Supporting information for:

Structural Variety of Zinc and Copper Complexes Based on a 2,3-Disubstituted 1,2,3,4-Tetrahydroquinazoline Ligand

Jesús Sanmartín-Matalobos,* Cristina Portela-García, Luis Martínez-Rodríguez, Concepción González-Bello,* Emilio Lence, Ana M. García-Deibe and Matilde Fondo

jesus.sanmartin@usc.es

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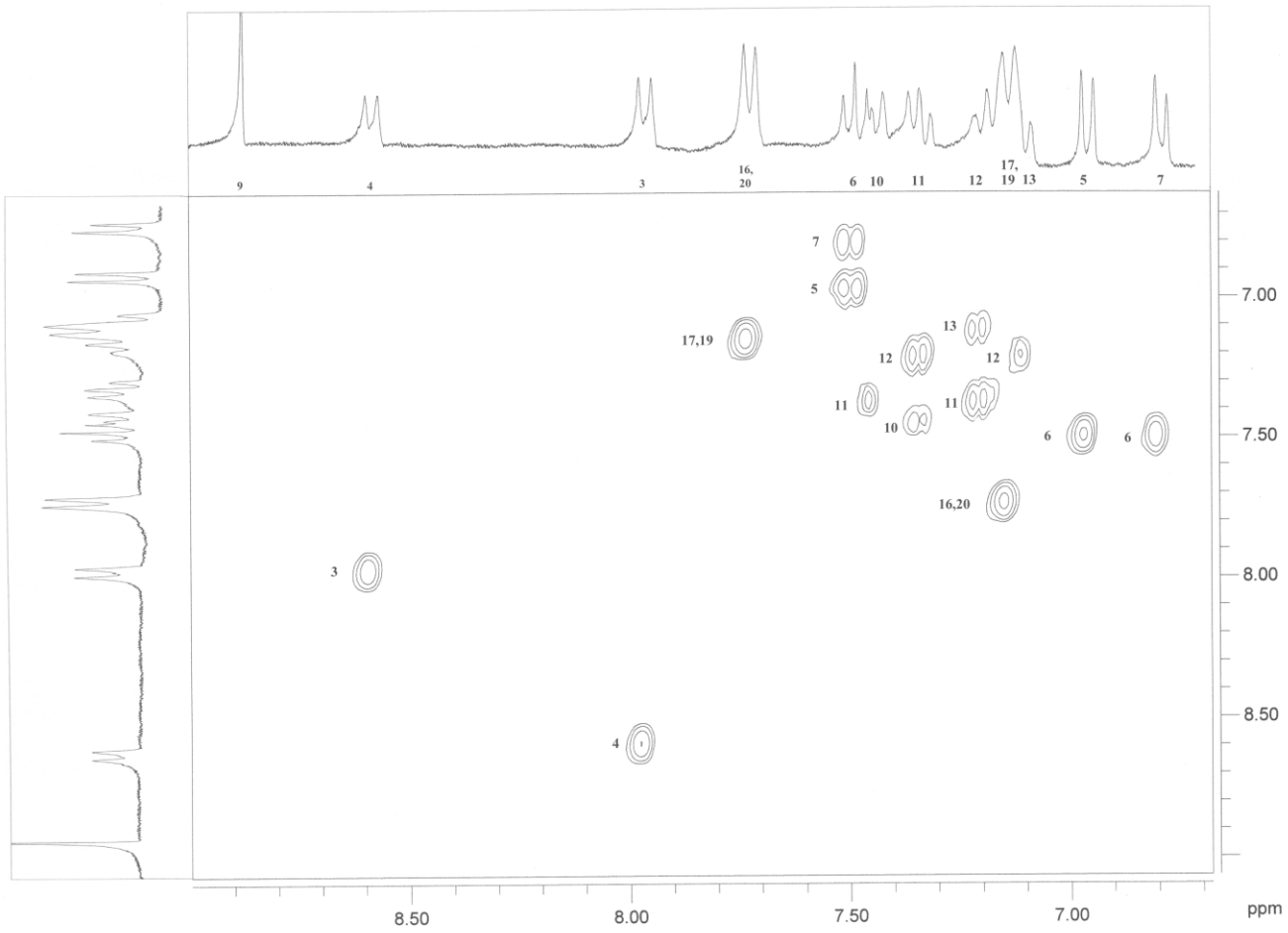


Fig. S1. Section of the COSY spectrum of $Zn_2(L^{chain})_2 \cdot 2MeOH$. Inset shows the numbering scheme of L^{chain} for the proton signals.

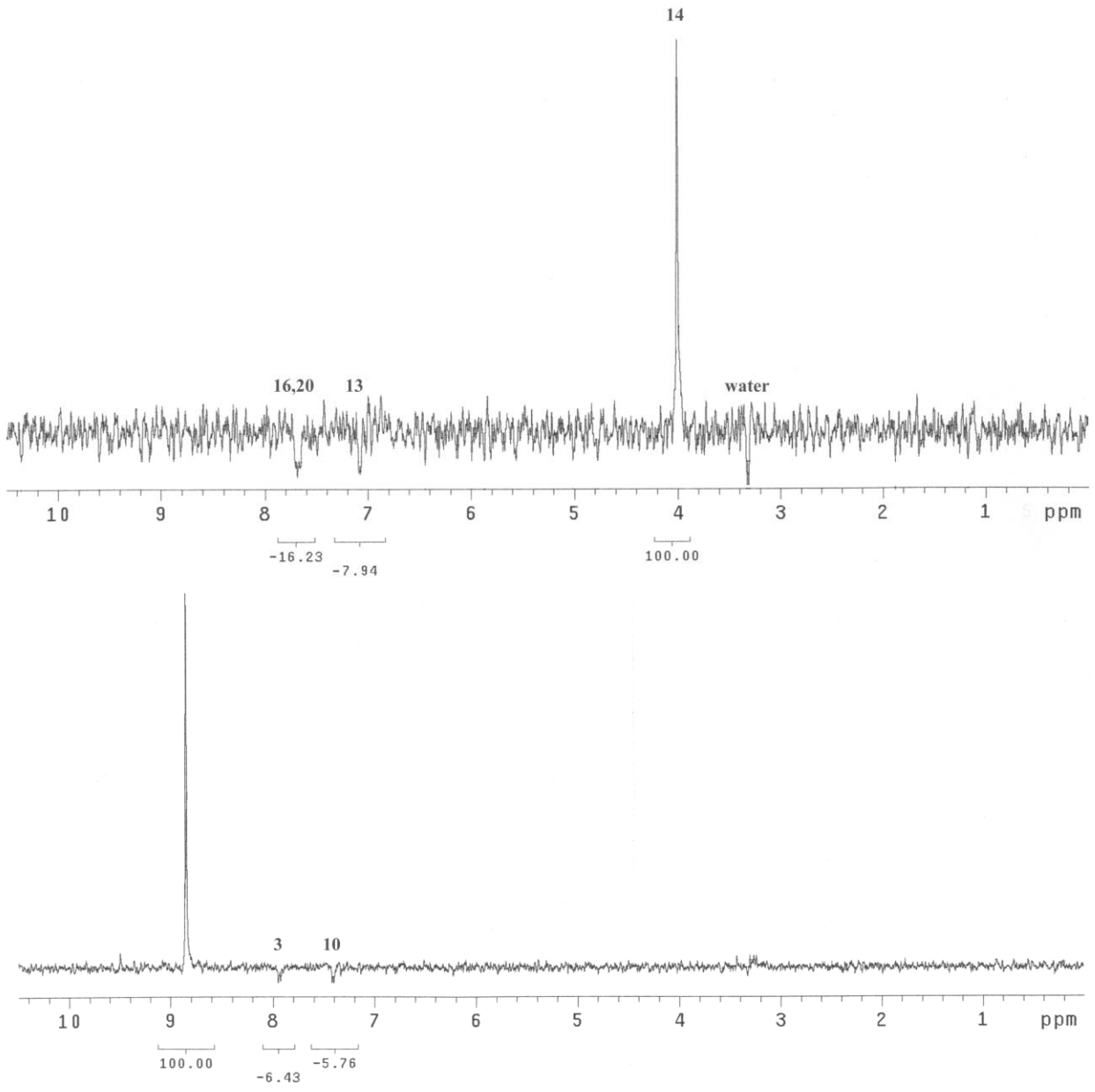


Fig.S2. 1D NOE spectra of $Zn_2(L^{chain})_2 \cdot 2MeOH$ at 298 K obtained after inversion of the imine proton H-9 (*bottom*) and the methylene protons H-14 (*top*). Inset shows the numbering scheme of L^{chain} for the proton signals.

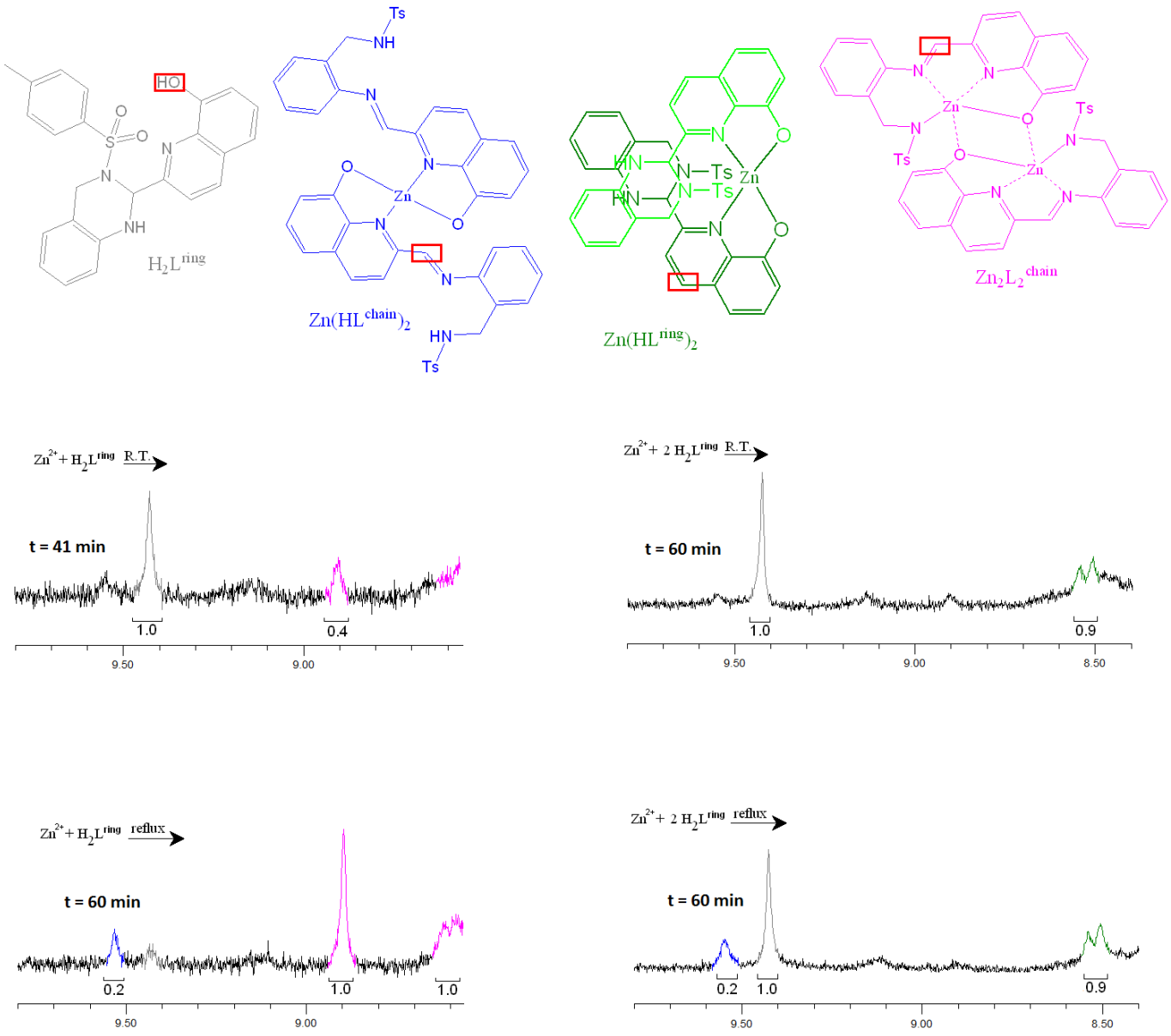
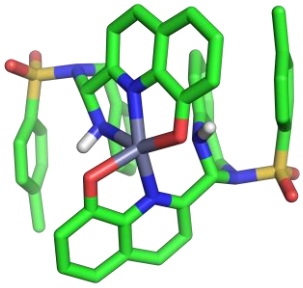
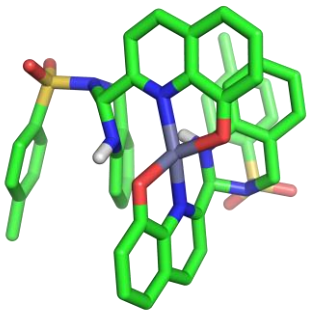
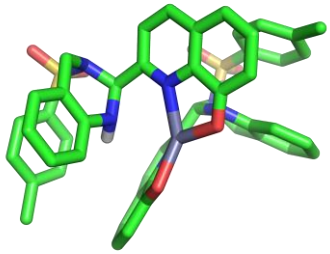
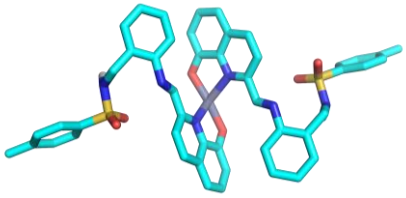


Fig. S3. Sections of the ^{1}H NMR spectra in dmso-d_6 (8.4–9.8 ppm) corresponding to the reactions at reflux/room temperature between H_2L^{ring} and $Zn(OAc)_2$ in a 1:1/2:1 molar ratios. The proton signals of each species that the figure is showing are marked by a red rectangle in the upper scheme.

Table S1. Energy (Hartrees)/Relative stability (kcal.mol^{-1}) for the most stable isomers of mononuclear complexes with tetrahedral geometry calculated at DFT/M06 level and represented as sticks.

Zn(II) complexes	in vacuum Energy/Relative Stability	in methanol Energy/Relative Stability
 **(*R*,*R*)-Zn(HL^{ring})$_2$**	-3493,08110509 / 0	-3493,08168124 / 0
 **(*R*,*S*)-Zn(HL^{ring})$_2$**	-3493,04610843 /4,00	-3493,08019334 / 0,93
 **(*S*,*S*)-Zn(HL^{ring})$_2$**	-3493,03710651 / 9,65	-3493,07248906 / 5,77
 **Zn(HL^{chain})$_2$**	-3493,01690509 / 22,33	-3493,05288133 / 18,07

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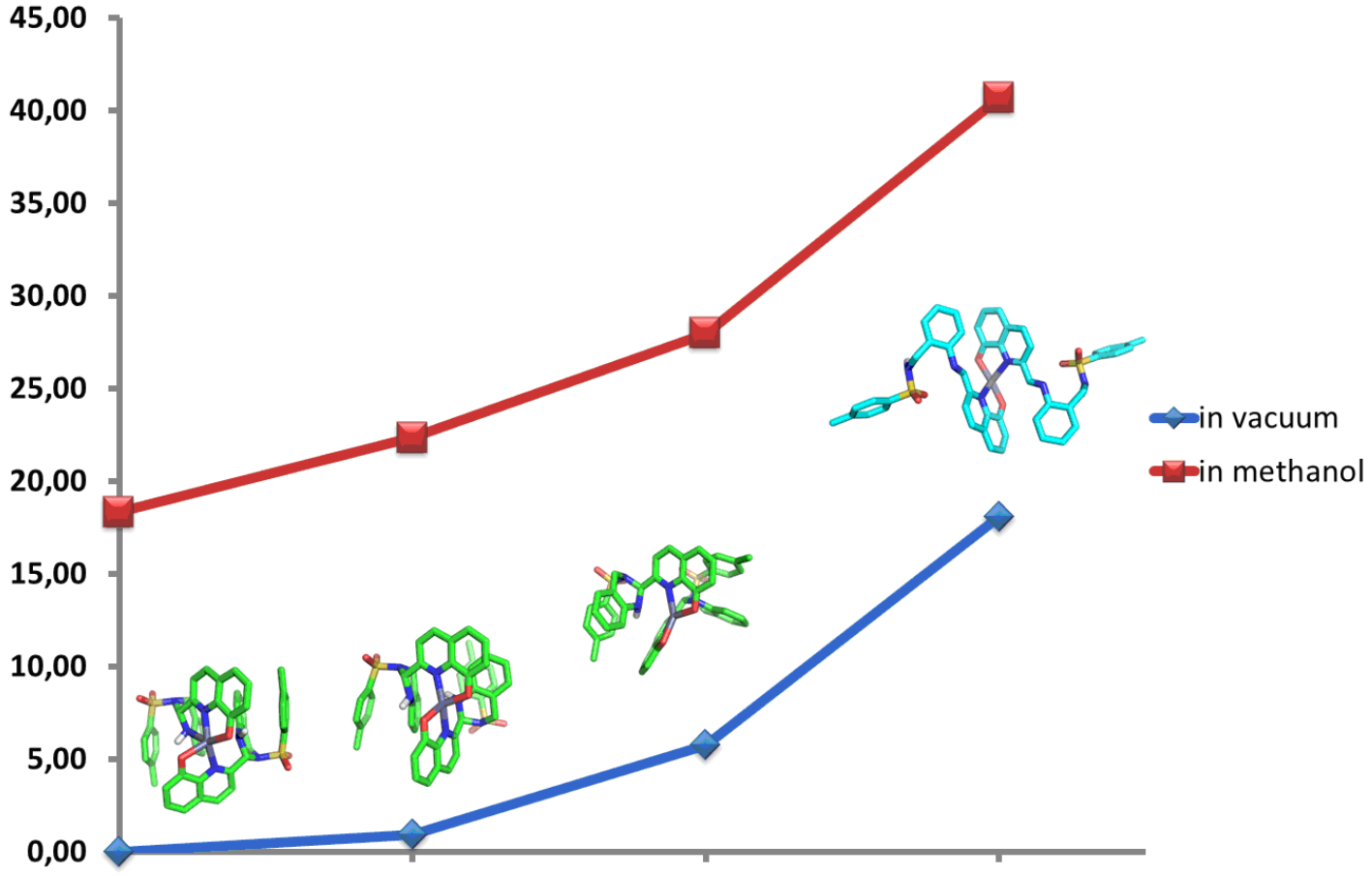
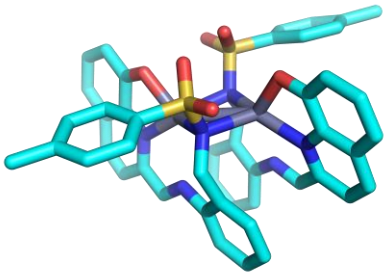
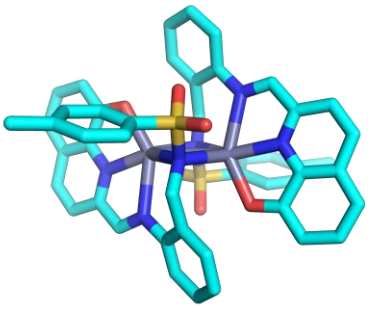
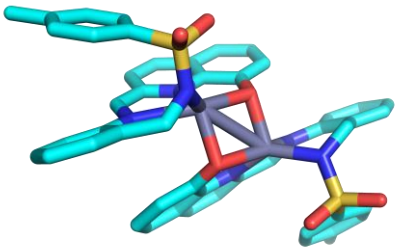
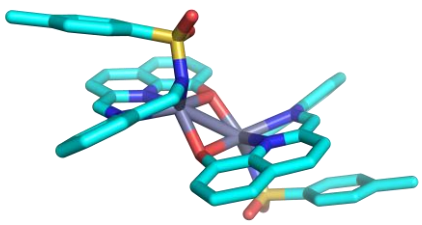


Figure S4. Comparison of the solvent effect in the relative stability of tetrahedral Zn(II) complexes calculated at DFT/M06 level in vacuum and methanol. The complexes represented (from left to right) are (*R*,*R*)-Zn(HL^{ring})$_2$, (*R*,*S*)-Zn(HL^{ring})$_2$, (*S*,*S*)-Zn(HL^{ring})$_2$ and Zn(HL^{chain})$_2$.

Table S2. Gibbs free energy (Hartrees) for the most stable conformers of $Zn_2(L^{chain})_2$ calculated at DFT/M06 level in methanol and represented as sticks. Relative stability to the most stable complex of all series is included. Two *N*-bridged complexes (**N1**–**N2)** and two *O*-bridged compounds **(O1**–**O2)** were studied.

N-bridged	G (Hartree)	Relative G (kcal.mol^{-1})
 **N1**	-3556,696311	16,24
 **N2**	-3556,703228	11,90
O-bridged		
 **O1**	-3556,722190	0,00
 **O2**	-3556,715099	4,45

Energy details and coordinates for all the compounds studied:

$Zn_2(L^{chain})_2$

```
Zero-point correction=                           0.772779 (Hartree/Particle)
Thermal correction to Energy=                    0.827059
Thermal correction to Enthalpy=                  0.828003
Thermal correction to Gibbs Free Energy=         0.685286
Sum of electronic and zero-point Energies=      -3556.634697
Sum of electronic and thermal Energies=         -3556.580416
Sum of electronic and thermal Enthalpies=       -3556.579472
Sum of electronic and thermal Free Energies=    -3556.722190
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	4.690161	2.299537	-0.249612
4	6	0	5.541935	2.429447	0.842716
5	6	0	6.728088	1.695230	0.922979
6	6	0	7.059464	0.844277	-0.137885
7	16	0	3.862672	1.125673	-2.601498
8	8	0	2.972681	2.296158	-2.637189
9	6	0	7.635022	1.819082	2.109634
10	7	0	2.951110	-0.132625	-2.176394
11	6	0	3.530885	-1.466218	-2.281562
12	6	0	4.463158	-1.977405	-1.194614
13	6	0	4.313775	-1.728034	0.184443
14	6	0	5.139393	-2.380931	1.109135
15	6	0	6.151811	-3.228578	0.684857
16	6	0	6.348114	-3.434684	-0.677621
17	6	0	5.501839	-2.820498	-1.593793
18	7	0	3.332200	-0.810189	0.602511
19	6	0	3.500820	-0.098433	1.652153
20	6	0	2.508865	0.928802	1.988671
21	7	0	1.571214	1.131760	1.077756
22	6	0	0.642481	2.090177	1.228591
23	6	0	0.624090	2.935132	2.372857
24	6	0	1.633077	2.706510	3.338731
25	6	0	2.571827	1.715880	3.155773
26	6	0	-0.374478	3.928684	2.462375
27	6	0	-1.283626	4.054858	1.433970
28	6	0	-1.258100	3.222191	0.294776
29	6	0	-0.317147	2.213721	0.168206
30	30	0	1.560321	0.118634	-0.756237

31	8	0	-0.257693	1.354908	-0.842297
32	30	0	-1.528274	-0.285895	-0.672636
33	8	0	0.290821	-1.505653	-0.600847
34	6	0	0.389561	-2.185948	0.535288
35	6	0	-0.530534	-1.882471	1.592800
36	6	0	-0.474096	-2.530086	2.858165
37	6	0	0.527348	-3.501407	3.074412
38	6	0	1.396816	-3.802463	2.048674
39	6	0	1.330827	-3.168822	0.789260
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41	6	0	-2.386657	-0.622368	2.203855
42	6	0	-2.410313	-1.207838	3.485858
43	6	0	-1.456081	-2.148670	3.802527
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45	7	0	-3.264930	0.854575	0.569353
46	6	0	-4.271487	1.677093	0.029065
47	6	0	-5.115380	2.434707	0.851939
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51	6	0	-4.424363	1.726698	-1.371903
52	6	0	-3.486462	1.068391	-2.370198
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67	1	0	-3.178600	-0.917675	4.199293
68	1	0	3.357906	1.537370	3.886737
69	1	0	0.593596	-4.003085	4.038020
70	1	0	-0.410690	4.579083	3.334397
71	1	0	2.166898	-4.556715	2.205039
72	1	0	-2.056246	4.820079	1.496129
73	1	0	2.047105	-3.428364	0.010559
74	1	0	-2.003946	3.352695	-0.488875
75	1	0	-4.282620	0.477683	2.361972
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78	1	0	4.961488	-2.239783	2.174473
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88	1	0	2.674548	-2.158703	-2.335787
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96	1	0	7.982660	0.265351	-0.091913
97	1	0	-8.971148	-1.704026	1.834943
98	1	0	8.528431	2.411058	1.867079
99	1	0	-7.663199	-1.678525	3.032732
100	1	0	7.132079	2.310299	2.950980
101	1	0	-8.255306	-0.166188	2.315738
102	1	0	7.986816	0.835665	2.447103

Zn(HL^{ring})(HL^{chain})

Zero-point correction= 0.797081 (Hartree/Particle)
Thermal correction to Energy= 0.849870
Thermal correction to Enthalpy= 0.850814
Thermal correction to Gibbs Free Energy= 0.713020
Sum of electronic and zero-point Energies= -3492.257497
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Sum of electronic and thermal Enthalpies= -3492.203764
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6	6	0	6.802127	0.034956	-0.743761
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17	6	0	3.557214	-2.752471	-0.437866
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35	6	0	-0.587962	-3.640691	0.737456
36	6	0	-0.238411	-4.893287	0.189582
37	6	0	-0.129830	-5.006200	-1.182810
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40	6	0	-1.306041	-1.108603	1.618314
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43	6	0	-1.697773	0.308894	1.970595
44	7	0	-3.075053	0.610181	1.536220
45	6	0	-3.507161	2.027979	1.560195
46	6	0	-2.361758	2.995876	1.524846
47	6	0	-1.049549	2.561982	1.352600
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49	6	0	-2.607563	4.364475	1.635749
50	6	0	-1.570066	5.285083	1.558016
51	6	0	-0.261353	4.835497	1.379876
52	6	0	0.003659	3.476699	1.291367
53	16	0	-4.287867	-0.456010	2.017704
54	8	0	-4.004534	-0.969661	3.359737
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56	6	0	-4.117204	-3.102824	1.339889
57	6	0	-4.060365	-4.144350	0.418621
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61	6	0	-3.986680	-5.011517	-1.944951

62	8	0	-5.539669	0.262361	1.791727
63	8	0	4.024127	1.087902	3.294201
64	1	0	2.213542	4.032776	-2.113754
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66	1	0	-2.132815	6.220172	-2.450063
67	1	0	0.401711	5.727437	-2.359647
68	1	0	-4.428486	5.297495	-2.328521
69	1	0	2.836270	1.541365	-1.971906
70	1	0	2.610301	-0.629520	-3.514637
71	1	0	4.179297	-2.535404	-3.766067
72	1	0	3.826409	-3.337684	0.442326
73	1	0	4.773310	-3.919440	-1.776704
74	1	0	1.361975	-0.619405	1.037058
75	1	0	1.755783	-2.263100	1.555336
76	1	0	4.657093	0.195864	-0.822896
77	1	0	6.447226	0.622037	3.068437
78	1	0	6.897268	-0.136036	-1.816358
79	1	0	8.695957	0.296188	2.059887
80	1	0	9.320855	-0.992096	-1.232596
81	1	0	9.582245	0.750801	-1.167774
82	1	0	10.080101	-0.261200	0.198636
83	1	0	3.001859	-1.104911	3.009061
84	1	0	-0.244724	-4.064332	-3.133428
85	1	0	-0.057026	-5.741185	0.847690
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88	1	0	1.023268	3.105305	1.167821
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90	1	0	-3.634769	4.705770	1.773408
91	1	0	-1.779575	6.349981	1.635915
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93	1	0	-4.143244	2.180157	0.675778
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95	1	0	-4.295146	-0.482093	-0.842867
96	1	0	-3.969382	-5.170742	0.773951
97	1	0	-4.222861	-2.361529	-2.464427
98	1	0	-3.684392	-5.948500	-1.462411
99	1	0	-4.946562	-5.185831	-2.450382
100	1	0	-3.247659	-4.778141	-2.723338
101	1	0	-1.591217	0.477433	3.058493
102	1	0	-1.218720	-1.909906	3.624410
103	1	0	0.163651	0.957791	1.384746

$Zn(HL^{chain})_2$

Zero-point correction= 0.794064 (Hartree/Particle)
Thermal correction to Energy= 0.848239
Thermal correction to Enthalpy= 0.849184

Thermal correction to Gibbs Free Energy= 0.706231
Sum of electronic and zero-point Energies= -3492.255398
Sum of electronic and thermal Energies= -3492.201222
Sum of electronic and thermal Enthalpies= -3492.200278
Sum of electronic and thermal Free Energies= -3492.343230

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.567045	-2.266297	-2.568368
2	6	0	4.002244	-1.411706	-1.563959
3	6	0	5.192642	-1.647114	-0.877058
4	6	0	5.935344	-2.774709	-1.189372
5	6	0	5.507651	-3.668601	-2.179381
6	6	0	4.325156	-3.391988	-2.868285
7	16	0	3.049142	0.020792	-1.151058
8	8	0	1.843045	0.021793	-1.982263
9	6	0	6.288744	-4.913102	-2.469095
10	7	0	2.705425	-0.196820	0.469737
11	6	0	1.476016	-0.929417	0.831116
12	6	0	1.460008	-2.328614	0.289210
13	6	0	0.488909	-2.729097	-0.641498
14	6	0	0.555696	-4.003192	-1.215711
15	6	0	1.573193	-4.879998	-0.860817
16	6	0	2.528894	-4.497513	0.077389
17	6	0	2.465605	-3.228816	0.640696
18	7	0	-0.611590	-1.896894	-0.928895
19	6	0	-0.868081	-1.548388	-2.133595
20	6	0	-2.131477	-0.859478	-2.422090
21	7	0	-3.002080	-0.877284	-1.426192
22	6	0	-4.220376	-0.344577	-1.534096
23	6	0	-4.655277	0.275133	-2.742190
24	6	0	-3.710380	0.307026	-3.798593
25	6	0	-2.463088	-0.260494	-3.654502
26	6	0	-5.965975	0.785738	-2.797496
27	6	0	-6.775776	0.651129	-1.681997
28	6	0	-6.353173	0.042426	-0.488599
29	6	0	-5.058667	-0.472858	-0.354500
30	30	0	-2.557606	-1.543484	0.510480
31	8	0	-4.581503	-1.038165	0.704968
32	7	0	-2.070588	0.901313	0.922278
33	6	0	-1.624194	1.067717	2.106779
34	6	0	-1.150901	-0.112584	2.843381
35	7	0	-1.490417	-1.275978	2.312178
36	6	0	-1.064738	-2.437689	2.824869
37	6	0	-0.202833	-2.478912	3.960165
38	6	0	0.132588	-1.226417	4.533462
39	6	0	-0.339699	-0.050312	3.993260
40	6	0	0.244048	-3.732222	4.420458
41	6	0	-0.177176	-4.869919	3.754068
42	6	0	-1.039594	-4.838411	2.645582

43	6	0	-1.523790	-3.629207	2.133790
44	8	0	-2.318116	-3.513712	1.120909
45	6	0	-2.594790	1.976803	0.176266
46	6	0	-1.881975	2.499195	-0.913728
47	6	0	-2.495067	3.470991	-1.705540
48	6	0	-3.773568	3.938891	-1.423648
49	6	0	-4.459873	3.429996	-0.325148
50	6	0	-3.877170	2.447494	0.466649
51	6	0	-0.456473	2.110795	-1.197216
52	7	0	0.542220	3.141600	-0.825510
53	16	0	0.792099	3.411192	0.807094
54	8	0	1.244998	2.128787	1.360784
55	6	0	2.128199	4.563792	0.751513
56	6	0	3.356405	4.158984	0.231233
57	6	0	4.404612	5.069076	0.223444
58	6	0	4.245526	6.363378	0.729843
59	6	0	3.000028	6.737291	1.244341
60	6	0	1.936718	5.845103	1.261739
61	6	0	5.388233	7.331069	0.737751
62	8	0	-0.346614	4.047296	1.474168
63	8	0	3.926149	1.195887	-1.182146
64	1	0	-1.740304	-0.252410	-4.468016
65	1	0	-7.033968	-0.031787	0.358503
66	1	0	-6.326965	1.262943	-3.706897
67	1	0	-3.991382	0.776039	-4.741286
68	1	0	-7.794578	1.036724	-1.726391
69	1	0	-0.078670	0.915977	4.420365
70	1	0	-1.339236	-5.765205	2.158097
71	1	0	0.906856	-3.790442	5.282050
72	1	0	0.777692	-1.205934	5.411560
73	1	0	0.171124	-5.841422	4.105159
74	1	0	-1.547997	2.056620	2.579473
75	1	0	-0.187869	-1.766685	-2.967986
76	1	0	-0.219610	-4.304382	-1.919508
77	1	0	1.614883	-5.868595	-1.314823
78	1	0	3.225010	-2.906029	1.353897
79	1	0	3.331192	-5.178822	0.356075
80	1	0	-4.417068	2.008596	1.304852
81	1	0	-1.947455	3.871884	-2.560836
82	1	0	-5.462975	3.782489	-0.090843
83	1	0	-4.230861	4.695993	-2.057550
84	1	0	0.578827	-0.380802	0.510408
85	1	0	1.480301	-0.938119	1.930717
86	1	0	-0.166573	1.182201	-0.694005
87	1	0	-0.300367	1.946085	-2.271213
88	1	0	2.641450	-2.055788	-3.099673
89	1	0	5.523445	-0.961824	-0.098250
90	1	0	3.986561	-4.075076	-3.646898
91	1	0	6.864745	-2.973206	-0.655873
92	1	0	0.967514	6.133115	1.662320
93	1	0	3.491103	3.154492	-0.173686

94	1	0	2.864041	7.744488	1.637453
95	1	0	5.370113	4.771265	-0.184247
96	1	0	5.063037	8.335570	0.440049
97	1	0	5.818227	7.419860	1.744955
98	1	0	6.191030	7.013170	0.062947
99	1	0	5.982931	-5.727106	-1.796206
100	1	0	6.126839	-5.262384	-3.495500
101	1	0	7.364346	-4.759218	-2.320493
102	1	0	2.671717	0.743178	0.879740
103	1	0	0.350424	4.038305	-1.279103

$Zn(HL^{ring})_2$

Zero-point correction= 0.800202 (Hartree/Particle)
Thermal correction to Energy= 0.851957
Thermal correction to Enthalpy= 0.852901
Thermal correction to Gibbs Free Energy= 0.716301
Sum of electronic and zero-point Energies= -3492.279991
Sum of electronic and thermal Energies= -3492.228236
Sum of electronic and thermal Enthalpies= -3492.227292
Sum of electronic and thermal Free Energies= -3492.363892

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.510493	-0.974849	-2.567696
2	6	0	4.579861	-1.645693	-1.346618
3	6	0	5.268957	-1.107443	-0.262491
4	6	0	5.872378	0.136753	-0.403634
5	6	0	5.791002	0.845013	-1.605101
6	6	0	5.117206	0.264477	-2.686638
7	16	0	3.652550	-3.135294	-1.138977
8	8	0	4.205843	-3.871134	-0.008499
9	6	0	6.397923	2.206111	-1.744736
10	7	0	2.095055	-2.694890	-0.655963
11	6	0	1.957754	-2.069127	0.649054
12	7	0	1.910873	-0.598825	0.580091
13	6	0	1.856195	0.040603	-0.671495
14	6	0	1.395793	-0.656868	-1.797412
15	6	0	1.180166	-2.137266	-1.660239
16	6	0	2.210225	1.388597	-0.787774
17	6	0	2.043857	2.050015	-1.997469
18	6	0	1.542154	1.375637	-3.111880
19	6	0	1.246717	0.020044	-3.008083
20	6	0	0.735548	-2.651340	1.346034
21	7	0	-0.065349	-1.825051	1.981050

22	6	0	-1.137256	-2.278654	2.677537
23	6	0	-1.437066	-3.664055	2.754294
24	6	0	-0.563966	-4.534537	2.056771
25	6	0	0.514135	-4.044014	1.360487
26	6	0	-1.950650	-1.273460	3.323955
27	6	0	-3.033057	-1.756577	4.066134
28	6	0	-3.320764	-3.129077	4.141703
29	6	0	-2.556763	-4.085362	3.501181
30	30	0	-0.011111	0.269447	2.023710
31	8	0	-1.654440	-0.015845	3.195072
32	7	0	0.153539	2.250760	1.387264
33	6	0	-0.486534	2.825100	0.397771
34	6	0	-0.323498	4.198704	0.116610
35	6	0	0.537714	4.934962	0.891535
36	6	0	1.264083	4.328510	1.947826
37	6	0	1.030634	2.945011	2.155685
38	6	0	2.200489	4.995749	2.764368
39	6	0	2.876437	4.267994	3.724563
40	6	0	2.670277	2.891396	3.914916
41	6	0	1.748863	2.174950	3.143683
42	6	0	-1.315036	1.956434	-0.532259
43	7	0	-2.631024	2.548060	-0.687464
44	6	0	-3.542545	2.187459	0.412419
45	6	0	-3.716679	0.701262	0.459496
46	6	0	-2.610098	-0.080867	0.116403
47	7	0	-1.349780	0.536108	-0.107667
48	6	0	-4.934607	0.086901	0.734161
49	6	0	-5.064846	-1.296394	0.665940
50	6	0	-3.967164	-2.067125	0.290747
51	6	0	-2.744644	-1.465951	0.017480
52	16	0	-3.240901	2.630696	-2.260070
53	8	0	-4.565895	3.223109	-2.130369
54	8	0	1.530403	0.898057	3.248147
55	6	0	-3.398320	0.975105	-2.859090
56	6	0	-2.279820	0.343594	-3.399175
57	6	0	-2.352947	-1.010100	-3.701595
58	6	0	-3.528772	-1.733072	-3.480838
59	6	0	-4.652465	-1.059344	-2.988960
60	6	0	-4.594321	0.286749	-2.663740
61	6	0	-3.584224	-3.208365	-3.723069
62	8	0	-2.195776	3.290981	-3.035750
63	8	0	3.484942	-3.772963	-2.438392
64	1	0	2.554270	-0.152449	1.232110
65	1	0	-0.787790	-0.020201	-0.753168
66	1	0	-0.868072	4.643936	-0.713390
67	1	0	0.686846	5.995963	0.690963
68	1	0	2.383630	6.059246	2.620399
69	1	0	3.606453	4.773141	4.356686
70	1	0	3.237728	2.352752	4.673122
71	1	0	-0.807322	2.007639	-1.508252
72	1	0	-1.889761	-2.079177	-0.277314

73	1	0	-4.055683	-3.150322	0.215222
74	1	0	-6.021261	-1.768272	0.881822
75	1	0	-5.793386	0.709733	0.986855
76	1	0	-1.364503	0.905177	-3.584543
77	1	0	-1.483149	-1.519111	-4.117785
78	1	0	-5.579986	-1.610117	-2.833096
79	1	0	-5.461121	0.799558	-2.251751
80	1	0	-3.078946	2.587139	1.329328
81	1	0	-4.492133	2.713880	0.274818
82	1	0	-3.548674	-3.749088	-2.765581
83	1	0	-4.516614	-3.501823	-4.220911
84	1	0	-2.741325	-3.553692	-4.332055
85	1	0	1.196731	-4.701105	0.826372
86	1	0	-0.757072	-5.606936	2.083628
87	1	0	-2.794668	-5.145663	3.567954
88	1	0	-4.183566	-3.444285	4.728596
89	1	0	-3.670152	-1.034181	4.575245
90	1	0	2.834148	-2.358546	1.245853
91	1	0	2.605625	1.916371	0.082241
92	1	0	2.307183	3.104209	-2.067948
93	1	0	1.413661	1.893649	-4.059975
94	1	0	0.916819	-0.539335	-3.885398
95	1	0	5.337751	-1.655876	0.675090
96	1	0	6.414275	0.569613	0.436389
97	1	0	5.064729	0.800827	-3.634011
98	1	0	3.986109	-1.423312	-3.409527
99	1	0	0.160865	-2.396780	-1.325252
100	1	0	1.332470	-2.661141	-2.610151
101	1	0	6.998616	2.475572	-0.869019
102	1	0	5.615536	2.969130	-1.863400
103	1	0	7.037936	2.267730	-2.634125