Supporting Information

Transition Metal-Mediated Hydrolysis of the Imine Bond in 2-Azomethine Benzothiazoles

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1. X-ray crystal structure determination

Table S1. Experimental data for the X-ray diffraction studies.

Compound	**3**	**1a**	**2a**	**2b**	**2c**
Formula	$C_{14}H_9BrN_2OS$	$C_{22}H_{17}N_5O_5S_2Zn$	$C_{21}H_{14}CuFN_5O_4S_2$	$C_{14}H_8CuF_2O_4$	$C_{14}H_{10}CuF_2O_5$
F_w (g mol^{-1})	333.20	560.89	547.03	341.74	359.76
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P\bar{1}$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	17.9824(3)	8.0897(7)	7.9378(2)	12.5165(5)	12.9621(1)
b (Å)	6.3691(1)	11.7385(10)	13.4701(3)	3.8555(2)	6.9497(1)
c (Å)	11.8792(2)	12.9843(10)	20.3168(6)	12.6338(5)	14.6724(1)
α (°)	90	98.819(7)	90	90	90
β (°)	105.743(2)	101.722(7)	99.617(3)	94.421(4)	92.061(1)
γ (°)	90	100.623(7)	90	90	90
V (Å^3)	1309.51(4)	1163.05(17)	2141.80(10)	607.86(5)	1320.87(2)
Z	4	2	4	2	4
Z'	1	1	1	0.5	1
D_{calc} (g cm^{-3})	1.690	1.602	1.696	1.867	1.809
F(000)	664	572	1108	342	724
Reflections collected	5768	12137	7761	4215	6296
Independent reflections	2681	4783	4127	1252	2731
R_{init}	0.0236	0.0637	0.0390	0.0338	0.0192
Reflections observed	2415	3395	3448	1194	2498
Parameters	176	325	313	97	207
R_1 [$I > 2\sigma(I)$][a]	0.0542	0.0619	0.0589	0.0743	0.0348
wR_2 (all data) [b]	0.1543	0.1843	0.1661	0.2288	0.1152
Goof, S[c]	1.068	1.056	1.041	1.147	1.096
Maximum/minimum electron density (e Å^3)	1.516/-0.614	0.542/-0.939	0.544/-0.715	1.265/-0.612	0.476/-0.280

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. [c] $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$ where n is number of reflections and p is the total number of parameters refined.

2. Crystal packing

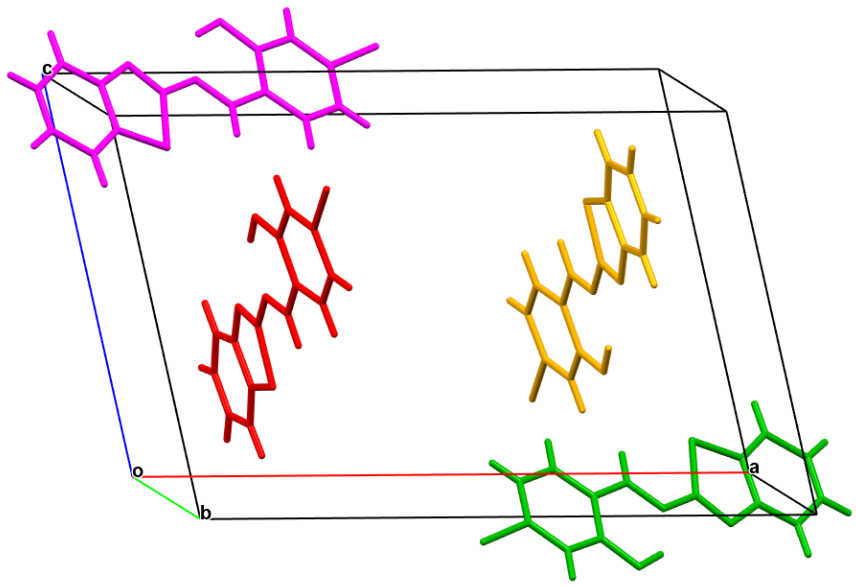


Figure S1. Crystal packing of molecules in **3**. One molecule in the asymmetric unit is given in red color.

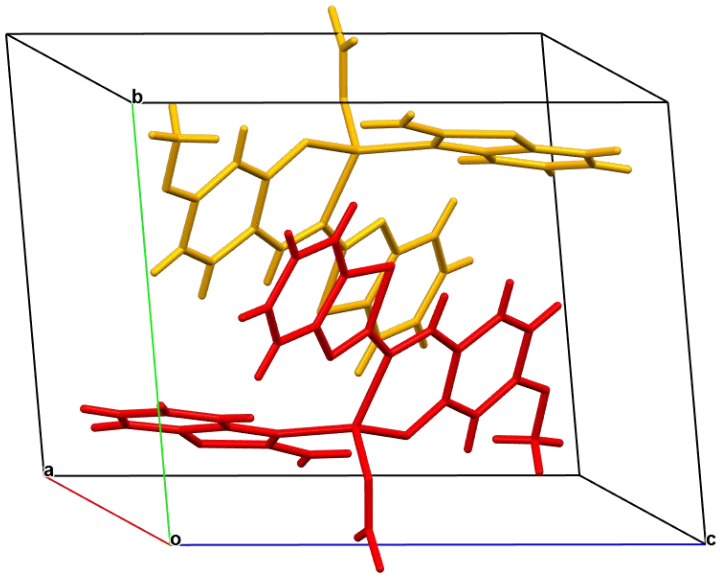


Figure S2. Crystal packing of complexes in **1a**. One complex in the asymmetric unit is given in red color.

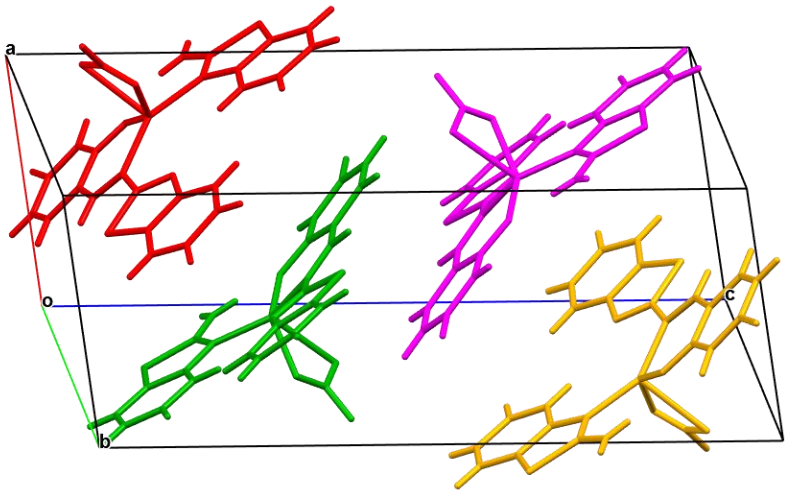


Figure S3. Crystal packing of complexes in **2a**. One complex in the asymmetric unit is given in red color.

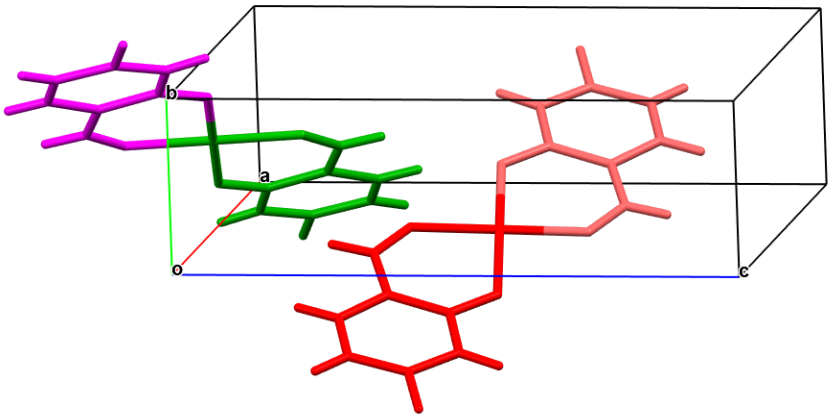


Figure S4. Crystal packing of complexes in **2b**. One half of complex in the asymmetric unit is given in red color.

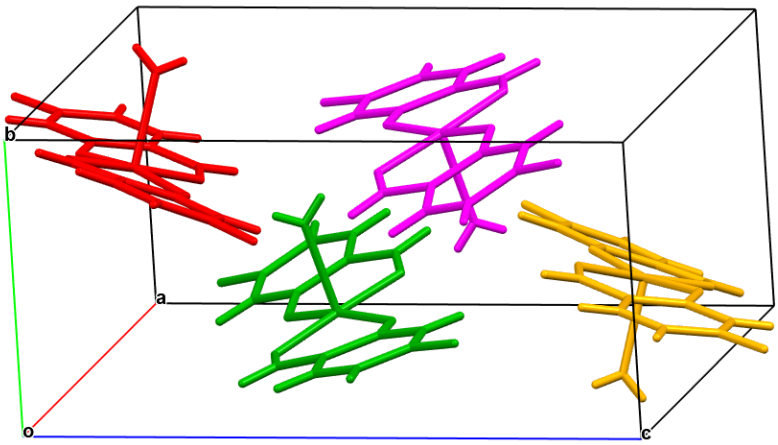
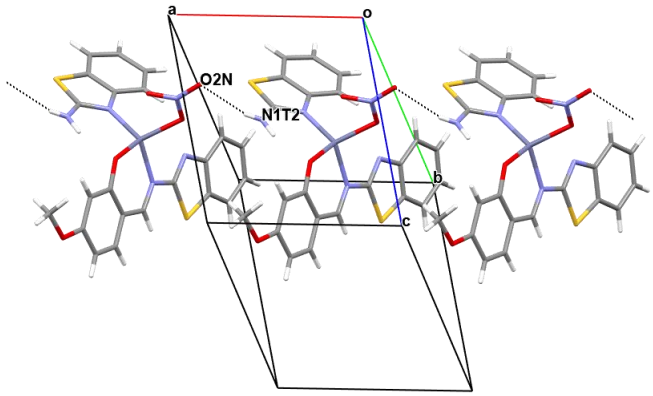
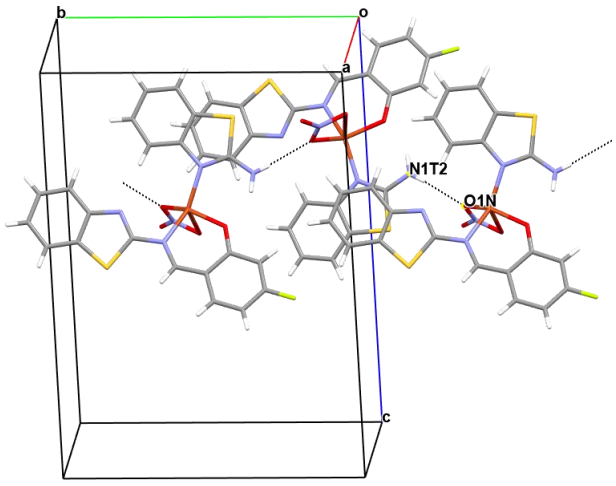


Figure S5. Crystal packing of molecules in **2c**. One complex in the asymmetric unit is given in red color.



a)



b)

Figure S6. One-dimensional hydrogen bonding motifs in **1a** (a) and **2a** (b), formed by intermolecular hydrogen bonds N1T2-HBT2···O2N^{i} for **1a** [symmetry code for **1a**: (i) *x*+1, *y*, *z*] and N1T2-HBT2···O1N^{i} for **2a** [symmetry code for **2a**: (i) −*x*+2, *y*−1/2, −*z*+1/2].

3. ^{1}H and ^{13}C NMR spectra of ligands **1–3**

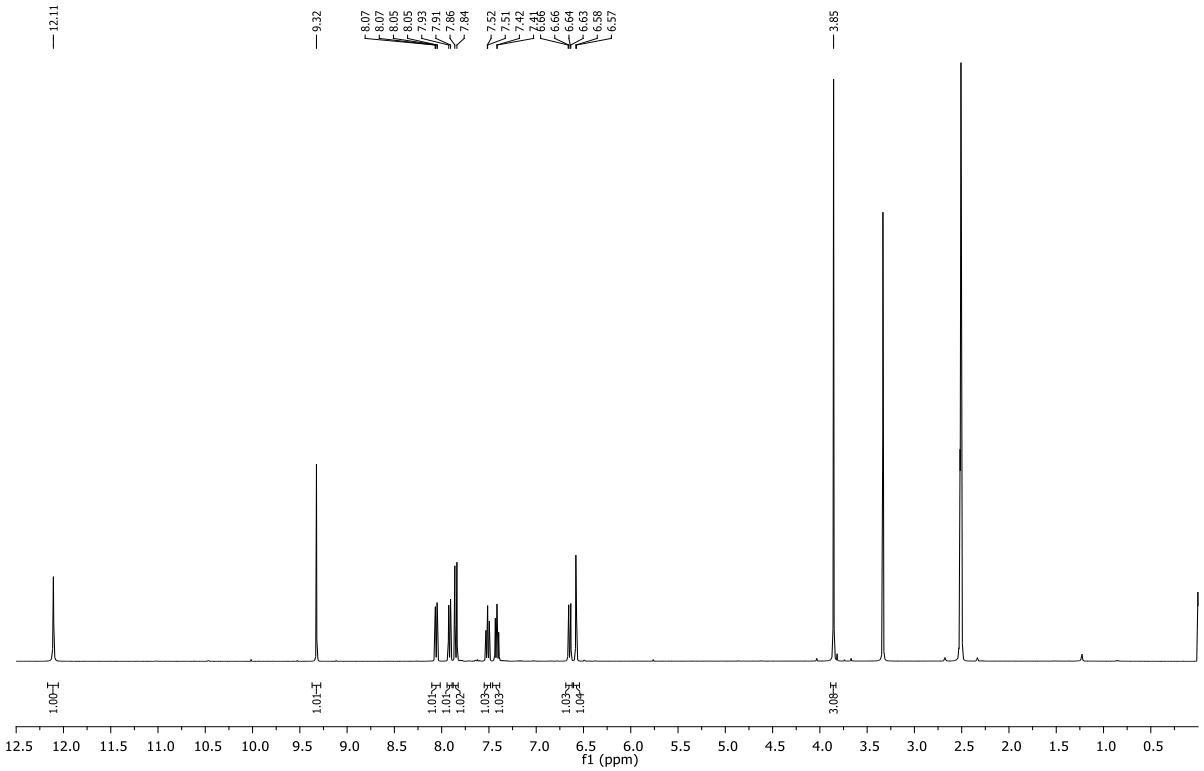


Figure S7. ^{1}H NMR spectrum of ligand **1**

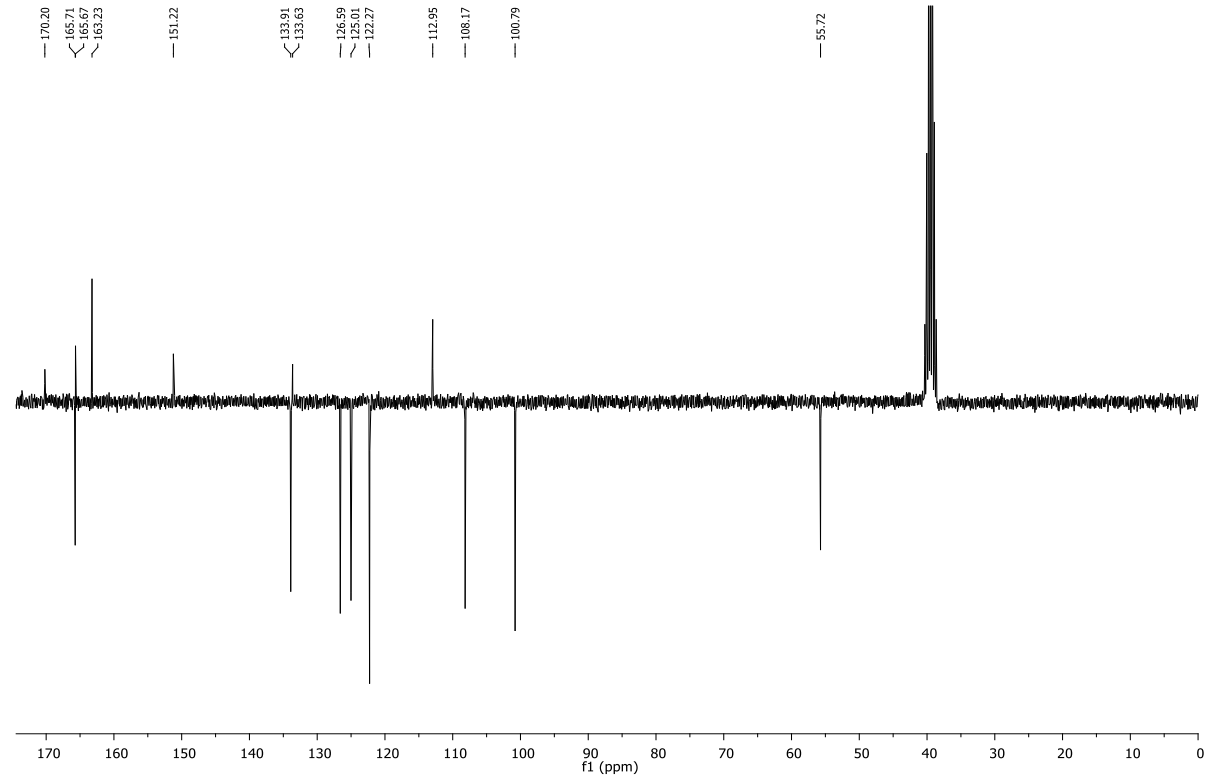


Figure S8. ^{13}C NMR spectrum of ligand **1**

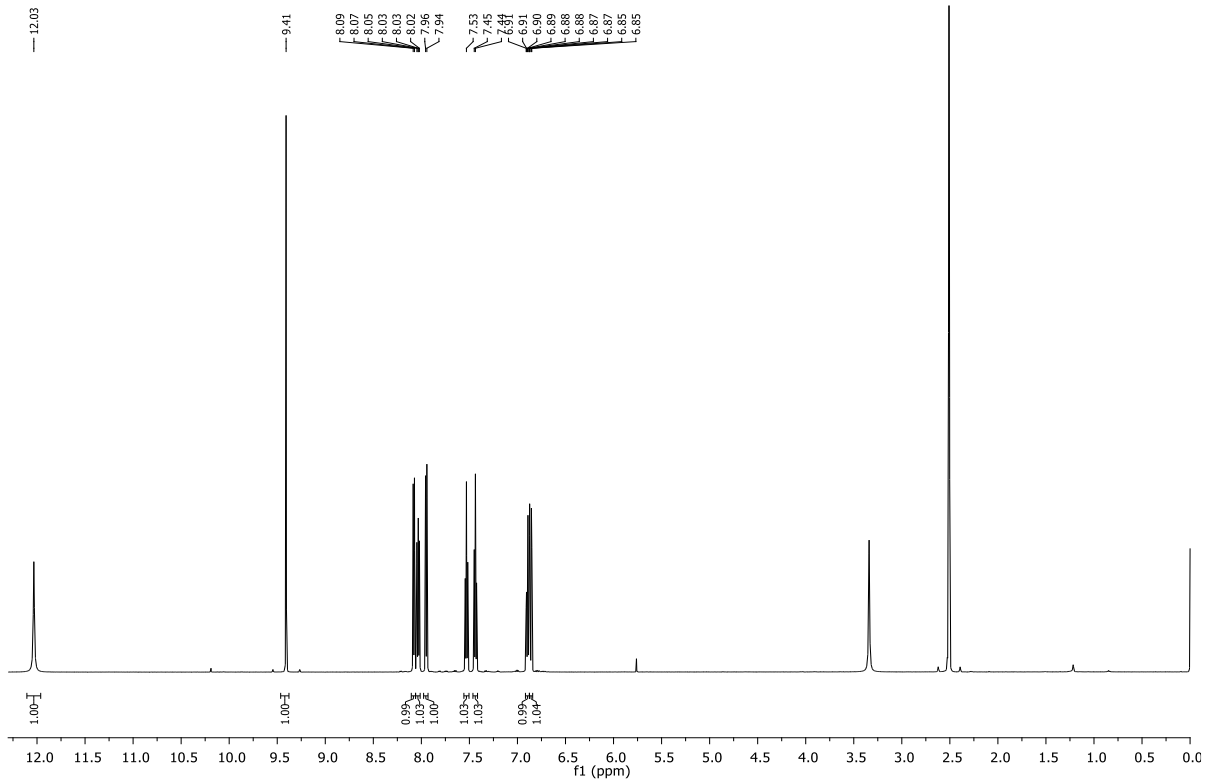


Figure S9. ^{1}H NMR spectrum of ligand **2**

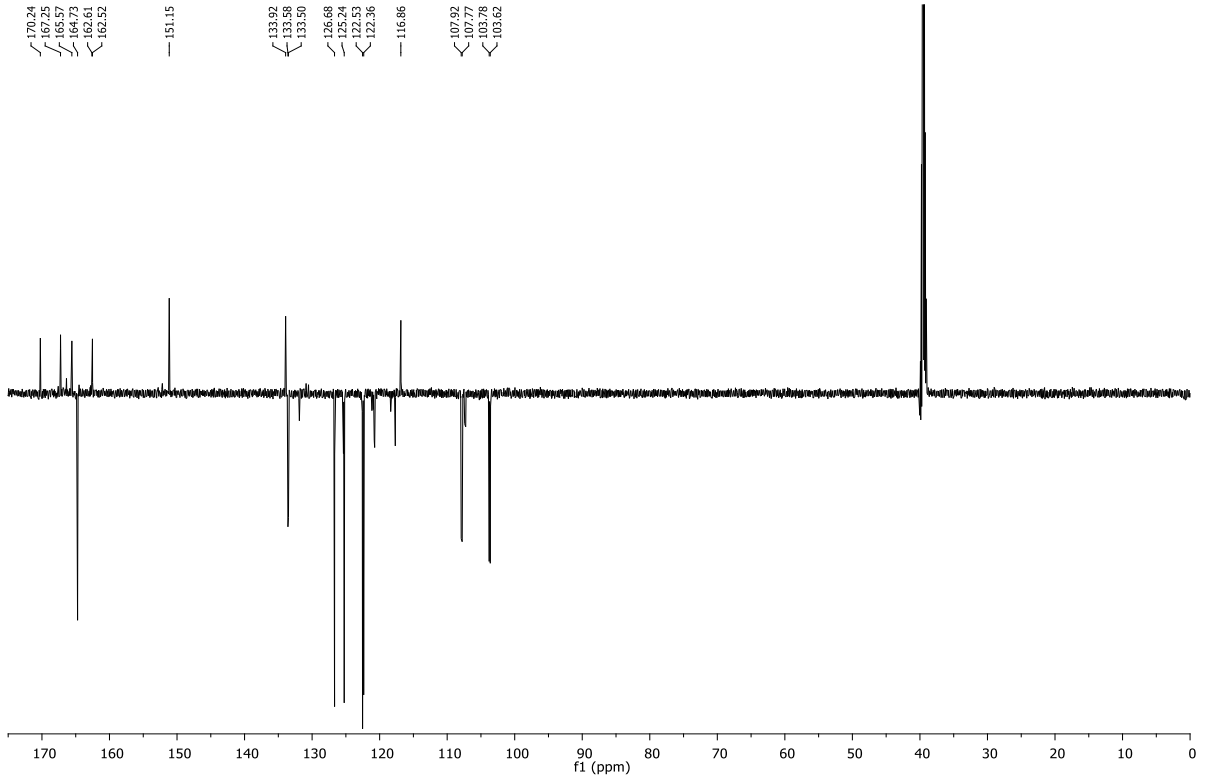


Figure S10. ^{13}C NMR spectrum of ligand **2**

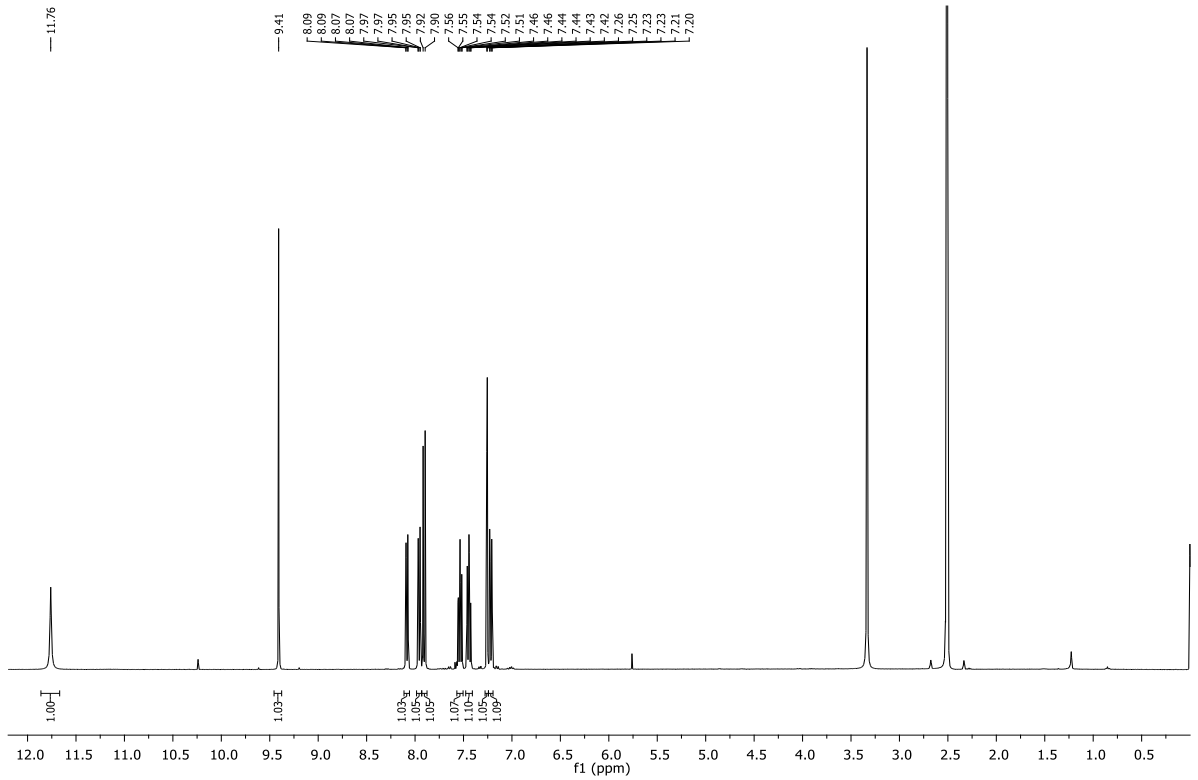


Figure S11. ^{1}H NMR spectrum of ligand **3**

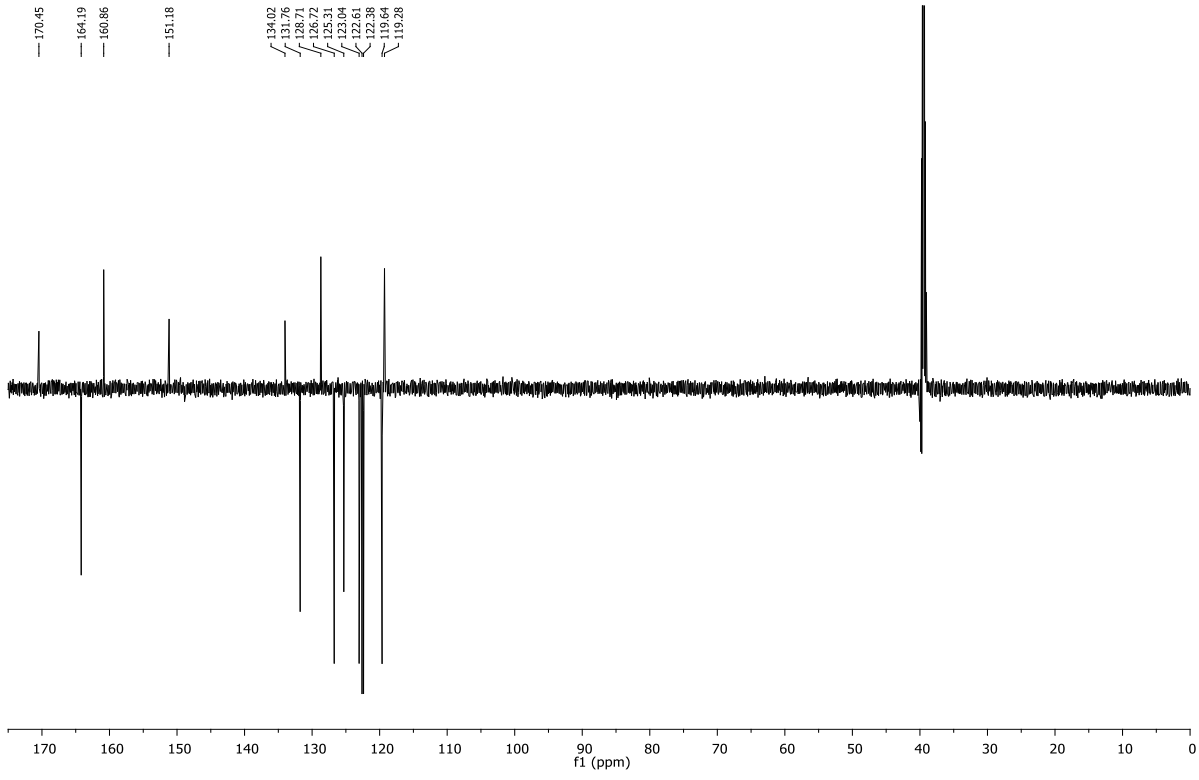


Figure S12. ^{13}C NMR spectrum of ligand **3**

4. IR(ATR) spectra of ligands **1–3**

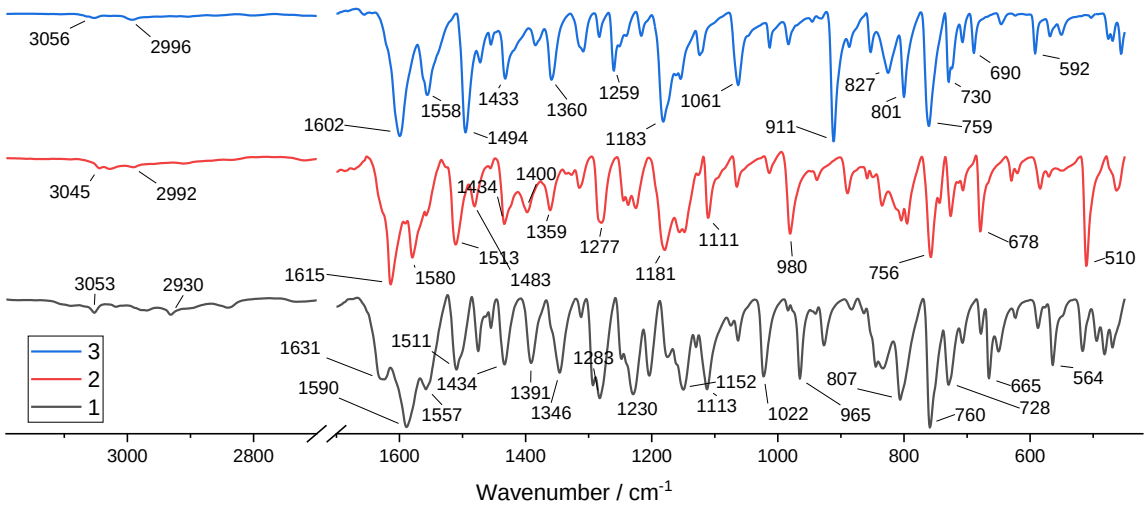


Figure S13. IR(ATR) spectra of ligands **1–3**