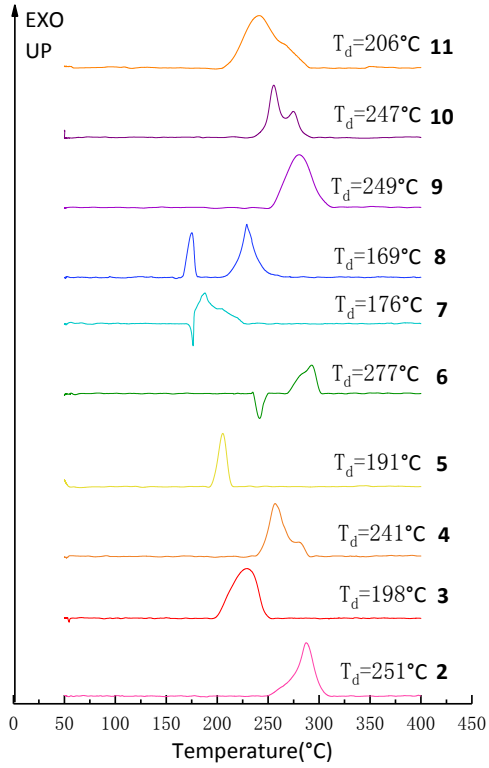

Figure S3 DSC plots for compounds **2**-**11**.

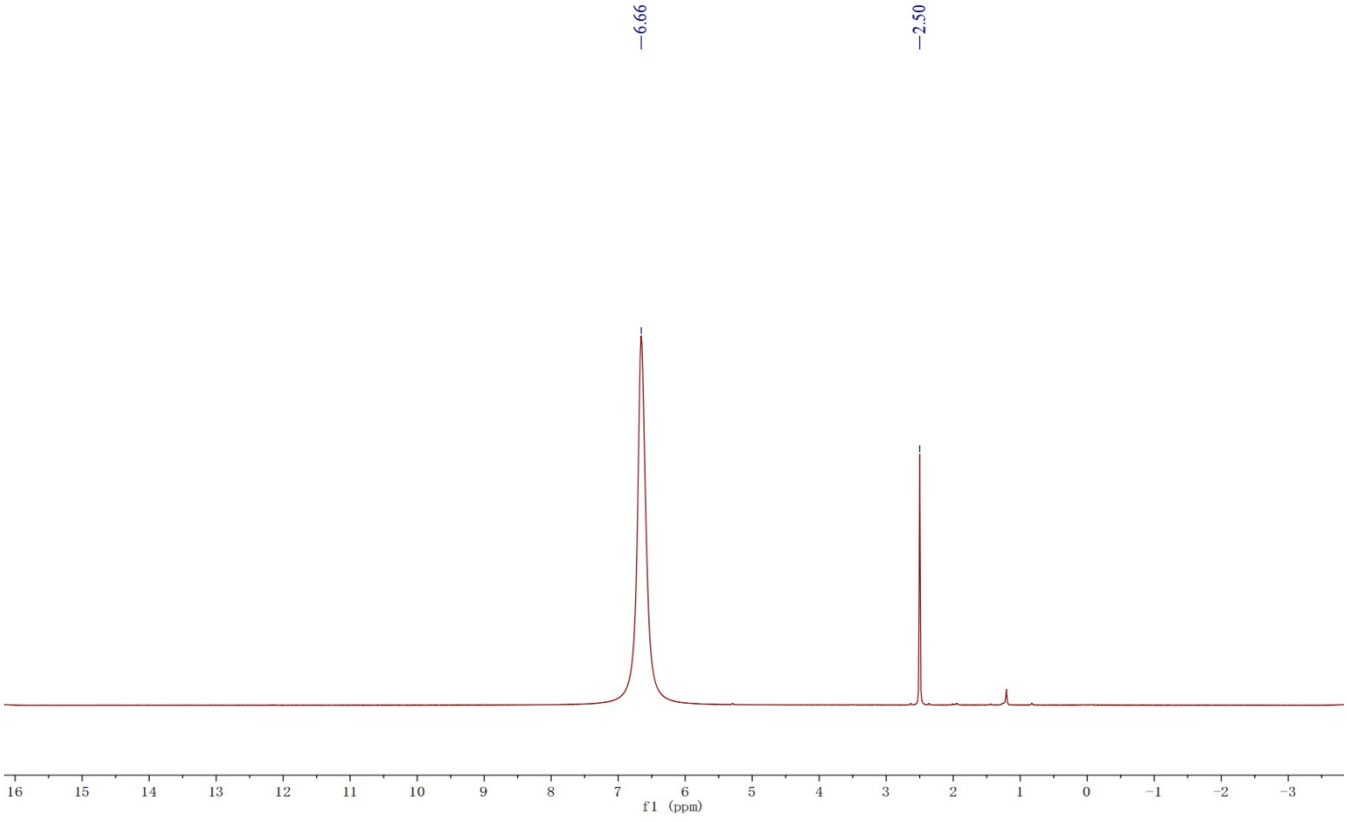

Figure S4 [1]HNMR spectra for compounds **3**.

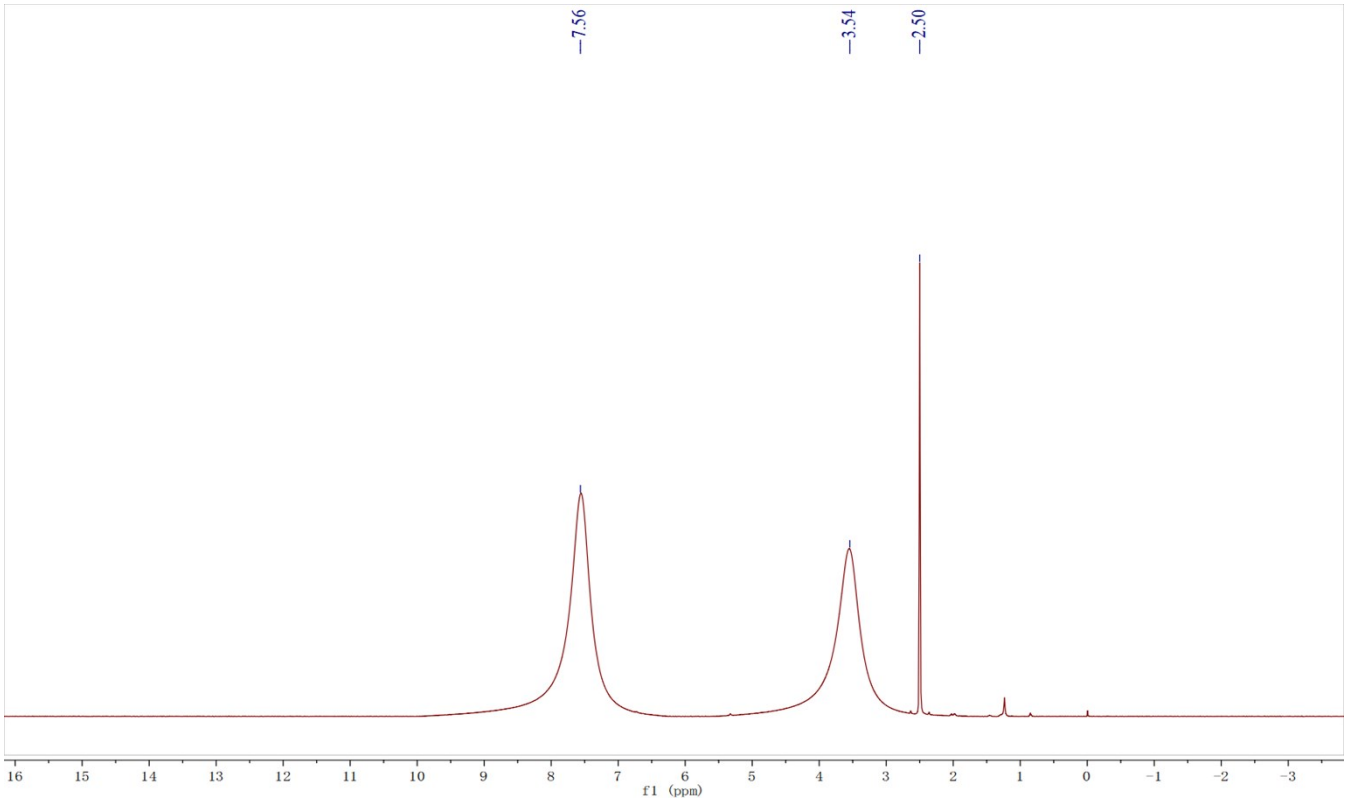

Figure S5 [1]HNMR spectra for compounds **5**.

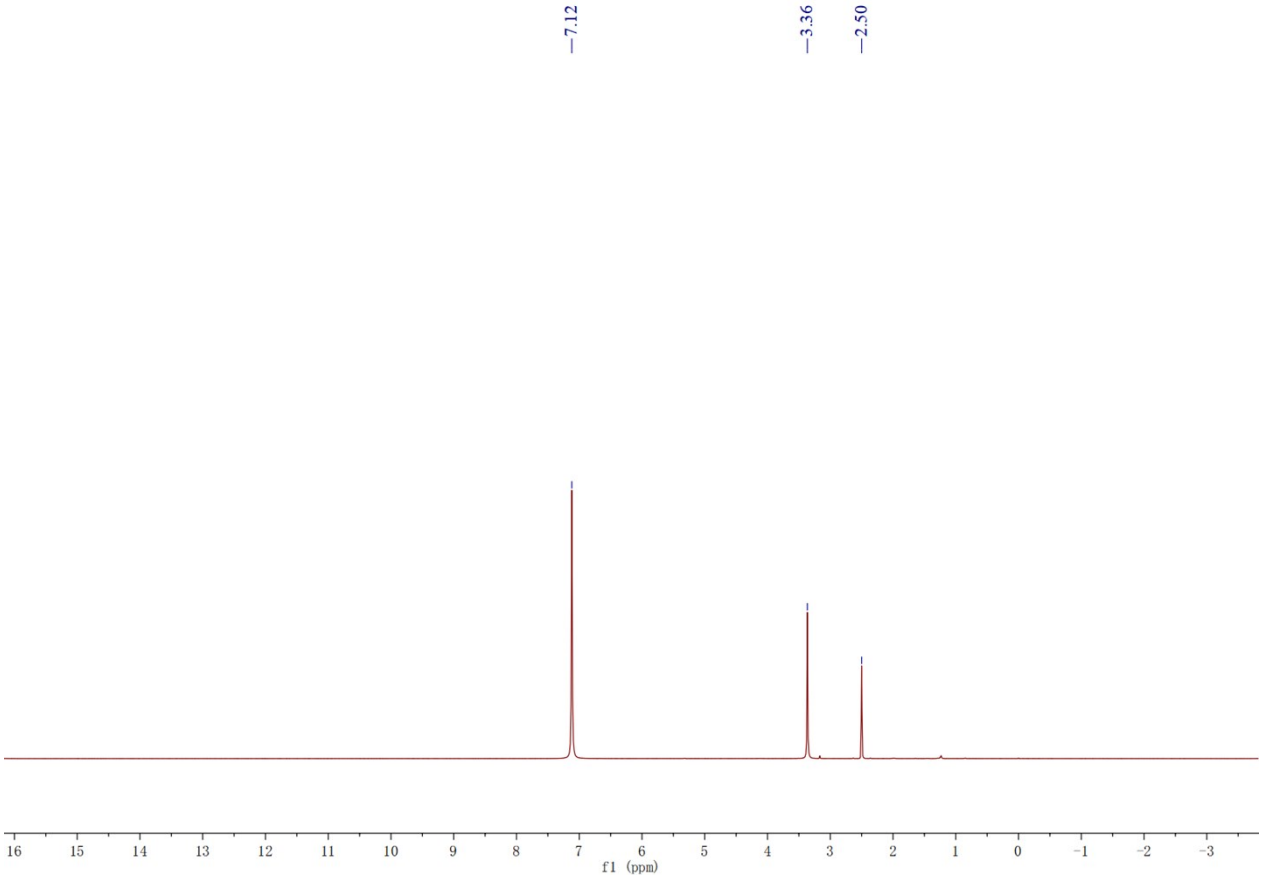

Figure S6 [1]HNMR spectra for compounds **6**.

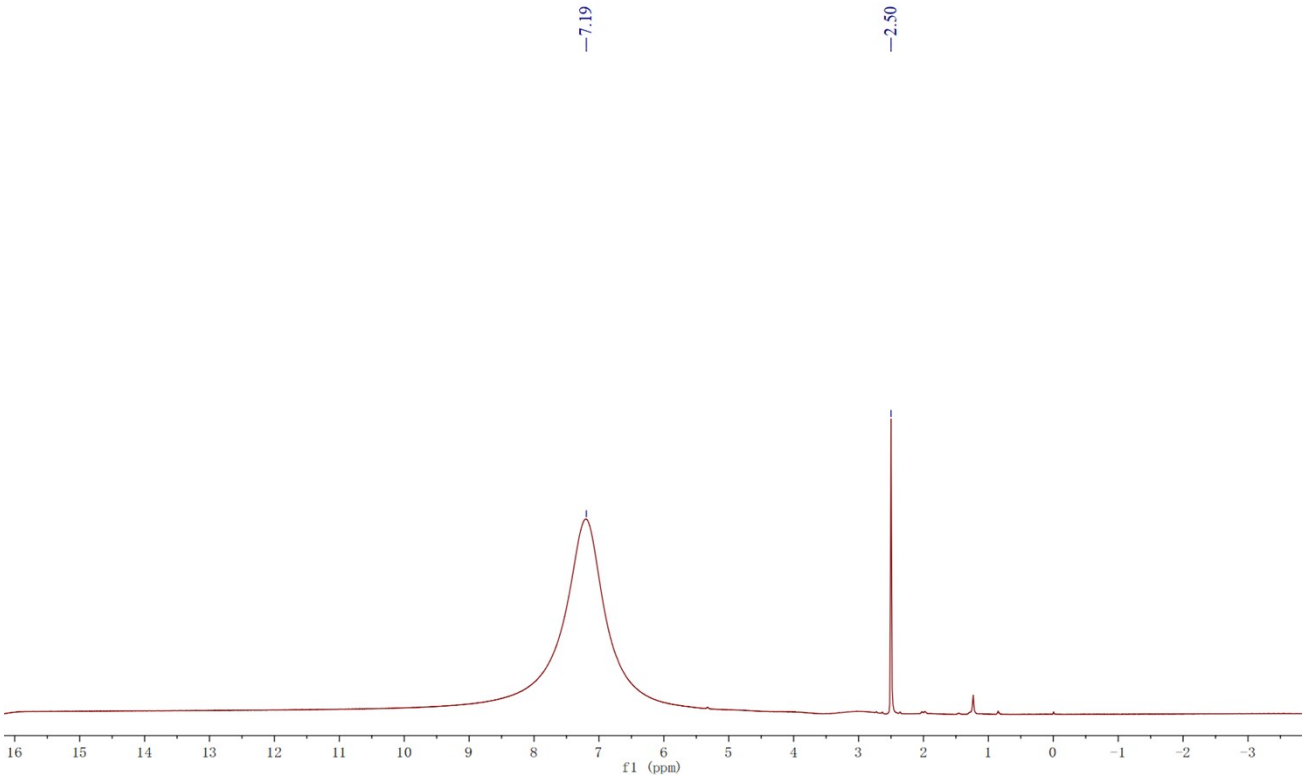

Figure S7 [1]HNMR spectra for compounds **7**.

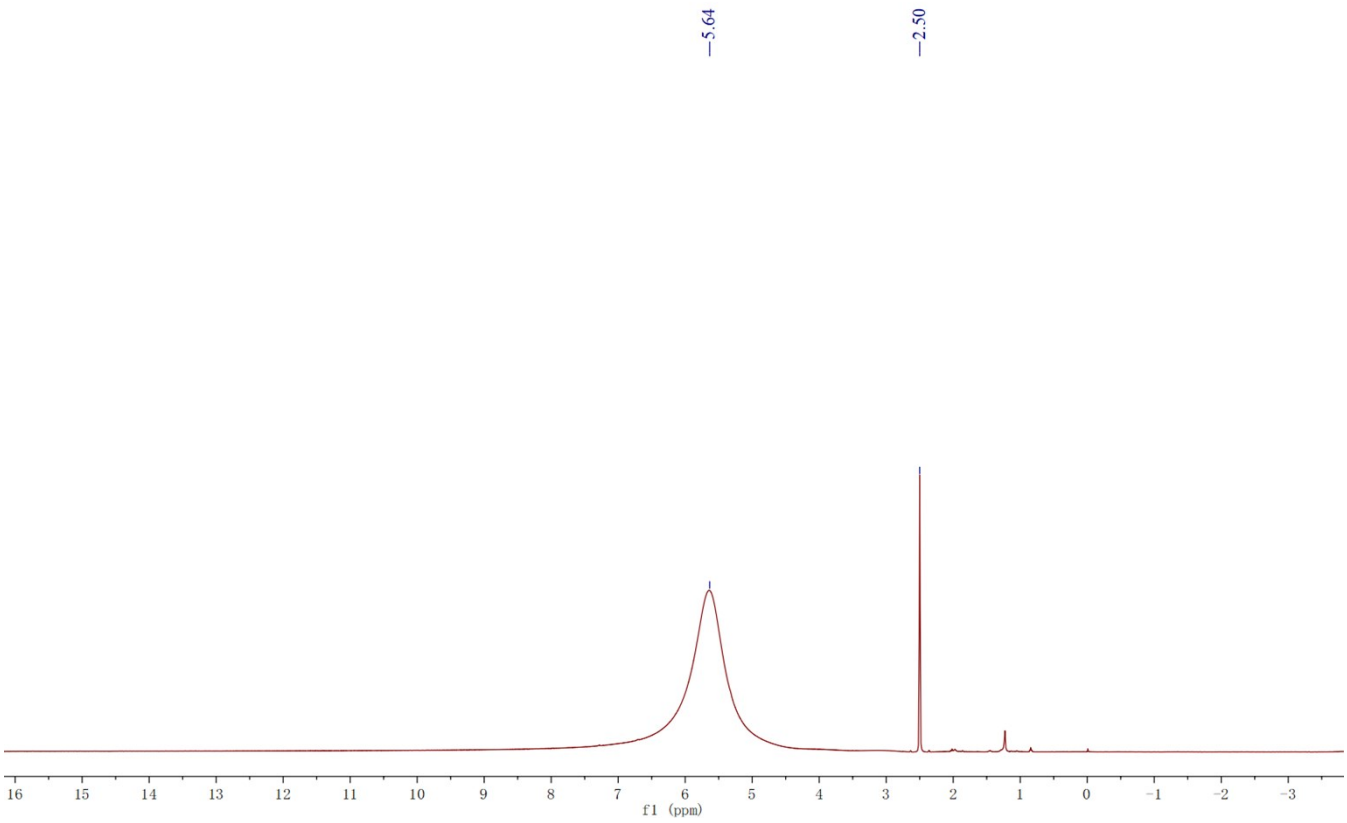

Figure S8 ^{1}H NMR spectra for compounds **8**.

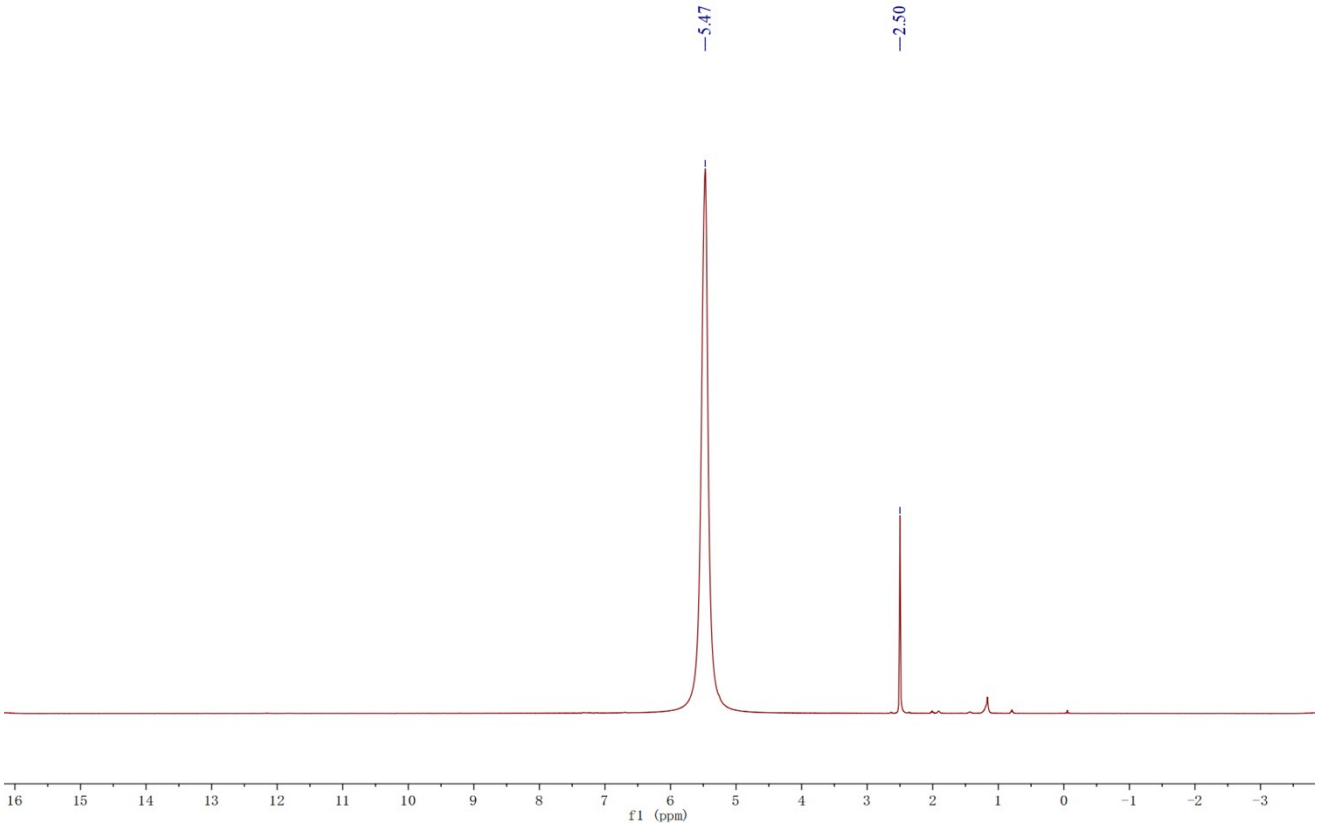

Figure S9 ^{1}H NMR spectra for compounds **9**.

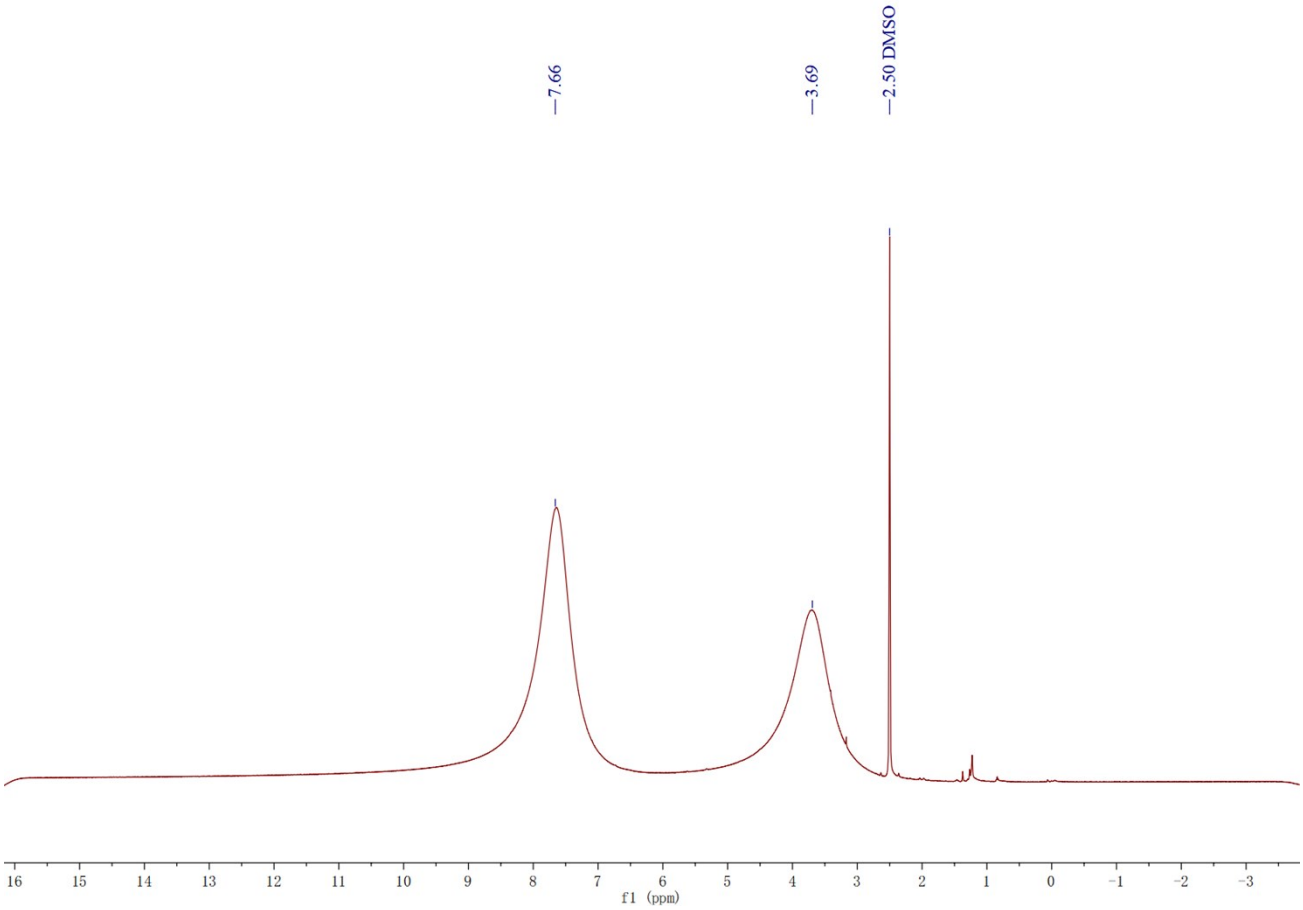

Figure S10 ^{1}H NMR spectra for compounds **11**.

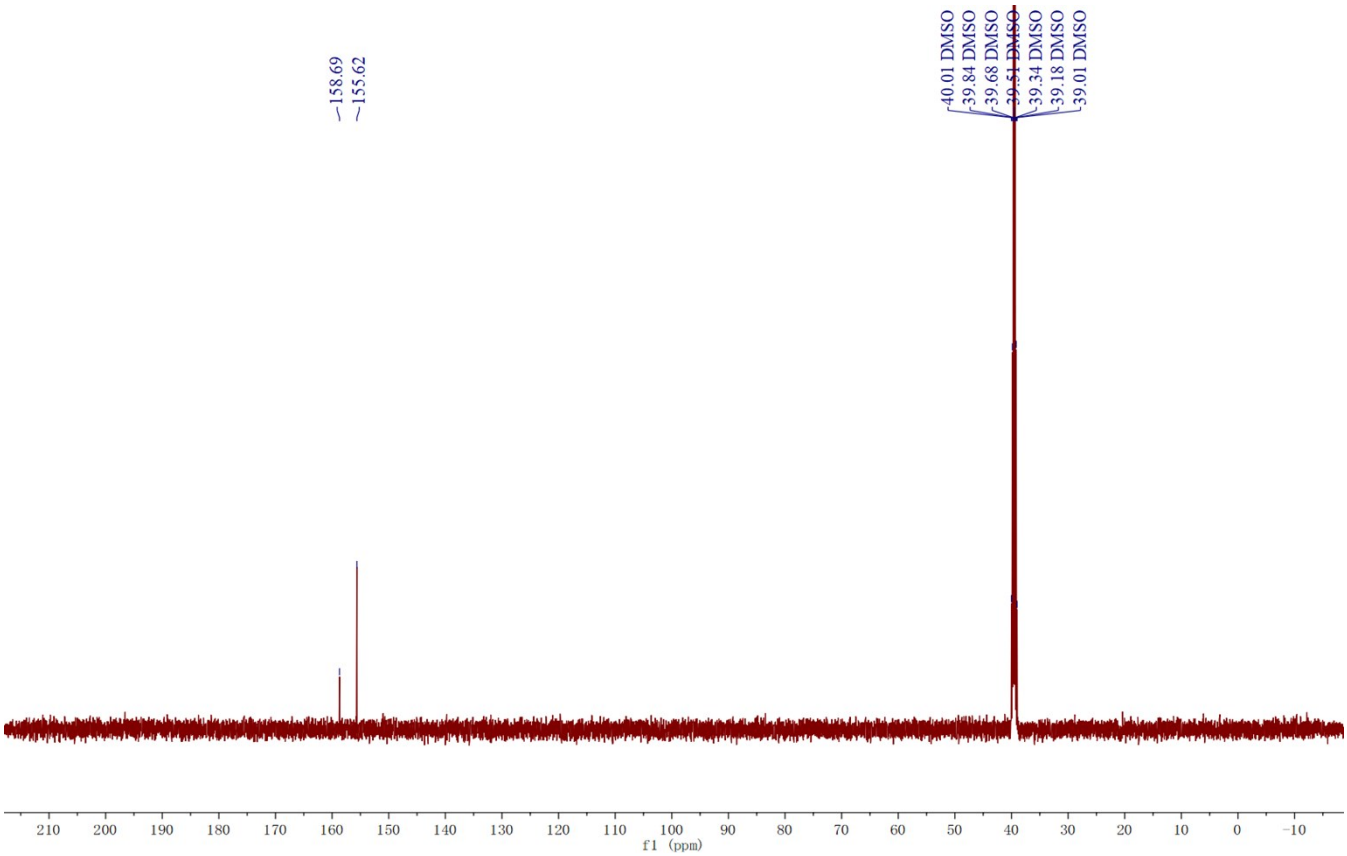

Figure S11 ^{13}C NMR spectra for compounds **2**.

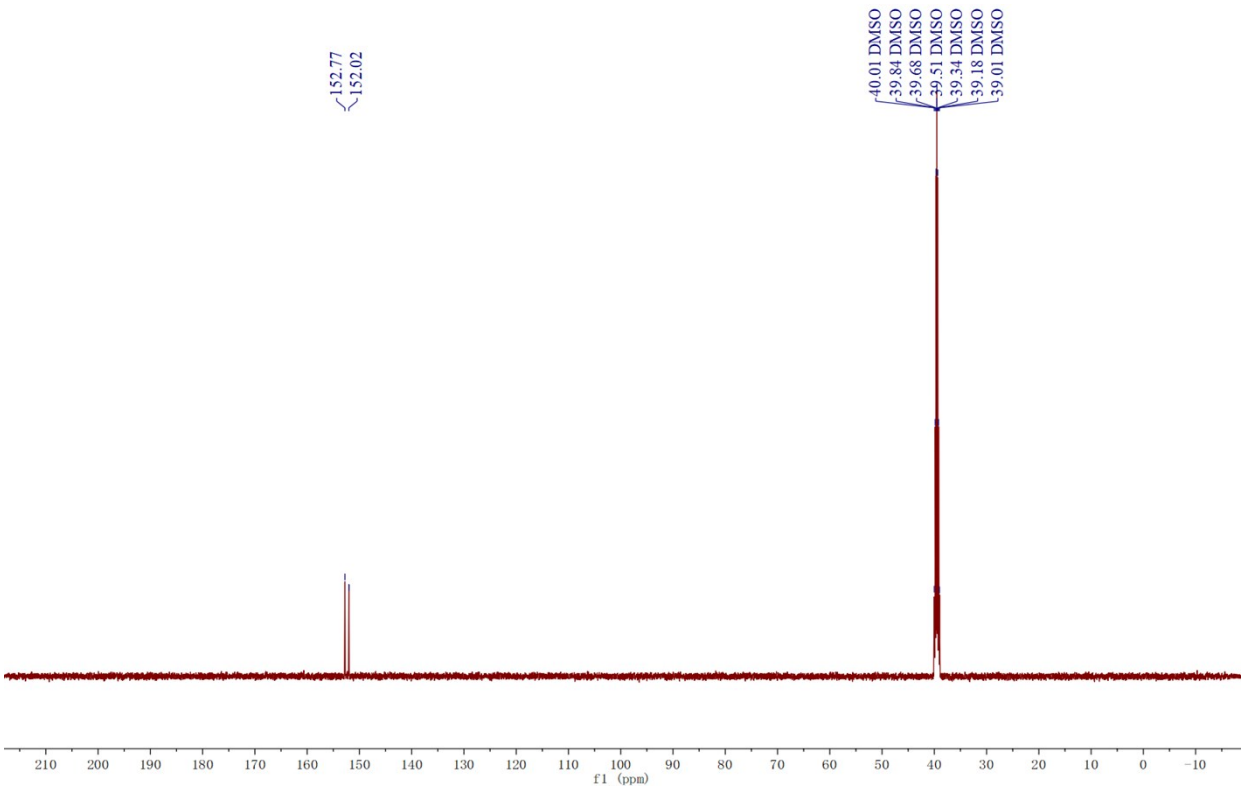

Figure S12 ^{13}C NMR spectra for compounds **3**.

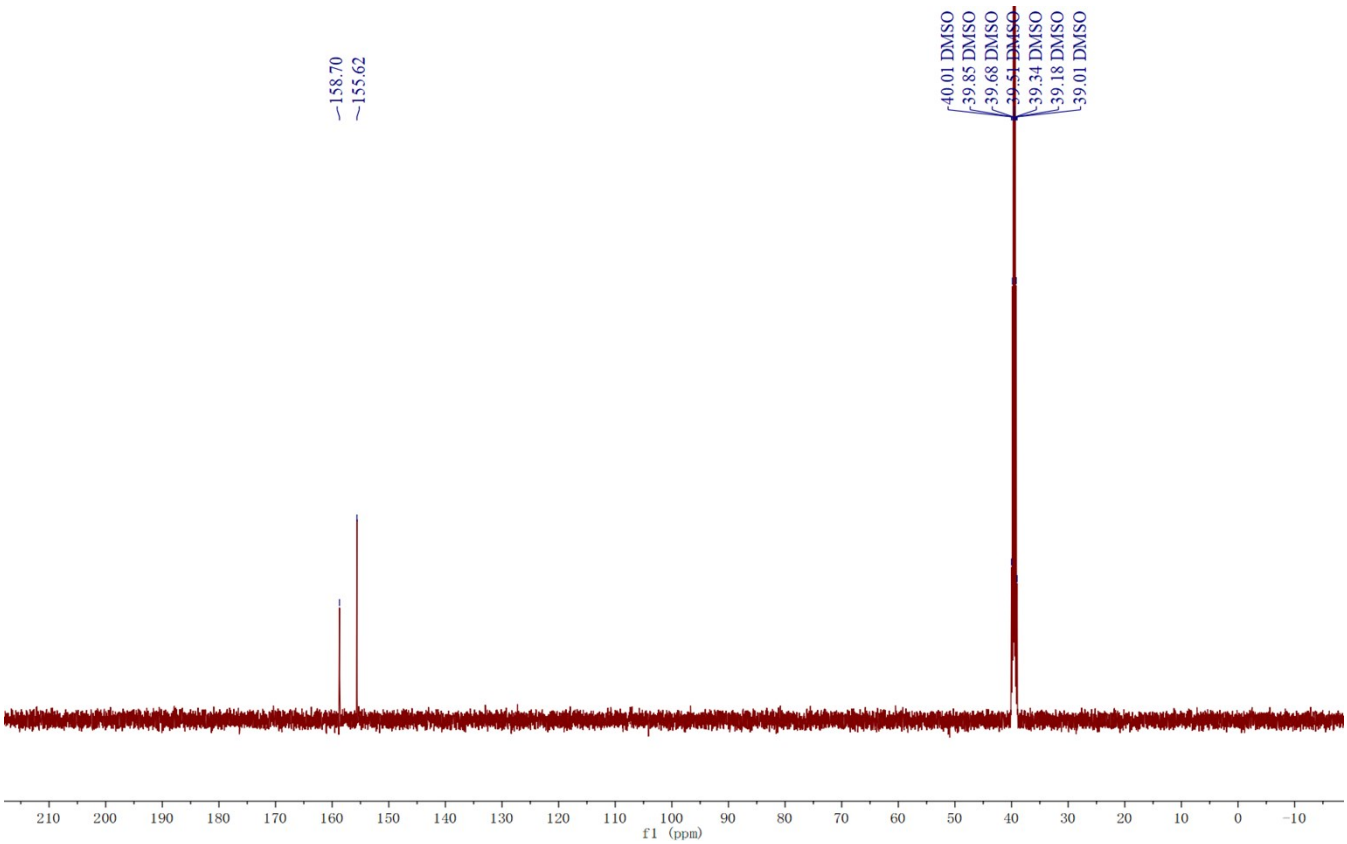

Figure S13 ^{13}C NMR spectra for compounds **4**.

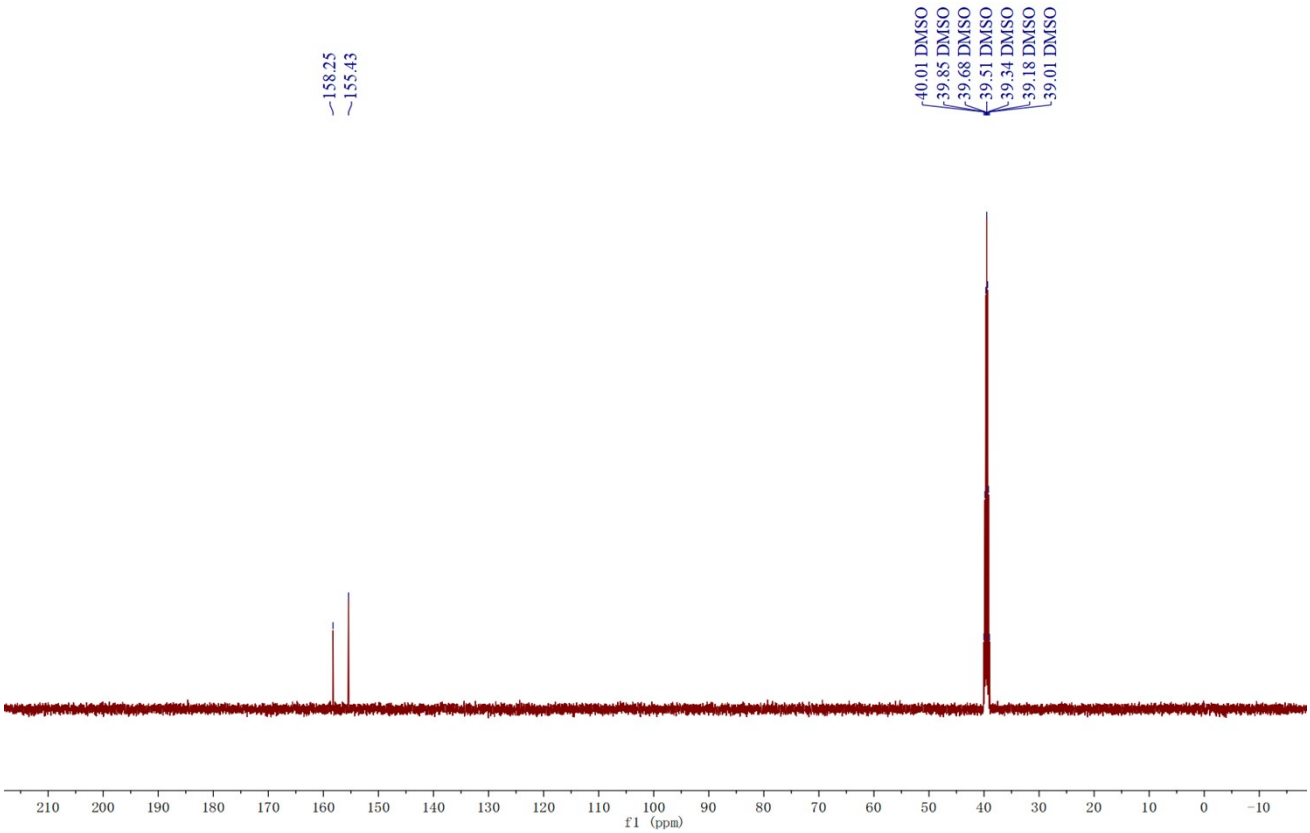

Figure S14 ^{13}C NMR spectra for compounds **5**.

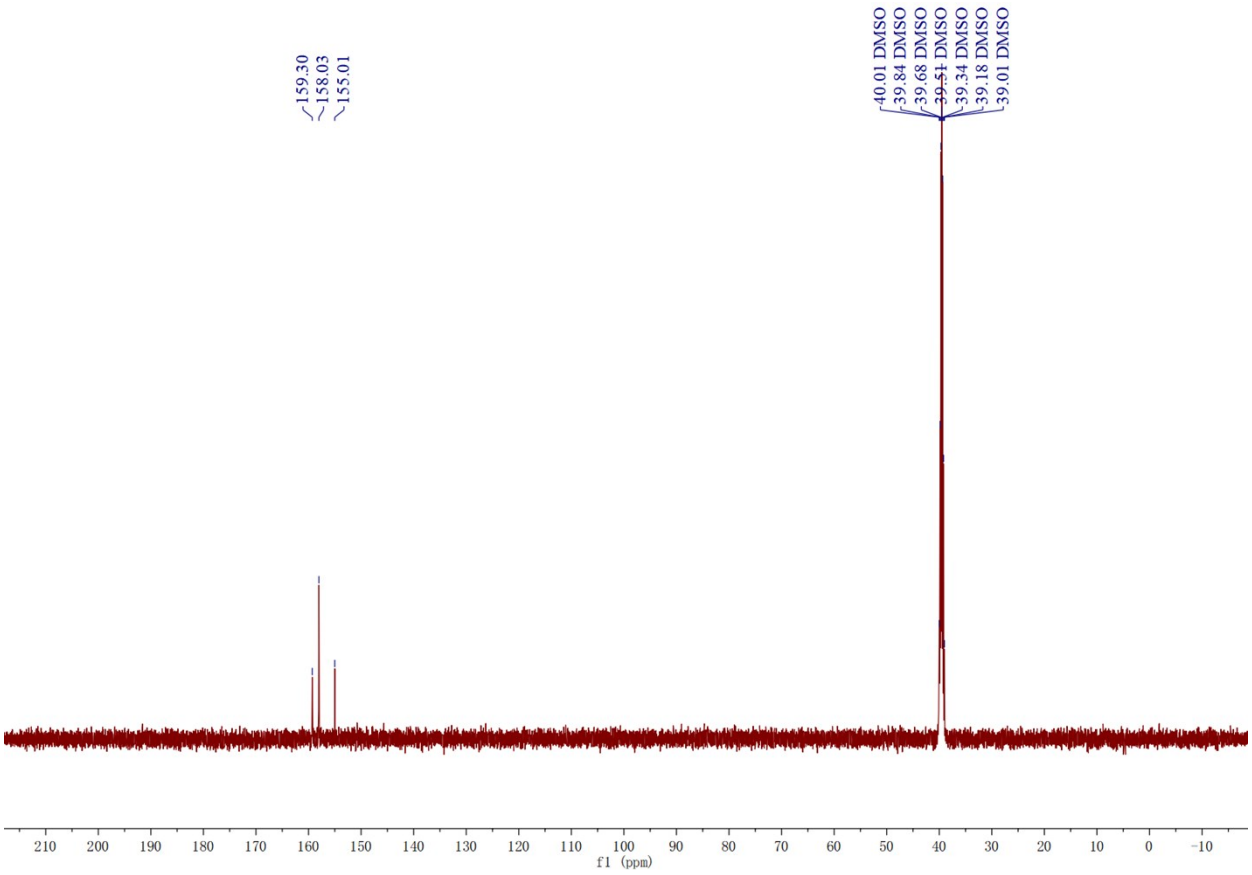

Figure S15 ^{13}C NMR spectra for compounds **6**.

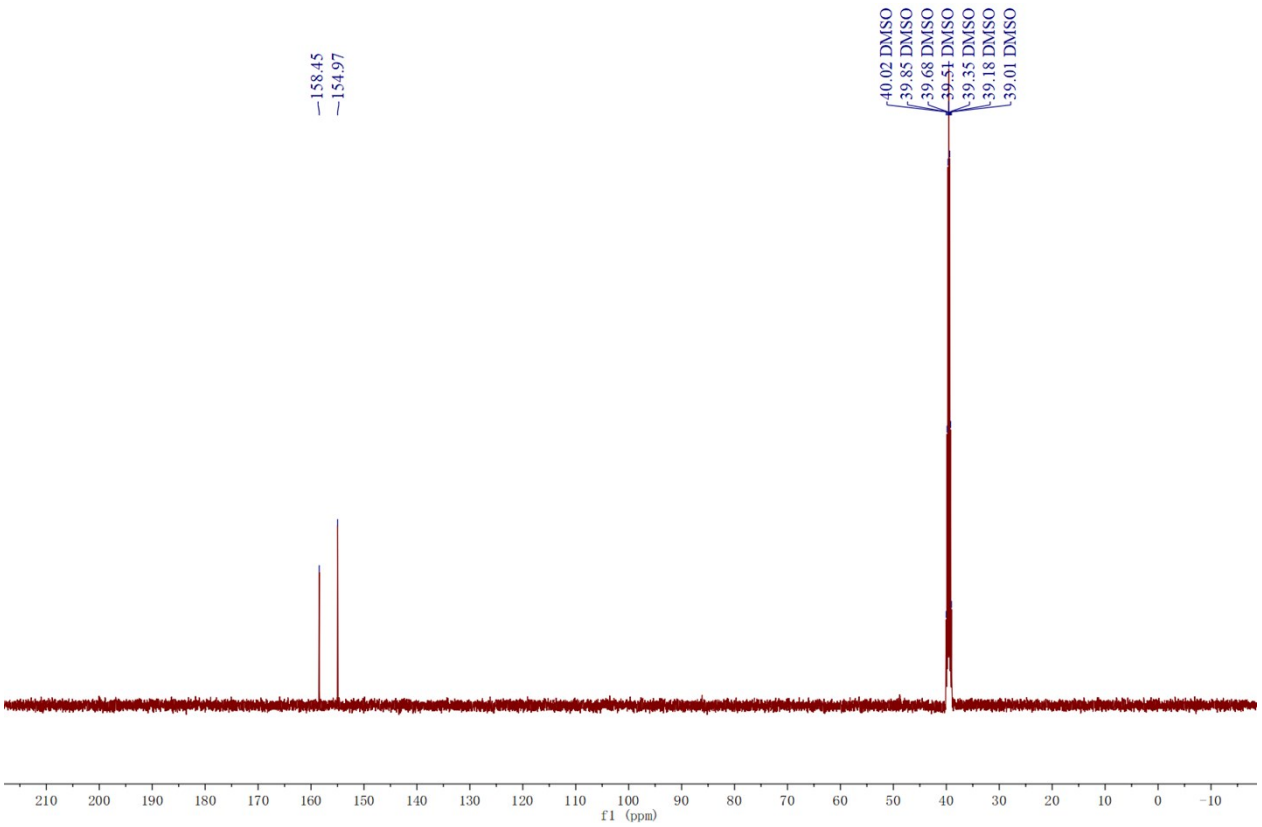

Figure S16 ^{13}C NMR spectra for compounds **7**.

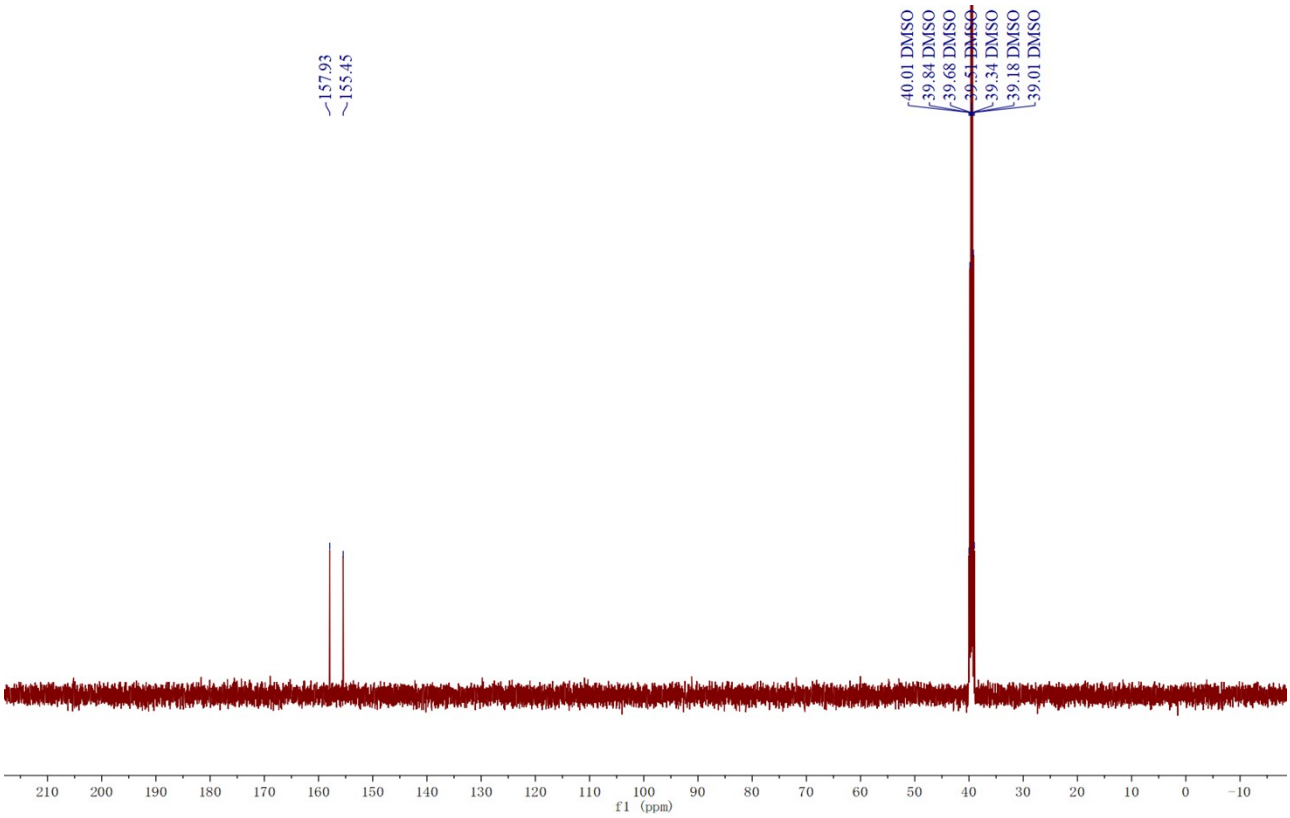

Figure S17 ^{13}C NMR spectra for compounds **8**.

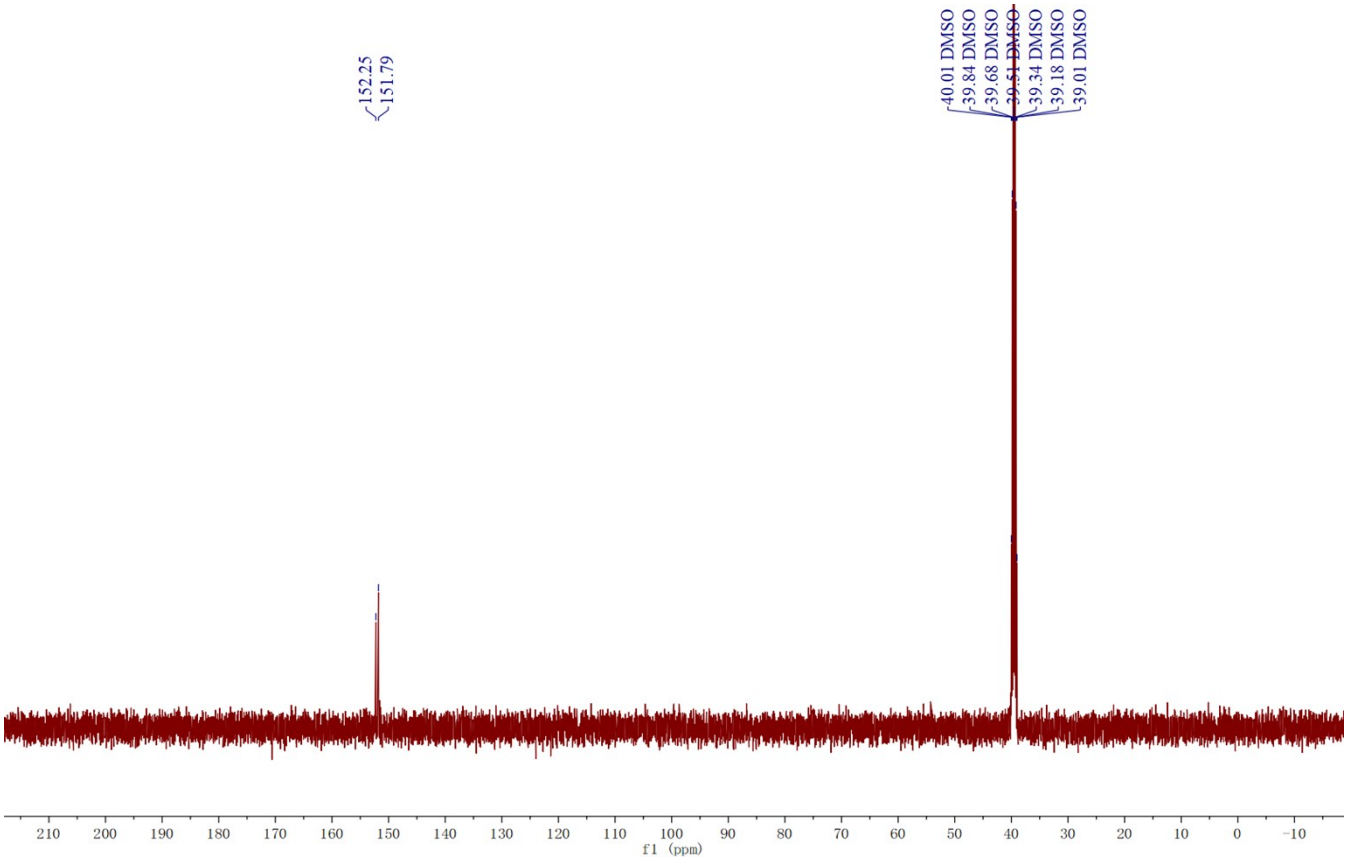

Figure S18 ^{13}C NMR spectra for compounds **9**.

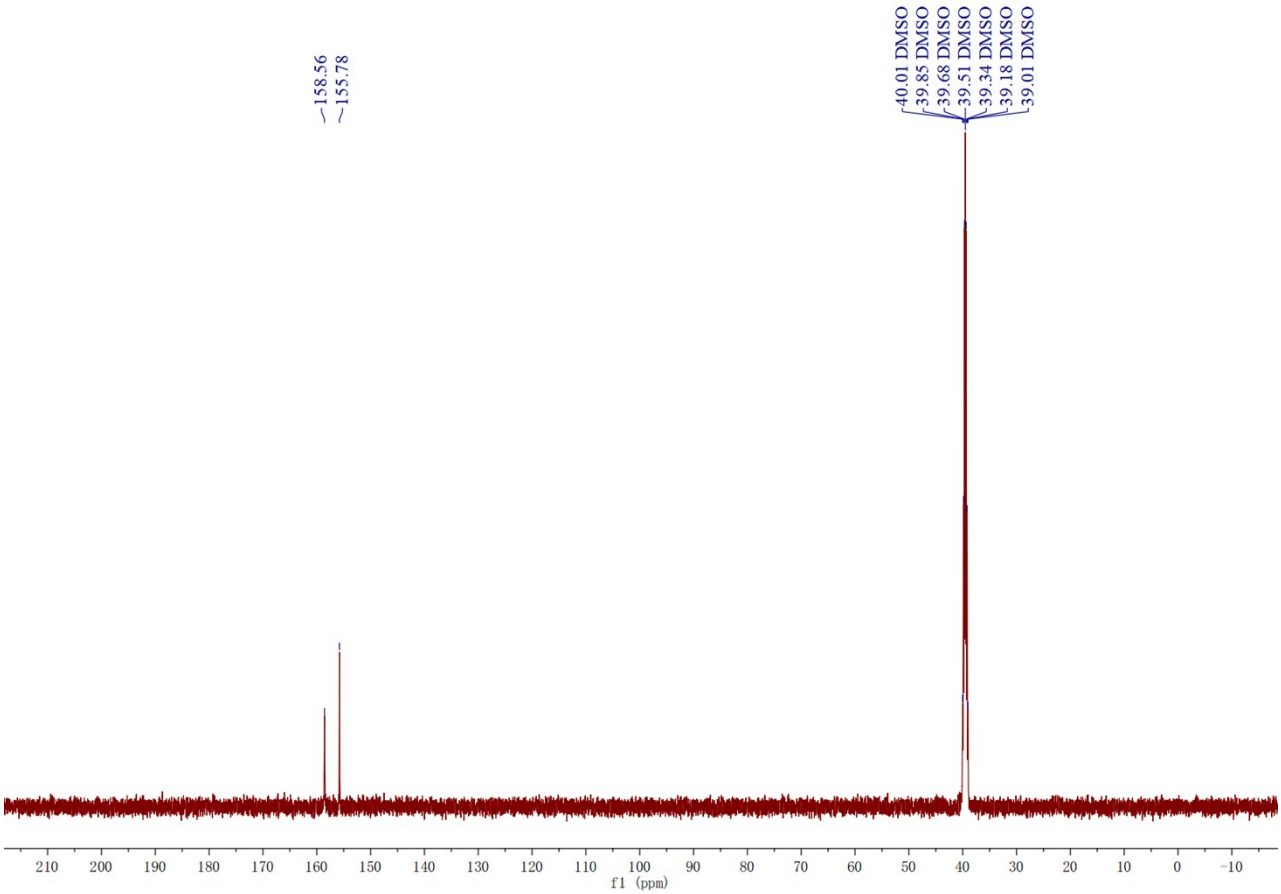

Figure S19 ^{13}C NMR spectra for compounds **10**.

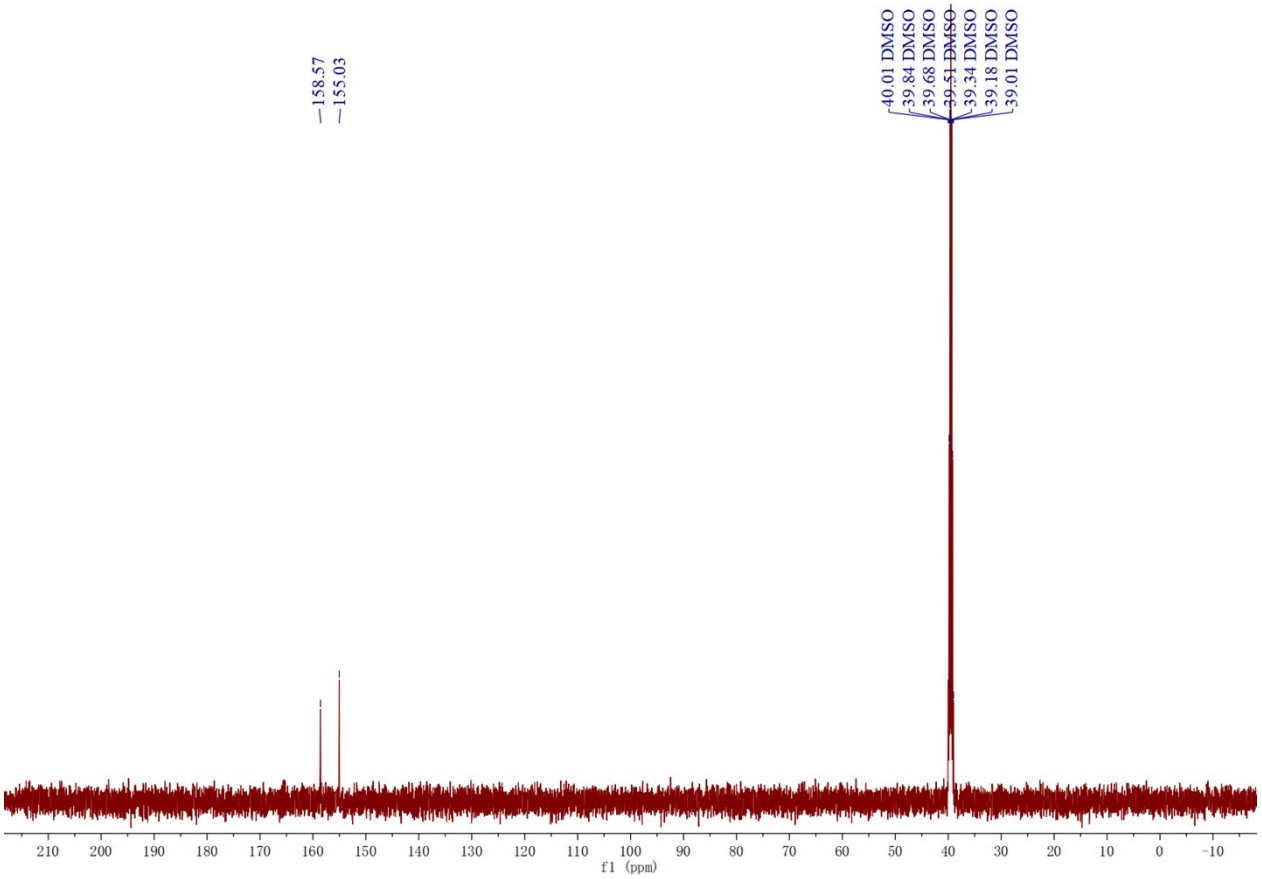

Figure S20 ^{13}C NMR spectra for compounds **11**.

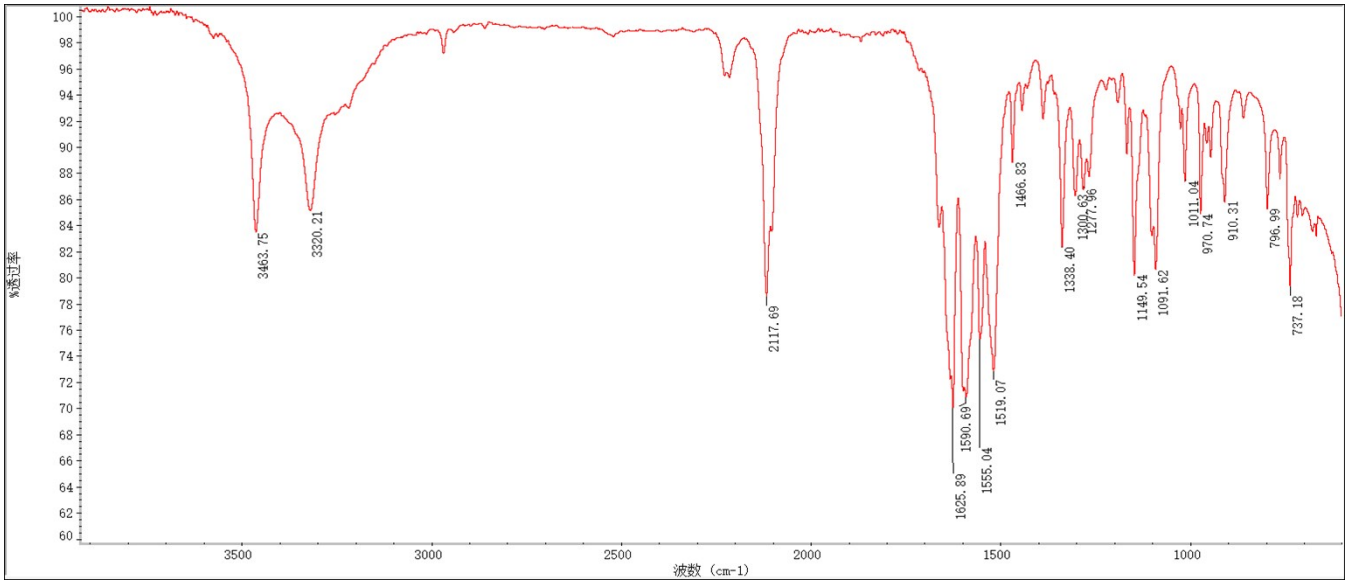

Figure S21 IR spectra for **2**.

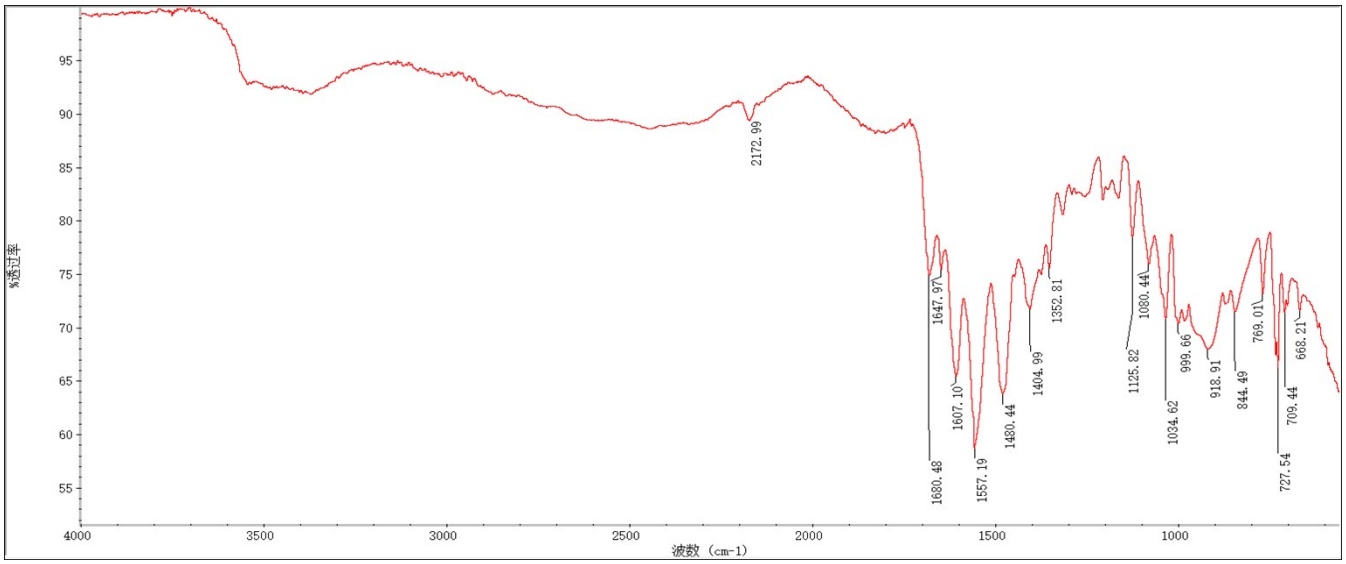

Figure S22 IR spectra for **3**.

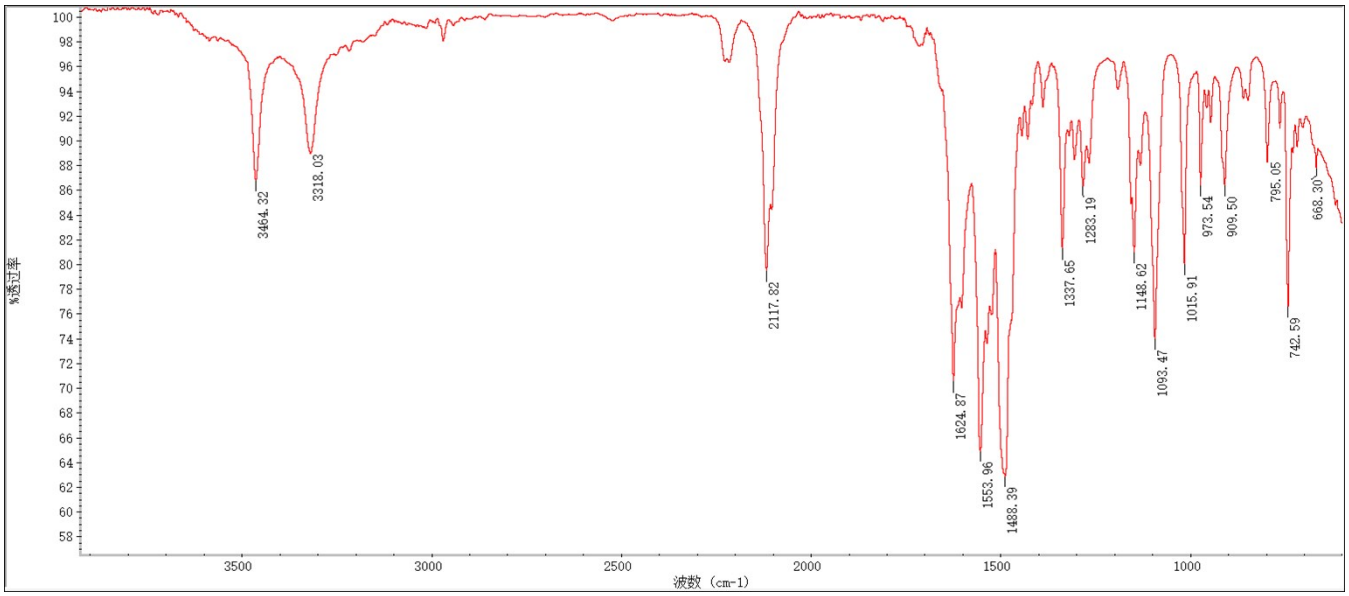

Figure S23 IR spectra for **4**.

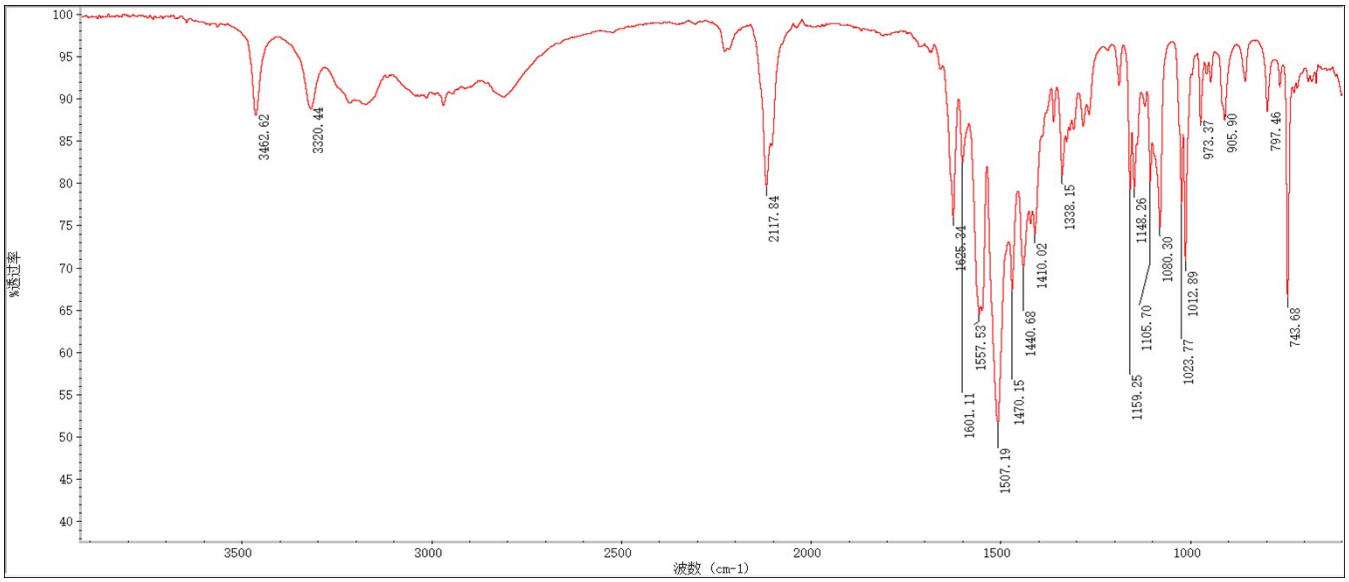

Figure S24 IR spectra for **5**.

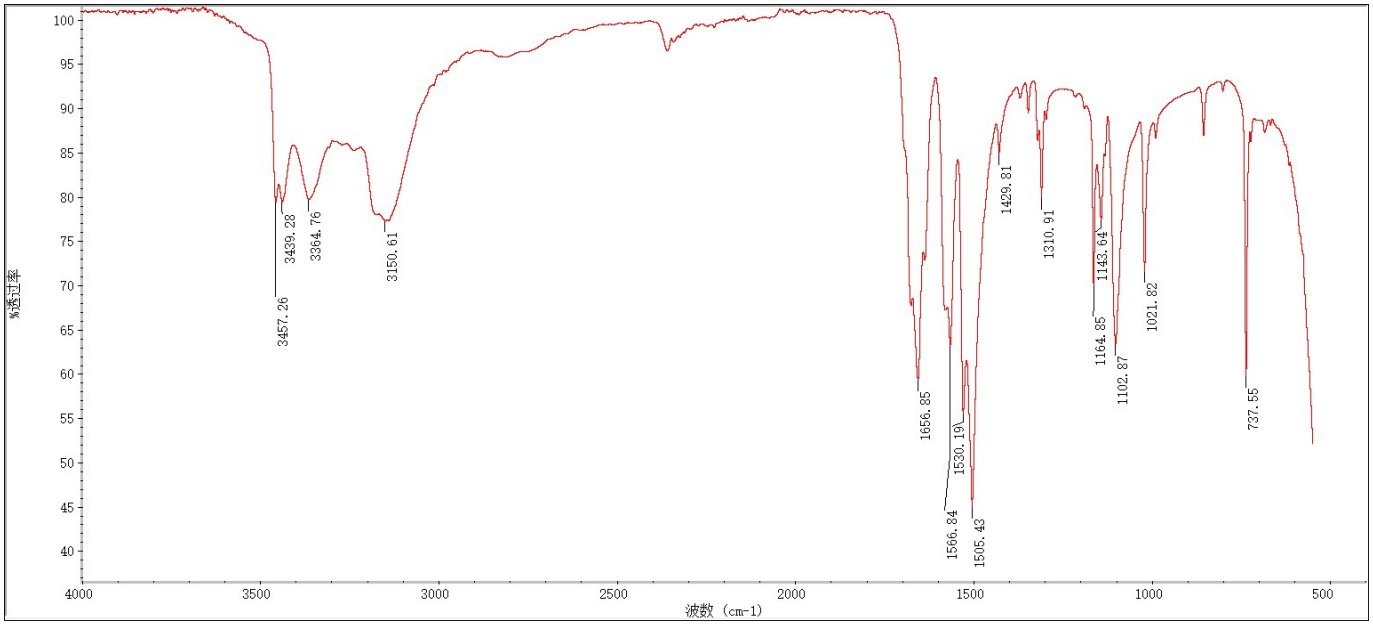

Figure S25 IR spectra for **6.**

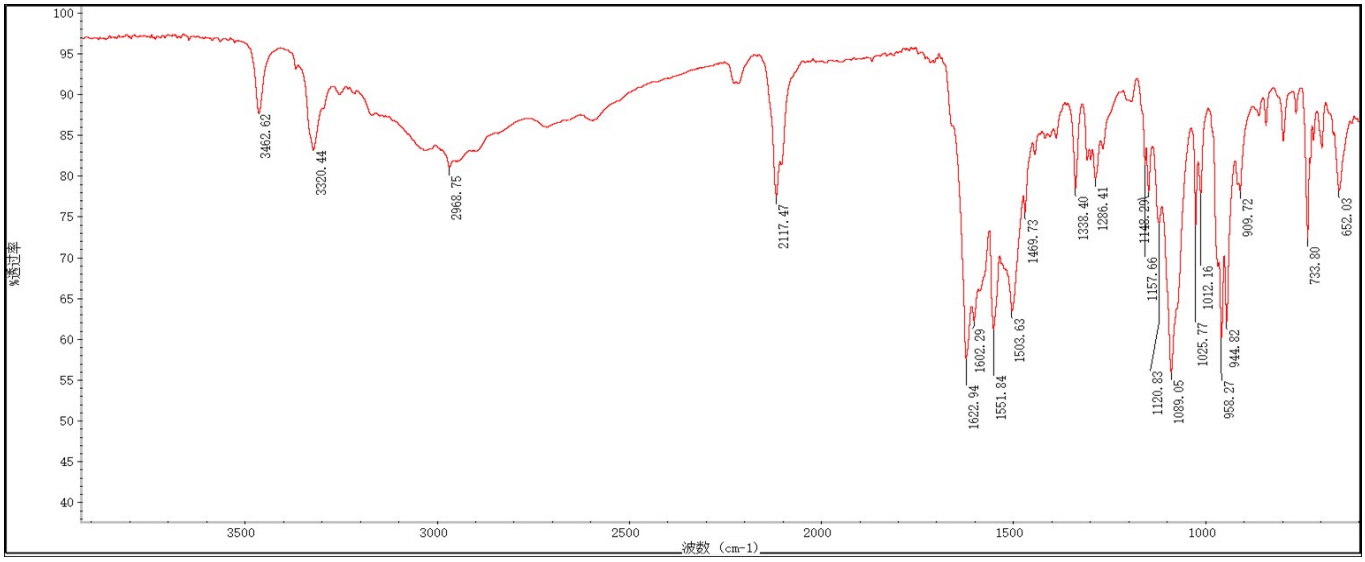

Figure S26 IR spectra for **7**.

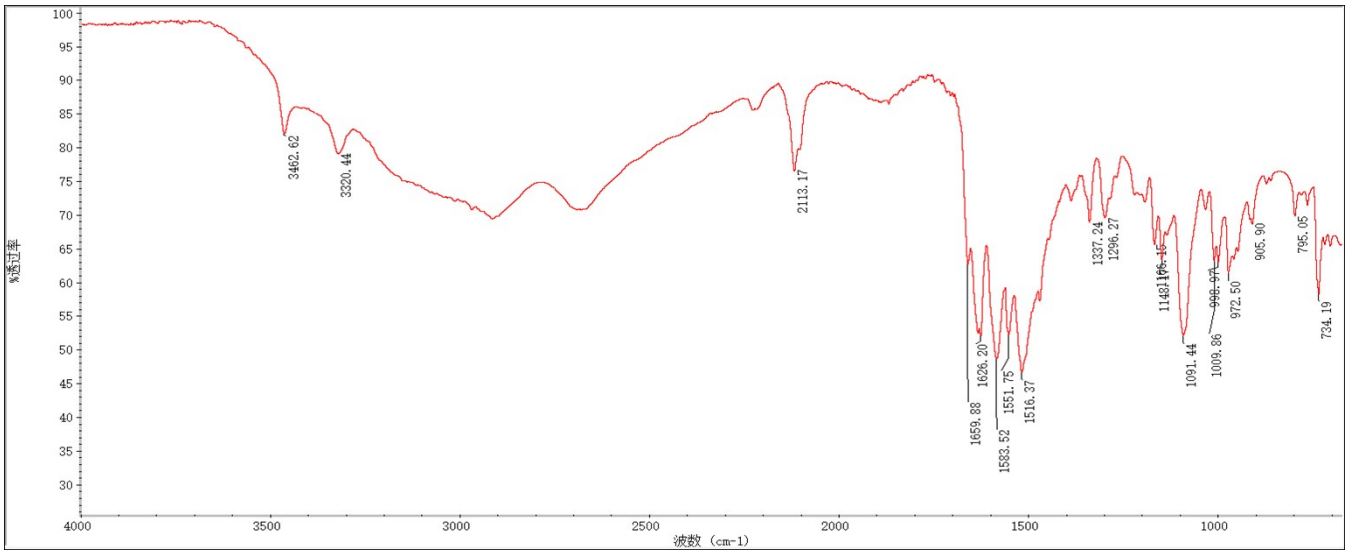

Figure S27 IR spectra for **8**.

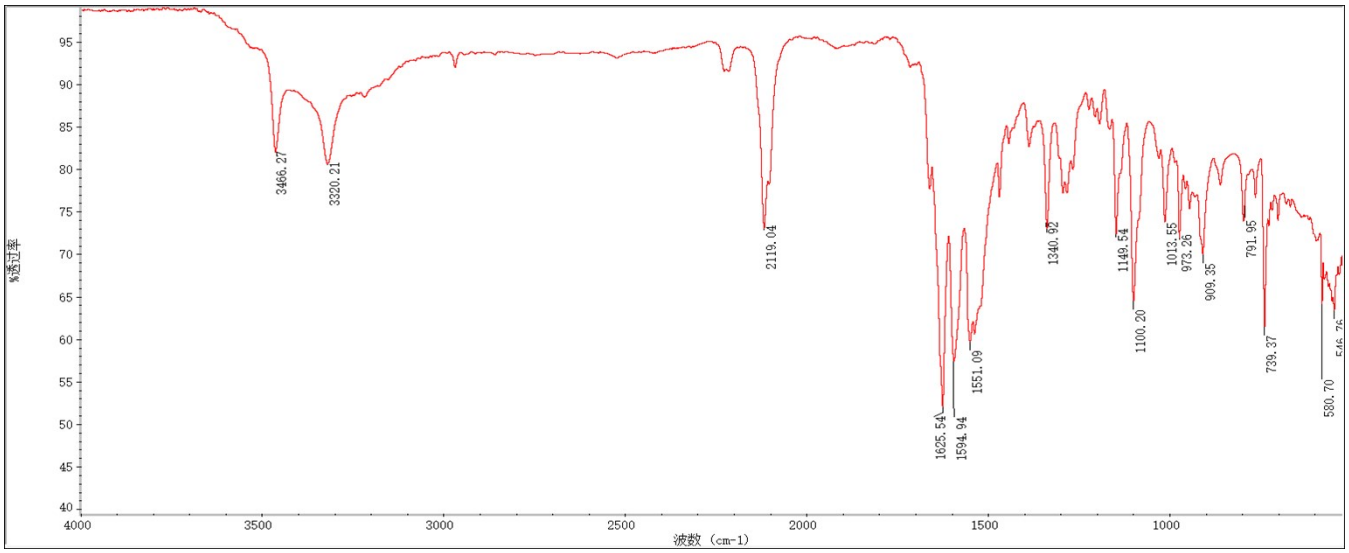

Figure S28 IR spectra for **9**.

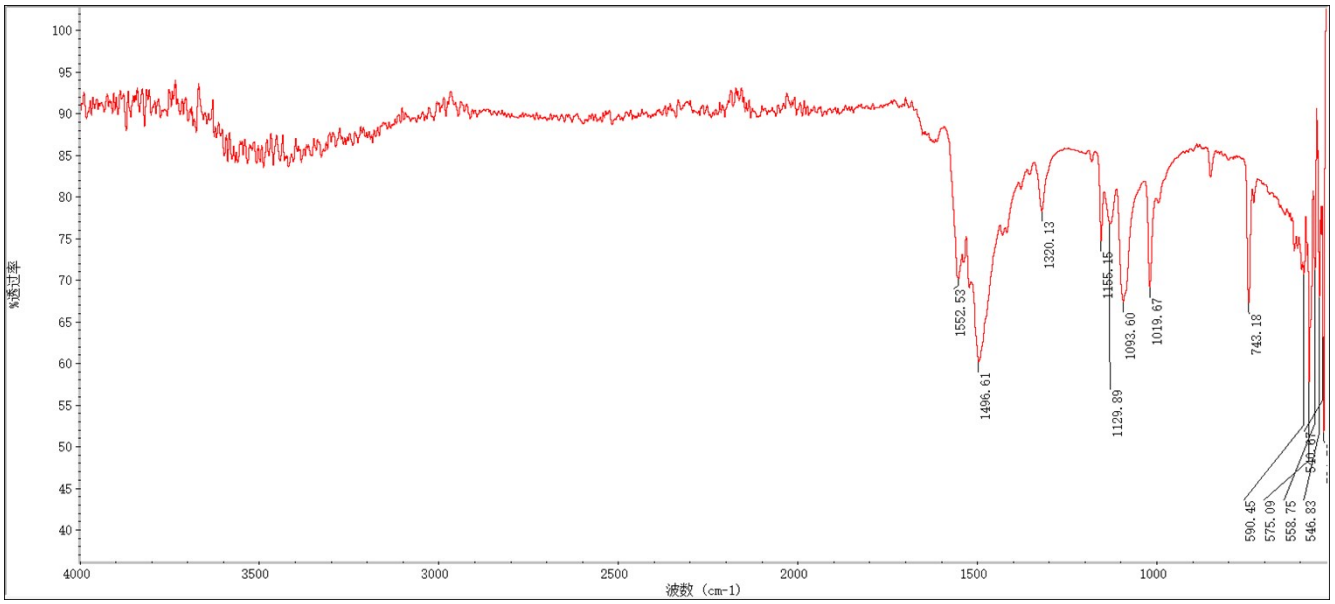

Figure S29 IR spectra for **10**.

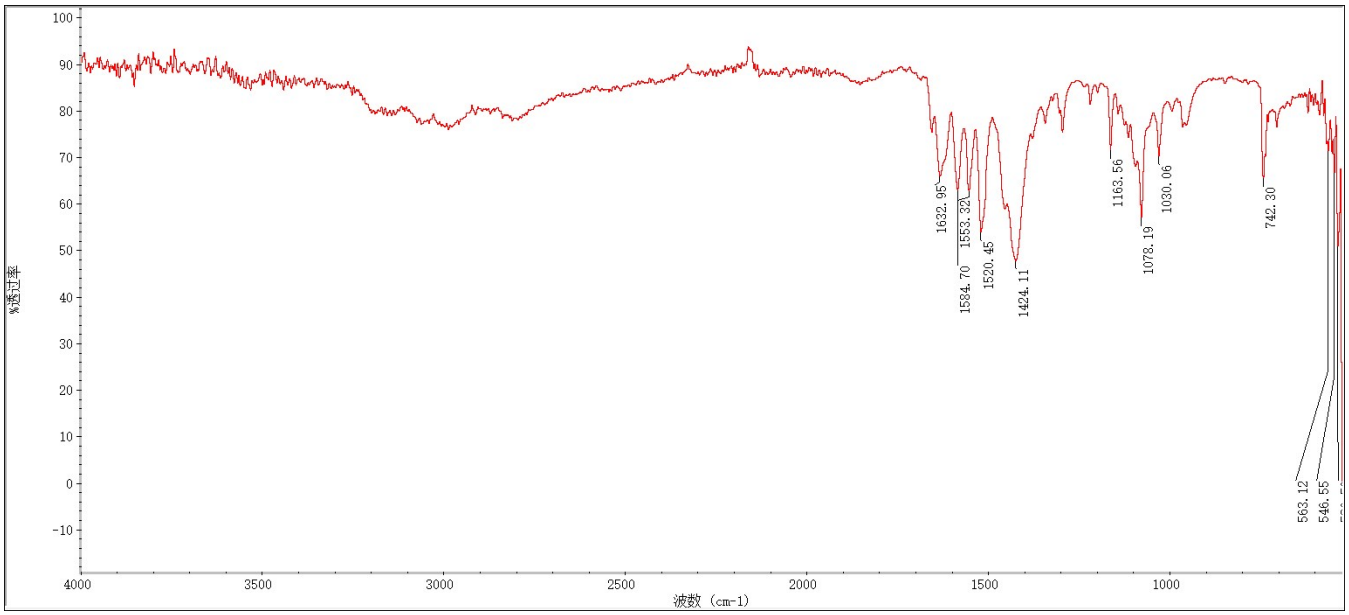

Figure S30 IR spectra for **11**.

References

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery Jr, T. V. Reven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Sal-vador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Ba-

boul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2009.

[2] H. D. B. Jenkins, D. Tudela, L. Glasser, *Inorg. Chem*., 2002, **41**, 2364-2367.

[3] P. C. Hariharan and J. A. Pople, Theor. *Chim. Acta.,* 1973, **28**, 213-222.