

## Supporting Information

### Role of hydrazone substituents in determining the nuclearity and antibacterial activity of Zn(II) complexes with pyrazolone-based hydrazones

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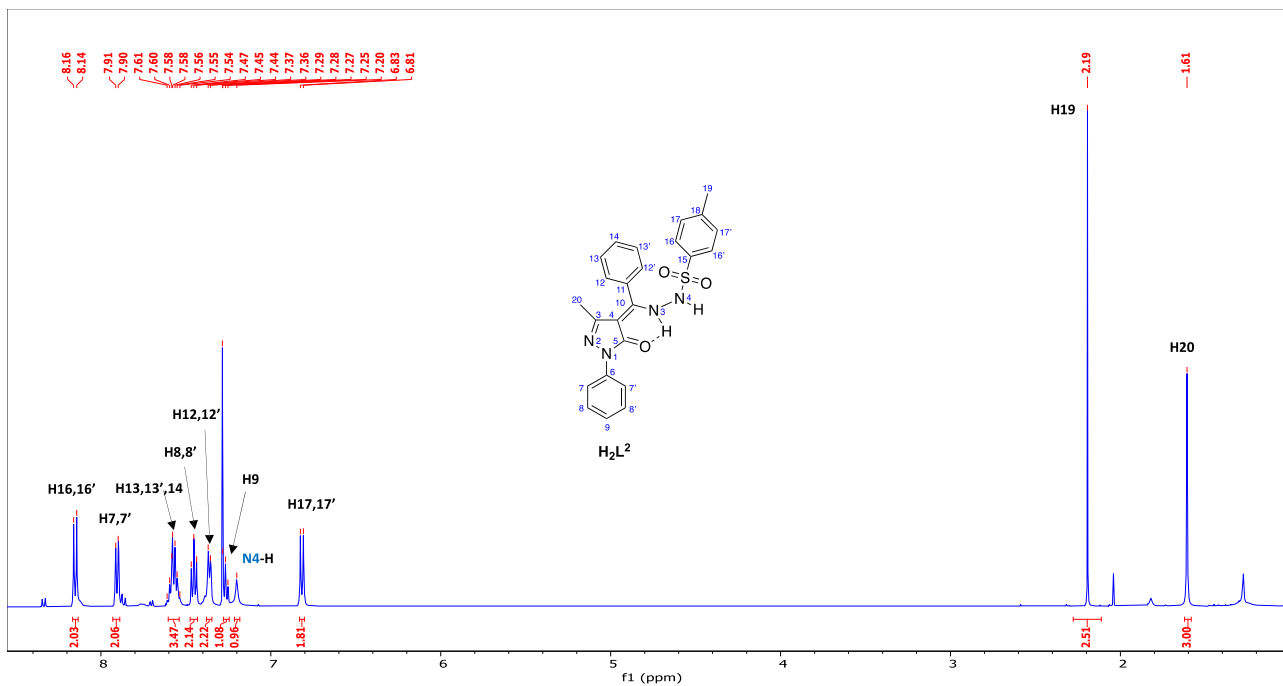


Figure S1.  $^1H$  NMR  $H_2L^2$  in  $CDCl_3$  at 298 K.

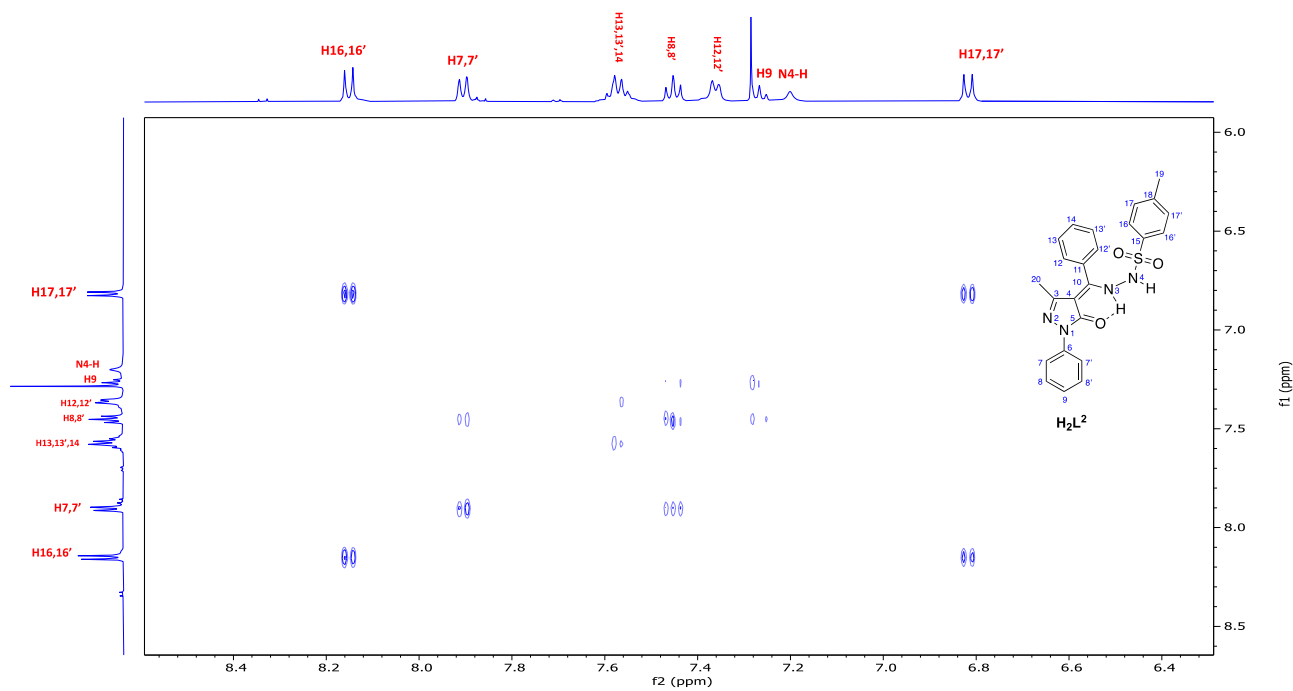


Figure S2.  $\{^1H,^1H\}$ -COSY  $H_2L^2$  in  $CDCl_3$  at 298 K.

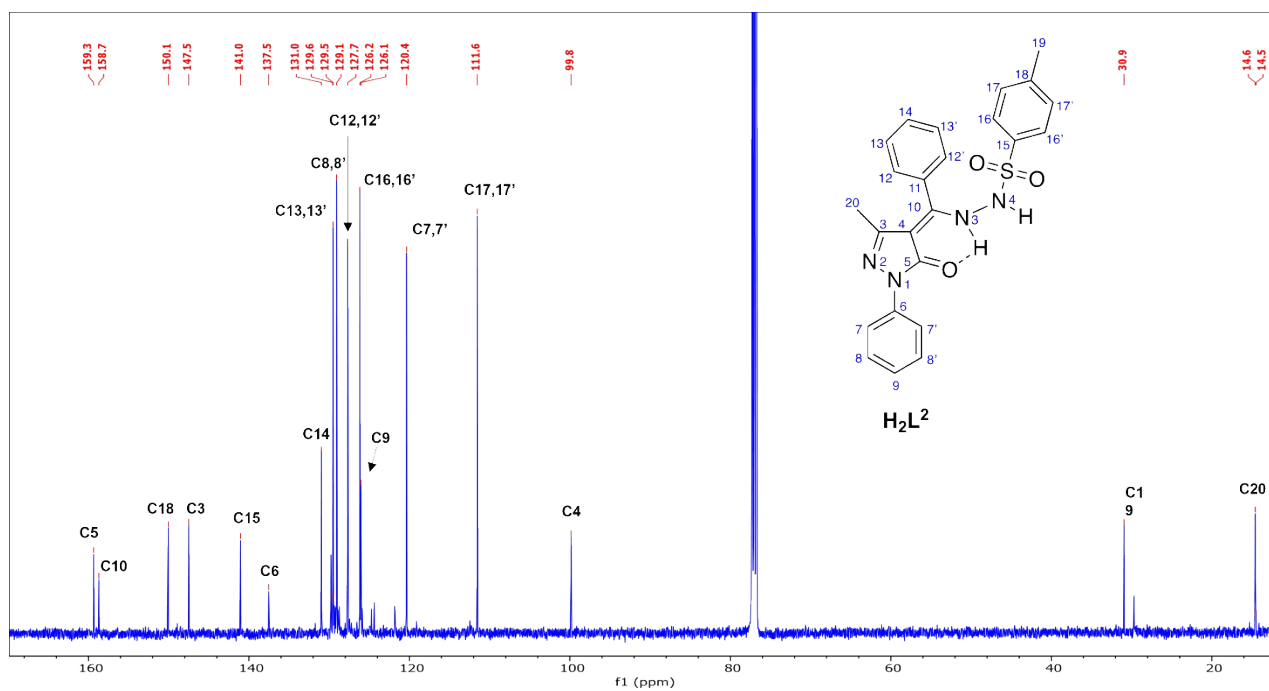


Figure S3.  $^{13}\text{C}\{^1\text{H}\}$  NMR  $\text{H}_2\text{L}^2$  in  $\text{CDCl}_3$  at 298 K.

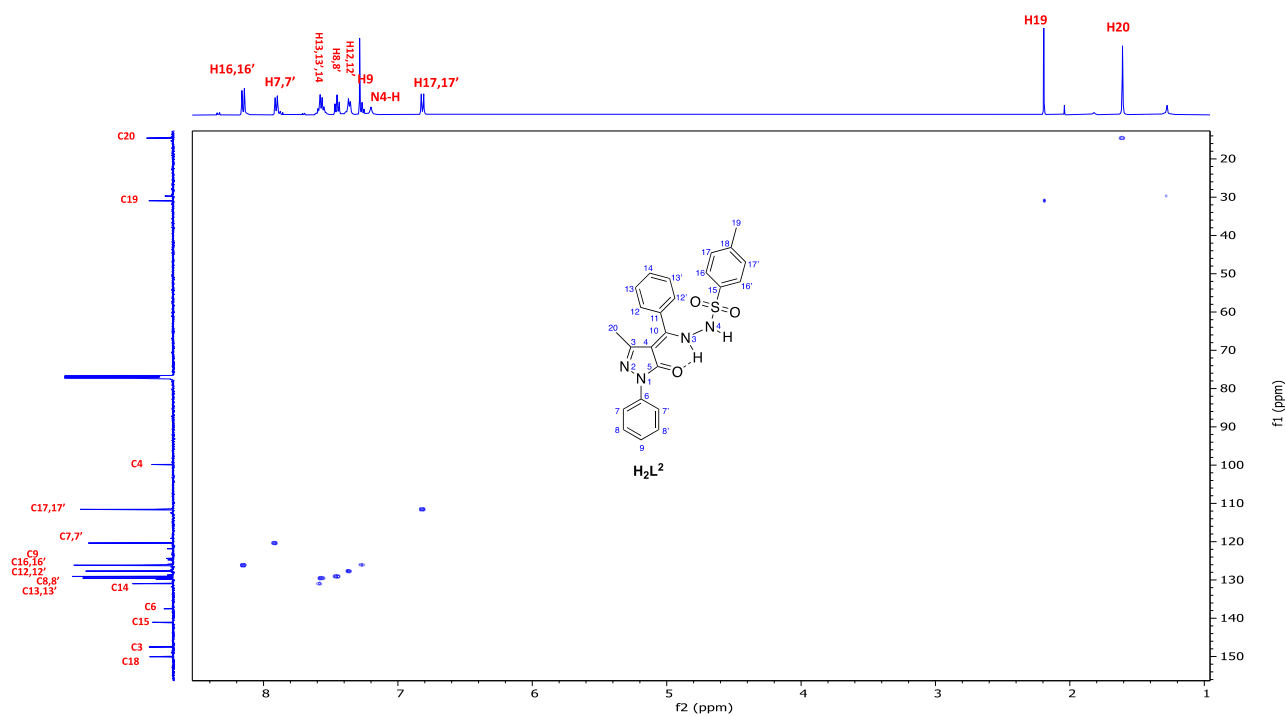


Figure S4.  $\{^1\text{H}, ^{13}\text{C}\}$ -HSQC  $\text{H}_2\text{L}^2$  in  $\text{CDCl}_3$  at 298 K.

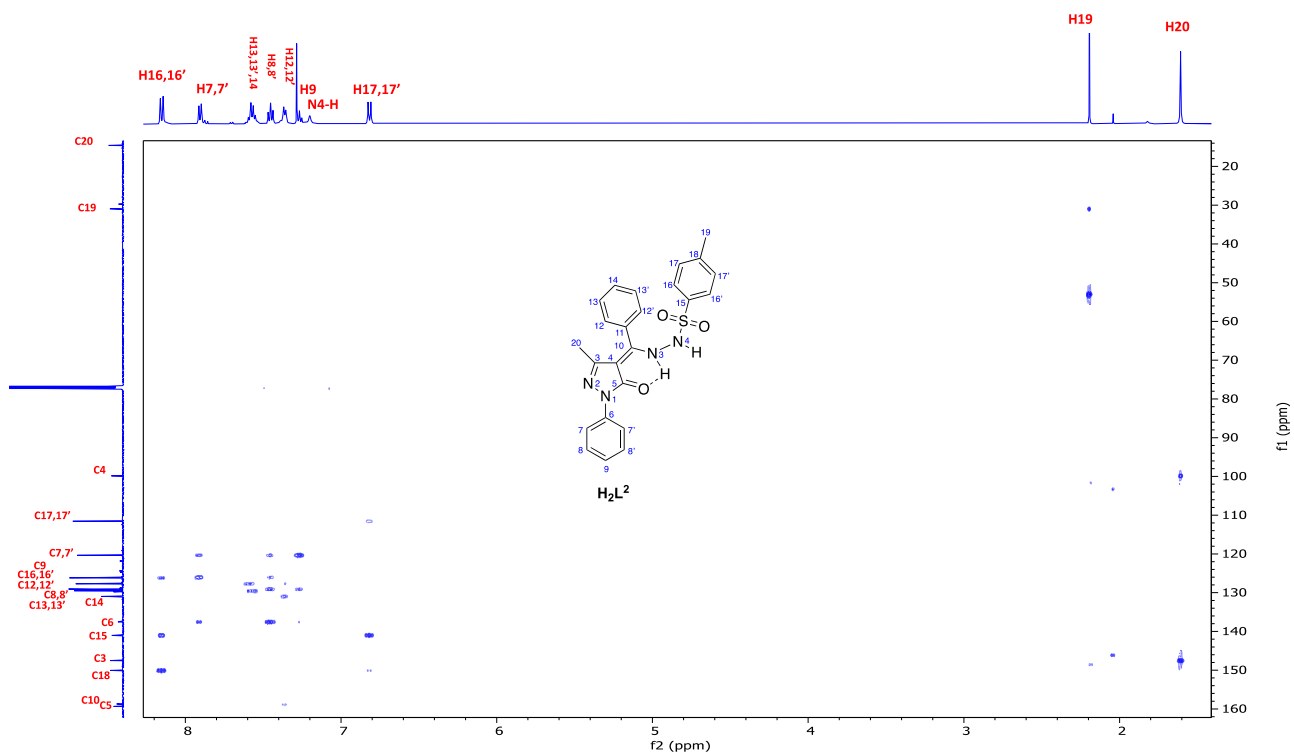


Figure S5.  $\{^1\text{H}, ^{13}\text{C}\}$ -HMBC  $\text{H}_2\text{L}^2$  in  $\text{CDCl}_3$  at 298 K.

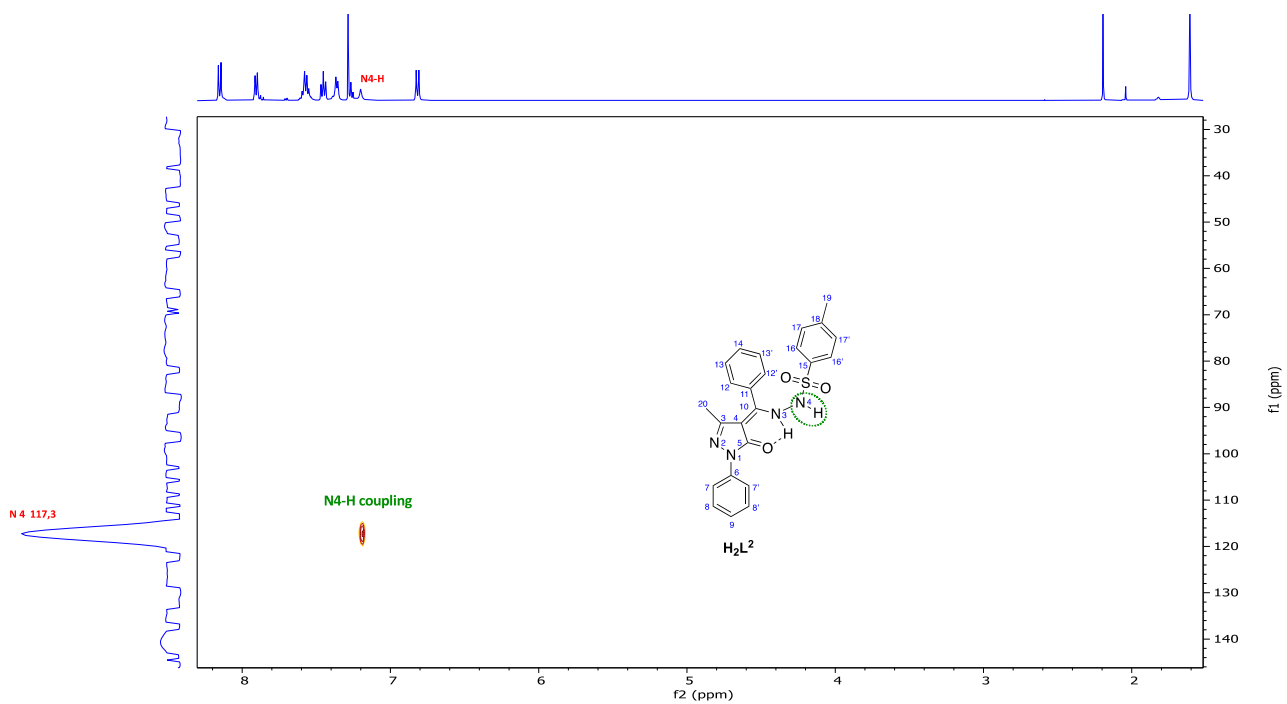


Figure S6.  $\{^1\text{H}, ^{15}\text{N}\}$ -HSQC  $\text{H}_2\text{L}^2$  in  $\text{CDCl}_3$  at 298 K.

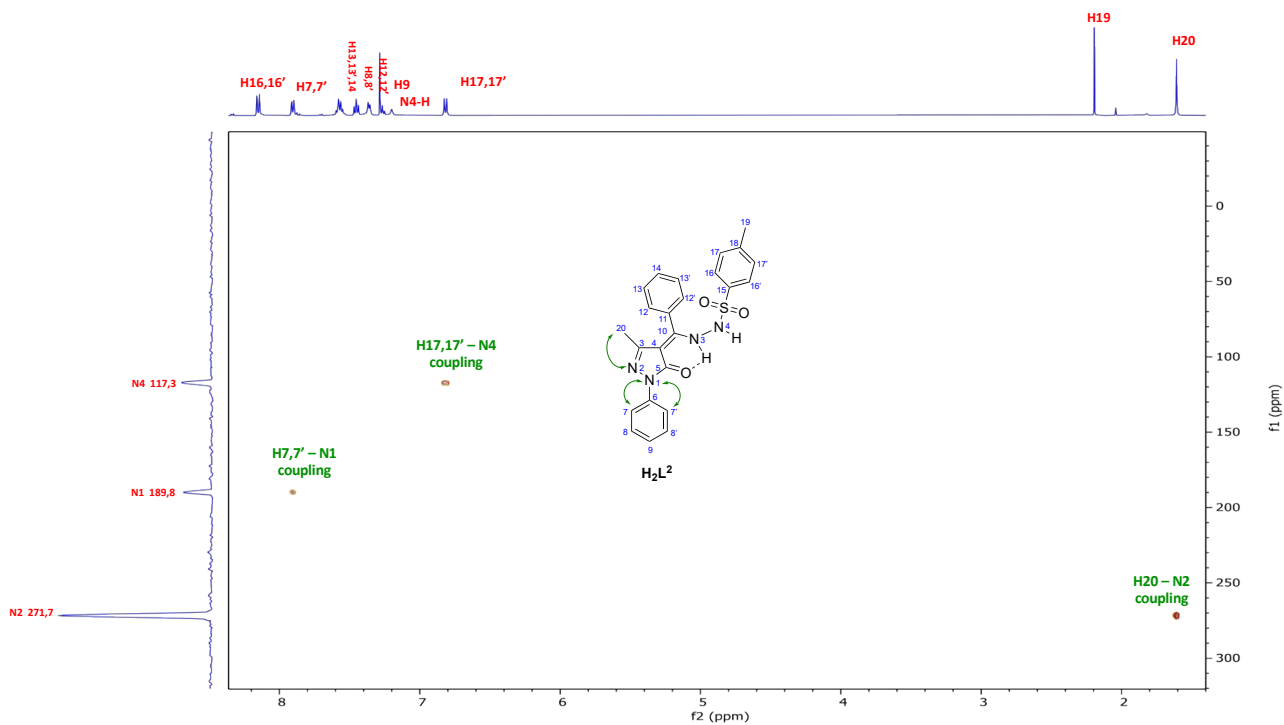


Figure S7.  $\{^1\text{H}, ^{15}\text{N}\}$ -HMBC  $\text{H}_2\text{L}^2$  in  $\text{CDCl}_3$  at 298 K.

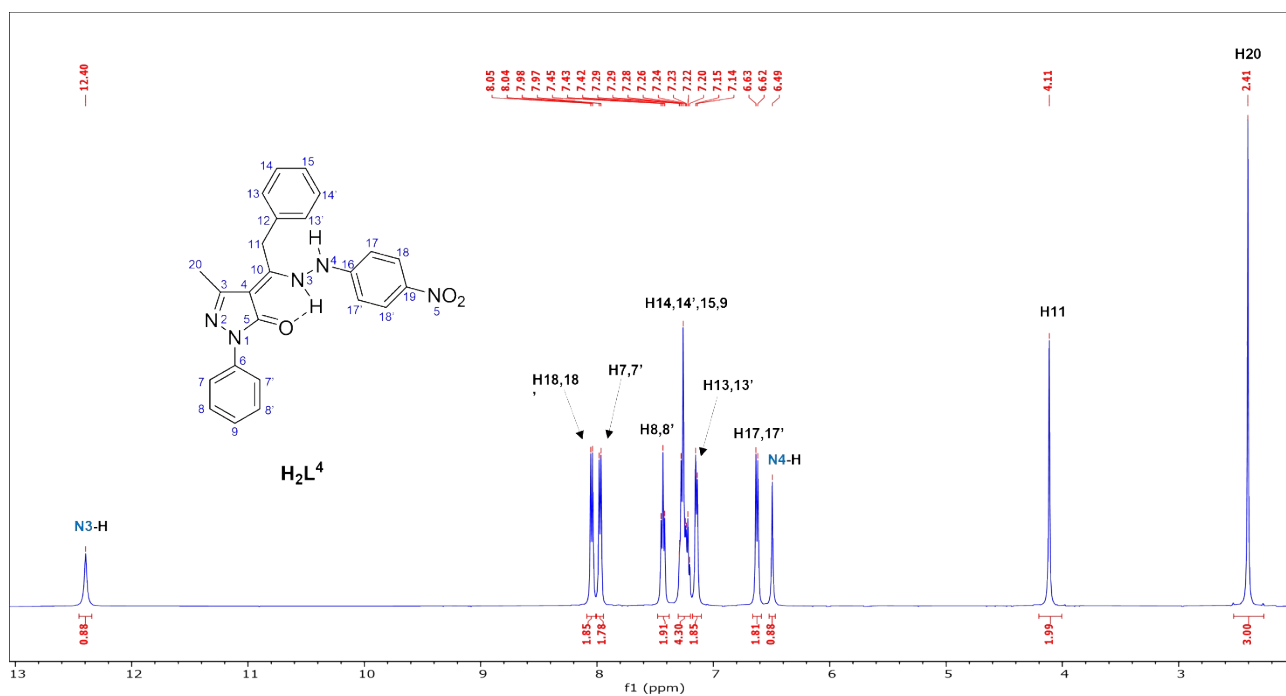


Figure S8.  $^1\text{H}$  NMR  $\text{H}_2\text{L}^4$  in  $\text{CDCl}_3$  at 298 K.

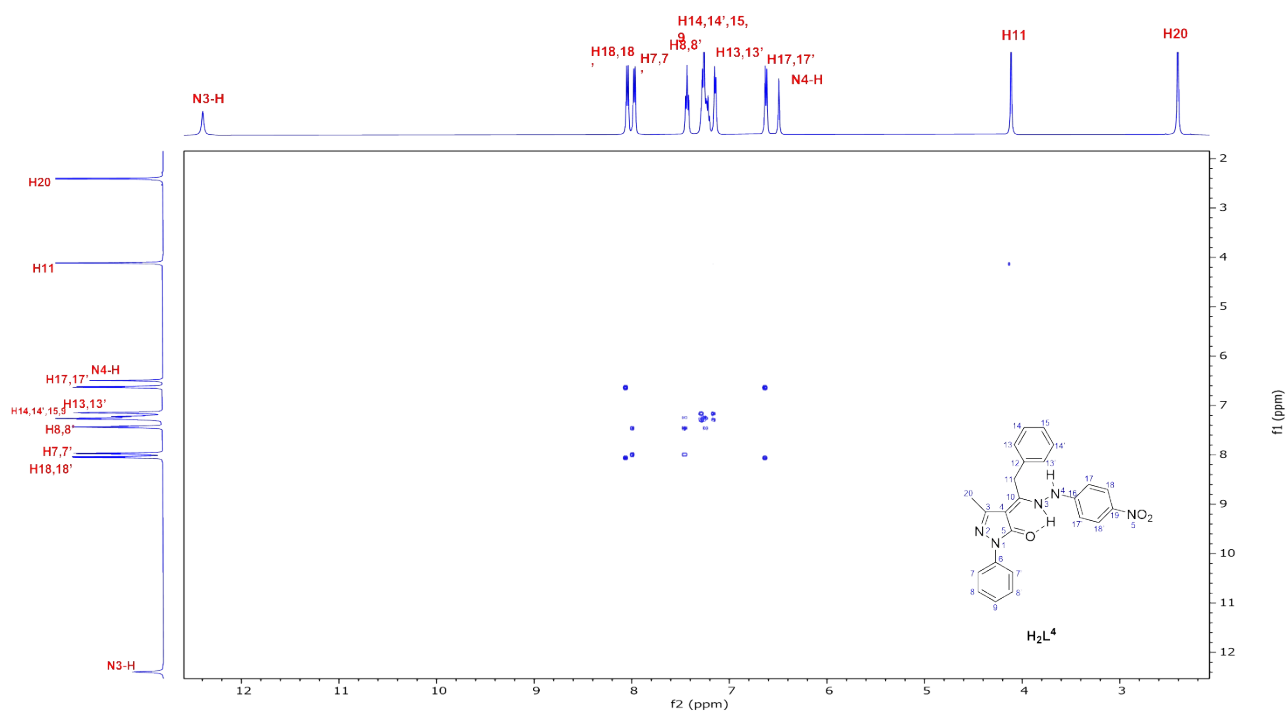


Figure S9.  $\{^1\text{H},^1\text{H}\}$ -COSY  $\text{H}_2\text{L}^4$  in  $\text{CDCl}_3$  at 298 K.

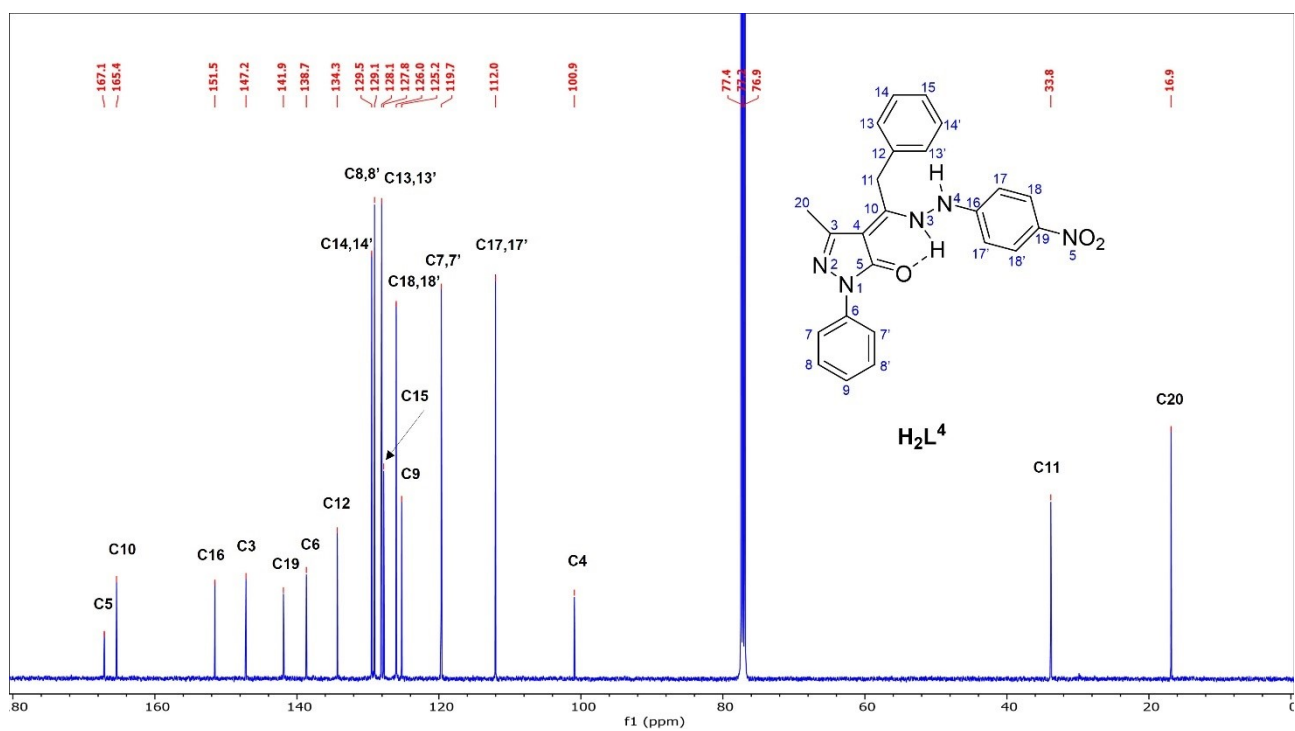


Figure S10.  $^{13}\text{C}\{^1\text{H}\}$  NMR  $\text{H}_2\text{L}^4$  in  $\text{CDCl}_3$  at 298 K.

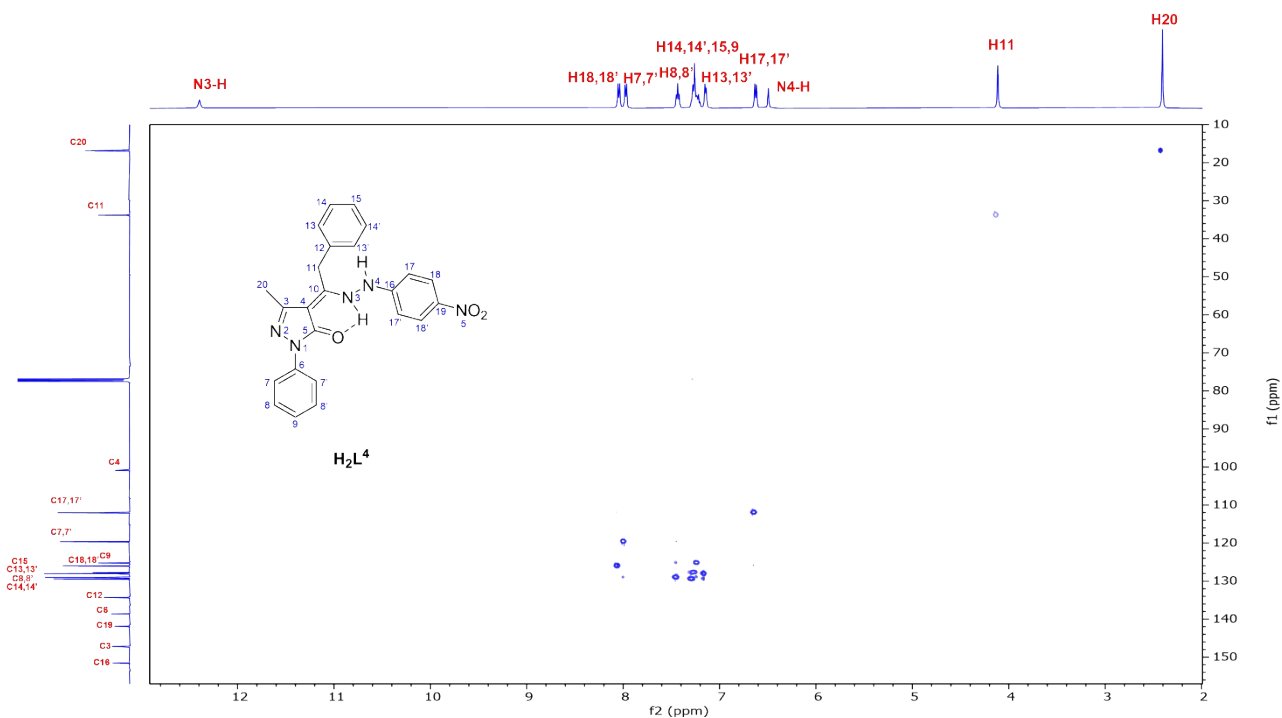


Figure S11.  $\{^1\text{H}, ^{13}\text{C}\}$ -HSQC  $\text{H}_2\text{L}^4$  in  $\text{CDCl}_3$  at 298 K.

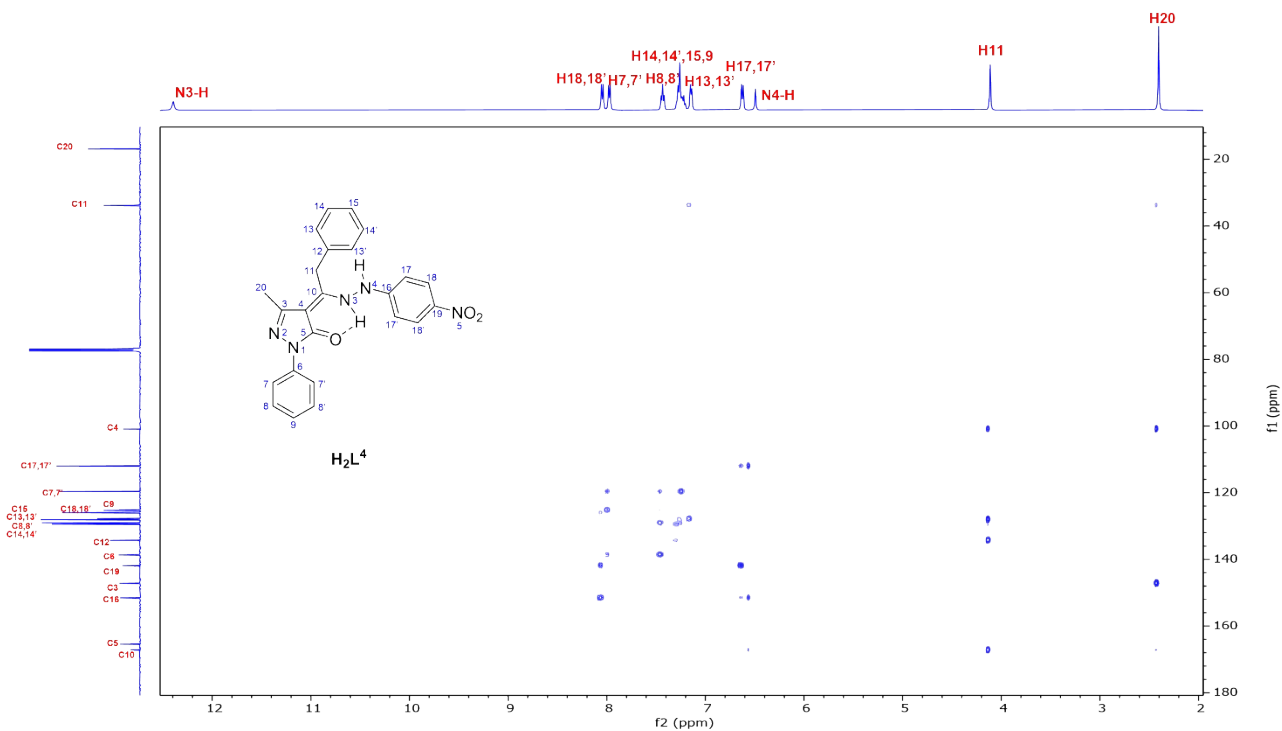


Figure S12.  $\{^1\text{H}, ^{13}\text{C}\}$ -HMBC  $\text{H}_2\text{L}^4$  in  $\text{CDCl}_3$  at 298 K.



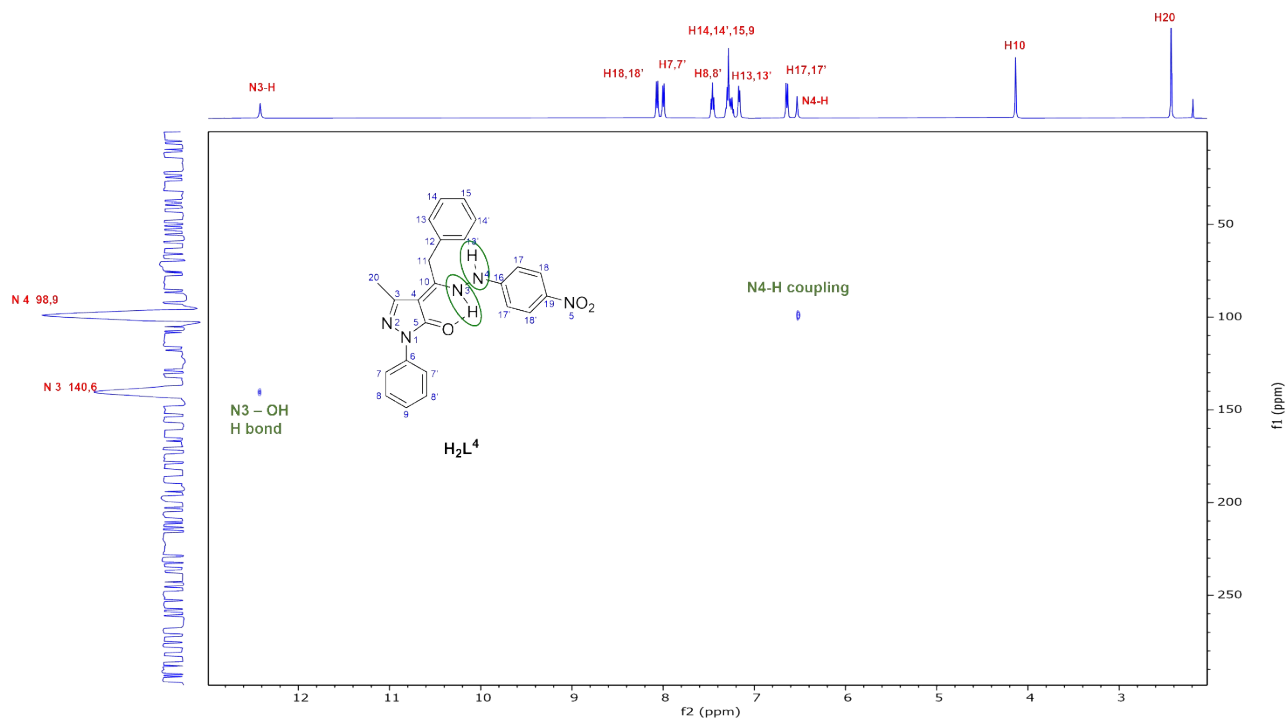


Figure S13.  $\{^1\text{H}-^{15}\text{N}\}$ -HSQC  $\text{H}_2\text{L}^4$  in  $\text{CDCl}_3$  at 298 K.

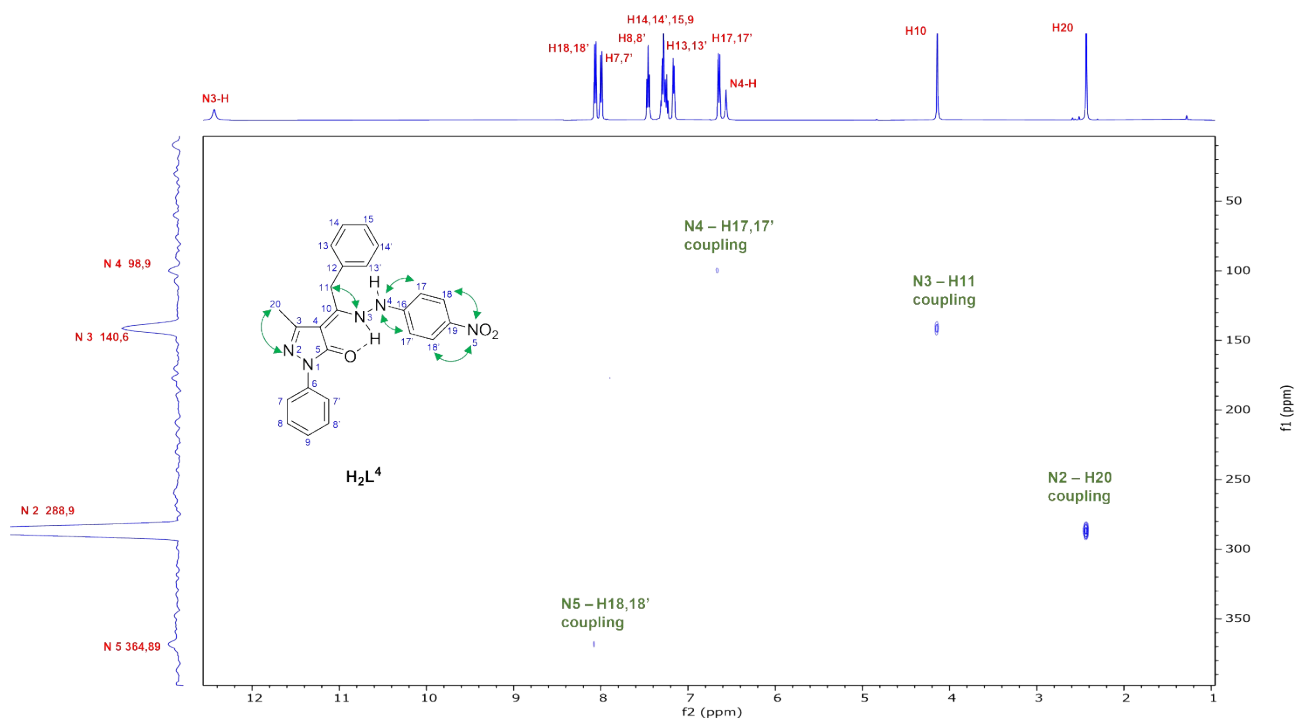
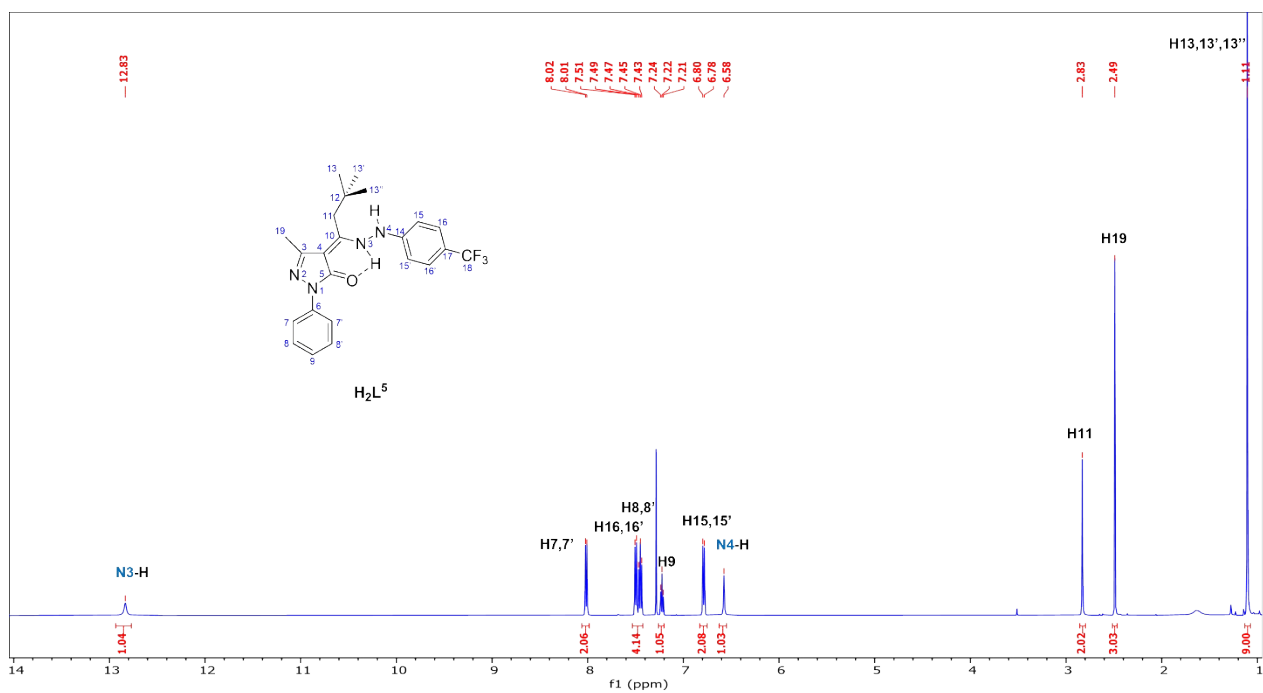
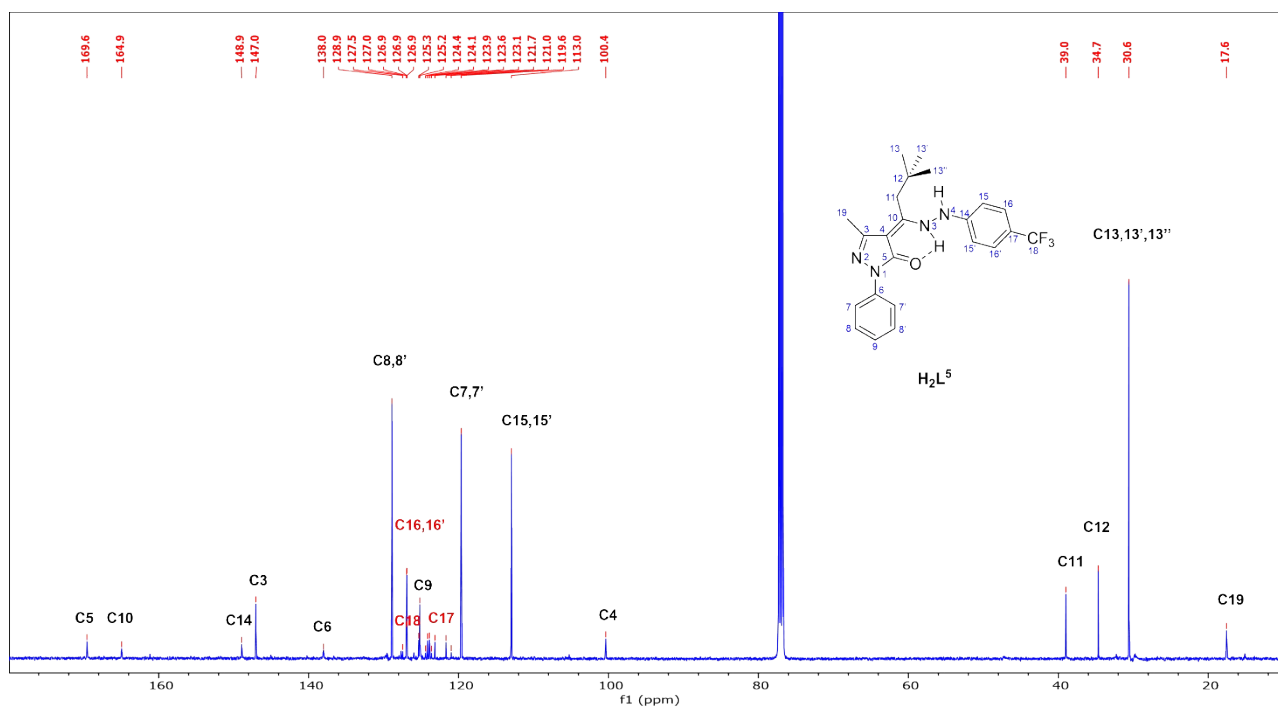


Figure S14.  $\{^1\text{H}, ^{15}\text{N}\}$ -HMBC  $\text{H}_2\text{L}^4$  in  $\text{CDCl}_3$  at 298 K.



**Figure S15.  $^1\text{H}$  NMR  $\text{H}_2\text{L}^5$  in  $\text{CDCl}_3$  at 298 K.**



**Figure S16.  $^{13}\text{C}\{^1\text{H}\}$  NMR  $\text{H}_2\text{L}^5$  in  $\text{CDCl}_3$  at 298 K.**

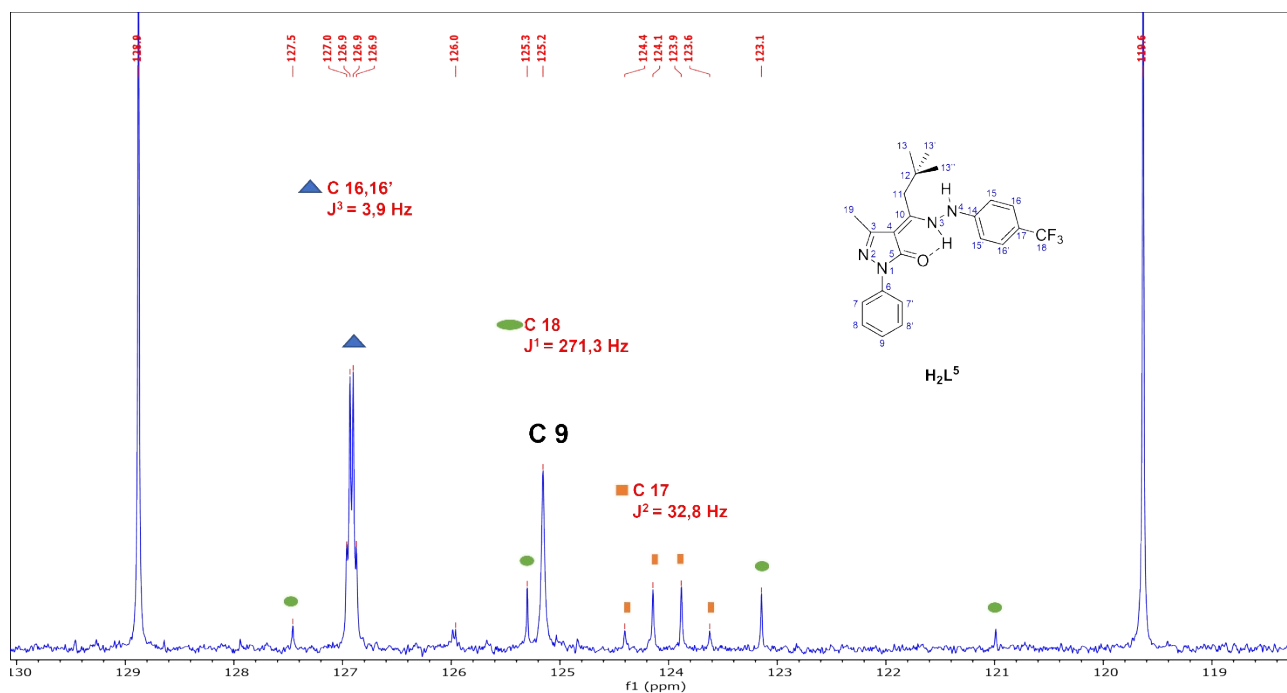


Figure S17. Magnification  $^{13}\text{C}\{^1\text{H}\}$  NMR  $\text{H}_2\text{L}^5$  in  $\text{CDCl}_3$  at 298 K.

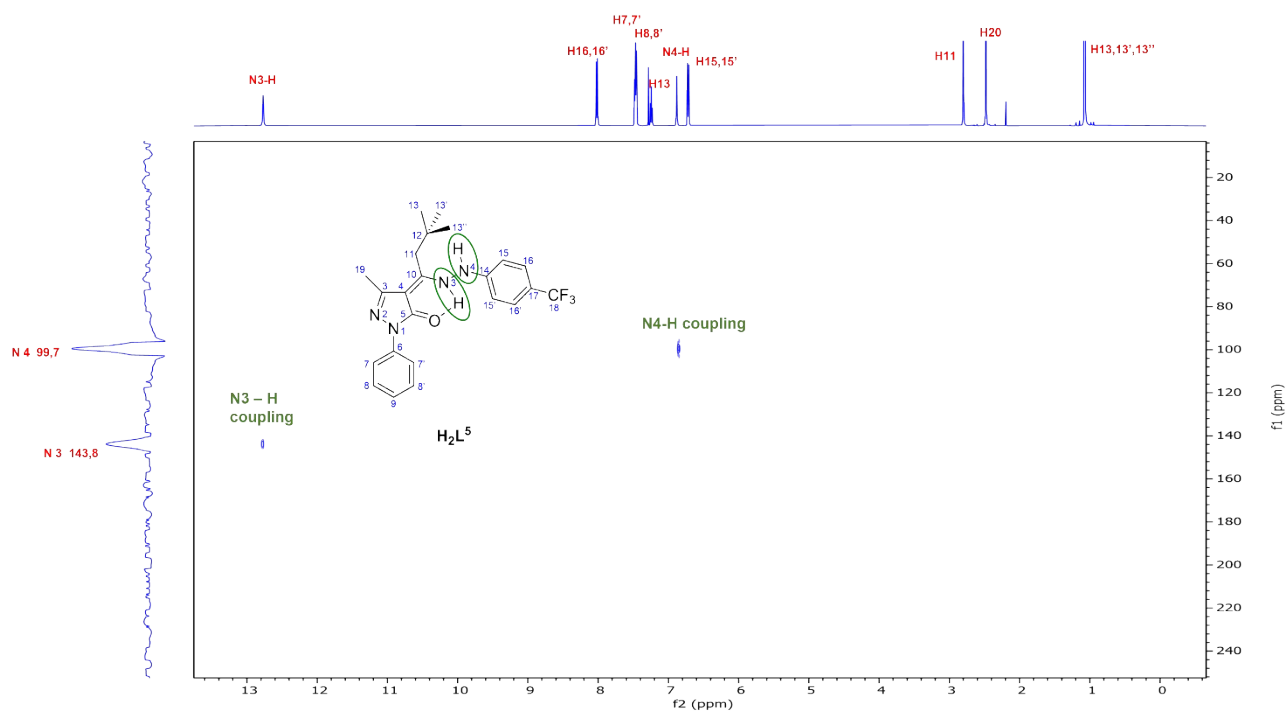


Figure S18.  $\{^1\text{H}, ^{15}\text{N}\}$ -HSQC  $\text{H}_2\text{L}^5$  in  $\text{CDCl}_3$  at 298 K.

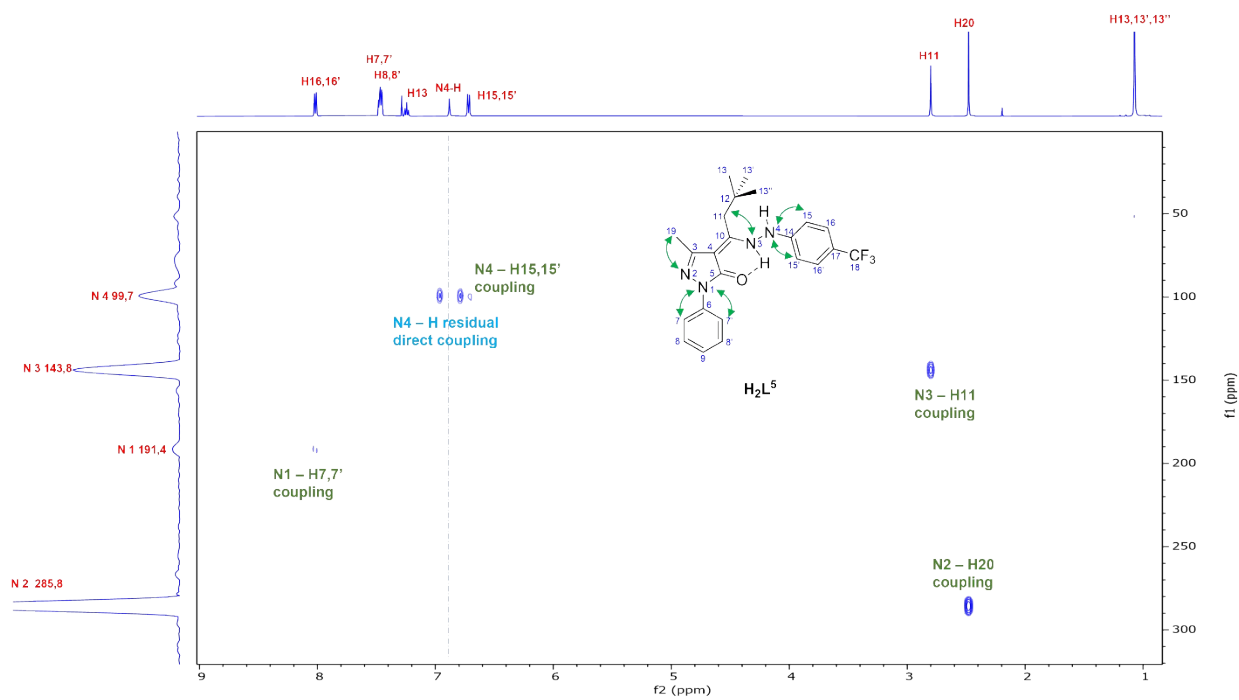


Figure S19.  $\{^1\text{H}, ^{15}\text{N}\}$ -HMBC  $\text{H}_2\text{L}^5$  in  $\text{CDCl}_3$  at 298 K.

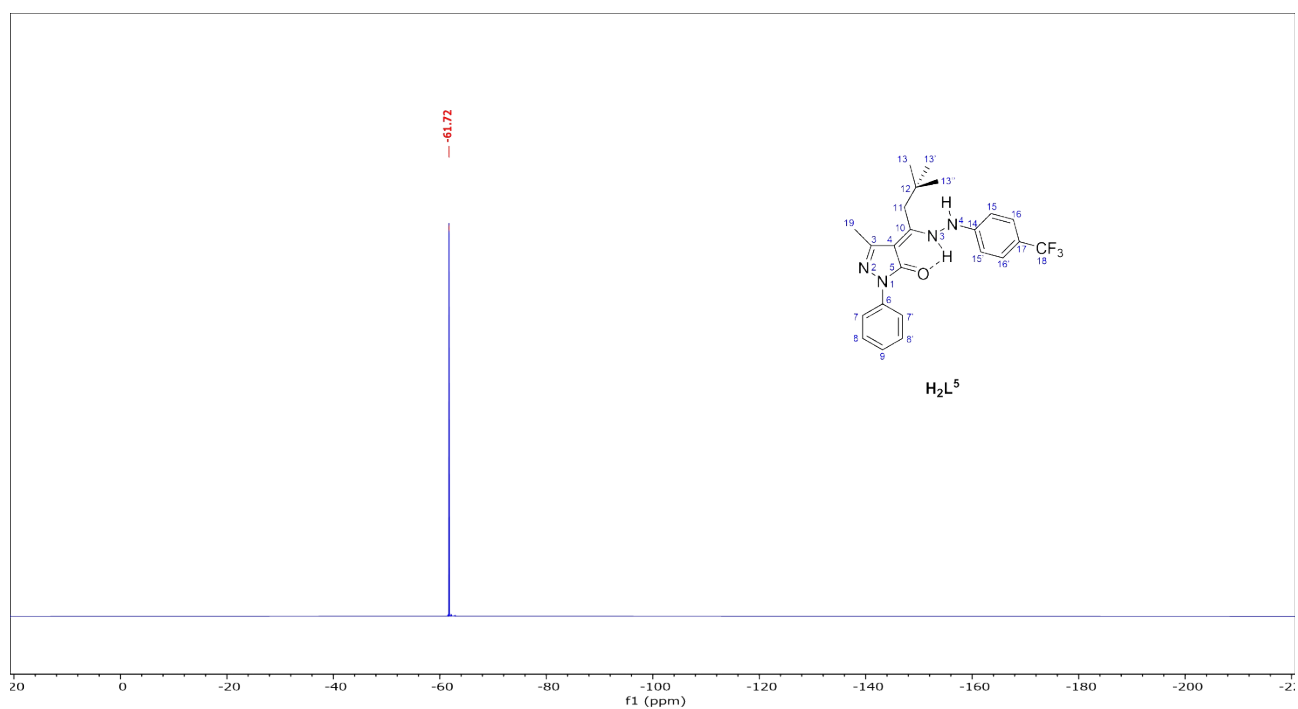
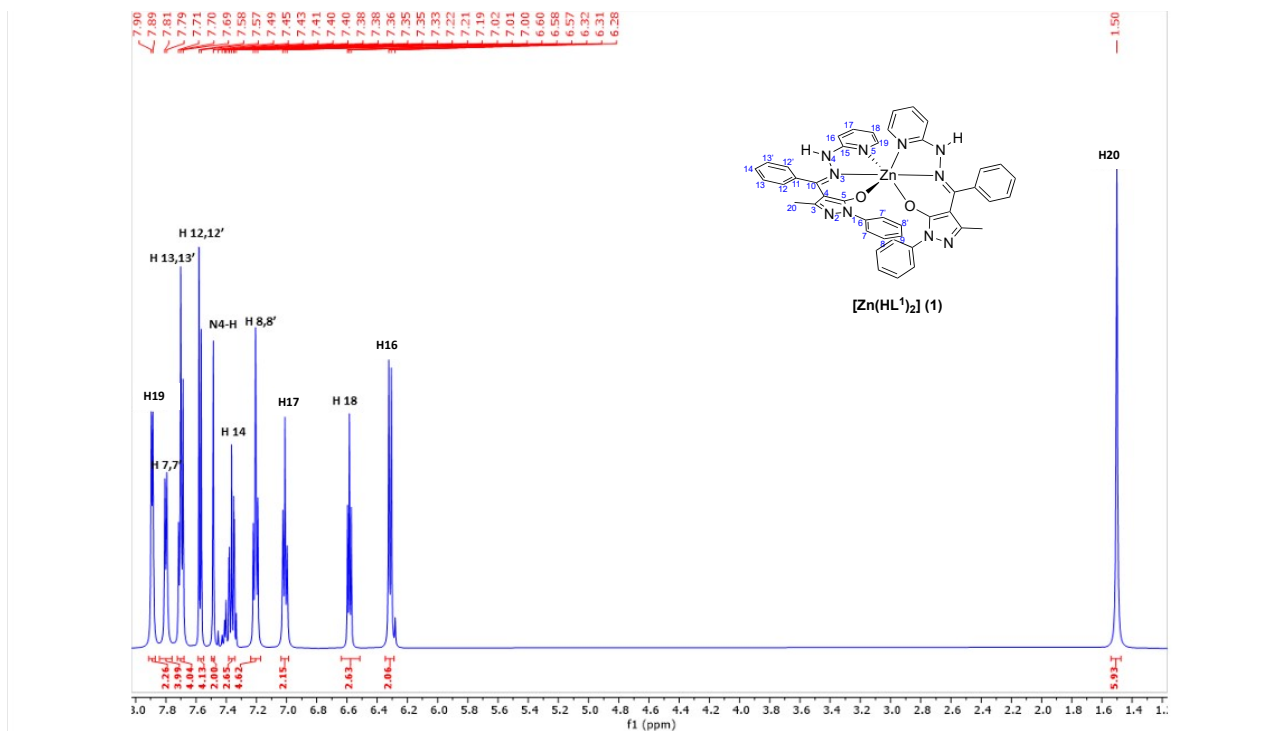
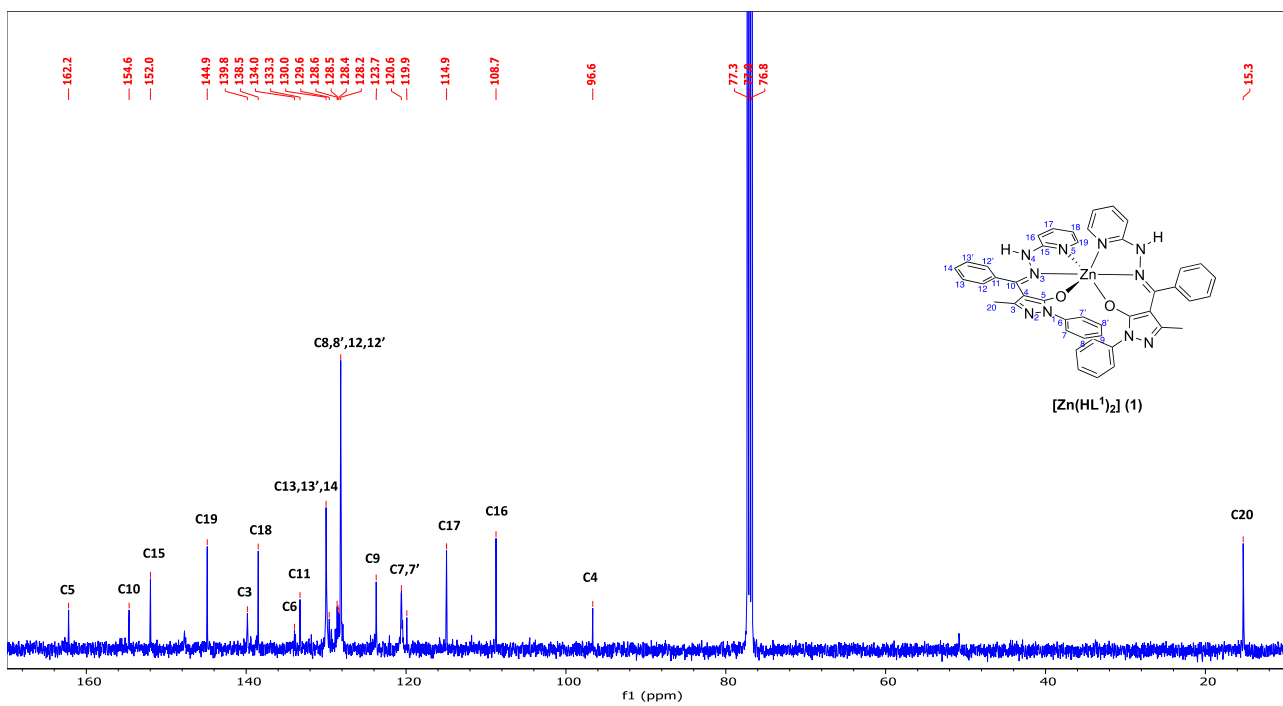


Figure S20.  $^{19}\text{F}\{^1\text{H}\}$  NMR  $\text{H}_2\text{L}^5$  in  $\text{CDCl}_3$  at 298 K.



**Figure S21.**  $^1\text{H}$  NMR  $[\text{Zn}(\text{HL}^1)_2]$  (**1**) in  $\text{CDCl}_3$  at 298 K.



**Figure S22.**  $^{13}\text{C}\{^1\text{H}\}$  NMR  $[\text{Zn}(\text{HL}^1)_2]$  (**1**) in  $\text{CDCl}_3$  at 298 K.

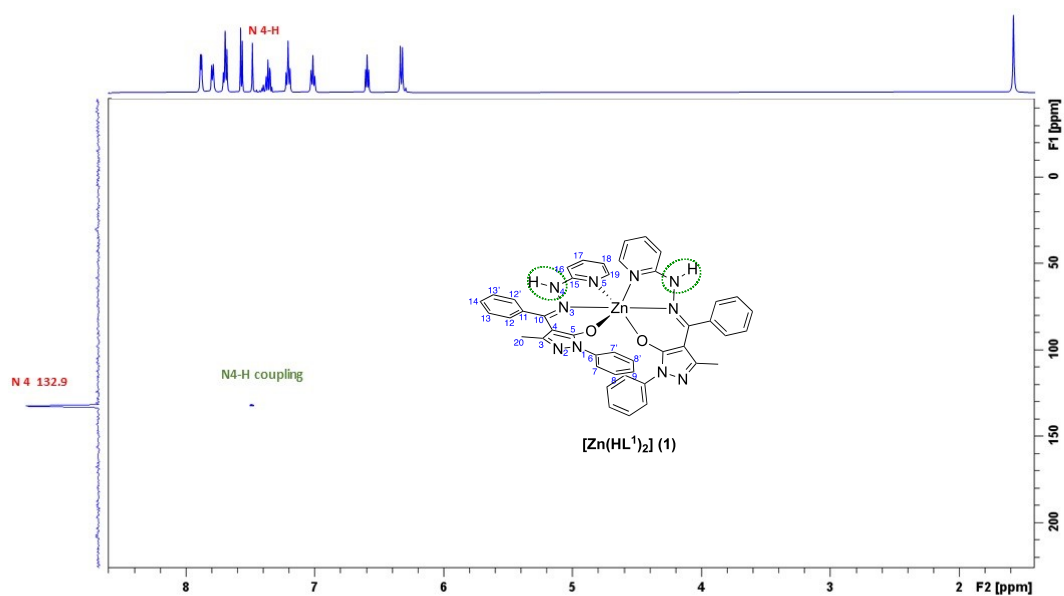


Figure S23.  $\{^1\text{H}, ^{15}\text{N}\}$ -HSQC  $[\text{Zn}(\text{HL}^1)_2]$  (1) in  $\text{CDCl}_3$  at 298 K.

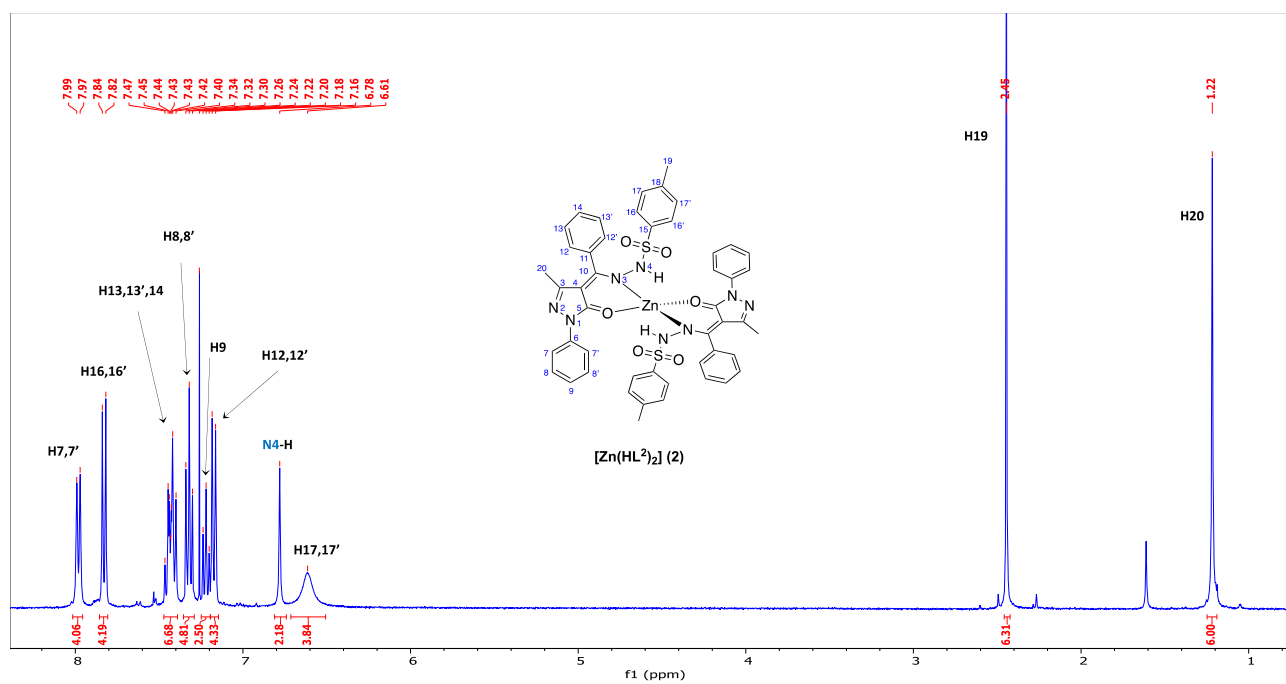


Figure S24.  $^1\text{H}$  NMR  $[\text{Zn}(\text{HL}^2)_2]$  (2) in  $\text{CDCl}_3$  at 298 K.

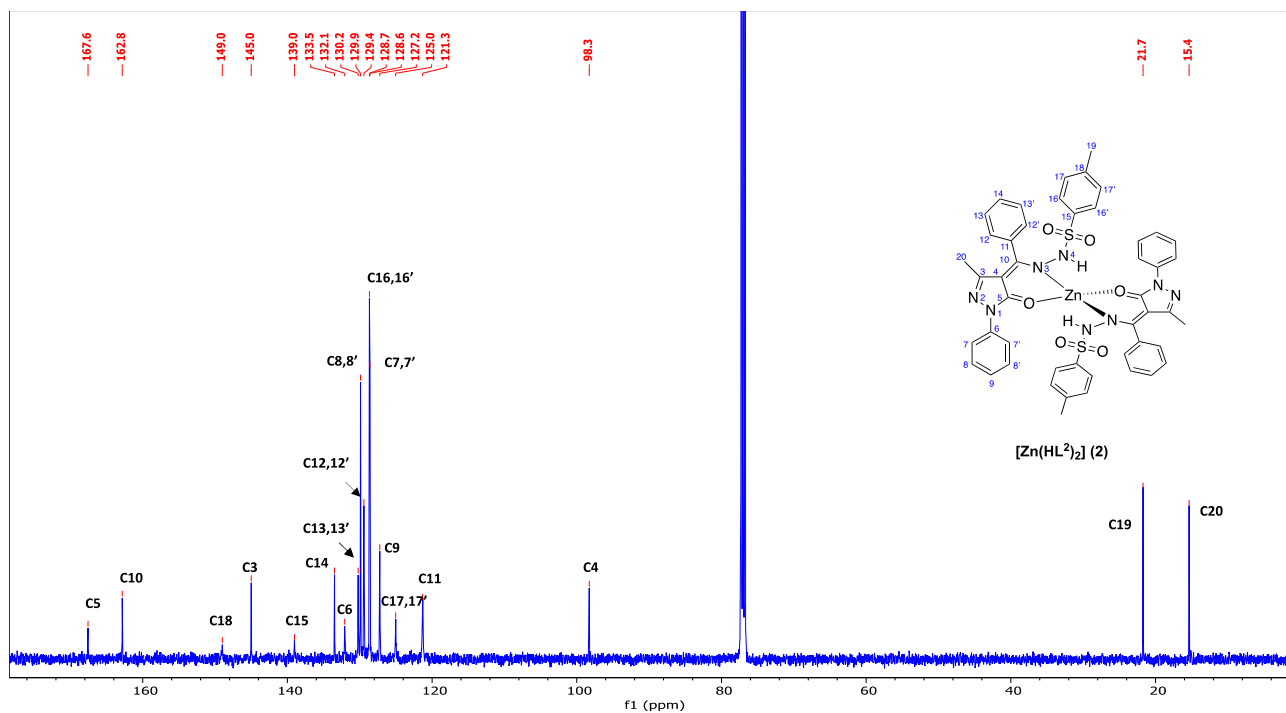


Figure S25.  $^{13}\text{C}\{^1\text{H}\}$  NMR  $[\text{Zn}(\text{HL}^2)_2]$  (**2**) in  $\text{CDCl}_3$  at 298 K.

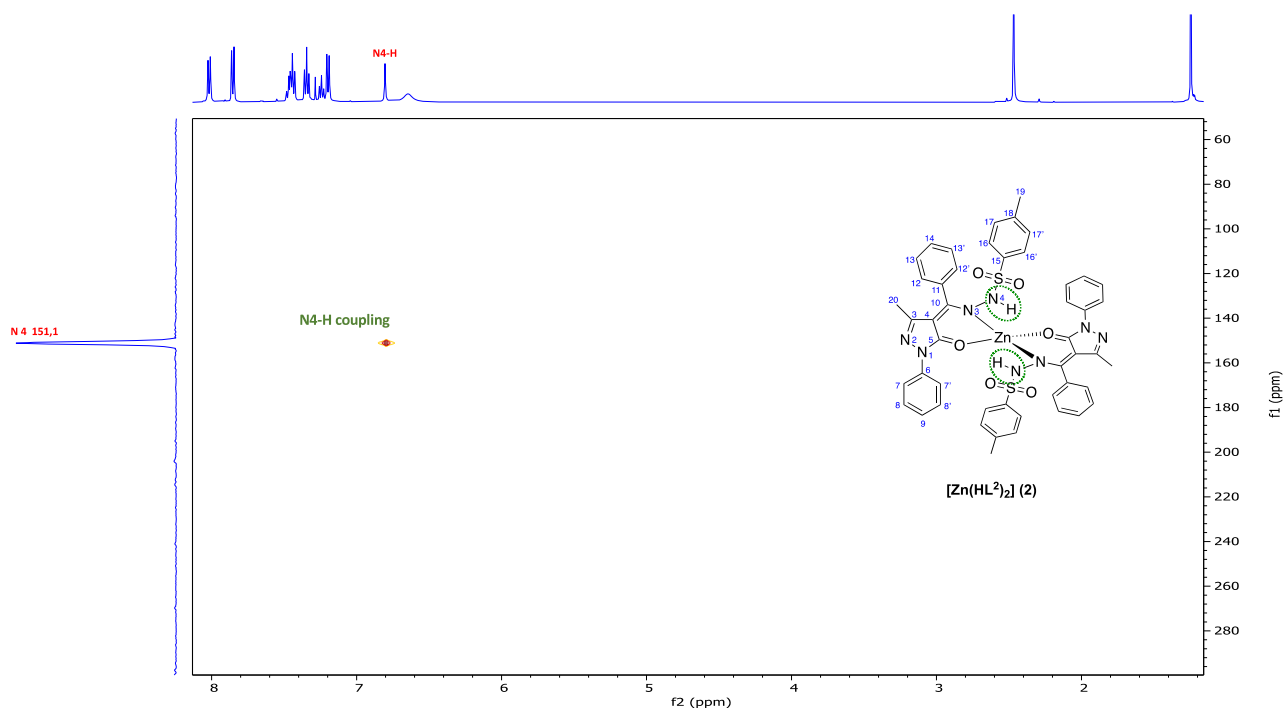


Figure S26.  $\{^1\text{H}, ^{15}\text{N}\}$ -HSQC  $[\text{Zn}(\text{HL}^2)_2]$  (**2**) in  $\text{CDCl}_3$  at 298 K.

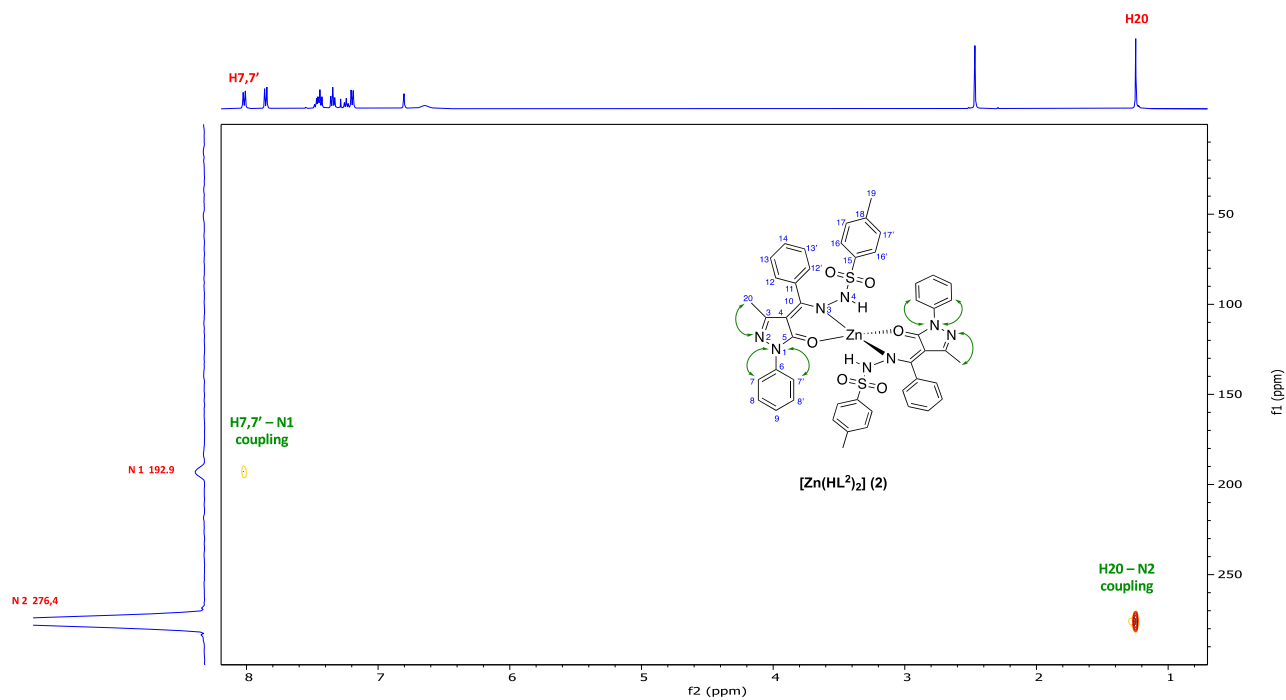


Figure S27.  $\{^1\text{H}, ^{15}\text{N}\}$ -HMBC  $[\text{Zn}(\text{HL}^2)_2]$  (2) in  $\text{CDCl}_3$  at 298 K.

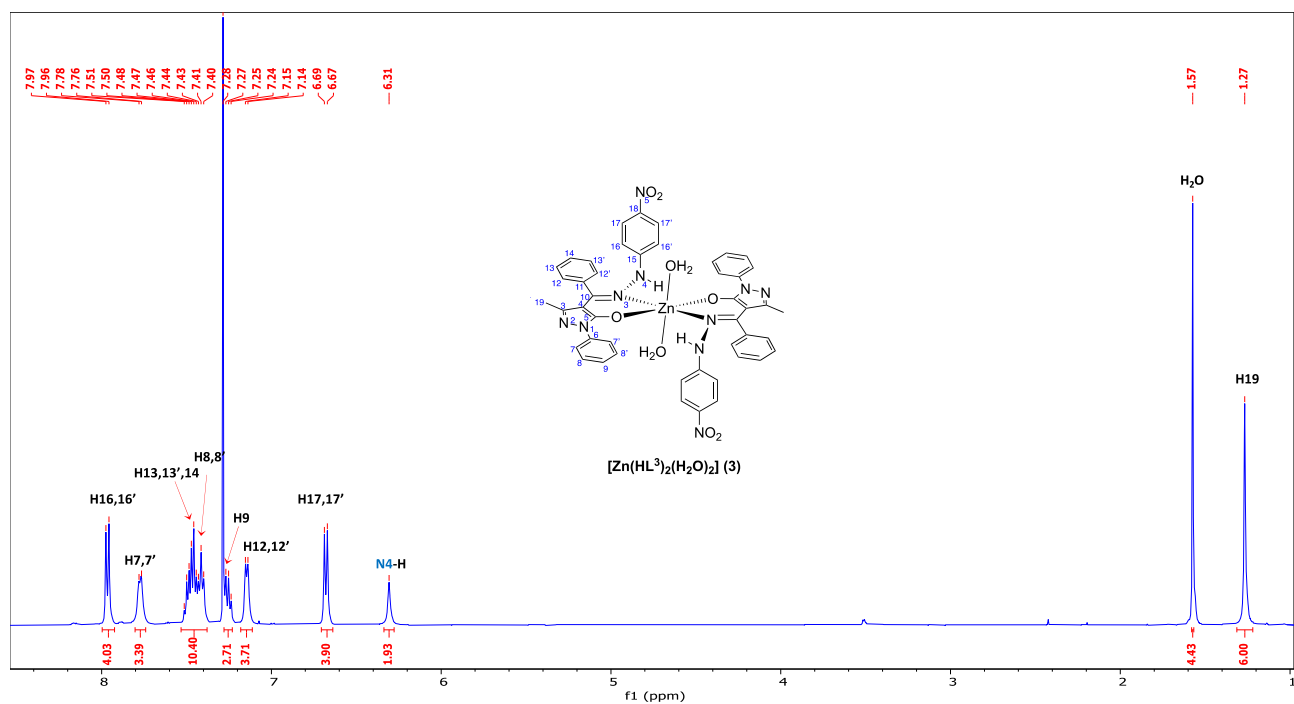


Figure S28.  $^1\text{H}$  NMR  $[\text{Zn}(\text{HL}^3)_2(\text{H}_2\text{O})_2]$  (3) in  $\text{CDCl}_3$  at 298 K.



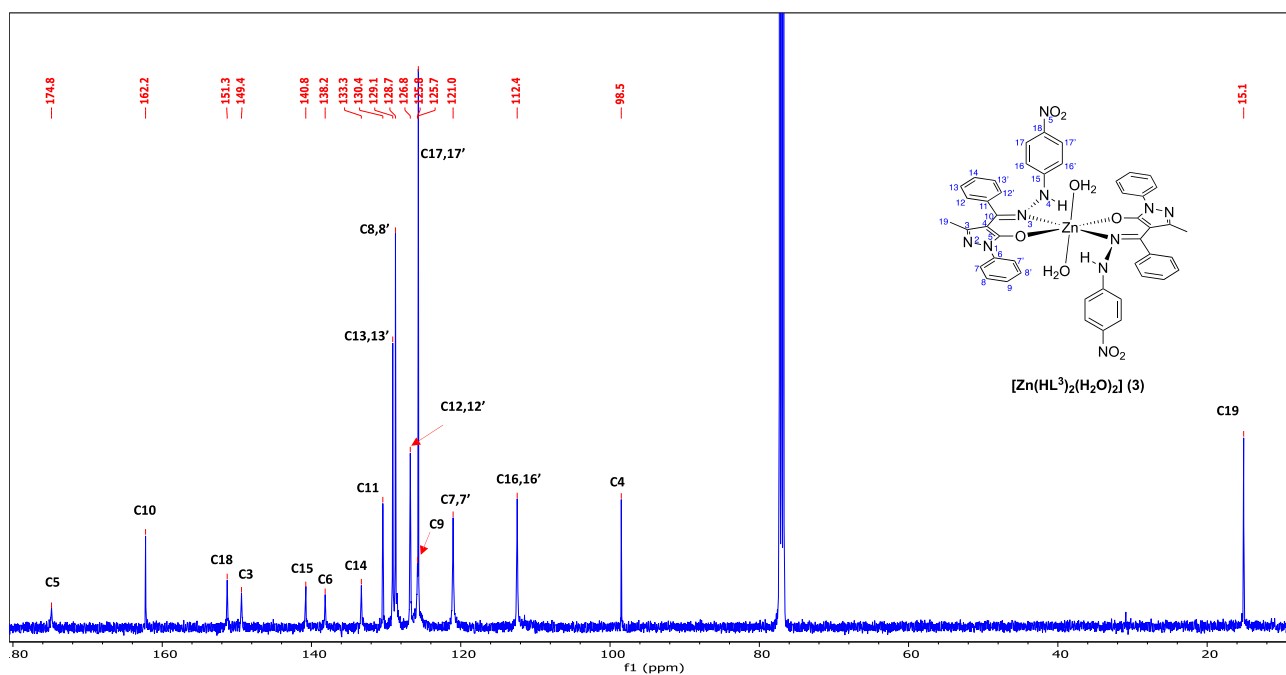


Figure S29.  $^{13}\text{C}\{^1\text{H}\}$  NMR  $[\text{Zn}(\text{HL}^3)_2(\text{H}_2\text{O})_2]$  (**3**) in  $\text{CDCl}_3$  at 298 K.

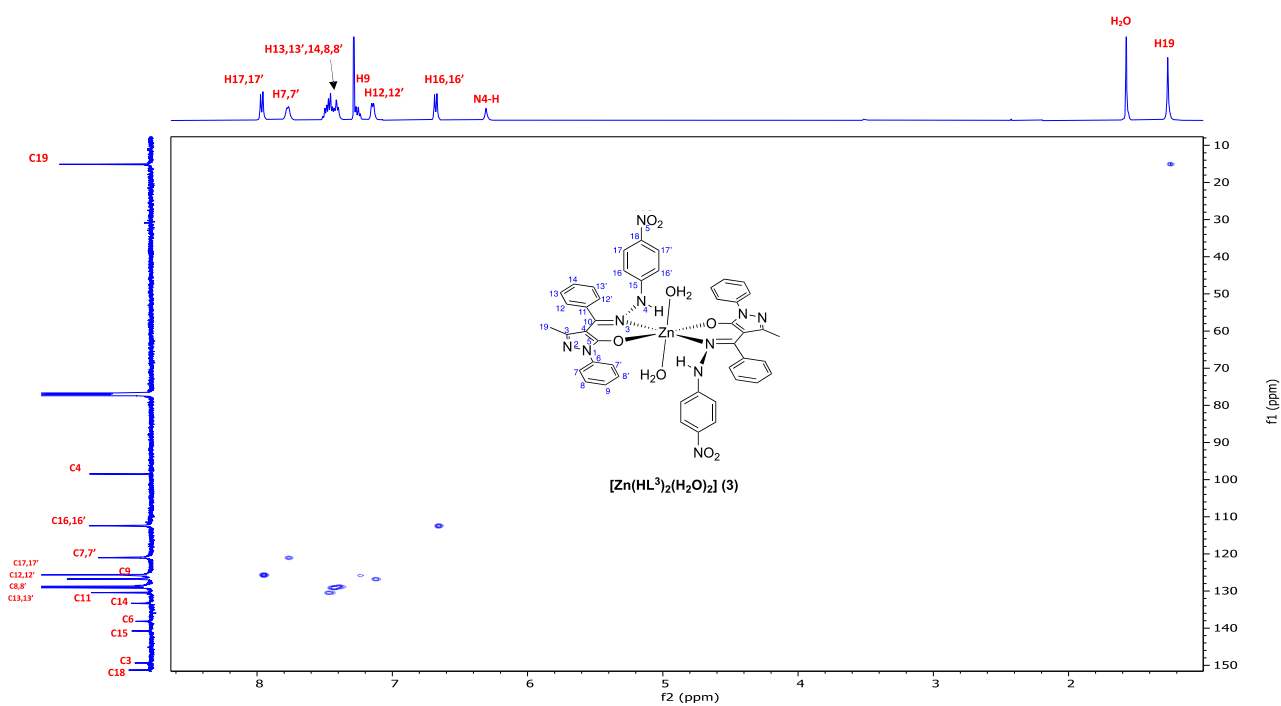


Figure S30.  $\{^1\text{H}, ^{13}\text{C}\}$ -HSQC  $[\text{Zn}(\text{HL}^3)_2(\text{H}_2\text{O})_2]$  (**3**) in  $\text{CDCl}_3$  at 298 K.

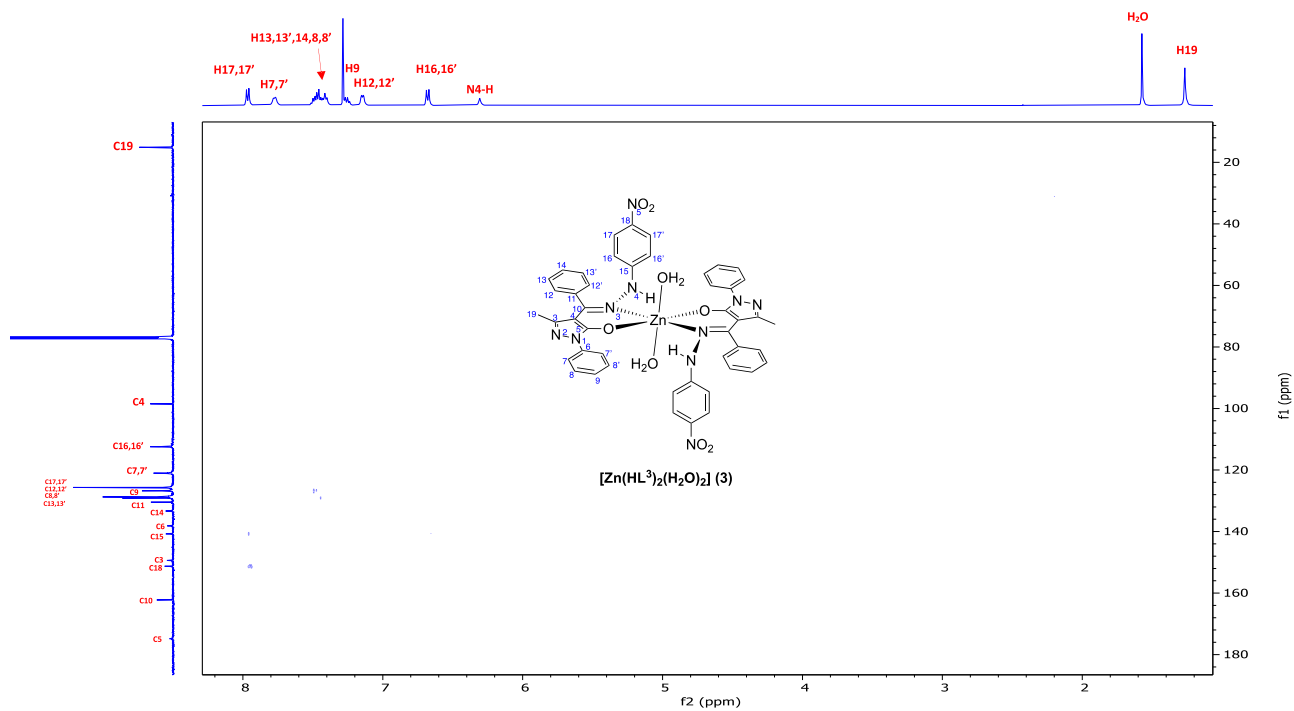


Figure S31.  $\{^1\text{H}, ^{13}\text{C}\}$ -HMBC  $[\text{Zn}(\text{HL}^3)_2(\text{H}_2\text{O})_2]$  (**3**) in  $\text{CDCl}_3$  at 298 K.

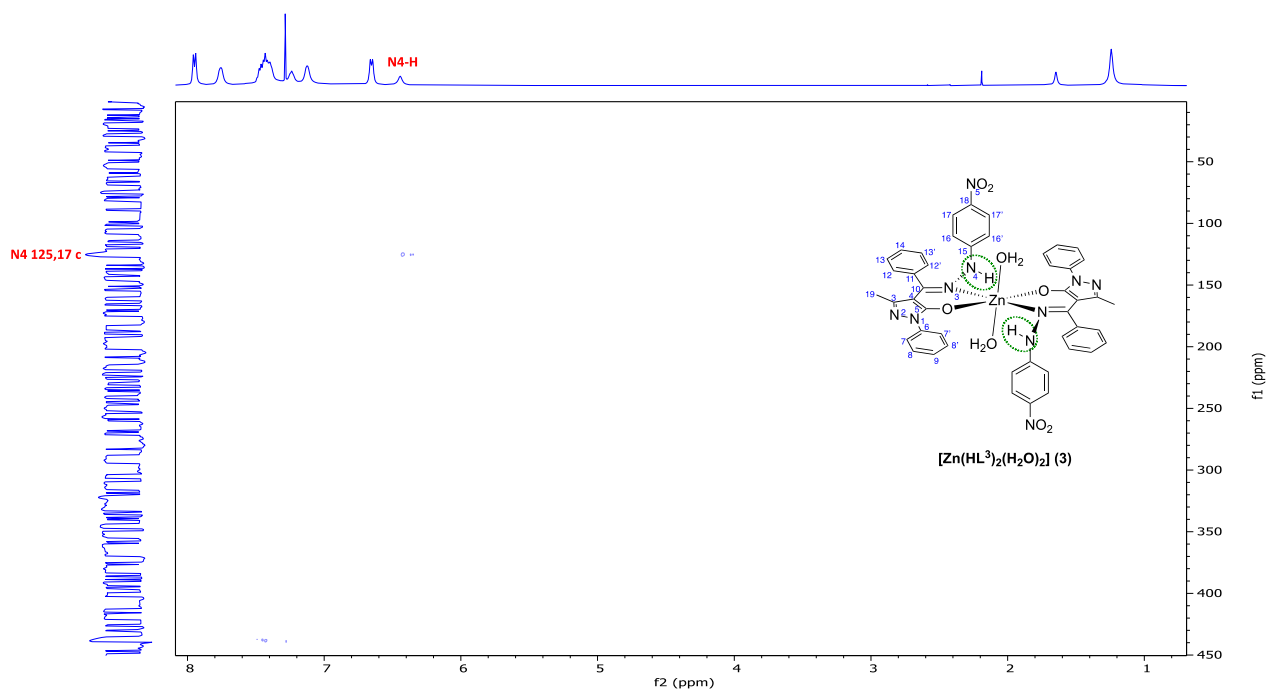


Figure S32.  $\{^1\text{H}, ^{15}\text{N}\}$ -HSQC  $[\text{Zn}(\text{HL}^3)_2(\text{H}_2\text{O})_2]$  (**3**) in  $\text{CDCl}_3$  at 298 K.

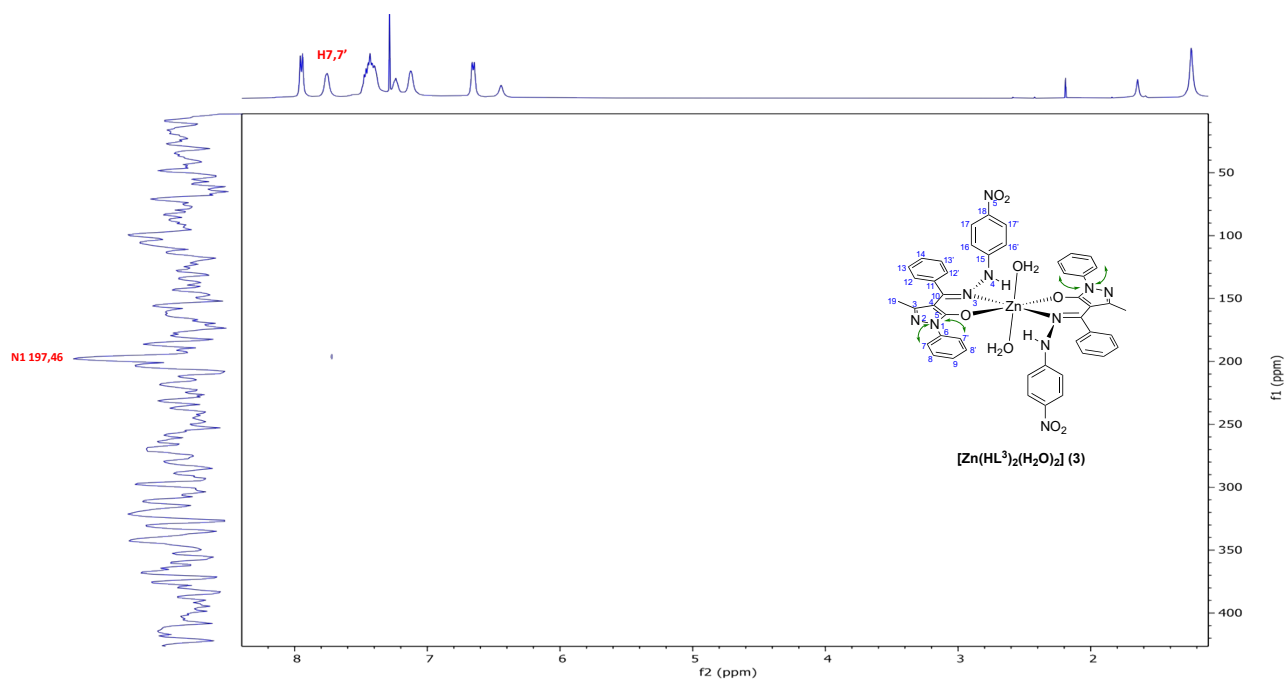


Figure S33.  $\{^1\text{H}, ^{15}\text{N}\}$ -HMBC  $[\text{Zn}(\text{HL}^3)_2(\text{H}_2\text{O})_2]$  (**3**) in  $\text{CDCl}_3$  at 298 K.

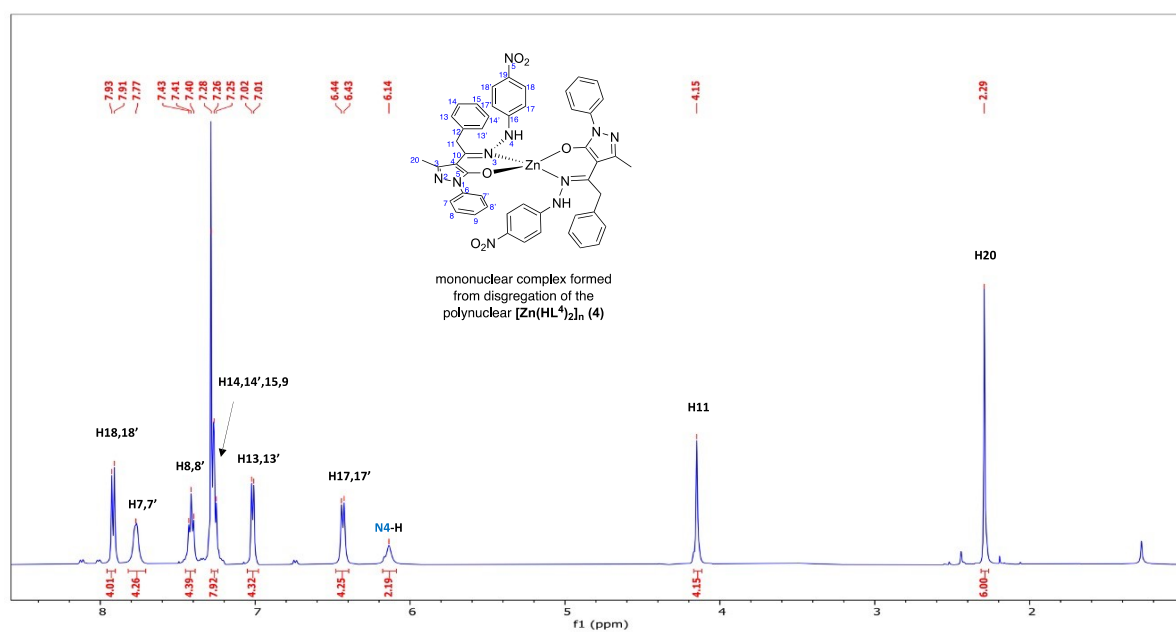


Figure S34.  $^1\text{H}$  NMR  $[\text{Zn}(\text{HL}^4)_2]$  (**4**) in  $\text{CDCl}_3$  at 298 K.

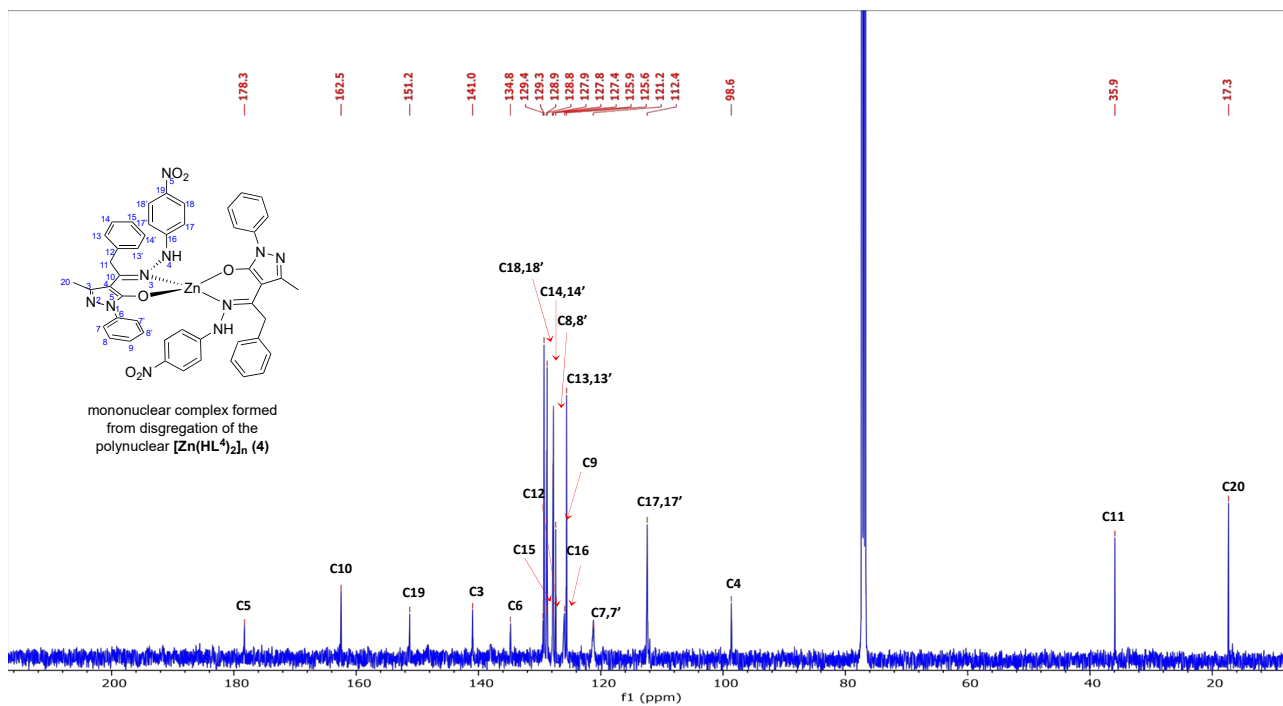


Figure S35.  $^{13}\text{C}\{^1\text{H}\}$  NMR  $[\text{Zn}(\text{HL}^4)_2]$  (**4**) in  $\text{CDCl}_3$  at 298 K.

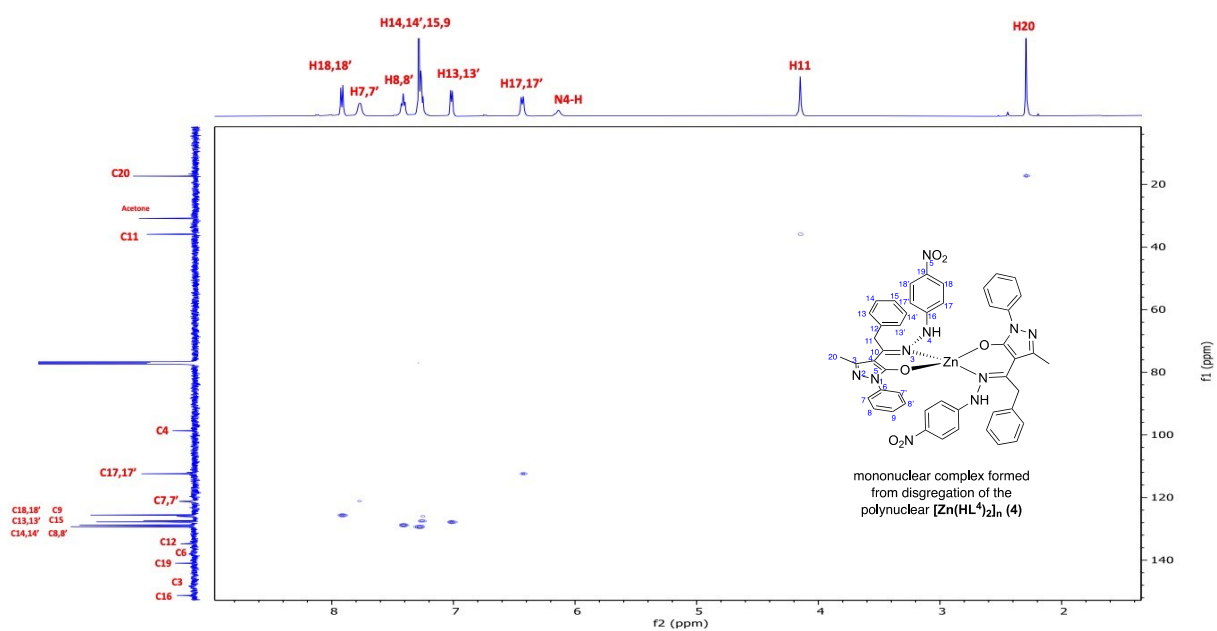


Figure S36.  $\{^1\text{H}, ^{13}\text{C}\}$ -HSQC  $[\text{Zn}(\text{HL}^4)_2]$  (**4**) in  $\text{CDCl}_3$  at 298 K.

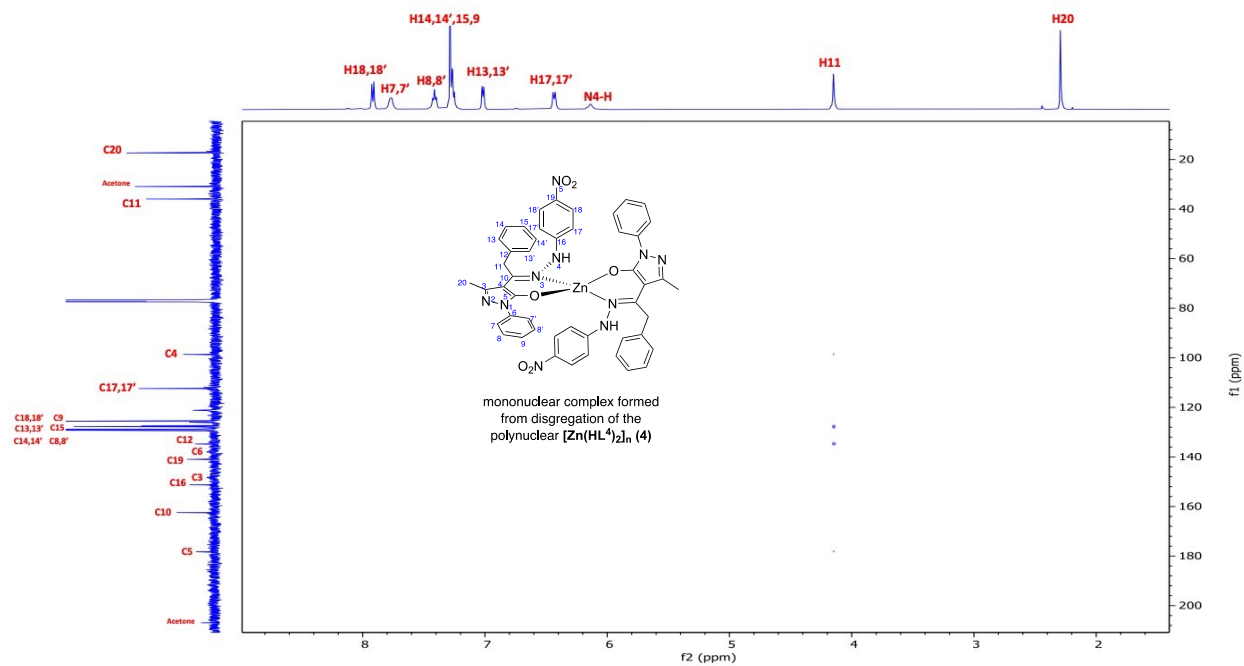


Figure S37.  $\{^1\text{H}, ^{13}\text{C}\}$ -HMBC  $[\text{Zn}(\text{HL}^4)_2]$  (**4**) in  $\text{CDCl}_3$  at 298 K.

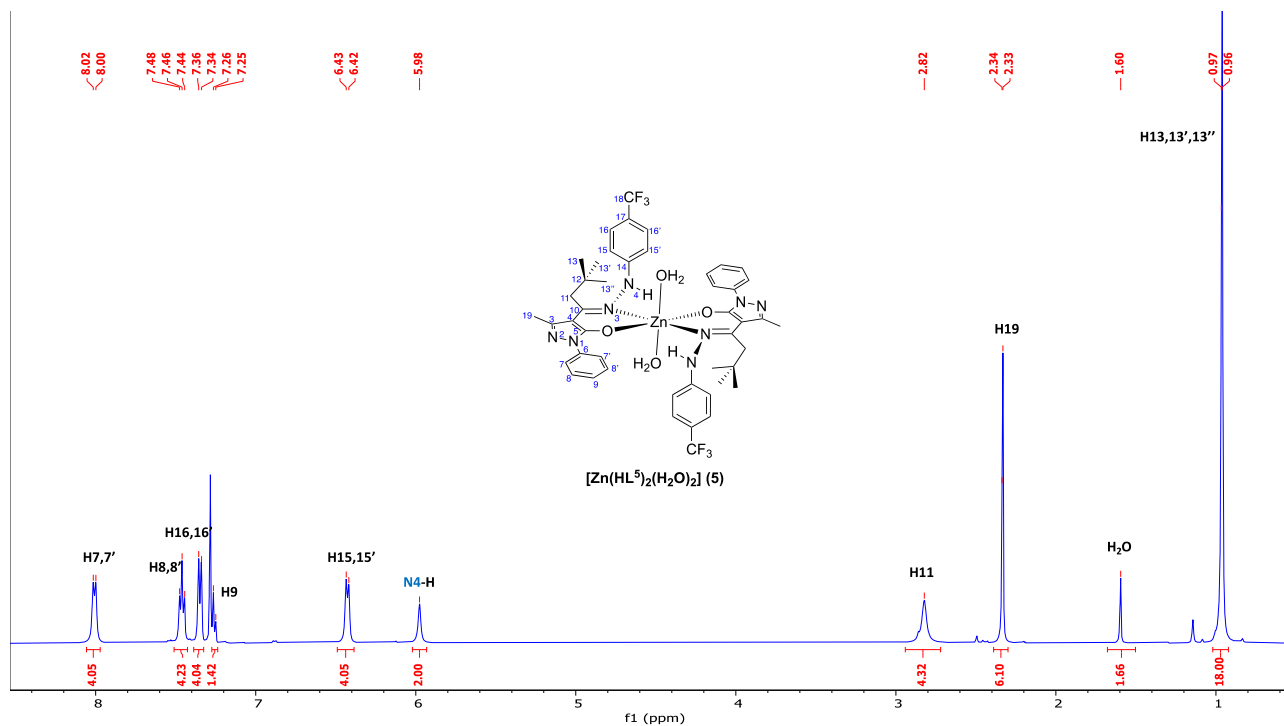


Figure S38.  $^1\text{H}$  NMR  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (**5**) in  $\text{CDCl}_3$  at 298 K.

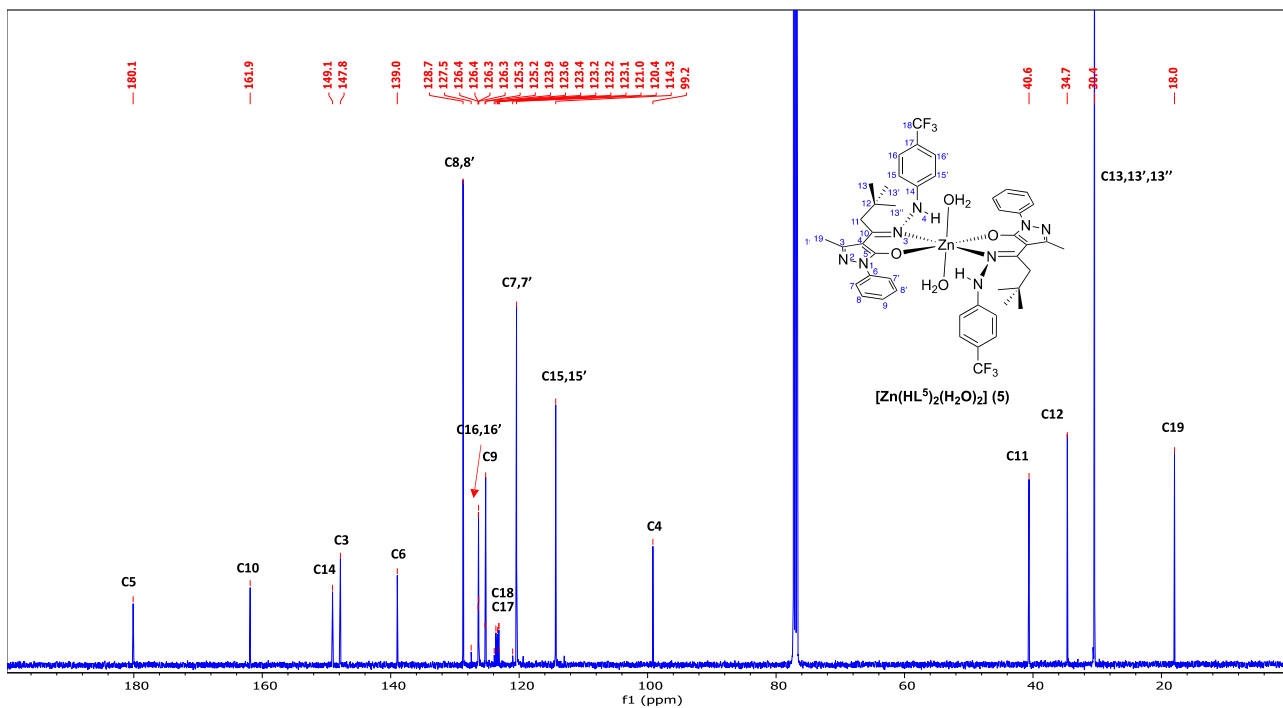


Figure S39.  $^{13}\text{C}\{^1\text{H}\}$  NMR  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (5) in  $\text{CDCl}_3$  at 298 K.

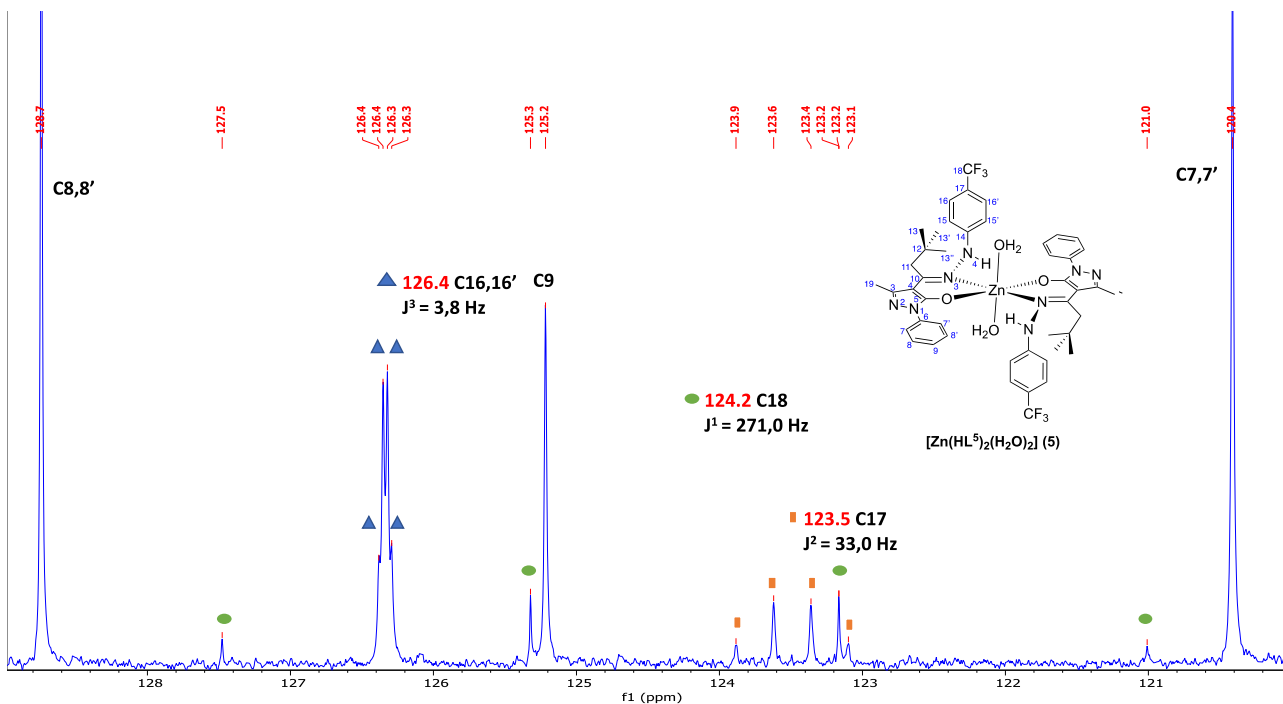


Figure S40. Magnification  $^{13}\text{C}\{^1\text{H}\}$  NMR  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (5) in  $\text{CDCl}_3$  at 298 K.

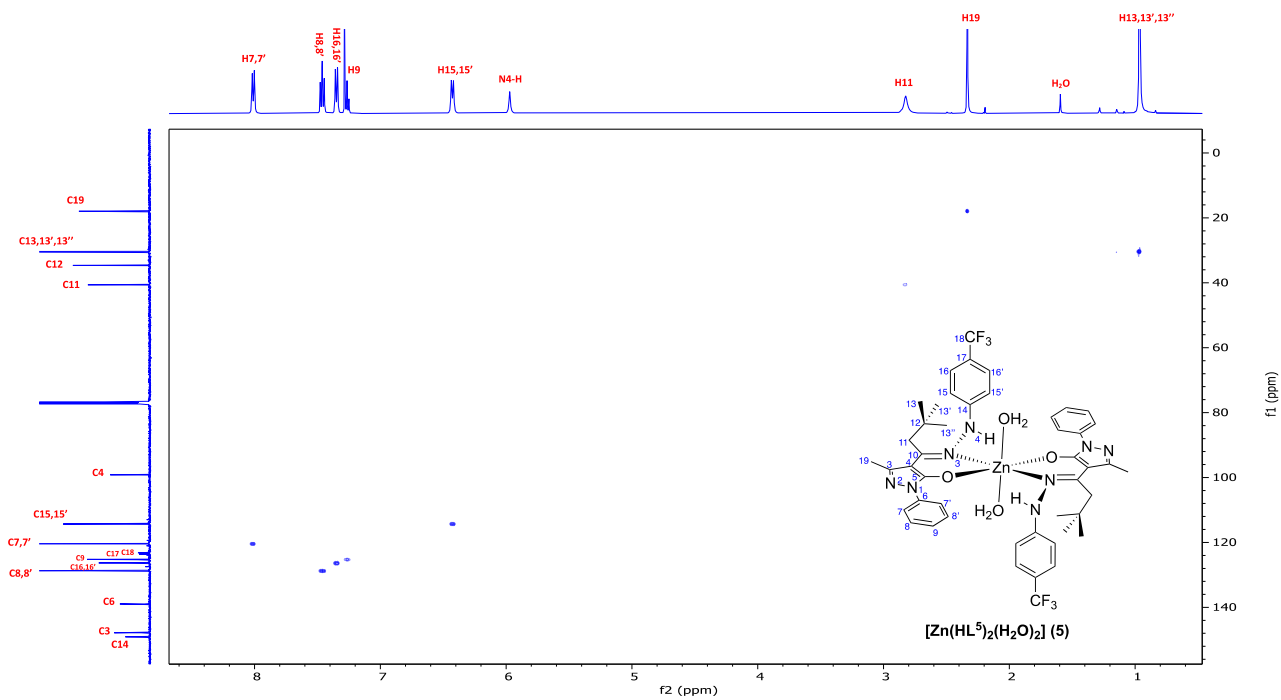


Figure S41.  $\{^1\text{H}, ^{13}\text{C}\}$ -HSQC  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (**5**) in  $\text{CDCl}_3$  at 298 K.

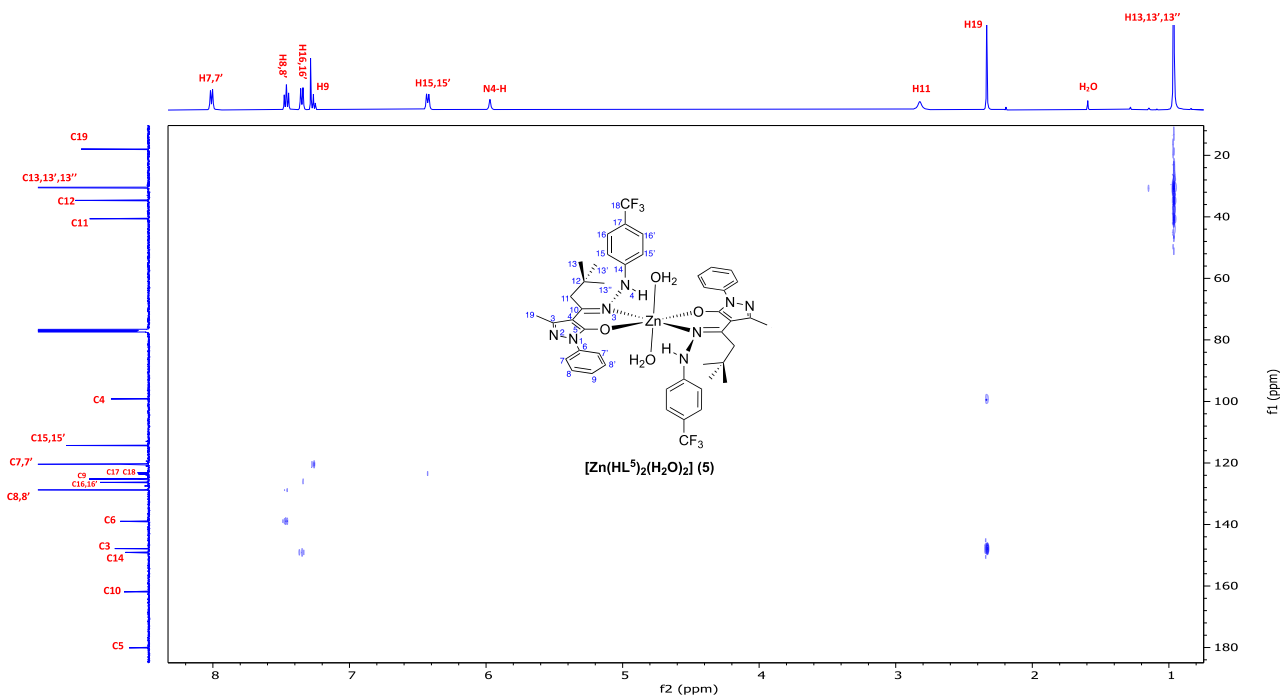
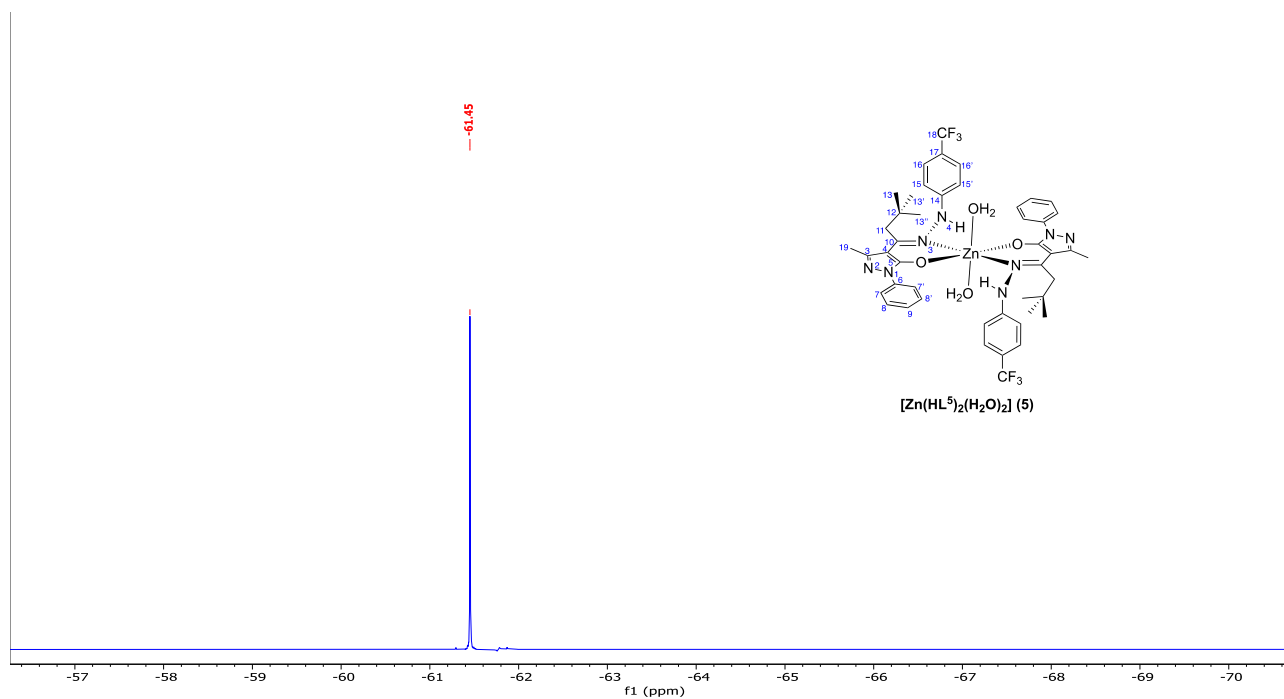
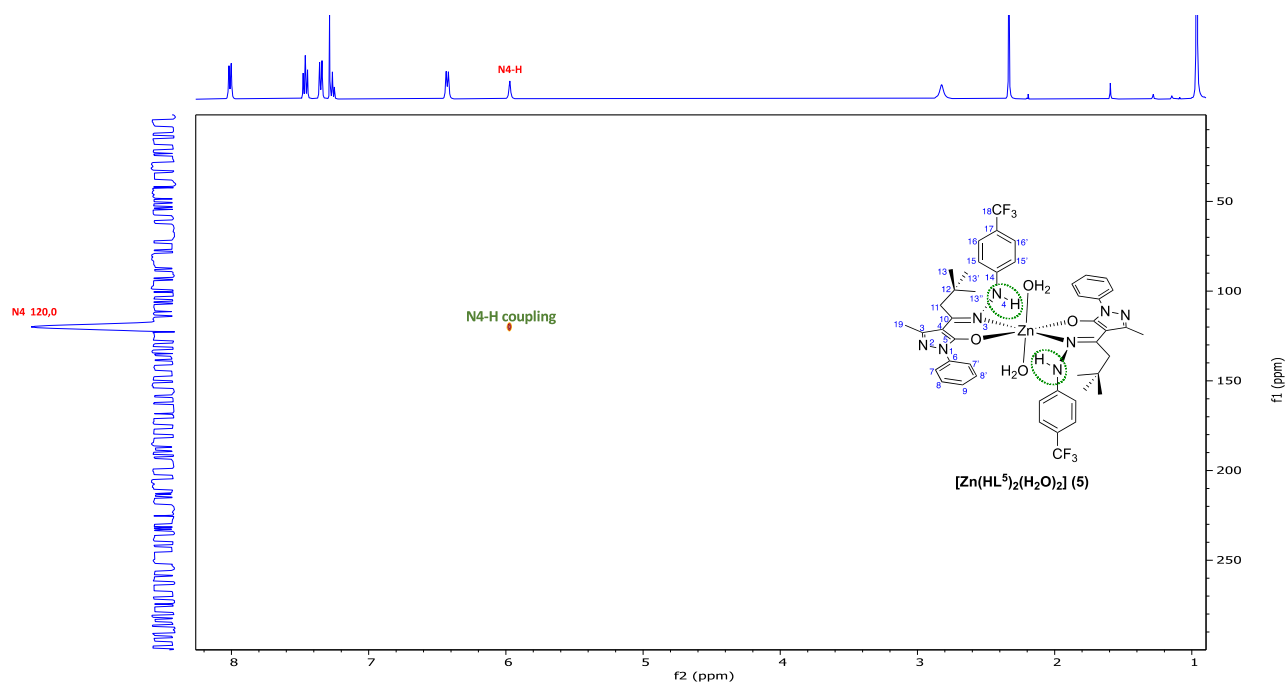


Figure S42.  $\{^1\text{H}, ^{13}\text{C}\}$ -HMBC  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (**5**) in  $\text{CDCl}_3$  at 298 K.

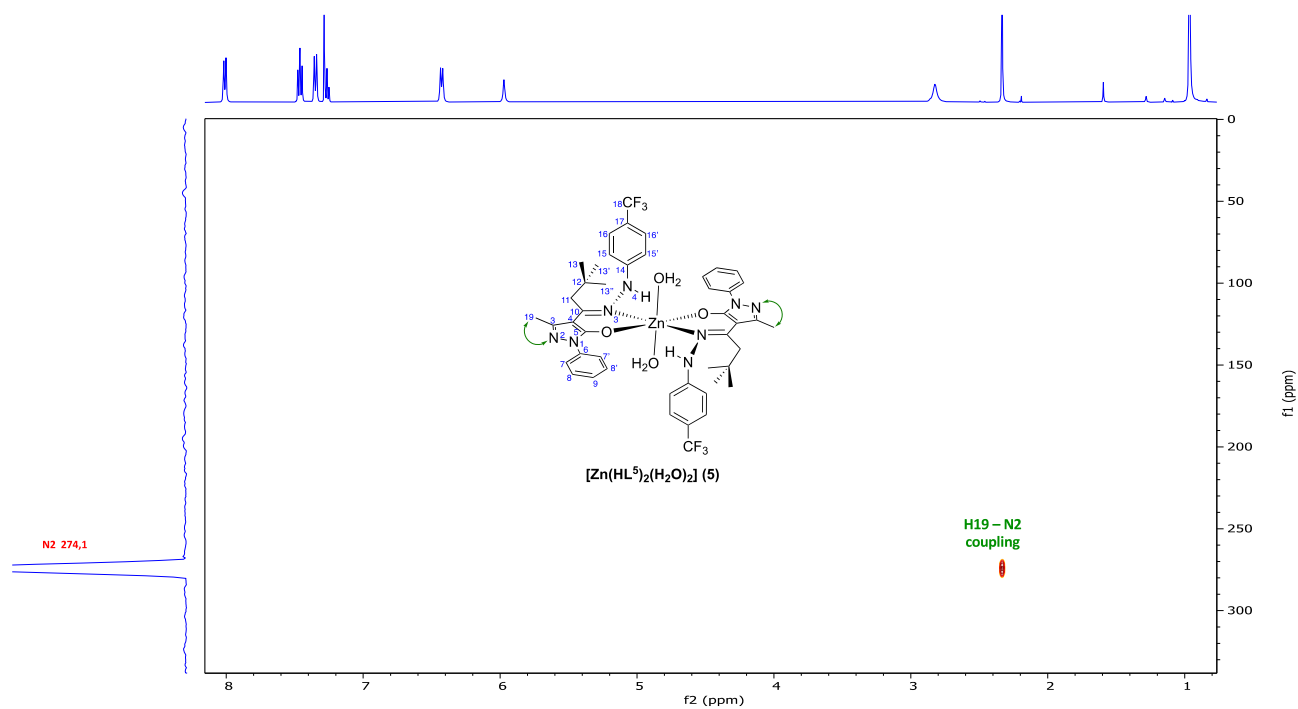


**Figure S43.**  $^{19}\text{F}\{^1\text{H}\}$  NMR  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (5) in  $\text{CDCl}_3$  at 298 K.

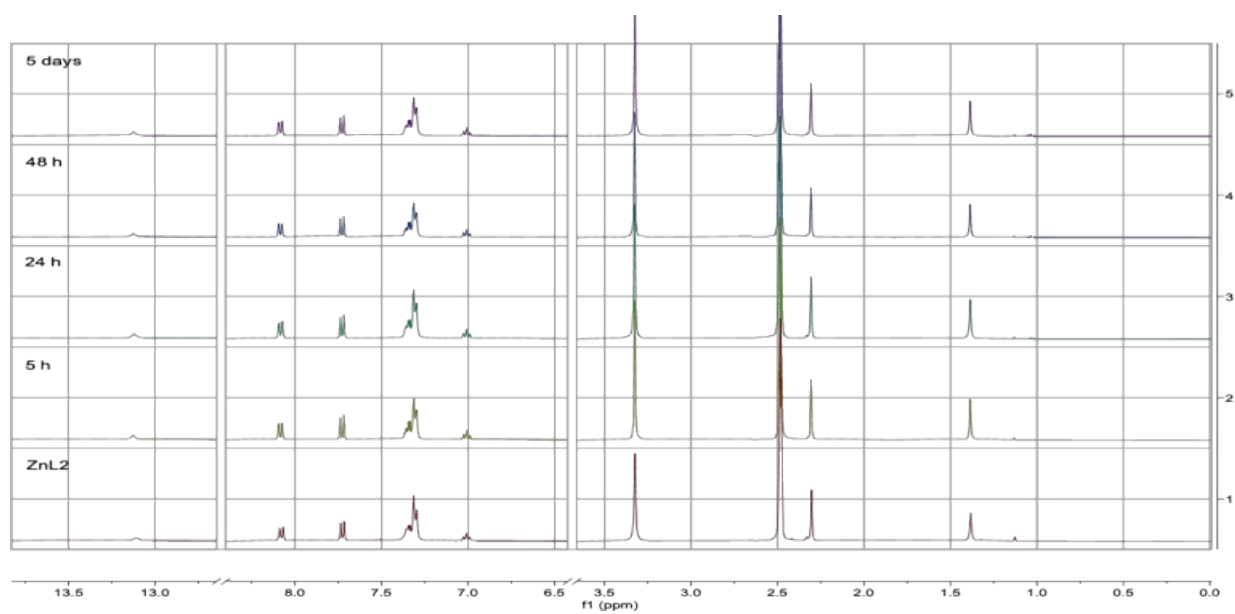


**Figure S44.**  $\{^1\text{H}, ^{15}\text{N}\}$ -HSQC  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (5) in  $\text{CDCl}_3$  at 298 K.

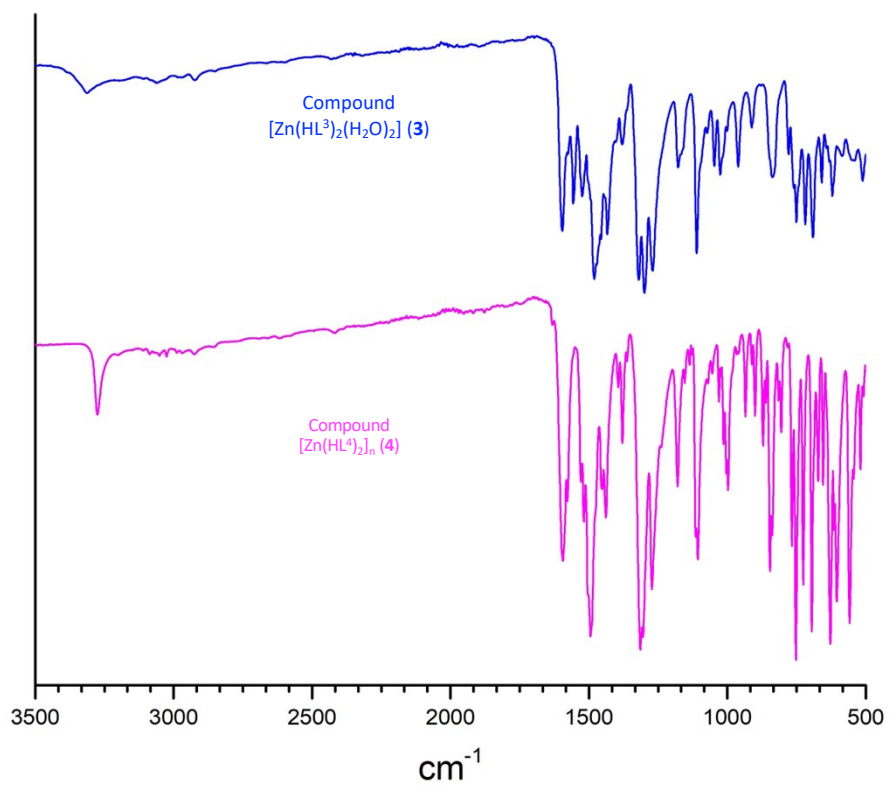




**Figure S45.**  $\{^1\text{H}, ^{15}\text{N}\}$ -HMBC  $[\text{Zn}(\text{HL}^5)_2(\text{H}_2\text{O})_2]$  (**5**) in  $\text{CDCl}_3$  at 298 K.



**Figure S46.** Stability study of  $[\text{Zn}(\text{HL}^2)_2]$  (**2**) in  $\text{DMSO-d}_6$ .



**Figure S47.** Comparison of IR spectra of  $[\text{Zn}(\text{HL}^3)_2(\text{H}_2\text{O})_2]$  (**3**) and  $[\text{Zn}(\text{HL}^3)_2]_n$  (**4**).

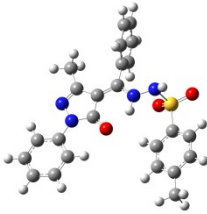
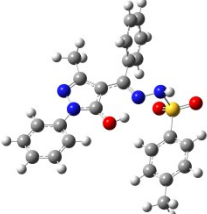
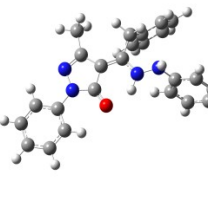
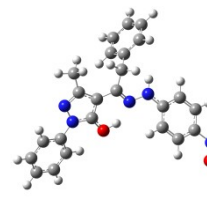
**Table S1.** Crystallographic data and structure refinement details of proligands H<sub>2</sub>L<sup>2</sup> and H<sub>2</sub>L<sup>4</sup>.

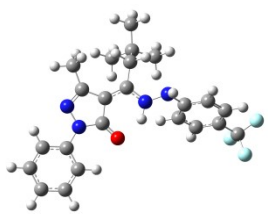
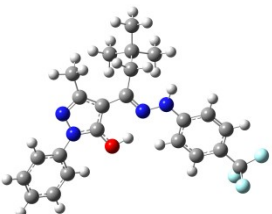
Compound	H <sub>2</sub> L <sup>2</sup>	H <sub>2</sub> L <sup>4</sup>
Formula	C <sub>24</sub> H <sub>24.4</sub> N <sub>4</sub> O <sub>4.2</sub> S	C <sub>24</sub> H <sub>21</sub> N <sub>5</sub> O <sub>3</sub>
CCDC	2158177	2158178
M <sub>r</sub> (g mol <sup>-1</sup> )	468.13	427.46
Crystal system	Monoclinic	Triclinic
Space group	C2/c	P-1
a (Å)	24.3936(19)	8.8530(8)
b (Å)	10.9327(7)	9.6590(8)
c (Å)	17.3895(12)	12.8829(12)
α (°)	90	85.651(3)
β (°)	92.135(4)	74.757(3)
γ (°)	90	78.819(3)
V (Å <sup>3</sup> )	4634.3(6)	1042.34(16)
Z	8	2
T (K)	120(2)	293(2)
ρ <sub>calc</sub> (g cm <sup>-3</sup> )	1.342	1.362
F (000)	1968	448
μ (Mo Kα) (mm <sup>-1</sup> )	0.179	0.093
GoF on F <sup>2</sup>	1.007	1.068
Final R indexes [I > 2σ(I)]	R <sub>1</sub> = 0.0500; wR <sub>2</sub> = 0.1102	R <sub>1</sub> = 0.0451; wR <sub>2</sub> = 0.1020
Final R indexes [all data]	R <sub>1</sub> = 0.0820; wR <sub>2</sub> = 0.1249	R <sub>1</sub> = 0.0674; wR <sub>2</sub> = 0.1116

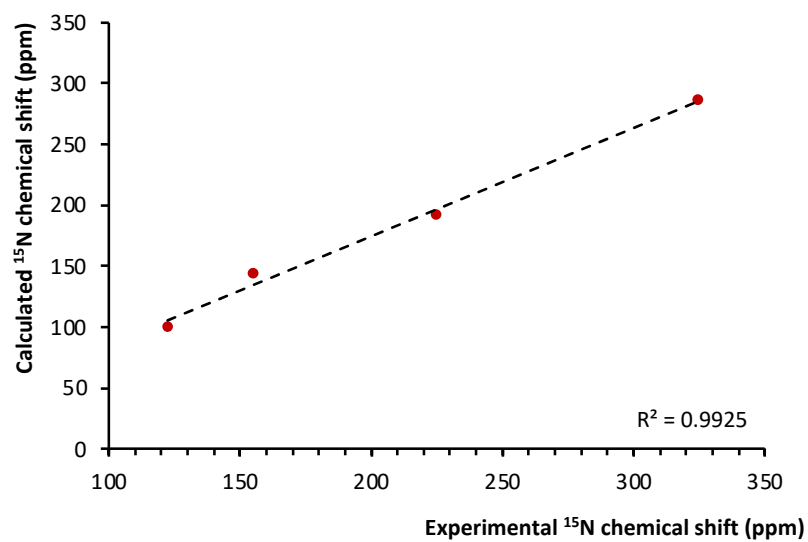
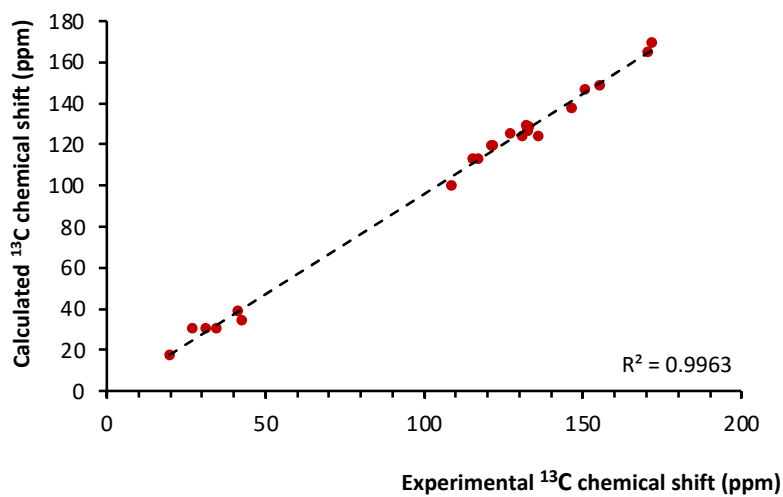
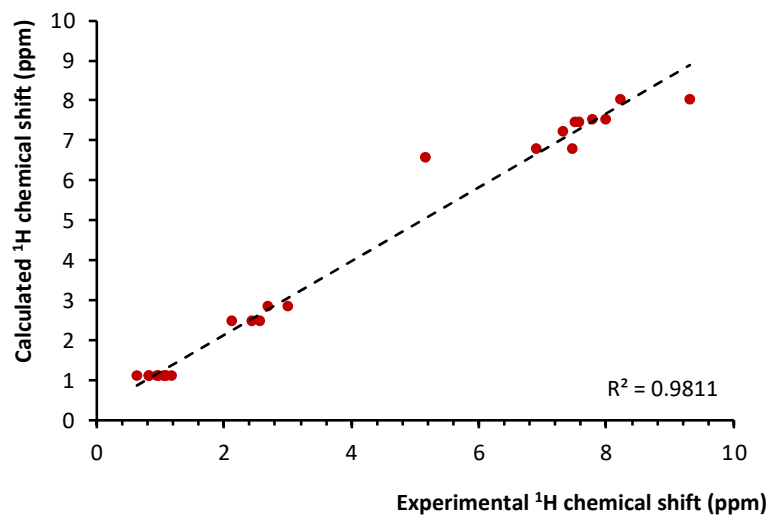
**Table S2.** Crystallographic data and structure refinement details of complexes **1**, **2**, and **4**.

Compound	Complex 1	Complex 2	Complex 4
Formula	C <sub>44</sub> H <sub>38</sub> N <sub>10</sub> O <sub>2</sub> Zn	C <sub>50</sub> H <sub>52</sub> N <sub>8</sub> O <sub>6</sub> S <sub>2</sub> Zn	C <sub>48</sub> H <sub>40</sub> N <sub>10</sub> O <sub>6</sub> Zn
CCDC	2158179	2158180	2158176
M <sub>r</sub> (g mol <sup>-1</sup> )	804.21	1022.48	918.27
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	P-1	C2/c	P-1
a (Å)	9.8944(6)	17.44(3)	9.8009(8)
b (Å)	11.3405(6)	13.34(2)	9.9718(9)
c (Å)	18.1843(10)	22.28(4)	12.2060(12)
α (°)	89.300(2)	90	88.090(3)
β (°)	86.246(2)	105.95(3)	70.399(3)
γ (°)	67.2918(18)	90	73.834(3)
V (Å <sup>3</sup> )	1878.02(18)	4987(16)	1076.97(17)
Z	2	4	1
T (K)	100(2)	273.15	298(2)
ρ <sub>calc</sub> (g cm <sup>-3</sup> )	1.422	1.362	1.416
F (000)	836	2136	476
μ (Mo Kα) (mm <sup>-1</sup> )	0.708	0.637	0.634
GoF on F <sup>2</sup>	1.060	1.048	1.017
Final R indexes [I ≥ 2σ]	R <sub>1</sub> = 0.0561; wR <sub>2</sub> = 0.1450	R <sub>1</sub> = 0.0561; wR <sub>2</sub> = 0.1367	R <sub>1</sub> = 0.0739; wR <sub>2</sub> = 0.1476
Final R indexes [all data]	R <sub>1</sub> = 0.0731; wR <sub>2</sub> = 0.1538	R <sub>1</sub> = 0.0773; wR <sub>2</sub> = 0.1585	R <sub>1</sub> = 0.1479; wR <sub>2</sub> = 0.1765

**Table S3.** Energies (Hartree) and relative energy differences (kcal/mol) for the tautomers I and II of proligands  $H_2L^2$ ,  $H_2L^4$  and  $H_2L^5$ .

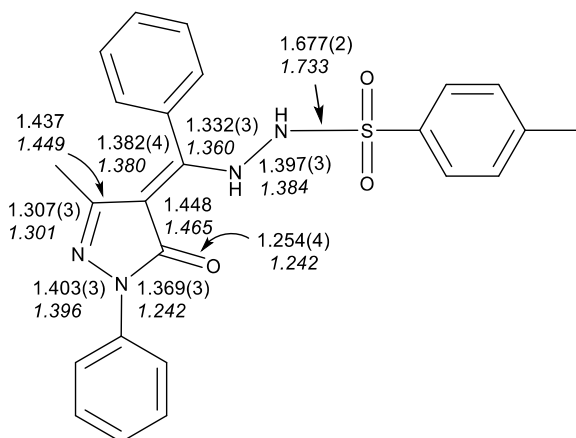
	$H_2L^2$		$H_2L^4$	
	Tautomer I	Tautomer II	Tautomer I	Tautomer II
				
E	-1770.946848	-1770.937687	-1426.865589	-1426.864598
$E_o$	-1770.526114	-1770.517408	-1426.450842	-1426.450241
$E_t$	-1770.497523	-1770.48903	-1426.423841	-1426.423223
H	-1770.496579	-1770.488085	-1426.422897	-1426.422279
G	-1770.590327	-1770.58033	-1426.513320	-1426.512049
$\Delta E$	0.0	5.7	0.0	0.6
$\Delta G$	0.0	6.3	0.0	0.8
$\Delta E_{(CHCl_3)}$	0.0	6.6	0.0	2.8
$\Delta G_{(CHCl_3)}$	0.0	7.1	0.0	2.9

	$H_2L^5$	
	Tautomer I	Tautomer II
		
E	-1485.635608	-1485.630883
$E_o$	-1485.187451	-1485.183379
$E_t$	-1485.158598	-1485.154414
H	-1485.157654	-1485.153470
G	-1485.250309	-1485.245797
$\Delta E$	0	3.0
$\Delta G$	0	2.8
$\Delta E_{(CHCl_3)}$	0	4.3
$\Delta G_{(CHCl_3)}$	0	4.2

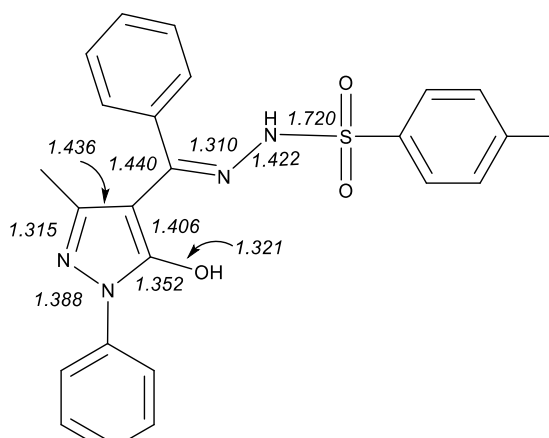


**Figure S48.** Comparison of the calculated (tautomer I) and experimental  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  NMR spectra of  $\text{H}_2\text{L}^5$ .

**H<sub>2</sub>L<sup>2</sup>**

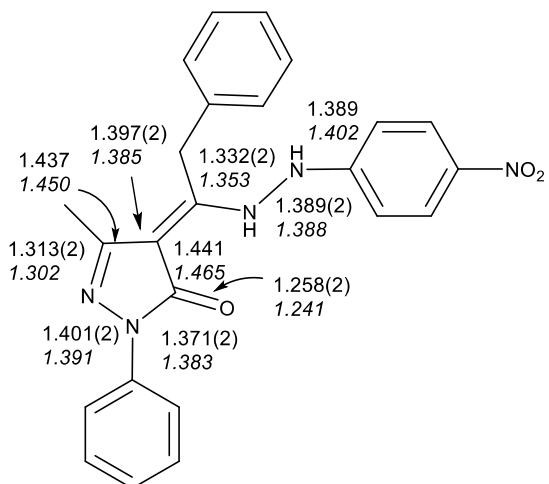


**I**

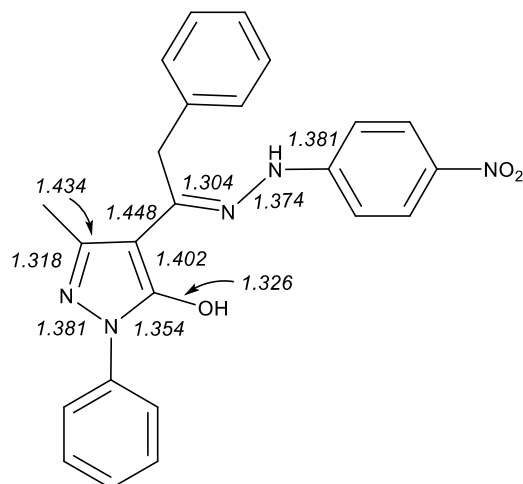


**II**

**H<sub>2</sub>L<sup>4</sup>**

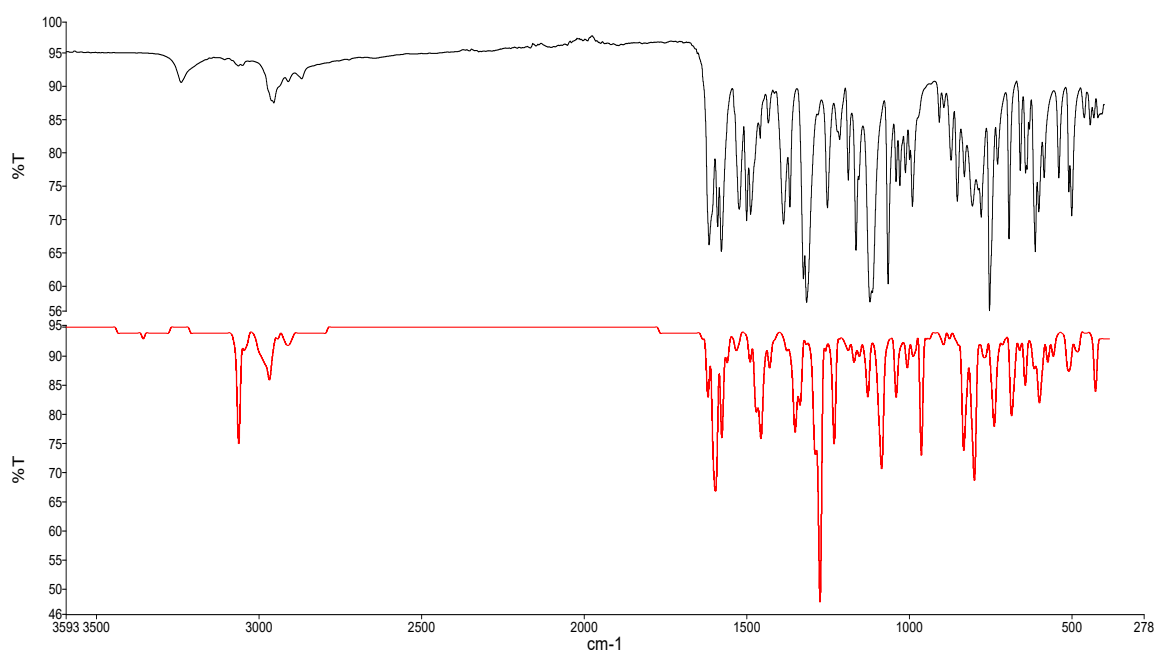


**I**



**II**

**Figure S49.** Comparison of selected bond distances of H<sub>2</sub>L<sup>2</sup> and H<sub>2</sub>L<sup>4</sup>: calculated tautomers I and II (*italic*) and experimental.

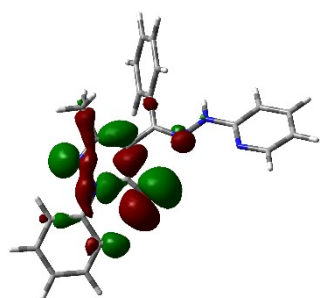


**Figure S50.** Comparison of experimental (black line) and calculated (tautomer I, red line) IR spectrum of  $H_2L^5$ .

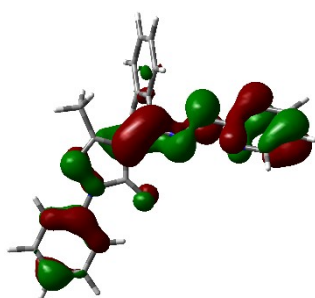
**Table S4.** Selected stretching assignments of the IR spectrum of  $H_2L^5$ .

IR band ( $cm^{-1}$ )	Experimental	Calculated
$\nu(N3-H)$	3064	3062
$\nu(C=N2)$	1524	1530
$\nu(C=O)$	1615	1618
$\nu_{as}(C-F)$	1315, 1065	1274, 1084
$\nu_s(C-F)$	1163	1127

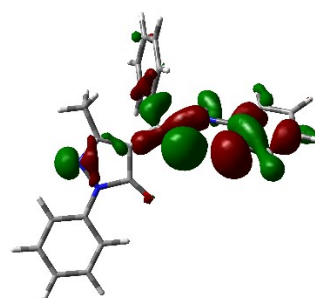
*Optimized [HL<sup>1</sup>]*



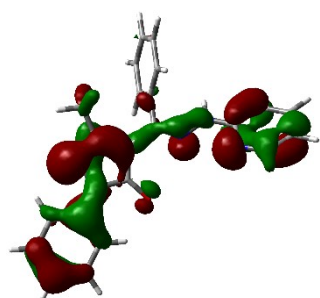
HOMO-2



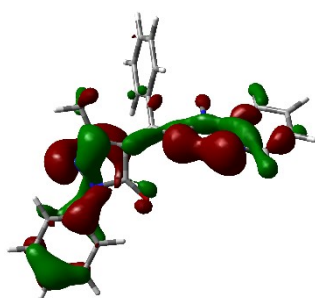
HOMO-3



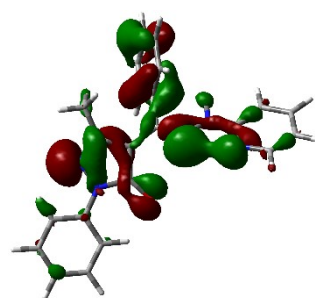
HOMO-5



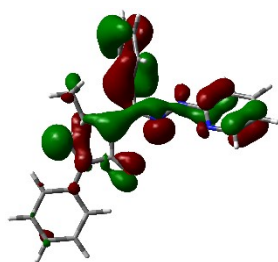
HOMO-6



HOMO-7

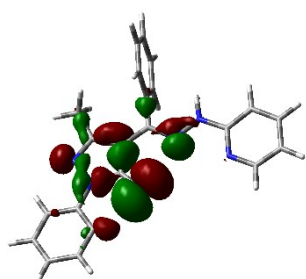


HOMO-8

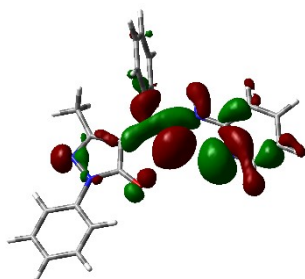


HOMO-9

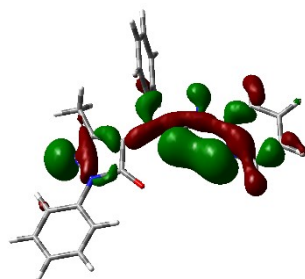
*Single point calculation of [HL<sup>1</sup>] from the optimization of 1.*



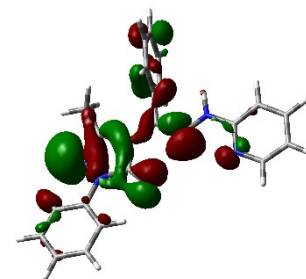
HOMO-2



HOMO-4



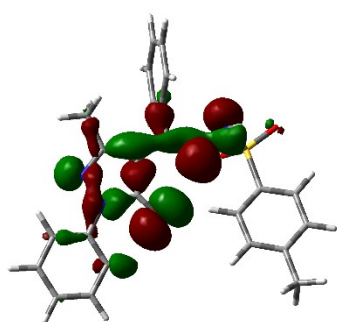
HOMO-6



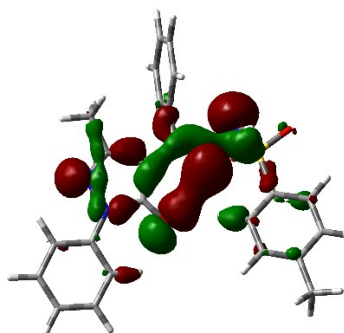
HOMO-8



*Optimized [HL<sup>2-</sup>]*

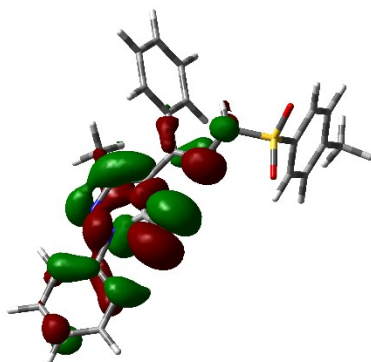


HOMO-2

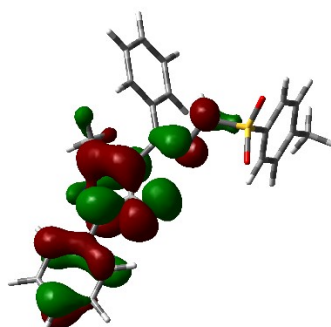


HOMO-3

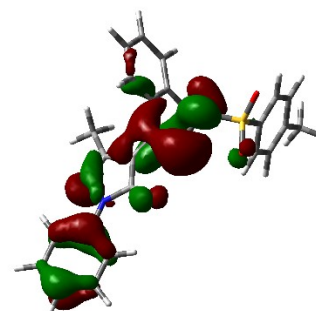
*Single point calculation of [HL<sup>2-</sup>] from the optimization of 2.*



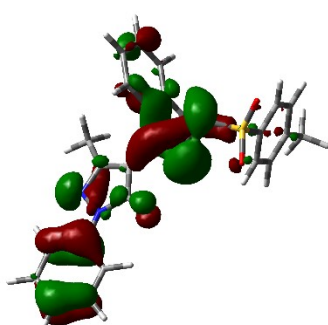
HOMO-1



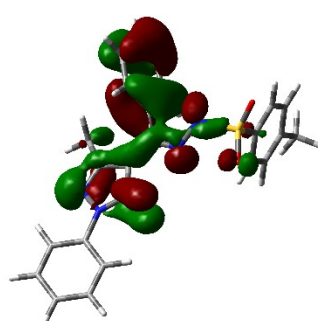
HOMO-2



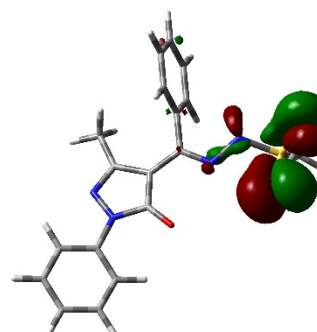
HOMO-3



HOMO-5

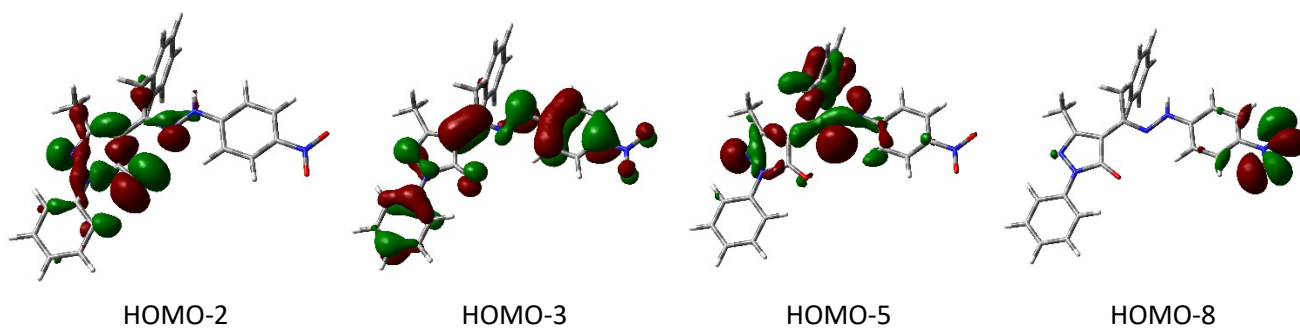


HOMO-8

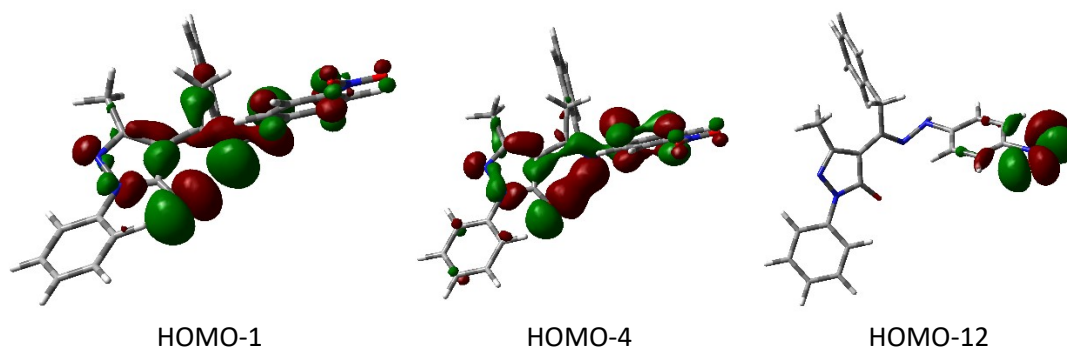


HOMO-13

*Optimized [HL<sup>4-</sup>]*



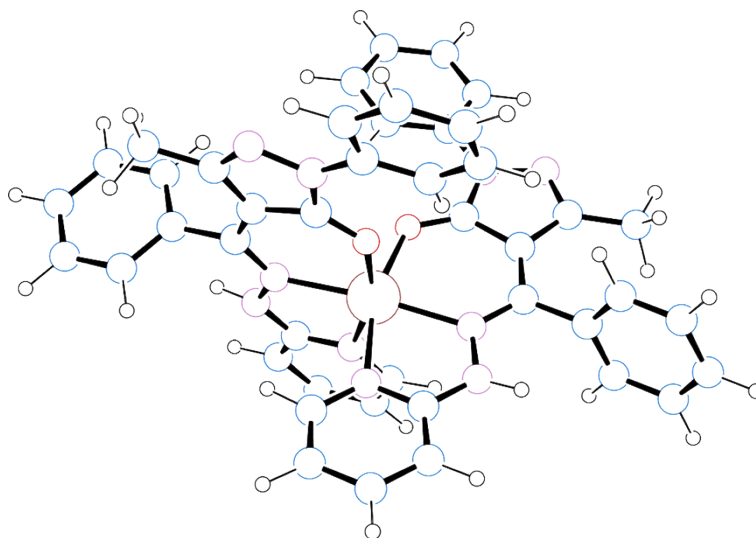
*Single point calculation of [HL<sup>4-</sup>] from the optimization of 4.*



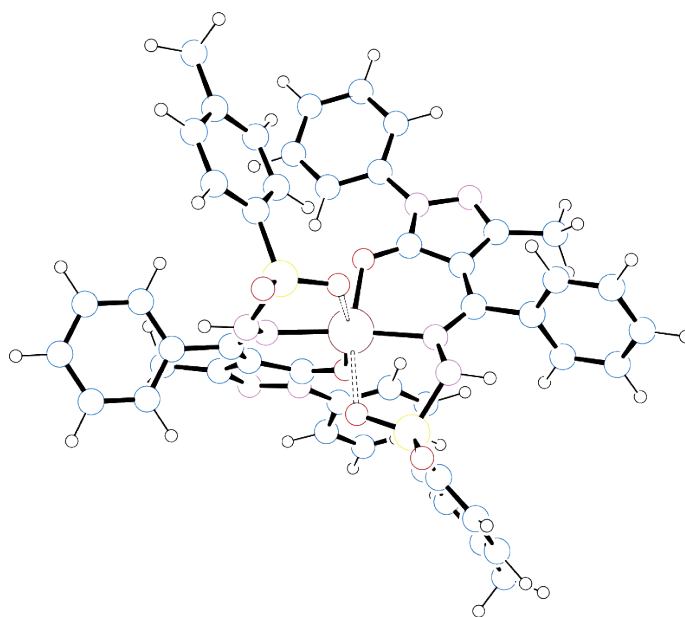
**Figure S51.** MOs of anionic ligands [HL<sup>1-</sup>], [HL<sup>2-</sup>] and [HL<sup>4-</sup>], involved in the coordination to metal centers.

**Figure S52.** Optimized structures of complexes **1** and **2**.

Complex **1** -  $[\text{Zn}(\text{HL}^1)]_2$



Complex **2** -  $[\text{Zn}(\text{HL}^2)]_2$



**Table S5.** Comparison of selected experimental and calculated structural parameters of complexes **1** and **2**.

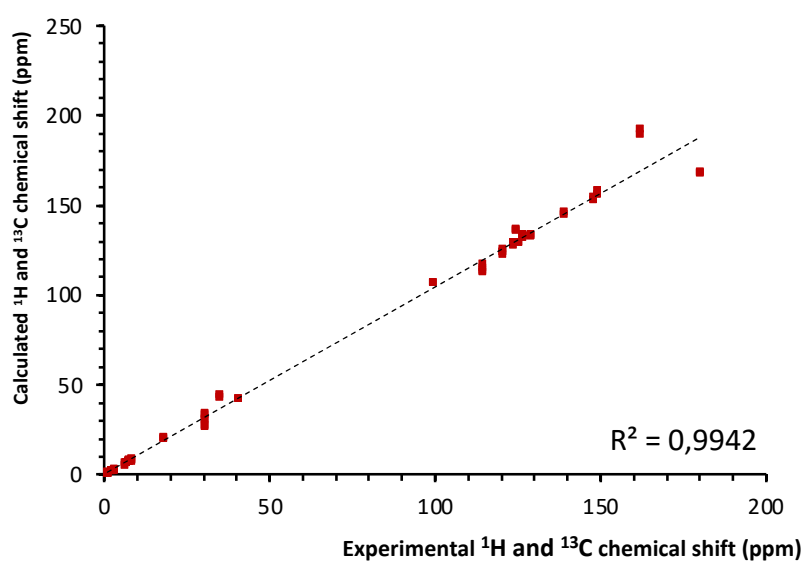
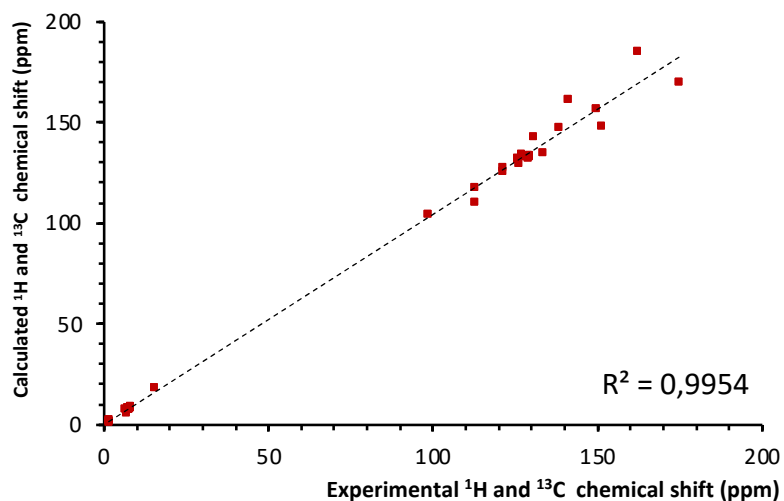
**1, [Zn(HL<sup>1</sup>)]<sub>2</sub>**

Bond distances (Å) and angles (°) *	Experimental	Calculated
Zn-N3 <sub>A</sub>	2.151(2)	2.178
Zn-N5 <sub>A</sub>	2.132(2)	2.183
Zn-O <sub>A</sub>	2.051(2)	2.053
Zn-N3 <sub>B</sub>	2.143(2)	2.176
Zn-N5 <sub>B</sub>	2.142(2)	2.183
Zn-O <sub>B</sub>	2.049(2)	2.053
C-O	1.270	1.262
C-N3	1.310	1.318
N3 <sub>A</sub> -Zn-N5 <sub>A</sub>	76.33(9)	76.0
N3 <sub>A</sub> -Zn-N5 <sub>B</sub>	98.99(9)	100.3
N3 <sub>A</sub> -Zn-O <sub>A</sub>	87.22(8)	86.7
O <sub>A</sub> -Zn-O <sub>B</sub>	88.80(8)	94.5
O <sub>A</sub> -Zn-N5 <sub>B</sub>	90.30(9)	88.7
O <sub>A</sub> -Zn-N5 <sub>A</sub>	163.54(8)	162.6

\* A and B are the two ligands of the complex (see Table S1).

**2, [Zn(HL<sup>2</sup>)]<sub>2</sub>**

Bond distances (Å) and angles (°)	Experimental	Calculated
Zn-N	1.998(4)	2.109
Zn-O	1.958(3)	2.032
O <sub>SO2</sub> -Zn	2.770	2.277
C-O	1.275	1.270
C-N	1.330	1.317
N3-N4	1.432	1.403
C4-C10	1.425	1.425
O-Zn-N	96.95(12)	90.1
O-Zn-O <sub>SO2</sub>	163.26	167.7



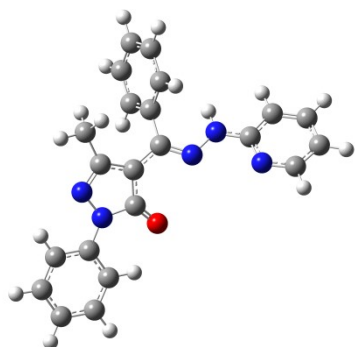
**Figure S53.** Comparison of the calculated and experimental  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of complexes **3** (top) and **5** (bottom).

**Table S6.** Comparison of selected experimental and calculated structural parameters of complex **4**.

Bond distances (Å) and angles (°)	4, $[\text{Zn}(\text{HL}^4)]_n$	
	Experimental	$[\text{Zn}(\text{HL}^4)]_3$ Calculated
Zn-N	2.069(3)	2.109
Zn-O	2.004(3)	2.032
Zn-O <sub>NO2</sub>	2.342(3)	2.383
C-O	1.274	1.271
C-N	1.312	1.325
N-Zn-N	180.0	180.0
O-Zn-O	180.0	180.0
Centroid-Centroid ( $\pi$ stacking)	4.155	4.449

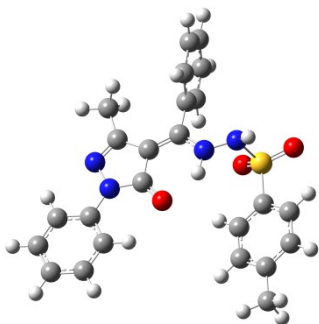
**Table S7.** Coordinates of the optimized compounds.

**[HL<sup>1</sup>]<sup>-</sup>**



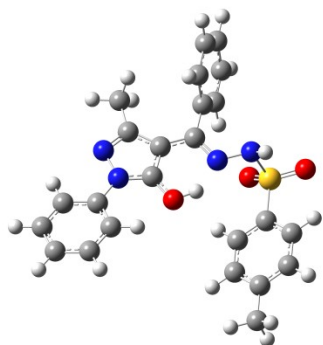
C	-4.08636500	-3.65555600	-0.78749500
H	-3.72917400	-4.52104100	-1.34362300
C	-5.37596900	-3.65012800	-0.26684200
H	-6.03753100	-4.49700600	-0.40300800
C	-5.77240400	-2.50542200	0.43768200
H	-6.76519300	-2.43938100	0.87230000
C	-4.88752200	-1.45896400	0.58660000
H	-5.16454800	-0.56590200	1.13783300
C	-3.59217300	-1.56862300	0.01138900
C	-0.73765500	0.55263500	-0.15308500
C	-1.41182700	1.87237100	0.13002000
C	-2.39194000	2.39058400	-0.72894500
H	-2.66531500	1.82708000	-1.61429900
C	-2.99831000	3.61666200	-0.46598200
H	-3.74219300	4.00825900	-1.15244400
C	-2.64822000	4.34193100	0.67225900
H	-3.12038200	5.29688000	0.87838600
C	-1.68421900	3.83256400	1.54099500
H	-1.40482800	4.38998300	2.42929200
C	-1.06916800	2.61230800	1.26881000
H	-0.30269000	2.22235700	1.92885000
C	1.18522000	2.87746200	-1.44453200
H	0.74726900	3.57759800	-0.72666400
H	0.45500700	2.74659000	-2.24972800
H	2.08958800	3.32596900	-1.86078800
C	1.55049000	1.56523200	-0.81296800
C	0.69785800	0.54923300	-0.28627000
C	1.57473300	-0.52398600	0.13160300
C	4.11825300	-0.61693000	0.01568200
C	5.29319100	0.06852600	-0.35209400
H	5.19202200	1.05244800	-0.78690900
C	6.53907200	-0.51491400	-0.15826300
H	7.42925100	0.03483500	-0.45133400
C	6.65856300	-1.78658700	0.40301200
H	7.63430800	-2.23761400	0.55203200
C	5.49550800	-2.46489100	0.76706600
H	5.56286500	-3.45676000	1.20492100
C	4.23704300	-1.90185300	0.58284200
H	3.33413200	-2.42264600	0.86453500
N	-3.20912500	-2.65846900	-0.67269400
N	-2.73414400	-0.51408500	0.14527300
N	-1.40769300	-0.56584200	-0.21081000
N	2.82581300	1.24282800	-0.77365300
N	2.87759800	-0.01442700	-0.18592900
O	1.36758300	-1.60757400	0.67722200
H	-3.08535900	0.29898000	0.63865800

## H<sub>2</sub>L<sup>2</sup> (tautomer I)



C	-4.15349400	-0.16963400	-0.01831600
C	-4.23492400	1.18087400	-0.38463400
H	-3.34614100	1.69971400	-0.70894400
C	-5.46360700	1.83274900	-0.32580000
H	-5.51695500	2.87732300	-0.61279700
C	-6.61245700	1.16535300	0.09036500
H	-7.56400200	1.68269600	0.13206000
C	-6.52234100	-0.17742300	0.45148300
H	-7.40667900	-0.71372500	0.77761300
C	-5.30557900	-0.84750800	0.40068700
H	-5.22872000	-1.88843200	0.67809800
C	-1.66270100	-0.39966600	-0.39125200
C	-0.79131300	-1.56839000	-0.24775200
C	-1.67402100	-2.64533200	0.15299100
C	-1.35990500	-4.07910700	0.43824400
H	-2.28516800	-4.59777400	0.69001500
H	-0.65928900	-4.17626600	1.27110000
H	-0.90072400	-4.56729300	-0.42498200
C	0.57101000	-1.50815200	-0.45716800
C	1.48244100	-2.67548600	-0.28269800
C	2.02529100	-2.97685100	0.96811000
H	1.81872700	-2.32969400	1.81071500
C	2.85584700	-4.08501500	1.11378300
H	3.28062400	-4.31069300	2.08506600
C	3.14796300	-4.89372600	0.01760800
H	3.79494900	-5.75552100	0.13533100
C	2.61225600	-4.58948400	-1.23198400
H	2.83918500	-5.21318700	-2.08909900
C	1.78324900	-3.48131800	-1.38439100
H	1.36348400	-3.24440800	-2.35565900
C	2.36902300	2.45121500	0.28723700
C	1.11826800	2.70920200	0.84622200
H	0.60180100	1.94484300	1.41062900
C	0.55279000	3.96801900	0.67528900
H	-0.42457800	4.16781500	1.09992000
C	1.21767600	4.97208500	-0.03666700
C	2.47589100	4.68448900	-0.58116700
H	3.00943200	5.45290300	-1.13025400
C	3.05635000	3.43127900	-0.42929200
H	4.03684700	3.21746700	-0.83599000
C	0.60730000	6.34256000	-0.18846100
H	-0.48330300	6.29302600	-0.19900300
H	0.93781300	6.82657000	-1.10972400
H	0.89900400	6.98958800	0.64584200
N	-2.92162900	-0.86761300	-0.06391900
N	-2.90100500	-2.22637700	0.25674700
N	1.10200300	-0.33668300	-0.89788900
H	0.43859800	0.44561200	-0.99405400
N	2.46812800	-0.11580700	-0.87668000
O	-1.34970100	0.75453100	-0.72559200
O	2.55190000	0.19384900	1.64297100
O	4.51372400	0.90647400	0.15257800
S	3.09018400	0.81900800	0.44389900
H	2.82221300	0.23743800	-1.76035900

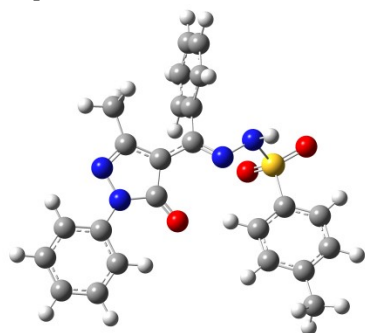
## H<sub>2</sub>L<sup>2</sup> (tautomer II)



C	-4.13518700	-0.32659200	-0.04186600
C	-4.29446700	0.89196400	-0.70948000
H	-3.45946400	1.34765000	-1.21926400
C	-5.54086900	1.51274800	-0.70902900
H	-5.65822200	2.45684500	-1.22893800
C	-6.62748200	0.93269500	-0.06054900
H	-7.59453700	1.42183500	-0.06819000
C	-6.45941900	-0.28537700	0.59536100
H	-7.29698300	-0.75036500	1.10289400
C	-5.22169400	-0.91741400	0.61094200
H	-5.07885500	-1.86454500	1.11026800
C	-1.64128000	-0.54781200	-0.31053100
C	-0.73754500	-1.60795100	-0.12005300
C	-1.56722800	-2.68998600	0.33105200
C	-1.19664200	-4.07942600	0.74397600
H	-2.07752600	-4.56831600	1.16051700
H	-0.40263500	-4.07179300	1.49407300
H	-0.83390100	-4.66871000	-0.10101100
C	0.67794000	-1.44463500	-0.32819000
C	1.59404200	-2.62170500	-0.24905200
C	2.52394000	-2.75920600	0.78575400
H	2.60773500	-1.98571800	1.53834500
C	3.34952700	-3.87965800	0.82959400
H	4.06714100	-3.98150000	1.63559600
C	3.26814700	-4.85597200	-0.16135900
H	3.91984700	-5.72168500	-0.12639500
C	2.35172900	-4.71368000	-1.20076200
H	2.28900600	-5.46506300	-1.97978100
C	1.51043500	-3.60506700	-1.24009400
H	0.79292900	-3.49678300	-2.04610500
C	2.30193800	2.55395800	0.23337700
C	1.17682600	2.74416400	1.03328600
H	0.86948700	1.97271700	1.72650000
C	0.47729800	3.94256700	0.93989200
H	-0.40067600	4.09227500	1.55881400
C	0.88513200	4.95429600	0.06312800
C	2.02138100	4.73596400	-0.72520800
H	2.35762900	5.51175400	-1.40487300
C	2.73193800	3.54334800	-0.64942500
H	3.62222700	3.38676300	-1.24580200
C	0.13805800	6.26270700	-0.00466500
H	-0.92586700	6.12499900	0.19951000
H	0.24073400	6.73082100	-0.98584300
H	0.52571000	6.96821100	0.73818400
N	-2.88172900	-0.99999300	-0.01978800
N	-2.82907000	-2.32526700	0.38847400
N	1.06049400	-0.22927700	-0.63242900
N	2.45702500	-0.05614400	-0.83845000
O	-1.36597300	0.68761400	-0.68695300
O	2.94841200	0.40215100	1.61176700
O	4.53321500	1.21063600	-0.22747400
S	3.19286300	0.99768400	0.30419600
H	2.61745000	0.33854000	-1.76305500
H	-0.35840700	0.69110700	-0.76255500

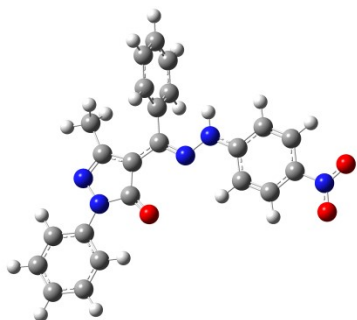


[HL<sup>2-</sup>]



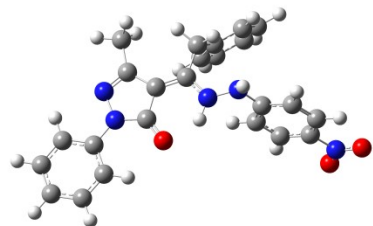
C	4.18599500	-0.84309200	0.06144900
C	3.94473900	-2.22161600	0.21485600
H	2.92402400	-2.57112400	0.19672000
C	5.01225100	-3.09737900	0.38605100
H	4.80367600	-4.15674300	0.50299000
C	6.32958300	-2.64228900	0.41078800
H	7.15332300	-3.33546900	0.54551600
C	6.56611400	-1.27596200	0.25992100
H	7.58338900	-0.89581100	0.27660100
C	5.51609400	-0.38276900	0.08756500
H	5.69099000	0.67668000	-0.03029800
C	1.74584000	-0.16507200	-0.18542300
C	1.18718000	1.16159200	-0.37209200
C	2.31403200	2.04941400	-0.39738300
C	2.36835400	3.53505800	-0.60326700
H	3.41670300	3.83724100	-0.64209600
H	1.87155200	4.08121300	0.20246500
H	1.87984600	3.83216900	-1.53568800
C	-0.20677500	1.45328800	-0.49392000
C	-0.68115200	2.85256000	-0.20770400
C	-0.71159100	3.33237600	1.10344400
H	-0.40874200	2.67654800	1.91049300
C	-1.14824400	4.62775700	1.37164100
H	-1.17871600	4.98274500	2.39654600
C	-1.54940100	5.46372600	0.33123900
H	-1.88512100	6.47416600	0.54056900
C	-1.52451800	4.99035300	-0.97949700
H	-1.84040900	5.63201300	-1.79586800
C	-1.10116300	3.69069300	-1.24409600
H	-1.09052500	3.31852100	-2.26275900
C	-3.05335700	-1.71190200	0.19585800
C	-1.78438400	-2.29649800	0.18301600
H	-0.88240600	-1.71059400	0.32254800
C	-1.68781400	-3.65972000	-0.07922600
H	-0.70019200	-4.10837900	-0.11144300
C	-2.82082300	-4.44831800	-0.30923300
C	-4.07581900	-3.83255200	-0.28969400
H	-4.96794900	-4.42436700	-0.47183900
C	-4.19893800	-2.46724300	-0.04547900
H	-5.16685700	-1.98203000	-0.04074700
C	-2.68701700	-5.93231500	-0.55645600
H	-1.85075300	-6.14881800	-1.22682300
H	-3.59522200	-6.34753100	-1.00032000
H	-2.49926600	-6.47159500	0.37886400
N	3.14566200	0.07450600	-0.11567600
N	3.45728500	1.42026100	-0.26303800
N	-1.03477000	0.50138600	-0.85170800
N	-2.42188300	0.88778700	-0.73780800
O	1.22932300	-1.27938400	-0.05259600
O	-2.57619200	0.38263200	1.75989400
O	-4.66297200	0.37761600	0.30129600
S	-3.24624200	0.05613500	0.50618200
H	-2.89790800	0.62797200	-1.59964300

[HL<sup>3-</sup>]



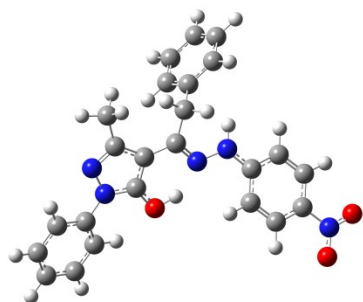
C	-2.87099600	1.50351000	-0.18435300
C	-1.65087800	0.75870200	-0.08125700
C	-2.05389300	-0.63675800	0.00094200
N	-3.93658300	0.73527400	-0.16825700
N	-3.47728600	-0.56769500	-0.04909800
C	-4.40572200	-1.61184000	0.00348000
C	-5.78161400	-1.31811000	-0.04049500
C	-4.00357800	-2.95764400	0.10056300
C	-6.72080200	-2.34068800	0.01051900
H	-6.08051300	-0.28265100	-0.11530200
C	-4.96236500	-3.96467300	0.14994100
H	-2.94789800	-3.17976100	0.13605100
C	-6.32528000	-3.67471600	0.10609900
H	-7.77662800	-2.08838800	-0.02508300
H	-4.63075200	-4.99602900	0.22433500
H	-7.06263300	-4.46962300	0.14543300
C	-3.10283300	2.98023300	-0.32993500
H	-4.17670400	3.14564000	-0.43439000
H	-2.74448600	3.54523900	0.53511800
H	-2.59769100	3.39008700	-1.20940800
O	-1.40988400	-1.68023100	0.10199700
C	-0.29526000	1.20963600	-0.06084700
C	-0.00503500	2.68626800	0.02071900
C	-0.02049500	3.34571500	1.25534400
C	0.34760300	3.41317700	-1.12283200
C	0.28854700	4.70175000	1.34227700
H	-0.28683800	2.78676600	2.14551900
C	0.65320000	4.77066100	-1.03823600
H	0.36903000	2.90787800	-2.08234000
C	0.62225600	5.41919300	0.19477000
H	0.26611800	5.19884700	2.30637700
H	0.91306200	5.32171200	-1.93597600
H	0.85925800	6.47562100	0.26149100
N	0.69094000	0.34802400	-0.08969700
N	1.97076000	0.82448000	-0.01455200
H	2.14966900	1.82220500	0.04752100
C	3.02903700	-0.02499300	-0.01123900
C	4.34775000	0.49562200	0.04866500
C	2.84752200	-1.43171600	-0.06755800
C	5.43617600	-0.34679500	0.05016900
H	4.49488900	1.57032800	0.09239600
C	3.94426800	-2.26465300	-0.06593900
H	1.83618200	-1.81372700	-0.10519900
C	5.24319800	-1.73462200	-0.00851100
H	6.44562300	0.03765500	0.09489100
H	3.82388300	-3.33856000	-0.10664300
N	6.38341900	-2.61257400	-0.00775500
O	6.19060200	-3.83287900	-0.06202200
O	7.51464000	-2.11055900	0.04715100

## H<sub>2</sub>L<sup>4</sup> (tautomer I)



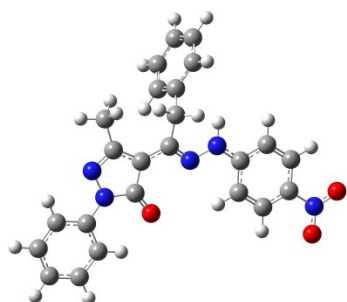
C	2.81499000	1.90791300	-0.32586400
C	1.80311000	0.94045900	-0.70200000
C	2.45578200	-0.36156000	-0.54214500
N	3.92197300	1.31493000	0.01606900
N	3.73301900	-0.05827000	-0.10574500
C	4.80258500	-0.93248700	0.21644700
C	6.01654800	-0.38959500	0.65583400
C	4.66094400	-2.32174800	0.10104700
C	7.07486500	-1.23230500	0.97545700
H	6.11191300	0.68295800	0.73938500
C	5.73352500	-3.14732100	0.42687700
H	3.72455000	-2.73715600	-0.23769800
C	6.94326700	-2.61496600	0.86436400
H	8.00983000	-0.80004100	1.31452100
H	5.61436700	-4.22125800	0.33511800
H	7.77165000	-3.26727800	1.11540700
C	2.76809300	3.40502800	-0.29563400
H	3.71893900	3.77276700	0.09025200
H	2.62194800	3.82393700	-1.29634800
H	1.96501300	3.78055000	0.34458000
O	1.97851600	-1.48894300	-0.74613900
N	-0.17982900	-0.08751900	-1.41181100
N	-1.46223100	-0.09033500	-1.94164300
H	-1.46728700	-0.29201500	-2.93506800
C	-2.48303300	-0.73248400	-1.22614700
C	-3.65584400	-1.09048900	-1.91244400
C	-2.38148000	-0.97917400	0.14939000
C	-4.71088500	-1.67610100	-1.23638900
H	-3.73620100	-0.90354100	-2.97804600
C	-3.43880200	-1.56708600	0.82666700
H	-1.47998300	-0.70846100	0.68086100
C	-4.59475100	-1.90901500	0.13240500
H	-5.62081700	-1.95926800	-1.74652200
H	-3.38133500	-1.76516500	1.88776500
C	0.49020200	1.05352500	-1.12949400
C	-0.24551900	2.36238400	-1.27470200
H	-0.80537000	2.34904800	-2.21101600
H	0.48566300	3.16566500	-1.34817400
C	-1.21253300	2.65067400	-0.13077700
C	-2.51668700	3.06760900	-0.40707000
C	-0.80816100	2.54947000	1.20457100
C	-3.39734800	3.38375700	0.62488000
H	-2.84734000	3.14381800	-1.43752600
C	-1.68851300	2.86237100	2.23773400
H	0.19673600	2.21794100	1.44213700
C	-2.98569200	3.28172200	1.95126100
H	-4.40639500	3.70424700	0.39153800
H	-1.35928100	2.77757800	3.26721400
H	-3.67106800	3.52341700	2.75536800
N	-5.71386900	-2.52972900	0.85293100
O	-5.58109100	-2.72226500	2.05576800
O	-6.71642900	-2.81724200	0.20831600
H	0.34506200	-0.96717100	-1.29153100

## H<sub>2</sub>L<sup>4</sup> (tautomer II)



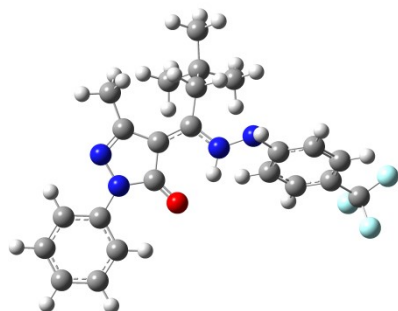
C	3.01283400	1.47956900	-0.95031700
C	1.77070100	0.82019800	-0.66771600
C	2.16794100	-0.43298300	-0.17928700
N	4.04010600	0.70618900	-0.66319500
N	3.52118400	-0.47862000	-0.18018800
C	4.40713600	-1.53064000	0.19022800
C	5.73329500	-1.47009600	-0.24893000
C	3.97724400	-2.59867200	0.98348900
C	6.62098800	-2.47934200	0.10456600
H	6.04712000	-0.63011500	-0.85142000
C	4.87931800	-3.60424400	1.32138700
H	2.95605600	-2.64604200	1.32913300
C	6.20081900	-3.55302900	0.88748000
H	7.64770900	-2.42531700	-0.23922700
H	4.53968700	-4.43049600	1.93546400
H	6.89629300	-4.33906400	1.15748700
C	3.29060000	2.84867000	-1.49293400
H	4.36993000	3.00050400	-1.51316100
H	2.91205400	2.96706100	-2.51280300
H	2.84530500	3.63356800	-0.87515500
O	1.39620200	-1.42948100	0.23362700
H	0.46938600	-1.07702700	0.13111000
N	-0.48960800	0.27988600	-0.44139500
N	-1.82543700	0.60086700	-0.46537400
H	-2.08085300	1.53406000	-0.16187900
C	-2.77858700	-0.38775300	-0.32022200
C	-4.09035700	-0.01864600	0.03990100
C	-2.48821600	-1.74277600	-0.56599900
C	-5.08083200	-0.97418500	0.15800000
H	-4.32118500	1.02374400	0.23166700
C	-3.48183200	-2.69857900	-0.44001000
H	-1.49175600	-2.03180200	-0.86870400
C	-4.77113800	-2.31354100	-0.07945500
H	-6.09010300	-0.70732700	0.43841400
H	-3.27718300	-3.74393000	-0.62500800
C	0.37640100	1.19511100	-0.77864800
C	-0.05485200	2.56405100	-1.26014100
H	-0.82204600	2.41229700	-2.02750800
H	0.78291100	3.05820900	-1.75083800
C	-0.61665100	3.48035400	-0.17822600
C	-1.72136600	4.29431400	-0.45452700
C	-0.02886400	3.55653300	1.08991100
C	-2.22400000	5.16709100	0.50879700
H	-2.18754000	4.24868500	-1.43395400
C	-0.53118000	4.42791200	2.05331500
H	0.82309200	2.92861600	1.32676200
C	-1.62929100	5.23623900	1.76618700
H	-3.07948900	5.79097200	0.27572200
H	-0.06367200	4.47407700	3.03033800
H	-2.01972900	5.91265800	2.51766900
N	-5.81850600	-3.32735700	0.04944000
O	-5.51461600	-4.49636700	-0.16695100
O	-6.94293900	-2.95083000	0.36704800

[HL<sup>4-</sup>]



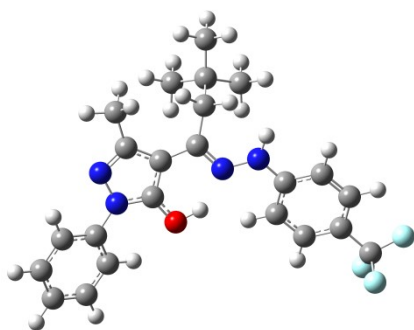
C	2.90180100	1.50229300	-0.61814500
C	1.72110100	0.69400800	-0.52887800
C	2.19806800	-0.64658900	-0.22194700
N	4.00450500	0.82019700	-0.40108700
N	3.61462800	-0.48815300	-0.17040400
C	4.59432000	-1.45199500	0.08892100
C	5.94978200	-1.07323700	0.11131700
C	4.26396300	-2.79953000	0.32808900
C	6.93884100	-2.01513400	0.36626900
H	6.19384000	-0.03727500	-0.07401900
C	5.27170400	-3.72493100	0.58092400
H	3.22377000	-3.08708600	0.31026300
C	6.61433600	-3.35060000	0.60395100
H	7.97761200	-1.69804500	0.37871400
H	4.99512900	-4.75911900	0.76304800
H	7.39052900	-4.08224200	0.80248800
C	3.07821200	2.97180100	-0.88706400
H	4.12319800	3.22453600	-0.69908600
H	2.85507800	3.23587300	-1.92750500
H	2.44941500	3.59595600	-0.24518000
O	1.61364300	-1.71585900	-0.05047700
N	-0.57435600	0.15773100	-0.34642200
N	-1.89235600	0.50351800	-0.50439000
H	-2.17655900	1.47768300	-0.50880300
C	-2.86689000	-0.42792300	-0.31832100
C	-4.22840900	-0.03283300	-0.32665600
C	-2.54876900	-1.79804200	-0.13626600
C	-5.23071500	-0.96306700	-0.16627900
H	-4.47883900	1.01507400	-0.45985200
C	-3.55965500	-2.72030900	0.02500100
H	-1.50439600	-2.08085500	-0.12166600
C	-4.90319200	-2.31489500	0.00868200
H	-6.27260500	-0.67453800	-0.16942300
H	-3.33557600	-3.76858200	0.16750100
C	0.33643900	1.03729100	-0.67337800
C	-0.06371400	2.39910300	-1.23611700
H	-0.79304600	2.23252700	-2.03853900
H	0.79664800	2.86030300	-1.71724900
C	-0.65305000	3.38846200	-0.23951900
C	-1.55207400	4.37220000	-0.67182700
C	-0.29413100	3.36751200	1.11312700
C	-2.07154600	5.31229100	0.21507600
H	-1.84597400	4.40001300	-1.71726100
C	-0.81302000	4.30668600	2.00231000
H	0.38688500	2.60166100	1.46691300
C	-1.70144700	5.28365300	1.55818500
H	-2.76744600	6.06425100	-0.14224700
H	-0.52398600	4.27005700	3.04718900
H	-2.10706700	6.01130900	2.25274800
N	-5.95418900	-3.28605500	0.17566200
O	-5.64373100	-4.47293300	0.32654900
O	-7.12815800	-2.89239100	0.16064200

## H<sub>2</sub>L<sup>5</sup> (tautomer I)



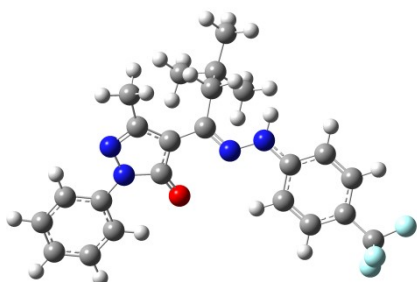
C	3.37087700	1.65464400	-0.23550200
C	2.07834100	1.02564600	-0.42166100
C	2.35809300	-0.40992500	-0.36370600
N	4.30582500	0.76283200	-0.06741100
N	3.71710000	-0.49437100	-0.12198000
C	4.52888700	-1.64451700	0.04756100
C	5.89556300	-1.48015300	0.30685200
C	3.98626300	-2.93367400	-0.03778800
C	6.70613500	-2.59645700	0.47753900
H	6.30073600	-0.48096200	0.36958000
C	4.81604100	-4.03785000	0.13686200
H	2.93322500	-3.05741500	-0.23734100
C	6.17532800	-3.88211000	0.39445100
H	7.76261700	-2.45573300	0.67781200
H	4.38650200	-5.03129600	0.06892700
H	6.81206000	-4.74889500	0.52872700
C	3.78598200	3.09305000	-0.30261200
H	4.86509800	3.14423800	-0.15668900
H	3.55295100	3.52956200	-1.27903300
H	3.30467600	3.70796000	0.46014400
O	1.56264900	-1.35620300	-0.49978800
N	-0.16128100	0.59325600	-0.92657300
N	-1.41318100	0.92895900	-1.43197200
H	-1.40313000	0.99552000	-2.44511800
C	-2.51686000	0.20082900	-0.94849300
C	-3.73007300	0.29614700	-1.64739900
C	-2.45538900	-0.56951200	0.21698600
C	-4.85642000	-0.36355600	-1.18629600
H	-3.78732300	0.89856800	-2.54794000
C	-3.59277200	-1.22734300	0.67368500
H	-1.52302700	-0.66395600	0.75721100
C	-4.79689800	-1.12839600	-0.01807300
H	-5.79030600	-0.27689400	-1.72751300
H	-3.53813100	-1.81943100	1.57830900
C	0.79509300	1.51253800	-0.65913400
C	0.43685600	2.97723700	-0.64141500
H	-0.28424800	3.17766900	-1.43676700
H	1.33809200	3.53961600	-0.87872000
C	-0.15991600	3.56351000	0.69121700
C	-1.59594300	3.07015100	0.93465600
C	0.69939600	3.20771900	1.91664300
C	-0.18685200	5.09450200	0.51435100
H	-2.24759700	3.29089800	0.08610200
H	-1.63403100	1.99505100	1.11567900
H	-2.01063900	3.56553300	1.81756100
H	1.71818600	3.59116600	1.83116500
H	0.25861000	3.64853100	2.81530600
H	0.75939400	2.12803200	2.07213900
H	-0.61885300	5.57330900	1.39736500
H	0.81950200	5.50006500	0.37326900
H	-0.79161400	5.38415100	-0.35057000
C	-6.00924100	-1.87918100	0.44576400
F	-7.15158500	-1.19689800	0.19884100
F	-6.13772500	-3.07599300	-0.17823100
F	-5.97470600	-2.13715800	1.77124000
H	0.15800300	-0.38975000	-0.94932600

## H<sub>2</sub>L<sup>5</sup> (tautomer II)



C	3.50878800	1.32090900	-0.57764800
C	2.13888500	0.93063600	-0.39869800
C	2.22629300	-0.44559100	-0.15087200
N	4.32435700	0.29490800	-0.42575200
N	3.53447300	-0.79983000	-0.15366400
C	4.14015500	-2.07374400	0.03251000
C	5.45684700	-2.25692900	-0.40131300
C	3.45019400	-3.12401400	0.64539600
C	6.07438100	-3.48921500	-0.22320900
H	5.97543900	-1.42814400	-0.86102200
C	4.08243200	-4.35391500	0.80839300
H	2.43557100	-2.98450400	0.98599600
C	5.39222100	-4.54550100	0.37801800
H	7.09568000	-3.62331200	-0.56140500
H	3.54146200	-5.16479700	1.28285400
H	5.87716900	-5.50553700	0.51113100
C	4.12540800	2.63672200	-0.94784700
H	5.20568300	2.50227700	-1.00766700
H	3.77289100	2.98762600	-1.92266300
H	3.91934300	3.42097700	-0.21636300
O	1.23377800	-1.31256800	0.01536100
H	0.41987800	-0.77032200	-0.17375800
N	-0.18836500	0.84387100	-0.42621700
N	-1.44598000	1.33793800	-0.57285000
H	-1.56984900	2.26047600	-0.96478600
C	-2.56623400	0.54323900	-0.41208800
C	-3.80647000	1.02029900	-0.87216000
C	-2.51481500	-0.70509800	0.23147600
C	-4.95681200	0.26766100	-0.70394600
H	-3.86151700	1.98344300	-1.36893300
C	-3.67206300	-1.45295400	0.38603000
H	-1.58059200	-1.06981600	0.63400200
C	-4.90060100	-0.97847400	-0.07664900
H	-5.90492000	0.64886700	-1.06111000
H	-3.62201400	-2.40972200	0.89133700
C	0.85721000	1.62322300	-0.47631600
C	0.79517400	3.13032500	-0.63473300
H	0.00854200	3.40312600	-1.35022700
H	1.72407300	3.45439200	-1.10133100
C	0.59133200	3.99055400	0.66362700
C	-0.83669000	3.85958800	1.22404600
C	1.58771700	3.58896100	1.76563900
C	0.83113500	5.46067400	0.26794600
H	-1.58867300	4.16100200	0.48681700
H	-1.06060900	2.84116300	1.54527400
H	-0.95538100	4.51554000	2.09132800
H	2.62415400	3.71440300	1.44570600
H	1.43823500	4.21695200	2.64861000
H	1.45492900	2.54836800	2.06985300
H	0.68214000	6.11940100	1.12812000
H	1.85028700	5.61484600	-0.09861900
H	0.13941500	5.77961700	-0.51839600
C	-6.12812100	-1.82404300	0.06175300
F	-7.26475900	-1.09508400	-0.01545200
F	-6.21272800	-2.77163800	-0.90637600
F	-6.15819900	-2.48815200	1.24134300

[HL<sup>5-</sup>]



C	3.18960200	1.16419100	-1.25276500
C	1.95689800	0.80869000	-0.63164100
C	2.18227100	-0.48777700	-0.03152300
N	4.12840900	0.25205900	-1.09882800
N	3.55423200	-0.75382900	-0.33696900
C	4.32483500	-1.86540900	0.00876800
C	5.66912900	-1.93422900	-0.40539400
C	3.79672000	-2.92791400	0.76811800
C	6.45353100	-3.03095600	-0.07068300
H	6.06476700	-1.11407400	-0.98684300
C	4.60172300	-4.01554500	1.09124700
H	2.76595500	-2.87003000	1.08417600
C	5.93251600	-4.08462800	0.68052000
H	7.48735600	-3.06027100	-0.40307500
H	4.17411100	-4.82415400	1.67689900
H	6.54941200	-4.93900100	0.93924900
C	3.53719500	2.35573300	-2.10001800
H	4.50432500	2.17159000	-2.57174600
H	2.79359800	2.52621400	-2.88578200
H	3.61808300	3.28055100	-1.51743100
O	1.45967100	-1.23434100	0.63654900
N	-0.38817800	0.78849900	-0.55941400
N	-1.61472900	1.37983500	-0.42428000
H	-1.72696900	2.38393500	-0.48927900
C	-2.74159300	0.61278100	-0.32387100
C	-4.01553100	1.22144900	-0.34855600
C	-2.66254800	-0.79120300	-0.17280000
C	-5.16450200	0.45918100	-0.23277400
H	-4.09241200	2.29881700	-0.46104000
C	-3.82089400	-1.53631500	-0.06120900
H	-1.68154500	-1.24530400	-0.13162700
C	-5.08580000	-0.92952500	-0.08666500
H	-6.13350500	0.94304600	-0.25020500
H	-3.74710800	-2.61059200	0.06453200
C	0.69318500	1.51324900	-0.57495500
C	0.68372800	3.03597200	-0.48139200
H	-0.23666700	3.44624300	-0.91884600
H	1.48831300	3.43111500	-1.10206400
C	0.85214600	3.65077800	0.94922900
C	-0.18701500	3.08550700	1.93434600
C	2.26155600	3.37074700	1.50281600
C	0.65890900	5.17460500	0.82668200
H	-1.20978500	3.32501900	1.62732100
H	-0.10572000	1.99934900	2.01430600
H	-0.03381400	3.51382000	2.93058800
H	3.03449900	3.78684400	0.84965200
H	2.37529700	3.82951400	2.49143700
H	2.44791500	2.30011900	1.59342000
H	0.78579800	5.66347800	1.79838900
H	1.38738300	5.61112300	0.13534900
H	-0.34298700	5.42078300	0.45799600
C	-6.31653900	-1.75990300	-0.01675000
F	-7.41305100	-1.04534600	0.35152600
F	-6.64403100	-2.34341200	-1.20863000
F	-6.20946500	-2.78860000	0.86535800



## Complex 1

Zn	0.00028200	0.00020400	0.90691600
C	0.57818800	-3.69213300	-2.47957900
C	-0.58015600	3.69319100	-2.47854000
C	-0.78853800	-3.40724700	-2.34986900
H	-1.10029700	-2.56303400	-1.75465100
C	0.78685900	3.41028100	-2.34749000
H	1.09929100	2.56710400	-1.75116600
C	-1.72334000	-4.21552500	-2.99172100
H	-2.77913400	-3.98318200	-2.88561100
C	1.72107000	4.21915600	-2.98944600
H	2.77709400	3.98836500	-2.88223600
C	-1.32643000	-5.30274500	-3.76541200
H	-2.06385400	-5.92437100	-4.26313500
C	1.32330400	5.30506600	-3.76453700
H	2.06027900	5.92717300	-4.26232500
C	0.03388800	-5.57703000	-3.89474400
H	0.36530700	-6.41788900	-4.49655000
C	-0.03727800	5.57741300	-3.89516000
H	-0.36936200	6.41724100	-4.49803400
C	0.98285600	-4.78437200	-3.26026600
H	2.03912200	-4.98975100	-3.36058500
C	-0.98567600	4.78412100	-3.26062000
H	-2.04213100	4.98804200	-3.36189800
C	1.42216300	-1.88321700	-0.92243900
C	-1.42288800	1.88370600	-0.92134300
C	2.76037200	-1.46035800	-0.61562300
C	-2.76080600	1.45990300	-0.61455100
C	3.60463200	-2.30986600	-1.41475900
C	-3.60564000	2.30875800	-1.41378300
C	5.09792000	-2.37489400	-1.52815500
H	5.35701600	-3.19112500	-2.20349000
H	5.57681300	-2.55797200	-0.56276300
H	5.52382200	-1.45042300	-1.92573500
C	-5.09896300	2.37259600	-1.52738700
H	-5.35860200	3.18840200	-2.20302700
H	-5.57814200	2.55561600	-0.56212800
H	-5.52407200	1.44765400	-1.92472100
C	3.09558200	-0.41365500	0.28786800
C	-3.09530100	0.41317700	0.28917400
C	4.52482200	0.03400800	0.41044700
C	-4.52435200	-0.03492700	0.41238100
C	5.04852800	0.96101600	-0.49762400
H	4.42397900	1.32555200	-1.30675800
C	-5.04795800	-0.96270800	-0.49495000
H	-4.42347900	-1.32758600	-1.30398400
C	6.36531500	1.40112200	-0.37569900
H	6.76202100	2.11523100	-1.08999100
C	-6.36457800	-1.40317200	-0.37243100
H	-6.76121200	-2.11788200	-1.08615900
C	7.17136400	0.92070100	0.65444300
H	8.19840400	1.25896100	0.74496100
C	-7.17053400	-0.92234300	0.65758400
H	-8.19744500	-1.26086800	0.74856800
C	6.65428500	0.00382800	1.56810400
H	7.27805200	-0.37544400	2.37111400
C	-6.65353300	-0.00470900	1.57053500
H	-7.27723300	0.37485500	2.37346000
C	5.33634300	-0.43259200	1.45083900
H	4.93629200	-1.14946100	2.16096200
C	-5.33577200	0.43207700	1.45267200
H	-4.93577100	1.14951700	2.16224100
C	1.61169700	1.93630600	2.52127800
C	-1.60982900	-1.93633500	2.52195000
C	1.99186600	3.03247800	3.32632000
H	3.03526000	3.32081700	3.39843000
C	-1.98938200	-3.03250700	3.32728300
H	-3.03273100	-3.32079700	3.40023100
C	1.00975000	3.71671200	4.00842500
H	1.27714500	4.56492500	4.63018300
C	-1.00675600	-3.71673800	4.00864700
H	-1.27367700	-4.56495000	4.63061100
C	-0.33038200	3.31657900	3.89190900
H	-1.12517100	3.83690500	4.41150400
C	0.33328300	-3.31657000	3.89115600
H	1.12846000	-3.83688600	4.41016600
C	-0.60939400	2.23649000	3.07795300
H	-1.62530600	1.88404900	2.93250000

C	0.61167200	-2.23645000	3.07703500
H	1.62745800	-1.88394700	2.93086800
N	1.56747400	-2.90153500	-1.84834100
N	-1.56888500	2.90196000	-1.84720800
N	2.90187700	-3.15370700	-2.12782700
N	-2.90346000	3.15308400	-2.12683200
N	2.16773400	0.18525800	1.00648800
N	-2.16698100	-0.18535900	1.00750000
N	2.55317100	1.20903000	1.84983100
N	-2.55187400	-1.20899100	1.85132900
N	0.33027700	1.55352200	2.40450300
N	-0.32850700	-1.55352500	2.40423900
O	0.30998500	-1.47426200	-0.48762900
O	-0.31044500	1.47551200	-0.48650100
H	-3.49545200	-1.56497500	1.78548300
H	3.49705700	1.56431200	1.78419200

## Complex 2

Zn	0.00000000	0.00000000	0.75120800
S	-0.54782600	2.40894800	2.83534500
O	-0.86358300	-1.18293500	-0.65675000
O	0.53568800	1.54906500	2.33226700
N	-1.84646300	0.96409500	1.07986200
N	-2.45374800	-1.49133000	-2.33890500
O	-0.73874400	2.66972700	4.25027500
N	-1.93604900	1.57503800	2.33930500
H	-2.79631400	2.08568400	2.52358600
N	-3.69770700	-0.99847300	-2.70018200
C	-1.96945100	-0.88158400	-1.20283900
C	-2.97982400	0.05798200	-0.81635200
C	-2.94400700	0.86114400	0.35965600
C	-1.87837300	-2.53411400	-3.10352400
C	-4.01260000	-0.08914700	-1.81147100
C	-2.71442100	-3.33620500	-3.89010900
H	-3.77672900	-3.13343700	-3.89677700
C	-0.46667500	3.97837200	1.98062600
C	-0.44852200	6.42801900	0.64483500
C	-0.49673500	-2.76320100	-3.10262500
H	0.15131000	-2.13512700	-2.50956600
C	-2.17214400	-4.36026000	-4.65815400
H	-2.83082100	-4.97286200	-5.26588200
C	-0.00033900	4.03494800	0.66690600
H	0.36771000	3.14746500	0.16374100
C	-0.92429100	5.12088300	2.63881500
H	-1.26429000	5.05761000	3.66540900
C	-0.79906000	-4.60218900	-4.65292100
H	-0.37956900	-5.40009700	-5.25715700
C	-0.90760700	6.33638100	1.96495500
H	-1.25193100	7.22981700	2.47725500
C	0.02925100	-3.79668900	-3.87452500
H	1.10275100	-3.95875600	-3.87497000
C	0.00000000	5.26276000	0.01200300
H	0.36242700	5.30662800	-1.01029400
C	-5.30737700	0.64442900	-1.98726100
H	-5.77289900	0.30554000	-2.91338700
H	-5.15889300	1.72547600	-2.04927900
H	-6.00241100	0.46367200	-1.16395000
C	-0.40287200	7.75676700	-0.06631000
H	-1.18067800	8.43458300	0.29269900
H	-0.52500000	7.63891500	-1.14504000
H	0.56042200	8.25190600	0.09755900
C	-4.19519900	1.55284600	0.81747900
C	-5.17948000	0.83892800	1.50914300
H	-5.03700600	-0.21984000	1.69768900
C	-6.33417600	1.48224700	1.94823300
H	-7.09222800	0.92036200	2.48380200
C	-6.51601700	2.84170800	1.69969500
H	-7.41810800	3.34036300	2.03861000
C	-5.53541100	3.55988500	1.01834600
H	-5.67153300	4.61855600	0.82331900
C	-4.37558900	2.92104000	0.58374000
H	-3.61165300	3.47938100	0.05204600
S	0.54782600	-2.40894800	2.83534500
O	0.86358300	1.18293500	-0.65675000
O	-0.53568800	-1.54906500	2.33226700
N	1.84646300	-0.96409500	1.07986200
N	2.45374800	1.49133000	-2.33890500

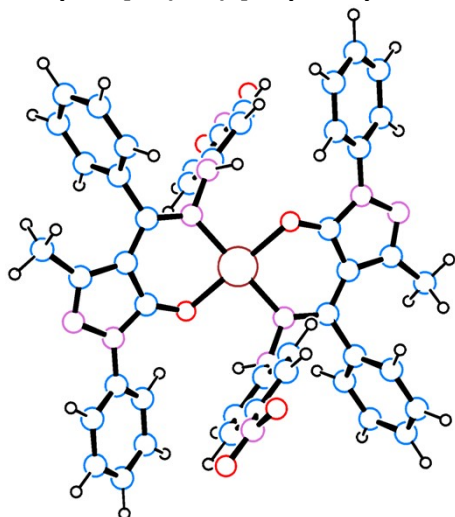
O	0.73874400	-2.66972700	4.25027500
N	1.93604900	-1.57503800	2.33930500
H	2.79631400	-2.08568400	2.52358600
N	3.69770700	0.99847300	-2.70018200
C	1.96945100	0.88158400	-1.20283900
C	2.97982400	-0.05798200	-0.81635200
C	2.94400700	-0.86114400	0.35965600
C	1.87837300	2.53411400	-3.10352400
C	4.01260000	0.08914700	-1.81147100
C	2.71442100	3.33620500	-3.89010900
H	3.77672900	3.13343700	-3.89677700
C	0.46667500	-3.97837200	1.98062600
C	0.44852200	-6.42801900	0.64483500
C	0.49673500	2.76320100	-3.10262500
H	-0.15131000	2.13512700	-2.50956600
C	2.17214400	4.36026000	-4.65815400
H	2.83082100	4.97286200	-5.26588200
C	0.00033900	-4.03494800	0.66690600
H	-0.36771000	-3.14746500	0.16374100
C	0.92429100	-5.12088300	2.63881500
H	1.26429000	-5.05761000	3.66540900
C	0.79906000	4.60218900	-4.65292100
H	0.37956900	5.40009700	-5.25715700
C	0.90760700	-6.33638100	1.96495500
H	1.25193100	-7.22981700	2.47725500
C	-0.02925100	3.79668900	-3.87452500
H	-1.10275100	3.95875600	-3.87497000
C	0.00000000	-5.26276000	0.01200300
H	-0.36242700	-5.30662800	-1.01029400
C	5.30737700	-0.64442900	-1.98726100
H	5.77289900	-0.30554000	-2.91338700
H	5.15889300	-1.72547600	-2.04927900
H	6.00241100	-0.46367200	-1.16395000
C	0.40287200	-7.75676700	-0.06631000
H	1.18067800	-8.43458300	0.29269900
H	0.52500000	-7.63891500	-1.14504000
H	-0.56042200	-8.25190600	0.09755900
C	4.19519900	-1.55284600	0.81747900
C	5.17948000	-0.83892800	1.50914300
H	5.03700600	0.21984000	1.69768900
C	6.33417600	-1.48224700	1.94823300
H	7.09222800	-0.92036200	2.48380200
C	6.51601700	-2.84170800	1.69969500
H	7.41810800	-3.34036300	2.03861000
C	5.53541100	-3.55988500	1.01834600
H	5.67153300	-4.61855600	0.82331900
C	4.37558900	-2.92104000	0.58374000
H	3.61165300	-3.47938100	0.05204600

### Complex 3

Zn	0.00001800	0.00028900	-0.00047100
C	-2.98060700	-3.51729200	1.76522800
C	-3.05223900	-2.62172500	2.83893700
H	-2.18616400	-2.03135900	3.10413900
C	-4.23629600	-2.51145400	3.56479100
H	-4.28396600	-1.81839200	4.39875900
C	-5.34416900	-3.29248700	3.24197900
H	-6.26135900	-3.20523400	3.81471700
C	-5.25717100	-4.19841700	2.18539400
H	-6.10873400	-4.82128500	1.93144200
C	-4.08508100	-4.31354600	1.44541100
H	-4.00445400	-5.01970700	0.62971500
C	-0.86892500	-2.66652500	0.71134700
C	0.10058400	-3.30688000	-0.13783800
C	-0.40505900	-4.65026500	-0.31383400
C	0.12286100	-5.78866100	-1.13212900
H	1.03552500	-6.21188900	-0.70714600
H	0.36184800	-5.48214600	-2.15297000
H	-0.63437400	-6.57262600	-1.16631600
C	1.30131900	-2.69084800	-0.59946000
C	3.68483300	-0.65891000	0.17397000
C	4.73968500	0.24678500	-0.07965800
H	4.76168600	0.79275700	-1.01683300
C	5.73636100	0.44534200	0.85373700
H	6.54467500	1.13917700	0.66566200
C	5.69968800	-0.25257600	2.06465300
C	4.66857900	-1.14323500	2.34176100

H	4.66424200	-1.67051700	3.28669200
C	3.66258800	-1.34652600	1.40514000
H	2.87126900	-2.05355500	1.61688600
N	-1.79451900	-3.63983400	1.00209700
N	-1.52156500	-4.83134400	0.34601300
N	1.47205600	-1.39254900	-0.43472400
N	2.73314700	-0.86115700	-0.81188300
H	2.58093200	-0.04060600	-1.38955600
N	6.75507900	-0.03985400	3.05506000
O	-0.94535900	-1.46796000	1.12191100
O	6.68436600	-0.66220900	4.11076700
O	7.65082600	0.75041700	2.77484000
C	2.98080400	3.51830100	-1.76585000
C	3.05316100	2.62213000	-2.83900800
H	2.18743400	2.03121700	-3.10413000
C	4.23746200	2.51200500	-3.56448600
H	4.28568700	1.81847900	-4.39803700
C	5.34486400	3.29377800	-3.24185000
H	6.26224700	3.20664300	-3.81429800
C	5.25712900	4.20031300	-2.18584800
H	6.10831000	4.82377000	-1.93206100
C	4.08478400	4.31532200	-1.44624900
H	4.00358000	5.02196000	-0.63102200
C	0.86934900	2.66710600	-0.71187900
C	-0.10066800	3.30747400	0.13669100
C	0.40423000	4.65122900	0.31194800
C	-0.12454700	5.78992300	1.12927100
H	-1.03796500	6.21163100	0.70441000
H	-0.36255700	5.48421900	2.15059200
H	0.63184100	6.57475600	1.16219500
C	-1.30111900	2.69121900	0.59860100
C	-3.68477200	0.65861900	-0.17341300
C	-4.73960600	-0.24681200	0.08124200
H	-4.76135200	-0.79208300	1.01882800
C	-5.73659000	-0.44598900	-0.85168800
H	-6.54489900	-1.13961500	-0.66283000
C	-5.70022700	0.25098400	-2.06316100
C	-4.66910600	1.14130200	-2.34130500
H	-4.66498600	1.66781000	-3.28666900
C	-3.66281400	1.34524700	-1.40514300
H	-2.87142200	2.05195200	-1.61769600
N	1.79443200	3.64074500	-1.00314300
N	1.52067400	4.83255900	-0.34793600
N	-1.47188500	1.39291300	0.43384300
N	-2.73275200	0.86162400	0.81193500
H	-2.58031600	0.04158600	1.39027100
N	-6.75594400	0.03759000	-3.05307800
O	0.94655500	1.46829600	-1.12161900
O	-6.68545700	0.65905400	-4.10932500
O	-7.65170600	-0.75234600	-2.77195500
O	1.15001700	0.72009600	1.77738300
H	1.94684700	0.22598800	2.01141400
O	-1.15007700	-0.72033500	-1.77734700
H	-1.94886100	-0.22886900	-2.01029500
H	1.34804100	1.66062600	1.84455600
H	-1.34461100	-1.66155300	-1.84528400
C	2.36284600	-3.51942500	-1.25470300
C	2.60917600	-3.37737700	-2.62446700
C	3.11090000	-4.43830200	-0.51619800
C	3.57998700	-4.15501700	-3.24665200
H	2.03465700	-2.65936200	-3.20015200
C	4.09721600	-5.20236800	-1.13710300
H	2.92316600	-4.55718600	0.54577700
C	4.32941800	-5.06646500	-2.50310700
H	3.75735700	-4.04478100	-4.31147600
H	4.68020300	-5.90615400	-0.55224600
H	5.09231700	-5.66686300	-2.98767700
C	-2.36249600	3.51954800	1.25439500
C	-3.11227700	4.43707600	0.51598400
C	-2.60692900	3.37855400	2.62460300
C	-4.09839400	5.20093800	1.13747300
H	-2.92598900	4.55515700	-0.54633400
C	-3.57763100	4.15590300	3.24730200
H	-2.03104100	2.66152400	3.20016900
C	-4.32875100	5.06607300	2.50388900
H	-4.68268800	5.90373200	0.55272900
H	-3.75357900	4.04647700	4.31244700
H	-5.09152900	5.66627600	2.98889200

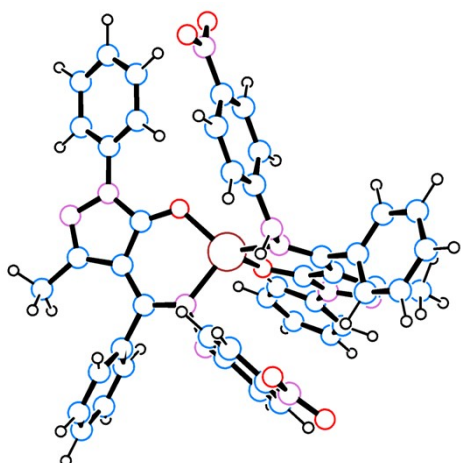
Complex  $[Zn(HL^3)_2]$ , square planar,  $3'_{sqp}$



Zn	0.00000300	0.00030600	-0.00024500
C	3.40900600	-3.00798300	-1.88446700
C	3.32699900	-2.09947600	-2.94501000
H	2.37944300	-1.63605200	-3.18350800
C	4.46498500	-1.81562600	-3.69698600
H	4.39501900	-1.11429100	-4.52231800
C	5.67810300	-2.43816900	-3.41044100
H	6.55967700	-2.21720200	-4.00274000
C	5.74541400	-3.35936300	-2.36578300
H	6.68205700	-3.85858200	-2.14027700
C	4.61983600	-3.64587700	-1.60047200
H	4.65898400	-4.36324100	-0.79156400
C	1.23907000	-2.47790400	-0.74641400
C	0.37313000	-3.26625100	0.08037700
C	1.04739400	-4.54026600	0.19581300
C	0.68342600	-5.75895900	0.98552600
H	-0.20036800	-6.25968500	0.58523500
H	0.46621800	-5.51394900	2.02787300
H	1.52014800	-6.45741900	0.95538800
C	-0.87954100	-2.81959400	0.56938100
C	-3.39854000	-0.95253100	-0.26782700
C	-4.59199600	-0.24262600	-0.02489300
H	-4.80131000	0.12854600	0.97256900
C	-5.49141900	-0.01096700	-1.04675800
H	-6.40698500	0.53741500	-0.87116500
C	-5.21065900	-0.48633600	-2.32949000
C	-4.03625300	-1.18224100	-2.59328900
H	-3.84179600	-1.53153100	-3.59859600
C	-3.13194600	-1.41696000	-1.56697700
H	-2.21212000	-1.94683700	-1.77479700
N	2.26907000	-3.30552000	-1.09674500
N	2.16295500	-4.54963900	-0.48752800
N	-1.20177800	-1.53434500	0.49439800
N	-2.54744300	-1.20879400	0.80867200
H	-2.55331900	-0.45273800	1.48397500
N	-6.16228400	-0.23978100	-3.41535500
O	1.13708800	-1.26056800	-1.11689000
O	-5.88200000	-0.66687700	-4.53110700
O	-7.18628300	0.38060600	-3.14807700
C	-3.40911300	3.00905200	1.88315500
C	-3.32746000	2.10063700	2.94380000
H	-2.37999900	1.63716900	3.18259600
C	-4.46567500	1.81691800	3.69547800
H	-4.39598700	1.11565300	4.52089300
C	-5.67867400	2.43950600	3.40852300
H	-6.56043000	2.21864700	4.00059100
C	-5.74563900	3.36060300	2.36375800
H	-6.68219400	3.85984300	2.13793200
C	-4.61982400	3.64698100	1.59874300
H	-4.65870000	4.36426600	0.78975200
C	-1.23896600	2.47869400	0.74565400
C	-0.37260700	3.26698900	-0.08074900
C	-1.04658000	4.54115500	-0.19621600
C	-0.68210700	5.75989500	-0.98562300
H	0.20175800	6.26028800	-0.58507000

H	-0.46477300	5.51502400	-2.02797800
H	-1.51863500	6.45858800	-0.95551100
C	0.88013600	2.82015800	-0.56940000
C	3.39840200	0.95207800	0.26834200
C	4.59175500	0.24193500	0.02558100
H	4.80140600	-0.12878800	-0.97197600
C	5.49062800	0.00945900	1.04774100
H	6.40610000	-0.53912600	0.87228500
C	5.20942700	0.48424400	2.33059600
C	4.03513000	1.18040300	2.59421000
H	3.84032900	1.52925000	3.59960400
C	3.13137000	1.41594200	1.56760400
H	2.21162100	1.94601900	1.77525800
N	-2.26892000	3.30645700	1.09575400
N	-2.16235600	4.55065200	0.48677200
N	1.20213400	1.53485000	-0.49443200
N	2.54782800	1.20910100	-0.80838100
H	2.55377400	0.45336600	-1.48404600
N	6.16045800	0.23679500	3.41677500
O	-1.13733000	1.26129600	1.11601900
O	5.87978100	0.66337500	4.53262400
O	7.18437600	-0.38378000	3.14964600
C	-1.85427100	-3.80406300	1.13326200
C	-2.15295500	-3.80162700	2.49955300
C	-2.46428600	-4.74269200	0.29862200
C	-3.03953100	-4.73645100	3.02354200
H	-1.68334700	-3.07282700	3.15174800
C	-3.36917700	-5.66398600	0.82202800
H	-2.23538600	-4.74914600	-0.76179800
C	-3.65346800	-5.66646500	2.18504500
H	-3.25700200	-4.73513000	4.08658600
H	-3.84793000	-6.38112500	0.16355800
H	-4.35162200	-6.38934500	2.59402000
C	1.85523200	3.80451200	-1.13285300
C	2.46531600	4.74277200	-0.29784900
C	2.15418400	3.80234700	-2.49908200
C	3.37054900	5.66396700	-0.82083700
H	2.23619800	4.74901200	0.76252500
C	3.04110800	4.73707700	-3.02265400
H	1.68451300	3.07384100	-3.15156100
C	3.65511500	5.66672000	-2.18379800
H	3.84935000	6.38081800	-0.16209000
H	3.25879400	4.73597100	-4.08565400
H	4.35353500	6.38952500	-2.59244900

### Complex $[\text{Zn}(\text{HL}^3)_2]$ , distorted tetrahedral, $3'T_d$

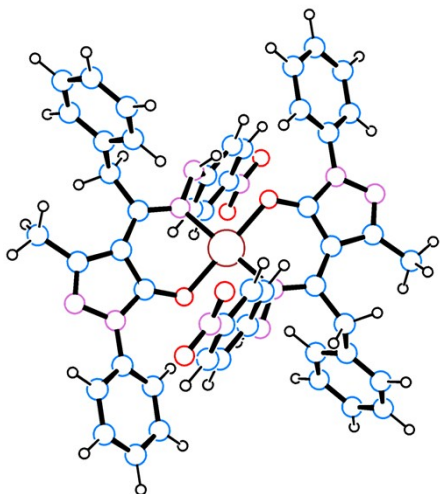


Zn	-0.28223300	-0.27823500	-0.35380600
C	-5.17493600	-0.36823700	-0.43883600
C	-4.89431900	0.97126200	-0.72329300
H	-3.94976000	1.40116200	-0.42393300
C	-5.84144200	1.74343500	-1.39185800
H	-5.62754100	2.78777500	-1.59474100
C	-7.06157600	1.19228700	-1.77647200
H	-7.79608800	1.80155800	-2.29257500
C	-7.33465600	-0.14285200	-1.48489400
H	-8.28414400	-0.58125600	-1.77504000

C	-6.39904100	-0.92641000	-0.81820900
H	-6.60728600	-1.95875400	-0.57148800
C	-2.88682200	-1.07736000	0.33431500
C	-2.45298100	-2.15895800	1.18169700
C	-3.67735900	-2.84477000	1.53584200
C	-3.90751300	-4.04405000	2.40213200
H	-3.51657800	-3.90030700	3.41178100
H	-3.42839400	-4.93927200	1.99935600
H	-4.98125700	-4.22239200	2.46572300
C	-1.11542700	-2.42204400	1.54962100
C	1.97345100	-1.08503200	2.15937100
C	3.37794500	-1.20406600	2.08283400
H	3.81722500	-2.00517900	1.49669200
C	4.19727700	-0.30564800	2.73801800
H	5.27460600	-0.38150800	2.67267600
C	3.62816200	0.72647500	3.48748500
C	2.24457400	0.84892600	3.59869800
H	1.83391500	1.64222200	4.21011100
C	1.41911500	-0.04479800	2.93547100
H	0.34329500	0.03804300	3.02208800
N	-4.24413900	-1.18057600	0.26774500
N	-4.71605200	-2.26431600	0.99707800
N	-0.13372300	-1.61706600	1.15173200
N	1.17251900	-2.00753000	1.52695100
H	1.62602400	-2.59257000	0.83631400
N	4.49319600	1.70283500	4.14639700
O	-2.21647300	-0.17642600	-0.27500500
O	3.96722700	2.52827700	4.88574600
O	5.69779500	1.64770900	3.91197800
C	2.15220900	-2.80218400	-3.85107300
C	0.88562500	-3.39541500	-3.78323800
H	0.07752000	-2.88656600	-3.28056400
C	0.68122300	-4.64159500	-4.37044100
H	-0.30499500	-5.09190800	-4.31808700
C	1.71582200	-5.30247900	-5.02706900
H	1.54521600	-6.27150400	-5.48427400
C	2.97096400	-4.70105200	-5.09692100
H	3.78669400	-5.19988100	-5.61036000
C	3.19562200	-3.45911500	-4.51397400
H	4.16361300	-2.98150100	-4.57277500
C	1.68454700	-0.84234900	-2.33645500
C	2.42657700	0.36426300	-2.07489400
C	3.59234300	0.25546400	-2.92832200
C	4.74740700	1.18710500	-3.12515200
H	4.42506800	2.16673500	-3.48399100
H	5.30011000	1.35482700	-2.19835100
H	5.42226400	0.75032800	-3.86175100
C	2.04097600	1.38410200	-1.17857400
C	-0.51675300	3.10160800	0.22534300
C	-0.99404700	3.90564500	1.28196200
H	-0.45562900	3.93168300	2.22435300
C	-2.13542900	4.66697500	1.12474300
H	-2.50997400	5.28716000	1.92808800
C	-2.82460500	4.62897800	-0.08908400
C	-2.36853900	3.84519200	-1.14571400
H	-2.91734500	3.83821000	-2.07776800
C	-1.21991100	3.08773800	-0.99394700
H	-0.86166700	2.48283100	-1.81625700
N	2.40869300	-1.53101600	-3.26926600
N	3.57183500	-0.85377800	-3.61709700
N	0.91973300	1.29598500	-0.45928600
N	0.65908300	2.39845500	0.38399200
H	0.99783100	2.27056700	1.32883500
N	-4.04398800	5.41784700	-0.25130000
O	0.59113100	-1.25789600	-1.83588600
O	-4.67249700	5.29302400	-1.30106000
O	-4.37440700	6.15992000	0.66682100
C	-0.78172000	-3.62344100	2.38031500
C	-0.59958400	-4.86444300	1.76457900
C	-0.63656500	-3.51394800	3.76532100
C	-0.27665200	-5.98441200	2.52763300
H	-0.71690100	-4.95502200	0.68917100
C	-0.31919200	-4.63609000	4.52586600
H	-0.77550400	-2.55258400	4.24900300
C	-0.13782300	-5.87275300	3.90924300
H	-0.13673300	-6.94421100	2.04124400
H	-0.21195200	-4.54325400	5.60157200
H	0.10988900	-6.74583900	4.50376600

C	2.91009300	2.59241700	-1.00303800
C	2.71573300	3.72966800	-1.78965800
C	3.91839900	2.58617000	-0.03560500
C	3.52614000	4.84804700	-1.60989500
H	1.93109900	3.74254200	-2.53901900
C	4.72673300	3.70637600	0.14271900
H	4.07299700	1.70417000	0.57713500
C	4.53195600	4.83905800	-0.64517900
H	3.36828000	5.72893000	-2.22338000
H	5.50411300	3.69065400	0.89952200
H	5.16063900	5.71229300	-0.50673600

### Complex mononuclear [Zn(HL<sup>4</sup>)<sub>2</sub>]

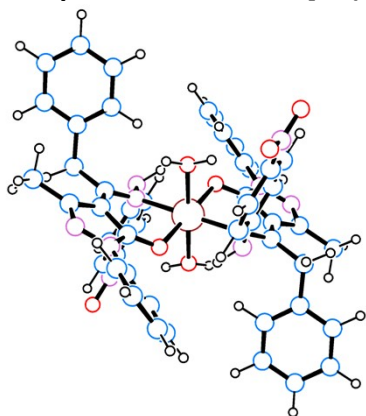


Zn	0.00001900	0.00107600	-0.00082100
C	-4.06720900	-0.54452000	2.70170600
C	-3.71991000	0.75029300	3.10087600
H	-2.67771700	1.02904000	3.17440800
C	-4.72245200	1.66445700	3.41767200
H	-4.44775000	2.66686100	3.72988800
C	-6.06451100	1.29521900	3.35398500
H	-6.84066200	2.00978600	3.60648200
C	-6.40090600	-0.00452300	2.97701600
H	-7.44227400	-0.30634400	2.93449200
C	-5.41101800	-0.92493500	2.64845500
H	-5.65987500	-1.93761800	2.36006300
C	-1.85978600	-1.27266400	1.76161900
C	-1.25142800	-2.56377900	1.62735900
C	-2.24117000	-3.47860000	2.15398500
C	-2.22981900	-4.97234900	2.26509400
H	-1.54508600	-5.32027100	3.04516000
H	-1.93709200	-5.45296500	1.32955200
H	-3.23143100	-5.30840100	2.53394700
C	0.07648100	-2.77108700	1.17296100
C	0.73325100	-4.12824100	1.30824200
H	0.33049700	-4.63409800	2.18433100
H	1.79790800	-3.97643300	1.48948200
C	0.57986800	-5.03378500	0.09024400
C	0.81348200	-6.40568000	0.24496200
H	1.06970600	-6.79767200	1.22541100
C	0.72317300	-7.27389600	-0.83835500
H	0.90791000	-8.33373800	-0.69504100
C	0.39112700	-6.78562800	-2.10126800
H	0.31436600	-7.46149400	-2.94652600
C	0.15403000	-5.42466200	-2.26667400
H	-0.11121000	-5.03308900	-3.24352800
C	0.24994600	-4.55554700	-1.17981600
H	0.05661600	-3.49890800	-1.33060800
C	3.03293000	-1.31547300	1.20426700
C	4.35308000	-1.12538700	0.74969400
H	4.62923300	-1.44707400	-0.24853600
C	5.29510100	-0.52609200	1.56317100
H	6.30919900	-0.36951500	1.22134200
C	4.92939000	-0.10795000	2.84398500
C	3.63118300	-0.28127000	3.31076400



H	3.37653800	0.05703300	4.30630700
C	2.68376300	-0.88496700	2.49562500
H	1.67184000	-1.01614800	2.85529000
N	-3.06764900	-1.49081300	2.36317800
N	-3.30560600	-2.84134600	2.56949300
N	0.75070700	-1.75766000	0.64086700
N	2.12860100	-1.98609900	0.37565000
H	2.31505600	-1.81590400	-0.60618400
N	5.92657500	0.53188800	3.70682200
O	-1.43340900	-0.11862500	1.41858200
O	5.56949000	0.89424500	4.82321100
O	7.06169800	0.66917800	3.26318000
C	4.06881600	0.54907300	-2.70066500
C	3.72222000	-0.74534700	-3.10167300
H	2.68015700	-1.02417500	-3.17684200
C	4.72529800	-1.65901500	-3.41819200
H	4.45115900	-2.66112600	-3.73184100
C	6.06721600	-1.28962000	-3.35239900
H	6.84380300	-2.00378600	-3.60469100
C	6.40293500	0.00975900	-2.97357500
H	7.44420200	0.31168800	-2.92939600
C	5.41247900	0.92965400	-2.64527500
H	5.66080800	1.94206400	-2.35546200
C	1.86042600	1.27595900	-1.76191900
C	1.25130700	2.56674600	-1.62790500
C	2.24102100	3.48217700	-2.15350600
C	2.22902100	4.97595100	-2.26422700
H	1.54479700	5.32374100	-3.04479700
H	1.93524300	5.45617900	-1.32881000
H	3.23069700	5.31257900	-2.53211500
C	-0.07707600	2.77327700	-1.17458000
C	-0.73452200	4.13003700	-1.31023200
H	-0.33118300	4.63634400	-2.18579500
H	-1.79889100	3.97746700	-1.49259200
C	-0.58308300	5.03546200	-0.09189700
C	-0.81824500	6.40710900	-0.24647300
H	-1.07430700	6.79899900	-1.22700500
C	-0.72970000	7.27520000	0.83708600
H	-0.91563400	8.33484700	0.69387900
C	-0.39789900	6.78706500	2.10011800
H	-0.32252100	7.46284400	2.94557000
C	-0.15925600	5.42635500	2.26538800
H	0.10582900	5.03489300	3.24233000
C	-0.25339300	4.55735800	1.17827400
H	-0.05883700	3.50092800	1.32898200
C	-3.03267700	1.31334500	-1.20563300
C	-4.35257900	1.12246500	-0.75068000
H	-4.62925900	1.44612700	0.24676600
C	-5.29366400	0.51980500	-1.56275700
H	-6.30755400	0.36256400	-1.22061500
C	-4.92725000	0.09906600	-2.84251700
C	-3.62927900	0.27317200	-3.30966000
H	-3.37410100	-0.06711700	-4.30438900
C	-2.68280100	0.88025800	-2.49594400
H	-1.67108100	1.01224200	-2.85589500
N	3.06862700	1.49484400	-2.36249400
N	3.30611500	2.84554200	-2.56828500
N	-0.75115200	1.75942000	-0.64310800
N	-2.12928300	1.98715300	-0.37865100
H	-2.31584000	1.81960500	0.60362100
N	-5.92342900	-0.54437100	-3.70385200
O	1.43434500	0.12164500	-1.41939200
O	-5.56567400	-0.90908500	-4.81925800
O	-7.05843100	-0.68205900	-3.26003400

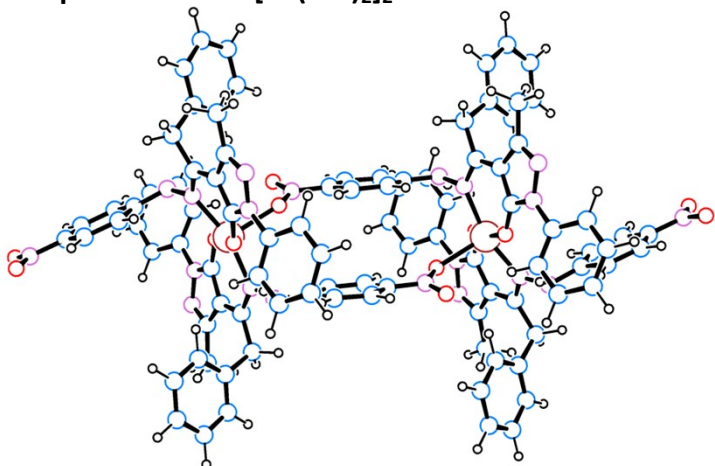
### Complex mononuclear [Zn(HL<sup>4</sup>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]



Zn	0.00000100	0.00005100	-0.00010100
C	-3.67906800	1.66772600	-2.83761700
C	-3.56176000	0.37386700	-3.35834200
H	-2.59229300	-0.10273200	-3.39913500
C	-4.69538400	-0.28251800	-3.83294700
H	-4.59674400	-1.28477900	-4.23742700
C	-5.94086700	0.34158300	-3.80740500
H	-6.81899800	-0.17325600	-4.18243700
C	-6.04536300	1.63984200	-3.30904000
H	-7.00753300	2.14147600	-3.29552700
C	-4.92424700	2.30432900	-2.82273300
H	-4.99281900	3.31487200	-2.44229300
C	-1.44422900	1.82917000	-1.70595600
C	-0.62713600	2.96005800	-1.35458300
C	-1.38857200	4.10270200	-1.81168000
C	-1.09743600	5.57088200	-1.73875800
H	-0.28414700	5.86146700	-2.41162300
H	-0.82338000	5.89029100	-0.73161400
H	-1.98971900	6.11534200	-2.04878500
C	0.68346400	2.86750700	-0.79308900
C	1.53447500	4.11074100	-0.61564300
H	1.34604700	4.79875700	-1.43857300
H	2.58465300	3.82402000	-0.67924100
C	1.32043600	4.83710200	0.70800800
C	1.65689900	6.19338600	0.79431200
H	2.02647500	6.71056300	-0.08687800
C	1.52627400	6.88929300	1.99249800
H	1.79302000	7.94048400	2.03589800
C	1.05024800	6.24002400	3.13022900
H	0.94342700	6.78116600	4.06462900
C	0.71143800	4.89219700	3.05568800
H	0.33884400	4.37554100	3.93466200
C	0.84757200	4.19417300	1.85556800
H	0.57708200	3.14445200	1.82428900
C	3.44712000	1.14875100	-0.85604300
C	4.64875800	0.61815800	-0.33727400
H	4.78331900	0.54878800	0.73679900
C	5.64886100	0.18403400	-1.18420200
H	6.56960100	-0.22776300	-0.79323100
C	5.46801500	0.26748400	-2.56764500
C	4.29334600	0.78346400	-3.10332100
H	4.18156300	0.84009300	-4.17814700
C	3.28366500	1.22169700	-2.25496300
H	2.37801500	1.64209300	-2.67350700
N	-2.54651900	2.35415500	-2.33520700
N	-2.51510200	3.73800100	-2.37087600
N	1.14336000	1.68284900	-0.43448000
N	2.48889500	1.62700500	0.02707500
H	2.50719400	1.14748900	0.92218000
N	6.52669600	-0.19833400	-3.46541000
O	-1.27900600	0.58600000	-1.49818200
O	6.32651200	-0.12342800	-4.67378800
O	7.55269500	-0.63884000	-2.95774800
C	3.67887400	-1.66749100	2.83773500
C	3.56144700	-0.37365400	3.35849900
H	2.59195900	0.10291000	3.39917800
C	4.69497700	0.28274700	3.83330000
H	4.59624100	1.28498700	4.23781200
C	5.94048900	-0.34130600	3.80791300

H	6.81854600	0.17354900	4.18309900
C	6.04510200	-1.63953700	3.30950600
H	7.00729100	-2.14113600	3.29610400
C	4.92407900	-2.30404500	2.82300900
H	4.99274800	-3.31456800	2.44253600
C	1.44414700	-1.82900800	1.70583700
C	0.62716300	-2.95993900	1.35432600
C	1.38863500	-4.10255400	1.81143100
C	1.09760500	-5.57074700	1.73838100
H	0.28426600	-5.86144100	2.41113800
H	0.82366300	-5.89010200	0.73118700
H	1.98989200	-6.11517200	2.04845600
C	-0.68345100	-2.86742300	0.79285400
C	-1.53444800	-4.11066300	0.61539500
H	-1.34608200	-4.79866900	1.43834800
H	-2.58462500	-3.82391600	0.67890300
C	-1.32031600	-4.83702600	-0.70823600
C	-1.65639000	-6.19340500	-0.79449400
H	-2.02571800	-6.71068500	0.08674000
C	-1.52570200	-6.88928400	-1.99269400
H	-1.79214800	-7.94055300	-2.03605200
C	-1.04999400	-6.23988800	-3.13048200
H	-0.94312400	-6.78100600	-4.06488900
C	-0.71155600	-4.89196200	-3.05598800
H	-0.33920500	-4.37520900	-3.93500700
C	-0.84776000	-4.19397200	-1.85586000
H	-0.57754600	-3.14417800	-1.82460900
C	-3.44713200	-1.14882800	0.85604400
C	-4.64874600	-0.61803300	0.33743700
H	-4.78332400	-0.54837900	-0.73661500
C	-5.64881500	-0.18409000	1.18450300
H	-6.56954000	0.22786200	0.79366200
C	-5.46795000	-0.26793300	2.56791700
C	-4.29329700	-0.78412400	3.10343600
H	-4.18151300	-0.84106100	4.17824700
C	-3.28365900	-1.22217300	2.25494000
H	-2.37802100	-1.64273400	2.67334400
N	2.54642500	-2.35395800	2.33515100
N	2.51510500	-3.73780800	2.37071100
N	-1.14336600	-1.68276600	0.43425500
N	-2.48894600	-1.62693600	-0.02721500
H	-2.50730700	-1.14725700	-0.92223700
N	-6.52658800	0.19769000	3.46582800
O	1.27885700	-0.58584100	1.49813000
O	-6.32637400	0.12243600	4.67418200
O	-7.55254800	0.63845200	2.95831000
O	1.21153600	-1.22610500	-1.43964700
H	1.83842200	-0.73559600	-1.98745400
O	-1.21148300	1.22612800	1.43954000
H	-1.83789300	0.73537800	1.98767200
H	1.64335900	-2.03154500	-1.13348500
H	-1.64405900	2.03106100	1.13310100

### Complex dinuclear $[Zn(HL^4)]_2$



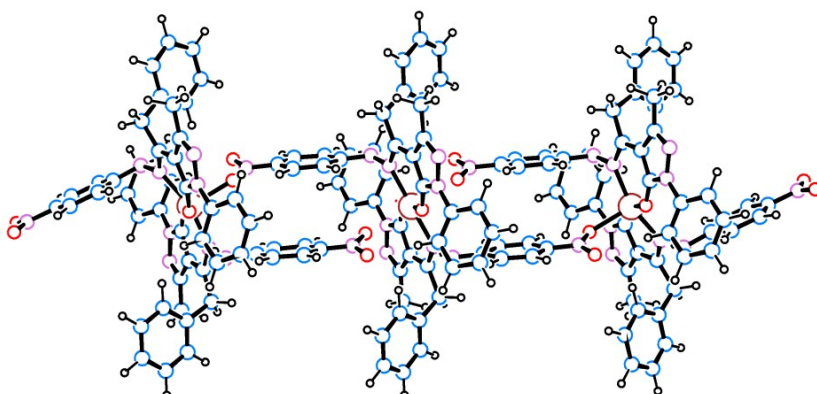
C	3.12591800	-0.12420900	5.11623600
C	3.50423300	1.22272500	5.11422400

H	4.38676900	1.53152300	4.57003800
C	2.75746900	2.15036800	5.83779100
H	3.06261800	3.19202700	5.83971400
C	1.64507800	1.74554600	6.57356500
H	1.07259500	2.47006000	7.14309600
C	1.28773400	0.39753700	6.58918300
H	0.43281100	0.06858700	7.17105500
C	2.01949700	-0.53731900	5.86433700
H	1.76040600	-1.58796200	5.88051900
C	4.49677200	-0.94012900	3.18143300
C	5.09423100	-2.21007500	2.89829000
C	4.69837300	-3.04354600	4.01062700
C	4.97267600	-4.48774300	4.29990800
H	6.01885300	-4.66024300	4.57229400
H	4.74338200	-5.13038800	3.44782600
H	4.35846000	-4.79413400	5.14709700
C	5.95465800	-2.45959900	1.78925100
C	6.73555100	-3.75746000	1.70061100
H	6.96987500	-4.10609100	2.70501600
H	7.68789800	-3.55788500	1.20879500
C	6.02532500	-4.86766900	0.93351100
C	6.34354000	-6.20024400	1.22109800
H	7.05823300	-6.42268100	2.00862300
C	5.76071000	-7.24546800	0.50992500
H	6.02317300	-8.27113300	0.74949700
C	4.84186400	-6.97575200	-0.50272400
H	4.38448200	-7.78896900	-1.05699800
C	4.51664300	-5.65428400	-0.79548200
H	3.80378100	-5.42722400	-1.58186800
C	5.10473300	-4.60868000	-0.08512900
H	4.83554200	-3.58874200	-0.33239700
C	8.29146300	-1.11506600	-0.00068900
C	9.11991900	-0.98422400	-1.13437600
H	8.77376000	-1.34683000	-2.09621800
C	10.36422300	-0.39418600	-1.03036200
H	11.00402200	-0.28458300	-1.89548000
C	10.80081900	0.07450200	0.21059500
C	9.99773500	-0.03999500	1.34063800
H	10.35942000	0.33833900	2.28751400
C	8.74748600	-0.63256000	1.23841700
H	8.11859400	-0.71106400	2.11520100
N	3.86904100	-1.08543400	4.39074000
N	3.96867300	-2.38038200	4.87361600
N	6.08237900	-1.53773200	0.84970700
N	7.07272700	-1.78064900	-0.14191200
H	6.66071000	-1.63400100	-1.05694200
N	12.11792000	0.70268000	0.32220100
O	4.48766900	0.14301300	2.50548700
O	12.79972500	0.78795600	-0.69457700
C	6.87715300	0.38115300	-3.95778000
C	6.36118000	-0.91935900	-3.99784500
H	5.46513400	-1.16282000	-3.44376600
C	7.00626500	-1.88905000	-4.76278400
H	6.60264500	-2.89615000	-4.78951400
C	8.14757700	-1.57374000	-5.49711700
H	8.64256900	-2.33349500	-6.09272400
C	8.64129800	-0.26993600	-5.46829200
H	9.52430300	-0.00933700	-6.04276700
C	8.01505900	0.70736600	-4.70192600
H	8.38708000	1.72288400	-4.67525600
C	5.56059600	1.24413800	-2.00497200
C	5.17363600	2.57092600	-1.61717200
C	5.75449100	3.42061200	-2.63557200
C	5.74746700	4.91044900	-2.79582900
H	4.75427500	5.29353500	-3.05220600
H	6.08015400	5.42351400	-1.89096900
H	6.42129500	5.17230100	-3.61182600
C	4.35181100	2.86288700	-0.50010200
C	3.93793100	4.29229600	-0.21245700
H	3.84226500	4.83296200	-1.15219300
H	2.94804100	4.29565300	0.24416900
C	4.89322200	5.05016600	0.70464500
C	4.80707200	6.44693300	0.75155900
H	4.08731500	6.96031000	0.11962400
C	5.62944700	7.18694700	1.59554300
H	5.54667200	8.26897400	1.61478200
C	6.56085100	6.54125600	2.40725600
H	7.20809200	7.11590700	3.06152100

C	6.65805700	5.15390600	2.36590000
H	7.38466000	4.64042600	2.98730500
C	5.82914800	4.41375100	1.52289800
H	5.92433200	3.33359800	1.50537300
C	1.70785300	2.07376500	1.16523000
C	0.87135400	2.15466300	2.30788800
H	1.31788800	2.28547400	3.28736800
C	-0.49348200	2.06184800	2.18252300
H	-1.13576300	2.12633300	3.05077400
C	-1.05879800	1.84347700	0.91516200
C	-0.25073700	1.75049500	-0.22393900
H	-0.70798400	1.57317600	-1.18803800
C	1.11639300	1.89234200	-0.10562400
H	1.74406000	1.82638100	-0.98380900
N	6.25216700	1.38588000	-3.17790000
N	6.38791000	2.71753300	-3.53859600
N	3.94726400	1.87414300	0.29175600
N	3.05906600	2.23105500	1.33477600
H	3.41809900	1.90699700	2.22787500
N	-2.47245000	1.68069700	0.80733300
O	5.36188500	0.12627300	-1.43323800
O	-3.19781900	2.03063900	1.73053200
Zn	-4.76650800	0.01303700	-0.48972300
O	12.46816800	1.10983800	1.42612400
C	-6.87991100	-0.38085400	3.95726800
C	-6.36395400	0.91965100	3.99758300
H	-5.46736400	1.16298000	3.44431400
C	-7.00971200	1.88948400	4.76177000
H	-6.60609700	2.89658200	4.78872000
C	-8.15170200	1.57430800	5.49511500
H	-8.64721900	2.33417200	6.09014700
C	-8.64541200	0.27050600	5.46607100
H	-9.52894000	0.01001500	6.03979100
C	-8.01848400	-0.70693400	4.70043700
H	-8.39049000	-1.72245500	4.67360700
C	-5.56227200	-1.24416200	2.00538200
C	-5.17447800	-2.57092300	1.61836200
C	-5.75530500	-3.42041400	2.63694100
C	-5.74755400	-4.91016600	2.79796700
H	-4.75420700	-5.29262900	3.05467300
H	-6.07988000	-5.42386600	1.89333300
H	-6.42136300	-5.17192800	3.61401100
C	-4.35215100	-2.86299800	0.50167900
C	-3.93818000	-4.29246500	0.21441000
H	-3.84245500	-4.83287200	1.15428900
H	-2.94832200	-4.29590800	-0.24227600
C	-4.89350000	-5.05058400	-0.70245000
C	-4.80770100	-6.44739500	-0.74868300
H	-4.08819200	-6.96065800	-0.11637300
C	-5.63011500	-7.18759700	-1.59247100
H	-5.54762100	-8.26965400	-1.61117800
C	-6.56119800	-6.54204800	-2.40466300
H	-7.20846800	-7.11684100	-3.05877600
C	-6.65804800	-5.15465000	-2.36398900
H	-7.38439600	-4.64127300	-2.98577700
C	-5.82910600	-4.41431900	-1.52118300
H	-5.92400500	-3.33413400	-1.50417500
C	-1.70787500	-2.07454100	-1.16361500
C	-0.87142100	-2.15599700	-2.30627200
H	-1.31801900	-2.28704000	-3.28569300
C	0.49344700	-2.06351700	-2.18097200
H	1.13568900	-2.12849200	-3.04921600
C	1.05883400	-1.84482900	-0.91370400
C	0.25083400	-1.75125600	0.22538400
H	0.70814900	-1.57373600	1.18941600
C	-1.11634200	-1.89284600	0.10715700
H	-1.74396800	-1.82653100	0.98534700
N	-6.25420700	-1.38569300	3.17811600
N	-6.38943000	-2.71723300	3.53939900
N	-3.94734800	-1.87438700	-0.29021400
N	-3.05912400	-2.23161200	-1.33313200
H	-3.41808000	-1.90760200	-2.22628500
N	2.47257600	-1.68255200	-0.80591800
O	-5.36408000	-0.12648100	1.43313500
O	2.92155900	-1.16836700	0.24964600
O	3.19786500	-2.03380200	-1.72868200
C	-3.12512600	0.12108900	-5.11533200
C	-3.50411200	-1.22565500	-5.11260100

H	-4.38680400	-1.53373400	-4.56826600
C	-2.75777300	-2.15406100	-5.83562900
H	-3.06342900	-3.19557200	-5.83697200
C	-1.64516000	-1.75019400	-6.57158800
H	-1.07301600	-2.47530200	-7.14070500
C	-1.28714400	-0.40237000	-6.58792300
H	-0.43203000	-0.07416100	-7.16993200
C	-2.01846500	0.53324200	-5.86361000
H	-1.75883700	1.58374200	-5.88033900
C	-4.49572900	0.93874700	-3.18107600
C	-5.09238500	2.20920600	-2.89855400
C	-4.69589100	3.04190700	-4.01124100
C	-4.96923100	4.48614700	-4.30122900
H	-6.01524100	4.65917700	-4.57392300
H	-4.73971700	5.12903500	-3.44939500
H	-4.35464600	4.79176700	-5.14842900
C	-5.95298100	2.45971100	-1.78985000
C	-6.73323400	3.75802600	-1.70201100
H	-6.96730100	4.10622000	-2.70662400
H	-7.68571300	3.55921300	-1.21014700
C	-6.02251400	4.86829600	-0.93547900
C	-6.33941300	6.20089900	-1.22439100
H	-7.05342700	6.42326400	-2.01255000
C	-5.75615900	7.24624500	-0.51374400
H	-6.01761500	8.27192200	-0.75436300
C	-4.83818700	6.97662100	0.49972100
H	-4.38046900	7.78991600	1.05360200
C	-4.51427300	5.65512700	0.79380500
H	-3.80211600	5.42815100	1.58085800
C	-5.10279000	4.60941000	0.08396700
H	-4.83467100	3.58945500	0.33231400
C	-8.29143300	1.11761700	-0.00086000
C	-9.12053200	0.98728400	1.13241800
H	-8.77445500	1.34932200	2.09450200
C	-10.36531300	0.39838700	1.02771500
H	-11.00558900	0.28913200	1.89252100
C	-10.80174400	-0.06962300	-0.21355600
C	-9.99804500	0.04440200	-1.34320800
H	-10.35961000	-0.33340400	-2.29034000
C	-8.74731400	0.63581400	-1.24028100
H	-8.11794900	0.71389700	-2.11676200
N	-3.86778200	1.08309400	-4.39037800
N	-3.96652400	2.37788500	-4.87385200
N	-6.08143200	1.53833100	-0.84994000
N	-7.07210000	1.78201600	0.14117900
H	-6.66072200	1.63438400	1.05634300
N	-12.11935300	-0.69664100	-0.32592100
O	-4.48741200	-0.14412600	-2.50467000
O	-12.46962300	-1.10288100	-1.43016000
O	-12.80154600	-0.78189600	0.69061400
Zn	4.76637400	-0.01319500	0.49040500
O	-2.92127800	1.16721300	-0.24866600

### Complex trinuclear $[Zn(HL^4)_2]_3$



C	1.70027800	0.08755800	-4.60626000
C	1.15669400	1.37454600	-4.51979900
H	0.27198000	1.54646200	-3.92085300
C	1.74902200	2.41853800	-5.22746100
H	1.31957900	3.41333900	-5.16279000
C	2.86744500	2.19036800	-6.02787700

H	3.31900000	3.00633400	-6.58242300
C	3.38870400	0.90054800	-6.12538800
H	4.25035500	0.70828000	-6.75651500
C	2.81266800	-0.15025500	-5.41845400
H	3.20028700	-1.15781100	-5.49658000
C	0.51618200	-0.96378600	-2.66617400
C	0.06404700	-2.30363100	-2.42521400
C	0.51686700	-3.04099400	-3.58554000
C	0.39888800	-4.49240500	-3.94053900
H	-0.63139100	-4.77752700	-4.17728700
H	0.74880000	-5.14417000	-3.13761200
H	1.00216900	-4.67842500	-4.82952200
C	-0.71229000	-2.69924100	-1.29974200
C	-1.24587900	-4.11944900	-1.20632900
H	-1.44666800	-4.48786300	-2.21032900
H	-2.20779900	-4.10675400	-0.69304000
C	-0.33478500	-5.10608000	-0.48557100
C	-0.38870400	-6.46025000	-0.83567900
H	-1.04331400	-6.78021600	-1.64166800
C	0.38156400	-7.40518500	-0.16283800
H	0.32368300	-8.45011400	-0.45091200
C	1.22584100	-7.00940200	0.87272100
H	1.82926700	-7.74328600	1.39713200
C	1.28846200	-5.66455300	1.22759600
H	1.93974000	-5.33987600	2.03278100
C	0.51339300	-4.72093500	0.55541900
H	0.57566500	-3.68170700	0.85286100
C	-3.17388500	-2.07614300	0.65666000
C	-3.91229800	-2.22770100	1.85915500
H	-3.38536700	-2.41184100	2.78876900
C	-5.28200100	-2.13367800	1.85515900
H	-5.84777200	-2.24881300	2.77005300
C	-5.95371200	-1.84808500	0.65408100
C	-5.24316500	-1.68346700	-0.54121800
H	-5.77883100	-1.45310900	-1.45198100
C	-3.87094000	-1.81963300	-0.54615000
H	-3.32098200	-1.69413500	-1.46889300
N	1.11541300	-0.98923500	-3.89803900
N	1.13982900	-2.26475500	-4.43717700
N	-0.98658500	-1.81057200	-0.35581300
N	-1.81597100	-2.24456800	0.70490100
H	-1.39352700	-2.00805400	1.59680000
N	-7.37001800	-1.69204300	0.67359800
O	0.44532800	0.08436000	-1.95084800
O	-8.01249400	-2.06583300	1.64843400
C	-1.70046500	-0.08712000	4.60744800
C	-1.15711100	-1.37419100	4.52081200
H	-0.27239300	-1.54617000	3.92188900
C	-1.74965100	-2.41818500	5.22829700
H	-1.32038700	-3.41305400	5.16348500
C	-2.86805600	-2.18993100	6.02871400
H	-3.31977800	-3.00589900	6.58312000
C	-3.38908000	-0.90003000	6.12640700
H	-4.25071400	-0.70770000	6.75753800
C	-2.81283500	0.15077500	5.41964800
H	-3.20027500	1.15838900	5.49790900
C	-0.51619900	0.96429300	2.66750900
C	-0.06380800	2.30407700	2.42674200
C	-0.51643800	3.04135200	3.58720100
C	-0.39815200	4.49268800	3.94240900
H	0.63217400	4.77752800	4.17929500
H	-0.74783000	5.14465300	3.13954300
H	-1.00146900	4.67873100	4.83136300
C	0.71250300	2.69974700	1.30127200
C	1.24648500	4.11982200	1.20818400
H	1.44739000	4.48791700	2.21228000
H	2.20841600	4.10696400	0.69491500
C	0.33572200	5.10694200	0.48768800
C	0.39069700	6.46111000	0.83766000
H	1.04587300	6.78069800	1.64334000
C	-0.37923400	7.40650000	0.16508300
H	-0.32053700	8.45141400	0.45304600
C	-1.22422600	7.01119500	-0.87008000
H	-1.82738600	7.74543900	-1.39429000
C	-1.28789900	5.66636100	-1.22481200
H	-1.93973300	5.34206300	-2.02970100
C	-0.51317100	4.72227600	-0.55289100
H	-0.57627900	3.68306700	-0.85022000

C	3.17363400	2.07668100	-0.65577000
C	3.91180900	2.22831100	-1.85839900
H	3.38471600	2.41269100	-2.78787300
C	5.28149500	2.13401300	-1.85472700
H	5.84707200	2.24917200	-2.76973700
C	5.95342400	1.84808400	-0.65385300
C	5.24311000	1.68340500	0.54158200
H	5.77893700	1.45279400	1.45218700
C	3.87091700	1.81983100	0.54684200
H	3.32114400	1.69426800	1.46968700
N	-1.11539200	0.98966600	3.89939000
N	-1.13954300	2.26510900	4.43872800
N	0.98649200	1.81124100	0.35710600
N	1.81575100	2.24537400	-0.70365200
H	1.39305700	2.00931100	-1.59554500
N	7.36968300	1.69172600	-0.67373000
O	-0.44556900	-0.08375600	1.95200700
O	8.01202200	2.06546000	-1.64867500
Zn	9.77559300	0.02927700	0.39672200
Zn	-9.77570100	-0.02954900	-0.39745300
C	-8.49403400	-0.10180700	-5.13971400
C	-8.88902100	1.23985100	-5.09947400
H	-9.72494100	1.53457100	-4.47946600
C	-8.21917500	2.18045500	-5.87907900
H	-8.53698100	3.21786500	-5.84897500
C	-7.16757200	1.79428400	-6.70820400
H	-6.65470200	2.52904600	-7.31988100
C	-6.79428600	0.45152400	-6.76019000
H	-5.98655300	0.13691900	-7.41313200
C	-7.44927100	-0.49641200	-5.98097600
H	-7.17797100	-1.54316900	-6.02420900
C	-9.70182000	-0.94009000	-3.10741100
C	-10.25774000	-2.21934100	-2.78387200
C	-9.92894200	-3.04686300	-3.92173400
C	-10.19899100	-4.49596200	-4.18984700
H	-11.25801600	-4.68539300	-4.39230600
H	-9.90421600	-5.13247200	-3.35344600
H	-9.63731400	-4.79531000	-5.07519500
C	-11.03829800	-2.47927200	-1.61948900
C	-11.80050700	-3.78386800	-1.48104500
H	-12.09561400	-4.13511800	-2.46839400
H	-12.72081500	-3.59195400	-0.92858400
C	-11.03219400	-4.88760400	-0.76177400
C	-11.36185300	-6.22277700	-1.02355500
H	-12.12956300	-6.45109600	-1.75776600
C	-10.72289300	-7.26287100	-0.35436400
H	-10.99536200	-8.29067800	-0.57280000
C	-9.73509500	-6.98527800	0.58892700
H	-9.23318000	-7.79447000	1.10958400
C	-9.39827100	-5.66121900	0.85547700
H	-8.63108700	-5.42767100	1.58687400
C	-10.04280900	-4.62068800	0.18777800
H	-9.76255300	-3.59885000	0.41359000
C	-13.25357100	-1.13594900	0.32269900
C	-14.00685700	-1.00552300	1.50782900
H	-13.60156900	-1.37395900	2.44405600
C	-15.25218400	-0.40884600	1.48592400
H	-15.83490300	-0.30006800	2.39059500
C	-15.76465500	0.06787300	0.27740600
C	-15.03592500	-0.04551900	-0.90223800
H	-15.45520500	0.33951300	-1.82226200
C	-13.78505800	-0.64482900	-0.88255900
H	-13.21309400	-0.72181700	-1.79759800
N	-9.16052700	-1.07593600	-4.35941900
N	-9.27368100	-2.37274600	-4.83458900
N	-11.10829900	-1.56017500	-0.67185600
N	-12.03185100	-1.80806900	0.38124800
H	-11.56022900	-1.66627900	1.26797300
N	-17.08289600	0.70250700	0.25248000
O	-9.66119200	0.14241300	-2.43226800
O	-17.50074700	1.11662700	-0.82515900
O	-17.69863500	0.78619900	1.31082600
C	-11.53269800	0.29757900	4.20915000
C	-11.02271600	-1.00579800	4.17980300
H	-10.17888900	-1.24158600	3.54597400
C	-11.60476800	-1.98747000	4.97923700
H	-11.20640900	-2.99664500	4.95135300
C	-12.67585500	-1.68161900	5.81612600



H	-13.12188900	-2.45076200	6.43785100
C	-13.16214100	-0.37529700	5.85552200
H	-13.98986400	-0.12216200	6.51012700
C	-12.59939600	0.61401900	5.05606000
H	-12.96596300	1.63156500	5.08131000
C	-10.38112300	1.19304500	2.16873700
C	-10.01812200	2.52432400	1.77589700
C	-10.50119700	3.35594900	2.85804700
C	-10.46003500	4.84108700	3.05308800
H	-9.44147100	5.20662900	3.22012400
H	-10.87265700	5.38134600	2.19844700
H	-11.04758200	5.08840900	3.93750200
C	-9.29243200	2.83502800	0.59725100
C	-8.90215200	4.26987500	0.30048700
H	-8.70578300	4.78879000	1.23690400
H	-7.96622700	4.27979500	-0.25797200
C	-9.94393300	5.04996900	-0.49496400
C	-9.91442500	6.44890700	-0.44940600
H	-9.17649300	6.94872200	0.17227700
C	-10.81680800	7.20858000	-1.18799000
H	-10.77737700	8.29202300	-1.13597800
C	-11.77238300	6.58010400	-1.98464100
H	-12.48207800	7.16950800	-2.55577800
C	-11.81267200	5.18993000	-2.03555400
H	-12.55659200	4.68908200	-2.64673200
C	-10.90432500	4.43089400	-1.29841000
H	-10.95524500	3.34882300	-1.34984400
C	-6.78965600	2.07007500	-1.28585500
C	-6.05035700	2.13471400	-2.49281300
H	-6.57529100	2.25485600	-3.43417600
C	-4.67820300	2.04166500	-2.47910100
H	-4.10967800	2.09538300	-3.39806800
C	-4.01109600	1.84266000	-1.26115400
C	-4.72155500	1.76335700	-0.06045600
H	-4.18669200	1.59970000	0.86545000
C	-6.09621700	1.90158800	-0.06785300
H	-6.64793300	1.84624600	0.86080200
N	-10.97196600	1.31485900	3.39809500
N	-11.06267700	2.63889900	3.79747700
N	-8.95588300	1.86053600	-0.24102800
N	-8.15415100	2.23340600	-1.34916400
H	-8.57599500	1.89141300	-2.20743600
N	-2.58323400	1.69455900	-1.26371000
O	-10.23981900	0.08450900	1.56281500
O	-2.04419800	1.19704000	-0.25578900
O	-1.94932700	2.05977300	-2.25099000
O	-7.91279500	-1.15959800	-0.32841300
C	11.53225400	-0.29825700	-4.20994300
C	11.02228600	1.00512800	-4.18066200
H	10.17847700	1.24096100	-3.54682600
C	11.60432100	1.98674700	-4.98017100
H	11.20597300	2.99592800	-4.95233000
C	12.67537800	1.68083700	-5.81707900
H	13.12140000	2.44993900	-6.43886200
C	13.16164500	0.37450700	-5.85641400
H	13.98934000	0.12132000	-6.51103400
C	12.59891900	-0.61475700	-5.05687400
H	12.96547600	-1.63230700	-5.08207500
C	10.38076100	-1.19355900	-2.16941500
C	10.01781600	-2.52480000	-1.77643500
C	10.50084200	-3.35652100	-2.85853100
C	10.45974000	-4.84168400	-3.05340500
H	9.44120400	-5.20728000	-3.22049900
H	10.87228800	-5.38183100	-2.19865600
H	11.04738100	-5.08909000	-3.93773100
C	9.29220700	-2.83541100	-0.59770900
C	8.90180900	-4.27021500	-0.30090300
H	8.70551800	-4.78916100	-1.23731900
H	7.96581000	-4.28004500	0.25743700
C	9.94342500	-5.05036500	0.49471100
C	9.91345000	-6.44931100	0.44960100
H	9.17527100	-6.94907800	-0.17183000
C	10.81567500	-7.20904700	1.18830400
H	10.77587900	-8.29249400	1.13664600
C	11.77156700	-6.58063400	1.98463200
H	12.48113900	-7.17009300	2.55586500
C	11.81232600	-5.19046100	2.03509200
H	12.55649400	-4.68966200	2.64600900

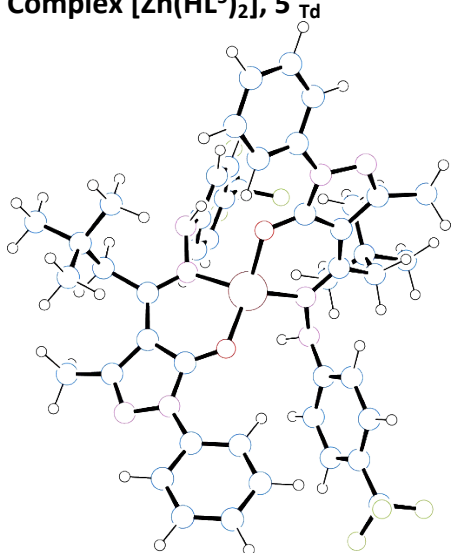
C	10.90412900	-4.43135600	1.29782600
H	10.95541600	-3.34928600	1.34891900
C	6.78973600	-2.07016000	1.28579600
C	6.05067800	-2.13465100	2.49290600
H	6.57578400	-2.25484900	3.43416500
C	4.67853600	-2.04136200	2.47947700
H	4.11019100	-2.09495200	3.39856400
C	4.01121100	-1.84226500	1.26166700
C	4.72143200	-1.76312200	0.06082000
H	4.18640900	-1.59939500	-0.86498100
C	6.09607300	-1.90159500	0.06793400
H	6.64760500	-1.84636900	-0.86083700
N	10.97153900	-1.31547300	-3.39880200
N	11.06228000	-2.63954900	-3.79805000
N	8.95580700	-1.86088200	0.24056900
N	8.15422200	-2.23370400	1.34883200
H	8.57626500	-1.89178400	2.20703500
N	2.58337900	-1.69384600	1.26452600
O	10.23945700	-0.08496700	-1.56359100
O	2.04425000	-1.19617400	0.25674300
O	1.94960600	-2.05894300	2.25194100
C	8.49479600	0.10167700	5.13928600
C	8.88986100	-1.23995900	5.09903900
H	9.72566500	-1.53466100	4.47886600
C	8.22024300	-2.18056200	5.87884000
H	8.53810700	-3.21795400	5.84871900
C	7.16879200	-1.79441500	6.70816800
H	6.65609900	-2.52917600	7.31999300
C	6.79543000	-0.45167600	6.76015800
H	5.98781800	-0.13708500	7.41325500
C	7.45018800	0.49626100	5.98075100
H	7.17882900	1.54300200	6.02398500
C	9.70212300	0.93990200	3.10668500
C	10.25791300	2.21917400	2.78296800
C	9.92925800	3.04675100	3.92083200
C	10.19924800	4.49589100	4.18878100
H	11.25829000	4.68541900	4.39105700
H	9.90429500	5.13230500	3.35236900
H	9.63768800	4.79527800	5.07419100
C	11.03829800	2.47906300	1.61846300
C	11.80048100	3.78365300	1.47983600
H	12.09566200	4.13500500	2.46712600
H	12.72075100	3.59170300	0.92732400
C	11.03209500	4.88731300	0.76051700
C	11.36173000	6.22251400	1.02218000
H	12.12946600	6.45090900	1.75634000
C	10.72271000	7.26254100	0.35294100
H	10.99516500	8.29037000	0.57129200
C	9.73487600	6.98485100	-0.59028200
H	9.23291400	7.79398600	-1.11098100
C	9.39807700	5.66076200	-0.85671800
H	8.63086500	5.42713800	-1.58806000
C	10.04267600	4.62029700	-0.18897300
H	9.76243800	3.59843600	-0.41469700
C	13.25335100	1.13562900	-0.32386800
C	14.00654900	1.00518600	-1.50905400
H	13.60118400	1.37360300	-2.44525500
C	15.25188100	0.40852000	-1.48723200
H	15.83453600	0.29972900	-2.39194200
C	15.76444800	-0.06816800	-0.27874000
C	15.03580800	0.04524300	0.90095600
H	15.45515800	-0.33976900	1.82095600
C	13.78493300	0.64454400	0.88136000
H	13.21303600	0.72153500	1.79644100
N	9.16106000	1.07580000	4.35879300
N	9.27420200	2.37265500	4.83384700
N	11.10816800	1.55991700	0.67086400
N	12.03161300	1.80773300	-0.38235700
H	11.55990300	1.66583600	-1.26901900
N	17.08269700	-0.70279100	-0.25390100
O	9.66144200	-0.14263800	2.43162300
O	17.50062500	-1.11690300	0.82371200
O	17.69834500	-0.78652300	-1.31229700
Zn	-0.00011900	0.00036500	0.00058100
O	7.91259000	1.15908600	0.32811800

## Complex 5

Zn	0.00028200	0.00016500	-0.00005200
C	-3.20081300	3.10970600	-2.19202400
C	-3.01608300	2.15129600	-3.19503300
H	-2.07624700	1.62227000	-3.26560100
C	-4.04039200	1.90219200	-4.10608600
H	-3.88751800	1.16144000	-4.88451900
C	-5.24121200	2.60510800	-4.03678400
H	-6.03271500	2.40890000	-4.75236700
C	-5.41000500	3.57316400	-3.04760500
H	-6.33587000	4.13642400	-2.98970900
C	-4.40012700	3.82681500	-2.12572200
H	-4.51687500	4.58365700	-1.36132200
C	-1.23443000	2.53532400	-0.73218500
C	-0.49694500	3.30946800	0.23099500
C	-1.11245100	4.62018300	0.16808100
C	-0.76767400	5.93111800	0.81392600
H	0.22838700	6.27844300	0.52290400
H	-0.80102100	5.90050800	1.90381400
H	-1.48957100	6.67335200	0.47222500
C	0.66769200	2.83915400	0.92748700
C	3.46625600	1.32022200	0.24721400
C	4.59696900	0.51518500	0.49317800
H	4.60793200	-0.14176100	1.35684800
C	5.68885300	0.55692300	-0.35495200
H	6.54986800	-0.06773300	-0.14613600
C	5.69188000	1.39742800	-1.47515800
C	4.57727300	2.19279000	-1.72769000
H	4.57066900	2.85566700	-2.58531200
C	3.47101200	2.15966000	-0.88169100
H	2.62409300	2.80374200	-1.08195200
N	-2.18242000	3.38677000	-1.24742400
N	-2.09981600	4.64915200	-0.69328600
N	1.12666000	1.63578400	0.63292900
N	2.40966900	1.29425100	1.15705000
H	2.33975600	0.39723400	1.62707200
O	-1.13558500	1.31598300	-1.08266400
C	3.20082000	-3.10959900	2.19211800
C	3.01618800	-2.15121000	3.19516300
H	2.07636400	-1.62217300	3.26582600
C	4.04058700	-1.90212500	4.10611700
H	3.88779700	-1.16139000	4.88458200
C	5.24139900	-2.60504800	4.03668100
H	6.03297000	-2.40885500	4.75219100
C	5.41009100	-3.57308900	3.04747500
H	6.33594600	-4.13635400	2.98947700
C	4.40011500	-3.82671800	2.12568600
H	4.51678400	-4.58355200	1.36126600
C	1.23453400	-2.53506900	0.73223400
C	0.49690500	-3.30918300	-0.23085400
C	1.11215600	-4.62002100	-0.16775800
C	0.76719200	-5.93096100	-0.81349800
H	-0.22894100	-6.27810200	-0.52250700
H	0.80061800	-5.90046000	-1.90338600
H	1.48894800	-6.67327500	-0.47167600
C	-0.66769000	-2.83879100	-0.92733100
C	-3.46610100	-1.31996700	-0.24725100
C	-4.59690900	-0.51503700	-0.49319500
H	-4.60787300	0.14203800	-1.35676500
C	-5.68887000	-0.55706500	0.35480900
H	-6.54994800	0.06751100	0.14600300
C	-5.69191400	-1.39777000	1.47487100
C	-4.57723600	-2.19303000	1.72737300
H	-4.57063700	-2.85605800	2.58487500
C	-3.47088100	-2.15960200	0.88150800
H	-2.62393500	-2.80366200	1.08172800
N	2.18231500	-3.38664500	1.24762900
N	2.09948900	-4.64907400	0.69363800
N	-1.12647300	-1.63530100	-0.63294300
N	-2.40943500	-1.29366000	-1.15695800
H	-2.33953400	-0.39652700	-1.62676500
O	1.13597700	-1.31565000	1.08252300
O	1.44275200	-0.31917600	-1.70107200
H	2.03750200	0.43006500	-1.84306000
O	-1.44224200	0.31926900	1.70120200
H	-2.03672000	-0.43025900	1.84282500
H	1.98619600	-1.11406900	-1.66633400
H	-1.98602400	1.11393500	1.66655400

C	6.85418700	1.39001600	-2.41864000
F	6.96628300	2.55024500	-3.10358700
F	6.75261800	0.40521800	-3.34936400
F	8.02874600	1.18558600	-1.77969100
C	-6.85435800	-1.39067400	2.41817900
F	-8.02889100	-1.18669600	1.77902900
F	-6.75327800	-0.40575300	3.34882700
F	-6.96616500	-2.55087700	3.10320400
C	-1.35877700	-3.71084400	-1.95795400
H	-1.15970500	-4.75465000	-1.73001900
H	-2.43608700	-3.56775600	-1.87236300
C	-0.97198300	-3.46583700	-3.46402700
C	-1.65621100	-4.58726400	-4.26919500
H	-1.29917800	-5.57680100	-3.96768500
H	-2.74184900	-4.56925900	-4.13338500
H	-1.45498100	-4.47522300	-5.33843800
C	0.54674400	-3.52735500	-3.70078000
H	0.98276600	-4.47805100	-3.38862600
H	0.76347500	-3.40515000	-4.76606900
H	1.06698400	-2.72608000	-3.17188300
C	-1.48066600	-2.10839400	-3.97838900
H	-0.97692800	-1.27492200	-3.48452600
H	-1.27737300	-2.02145200	-5.05044900
H	-2.55610600	-1.99727100	-3.82830400
C	1.35853800	3.71114500	1.95832500
H	1.15920200	4.75495100	1.73061300
H	2.43588600	3.56833500	1.87269100
C	0.97177800	3.46577000	3.46432500
C	-0.54698600	3.52702700	3.70099900
H	-0.98313700	4.47767800	3.38892400
H	-1.06709200	2.72574100	3.17199900
H	-0.76376900	3.40467300	4.76626100
C	1.65578500	4.58716000	4.26973300
H	1.29867400	5.57670200	3.96835200
H	1.45446800	4.47492600	5.33893700
H	2.74143000	4.56930000	4.13401600
C	1.48061600	2.10831700	3.97850900
H	2.55607100	1.99734900	3.82843200
H	1.27732000	2.02122300	5.05055400
H	0.97697900	1.27485200	3.48453300

### Complex $[Zn(HL^5)_2]$ , $5'_{Td}$



Zn	-0.11103700	0.47501200	0.44012200
C	-4.58517200	2.33779400	-0.37467700
C	-4.80484600	1.11657600	0.27025100
H	-3.99893000	0.40692000	0.37791900
C	-6.07220100	0.82573100	0.77021300
H	-6.24071700	-0.12777100	1.25781600
C	-7.12004800	1.73215600	0.63431000
H	-8.10390200	1.49306600	1.02432500
C	-6.89367800	2.94463900	-0.01394100
H	-7.70097700	3.66077000	-0.13038700
C	-5.63498600	3.25264500	-0.51666900

H	-5.45214300	4.18707700	-1.02883500
C	-2.06897000	2.20825600	-0.58778300
C	-1.13656200	3.00947900	-1.33195800
C	-1.97589400	3.89245200	-2.10845300
C	-1.64865200	4.86491200	-3.20406400
H	-1.02641100	4.40878200	-3.97970600
H	-1.13033600	5.75714400	-2.84707600
H	-2.58342500	5.18401600	-3.66562100
C	0.28487100	2.93913200	-1.21053200
C	2.92694500	0.92753500	-1.41167400
C	4.18360000	0.44275400	-1.00459300
H	4.57481200	0.71831100	-0.02993000
C	4.92446800	-0.37828800	-1.83640500
H	5.89099300	-0.74230500	-1.50782500
C	4.43422700	-0.73979700	-3.09529000
C	3.19289200	-0.25779900	-3.50626200
H	2.80911500	-0.52365400	-4.48447200
C	2.44237500	0.56947200	-2.67880400
H	1.48451300	0.94558100	-3.01511400
N	-3.31228800	2.68346500	-0.90999100
N	-3.24365000	3.68610900	-1.85956200
N	0.82272200	1.83989200	-0.70092500
N	2.24233700	1.81482600	-0.57948400
H	2.48772000	1.70836700	0.39905900
O	-1.87823800	1.25973000	0.25056300
C	2.85214800	0.40356100	4.37704300
C	2.26065200	1.67167200	4.37319300
H	1.38865400	1.85828700	3.76497500
C	2.80270500	2.68308100	5.16251100
H	2.33608800	3.66293200	5.15716200
C	3.91958500	2.44622000	5.95940000
H	4.33316700	3.23945400	6.57326400
C	4.49593700	1.17723500	5.96594800
H	5.36301200	0.97566400	6.58669900
C	3.97137800	0.15754100	5.17997800
H	4.40501100	-0.83315500	5.18741200
C	1.57763600	-0.60954100	2.45384100
C	1.39786000	-1.96987200	2.02923000
C	2.08348300	-2.74064300	3.04855200
C	2.17826300	-4.21699800	3.30357900
H	1.19025500	-4.67748600	3.39621200
H	2.72442500	-4.75577200	2.52759300
H	2.70365400	-4.36108700	4.24788600
C	0.67896000	-2.38258300	0.86573600
C	-2.24255600	-2.23332100	-0.56183100
C	-3.14456100	-2.30846500	-1.63631900
H	-2.79583500	-2.11844400	-2.64725500
C	-4.47536600	-2.62486500	-1.41801500
H	-5.16046200	-2.66979400	-2.25594200
C	-4.94043800	-2.86797700	-0.12355400
C	-4.05081600	-2.78212800	0.94694300
H	-4.40397000	-2.95443000	1.95742000
C	-2.71490200	-2.46703000	0.73799000
H	-2.04219400	-2.39101900	1.58192500
N	2.33127900	-0.66127400	3.59326700
N	2.62212300	-1.96341200	3.95333900
N	-0.07463900	-1.49838200	0.21536900
N	-0.88648200	-2.01981300	-0.82775900
H	-0.70402400	-1.54701400	-1.70252800
O	1.18704700	0.49005000	1.92882200
C	5.20252200	-1.69477300	-3.95339100
F	4.93240200	-1.53964500	-5.26782600
F	4.91462700	-2.99541300	-3.65868800
F	6.53835500	-1.56447400	-3.79720200
C	-6.36344800	-3.26336700	0.12224900
F	-7.18133200	-2.90862800	-0.89066500
F	-6.85839700	-2.69717300	1.25367900
F	-6.50467500	-4.60268100	0.28438600
C	0.76443200	-3.81750000	0.38811000
H	0.95315800	-4.45736700	1.24541500
H	-0.19951600	-4.11633900	-0.02198500
C	1.86066400	-4.13776200	-0.69495200
C	1.85365200	-5.66818700	-0.87307100
H	2.11429700	-6.18371500	0.05633800
H	0.87140000	-6.03032700	-1.19140800
H	2.58006300	-5.96973300	-1.63280200
C	3.26528700	-3.68654000	-0.26035800
H	3.58956300	-4.17392800	0.66167700

H	3.99137400	-3.93867700	-1.03762300
H	3.31906800	-2.60701400	-0.10558000
C	1.53626800	-3.48620100	-2.04943800
H	1.57006900	-2.39582600	-1.99247900
H	2.27965900	-3.78728500	-2.79222400
H	0.55059000	-3.78375800	-2.41363900
C	1.15123300	4.10499400	-1.63522000
H	0.69518000	4.58401500	-2.49931600
H	2.12237000	3.72512800	-1.95167000
C	1.40998900	5.21842000	-0.55408800
C	2.18051700	4.66894400	0.65792200
H	1.60494100	3.91497100	1.20184300
H	3.13134000	4.22183700	0.36298600
H	2.39485300	5.47906500	1.36126800
C	0.10790600	5.86615300	-0.05346400
H	-0.54720800	5.14624700	0.44116000
H	0.34065000	6.65234600	0.67075800
H	-0.46060000	6.33102300	-0.86193200
C	2.27348100	6.29282200	-1.24240200
H	1.76214000	6.72829200	-2.10640300
H	2.50078800	7.10754700	-0.54900500
H	3.22469300	5.87945800	-1.59079000