

# European Journal of Inorganic Chemistry

Supporting Information

## Correlating Structure and $KA^2$ Catalytic Activity of $Zn^{II}$ Hydrazone Complexes

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**Table S1.** Structural parameters correlating the geometry of five-coordinate Zn(II) complexes with tridentate NNS and/or NNO hydrazone-based ligands and monodentate ligands.

CCDC numbers of Zn(II) complexes with <b>NNS</b> hydrazone ligands	CSD Refcodes	$\beta$ ( $^\circ$ )	$\alpha$ ( $^\circ$ )	$\tau_5^1$	$\rho^2$ ( $\text{\AA}$ )	Refs.
[ZnL <sup>3</sup> (N <sub>3</sub> ) <sub>n</sub> ]		157.65	129.83	0.46	0.54092	This work
977550	COBRIW	154.14(10)	131.36(13)	0.38	0.5618(5)	[1]
977551	COBROC	153.82(6)	138.31(9)	0.26	0.4981(4)	[1]
916948	ZOJXIH	153.3(4)	135.6(5)	0.29	0.5734(17)	[2]
759085	UQENAG	153.5(5)	133.4(5)	0.34	0.6253(17)	[2]
732708	XUWGAY	149.09(7)	128.32(6)	0.35	0.6725(3)	[3]
721753	IGUGAT	151.46(4)	131.02(4)	0.34	0.6261(2)	[4]
664414	KOKBAO	152.96(8)	149.79(5)	0.05	0.4484(2)	[5]
609405	WEHVUB	155.13(6)	145.36(8)	0.16	0.40189	[6]
293428	XELLIK	156.09(13)	121.36(16)	0.58		[7]
257614	JAVJIA	149.94(5)	138.25(4)	0.19	0.5912(2)	[8]
236646	JAMHAH	150.44(5)	138.62(7)	0.20	0.60226	[9]
236647	JAMHEL	157.27(6)	157.01(7)	0.00	0.30925	[10]
234247	YACFUE	151.2(5)	125.6(6)	0.43	0.689(3)	[10]
210958	OJUHOQ	148.5(2)	142.7(2)	0.10	0.6109(11)	[10]
210959	OJUHUV	155.48(8)	145.25(10)	0.17	0.43479	[11]
1905866	TOQBIN	156.98(8)	147.84(10)	0.15	0.37709	[11]
1905869	TOQCAG	149.10(6)	141.91(6)	0.12	0.5993(3)	[12]
169261	ADABOW	153.54(7)	131.40(9)	0.37	0.50824	[12]
168862	EFOPOE	155.46(7)	120.19(8)	0.59		[13]
160137	MEVNEG	157.48(10)	151.64(9)	0.10	0.37510	[13]
1507965	EWUDAD	154.60(9)	135.01(11)	0.33	0.54090	[13]
1450935	UNIKIN	149.8(1)	142.3(1)	0.13	0.5793(6)	[14]
1450936	UNIKOT	156.58(6)	122.80(9)	0.56		[15]
1435302	YUQKEC	150.4(2)	135.65(19)	0.24	0.6340(10)	[16]
139785	MEMXIL	145.92(6)	144.44(6)	0.02	0.5886(3)	[17]
139784	MEMXEH	154.56(5)	132.71(5)	0.36	0.4593(2)	[18]
139783	MEMXAD	155.39(5)	136.84(5)	0.31	0.4508(2)	[18]
121260	NIZZEB	146.86(11)	137.02(11)	0.16	0.6511(5)	[18]
135740	HODZAB	153.14(10)	143.27(12)	0.16	0.4667(7)	[19]
135741	HODZIJ01	150.0(2)	136.3(3)	0.23	0.6617(13)	[20]
		148.4(1)	146.0(1)	0.04	0.5782(6)	[20]
		149.66(6)	141.78(6)	0.13	0.5982(5)	[20]
		158.4(5)	153.5(4)	0.08	0.33881	[21]
		153.3(4)	141.3(5)	0.20	0.48123	[21]
		155.94(7)	129.94(8)	0.43	0.5009(3)	[22]
		151.63(10)	135.52(12)	0.27	0.56726	[22]
CCDC numbers of Zn(II) complexes with <b>NNO</b> hydrazone ligands						
[ZnL <sup>4</sup> (N <sub>3</sub> ) <sub>2</sub> ]		146.88(7)	142.24(9)	0.08	0.5360(3)	This work
2021000	HUTYAZ	149.20(7)	127.42(10)	0.36	0.6091(3)	[23]
1835025	MIJNEB	147.9(2)	128.4(3)	0.32	0.6022(11)	[24]
1546080	CEHNAH	147.68(10)	129.4(2)	0.31	0.6165(5)	[25]
1546081	CEHNEL	146.98(8)	126.41(10)	0.34	0.6462(4)	[25]
1816621	REZKOZ	148.40(6)	128.68(8)	0.33	0.5648(2)	[26]
2064601	KAPGUH	150.0 (1)	128.5(1)	0.36	0.5778(4)	[27]
2110388	NAMYUZ	148.35(9)	130.7(1)	0.29	0.6113(4)	[27]
677454	VIWJUH	149.1(1)	123.3(2)	0.43	0.6646(5)	[28]
920181	NEPNON	147.07(6)	123.36(5)	0.40	0.6453(3)	[29]
1461711	OMOCOK	146.03(7)	126.09(5)	0.33	0.6715(2)	[30]
1461714	OMODEB	151.16(7)	133.96(8)	0.29	0.5154(3)	[31]
1461715	OMODIF	148.52(8)	131.46(6)	0.28	0.6628(3)	[31]
648484	BOJBAE	147.91(8)	131.83(6)	0.27	0.6528(3)	[31]
714809	LUNXIC	146.06(9)	129.81(8)	0.27	0.6677(4)	[32]
1438457	NABNAI	149.56(7)	134.73(6)	0.25	0.5025(3)	[33]
714808	LUNXEY	144.88(7)	133.36(6)	0.19	0.6438(3)	[34]
982944	FOKDEQ	143.18(9)	135.35(8)	0.13	0.6503(4)	[33]
		146.2(8)	131.3(7)	0.25	0.661(4)	[35]
		146.1(9)	132.3(8)	0.23	0.658(3)	[35]
		148.5(1)	128.31(9)	0.34	0.6628(5)	[36]
		144.8(1)	133.31(9)	0.19	0.6095(5)	[36]

846522	WARCOJ	148.8(2)	137.7(3)	0.19	0.5350(10)	[37]
		150.5(2)	126.7(3)	0.40	0.5723(11)	
773663	IBUWIN	144.82(9)	135.50(8)	0.16	0.6156(4)	[38]
701190	XOSCUE	144.02(9)	131.20(7)	0.21	0.6708(4)	[39]
695522	RUNVAY	146.5(1)	127.04(8)	0.32	0.6581(4)	[40]
695523	RUNVEC	149.7(3)	135.2(2)	0.24	0.5062(12)	[40]
650851	UGUZEC	145.99	140.47	0.09	0.02119	[41]
616443	CIRSIG	144.76(6)	124.90(5)	0.33	0.6995(2)	[42]
239078	IWOLAH	147.4(1)	127.9(1)	0.32	0.6217(3)	[43]
1959581	XUGREZ	150.92(5)	140.34(5)	0.18	0.4000(2)	[44]
1956330	JUCKIE	143.74(4)	135.51(4)	0.14	0.64544(19)	[45]
1956331	JUCKOK	145.81(8)	121.85(6)	0.40	0.7140(3)	[45]
1901649	HOPHEC	150.4(4)	140.6(4)	0.16	0.4913(17)	[46]
1901650	HOPHIG	152.23(7)	140.21(7)	0.20	0.4046(3)	[46]
1849711	YOXMIK	150.1(2)	147.4(2)	0.05	0.4589(12)	[47]
		149.4(3)	146.3(2)	0.05	0.4299(11)	
1821809	HIDMIT	146.61(7)	125.32(7)	0.35	0.6687(3)	[48]
		145.21(7)	133.40(7)	0.20	0.6442(5)	
1812963	FIRPOO	149.21(8)	149.20(9)	0.00	0.4317(4)	[49]
1524914	ZASVAT	145.73(14)	125.17(11)	0.34	0.7003(5)	[50]
1524915	NABNAI01	145.74(11)	124.45(10)	0.35	0.6956(5)	[50]
1524918	ZASVUN	143.54(6)	136.20(5)	0.12	0.6125(2)	[50]
		142.42(6)	139.62(5)	0.05	0.6116(2)	
1524920	ZASWEY	143.40(8)	138.59(7)	0.08	0.6053(3)	[50]
		142.01(8)	140.76(7)	0.02	0.6162(3)	
1519614	XATQIV	147.25(9)	125.33(7)	0.37	0.6701(4)	[51]
		146.13(9)	132.26(7)	0.23	0.6461(4)	
1519615	XATQOB	145.50(12)	132.40(10)	0.22	0.6492(5)	[51]
		146.83(12)	126.72(10)	0.34	0.6655(5)	
1494022	OBOROP	151.39(15)	126.67(12)	0.41	0.6143(5)	[52]
1494021	OBORIJ	150.93(7)	129.95(6)	0.35	0.5617(3)	[52]
1451166	PIKTUB	143.52(15)	134.17(12)	0.16	0.6759(6)	[53]
1451167	PIKVAJ	148.89(7)	137.60(8)	0.19	0.4862(3)	[53]
1451169	PIKVIR	147.29(18)	129.99(18)	0.29	0.6016(8)	[53]
1443982	AVONAC	150.64(13)	127.43(15)	0.39	0.6106(6)	[54]
1006340	GECVAO	147.83(8)	124.21(8)	0.39	0.5134(3)	[55]
1006344	GECVUI	145.59(5)	128.94(4)	0.28	0.6520(2)	[55]
210962	OJUJIM	145.74(11)	137.84(10)	0.13	0.5958(5)	[10]
210960	OJUJAE	142.32(13)	142.01(10)	0.01	0.5995(5)	[10]
		147.26(9)	128.57(8)	0.31	0.55147	[10]

<sup>1</sup>The parameter  $\tau_5$  ( $\tau_5 = (\beta - \alpha)/60$ , where  $\beta$  and  $\alpha$  are the two largest angles around the central atom) is an index of the degree of trigonality, within the structural continuum between trigonal bipyramidal and square-based pyramidal geometry (Addison, A.W.; Rao, T.N.; Reedijk, J.; van Rijn, J.; Verschoor, G.C.; *J. Chem. Soc. Dalton Trans.* **1984**,1349–1356.)

<sup>2</sup> $\rho$  (Å) is the distance of metal ion from the mean basal plane of square pyramid toward the apical ligand.

**Table S2.** Selected bond lengths (Å) and angles (°) of complexes **3** and **4**.

<b>3</b>		<b>4</b>	
Zn1–N5	2.085(2)	Zn1–N5	1.982(2)
Zn1–N7 <sup>i</sup>	2.097(2)	Zn1–N8	2.039(3)
Zn1–N2	2.1231(18)	Zn1–N2	2.0430(19)
Zn1–N1	2.1390(18)	Zn1–N1	2.1759(18)
Zn1–S2	2.3516(6)	Zn1–O1	2.2401(16)
N2–C4	1.290(3)	N2–C6	1.289(3)
N2–N3	1.369(2)	N2–N3	1.377(3)
N3–C6	1.327(3)	N3–C8	1.321(3)
S2–C6	1.736(2)	O1–C8	1.263(3)
N5–N6	1.178(3)	N5–N6	1.109(3)
N6–N7	1.167(3)	N6–N7	1.178(3)
		N8–N9	1.015(3)
		N9–N10	1.216(4)

N5–Zn1–N7 <sup>i</sup>	102.90(8)	N5–Zn1–N8	110.75(11)
N5–Zn1–N2	129.83(7)	N5–Zn1–N2	142.25(9)
N7–Zn1–N2 <sup>i</sup>	126.50(8)	N8–Zn1–N2	106.92(9)
N5–Zn1–N1	95.26(8)	N5–Zn1–N1	98.26(9)
N7–Zn1–N1 <sup>i</sup>	91.80(8)	N8–Zn1–N1	102.44(9)
N2–Zn1–N1	76.83(7)	N2–Zn1–N1	75.55(7)
N5–Zn1–S2	99.27(6)	N5–Zn1–O1	97.96(8)
N7–Zn1–S2 <sup>i</sup>	101.34(6)	N8–Zn1–O1	98.46(9)
N2–Zn1–S2	80.82(5)	N2–Zn1–O1	73.94(6)
N1–Zn1–S2	157.65(5)	N1–Zn1–O1	146.89(7)
N6–N5–Zn1	115.62(16)	N6–N5–Zn1	128.9(2)
N6–N7–Zn1 <sup>i</sup>	123.08(17)	N9–N8–Zn1	134.8(3)
N7–N6–N5	178.2(2)	N5–N6–N7	176.5(3)
		N8–N9–N10	177.0(4)

Symmetry codes:  $i = x, 1/2-y, -1/2+z$ .

**Table S3.** Hydrogen-bond parameters for complex **3**.

D–H...A	D–H (Å)	H...A (Å)	D...A (Å)	D–H...A (°)	Symm. operation on A
N4–H4NA...N5	0.85(2)	2.46(2)	3.232(3)	151(2)	1+x, y, z
N4–H4NB...N3	0.86(3)	2.34(3)	3.183(3)	169(2)	1–x, 1–y, –z
Intra C5–H5B...S1	0.96	2.67	3.212(2)	116	

**Table S4.** Hydrogen-bond parameters for complex **4**.

D–H...A	D–H (Å)	H...A (Å)	D...A (Å)	D–H...A (°)	Symm. operation on A
C1–H1...N7	0.93	2.62	3.308(4)	131	1–x, 1/2+y, 1/2–z
C9–H9A...N10	0.97	2.56	3.496(4)	163	x, –1+y, z
C10–H10...N7	0.93	2.62	3.303(4)	130	x, 1/2–y, –1/2+z
C14–H14...O1	0.93	2.58	3.438(3)	154	–x, 1–y, –z
Intra C7–H7A...N3	0.96	2.37	2.791(3)	106	

**Table S5.** Conceptual DFT reactivity descriptors (in a.u.) of studied complexes **1–6**. All descriptors are calculated at the CAM-B3LYP/TZP level of theory on BP86-D4/TZP optimized geometries based on finite difference linearisation (FDL) and frontier molecular orbital approximation (FMO).

		<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
FDL	$\mu$	-0.169	-0.154	-0.048	-0.165	-0.158	-0.163
	$\eta$	0.213	0.227	0.232	0.197	0.223	0.237
	S	4.689	4.396	4.314	5.073	4.491	4.215
	$\omega$	0.067	0.052	0.005	0.069	0.056	0.056
FMO	$\mu$	-0.169	-0.153	-0.051	-0.167	-0.157	-0.170
	$\eta$	0.174	0.189	0.203	0.156	0.188	0.216
	S	5.754	5.281	4.930	6.426	5.323	4.639
	$\omega$	0.082	0.062	0.006	0.089	0.066	0.067

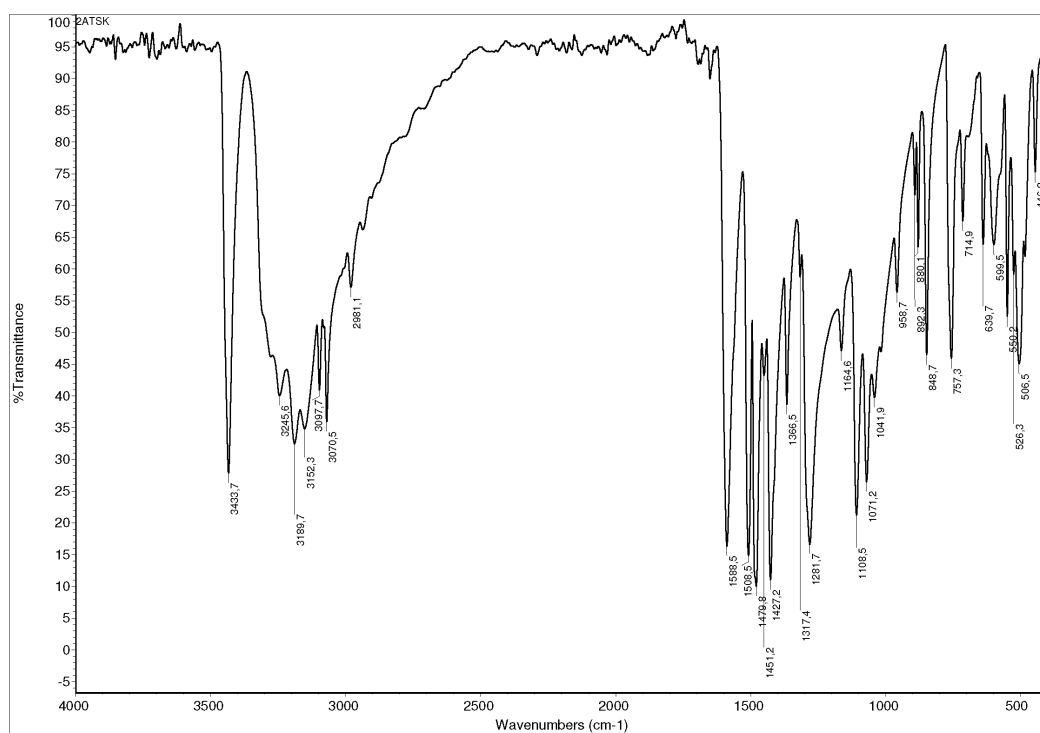


Figure S1. IR spectrum of HL<sup>3</sup> ligand.

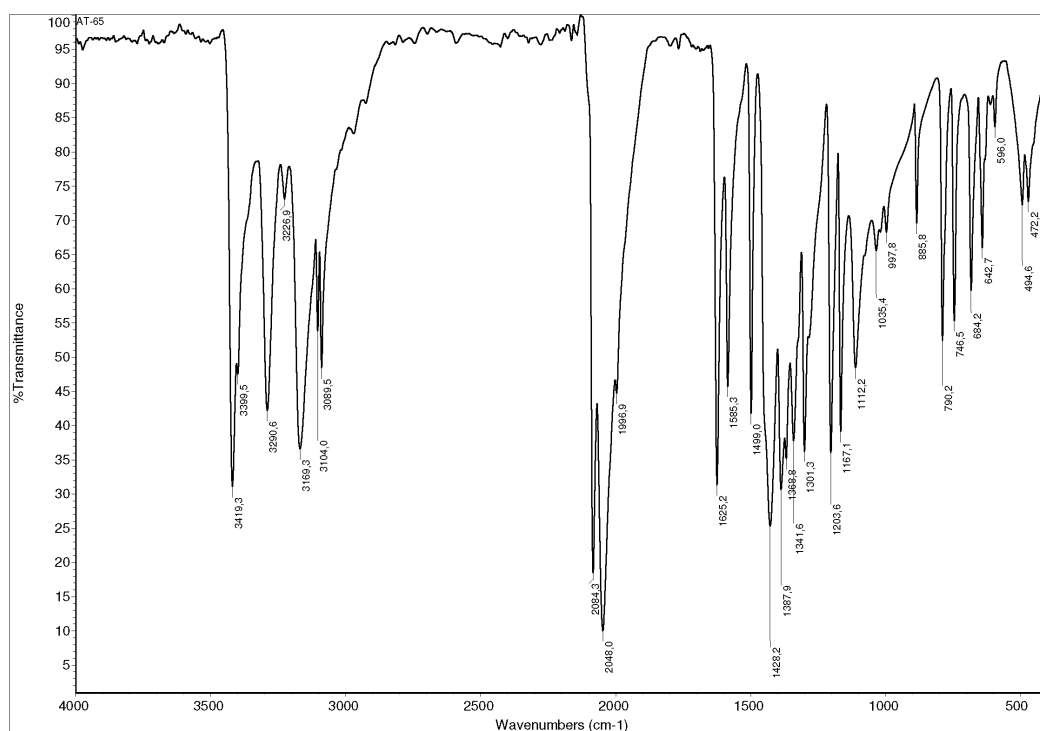


Figure S2. IR spectrum of complex 3.

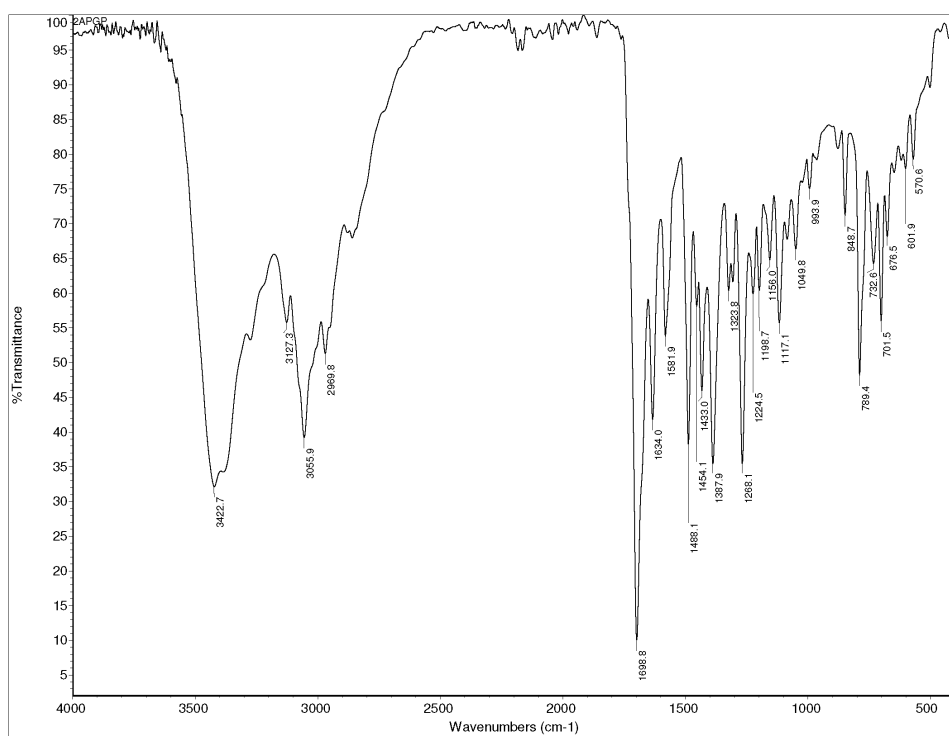


Figure S3. IR spectrum of HL<sup>4</sup>Cl ligand.

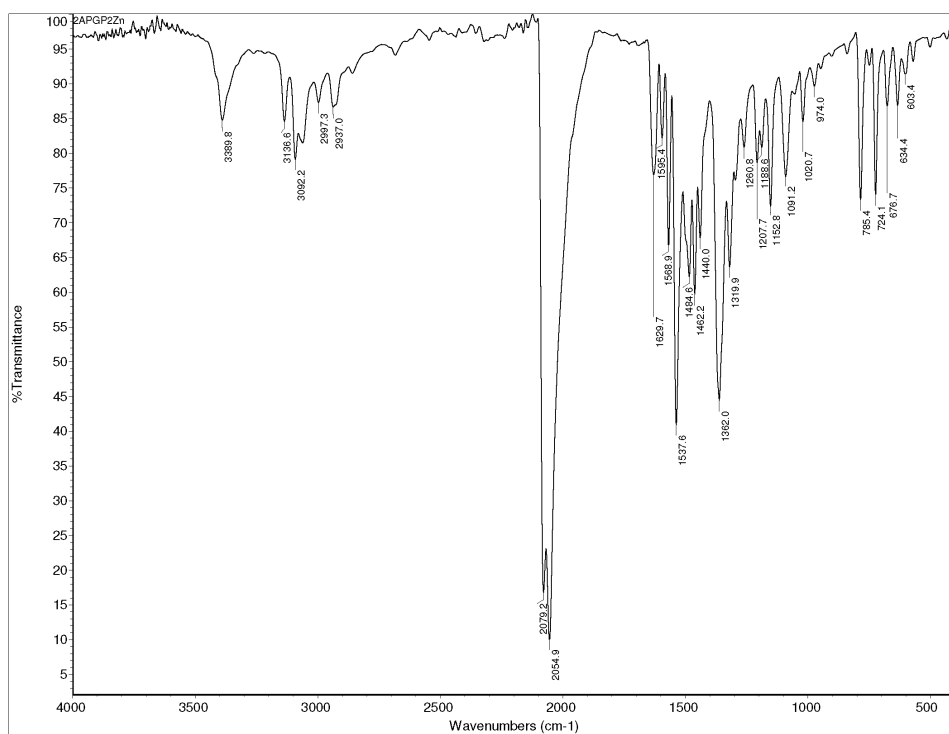


Figure S4. IR spectrum of complex 4.

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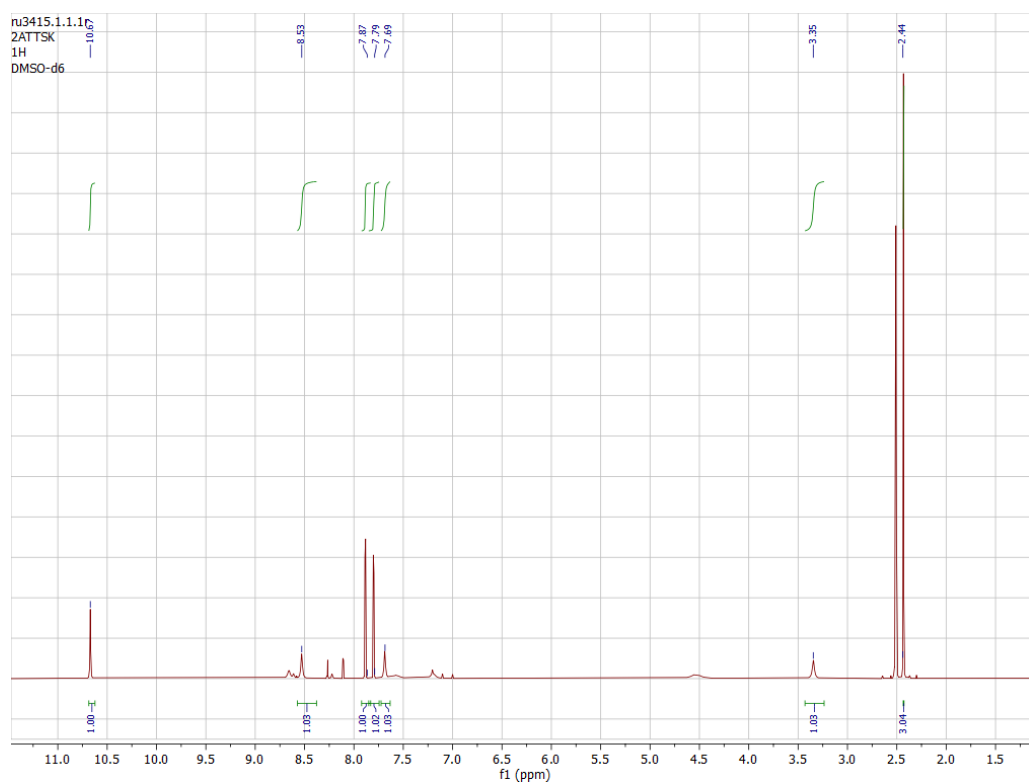


Figure S5.  $^1\text{H}$  NMR spectrum of  $\text{HL}^3$  ligand.

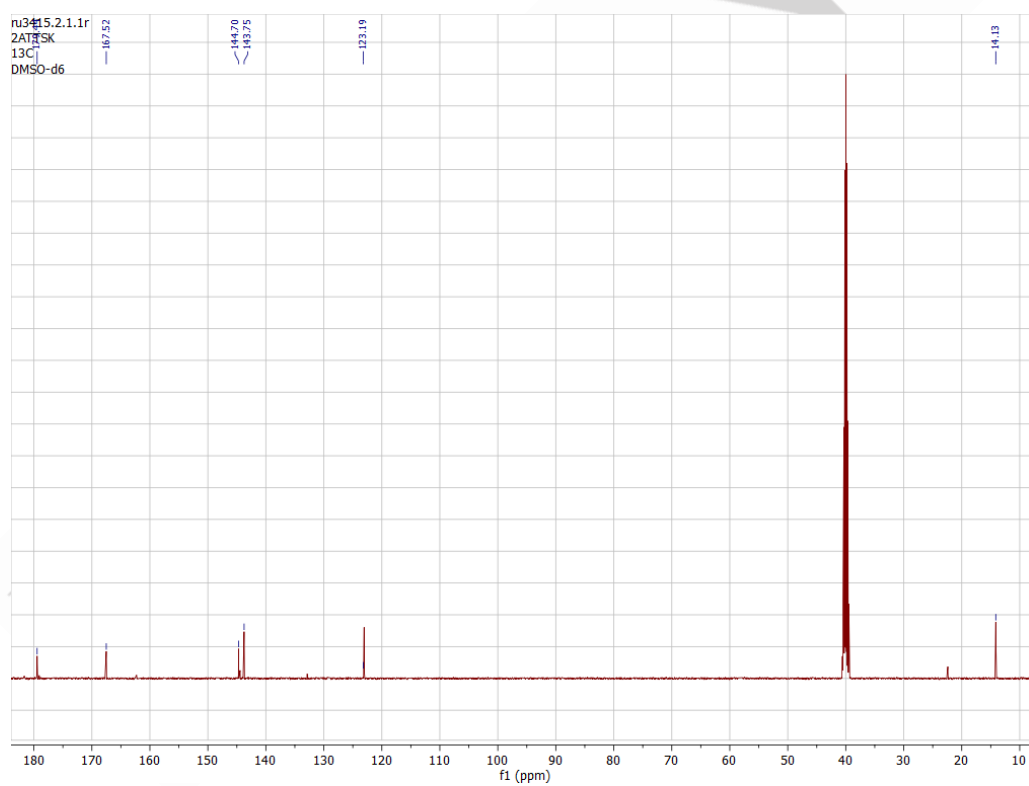


Figure S6.  $^{13}\text{C}$  NMR spectrum of  $\text{HL}^3$  ligand.



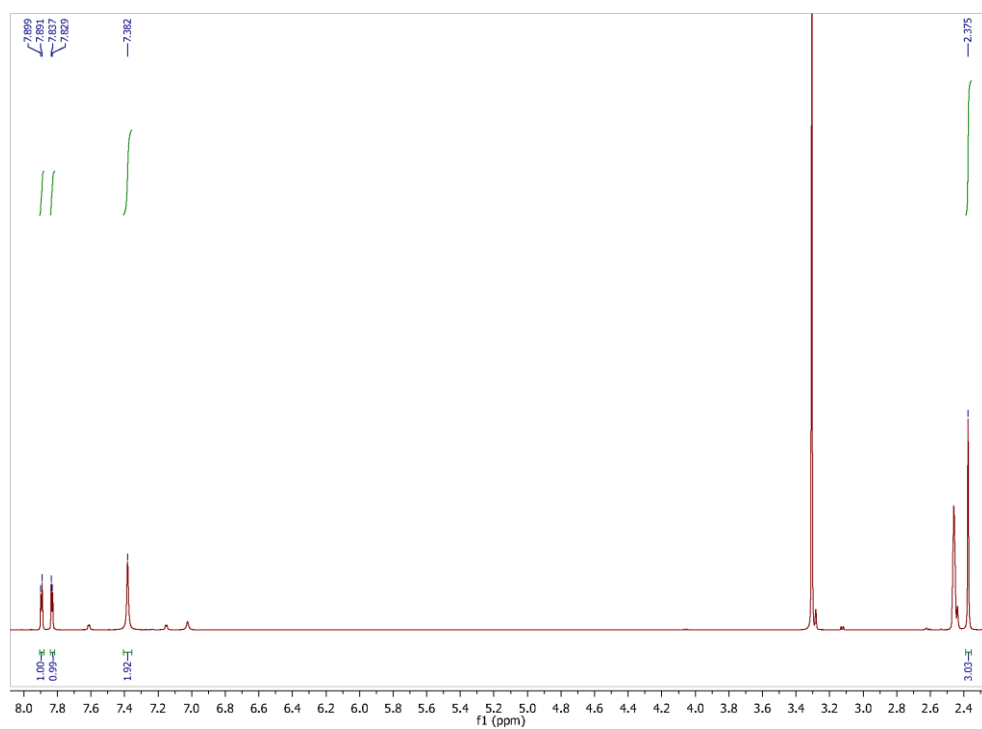


Figure S7. <sup>1</sup>H NMR spectrum of complex 3.

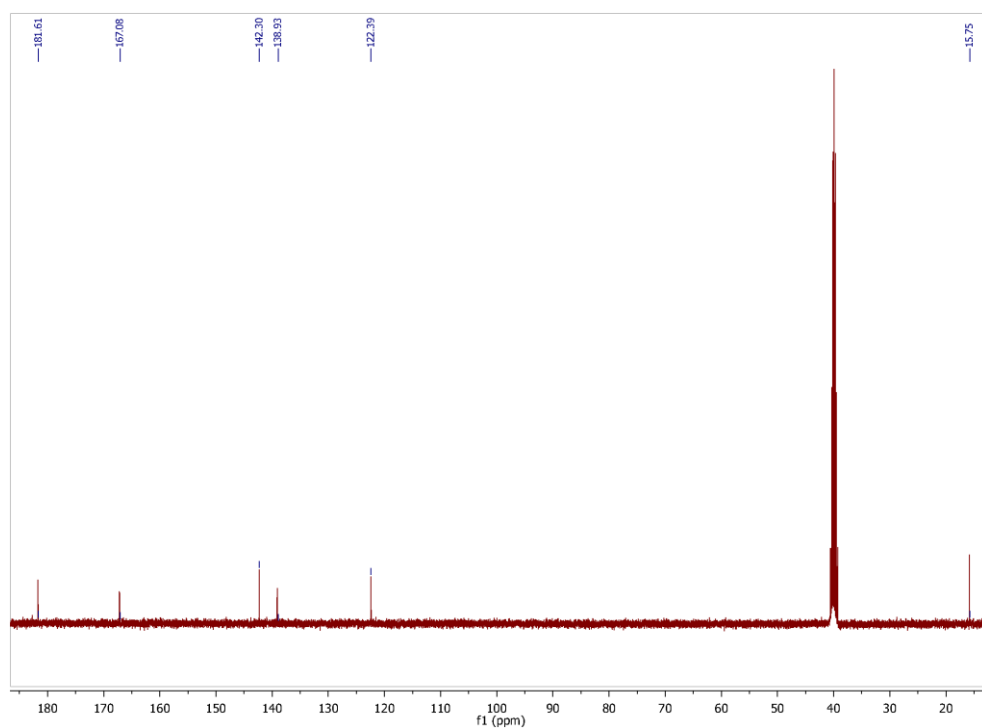


Figure S8. <sup>13</sup>C NMR spectrum of complex 3.

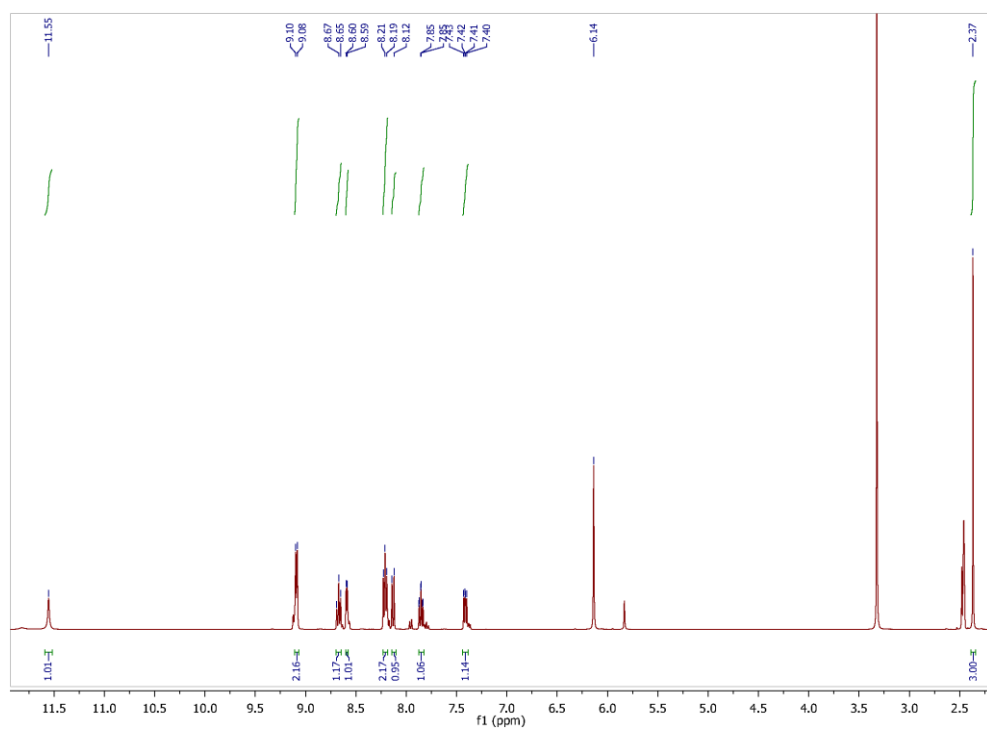


Figure S9.  $^1\text{H}$  NMR spectrum of  $\text{HL}^4\text{Cl}$  ligand.

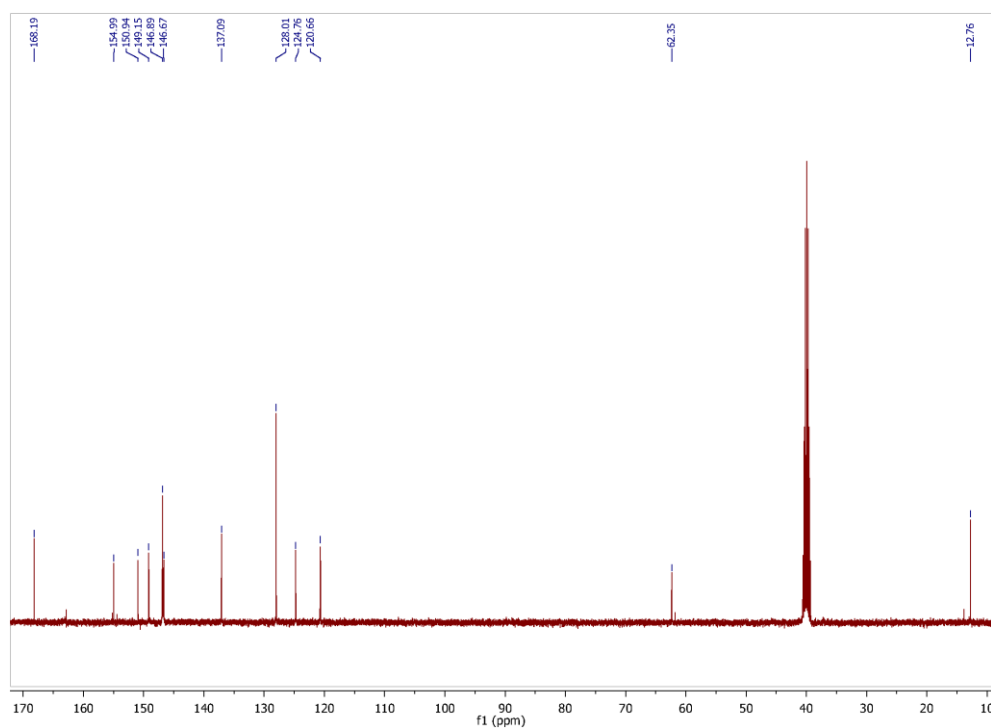


Figure S10.  $^{13}\text{C}$  NMR spectrum of  $\text{HL}^4\text{Cl}$  ligand.

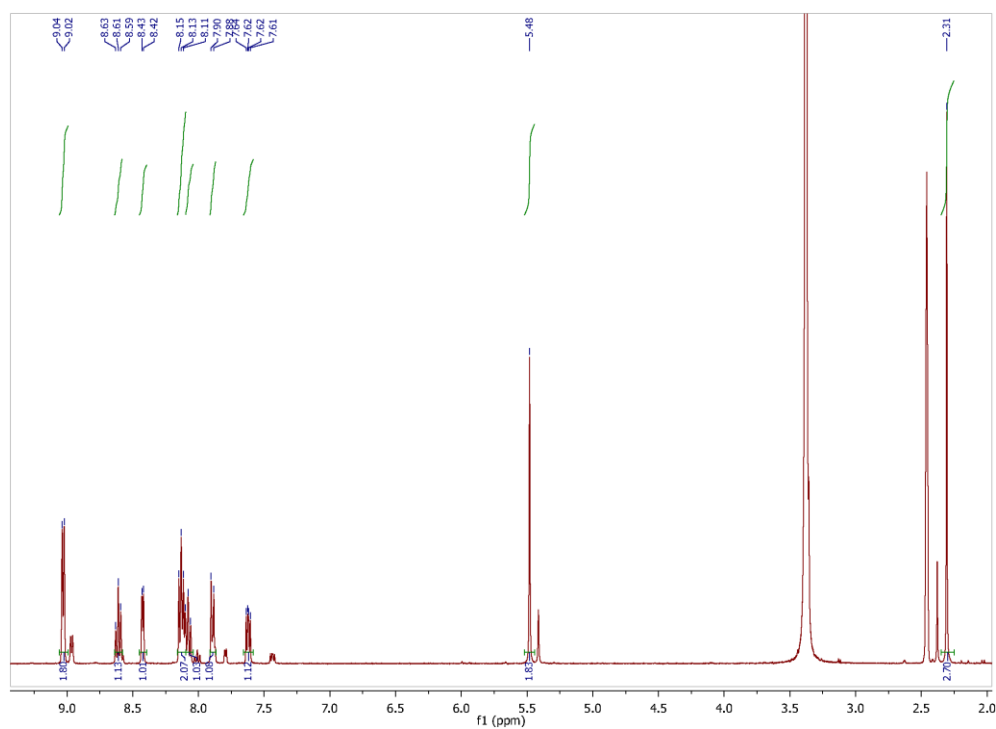


Figure S11. <sup>1</sup>H NMR spectrum of complex 4.

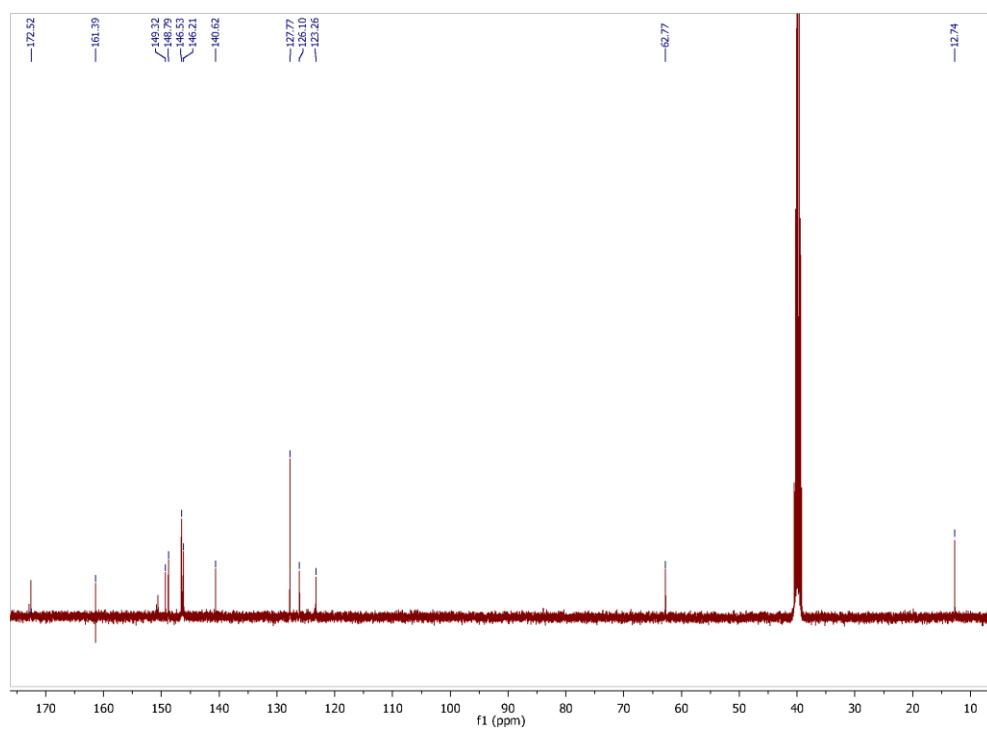
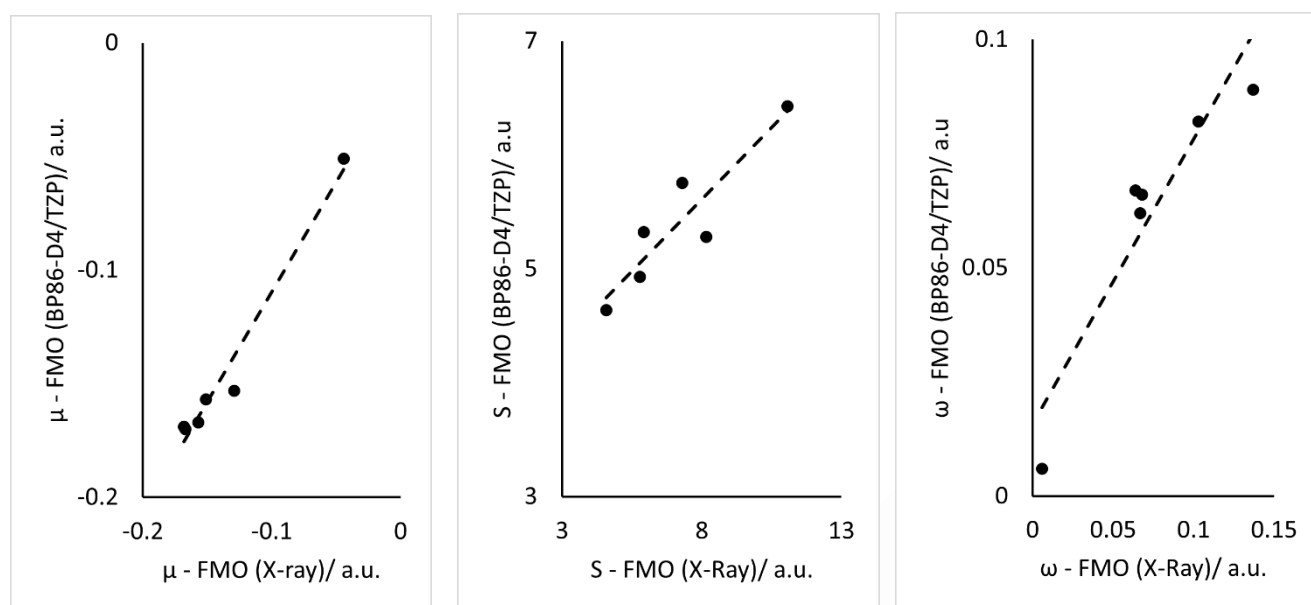


Figure S12. <sup>13</sup>C NMR spectrum of complex 4.



**Figure S13.** The linear relationship between a) the electronic chemical potential,  $\mu$ , calculated with FMO approach at optimized and X-ray geometries,  $R^2 = 0.9698$  (left), b) the molecular softness,  $S$ , calculated with FMO approach at optimized and X-ray geometries,  $R^2 = 0.8385$  (middle), c) the electrophilicity index,  $\omega$ , calculated with FMO approach at optimized and X-ray geometries,  $R^2 = 0.8735$  (right).

## Cartesian coordinates of all DFT optimized structures (BP86-D4/TZP level of theory)

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C19H14N6OS2Zn optimized with ADF in AMS. Complex 1.

Zn	2.26422678932648	4.15430469734538	16.24157300576683
S	1.06949166886428	6.47126374691802	12.58362707890126
S	5.37784205739051	0.76910124502888	17.21518190600092
O	0.58257139267423	3.21220816044064	17.43714362025301
N	3.83596897159240	5.76547910843758	16.09420503319517
N	2.28467616641119	5.04574549714857	18.12346860981599
N	1.61050909196357	4.46278350936583	19.14786732196369
N	1.24984114213012	1.34477878625635	19.54907458222689
N	1.29832451519918	4.60713375032142	14.66584366406221
N	3.34526987312286	2.53168263531113	16.40813650012448
C	3.87108303050538	6.51741090810758	17.20020799686022
C	4.65968645260462	7.69232225958577	17.29434937705410
C	5.40453565376981	8.08502108308033	16.20759833453619
C	5.38371802724506	7.31394519717434	15.02078755905568
C	4.56906359938405	6.12973530916838	15.00842451043692
C	4.53505271002771	5.32164805407209	13.84440236646742
C	5.27060576946189	5.68102642865386	12.73757423847015
C	6.06970505265059	6.85019950352650	12.74305896796303
C	6.12659565707975	7.65164680171341	13.86349645508411
C	3.05964766414707	6.06276239182052	18.32419424195457
C	0.82019794257566	3.49575163417228	18.64195577343040
C	0.33234419539107	2.49958701720840	19.69390176283203
C	1.12141084621439	0.54715983584761	18.45298091852507
C	2.08639698809370	-0.39384153875351	18.15382854224839
C	3.22183703095255	-0.50580386726693	18.96273224213528
C	3.33061315749918	0.32276279563319	20.09052281576325
C	2.34828498701262	1.25040347500168	20.35114356166067
C	1.20429427261268	5.41290042827105	13.78792273287034
C	4.21206677223583	1.80018662614078	16.75332899908797
H	1.96146333249613	-1.01051635764523	17.26657029361969
H	4.65696504092737	8.26817272378879	18.21989610376569
H	6.01557122338401	8.98840392031061	16.24730329356058
H	3.90705558440857	4.43248195860493	13.84409397019165
H	5.22929127338408	5.06313981319121	11.84080425316019
H	6.63869767410474	7.11681024058390	11.85212593700889
H	6.74092639638631	8.55341116228623	13.87434205274318
H	3.12812474883128	6.54943668563531	19.30235703192573
H	0.41912806038283	2.89384904294340	20.70994696431558
H	-0.68922618579904	2.16563945264889	19.48561386385465
H	0.24457648007420	0.72698859649145	17.83756077863839
H	3.97802320038664	-1.25625393814677	18.75207447238477
H	4.19719029705610	0.27123052782603	20.74585700264222
H	2.39271080251376	1.95505824473693	21.17760432003149

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C10H16N10OSZn optimized with ADF in AMS. Complex 2.

Zn	3.72382294564547	8.31994605800038	0.38359673969470
S	8.01598100595265	7.83478608312951	-1.30993754666825
N	5.85870345390002	7.67037741510877	0.08162345667759
N	4.33605675511538	9.30873442851078	-1.38846577563078
N	3.49822909590875	10.15465459769854	-2.03929766852337
N	0.97711328401161	12.32088873497448	-1.36621689433850
N	4.09107341580184	9.66130259310604	1.81026134930570
N	3.76021343495660	10.79251358125776	1.57991092242235
N	3.44506235016427	11.90751701145057	1.38869061373359
N	2.91677501406924	6.57814795761206	0.51523002087741
N	1.86704640126023	6.33636943942163	-0.05039354937684
N	0.87103921736662	6.03186313155230	-0.56669517778185
O	1.91972674245071	9.49673864483491	-0.41157040662205
C	6.75940651140953	6.83478649751986	0.67015381341377
C	7.99018370535363	6.78744655260816	0.06382215507577
C	6.35756844329387	8.27570563110569	-0.98612809445969
C	5.57533831458196	9.19654362666601	-1.79050908333072
C	6.15607172705052	9.94620534188467	-2.94643951377060
C	2.29052164764364	10.13828624757691	-1.43125346128096
C	1.27355792224773	11.02597483954237	-2.12709062530737
C	0.46263945401026	12.03669388364564	0.02653403979111
C	2.22559447508123	13.16248392693521	-1.26981647140611
C	-0.07183619714500	13.06616870594269	-2.13758387565858
H	0.30602031771367	13.27410773649075	-3.14390546472753

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H	-0.29140567965118	14.00388580041945	-1.61736099445650
H	-0.97430129535456	12.44924261276240	-2.19477090395341
H	2.93813878305139	12.65675165119479	-0.60531419974026
H	1.94672341362408	14.12898725692835	-0.83717699911486
H	2.63624883089369	13.29040686062432	-2.27586160684914
H	-0.36086257209251	11.32081595263864	-0.04502078893004
H	0.12237980800467	12.98704846476898	0.45137514637697
H	1.28369745452622	11.62895325596354	0.62483199113363
H	1.63470009009631	11.32541742930816	-3.11682186147516
H	0.31962938623420	10.49108800327394	-2.20549605735925
H	6.46042079599149	10.95663988522262	-2.63364394195802
H	5.39853569529390	10.06109313171928	-3.73020136143296
H	7.03664988237016	9.43605522238264	-3.35656109692403
H	8.86477435201308	6.20837274843283	0.34231712097617
H	6.46798096441215	6.27028960538447	1.55284262491561

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C6H7N10S2Zn optimized with ADF in AMS. Complex 3.

Zn	-0.07370305908341	6.05308180532341	1.42024473412339
S	-2.31166408912113	7.15213192706173	-2.53441416512509
S	1.86335956135464	6.88919897670580	2.65352444688448
N	-1.72465378140581	6.49265226255331	-0.11416882557811
N	0.72860870437279	7.52542846818103	0.00274981028711
N	1.98452847926368	7.98487588001002	0.11358005727785
N	3.79755895274948	8.27609566881681	1.46011641526809
N	-1.49585409412682	5.73284843915081	2.75682685194297
N	-1.32060163991857	5.63976159224609	3.95131342420197
N	-1.22124177687263	5.54071857774985	5.11098038603430
C	-3.48122635805200	6.27889987258973	-1.59566614418767
C	-2.97969603517927	6.01734930410697	-0.34592171977622
C	-1.21552248175884	7.11445018618151	-1.16481439457371
C	0.11490040730006	7.67581812280150	-1.14879396763871
C	0.73554267049922	8.32727864469285	-2.34252817434055
C	2.53332485821263	7.73459571018307	1.31599072937684
N	0.51830376691225	4.43770092198686	0.34415875790710
N	0.67895828994798	4.68538399026545	-2.01678528574505
N	0.59899152616799	4.57209910047804	-0.85187830217160
H	-4.44454766111692	6.00663987710763	-2.01481695059356
H	-3.48947845877721	5.47912993326840	0.45093296668669
H	1.22907583602721	9.26245302662479	-2.04698626011363
H	-0.00978840755866	8.53447301817537	-3.12107668175987
H	1.50594316781776	7.66584796946280	-2.76405478896449
H	4.37313936832728	7.82482922293332	2.16433274434161
H	4.25653746675989	8.48980685466303	0.57589309003649

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C14H14N10OZn optimized with ADF in AMS. Complex 4.

Zn	3.58910188898004	6.02510551514425	0.77232229123071
N	5.48684041980479	6.70301273028931	-0.07326606531526
N	3.54963493571233	5.40065860721603	-1.25099645202760
N	2.51699296971545	4.62743137136935	-1.66907092089142
N	0.69615317592222	2.73378856990294	-2.09422636739699
N	4.06182558539037	4.23074744801063	1.56340827852130
N	3.51270230112383	3.24599824009164	1.15806102413520
N	2.99388803812559	2.25773149530945	0.78764501750484
N	3.30654269376005	7.62533433878135	1.80331140248064
N	2.26364299702611	7.89363392041288	2.37044143119005
N	1.30355114580163	8.22353734114786	2.93326057418813
O	1.45234748981275	5.33673236229556	0.31061182057117
C	6.39634013097221	7.44883259444674	0.55715598497098
C	7.59037275454584	7.84430840483865	-0.05029709824314
C	7.82884057064859	7.44037640837132	-1.36428261159646
C	6.87429600104825	6.67375354605473	-2.0295252593499
C	5.69394640042886	6.32221761006765	-1.35763279576419
C	4.61971112759936	5.53617980094570	-1.98348409955641
C	4.78253935717188	4.93230575921693	-3.34331514527943
C	1.54428412490892	4.65165869407566	-0.73428795478759
C	0.41025946763220	3.64136965323944	-0.96787969380787
C	1.71327717977115	1.84478899102870	-1.94311115046913
C	2.08671793964307	1.04132086041953	-3.00960982786683
C	1.44321156513626	1.17413453399857	-4.23946587657853
C	0.41939642004651	2.11609013045521	-4.37446403643586
C	0.06526405259915	2.88853840420572	-3.28280276747683
H	-0.71545250671679	3.64478395219747	-3.31607095931623

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H	6.14131370690777	7.73671919774772	1.57887290557805
H	8.30865480570999	8.45193768880966	0.49832988175318
H	8.75078567984894	7.72579385055373	-1.87188356851612
H	7.03520153954458	6.35862101715849	-3.05931942199125
H	3.90010953620165	4.32838171987853	-3.57512253206669
H	5.67966383713079	4.29774631891858	-3.38795651814045
H	4.89073594623054	5.71127636437385	-4.11313739529468
H	0.32095983731133	3.04430197325107	-0.05266325405100
H	-0.53712732516253	4.15704392340915	-1.16018607024290
H	2.20350630057775	1.83984489764610	-0.95594574441861
H	2.89409017595410	0.32624357413128	-2.86318289285655
H	1.73492220384920	0.55445961403628	-5.08725771702200
H	-0.10598591100932	2.25764432260679	-5.31695610408700

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C15H18N10OZn optimized with ADF in AMS. Complex 5.

Zn	6.26804884295436	2.23189589722208	3.11390649977517
N	5.11603592902134	0.54742800540557	4.05902478399218
N	6.70995918327875	2.36919760411108	5.16063377856232
N	7.47608994743594	3.37113991133575	5.65959322523779
N	8.06377556772063	6.64678332455345	5.03963285112747
N	7.28752920497767	1.20591415961203	1.82422523024147
N	7.42341455733003	0.00831021609365	1.98500369591734
N	7.57817016720869	-1.14116744370801	2.08118534621331
N	4.77055476842916	3.45154349662041	2.65580982074603
N	4.78589219838176	4.55284060850913	3.13494640079640
N	4.77002415386898	5.63792814402090	3.58247350554553
O	7.72315247168870	4.01051014520285	3.39980745569247
C	5.35593487727290	0.45055151865863	5.37101803303299
C	4.83064855344619	-0.60371913255520	6.16172708116153
C	4.06409208903426	-1.57260613644037	5.55861375725565
C	3.80621032354368	-1.50508990391798	4.16813042924966
C	3.03484472728918	-2.46769350724788	3.47268314621793
C	2.82297868643956	-2.33966890996717	2.11613416610103
C	3.36981169341737	-1.24351264122697	1.40417973333672
C	4.12239147121374	-0.28691300758164	2.04756226538034
C	4.36218852874192	-0.39812440409199	3.44044171362474
C	6.19521890456455	1.48642644661541	5.95841820030135
C	7.91960011636289	4.13879238328658	4.63887701493164
C	8.77718218502145	5.29497164682948	5.12452610911511
C	8.98413936802134	7.67898137754672	5.62036043853650
C	7.75037675608448	7.00886860340104	3.60723908548703
C	6.78100036910622	6.61071883885826	5.83570170508338
H	6.40708220914036	7.63665437425812	5.91563758056316
H	6.99748870848403	6.19408705726048	6.82395826079515
H	6.04696440413271	5.99995334722246	5.29320530894981
H	6.38475670733076	1.51242100695611	7.03670463523028
H	2.23416880379897	-3.08691034137962	1.58348096014856
H	3.65281782204285	-2.40017205544015	6.13917349302261
H	5.04926745697674	-0.63457354482464	7.22937752829199
H	2.61747327545702	-3.31088460464365	4.02559199604495
H	3.19725681692882	-1.16139873058458	0.33088944329128
H	4.55765070235665	0.55523795068942	1.50986211093644
H	9.04500357564725	5.15114002395611	6.17677664040898
H	9.67537806921260	5.38296045057674	4.50172212610414
H	9.92209603133078	7.67625261878518	5.05580679421388
H	9.17624152945695	7.43351121308145	6.66986710567953
H	8.50468321644905	8.66022159299760	5.54525016543088
H	7.31647785652763	8.01419580144620	3.60641914662265
H	7.02854912295726	6.28672441825835	3.21463176075593
H	8.68110091349910	6.98508791320612	3.03261893286634

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C17H18N6O3Zn optimized with ADF in AMS. Complex 6.

Zn	0.95025882033367	13.07069538581947	2.18290028797881
N	2.15114299865605	11.40949192113374	1.20712086499696
N	0.41519586057670	13.12809667155725	0.13862662463167
N	-0.39556775238727	14.08958681134205	-0.37223153154315
N	-0.98776550659111	17.35818788681057	0.19765946635378
N	0.02948364767162	11.96635770637054	3.43356386541963
N	2.31282026894171	14.42094637445918	2.52264464997869
O	-0.66456108905964	14.77157744333168	1.87282713285048
O	-0.58012173163192	9.64829480712851	3.66389257745809
O	2.35311126094393	16.75769142987870	1.91699365093660

C	1.84199250388134	11.26003103348437	-0.08411936043466
C	2.34912502404240	10.19038730180772	-0.86790163219024
C	3.16943798092001	9.25993733497311	-0.27568884076444
C	3.49971147293260	9.38111309940796	1.09614618282129
C	4.32630238714321	8.45772868500920	1.78146681989847
C	4.60384764591647	8.63469432510585	3.12063781493519
C	4.07053747907226	9.74318593434183	3.82394540661745
C	3.26625660206510	10.66367790609402	3.18943065624345
C	2.95831516799181	10.50144086784040	1.81454559705148
C	0.93795322892751	12.24837654812899	-0.65700479205332
C	-0.86034512779309	14.86606437343465	0.63208555763332
C	-1.71501229160954	16.01174346080108	0.11193415592032
C	-1.83129292654454	18.38144913867902	-0.50270989873438
C	-0.79567076126492	17.76857139712303	1.63805902751347
C	0.35795689408837	17.27017034981489	-0.48366436511183
C	-0.26535199007735	10.80057409983198	3.52162868717247
C	-2.32135627825556	15.58140252344940	2.22030947185758
H	2.07155636052494	10.11581868728465	-1.91955394565438
H	3.56730923645014	8.42104548298580	-0.84941639478547
H	4.73329451570373	7.60508008438314	1.23523826721582
H	5.23463885838898	7.91717264059474	3.64609214537178
H	4.29623537509532	9.86475288397140	4.88362101019384
H	2.83960612409744	11.51348928267803	3.72053331880683
H	0.70593454853412	12.24141672576482	-1.72754309790588
H	-2.62608790209643	16.11608798189923	0.71314209663172
H	-1.95833054181521	15.85501968674196	-0.94436206527233
H	-2.82880269260616	18.38857841971002	-0.05164944404298
H	-1.90025857991393	18.11805698938548	-1.56299497653360
H	-1.36092665417913	19.36351139518222	-0.38806490169768
H	-0.20441440771333	18.68907466261200	1.65265732805805
H	-0.27246585569834	16.96200816438704	2.15759213576907
H	-1.78326849543293	17.93048339917824	2.08188956973778
H	0.72497257397188	18.29064739425036	-0.63340853448850
H	0.23086544193970	16.75176756517726	-1.43840275570741
H	1.05417091892889	16.73491689865484	0.17039159792744

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