Electronic Supporting Information for

Synthesis, dynamics and redox properties of eight-coordinate zirconium catecholate complexes

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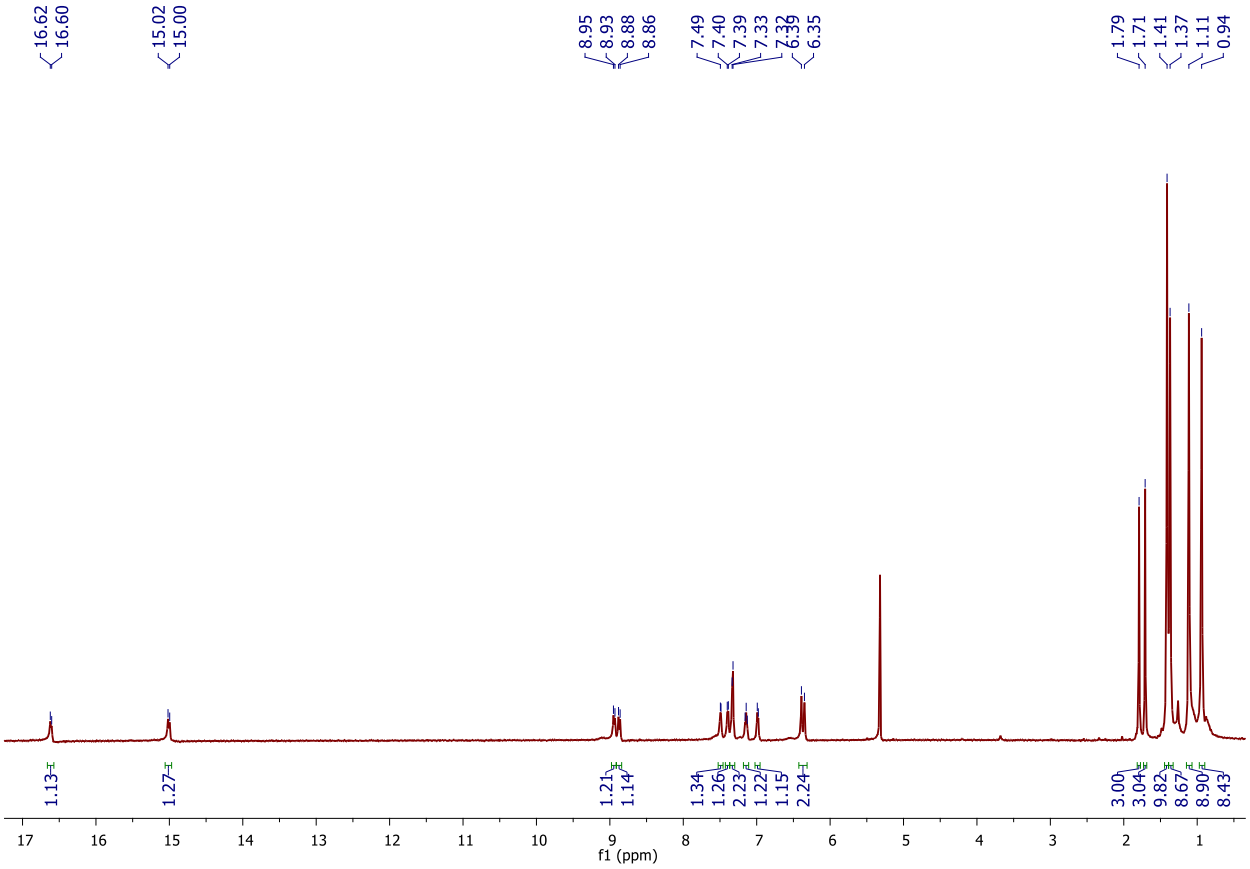
Contents:

I. ^{1}H and ^{13}C NMR Spectra

Figure S1. ^{1}H and ^{13}C NMR of $(XbicH_2)_2Zr$

^{1}H NMR (CD_2Cl_2, 500 MHz):



^{13}C NMR (C_6D_6):

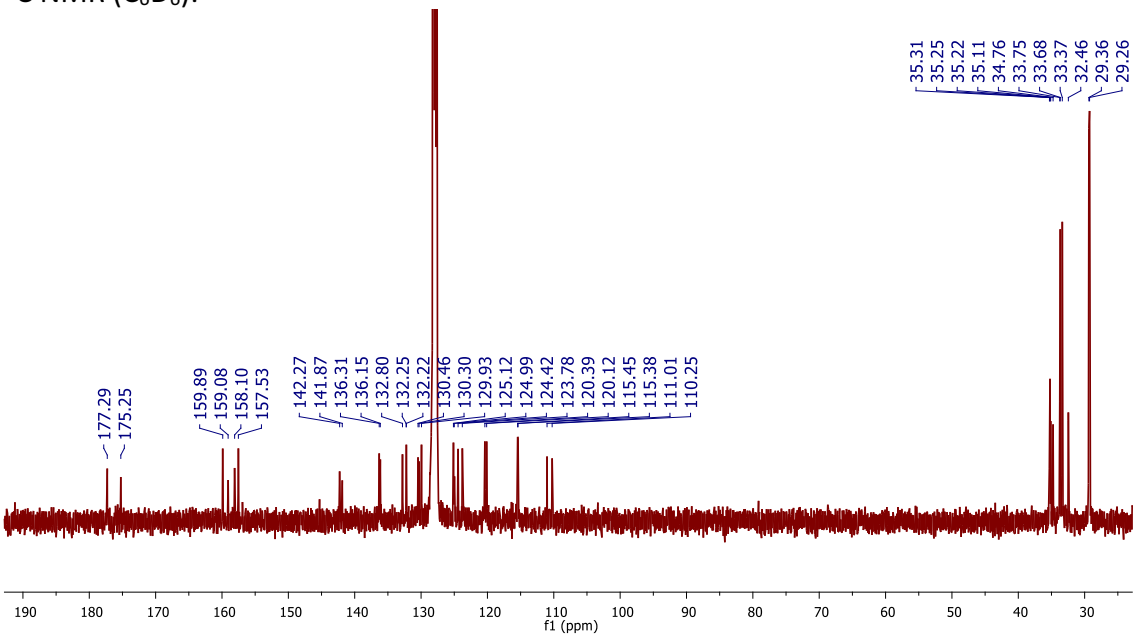
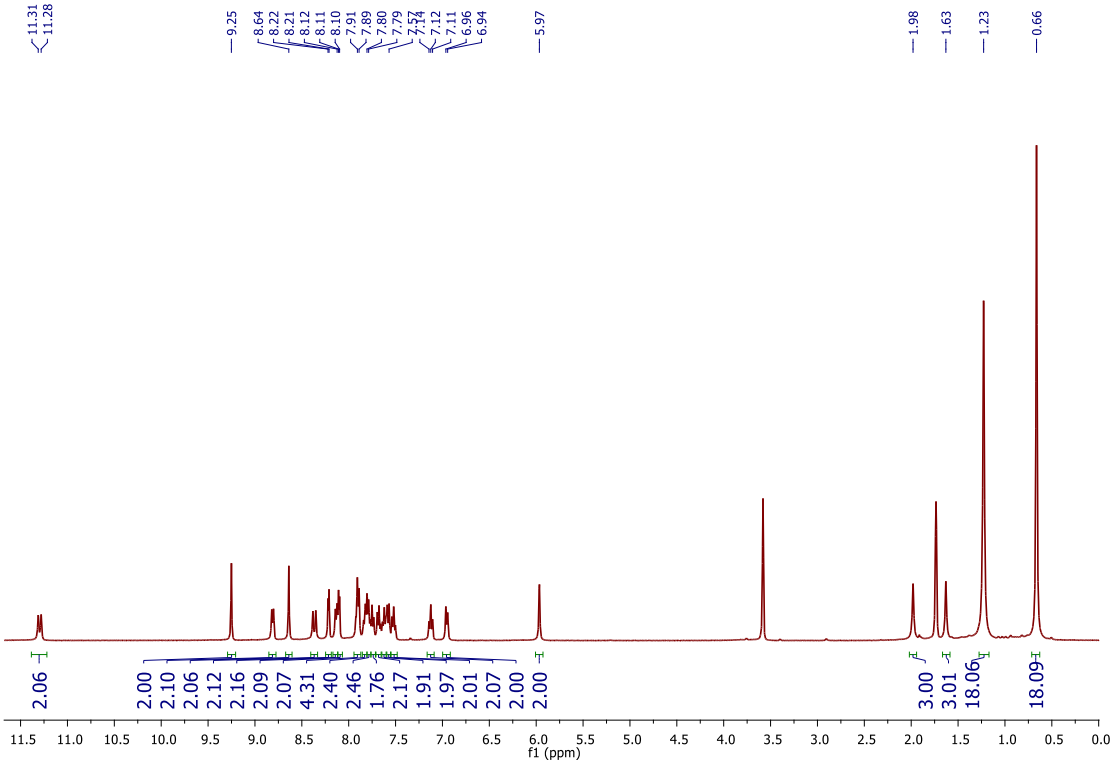
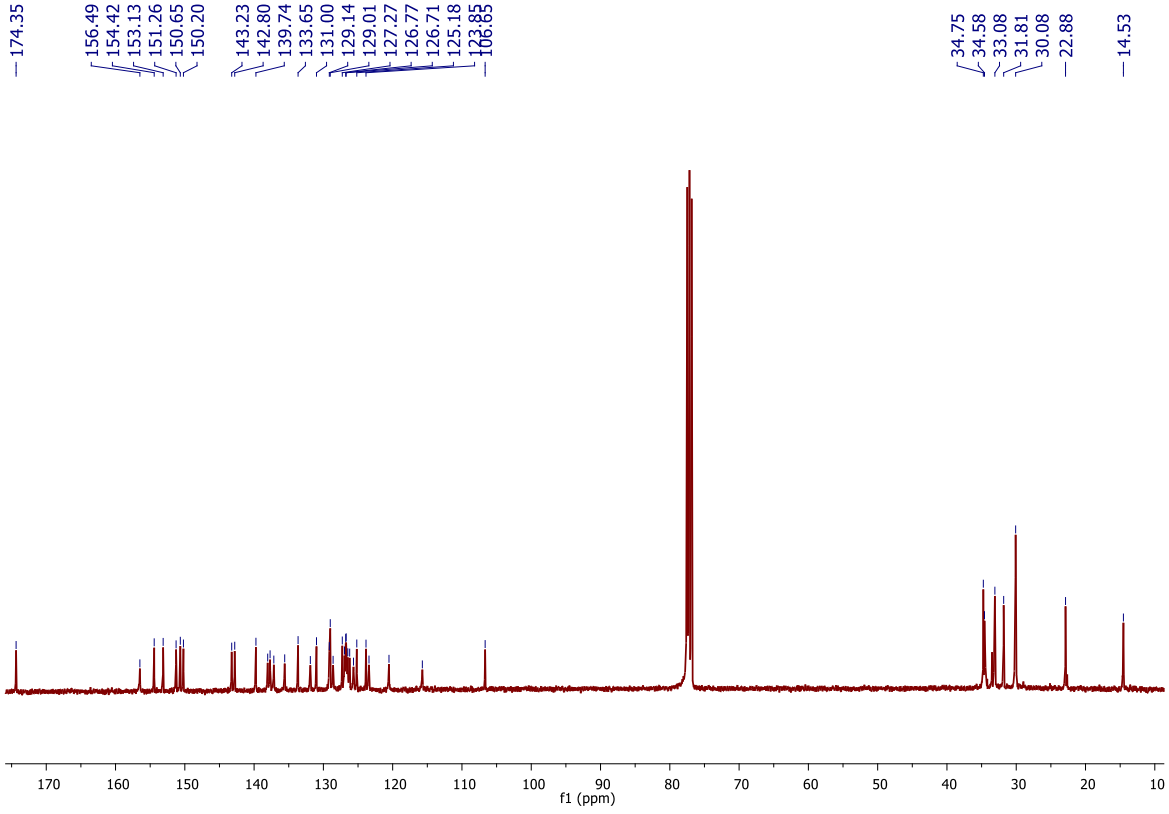


Figure S2. ^{1}H and ^{13}C NMR of (TPP)Zr(XbicH_2)

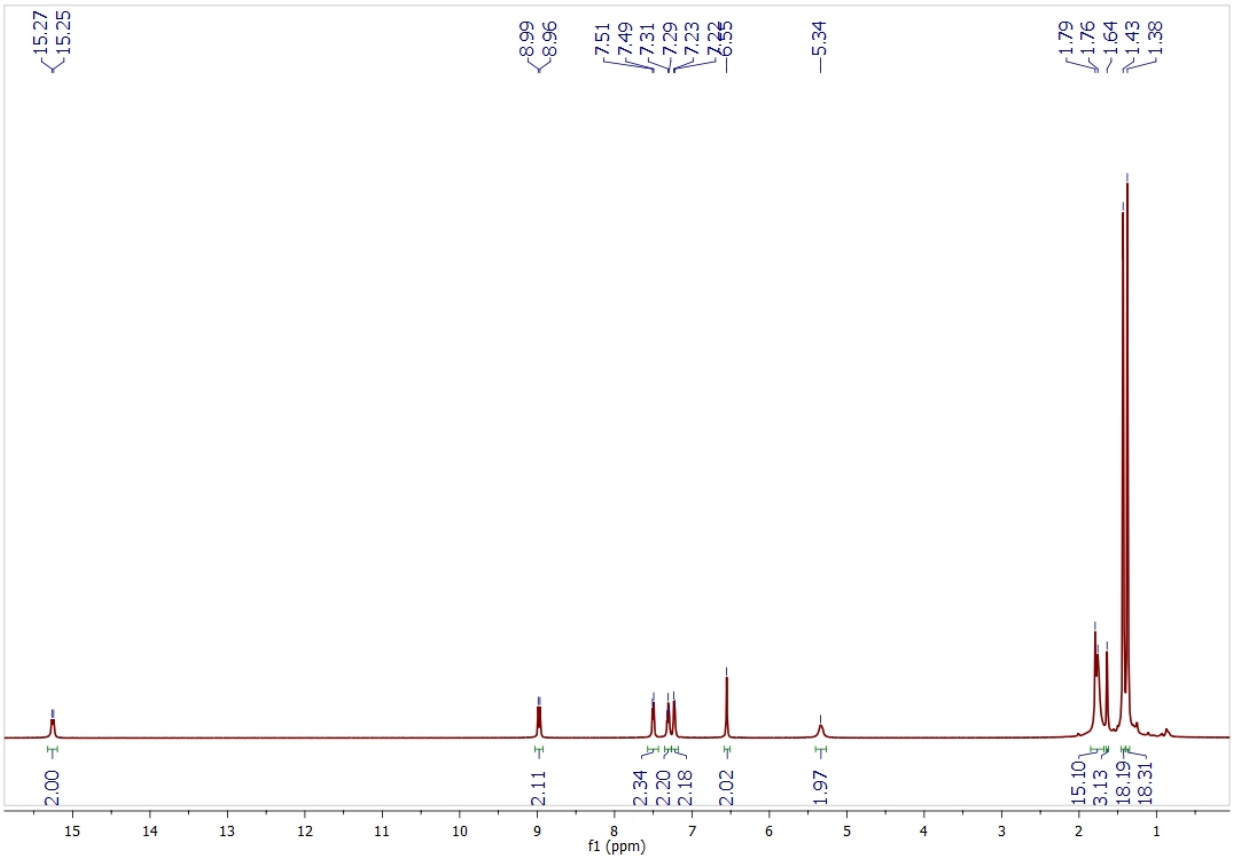
^{1}H NMR (400 MHz, THF-d_8, –58 °C):



^{13}C NMR ($CDCl_3$, –58 °C):

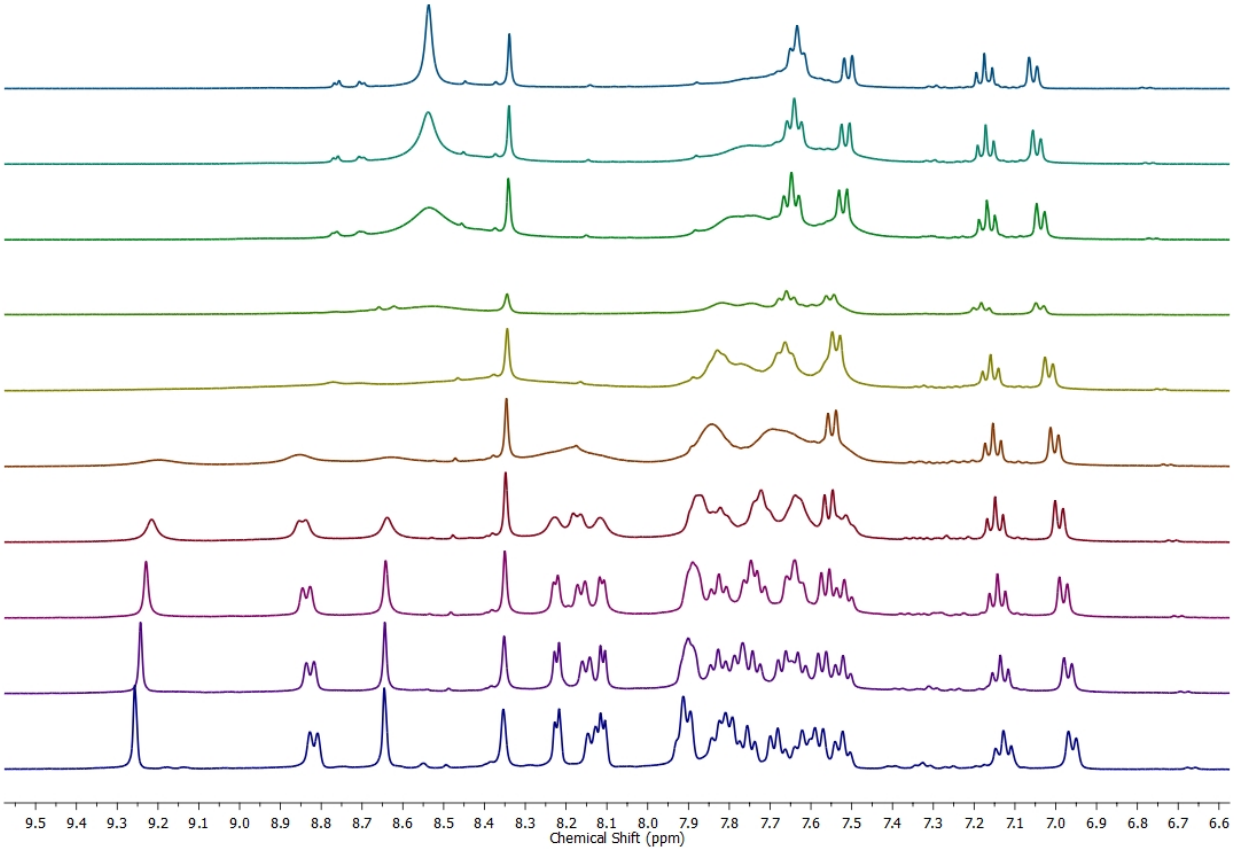


II. **Figure S3.** ^{1}H NMR spectrum of (XbicH_2)Zr(acac)$_2$ (500 MHz, CD_2Cl_2).

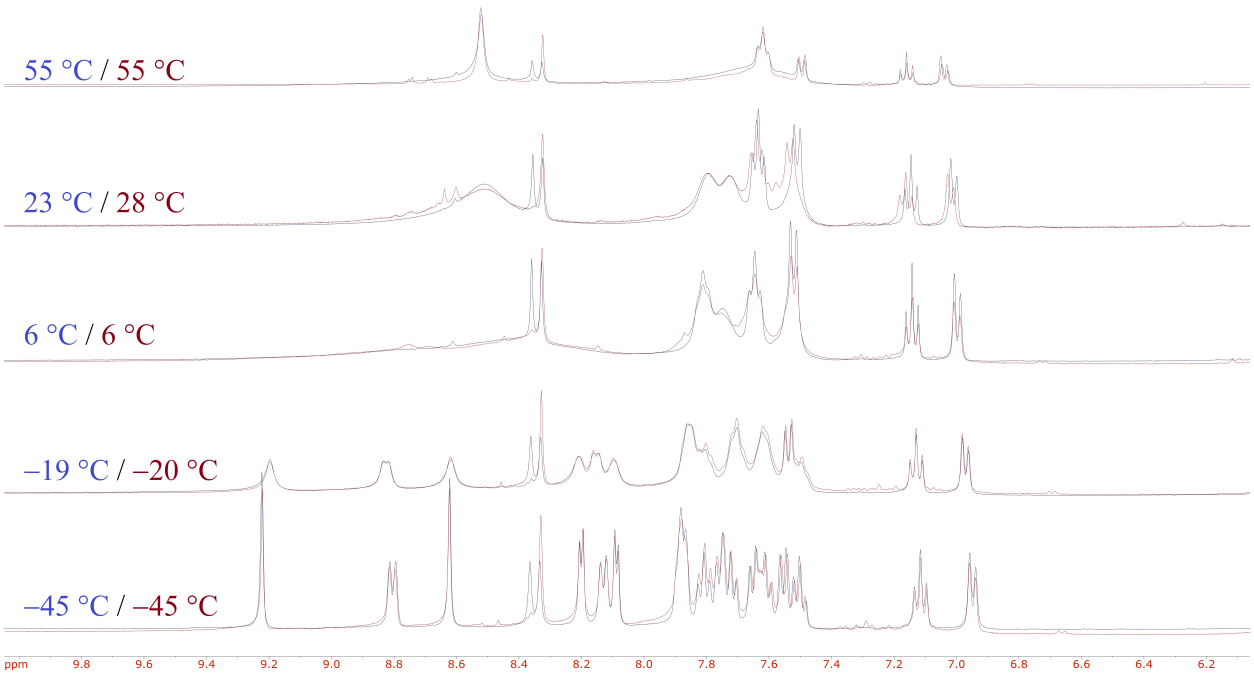


III. Fluxionality of ($XbicH_2$)Zr complexes

A. **Figure S4.** Variable-temperature ^{1}H NMR spectra (400 MHz, THF-d_8, aromatic region) of (TPP)Zr($XbicD_2$).



B. **Figure S5.** Overlay of variable-temperature ^{1}H NMR spectra (400 MHz, THF-d_8, aromatic region) of (TPP)Zr(XbicH$_2$) (blue) and (TPP)Zr(XbicD$_2$) (red).

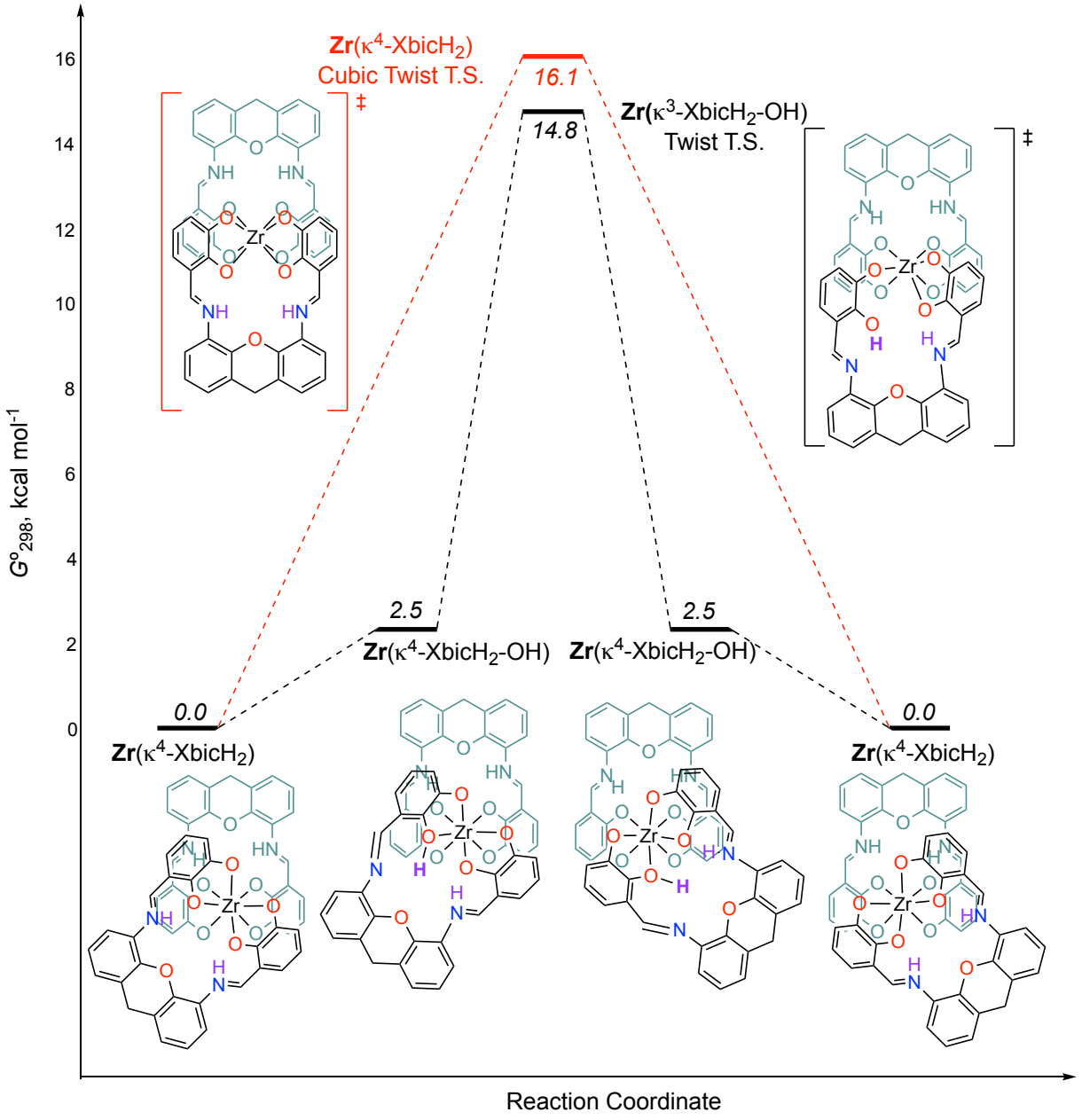


C. **Table S1.** Calculated *k* values for ring twisting in (TPP)Zr(XbicH$_2$) (blue) and (TPP)Zr(XbicD$_2$) (red) (THF-d_8).

T / K	k_H / s^{-1}	k_D / s^{-1}	k_H/k_D
266.6	79	75	1.06
279.3	310	290	1.07
306.2	2390	2390	1.00
317.5	6440	6200	1.04
328.8	23200	25000	0.93

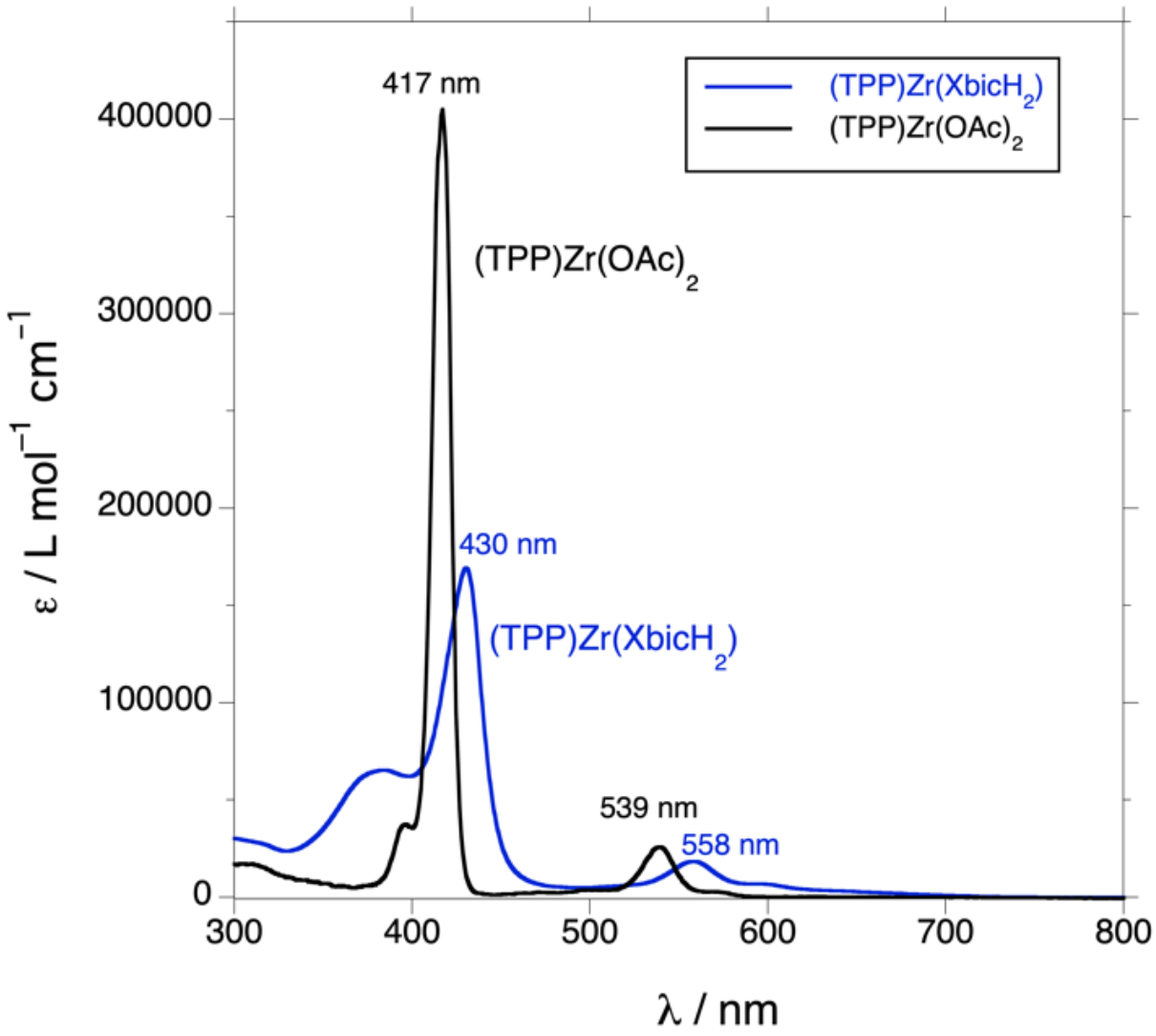
Average k_H/k_D = 1.02(6)

D. **Figure S6.** Calculated free energy landscape (B3LYP, SDD/6-31G*) for net ligand rotation in $(XbicH_2)_2Zr$. **Zr** = κ^4-$(XbicH_2)Zr$.

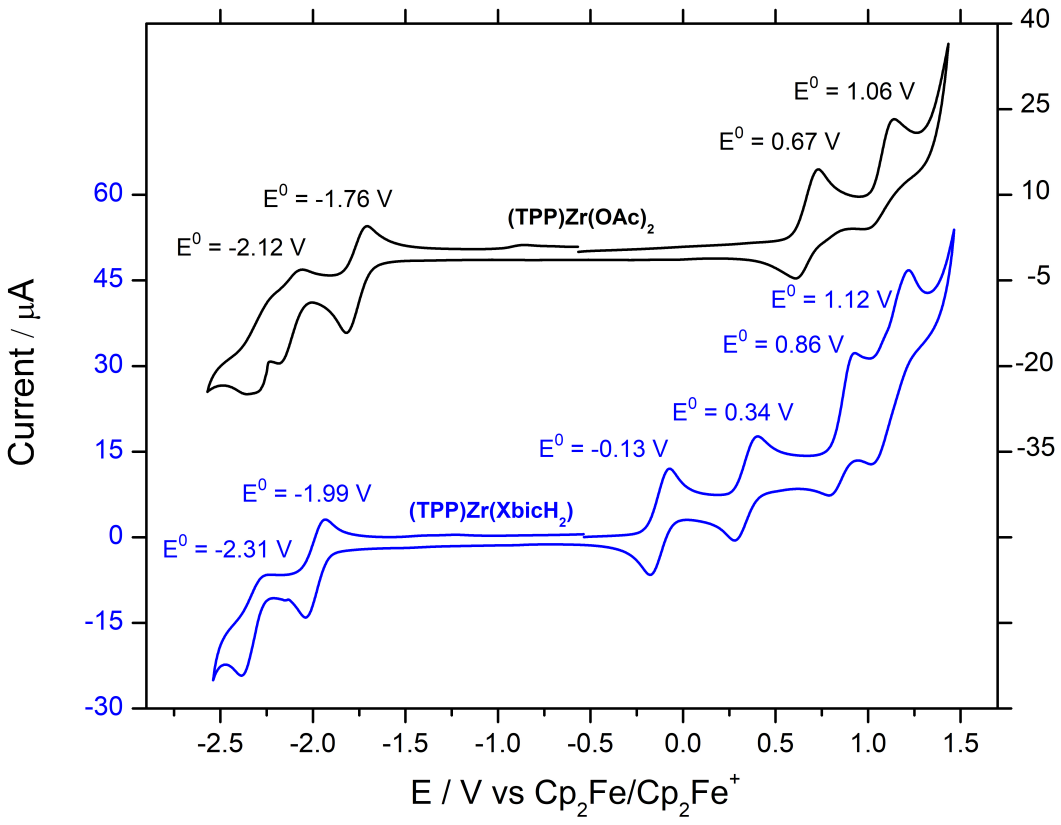


IV. Comparison of $(TPP)Zr(OAc)_2$ and $(TPP)Zr(XbicH_2)$

A. Figure S7. UV-visible spectra of $(TPP)Zr(OAc)_2$ (**black**) and $(TPP)Zr(XbicH_2)$ (blue) (CH_2Cl_2).

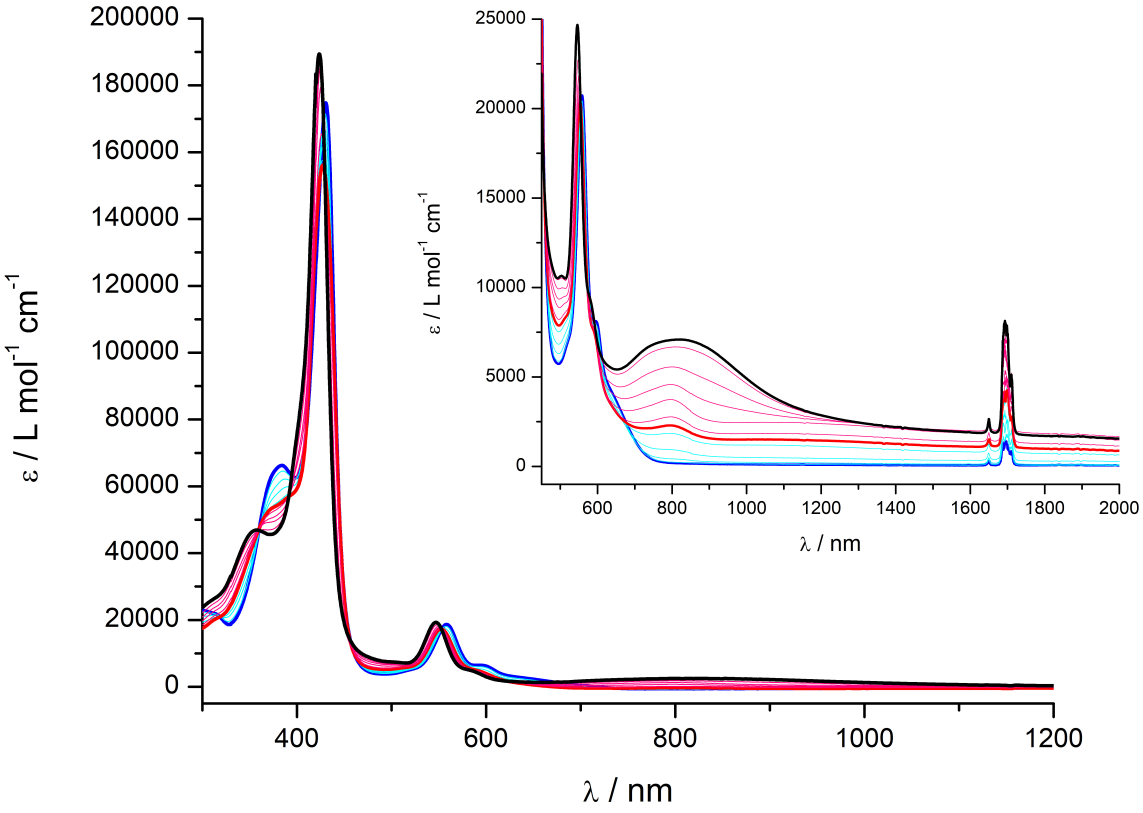


B. **Figure S8.** Cyclic voltammogram of (TPP)Zr(OAc)$_2$ (**black**) and (TPP)Zr(XbicH$_2$) (blue).

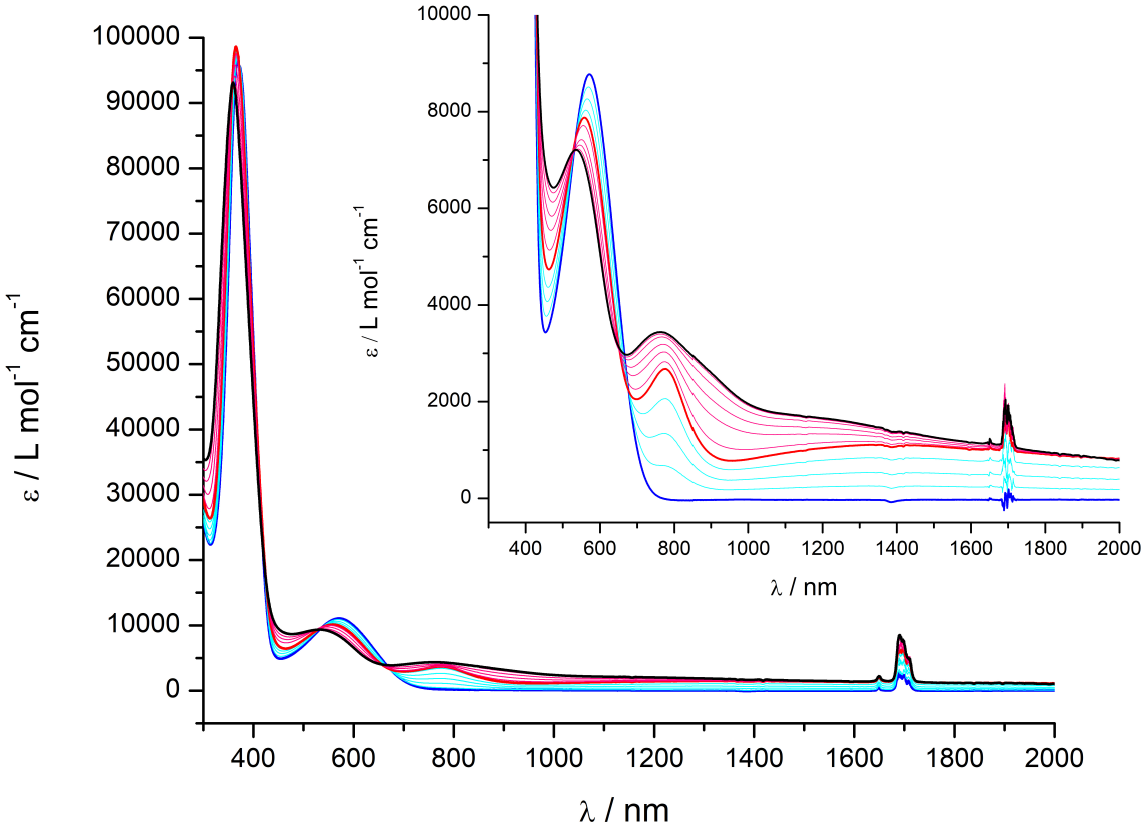


V. Redox titrations

A. Figure S9. Redox Titration of (TPP)Zr($XbicH_2$) with $AgPF_6$ in CH_2Cl_2 to generate first $[(TPP)Zr(XbicH_2)]^+$ and then to generate $[(TPP)Zr(XbicH_2)]^{2+}$. The initial spectrum is dark blue, with light blue spectra taken after aliquots of oxidant addition until 1.0 equiv, shown in red. Additions after 1.0 equiv are given in light red, with the final spectrum at 2.0 equiv oxidant shown in black. The concentration of (TPP)Zr($XbicH_2$) is 1.59×10^{-5} M in the main spectra and 6.34×10^{-5} M in the inset spectra.

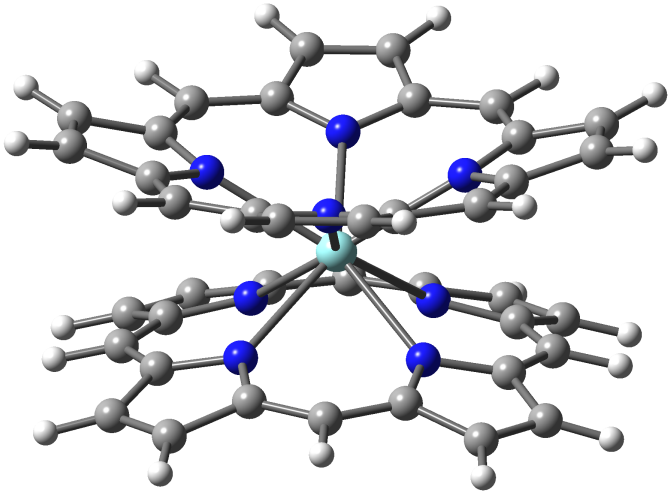


B. Figure S10. Redox Titration of $(XbicH_2)_2Zr$ (3.80×10^{-5} M; 1.14×10^{-4} M (expansion)) with $AcFcPF_6$ in CH_2Cl_2 to generate $[(XbicH_2)_2Zr]^+$ and then to generate $[(XbicH_2)_2Zr]^{2+}$. The initial spectrum is dark blue, with light blue spectra taken after aliquots of oxidant addition until 1.0 equiv, shown in red. Additions after 1.0 equiv are given in light red, with the final spectrum at 2.0 equiv oxidant shown in black. The concentration of $(XbicH_2)_2Zr$ is 3.80×10^{-5} M in the main spectra and 1.14×10^{-4} M in the inset spectra.



VI. Computational data (Cartesian coordinates, optimized energies, imaginary frequencies)

A. $(Por)_2Zr$



Optimized energy = –2023.94867302 a. u.

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4	1	-1.665969	1.585019	-5.112885
5	6	-0.705363	2.863119	-3.593199
6	1	-0.520345	3.815384	-4.074554
7	6	-0.435412	2.579823	-2.205235
8	6	-0.001462	3.545647	-1.306989
9	1	0.236050	4.524426	-1.713053
10	6	-0.000000	3.420367	0.075853
11	6	0.162840	4.543540	0.965600
12	1	0.377573	5.555868	0.646523
13	6	-0.072391	4.080502	2.223451
14	1	-0.091468	4.632365	3.155025
15	6	-0.378394	2.677054	2.095409
16	6	-0.839623	1.904586	3.153057
17	1	-0.861609	2.373400	4.132344
18	6	-1.425584	0.650717	3.041392
19	6	-2.164211	0.030822	4.113682
20	1	-2.258472	0.438305	5.112581
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22	1	-3.412803	-1.787139	4.073861
23	6	-2.354662	-1.141529	2.205091
24	6	-2.889006	-2.055636	1.306878
25	1	-3.548852	-2.816823	1.712492
26	6	-2.785102	-1.984917	-0.075970
27	6	-3.604347	-2.770293	-0.965764
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37	7	-2.015806	-1.084973	-0.781627
38	6	1.357919	-0.784076	-3.041107
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41	6	0.705363	-2.863119	-3.593199
42	1	0.520345	-3.815384	-4.074554
43	6	0.435412	-2.579823	-2.205235
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49	6	0.072391	-4.080502	2.223451
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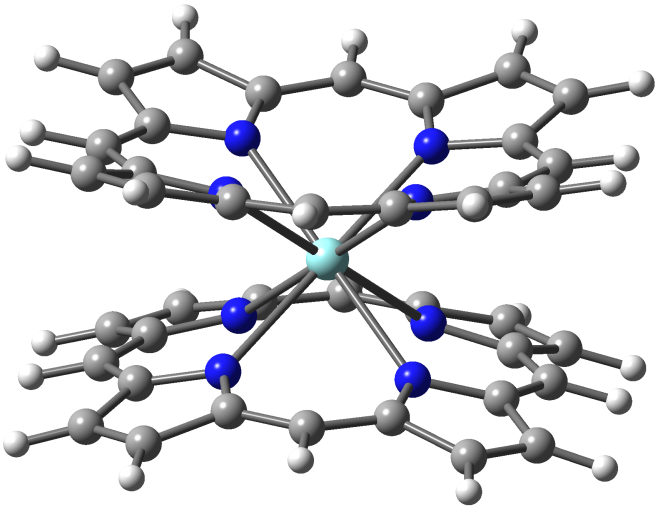
53	1	0.861609	-2.373400	4.132344
54	6	1.425584	-0.650717	3.041392
55	6	2.164211	-0.030822	4.113682
56	1	2.258472	-0.438305	5.112581
57	6	2.743206	1.085108	3.592690
58	1	3.412803	1.787139	4.073861
59	6	2.354662	1.141529	2.205091
60	6	2.889006	2.055636	1.306878
61	1	3.548852	2.816823	1.712492
62	6	2.785102	1.984917	-0.075970
63	6	3.604347	2.770293	-0.965764
64	1	4.303264	3.533418	-0.646589
65	6	3.364421	2.309660	-2.223602
66	1	3.824855	2.614698	-3.155098
67	6	2.400054	1.245119	-2.095601
68	6	2.039305	0.420554	-3.153009
69	1	2.433923	0.674155	-4.132412
70	7	0.796116	-1.288028	-1.887775
71	7	0.285798	-2.271387	0.781476
72	7	1.510431	0.099276	1.888086
73	7	2.015806	1.084973	-0.781627

B. $(Por)_2Zr$, twist transition state



Optimized energy = –2023.89134677 a. u.
Imaginary frequency = (44.9 cm^{-1})*i*

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8	6	-2.665984	-2.149367	-1.611422
9	1	-3.499956	-2.821838	-1.790025
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26	6	1.391145	2.703342	-1.600970
27	6	1.134001	4.076193	-1.960846
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32	6	-2.133260	2.640728	-1.798103
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37	7	0.213822	2.014971	-1.403011
38	6	2.708597	-1.392573	1.596853
39	6	4.082007	-1.136758	1.955856
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43	6	2.930371	0.776377	1.699949
44	6	2.648266	2.131488	1.792596
45	1	3.470253	2.793020	2.049814
46	6	1.384668	2.696427	1.700478
47	6	1.111183	4.073636	2.029773
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61	1	-3.465711	-2.787323	2.058311
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66	1	0.835352	-5.103007	2.184524
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69	1	2.818258	-3.496984	1.793434
70	7	2.021389	-0.214957	1.398975
71	7	0.221955	2.020723	1.398124
72	7	-2.018074	0.219767	1.400134
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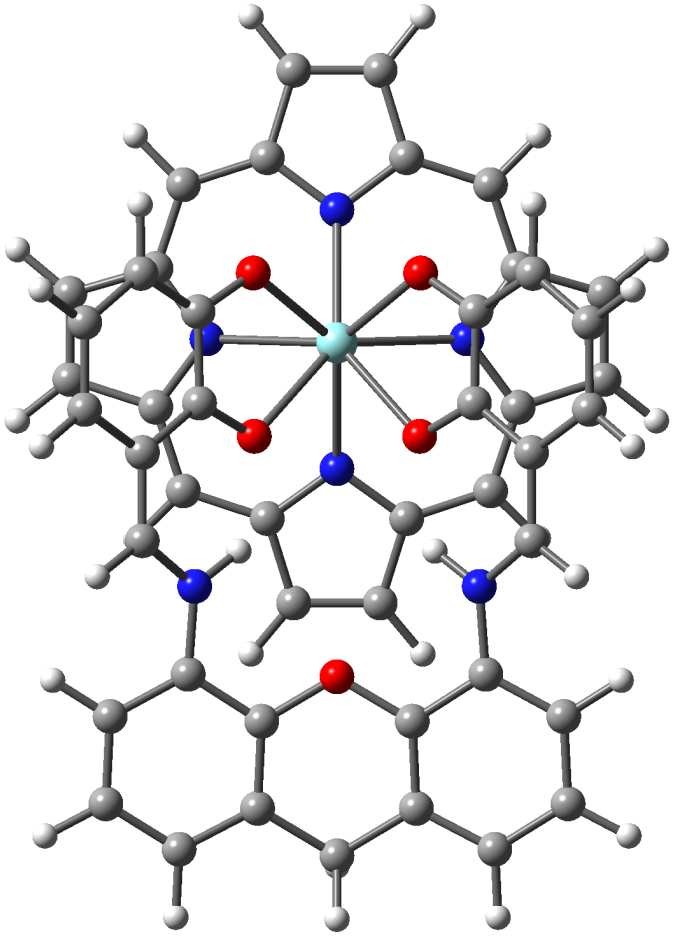
C. (Por)Zr(κ^4-XbicH$_2$)



Optimized energy = –2560.99630303 a. u.

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6	8	3.649653	0.000033	0.099994
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9	7	2.368326	-2.244416	0.930655
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12	7	-2.113383	-2.050818	-1.377987
13	7	-0.128716	-0.000127	-1.885188
14	7	-2.113377	2.050646	-1.378413
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17	6	0.480588	3.068499	2.203196
18	6	-0.000522	3.979852	3.208303
19	1	0.701480	4.660975	3.682187

20	6	-1.328586	3.978032	3.542323
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22	6	-2.254495	3.090473	2.920936
23	1	-3.301348	3.102418	3.210502
24	6	1.823293	3.070557	1.831785
25	1	2.502584	3.778293	2.301743
26	6	-1.845023	-2.189994	1.945204
27	6	-0.450616	-2.167569	1.574336
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30	1	0.701591	-4.660761	3.682302
31	6	-1.328439	-3.977651	3.542666
32	1	-1.695540	-4.665959	4.299354
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36	1	2.502635	-3.778228	2.301557
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38	6	4.341601	1.186827	-0.017862
39	6	5.635572	1.252184	-0.537809
40	6	6.287609	2.489329	-0.571501
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42	6	5.649080	3.644631	-0.127712
43	1	6.154836	4.603856	-0.178813
44	6	4.343333	3.576542	0.353969
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46	6	3.679069	-2.346768	0.430990
47	6	4.342992	-3.576593	0.353278
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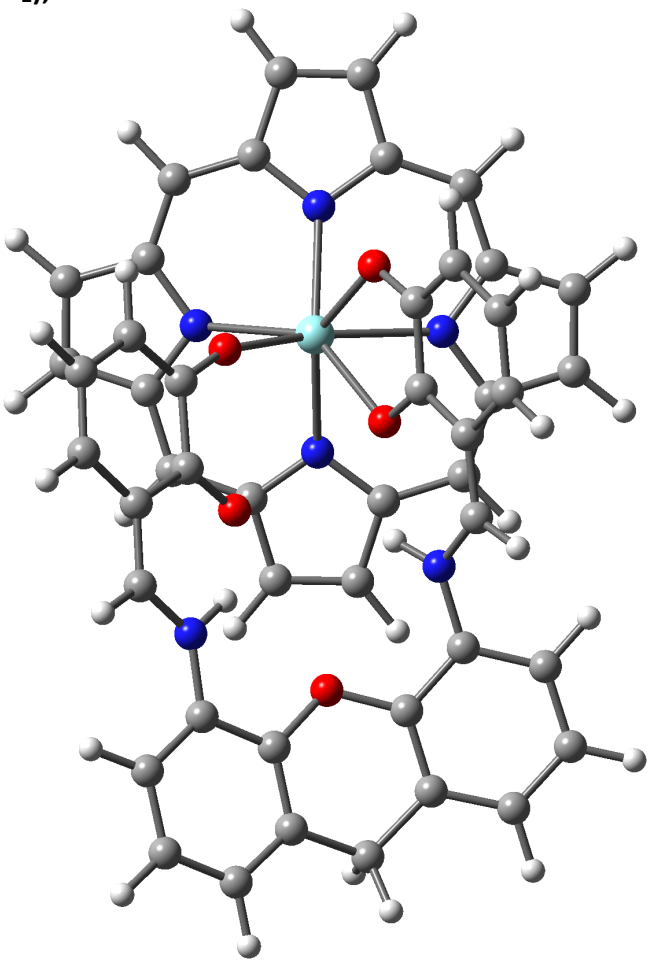
57	1	-7.101980	1.353248	-0.424413
58	6	-6.256414	-0.681172	-0.502248
59	1	-7.101973	-1.353260	-0.424059
60	6	-4.885690	-1.098696	-0.684151
61	6	-3.219256	-2.854161	-1.245669
62	6	-2.901614	-4.210199	-1.631084
63	1	-3.603500	-5.034994	-1.629595
64	6	-1.595155	-4.212488	-2.018924
65	1	-1.009292	-5.039082	-2.401998
66	6	-1.115793	-2.856610	-1.870662
67	6	0.586731	-1.099449	-2.306398
68	6	1.813822	-0.682576	-2.941119
69	1	2.544400	-1.354925	-3.374421
70	6	1.813820	0.682110	-2.941260
71	1	2.544390	1.354371	-3.374712
72	6	0.586730	1.099113	-2.306620
73	6	-1.115788	2.856352	-1.871226
74	6	-1.595164	4.212196	-2.019771
75	1	-1.009297	5.038723	-2.402980
76	6	-2.901634	4.209963	-1.631976
77	1	-3.603537	5.034746	-1.630685

78	6	-3.219267	2.853998	-1.246300
79	6	6.285297	0.000022	-1.078047
80	1	7.357178	-0.000070	-0.844889
81	1	6.217062	0.000170	-2.177597
82	6	-4.489418	-2.420522	-0.869905
83	1	-5.265235	-3.177920	-0.799777
84	6	0.152297	-2.423424	-2.250607
85	1	0.833347	-3.177391	-2.636619
86	6	0.152302	2.423100	-2.251087
87	1	0.833352	3.176992	-2.637240
88	6	-4.489432	2.420416	-0.870486
89	1	-5.265264	3.177818	-0.800552

D. (Por)Zr(κ^3-XbicH$_2$), NH tautomer



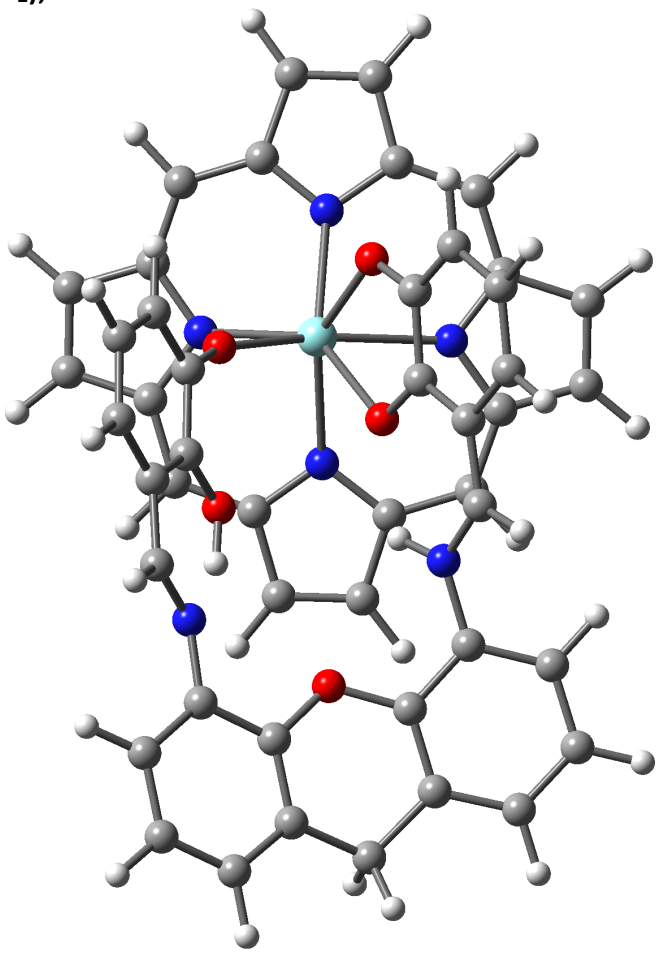
Optimized energy = –2560.98568823 a.u.

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	40	2.230917	0.065502	-0.245471
2	8	-4.071566	-0.119952	-0.285543
3	6	-6.580209	-0.907923	-1.388660
4	1	-7.599587	-1.279775	-1.232142
5	1	-6.464139	-0.788052	-2.477844
6	8	2.750946	-0.728445	1.670026
7	8	0.402134	-1.005720	0.595379
8	7	-2.192207	-1.892839	0.733634
9	1	-1.586333	-1.201965	0.276508
10	6	1.845744	-1.356972	2.396781
11	6	0.548069	-1.498430	1.777468
12	6	-0.501316	-2.193251	2.475900
13	6	-0.235552	-2.725518	3.787602
14	1	-1.029787	-3.251303	4.311372
15	6	0.997926	-2.557565	4.355242
16	1	1.197244	-2.953027	5.347417
17	6	2.042818	-1.872907	3.666743
18	1	3.017088	-1.752402	4.132100

19	6	-1.749174	-2.401140	1.889194
20	1	-2.464854	-3.036849	2.407450
21	6	-3.389565	-2.356467	0.127762
22	6	-3.650307	-3.730138	0.061060
23	1	-2.888193	-4.424083	0.402201
24	6	-4.861119	-4.199114	-0.446583
25	1	-5.051523	-5.267026	-0.489546
26	6	-5.816619	-3.295414	-0.906988
27	1	-6.763877	-3.655802	-1.300147
28	6	-5.572789	-1.918891	-0.881461
29	6	-4.356391	-1.460068	-0.365283
30	8	1.518486	1.672529	0.777934
31	8	-1.147990	1.469683	0.292174
32	7	-3.533125	2.251058	0.713172
33	1	-2.778517	1.633169	0.337754
34	6	0.683825	2.472516	1.416215
35	6	-0.745961	2.343163	1.113664
36	6	-1.662254	3.266410	1.796442
37	6	-1.155690	4.236735	2.727257
38	1	-1.856533	4.905376	3.222450
39	6	0.184350	4.301813	2.981089
40	1	0.573806	5.029557	3.687689
41	6	1.100696	3.421615	2.326968
42	1	2.163970	3.492195	2.539622
43	6	-3.028640	3.176864	1.540935
44	1	-3.725599	3.853358	2.032721
45	6	-4.851398	2.026070	0.328194
46	6	-5.893639	2.954065	0.439138
47	1	-5.698222	3.939560	0.849857
48	6	-7.175273	2.617828	0.000904
49	1	-7.977927	3.343358	0.093874
50	6	-7.427261	1.372822	-0.575751
51	1	-8.423754	1.126612	-0.932761
52	6	-6.397288	0.434469	-0.715134
53	6	-5.133402	0.767377	-0.239899
54	6	0.531957	-2.606476	-2.121445
55	1	-0.112328	-3.400271	-2.489986
56	6	5.067544	2.358736	-0.667543
57	1	5.831595	3.120474	-0.541870
58	7	2.837918	1.904344	-1.589002
59	7	0.853220	-0.163580	-2.084463
60	6	3.904867	2.731666	-1.340908
61	6	3.665903	4.038748	-1.909837
62	1	4.360532	4.868564	-1.869891
63	6	2.440891	3.989725	-2.503851
64	1	1.928070	4.771230	-3.050682
65	6	1.930049	2.652905	-2.298267
66	6	0.710130	2.191182	-2.789799
67	1	0.102334	2.906308	-3.336840
68	6	0.232316	0.882991	-2.728924
69	6	-0.921938	0.402929	-3.447443
70	1	-1.578750	1.022426	-4.045324
71	6	-0.966922	-0.948979	-3.267821
72	1	-1.666531	-1.658342	-3.692789
73	6	0.156152	-1.299720	-2.432639
74	7	4.532638	-0.012171	-0.292449
75	7	2.633750	-2.133203	-0.945426
76	6	5.373782	1.076423	-0.216130

77	6	6.658604	0.670388	0.299510
78	1	7.502119	1.332779	0.448647
79	6	6.597379	-0.677681	0.496276
80	1	7.382015	-1.340471	0.839455
81	6	5.273660	-1.101413	0.109479
82	6	4.859847	-2.431590	0.055258
83	1	5.577254	-3.175473	0.390688
84	6	3.663644	-2.913024	-0.477064
85	6	3.360247	-4.309934	-0.688539
86	1	4.011733	-5.132887	-0.421843
87	6	2.145447	-4.361168	-1.306914
88	1	1.604157	-5.234896	-1.648584
89	6	1.702926	-2.995731	-1.471988

E. (Por)Zr(κ^3-XbicH$_2$), OH tautomer



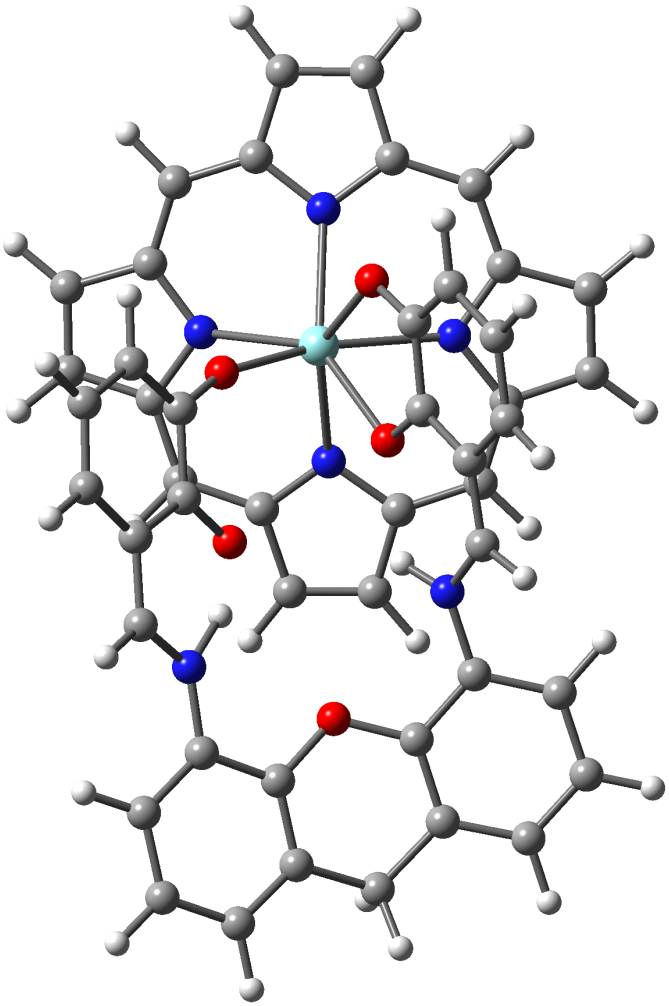
Optimized energy = –2560.98981605 a. u.

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	40	2.253002	0.104992	-0.276187
2	8	-4.104636	-0.053580	-0.330134
3	6	-6.647656	-0.787640	-1.406473
4	1	-7.665190	-1.154444	-1.226091
5	1	-6.566676	-0.642515	-2.495854
6	8	2.676766	-0.621219	1.682584
7	8	0.347443	-0.871841	0.553071
8	7	-2.232240	-1.852484	0.604646
9	1	-1.615327	-1.170792	0.150602
10	6	1.752873	-1.258021	2.380076
11	6	0.471221	-1.392872	1.729396
12	6	-0.582345	-2.115017	2.391055
13	6	-0.344700	-2.659230	3.702742
14	1	-1.146053	-3.201823	4.197714
15	6	0.871617	-2.486566	4.305251
16	1	1.049752	-2.891963	5.297343
17	6	1.925333	-1.787084	3.648407
18	1	2.889132	-1.665913	4.134953

19	6	-1.812805	-2.344235	1.772960
20	1	-2.532181	-2.987171	2.276763
21	6	-3.436831	-2.300386	-0.005527
22	6	-3.700422	-3.669945	-0.109795
23	1	-2.936647	-4.376035	0.202033
24	6	-4.921486	-4.117668	-0.613380
25	1	-5.117955	-5.182732	-0.687833
26	6	-5.881576	-3.194919	-1.025267
27	1	-6.837563	-3.539856	-1.411444
28	6	-5.634596	-1.820326	-0.958041
29	6	-4.406041	-1.382112	-0.451551
30	8	1.517879	1.775655	0.642233
31	8	-1.088043	1.747543	0.003569
32	1	-2.088747	1.797782	-0.039538
33	7	-3.507117	2.299904	0.666200
34	6	0.658864	2.361442	1.466788
35	6	-0.724987	2.366813	1.137424
36	6	-1.660847	2.999303	2.001009
37	6	-1.203088	3.643040	3.176601
38	1	-1.927696	4.119838	3.832445
39	6	0.145223	3.651827	3.482349
40	1	0.500388	4.145405	4.382509
41	6	1.067237	3.012076	2.634397
42	1	2.127274	3.005980	2.871201
43	6	-3.075664	2.911014	1.722452
44	1	-3.768215	3.332582	2.464402
45	6	-4.844663	2.091458	0.344947
46	6	-5.878344	3.025728	0.490431
47	1	-5.652995	4.000210	0.913966
48	6	-7.171501	2.718348	0.061605
49	1	-7.964831	3.451312	0.176617
50	6	-7.444632	1.486474	-0.532336
51	1	-8.449245	1.258457	-0.879729
52	6	-6.429572	0.536449	-0.705604
53	6	-5.152793	0.848875	-0.248999
54	6	0.506589	-2.555239	-2.118671
55	1	-0.156311	-3.334235	-2.485775
56	6	5.190630	2.275660	-0.649709
57	1	5.978009	3.011567	-0.515028
58	7	2.978383	1.878614	-1.636039
59	7	0.928715	-0.127637	-2.147626
60	6	4.064988	2.674292	-1.369319
61	6	3.892065	3.974569	-1.975700
62	1	4.613461	4.780840	-1.929406
63	6	2.688453	3.952742	-2.613580
64	1	2.223584	4.737676	-3.197075
65	6	2.123813	2.639979	-2.396716
66	6	0.908952	2.208785	-2.925936
67	1	0.350224	2.930554	-3.514814
68	6	0.378357	0.921883	-2.849272
69	6	-0.766466	0.465671	-3.597481
70	1	-1.373525	1.091078	-4.240059
71	6	-0.876314	-0.876626	-3.376323
72	1	-1.589492	-1.569675	-3.805535
73	6	0.197839	-1.245632	-2.486855
74	7	4.550829	-0.062360	-0.237597
75	7	2.583460	-2.128101	-0.881400
76	6	5.432028	0.993637	-0.159603

77	6	6.680941	0.551770	0.411890
78	1	7.544972	1.184186	0.573094
79	6	6.557822	-0.786381	0.643663
80	1	7.302237	-1.469610	1.033212
81	6	5.231528	-1.167935	0.222840
82	6	4.763954	-2.481077	0.198899
83	1	5.439212	-3.241522	0.581375
84	6	3.565463	-2.932480	-0.354602
85	6	3.212272	-4.322019	-0.532694
86	1	3.820670	-5.161192	-0.219014
87	6	2.017424	-4.345084	-1.190786
88	1	1.453336	-5.207467	-1.524265
89	6	1.636319	-2.969712	-1.413820

F. (Por)Zr(κ^3-XbicH$_2$), tautomerization transition state



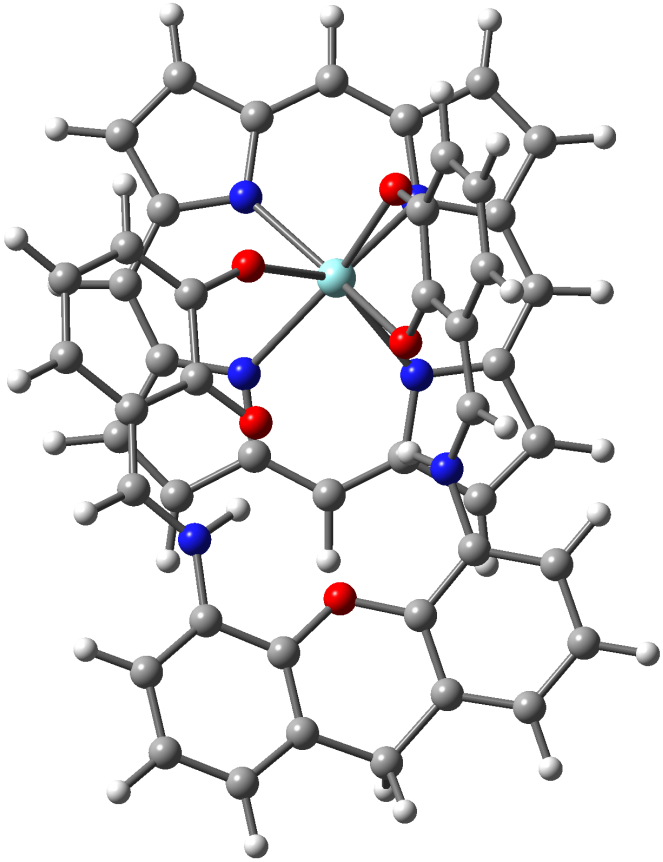
Optimized energy = –2560.98241511 a.u.
Imaginary frequency = (1167.7 cm^{-1})*i*

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	40	2.216084	0.085900	-0.270918
2	8	-4.018830	-0.118044	-0.278827
3	6	-6.512739	-0.872439	-1.442285
4	1	-7.540987	-1.228369	-1.307865
5	1	-6.371153	-0.755882	-2.528878
6	8	2.741718	-0.668870	1.657380
7	8	0.386005	-0.964203	0.601571
8	7	-2.176867	-1.902085	0.743415
9	1	-1.576088	-1.203376	0.291013
10	6	1.848380	-1.309018	2.389721
11	6	0.548382	-1.463759	1.780277
12	6	-0.484133	-2.179416	2.481690
13	6	-0.202978	-2.711359	3.789639
14	1	-0.985703	-3.251744	4.315855
15	6	1.031318	-2.526236	4.350798
16	1	1.242668	-2.921474	5.340541

17	6	2.061375	-1.825257	3.657169
18	1	3.037386	-1.692898	4.115642
19	6	-1.730414	-2.407550	1.897132
20	1	-2.436280	-3.055591	2.413573
21	6	-3.372260	-2.360668	0.132126
22	6	-3.645978	-3.731190	0.062771
23	1	-2.896929	-4.434027	0.414617
24	6	-4.854359	-4.185583	-0.464186
25	1	-5.056992	-5.251126	-0.510087
26	6	-5.790530	-3.270742	-0.942687
27	1	-6.734146	-3.620651	-1.353752
28	6	-5.531695	-1.896981	-0.912941
29	6	-4.320737	-1.451934	-0.373124
30	8	1.464093	1.702030	0.706915
31	8	-1.233228	1.563508	0.243815
32	7	-3.477605	2.255957	0.745780
33	1	-2.486911	1.727488	0.309667
34	6	0.633958	2.413176	1.453548
35	6	-0.782133	2.345197	1.176950
36	6	-1.673899	3.170371	1.961302
37	6	-1.164855	4.015095	2.991118
38	1	-1.858244	4.621181	3.569904
39	6	0.185500	4.046499	3.236261
40	1	0.588141	4.682695	4.019365
41	6	1.075901	3.250326	2.469297
42	1	2.144190	3.286036	2.664463
43	6	-3.057975	3.081280	1.686536
44	1	-3.774856	3.669567	2.264398
45	6	-4.786628	2.037980	0.325127
46	6	-5.822687	2.978206	0.402899
47	1	-5.620612	3.961752	0.816163
48	6	-7.095597	2.662249	-0.072649
49	1	-7.891237	3.398474	-0.006305
50	6	-7.344740	1.418818	-0.654026
51	1	-8.333542	1.183908	-1.039526
52	6	-6.323796	0.467461	-0.764891
53	6	-5.066621	0.784873	-0.257360
54	6	0.493685	-2.600093	-2.100846
55	1	-0.156255	-3.395244	-2.456268
56	6	5.065180	2.360440	-0.727806
57	1	5.833337	3.119844	-0.613782
58	7	2.829035	1.905691	-1.632559
59	7	0.828983	-0.159261	-2.096924
60	6	3.900136	2.731678	-1.397977
61	6	3.661852	4.034371	-1.976902
62	1	4.359170	4.862387	-1.948151
63	6	2.433396	3.983737	-2.563816
64	1	1.920100	4.761936	-3.114897
65	6	1.919538	2.650527	-2.343868
66	6	0.696009	2.188746	-2.826135
67	1	0.088963	2.901368	-3.377209
68	6	0.211911	0.883536	-2.750990
69	6	-0.947182	0.401400	-3.460235
70	1	-1.603109	1.017632	-4.062393
71	6	-0.999276	-0.948106	-3.264694
72	1	-1.704827	-1.658146	-3.678499
73	6	0.124335	-1.295601	-2.428943
74	7	4.518814	-0.002740	-0.323955

75	7	2.601777	-2.122659	-0.936820
76	6	5.366988	1.081218	-0.264572
77	6	6.651543	0.673617	0.250672
78	1	7.499872	1.332434	0.387857
79	6	6.582409	-0.671308	0.465353
80	1	7.364144	-1.334630	0.814091
81	6	5.254147	-1.091376	0.089940
82	6	4.831167	-2.419460	0.057505
83	1	5.545584	-3.162880	0.400279
84	6	3.629332	-2.901702	-0.461518
85	6	3.316983	-4.299436	-0.652416
86	1	3.964719	-5.122419	-0.376870
87	6	2.099744	-4.352272	-1.266102
88	1	1.552616	-5.227610	-1.594059
89	6	1.664143	-2.987034	-1.448796

G. (Por)Zr(κ^3-XbicH$_2$), NH tautomer, twist transition state



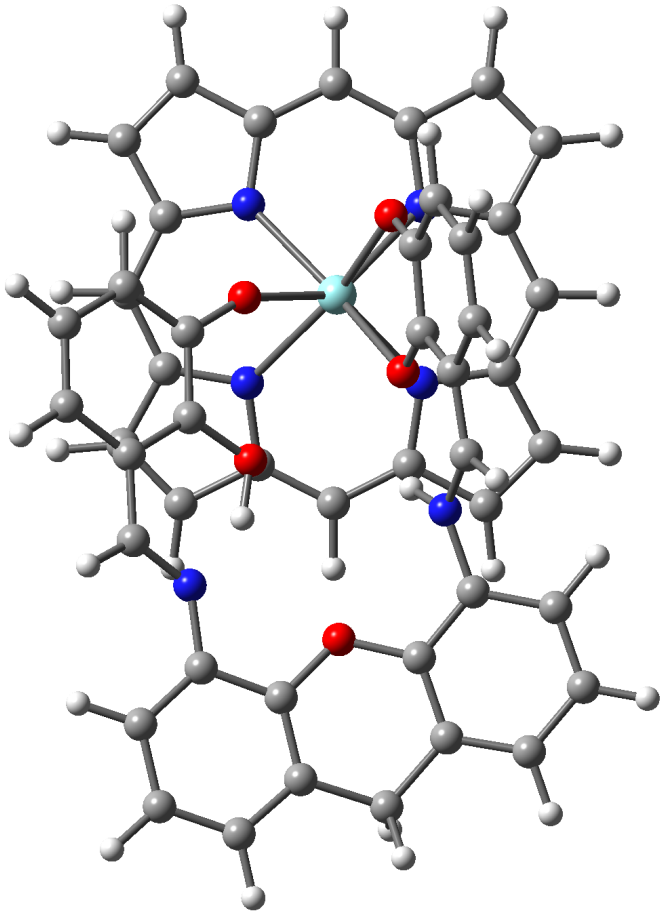
Optimized energy = –2560.97761735 a.u.
Imaginary frequency = (14.0 cm^{-1})*i*

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	40	2.196318	0.104042	0.251184
2	8	-4.015923	0.232986	0.251232
3	6	-6.531993	1.083444	1.280357
4	1	-7.569747	1.388257	1.101709
5	1	-6.383602	1.134617	2.371076
6	8	2.822118	0.978607	-1.601812
7	8	0.432367	1.217687	-0.672129
8	7	-2.204859	1.908701	-1.021689
9	1	-1.582396	1.313304	-0.463913
10	6	1.912161	1.382727	-2.465320
11	6	0.581968	1.524128	-1.916146
12	6	-0.476474	2.038884	-2.742622
13	6	-0.191014	2.379882	-4.111397
14	1	-0.994391	2.763372	-4.735221
15	6	1.071993	2.205914	-4.610844
16	1	1.284229	2.454235	-5.647068
17	6	2.129126	1.709761	-3.793743
18	1	3.128295	1.591845	-4.203532
19	6	-1.753326	2.266241	-2.227766
20	1	-2.479633	2.786780	-2.849533
21	6	-3.425219	2.408745	-0.497967

22	6	-3.743329	3.764568	-0.639349
23	1	-3.011138	4.430166	-1.085907
24	6	-4.970412	4.255269	-0.195758
25	1	-5.205347	5.308469	-0.314342
26	6	-5.882340	3.395933	0.414046
27	1	-6.839249	3.774732	0.764114
28	6	-5.580368	2.043117	0.596790
29	6	-4.352583	1.559331	0.133605
30	8	1.593564	-1.417345	-1.002625
31	8	-1.077518	-1.232071	-0.417678
32	7	-3.423281	-2.225399	-0.475016
33	1	-2.695893	-1.500478	-0.287696
34	6	0.768499	-2.378500	-1.374225
35	6	-0.655205	-2.250878	-1.037987
36	6	-1.547700	-3.344820	-1.447310
37	6	-1.031001	-4.469855	-2.177306
38	1	-1.714209	-5.262813	-2.473943
39	6	0.297072	-4.524256	-2.488936
40	1	0.694669	-5.367688	-3.047179
41	6	1.190062	-3.482755	-2.089367
42	1	2.244247	-3.547917	-2.344628
43	6	-2.900039	-3.275885	-1.125111
44	1	-3.572420	-4.081782	-1.413350
45	6	-4.730881	-2.001621	-0.057548
46	6	-5.738309	-2.972836	0.000581
47	1	-5.520206	-3.997308	-0.283288
48	6	-7.017818	-2.625786	0.435720
49	1	-7.792184	-3.386284	0.472676
50	6	-7.305380	-1.321279	0.837398
51	1	-8.301523	-1.062081	1.185945
52	6	-6.310075	-0.336885	0.808829
53	6	-5.045847	-0.688964	0.348930
54	6	-0.413276	0.158001	2.862166
55	1	-1.336900	0.191450	3.433089
56	6	5.871640	-0.019915	0.023387
57	1	6.903786	-0.047247	-0.313636
58	7	3.930774	-1.392616	0.630350
59	7	1.258904	-1.321757	1.854291
60	6	5.233925	-1.243768	0.217265
61	6	5.868099	-2.535621	0.103037
62	1	6.896194	-2.696387	-0.196548
63	6	4.944140	-3.462903	0.484909
64	1	5.064943	-4.536287	0.562764
65	6	3.741407	-2.741548	0.829474
66	6	2.603672	-3.330019	1.380713
67	1	2.624622	-4.410894	1.488779
68	6	1.482599	-2.677947	1.895165
69	6	0.426713	-3.330484	2.635062
70	1	0.371382	-4.395165	2.825259
71	6	-0.422903	-2.351753	3.057994
72	1	-1.315615	-2.453380	3.662609
73	6	0.112997	-1.100018	2.578461
74	7	4.043754	1.458620	0.734540
75	7	1.368201	1.538908	1.869589
76	6	5.326055	1.232570	0.295701
77	6	6.044058	2.481492	0.191434
78	1	7.078694	2.576866	-0.113664
79	6	5.180999	3.465126	0.569996

80	1	5.365540	4.529813	0.641669
81	6	3.935432	2.817772	0.912570
82	6	2.812631	3.479770	1.406674
83	1	2.882221	4.560483	1.493118
84	6	1.644519	2.888318	1.887786
85	6	0.590640	3.598788	2.569291
86	1	0.575467	4.668295	2.739049
87	6	-0.310918	2.664040	2.987581
88	1	-1.213443	2.815802	3.566797
89	6	0.184265	1.379717	2.556625

H. (Por)Zr(κ^3-XbicH$_2$), OH tautomer, twist transition state



Optimized energy = –2560.98047193 a.u.
Imaginary frequency = (13.7 cm^{-1})*i*

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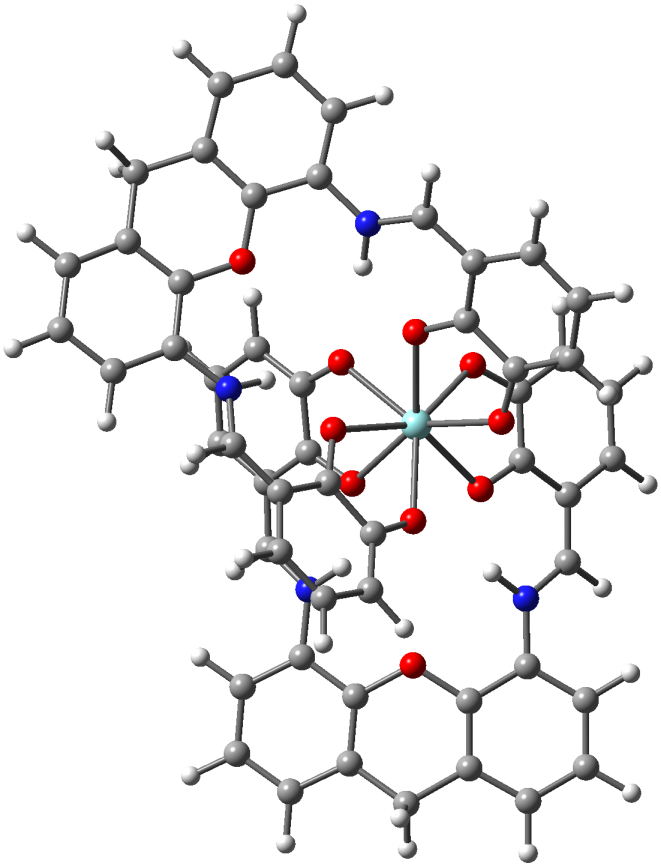
2	8	-4.054808	-0.234463	-0.212265
3	6	-6.602616	-1.078089	-1.206208
4	1	-7.635068	-1.365620	-0.973625
5	1	-6.507880	-1.154284	-2.301542
6	8	2.802175	-0.944530	1.607434
7	8	0.419539	-1.198054	0.651380
8	7	-2.222307	-1.924744	0.993407
9	1	-1.583010	-1.371253	0.413116
10	6	1.880988	-1.337598	2.464538
11	6	0.558414	-1.491446	1.902960
12	6	-0.503427	-2.000989	2.727113
13	6	-0.231373	-2.317948	4.103904
14	1	-1.040003	-2.695848	4.724314
15	6	1.025200	-2.130608	4.615246
16	1	1.227424	-2.361423	5.657428

17	6	2.086609	-1.643367	3.800438
18	1	3.081930	-1.514732	4.216361
19	6	-1.778575	-2.243021	2.210853
20	1	-2.509279	-2.742423	2.844530
21	6	-3.457263	-2.418046	0.489055
22	6	-3.770237	-3.774492	0.625665
23	1	-3.028123	-4.442197	1.052629
24	6	-5.006662	-4.261511	0.204148
25	1	-5.240333	-5.315538	0.317452
26	6	-5.929969	-3.394005	-0.376070
27	1	-6.894534	-3.768833	-0.709480
28	6	-5.634181	-2.038684	-0.550302
29	6	-4.396759	-1.556290	-0.109411
30	8	1.559214	1.434773	0.952482
31	8	-1.051427	1.279084	0.233791
32	1	-2.040670	1.394175	0.087878
33	7	-3.410291	2.240685	0.384150
34	6	0.715970	2.364820	1.367445
35	6	-0.661210	2.303638	1.007769
36	6	-1.571761	3.292762	1.473044
37	6	-1.101576	4.344806	2.297661
38	1	-1.806485	5.093350	2.651659
39	6	0.235670	4.406642	2.641780
40	1	0.602177	5.209988	3.274892
41	6	1.131969	3.424705	2.182287
42	1	2.182452	3.462402	2.456178
43	6	-2.973525	3.195123	1.145009
44	1	-3.650382	3.936711	1.591229
45	6	-4.733625	2.027170	0.018605
46	6	-5.732316	3.006920	-0.083004
47	1	-5.487529	4.039763	0.146626
48	6	-7.018479	2.665937	-0.501518
49	1	-7.782391	3.434566	-0.575800
50	6	-7.322487	1.348094	-0.842830
51	1	-8.322541	1.088014	-1.180749
52	6	-6.343395	0.349291	-0.776553
53	6	-5.069774	0.701288	-0.337171
54	6	-0.327581	-0.139874	-2.954206
55	1	-1.232440	-0.166222	-3.554786
56	6	5.874697	-0.014176	0.049788
57	1	6.899548	0.003216	0.409032
58	7	3.960422	1.377438	-0.597494
59	7	1.330789	1.326208	-1.904536
60	6	5.252978	1.215633	-0.155158
61	6	5.895235	2.501569	-0.023644
62	1	6.917619	2.652836	0.299455
63	6	4.988209	3.437924	-0.424144
64	1	5.120481	4.510294	-0.496991
65	6	3.787896	2.728091	-0.799119
66	6	2.670574	3.325725	-1.382172
67	1	2.702640	4.406528	-1.488725
68	6	1.563947	2.681063	-1.935700
69	6	0.538117	3.341188	-2.710658
70	1	0.495881	4.406407	-2.901110
71	6	-0.302921	2.368742	-3.163362
72	1	-1.174972	2.476963	-3.796218
73	6	0.207391	1.113115	-2.665698
74	7	4.048421	-1.477509	-0.698027

75	7	1.399253	-1.536217	-1.888165
76	6	5.323105	-1.262082	-0.232731
77	6	6.025430	-2.517627	-0.105140
78	1	7.052334	-2.621782	0.222355
79	6	5.159486	-3.495019	-0.493373
80	1	5.333602	-4.562220	-0.552393
81	6	3.928521	-2.837002	-0.866452
82	6	2.807516	-3.490810	-1.375555
83	1	2.865933	-4.573014	-1.450702
84	6	1.657480	-2.889818	-1.886929
85	6	0.613046	-3.591977	-2.590612
86	1	0.587251	-4.662776	-2.750530
87	6	-0.261778	-2.648637	-3.045190
88	1	-1.148626	-2.793320	-3.649823
89	6	0.239607	-1.367082	-2.613636

I. $(XbicH_2)_2Zr$, ground state



Optimized energy = –3098.01485290 a.u.

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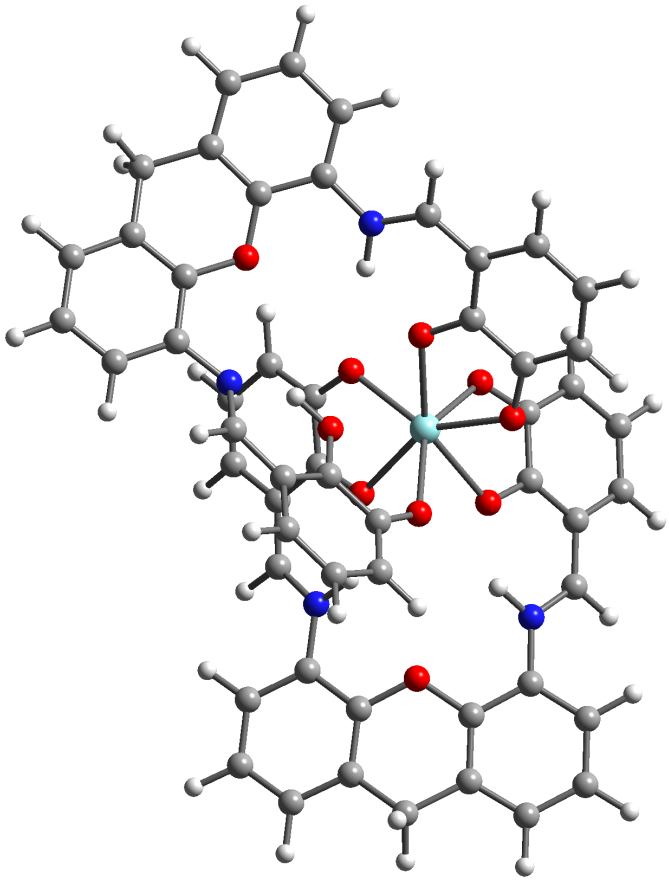
3	1	0.054018	-3.807979	1.333371
4	8	0.416998	-2.122062	1.798942
5	1	1.015289	-2.760728	-1.468485
6	8	1.541550	1.285122	0.187382
7	8	1.114016	-1.150181	-0.589515
8	8	0.023864	-5.003152	-0.932664
9	7	0.217099	-4.729389	1.772135
10	7	1.530511	-3.151976	-2.270386
11	6	1.744395	-1.029557	3.367091
12	6	1.165586	-2.243238	2.842711
13	6	1.453152	-3.512228	3.454863
14	6	2.290068	-3.545591	4.624313
15	1	2.501116	-4.501418	5.097026
16	6	2.806807	-2.376701	5.117590
17	1	3.438192	-2.397359	6.002008
18	6	2.547480	-1.119333	4.494818
19	1	2.986334	-0.210780	4.897594
20	6	0.949447	-4.683809	2.890372
21	1	1.177922	-5.642216	3.352255
22	6	2.372898	0.808300	-0.705034

23	6	2.106701	-0.545052	-1.145117
24	6	2.918556	-1.160111	-2.163336
25	6	4.044947	-0.431844	-2.687349
26	1	4.668839	-0.895540	-3.447095
27	6	4.295261	0.835599	-2.233602
28	1	5.142123	1.390886	-2.628877
29	6	3.468602	1.463119	-1.253684
30	1	3.695904	2.470669	-0.916140
31	6	2.572258	-2.409306	-2.674686
32	1	3.173937	-2.831708	-3.475666
33	6	-0.360250	-5.894091	1.236355
34	6	-0.474956	-6.034850	-0.161466
35	6	-1.050992	-7.177471	-0.719821
36	6	-1.483889	-8.201814	0.128873
37	1	-1.924119	-9.094848	-0.307399
38	6	-1.374805	-8.078413	1.511374
39	1	-1.734782	-8.868963	2.162543
40	6	-0.830397	-6.920653	2.062794
41	1	-0.792227	-6.791528	3.139582
42	6	1.030931	-4.273218	-2.959012
43	6	1.276084	-4.461463	-4.325717
44	1	1.828998	-3.709756	-4.878202
45	6	0.783181	-5.581966	-4.989234
46	1	0.987831	-5.714032	-6.047237
47	6	-0.000000	-6.505915	-4.303552
48	1	-0.408401	-7.370093	-4.821080
49	6	-0.297753	-6.323851	-2.949615
50	6	0.237791	-5.221903	-2.278351
51	6	-1.218267	-7.270869	-2.216970
52	1	-2.262244	-7.039816	-2.482531
53	1	-1.044887	-8.300790	-2.552956
54	8	-1.459417	-0.054955	2.683298
55	1	-0.054018	3.807979	1.333371
56	8	-0.416998	2.122062	1.798942
57	1	-1.015289	2.760728	-1.468485
58	8	-1.541550	-1.285122	0.187382
59	8	-1.114016	1.150181	-0.589515
60	8	-0.023864	5.003152	-0.932664
61	7	-0.217099	4.729389	1.772135
62	7	-1.530511	3.151976	-2.270386
63	6	-1.744395	1.029557	3.367091
64	6	-1.165586	2.243238	2.842711
65	6	-1.453152	3.512228	3.454863
66	6	-2.290068	3.545591	4.624313
67	1	-2.501116	4.501418	5.097026
68	6	-2.806807	2.376701	5.117590
69	1	-3.438192	2.397359	6.002008
70	6	-2.547480	1.119333	4.494818
71	1	-2.986334	0.210780	4.897594
72	6	-0.949447	4.683809	2.890372
73	1	-1.177922	5.642216	3.352255
74	6	-2.372898	-0.808300	-0.705034
75	6	-2.106701	0.545052	-1.145117
76	6	-2.918556	1.160111	-2.163336
77	6	-4.044947	0.431844	-2.687349
78	1	-4.668839	0.895540	-3.447095
79	6	-4.295261	-0.835599	-2.233602
80	1	-5.142123	-1.390886	-2.628877

81	6	-3.468602	-1.463119	-1.253684
82	1	-3.695904	-2.470669	-0.916140
83	6	-2.572258	2.409306	-2.674686
84	1	-3.173937	2.831708	-3.475666
85	6	0.360250	5.894091	1.236355
86	6	0.474956	6.034850	-0.161466
87	6	1.050992	7.177471	-0.719821
88	6	1.483889	8.201814	0.128873
89	1	1.924119	9.094848	-0.307399
90	6	1.374805	8.078413	1.511374
91	1	1.734782	8.868963	2.162543
92	6	0.830397	6.920653	2.062794
93	1	0.792227	6.791528	3.139582
94	6	-1.030931	4.273218	-2.959012
95	6	-1.276084	4.461463	-4.325717
96	1	-1.828998	3.709756	-4.878202
97	6	-0.783181	5.581966	-4.989234
98	1	-0.987831	5.714032	-6.047237
99	6	0.000000	6.505915	-4.303552
100	1	0.408401	7.370093	-4.821080
101	6	0.297753	6.323851	-2.949615
102	6	-0.237791	5.221903	-2.278351
103	6	1.218267	7.270869	-2.216970
104	1	2.262244	7.039816	-2.482531
105	1	1.044887	8.300790	-2.552956

J. $(XbicH_2)_2Zr$, OH tautomer



Optimized energy = –3098.00907317 a.u.

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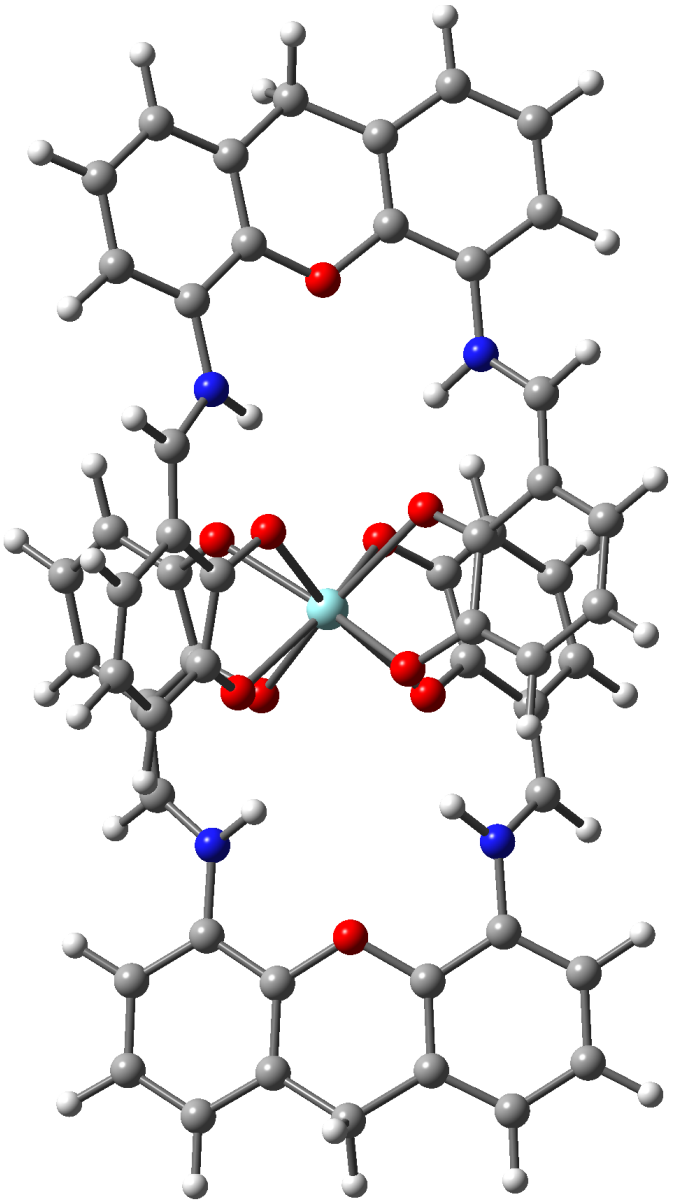
3	6	7.410886	-2.162830	-1.102169
4	1	8.435273	-2.467680	-0.851945
5	1	7.272597	-2.425790	-2.163110
6	8	-0.129927	2.838124	1.285148
7	8	2.060655	1.794709	0.441466
8	7	4.714411	1.744614	0.300766
9	1	3.810449	1.286330	0.115644
10	6	0.967193	3.468875	1.634083
11	6	2.187018	2.867935	1.159569
12	6	3.458022	3.442454	1.491820
13	6	3.494685	4.629082	2.303085
14	1	4.456760	5.068640	2.553306
15	6	2.321054	5.185765	2.740667
16	1	2.344450	6.084272	3.351564
17	6	1.057403	4.613975	2.415329
18	1	0.141262	5.069580	2.780479
19	6	4.640640	2.860167	1.028430
20	1	5.591958	3.325062	1.278412
21	6	5.904947	1.241377	-0.264839
22	6	6.910093	2.103336	-0.715130

23	1	6.745168	3.175369	-0.678569
24	6	8.095217	1.591374	-1.239334
25	1	8.870432	2.268277	-1.584781
26	6	8.264392	0.213502	-1.345550
27	1	9.180105	-0.192787	-1.767959
28	6	7.260873	-0.670256	-0.934967
29	6	6.086834	-0.152126	-0.381987
30	8	-1.135735	0.243302	1.554288
31	8	1.140252	-0.740031	0.911040
32	1	2.042095	-1.146476	0.753197
33	7	3.146981	-2.355682	1.401953
34	6	-0.647192	-0.659581	2.377542
35	6	0.610724	-1.225930	2.066962
36	6	1.251752	-2.178598	2.871576
37	6	0.592444	-2.601148	4.053566
38	1	1.068728	-3.338818	4.694065
39	6	-0.648044	-2.070693	4.374829
40	1	-1.152392	-2.394324	5.281639
41	6	-1.268265	-1.112022	3.553256
42	1	-2.233075	-0.690925	3.821550
43	6	2.534325	-2.721050	2.485775
44	1	2.974297	-3.471282	3.155869
45	6	4.307023	-3.015816	0.976679
46	6	4.504743	-4.393190	1.165381
47	1	3.731181	-4.967952	1.664807
48	6	5.644645	-5.031504	0.682416
49	1	5.776094	-6.098226	0.838856
50	6	6.596211	-4.303102	-0.025187
51	1	7.480314	-4.795919	-0.422386
52	6	6.420256	-2.935235	-0.262273
53	6	5.286515	-2.300127	0.249210
54	8	1.259205	0.291351	-1.614518
55	1	-2.751651	-1.455377	-1.051696
56	8	-1.166711	-0.527771	-1.170945
57	1	-3.862021	1.285904	0.018442
58	8	-0.112865	2.690329	-1.585499
59	8	-2.205987	1.800518	-0.394296
60	8	-4.972811	-1.019283	0.033237
61	7	-3.130189	-2.259917	-1.571542
62	7	-4.801828	1.696811	-0.106191
63	6	0.778130	-0.593144	-2.458194
64	6	-0.562794	-1.057482	-2.180728
65	6	-1.170498	-2.074576	-2.998003
66	6	-0.451508	-2.565656	-4.144556
67	1	-0.910858	-3.324168	-4.773068
68	6	0.803719	-2.085862	-4.407106
69	1	1.353277	-2.457367	-5.268074
70	6	1.426120	-1.110077	-3.571868
71	1	2.425990	-0.754152	-3.804259
72	6	-2.399249	-2.624219	-2.635546
73	1	-2.810744	-3.427188	-3.241937
74	6	-1.220953	3.366674	-1.804411
75	6	-2.388196	2.832159	-1.147648
76	6	-3.681096	3.417391	-1.376479
77	6	-3.777882	4.581698	-2.215047
78	1	-4.751720	5.036044	-2.378678
79	6	-2.647540	5.091505	-2.797234
80	1	-2.716651	5.971928	-3.430447

81	6	-1.368949	4.486905	-2.606617
82	1	-0.492460	4.897335	-3.099969
83	6	-4.817594	2.820305	-0.830029
84	1	-5.797035	3.254643	-1.019960
85	6	-4.212571	-2.995802	-1.052081
86	6	-5.153857	-2.366518	-0.209218
87	6	-6.212709	-3.087704	0.348360
88	6	-6.361311	-4.439181	0.023017
89	1	-7.192380	-4.995251	0.448988
90	6	-5.444312	-5.074430	-0.809294
91	1	-5.548515	-6.131135	-1.035324
92	6	-4.364644	-4.362015	-1.324149
93	1	-3.615134	-4.876466	-1.915273
94	6	-5.928520	1.107586	0.494737
95	6	-6.967796	1.886569	1.014686
96	1	-6.878713	2.967983	0.994720
97	6	-8.086216	1.281774	1.584197
98	1	-8.887643	1.895668	1.983366
99	6	-8.155500	-0.106387	1.667547
100	1	-9.016787	-0.584151	2.127419
101	6	-7.116269	-0.907938	1.183414
102	6	-6.014591	-0.296412	0.582217
103	6	-7.147137	-2.410372	1.322478
104	1	-6.862098	-2.687284	2.350044
105	1	-8.169975	-2.782055	1.184778

K. $(XbicH_2)_2Zr$, twist transition state



Optimized energy = –3097.99117681 a.u.

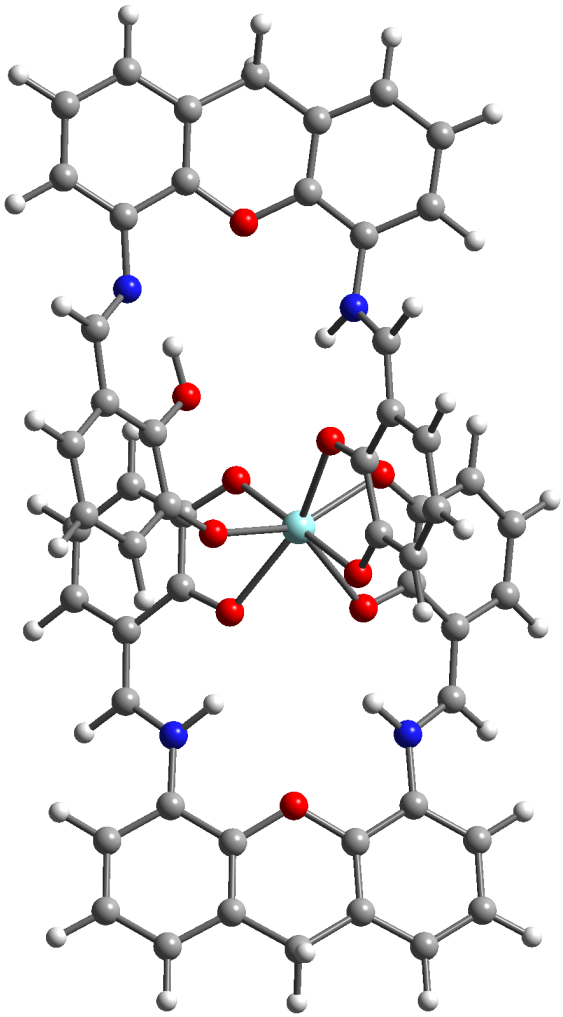
Imaginary frequency = (13.1 cm^{-1})*i*

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	40	0.000065	0.129465	0.000866
2	8	-0.354981	-0.907389	1.901518
3	1	3.372724	-1.687381	-0.091357
4	8	1.672923	-1.415314	0.377949
5	1	3.607515	1.309974	0.901494
6	8	-0.783302	1.689993	1.293337
7	8	1.766062	1.105780	1.097893
8	8	5.355448	-0.013217	-0.241640
9	7	4.092696	-2.388306	0.145056
10	7	4.285571	1.931421	1.359648

11	6	0.402485	-1.909749	2.272913
12	6	1.555171	-2.152223	1.434572
13	6	2.524249	-3.147442	1.810518
14	6	2.268044	-3.977023	2.957850
15	1	2.991520	-4.741248	3.229930
16	6	1.136898	-3.766578	3.701014
17	1	0.941012	-4.385251	4.573014
18	6	0.210370	-2.732535	3.375994
19	1	-0.660256	-2.564078	4.003912
20	6	3.743873	-3.212915	1.136002
21	1	4.500822	-3.929047	1.451038
22	6	0.029427	2.290155	2.133264
23	6	1.440876	1.999639	1.962964
24	6	2.429662	2.728360	2.720384
25	6	1.988463	3.621080	3.762512
26	1	2.730257	4.149769	4.355547
27	6	0.648528	3.815414	3.956810
28	1	0.309542	4.494579	4.734874
29	6	-0.331756	3.169297	3.142888
30	1	-1.387412	3.370858	3.302370
31	6	3.772543	2.668456	2.360682
32	1	4.480802	3.289442	2.902496
33	6	5.347891	-2.375352	-0.493585
34	6	5.993700	-1.144043	-0.712071
35	6	7.232552	-1.090151	-1.353138
36	6	7.843797	-2.287626	-1.739977
37	1	8.813101	-2.248197	-2.230426
38	6	7.222020	-3.514370	-1.517522
39	1	7.699378	-4.435686	-1.836678
40	6	5.968515	-3.556674	-0.908625
41	1	5.449713	-4.500223	-0.769794
42	6	5.555785	2.125776	0.786166
43	6	6.291777	3.300897	0.993707
44	1	5.864681	4.106554	1.579904
45	6	7.551815	3.462760	0.423609
46	1	8.107293	4.378299	0.602519
47	6	8.078133	2.471577	-0.400124
48	1	9.051186	2.603308	-0.865937
49	6	7.349795	1.307924	-0.663344
50	6	6.106068	1.132668	-0.052379
51	6	7.856979	0.257183	-1.624035
52	1	7.625108	0.566115	-2.655957
53	1	8.949950	0.188581	-1.567858
54	8	0.783904	1.690125	-1.291283
55	1	-3.607106	1.309958	-0.901247
56	8	-1.765683	1.106152	-1.096402
57	1	-3.373024	-1.687405	0.092199
58	8	0.355497	-0.906641	-1.900087
59	8	-1.673450	-1.414607	-0.377359
60	8	-5.355553	-0.012880	0.241848
61	7	-4.285079	1.931334	-1.359667
62	7	-4.093151	-2.387890	-0.145071
63	6	-0.028563	2.289957	-2.131729
64	6	-1.440128	1.999698	-1.961675
65	6	-2.428645	2.728220	-2.719681
66	6	-1.987077	3.620433	-3.762079
67	1	-2.728651	4.148941	-4.355548
68	6	-0.647064	3.814396	-3.956207

69	1	-0.307790	4.493103	-4.734546
70	6	0.332940	3.168505	-3.141770
71	1	1.388659	3.369781	-3.301192
72	6	-3.771683	2.668309	-2.360571
73	1	-4.479808	3.289111	-2.902768
74	6	-0.402507	-1.908293	-2.272361
75	6	-1.555565	-2.150841	-1.434483
76	6	-2.524830	-3.145534	-1.811349
77	6	-2.268696	-3.974361	-2.959237
78	1	-2.992397	-4.738134	-3.231983
79	6	-1.137270	-3.763867	-3.701958
80	1	-0.941378	-4.382035	-4.574315
81	6	-0.210410	-2.730458	-3.375924
82	1	0.660556	-2.562002	-4.003371
83	6	-3.744498	-3.211433	-1.136940
84	1	-4.501562	-3.927115	-1.452735
85	6	-5.555572	2.125751	-0.786809
86	6	-6.106096	1.132945	0.051914
87	6	-7.350104	1.308255	0.662280
88	6	-8.078565	2.471625	0.398165
89	1	-9.051875	2.603382	0.863434
90	6	-7.552067	3.462501	-0.425838
91	1	-8.107677	4.377812	-0.605502
92	6	-6.291715	3.300634	-0.995248
93	1	-5.864523	4.106088	-1.581653
94	6	-5.348568	-2.375027	0.493184
95	6	-5.969470	-3.556333	0.907826
96	1	-5.450769	-4.499936	0.768944
97	6	-7.223149	-3.513912	1.516381
98	1	-7.700744	-4.435201	1.835262
99	6	-7.844823	-2.287105	1.738837
100	1	-8.814273	-2.247621	2.228992
101	6	-7.233277	-1.089664	1.352359
102	6	-5.994236	-1.143682	0.711689
103	6	-7.857447	0.257799	1.623200
104	1	-7.625378	0.566828	2.655048
105	1	-8.950435	0.189408	1.567162

L. $(XbicH_2)_2Zr$, OH tautomer, twist transition state



Optimized energy = –3097.99025870 a.u.

Imaginary frequency = (11.2 cm^{-1})*i*

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	40	-0.323921	0.406232	-0.239866
2	8	5.835350	0.011180	-0.317744
3	6	8.412214	0.626709	-1.410539
4	1	9.471966	0.825053	-1.208714
5	1	8.292830	0.706099	-2.503147
6	8	-0.879763	1.307112	1.628002
7	8	1.574565	1.127861	0.742876
8	7	4.211066	1.847057	0.949247
9	1	3.542088	1.271706	0.426366
10	6	0.071344	1.731629	2.439709
11	6	1.419446	1.654805	1.911413
12	6	2.510491	2.199793	2.673998
13	6	2.253092	2.728859	3.988066
14	1	3.084152	3.125685	4.565578
15	6	0.977925	2.734111	4.484203

16	1	0.782942	3.130651	5.476933
17	6	-0.116326	2.244040	3.712943
18	1	-1.125890	2.280122	4.113204
19	6	3.792218	2.309065	2.131143
20	1	4.551585	2.835445	2.706069
21	6	5.454660	2.238769	0.386187
22	6	5.879673	3.568446	0.482266
23	1	5.210560	4.303961	0.917945
24	6	7.133668	3.946830	0.005254
25	1	7.453394	4.981055	0.087239
26	6	7.962165	2.999128	-0.592073
27	1	8.940291	3.289462	-0.967669
28	6	7.549815	1.670767	-0.734153
29	6	6.294576	1.297875	-0.241306
30	8	0.067813	-1.328395	0.835459
31	8	2.604607	-1.481393	-0.063778
32	1	3.583507	-1.629147	-0.216868
33	7	4.981444	-2.411961	0.253760
34	6	0.898522	-2.183588	1.404862
35	6	2.246328	-2.281451	0.950704
36	6	3.150967	-3.181656	1.575794
37	6	2.698199	-4.010376	2.632693
38	1	3.400192	-4.693343	3.105355
39	6	1.384305	-3.934500	3.054297
40	1	1.030862	-4.567515	3.863780
41	6	0.497392	-3.025482	2.448838
42	1	-0.532275	-2.948258	2.787247
43	6	4.543196	-3.185561	1.195256
44	1	5.224848	-3.827661	1.770871
45	6	6.314985	-2.299988	-0.125862
46	6	7.219795	-3.363404	-0.243122
47	1	6.884428	-4.368402	-0.003840
48	6	8.520795	-3.137454	-0.696684
49	1	9.212427	-3.970295	-0.786441
50	6	8.928009	-1.853255	-1.055262
51	1	9.936491	-1.682555	-1.423963
52	6	8.042701	-0.771164	-0.965225
53	6	6.756954	-1.008769	-0.487710
54	8	0.268860	-0.551663	-2.052667
55	1	-3.679572	-1.584994	-0.483734
56	8	-2.010823	-1.040727	-0.900423
57	1	-4.062849	1.473964	-0.438717
58	8	0.204500	2.175593	-1.338121
59	8	-2.239408	1.523057	-0.762575
60	8	-5.689773	-0.314015	0.271903
61	7	-4.260198	-2.397916	-0.736241
62	7	-4.835376	2.102153	-0.696540
63	6	-0.379826	-1.616514	-2.477154
64	6	-1.654811	-1.857992	-1.835912
65	6	-2.479611	-2.955737	-2.272668
66	6	-2.005822	-3.813302	-3.326017
67	1	-2.627023	-4.645264	-3.647724
68	6	-0.786740	-3.571524	-3.899718
69	1	-0.423389	-4.219831	-4.692407
70	6	0.026455	-2.475282	-3.486118
71	1	0.983825	-2.293879	-3.965981
72	6	-3.725678	-3.172513	-1.687394
73	1	-4.334228	-4.008315	-2.024732

74	6	-0.738032	2.919399	-1.879387
75	6	-2.090012	2.558547	-1.521813
76	6	-3.200609	3.339084	-1.999303
77	6	-2.944490	4.437129	-2.894404
78	1	-3.782142	5.021687	-3.265763
79	6	-1.655429	4.738506	-3.243095
80	1	-1.457857	5.570129	-3.914036
81	6	-0.549586	3.991847	-2.737956
82	1	0.464215	4.257858	-3.023190
83	6	-4.492956	3.080186	-1.546159
84	1	-5.304109	3.719136	-1.886061
85	6	-5.459995	-2.657543	-0.052996
86	6	-6.199745	-1.582416	0.480539
87	6	-7.389437	-1.806946	1.175162
88	6	-7.860145	-3.117415	1.307514
89	1	-8.791210	-3.290427	1.840920
90	6	-7.140002	-4.189665	0.787977
91	1	-7.499426	-5.205724	0.917935
92	6	-5.935733	-3.961850	0.126481
93	1	-5.343577	-4.798594	-0.228685
94	6	-6.074784	2.014167	-0.033707
95	6	-6.880526	3.144350	0.156814
96	1	-6.527354	4.114601	-0.174662
97	6	-8.108549	3.040429	0.804410
98	1	-8.722551	3.925438	0.939265
99	6	-8.524190	1.811911	1.309474
100	1	-9.470364	1.728327	1.837750
101	6	-7.722235	0.674783	1.173105
102	6	-6.512205	0.776070	0.482311
103	6	-8.122209	-0.641972	1.794251
104	1	-7.911274	-0.611915	2.875094
105	1	-9.205861	-0.787231	1.704855