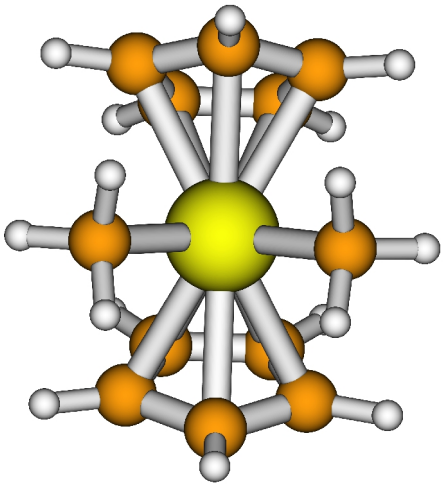
Supplementary Information

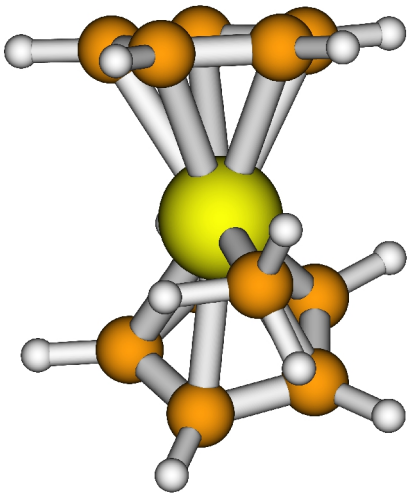
Cartesian coordinates (in Å) of compound Cp_2TiMe_2 (**II**)
(B3LYP/ECP11)



Ti	0.138164	0.211658	-0.032994
C	0.386886	-0.146635	2.369423
C	1.691099	-0.166831	1.827302
C	1.792860	-1.281030	0.965029
C	0.547558	-1.947365	0.964076
C	-0.324772	-1.243550	1.835476
H	-1.343322	-1.510945	2.069064
H	0.311400	-2.846095	0.416326
H	2.662576	-1.560544	0.391377
H	2.462616	0.565478	2.008105
H	-0.003061	0.590187	3.054001
C	-1.103942	1.066613	-1.967289
C	-0.623153	-0.215800	-2.313086
C	-1.241843	-1.157976	-1.462026
C	-2.113453	-0.453027	-0.590826
C	-2.027997	0.920386	-0.909036
H	-2.558354	1.720109	-0.416316
H	-2.748092	-0.889065	0.164564
H	-1.094827	-2.226256	-1.488006
H	0.105167	-0.433966	-3.078312
H	-0.788489	2.000053	-2.407042
C	1.905803	0.692832	-1.179083
H	2.696508	1.040193	-0.508931
H	2.289844	-0.166011	-1.740765
H	1.677494	1.489118	-1.892501
C	0.000724	2.230677	0.724800
H	-0.107613	2.930491	-0.107946
H	0.911659	2.480750	1.274852
H	-0.851736	2.370267	1.398846

Cartesian coordinates (in Å) of compound $[Cp_2TiMe]^+$ (**III**)
(B3LYP/ECP11)

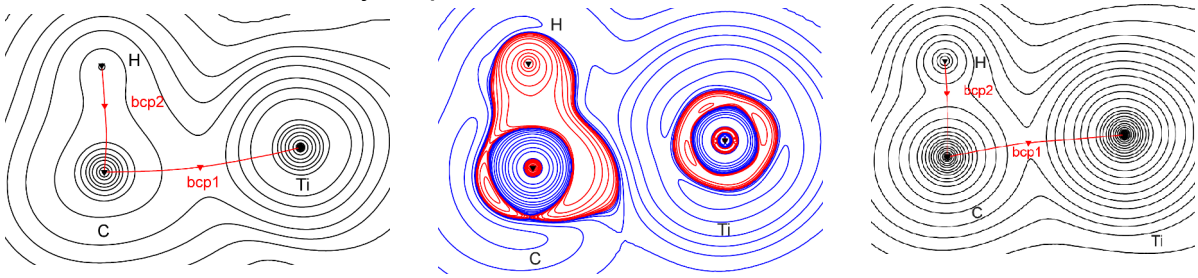
C	-1.915037	-0.641870	-1.147313
C	-2.310702	0.576805	-0.530833
C	-2.150037	0.435160	0.866251
C	-1.640385	-0.867991	1.117579
C	-1.522657	-1.539503	-0.129633
Ti	0.000508	0.275282	-0.093030
C	2.272002	0.490688	-0.695395
C	2.195823	0.556332	0.715817
C	1.707056	-0.693783	1.183839
C	1.524141	-1.541433	0.059319
C	1.850510	-0.805758	-1.101459
C	-0.008093	2.352072	0.021941
H	1.195439	-2.568243	0.088744
H	1.554814	-0.968979	2.217734
H	-1.930973	-0.851069	-2.208592
H	-2.668580	1.458247	-1.042220
H	-2.367632	1.186825	1.609857
H	-1.198731	-2.557733	-0.275810
H	2.466518	1.401017	1.329416
H	2.596898	1.286947	-1.349921
H	1.807049	-1.170523	-2.118789
H	-1.434206	-1.293210	2.089194
H	-0.896019	2.888810	0.348029
H	0.885869	2.905995	0.297437
H	-0.037346	2.301396	-1.099096



	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.1048	0.1031
$\nabla^2\rho(\mathbf{r})$	-0.0311	-0.0248
bcp2, $\rho(\mathbf{r})$	0.2439	0.2454
$\nabla^2\rho(\mathbf{r})$	0.1777	0.1831

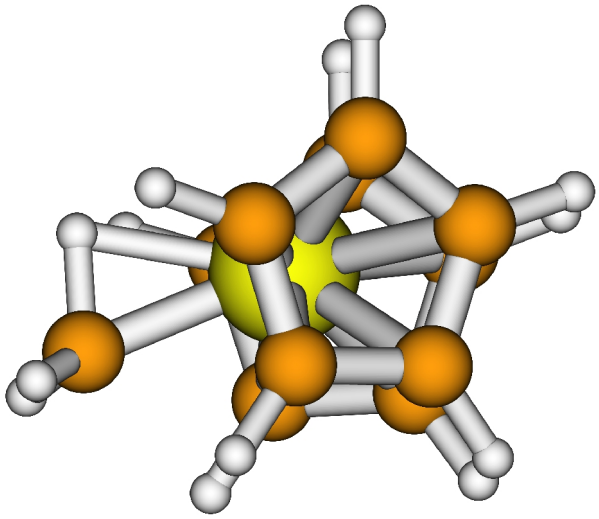
Bader analysis:

Table S1: Electron density, Laplacian and Virial Field Function of **III**



Plane through Ti-C-H

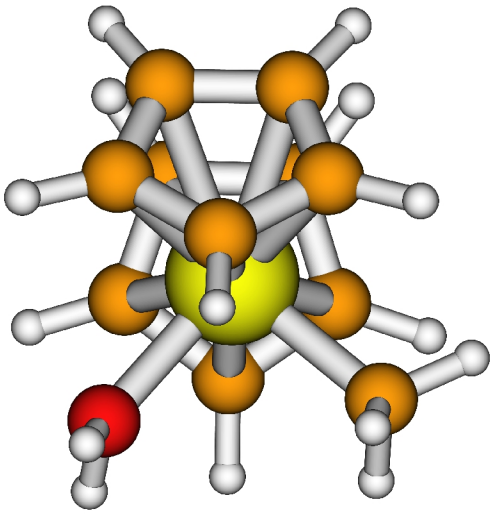
Cartesian coordinates (in Å) of compound $[Cp_2TiMe]^+$ (**III-MP2**)
(MP2/ECP11)



C	-1.938087	0.695565	-1.111809
C	-2.274803	-0.580134	-0.576511
C	-2.059934	-0.541544	0.832050
C	-1.569163	0.754330	1.159967
C	-1.504555	1.522294	-0.044393
Ti	0.002212	-0.252244	-0.204197
C	-0.002147	-2.330073	0.062108
C	1.964205	0.693135	-1.066588
C	2.286848	-0.582951	-0.523603
C	2.039416	-0.544032	0.879595
C	1.542765	0.752459	1.196019
C	1.507048	1.520445	-0.009530
H	-1.199821	2.556981	-0.125046
H	-1.328933	1.110142	2.153848
H	2.030480	0.975571	-2.112399
H	2.649974	-1.438519	-1.080991
H	2.211069	-1.349243	1.580775
H	1.205534	2.555501	-0.097248
H	-2.248795	-1.346553	1.529025
H	-2.625954	-1.435246	-1.142209
H	-1.979746	0.978101	-2.158861
H	1.279985	1.108610	2.184055
H	0.893714	-2.912278	0.279348
H	-0.903517	-2.911179	0.258497
H	0.010984	-2.090473	-1.057050

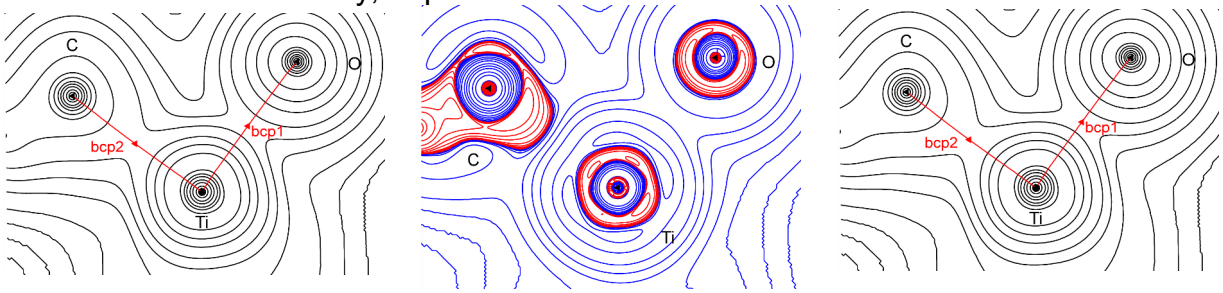
Cartesian coordinates (in Å) of compound $[Cp_2TiMe(OH_2)]^+$ (**1**)
(B3LYP/ECP11)

Ti	-0.000037	0.215635	0.021862
C	-2.043592	-0.257179	-1.183832
C	-2.382642	0.539972	-0.060477
C	-2.089247	-0.199478	1.108008
C	-1.540657	-1.441183	0.709008
C	-1.522949	-1.477685	-0.713031
H	-1.200678	-2.305046	-1.324635
H	-1.249551	-2.244287	1.367934
H	-2.259216	0.123170	2.122528
H	-2.818724	1.528744	-0.082179
H	-2.153602	0.018917	-2.223118
C	2.382115	0.540500	-0.065528
C	2.091294	-0.194892	1.106071
C	1.542423	-1.438234	0.712512
C	1.522523	-1.479976	-0.709350
C	2.041450	-0.260873	-1.185509
H	2.149430	0.011651	-2.225948
H	1.199525	-2.309763	-1.317280
H	1.252812	-2.239055	1.374875
H	2.263119	0.131379	2.119100
H	2.817951	1.529297	-0.091514
C	-0.000180	1.630300	1.643385
H	-0.891301	2.258047	1.572087
H	0.002965	1.166188	2.632866
H	0.888491	2.261179	1.568063
O	-0.000361	1.847833	-1.379365
H	0.780254	2.387678	-1.553177
H	-0.781005	2.387634	-1.553178

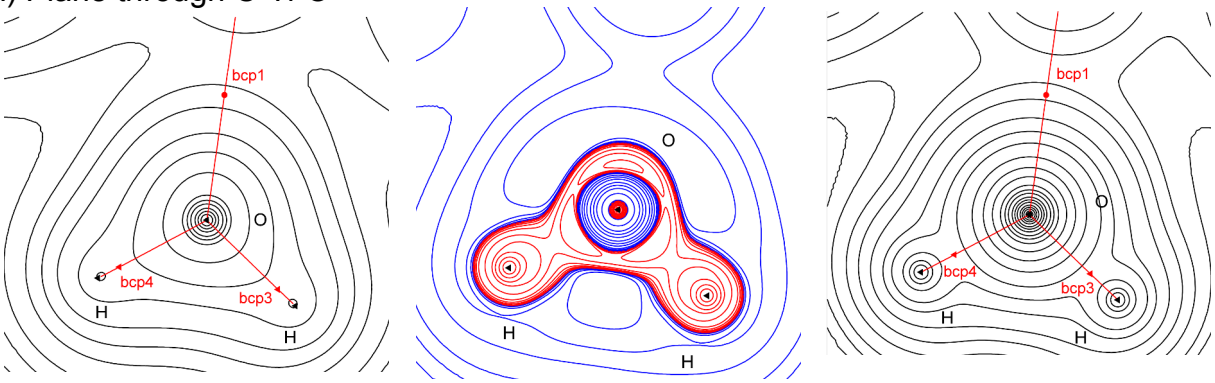


	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.0536	0.0555
$\nabla^2\rho(\mathbf{r})$	-0.0804	-0.0711
bcp2, $\rho(\mathbf{r})$	0.0952	0.09632
$\nabla^2\rho(\mathbf{r})$	-0.0222	-0.0121
bcp3, $\rho(\mathbf{r})$	0.3580	0.3808
$\nabla^2\rho(\mathbf{r})$	0.6394	0.3151
bcp4, $\rho(\mathbf{r})$	0.3580	0.3808
$\nabla^2\rho(\mathbf{r})$	0.6394	0.3151

Table S2: Electron density, Laplacian and Virial Field Function of **1**



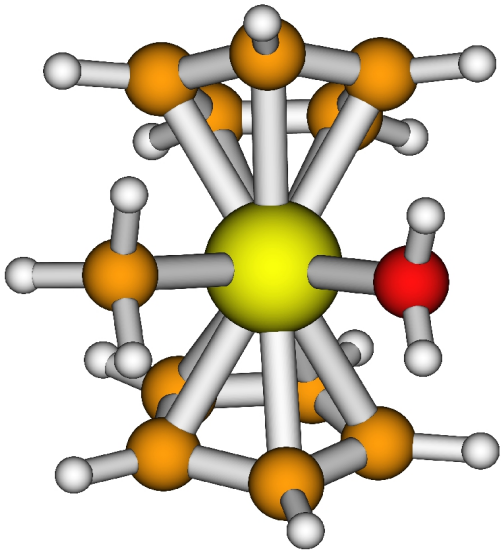
a) Plane through C-Ti-O



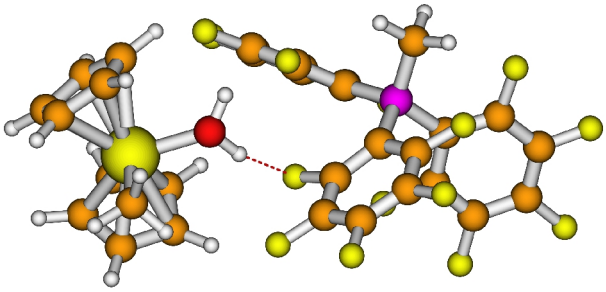
b) Plane through H-O-H

Cartesian coordinates (in Å) of compound $[Cp_2TiMe(OH_2)]^+$ (**1-MP2**) (MP2/ECP11)

C	-1.969489	0.306658	-1.184541
C	-2.326403	-0.560026	-0.112728
C	-2.057550	0.108893	1.109807
C	-1.509675	1.380878	0.795163
C	-1.465289	1.505648	-0.626603
Ti	-0.002117	-0.226274	0.003757
O	-0.019942	-1.953026	-1.253466
C	2.056071	0.030347	-1.150548
C	2.339887	-0.553246	0.112226
C	1.981909	0.380094	1.122642
C	1.454707	1.532346	0.481383
C	1.490814	1.310668	-0.929985
C	0.034543	-1.524843	1.772474
H	1.191831	2.011080	-1.697959
H	1.120436	2.437072	0.970972
H	2.088442	0.233490	2.188867
H	2.756472	-1.537712	0.287688
H	2.205542	-0.428836	-2.121120
H	-2.036110	0.081260	-2.242931
H	-1.125111	2.371259	-1.178429
H	-1.218179	2.137048	1.512185
H	-2.245069	-0.275418	2.102095
H	-2.745267	-1.556195	-0.200736
H	0.955433	-2.118202	1.757462
H	-0.012837	-0.994535	2.729910
H	-0.829630	-2.198053	1.712574
H	-0.792095	-2.528648	-1.314680
H	0.751707	-2.527350	-1.333125



Cartesian coordinates (in Å) of compound $[Cp_2TiMe(OH_2)][MeB(C_6F_5)_3]$ (**2**)
(B3LYP/ECP11)

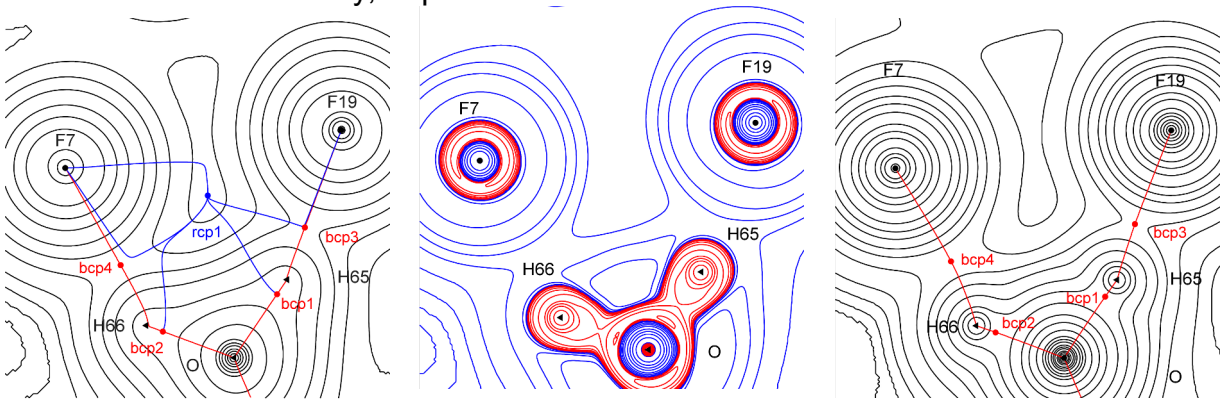


Ti	-4.455621	-0.423407	-0.341201
C	-6.488659	-0.796356	0.872193
C	-5.449745	-0.823579	1.836187
C	-4.859355	0.460601	1.881435
C	-5.511398	1.283106	0.933516
C	-6.530043	0.505707	0.314469
H	-7.230107	0.854610	-0.431851
H	-5.282790	2.321440	0.737653
H	-4.030881	0.767198	2.505449
H	-5.143099	-1.684679	2.415211
H	-7.126001	-1.626784	0.601337
C	-4.713860	-2.550557	-0.538865
H	-4.714755	-2.987951	0.464113
H	-5.631685	-2.857151	-1.052763
H	-3.853595	-2.944103	-1.089788
C	-5.264525	0.296420	-2.446952
C	-4.439291	-0.826163	-2.702753
C	-3.114806	-0.487106	-2.336795
C	-3.114328	0.860990	-1.888304
C	-4.436961	1.345910	-1.951525
H	-4.762901	2.338936	-1.674405
H	-2.255760	1.408984	-1.520094
H	-2.258509	-1.148524	-2.369631
H	-4.765551	-1.777358	-3.097296
H	-6.327587	0.356596	-2.637640
C	-0.233889	1.459617	1.381367
C	1.061339	1.475057	0.865130
B	2.145322	0.241181	1.181136
C	3.515377	0.365477	0.259005
C	3.432458	0.297080	-1.135433
C	4.524410	0.316929	-1.994502
C	5.804710	0.408236	-1.455739
C	5.950885	0.482503	-0.076606
C	4.821062	0.460349	0.745281
F	5.074902	0.546760	2.066721
F	7.179721	0.575099	0.457734
F	6.878870	0.428691	-2.258323
F	4.359706	0.253581	-3.327303
F	2.211919	0.227191	-1.727593
C	2.382919	0.335171	2.803439
H	2.762214	1.324624	3.088228
H	1.436219	0.191166	3.341097
H	3.091153	-0.398949	3.190648
C	1.556501	-1.274808	0.754218
C	2.233846	-2.430838	1.178486
C	1.862869	-3.733209	0.842549
C	0.765027	-3.953067	0.014969
C	0.078242	-2.847488	-0.463255
C	0.499208	-1.573836	-0.095090
F	-0.274630	-0.562852	-0.658665

F	-1.001207	-3.005837	-1.268061
F	0.384183	-5.194019	-0.312016
F	2.558124	-4.780485	1.304875
F	3.335228	-2.333632	1.944486
C	1.364384	2.680052	0.215670
C	0.461891	3.734842	0.045282
C	-0.827925	3.632112	0.550579
C	-1.169482	2.475745	1.239248
F	-2.428770	2.334282	1.730438
F	-1.725806	4.615167	0.381861
F	0.828205	4.844866	-0.608718
F	2.584839	2.907678	-0.300183
F	-0.694937	0.355563	2.073567
O	-2.614174	-0.672100	0.547039
H	-1.805769	-0.717321	-0.016534
H	-2.288448	-0.316760	1.398106

	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.3183	0.3207
$\nabla^2\rho(\mathbf{r})$	0.4304	0.3703
bcp2, $\rho(\mathbf{r})$	0.3259	0.3281
$\nabla^2\rho(\mathbf{r})$	0.4462	0.3857
bcp3, $\rho(\mathbf{r})$	0.0437	0.0444
$\nabla^2\rho(\mathbf{r})$	-0.0366	-0.0400
bcp4, $\rho(\mathbf{r})$	0.0285	0.0290
$\nabla^2\rho(\mathbf{r})$	-0.0251	-0.0268

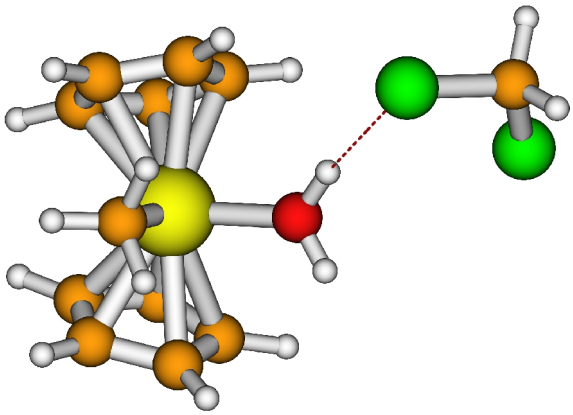
Table S3: Electron density, Laplacian and Virial Field Function of **2**



Plane through H-O-H

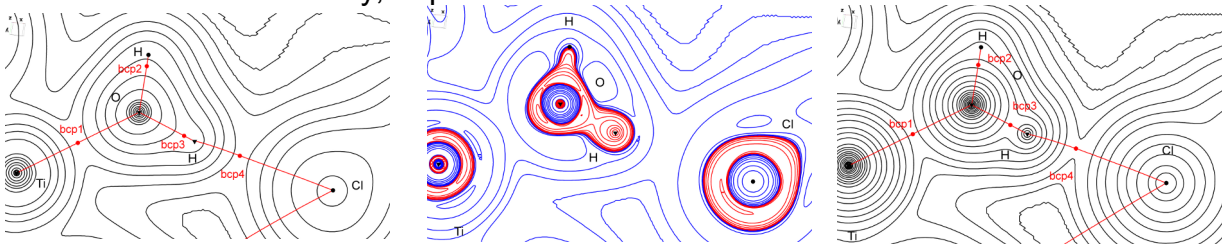
Cartesian coordinates (in Å) of compound {[$Cp_2TiMe(OH_2)$](CH_2Cl_2)}$^+$ (**3**) (B3LYP/ECP11)

C	-3.489657	-0.865213	-0.254245
C	-3.128836	-1.267153	1.053152
C	-2.008929	-2.124095	0.950034
C	-1.695376	-2.275035	-0.423869
C	-2.601799	-1.496082	-1.169367
Ti	-1.348496	0.054818	0.151854
O	0.621374	-0.704507	0.394258
C	-1.507401	2.441319	0.067331
C	-0.175101	2.109429	-0.268074
C	-0.193278	1.394894	-1.493207
C	-1.533538	1.266238	-1.904600
C	-2.352644	1.905515	-0.932417
C	-1.394943	0.639391	2.224249
Cl	4.027210	-1.258186	-1.007774
C	4.705334	0.009024	0.044087
Cl	3.446345	0.793642	1.090212
H	-3.424343	2.019803	-0.980875
H	-1.875121	0.792916	-2.811191
H	0.666139	0.998258	-2.014613
H	0.702249	2.378221	0.301922
H	-1.823748	3.006596	0.928907
H	-4.329564	-0.240448	-0.514660
H	-2.637299	-1.424459	-2.244639
H	-0.896239	-2.873528	-0.838354
H	-1.502203	-2.595753	1.779832
H	-3.622109	-0.975285	1.966342
H	-0.578361	1.339459	2.414937
H	-2.327857	1.118949	2.530599
H	-1.253555	-0.248801	2.844021
H	0.808452	-1.574540	0.765183
H	1.433044	-0.172082	0.480867
H	5.430367	-0.439871	0.712805
H	5.132630	0.788461	-0.575837



	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.0576	0.0595
$\nabla^2\rho(\mathbf{r})$	-0.0861	-0.0764
bcp2, $\rho(\mathbf{r})$	0.3591	0.3815
$\nabla^2\rho(\mathbf{r})$	0.6387	0.3154
bcp3, $\rho(\mathbf{r})$	0.3451	0.3688
$\nabla^2\rho(\mathbf{r})$	0.6125	0.2940
bcp4, $\rho(\mathbf{r})$	0.0180	0.0185
$\nabla^2\rho(\mathbf{r})$	-0.0136	-0.0128

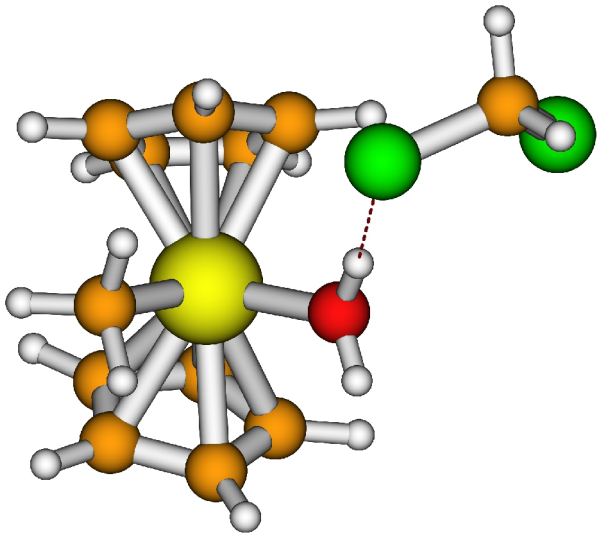
Table S4: Electron density, Laplacian and Virial Field Function of **3**



Plane through Ti-O-H

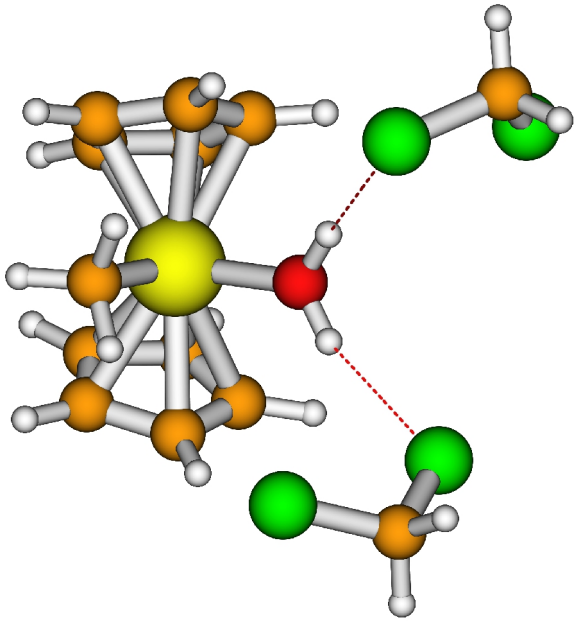
Cartesian coordinates (in Å) of compound {[$Cp_2TiMe(OH_2)$](CH_2Cl_2)}$^+$ (**3-MP2**) (MP2/ECP11)

C	-2.042947	-1.618470	1.299004
C	-1.392296	-2.281740	0.225568
C	-0.016641	-1.925793	0.264360
C	0.184558	-1.055377	1.366115
C	-1.067973	-0.841935	1.996886
Ti	-1.269156	0.048805	-0.145210
C	-1.224175	-0.778521	-2.177996
C	-3.555250	0.547422	-0.054740
C	-3.077165	1.035403	-1.299717
C	-2.129126	2.055398	-1.028539
C	-2.037225	2.216870	0.383201
C	-2.918136	1.287941	0.986475
O	0.551252	1.057954	-0.501525
Cl	3.145806	-0.611289	-1.326636
C	4.380436	-0.260915	-0.083341
Cl	3.733920	0.667839	1.268415
H	-3.088350	-1.705427	1.562686
H	-1.240301	-0.238330	2.878164
H	1.120116	-0.589098	1.649816
H	0.740139	-2.259058	-0.432963
H	-1.858074	-2.935759	-0.499533
H	-4.301082	-0.225793	0.074775
H	-3.088272	1.167503	2.047866
H	-1.383605	2.902156	0.910837
H	-1.581942	2.614660	-1.778935
H	-3.386522	0.695144	-2.277376
H	-0.342304	-1.420117	-2.280573
H	-2.106968	-1.368062	-2.449150
H	-1.142503	0.059919	-2.880736
H	0.596025	1.846066	-1.055094
H	1.377113	0.568464	-0.663753
H	5.166322	0.315703	-0.562155
H	4.747185	-1.214525	0.284953



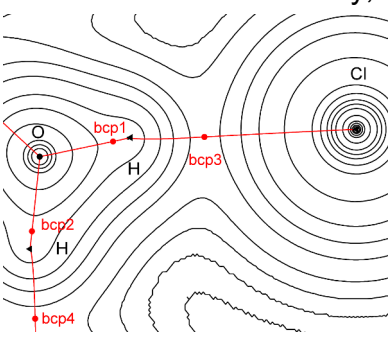
Cartesian coordinates (in Å) of compound $\{[Cp_2TiMe(OH_2)](CH_2Cl_2)_2\}^+$ (**4**) (B3LYP/ECP11)

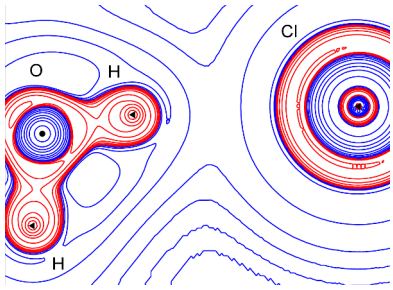
Ti	1.787883	0.010415	0.130386
C	3.547989	1.327429	-0.757900
C	2.771136	2.192422	0.047690
C	1.491386	2.302758	-0.542186
C	1.486099	1.527866	-1.729204
C	2.750328	0.921569	-1.863280
H	3.066254	0.289663	-2.677870
H	0.655677	1.406638	-2.409890
H	0.668836	2.885102	-0.153910
H	3.098137	2.682971	0.950199
H	4.582776	1.070951	-0.593850
O	-0.313981	-0.074327	-0.083300
H	-0.891047	0.667052	-0.332197
H	-0.882608	-0.765850	0.296194
C	2.802663	-1.714719	1.444562
C	1.520687	-2.185061	1.077126
C	1.497879	-2.346988	-0.330594
C	2.752450	-1.955396	-0.837164
C	3.562737	-1.557798	0.262461
H	4.594687	-1.248017	0.210968
H	3.053782	-1.985580	-1.872102
H	0.659630	-2.688725	-0.920628
H	0.709359	-2.397451	1.757674
H	3.141846	-1.514261	2.448014
C	1.586525	0.731236	2.149971
H	1.032159	-0.007130	2.733648
H	2.537585	0.916818	2.654954
H	1.022408	1.666109	2.132285
Cl	-2.528637	-3.045080	-1.441034
C	-3.238715	-3.215007	0.183974
Cl	-2.495514	-2.089895	1.395650
H	-4.292439	-2.967968	0.130913
H	-3.063343	-4.223521	0.539701
Cl	-2.630836	1.971566	-1.285368
C	-3.145622	3.266900	-0.125924
Cl	-2.084769	3.374293	1.300724
H	-3.105278	4.205866	-0.665582
H	-4.147410	3.016518	0.202685

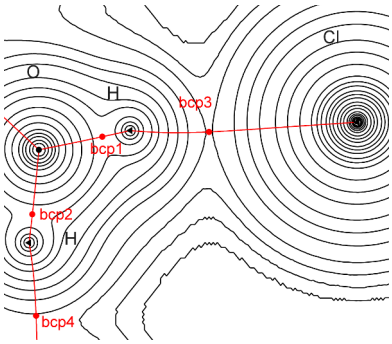


	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.3481	0.3714
$\nabla^2\rho(\mathbf{r})$	0.6173	0.2978
bcp2, $\rho(\mathbf{r})$	0.3486	0.3720
$\nabla^2\rho(\mathbf{r})$	0.6187	0.2988
bcp3, $\rho(\mathbf{r})$	0.0161	0.0163
$\nabla^2\rho(\mathbf{r})$	-0.0126	-0.0119
bcp4, $\rho(\mathbf{r})$	0.0155	0.0157
$\nabla^2\rho(\mathbf{r})$	-0.0123	-0.0117

Table S5: Electron density, Laplacian and Virial Field Function of **4**

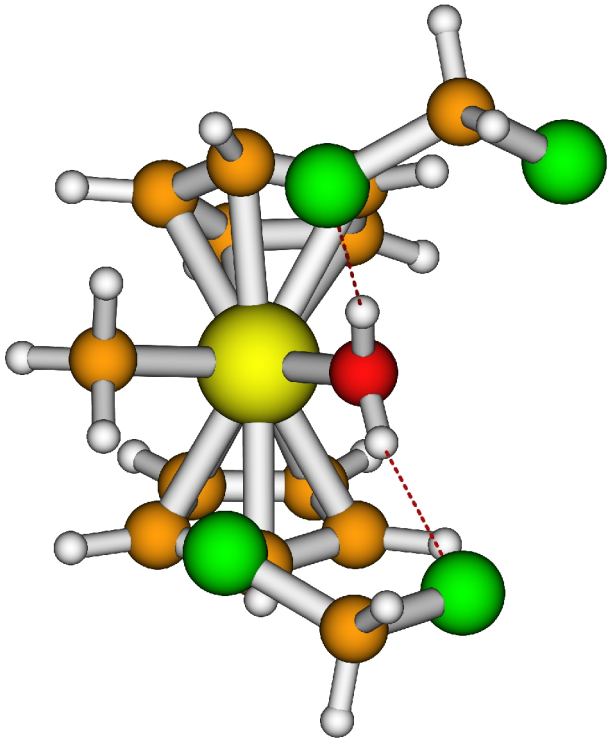






Plane through H-O-Hl

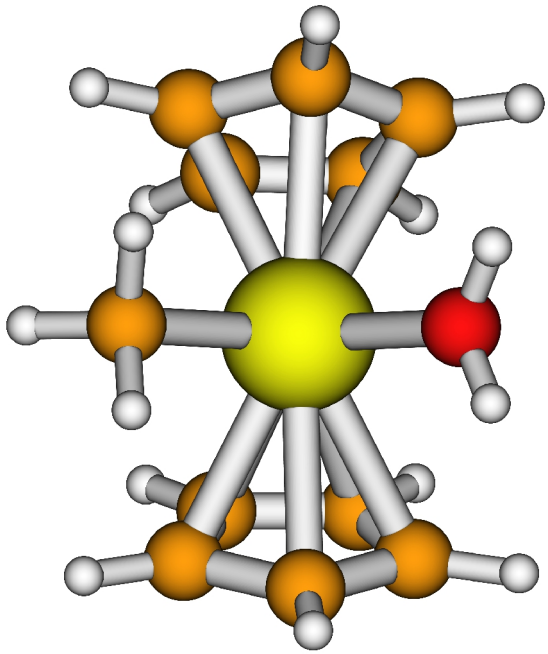
Cartesian coordinates (in Å) of compound {[$Cp_2TiMe(OH_2)$]$(CH_2Cl_2)_2$]$^+$ (**4-MP2**) (MP2/ECP11)



C	-3.476783	-1.500183	-0.064971
C	-2.819458	-1.628272	-1.316153
C	-1.509852	-2.125372	-1.070725
C	-1.363598	-2.314809	0.326501
C	-2.566236	-1.905104	0.958074
Ti	-1.686046	0.007495	-0.039261
C	-1.276181	0.622542	-2.106991
C	-3.512198	1.412003	0.392493
C	-2.527100	2.201974	-0.256604
C	-1.388448	2.255147	0.587740
C	-1.676763	1.518912	1.771372
C	-2.986402	0.994558	1.652706
O	0.355746	-0.076124	0.399391
Cl	2.343213	2.201832	1.566469
C	2.929197	3.092397	0.136248
Cl	2.050232	2.658459	-1.331996
Cl	2.248790	-1.777666	-1.545290
C	2.987330	-3.035250	-0.516261
Cl	2.433953	-2.951955	1.156598
H	-3.504087	0.395429	2.389703
H	-1.002583	1.350134	2.603403
H	-0.456744	2.750363	0.348438
H	-2.628833	2.678973	-1.220726
H	-4.501719	1.199083	0.010572
H	0.898474	0.690967	0.641503
H	0.945038	-0.672293	-0.092491
H	-4.497106	-1.177229	0.089862
H	-2.771208	-1.942930	2.019765
H	-0.470647	-2.656704	0.834526
H	-0.757126	-2.315170	-1.823878
H	-3.234958	-1.385756	-2.285041
H	-0.695977	-0.167141	-2.597389
H	-2.168144	0.816476	-2.712849
H	-0.676851	1.538922	-2.067885
H	4.062173	-2.881203	-0.536834
H	2.712352	-4.000577	-0.931219
H	2.789114	4.151838	0.330421
H	3.978101	2.843985	0.003314

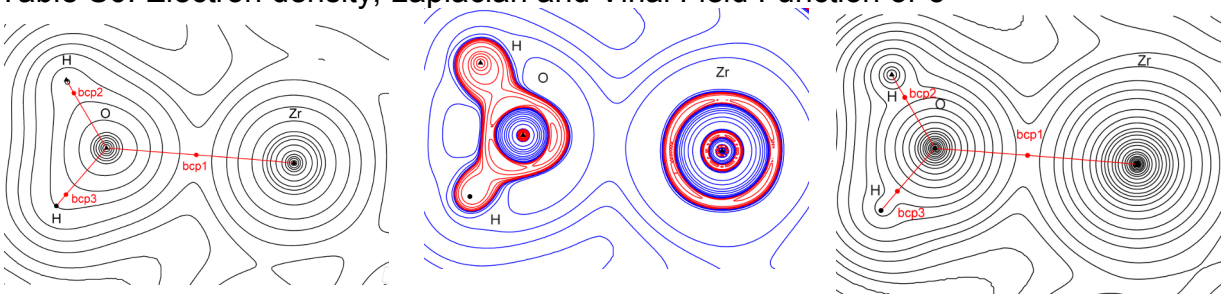
Cartesian coordinates (in Å) of compound $[Cp_2ZrMe(OH_2)]^+$ (**5**)
(B3LYP/ECP11)

C	1.660622	-1.496213	-0.814020
C	2.196117	-0.250283	-1.209523
C	2.547705	0.471725	-0.036244
C	2.248518	-0.338910	1.085047
C	1.683204	-1.549081	0.608986
Zr	0.000000	0.223294	0.027715
C	-0.000006	1.482663	1.915244
C	-1.683156	-1.549168	0.608845
C	-2.248459	-0.339065	1.085092
C	-2.547720	0.471709	-0.036080
C	-2.196182	-0.250142	-1.209468
C	-1.660643	-1.496116	-0.814154
O	0.000001	2.041994	-1.370954
H	-1.390148	-2.393356	1.215412
H	-1.335928	-2.285170	-1.475214
H	-2.338791	0.077252	-2.230201
H	-3.014309	1.446280	0.001486
H	-2.430925	-0.085836	2.117572
H	2.338661	0.076987	-2.230305
H	1.335882	-2.285357	-1.474960
H	1.390237	-2.393194	1.215676
H	2.431038	-0.085548	2.117485
H	3.014292	1.446304	0.001172
H	-0.888415	2.123490	1.935017
H	0.000036	0.911011	2.849051
H	0.888364	2.123545	1.934975
H	-0.780986	2.556560	-1.610270
H	0.780983	2.556590	-1.610221



	Electron Density	Virial Field Function
bcp3, $\rho(\mathbf{r})$	0.0508	0.0524
$\nabla^2\rho(\mathbf{r})$	-0.0641	-0.0608
bcp3, $\rho(\mathbf{r})$	0.3565	0.3794
$\nabla^2\rho(\mathbf{r})$	0.6374	0.3131
bcp3, $\rho(\mathbf{r})$	0.3565	0.3794
$\nabla^2\rho(\mathbf{r})$	0.6374	0.3131

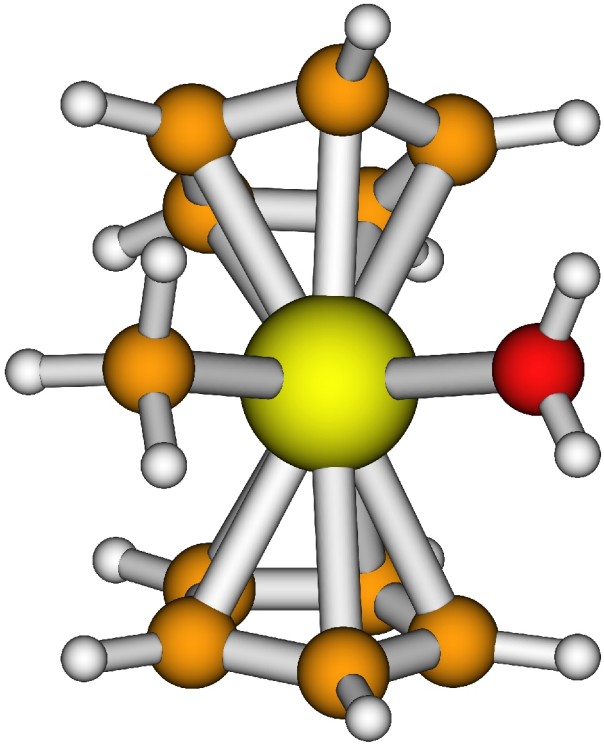
Table S6: Electron density, Laplacian and Virial Field Function of **5**



Plane through Zr-O-H

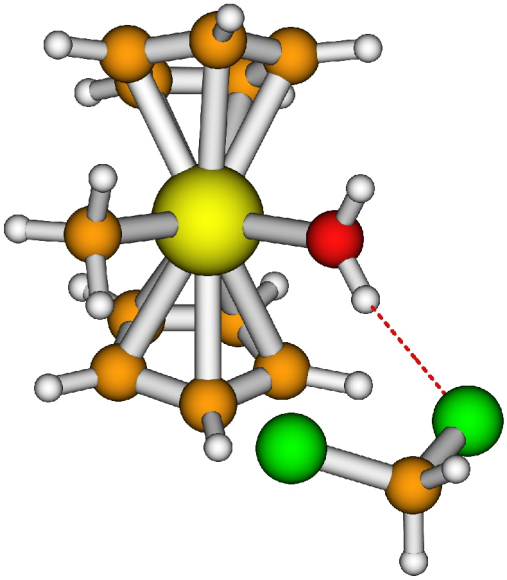
Cartesian coordinates (in Å) of compound $[Cp_2ZrMe(OH_2)]^+$ (**5-MP2**)
(MP2/ECP11)

C	-1.630846	1.424976	-0.927382
C	-2.179676	0.145765	-1.204378
C	-2.525713	-0.464845	0.036563
C	-2.209771	0.446110	1.081228
C	-1.641869	1.608153	0.488662
Zr	-0.000320	-0.227328	0.046946
C	0.014583	-1.241034	2.083734
C	1.660674	1.597526	0.458966
C	2.231499	0.431899	1.041602
C	2.522906	-0.481202	-0.008309
C	2.158811	0.131496	-1.243037
C	1.623272	1.414260	-0.956616
O	-0.017358	-2.260252	-1.122647
H	1.366510	2.494036	0.990495
H	1.291243	2.142007	-1.685714
H	2.293024	-0.289666	-2.233296
H	2.988839	-1.452407	0.114880
H	2.420798	0.272572	2.094644
H	-2.334192	-0.274301	-2.192140
H	-1.307134	2.150729	-1.662185
H	-1.332499	2.502617	1.014979
H	-2.381334	0.287773	2.137453
H	-2.995669	-1.433039	0.167907
H	0.903852	-1.879045	2.172875
H	0.024383	-0.549944	2.935424
H	-0.877030	-1.873336	2.188736
H	0.754740	-2.821111	-1.280896
H	-0.795762	-2.816122	-1.266996



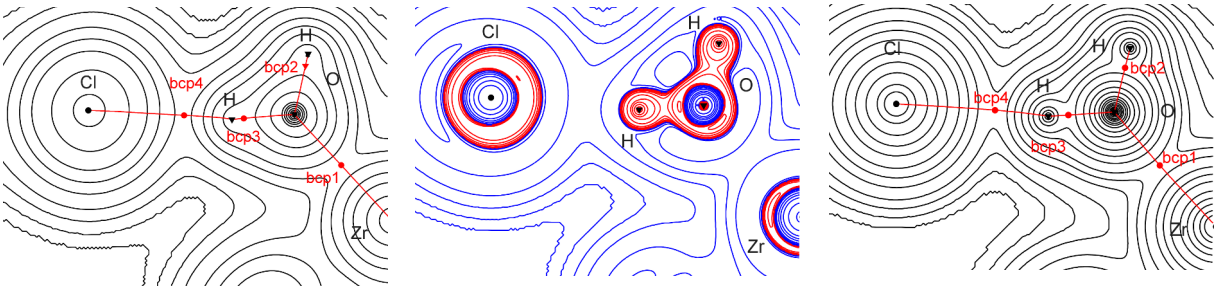
Cartesian coordinates (in Å) of compound {[$Cp_2ZrMe(OH_2)$](CH_2Cl_2)}$^+$ (**6**) (B3LYP/ECP11)

C	-0.059163	1.891656	-1.124704
C	-0.452127	2.001667	0.236210
C	0.691292	2.343645	0.997228
C	1.797626	2.416770	0.113494
C	1.329284	2.143764	-1.203155
Zr	1.125966	-0.008054	0.119637
Cl	-3.672159	-0.327898	-1.543214
C	-4.781865	-0.283094	-0.104372
Cl	-3.901149	-0.356361	1.439516
C	3.119309	-1.403516	0.882063
C	2.319580	-2.278555	0.107577
C	2.341045	-1.820789	-1.237086
C	3.131525	-0.651070	-1.290814
C	3.609588	-0.387209	0.024615
C	0.693598	-0.361199	2.321234
O	-0.678909	-1.161390	-0.635675
H	4.285465	0.406601	0.305442
H	3.370983	-0.087898	-2.179920
H	1.860215	-2.293189	-2.082522
H	1.826205	-3.167881	0.474051
H	3.327600	-1.501314	1.935829
H	-0.708981	1.676644	-1.961465
H	1.919828	2.171513	-2.106299
H	2.804882	2.699281	0.381428
H	0.713997	2.526937	2.059875
H	-1.453375	1.881949	0.624211
H	0.683156	-1.436945	2.528670
H	1.413348	0.089587	3.012101
H	-0.291200	0.047542	2.572653
H	-5.430427	-1.147771	-0.182471
H	-5.323947	0.653732	-0.160191
H	-0.714929	-2.122905	-0.705183
H	-1.582075	-0.822628	-0.787157



	Electron Density	Virial Field Funktion
bcp1, $\rho(\mathbf{r})$	0.0519	0.0528
$\nabla^2\rho(\mathbf{r})$	-0.0685	-0.0666
bcp2, $\rho(\mathbf{r})$	0.3547	0.3765
$\nabla^2\rho(\mathbf{r})$	0.6265	0.3057
bcp3, $\rho(\mathbf{r})$	0.3288	0.3522
$\nabla^2\rho(\mathbf{r})$	0.5505	0.2299
bcp4, $\rho(\mathbf{r})$	0.0174	0.0177
$\nabla^2\rho(\mathbf{r})$	-0.0138	-0.0133

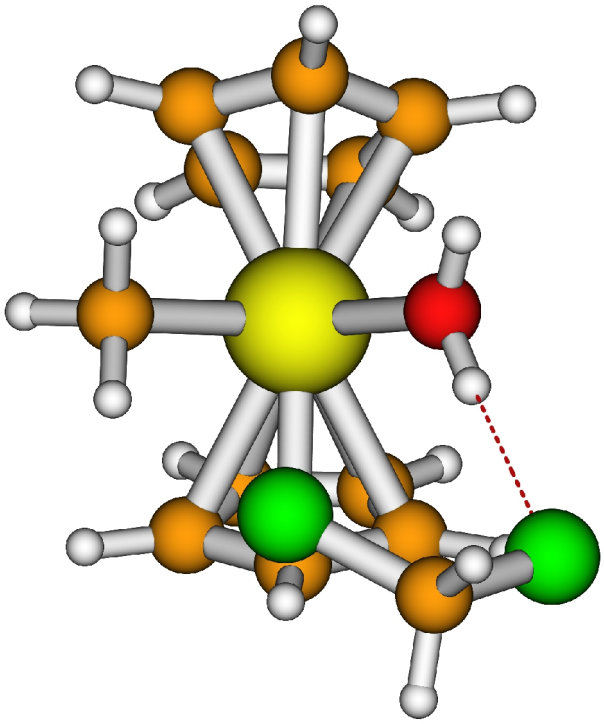
Table S7: Electron density, Laplacian and Virial Field Function of **6**



Plane through H-O-H

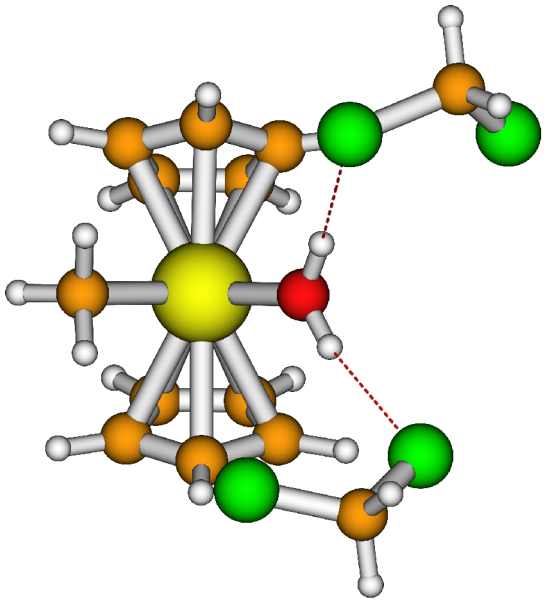
Cartesian coordinates (in Å) of compound $[Cp_2ZrMe(OH_2)(CH_2Cl_2)]^+$ (**6-MP2**) (MP2/ECP11)

C	3.516018	0.334363	-0.318060
C	2.941823	1.411719	-1.047784
C	2.274269	2.257966	-0.120965
C	2.461665	1.719905	1.186173
C	3.226968	0.531293	1.066180
Zr	1.039380	0.044456	-0.085686
O	-0.704525	1.299355	0.762143
C	-0.144088	-1.771205	1.237344
C	-0.573448	-1.912728	-0.113014
C	0.548395	-2.301992	-0.894712
C	1.677131	-2.376238	-0.032092
C	1.247464	-2.050298	1.290024
C	0.481338	0.338830	-2.273659
Cl	-3.566128	0.135651	1.475563
C	-4.496785	0.155548	-0.050980
Cl	-3.467972	0.401233	-1.460814
H	4.121345	-0.461587	-0.733680
H	3.565537	-0.093133	1.882893
H	2.103625	2.150449	2.114561
H	1.759793	3.179689	-0.368455
H	3.010301	1.565630	-2.116077
H	-0.770814	-1.521221	2.085715
H	1.859532	-2.065602	2.182674
H	2.675672	-2.684177	-0.316063
H	0.541824	-2.509451	-1.956548
H	-1.578691	-1.763095	-0.486221
H	0.437373	1.413739	-2.496621
H	1.182228	-0.112861	-2.986173
H	-0.507486	-0.096026	-2.465264
H	-5.209304	0.972585	0.014732
H	-4.994316	-0.806300	-0.135023
H	-0.765369	2.263526	0.740591
H	-1.607356	0.964695	0.927054



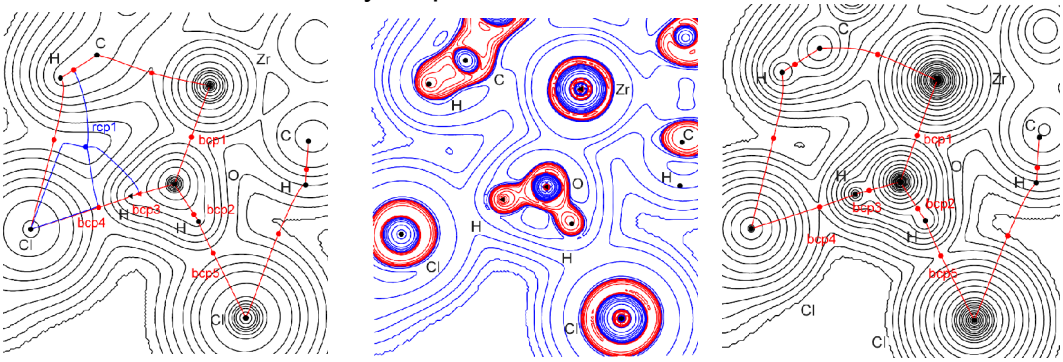
Cartesian coordinates (in Å) of compound {[$Cp_2ZrMe(OH_2)$][$(CH_2Cl_2)_2$}$^+$ (**7**) (B3LYP/ECP11)

C	3.396755	-1.812122	0.135112
C	2.667124	-2.024800	1.331075
C	1.358507	-2.433141	0.976250
C	1.287452	-2.503076	-0.440705
C	2.542000	-2.115715	-0.962901
Zr	1.618580	-0.027737	0.137206
C	1.663221	0.632690	2.310875
C	3.457030	1.358889	-0.879791
C	2.792293	2.232710	0.017155
C	1.485818	2.456289	-0.479638
C	1.350680	1.742202	-1.699537
C	2.563762	1.060228	-1.947463
O	-0.632897	-0.032755	-0.032386
Cl	-2.750511	2.146278	-1.269746
C	-3.209844	3.429286	-0.070853
Cl	-2.135435	3.459935	1.347694
Cl	-2.714781	-2.139983	1.387420
C	-3.496846	-3.215736	0.154341
Cl	-2.818008	-2.997314	-1.477777
H	2.788369	0.459567	-2.815770
H	0.481236	1.735903	-2.341756
H	0.736261	3.085182	-0.021514
H	3.210662	2.659942	0.914873
H	4.483019	1.031352	-0.802301
H	-1.200105	0.709789	-0.306960
H	-1.219532	-0.737895	0.295426
H	4.437986	-1.533762	0.069684
H	2.816545	-2.096399	-2.006671
H	0.429172	-2.810099	-1.021766
H	0.567180	-2.685207	1.667548
H	3.044176	-1.905840	2.334553
H	1.127543	-0.097504	2.927452
H	2.661764	0.747151	2.744419
H	1.158009	1.600012	2.405828
H	-4.548735	-2.956225	0.132553
H	-3.324940	-4.237192	0.473098
H	-3.139843	4.378947	-0.588441
H	-4.217977	3.206016	0.258037



	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.0562	0.0578
$\nabla^2\rho(\mathbf{r})$	-0.0699	-0.0661
bcp2, $\rho(\mathbf{r})$	0.3453	0.3688
$\nabla^2\rho(\mathbf{r})$	0.6120	0.2935
bcp3, $\rho(\mathbf{r})$	0.3453	0.3687
$\nabla^2\rho(\mathbf{r})$	0.6116	0.2933
bcp4, $\rho(\mathbf{r})$	0.0174	0.0178
$\nabla^2\rho(\mathbf{r})$	-0.0134	-0.0126
bcp5, $\rho(\mathbf{r})$	0.0174	0.0178
$\nabla^2\rho(\mathbf{r})$	-0.0134	-0.0126
rcp1, $\rho(\mathbf{r})$	0.0024	
$\nabla^2\rho(\mathbf{r})$	-0.0021	

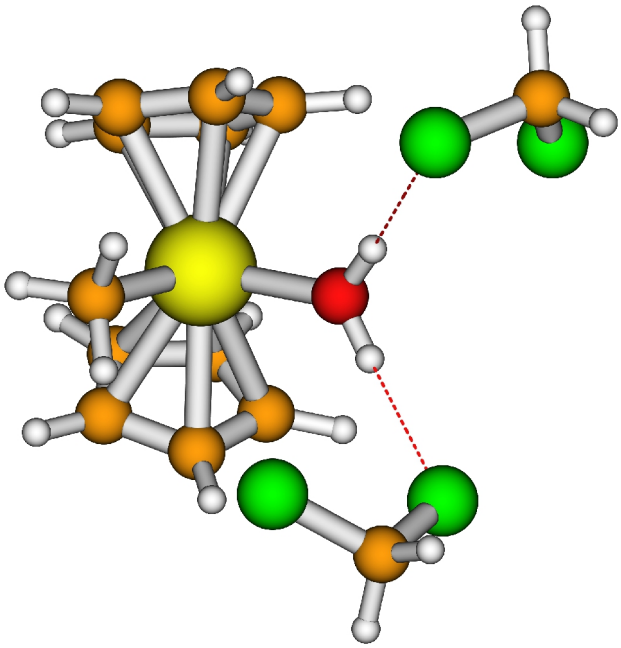
Table S8: Electron density, Laplacian and Virial Field Function of **7**



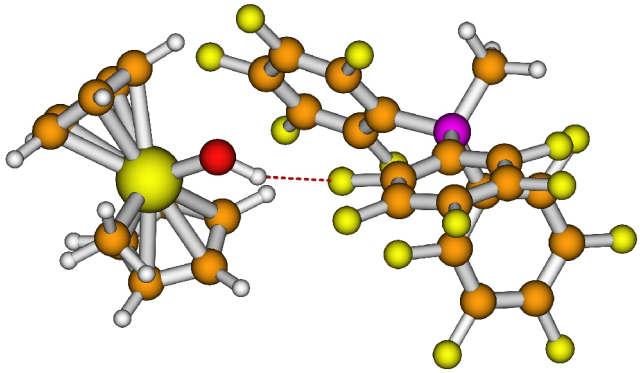
Plane through H-O-H

Cartesian coordinates (in Å) of compound {[$Cp_2ZrMe(OH_2)$]$(CH_2Cl_2)_2$}$^+$ (**7-MP2**) (MP2/ECP11)

C	2.444953	0.816560	-2.060709
C	3.333806	1.244939	-1.028427
C	2.661896	2.223015	-0.244467
C	1.353830	2.386189	-0.777329
C	1.226172	1.528822	-1.906911
Zr	1.474874	0.016934	0.118967
O	-0.793843	-0.030055	-0.077382
C	3.271677	-1.712861	0.375074
C	2.509163	-1.782744	1.573527
C	1.207161	-2.242354	1.235569
C	1.173065	-2.484810	-0.168272
C	2.445786	-2.154675	-0.702788
C	1.550106	0.946744	2.197479
Cl	-2.599689	2.327220	-1.228311
C	-2.872762	3.414428	0.163139
Cl	-1.779352	3.077908	1.504370
Cl	-2.677269	-2.196743	1.322196
C	-3.254677	-3.267030	0.014677
Cl	-2.501611	-2.906658	-1.538567
H	2.675660	0.113430	-2.850599
H	0.359111	1.444865	-2.551846
H	0.596063	3.056174	-0.391252
H	3.073468	2.753246	0.603910
H	4.360138	0.924159	-0.901799
H	-1.359992	0.705393	-0.374461
H	-1.385504	-0.710173	0.291725
H	4.315011	-1.432732	0.301914
H	2.748840	-2.259868	-1.736542
H	0.325728	-2.856892	-0.731648
H	0.394832	-2.408798	1.932835
H	2.859618	-1.536828	2.566817
H	0.982211	0.316036	2.895090
H	2.559468	1.063684	2.610099
H	1.087200	1.941275	2.173648
H	-4.327183	-3.120793	-0.073108
H	-3.009627	-4.286286	0.298798
H	-2.707291	4.429832	-0.185269
H	-3.895962	3.265875	0.495640



Cartesian coordinates (in Å) of compound $[Cp_2TiMe(OH)][MeB(C_6F_5)_3]^-$ (**8**)
(B3LYP/ECP11)

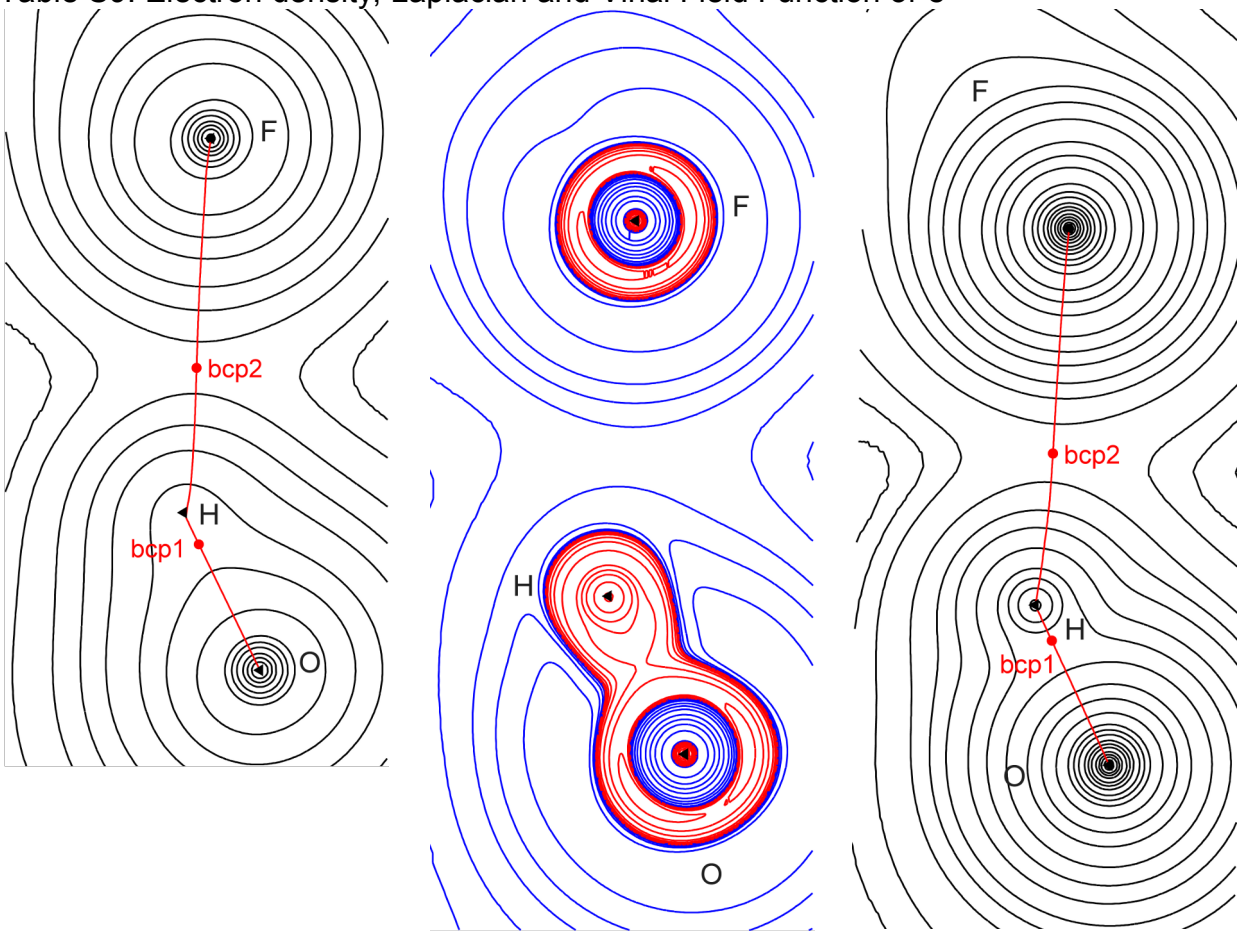


Ti	-4.296104	0.434739	0.801303
O	-3.133388	1.620822	0.011455
H	-2.203801	1.713576	0.269756
C	-3.363844	-1.745264	1.313805
C	-4.292979	-1.436678	2.344448
C	-3.793660	-0.325363	3.062218
C	-2.563005	0.057829	2.474648
C	-2.293179	-0.826586	1.403091
H	-1.435544	-0.783532	0.748370
H	-1.954184	0.902634	2.770006
H	-4.276423	0.157085	3.899918
H	-5.220070	-1.956256	2.547078
H	-3.451279	-2.541709	0.587879
C	-6.652999	0.453635	0.133840
C	-5.951102	1.270593	-0.797770
C	-5.071737	0.447003	-1.526367
C	-5.193397	-0.874595	-1.033461
C	-6.197687	-0.872248	-0.023857
H	-6.532858	-1.731728	0.540992
H	-4.631003	-1.728369	-1.384586
H	-4.338453	0.779225	-2.246189
H	-6.024341	2.346525	-0.881828
H	-7.391187	0.794449	0.847352
C	-5.171734	1.929030	2.119687
H	-5.585330	2.733033	1.501267
H	-5.961464	1.549450	2.780885
H	-4.370375	2.353070	2.736271
C	-1.428355	-1.351596	-2.274508
C	-0.256889	-0.625050	-2.088475
C	0.852661	-1.082082	-1.365794
C	0.699630	-2.381216	-0.872646
C	-0.458989	-3.146630	-1.025791
C	-1.535827	-2.623957	-1.726457
F	-2.685514	-3.325461	-1.842152
F	-0.545154	-4.380513	-0.493508
F	1.695109	-2.998538	-0.196838
B	2.249460	-0.177824	-1.296377
C	1.979430	1.412979	-0.836059
C	2.990909	2.371142	-0.992365
C	2.875353	3.710115	-0.620617
C	1.702205	4.162485	-0.027768
C	0.677188	3.251328	0.185874
C	0.844689	1.925324	-0.205361
F	-0.218055	1.126173	0.091570
F	-0.468370	3.648218	0.777635
F	1.569884	5.448472	0.340252
F	3.894466	4.568517	-0.816826
F	4.191640	2.027697	-1.510259
C	3.290139	-0.732344	-0.121938
C	2.884239	-0.761626	1.217118

C	3.695683	-1.138418	2.281630
C	5.010648	-1.515847	2.028627
C	5.470415	-1.509586	0.719177
C	4.615823	-1.124069	-0.317005
F	5.166951	-1.167038	-1.549292
F	6.740823	-1.877698	0.459725
F	5.821948	-1.884343	3.037151
F	3.229706	-1.145342	3.545451
F	1.612833	-0.420911	1.538075
C	2.838752	-0.249403	-2.830432
H	3.021852	-1.288567	-3.135064
H	2.101156	0.162287	-3.532257
H	3.771898	0.297469	-2.979141
F	-0.243884	0.608509	-2.642700
F	-2.473362	-0.829274	-2.948737

	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.3395	0.3407
$\nabla^2\rho(\mathbf{r})$	0.4432	0.4054
bcp2, $\rho(\mathbf{r})$	0.0159	0.0161
$\nabla^2\rho(\mathbf{r})$	-0.0155	-0.0159

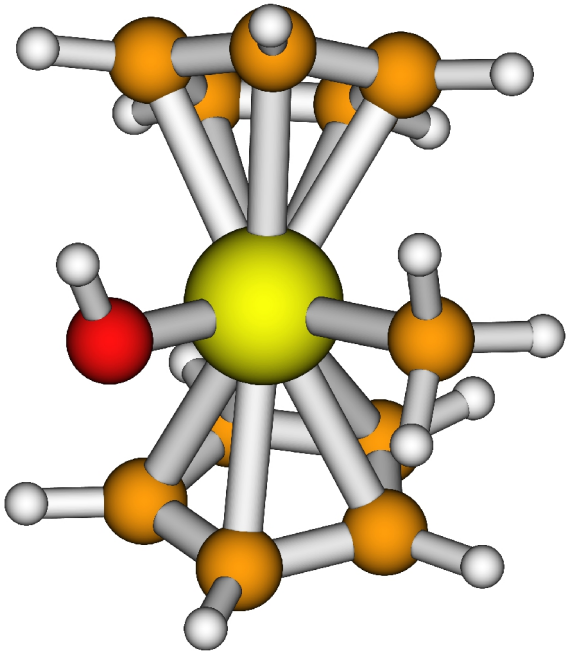
Table S9: Electron density, Laplacian and Virial Field Function of **8**



Plane through O-H-F

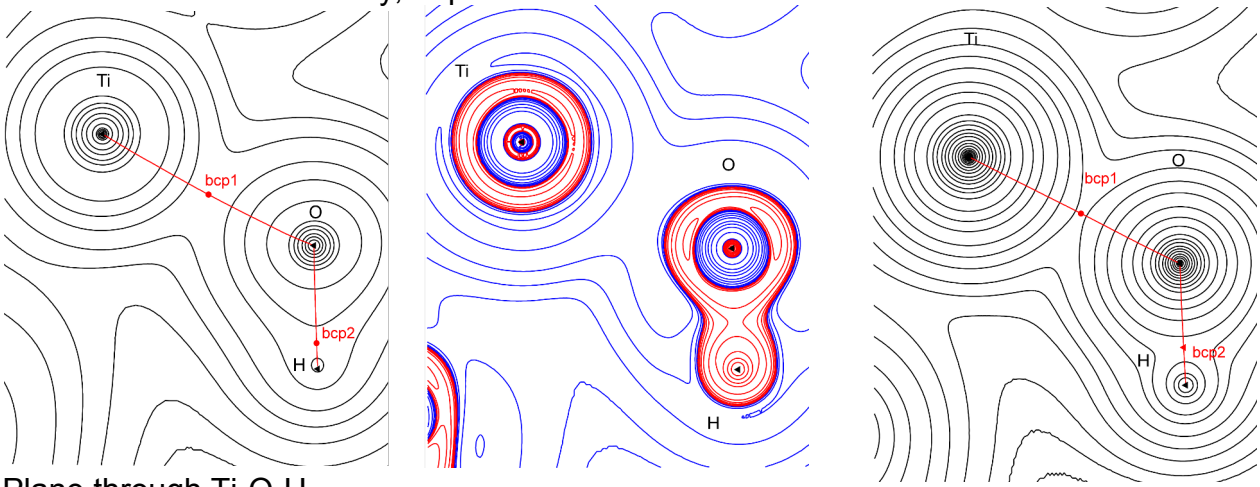
Cartesian coordinates (in Å) of compound [$Cp_2TiMe(OH)$] (**9**)
(B3LYP/ECP11)

C	-2.158388	-0.454099	1.055388
C	-2.443669	0.526952	0.084743
C	-2.041607	0.024027	-1.179343
C	-1.501646	-1.262146	-0.983943
C	-1.554004	-1.553191	0.406107
Ti	0.003892	0.279430	0.133287
O	0.073123	1.253463	1.719637
C	2.013901	-0.700857	1.080825
C	2.411334	0.466763	0.392991
C	2.171336	0.266265	-0.986027
C	1.617933	-1.023232	-1.151983
C	1.522441	-1.622628	0.129696
C	-0.014291	2.053272	-1.125633
H	1.151185	-2.613531	0.339728
H	1.329152	-1.471119	-2.090478
H	2.370245	0.973527	-1.774514
H	2.767514	1.375785	0.851175
H	2.027231	-0.837338	2.151096
H	-2.323857	-0.370189	2.119171
H	-1.230119	-2.465573	0.881733
H	-1.116473	-1.912522	-1.753375
H	-2.129459	0.539690	-2.122155
H	-2.873612	1.500508	0.267083
H	0.837255	2.675823	-0.841947
H	0.042295	1.847996	-2.198703
H	-0.929455	2.618083	-0.930837
H	-0.732552	1.636937	2.075693



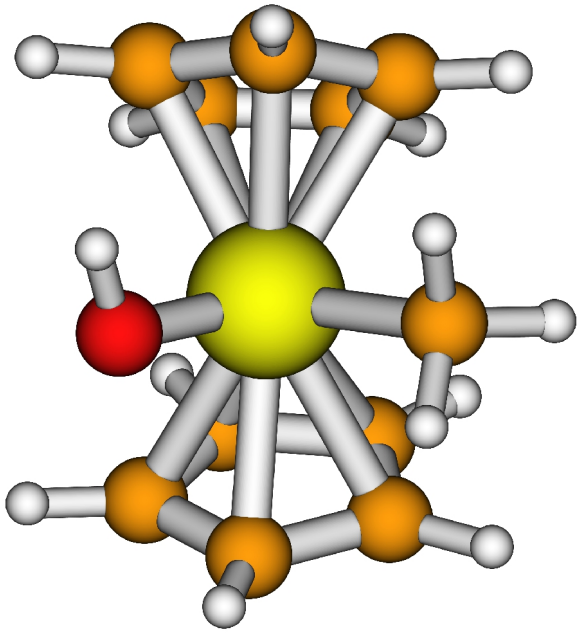
	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.1250	0.1272
$\nabla^2\rho(\mathbf{r})$	-0.1514	-0.1379
bcp2, $\rho(\mathbf{r})$	0.3642	0.3824
$\nabla^2\rho(\mathbf{r})$	0.6060	0.3045

Table S10: Electron density, Laplacian and Virial Field Function of **9**



Plane through Ti-O-H

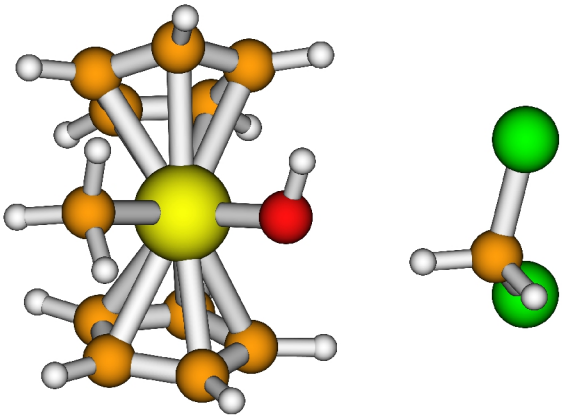
Cartesian coordinates (in Å) of compound [$Cp_2TiMe(OH)$] (**9-MP2**) (MP2/ECP11)



C	1.471771	1.580829	-0.330187
C	1.971571	0.521939	-1.127087
C	2.333833	-0.540462	-0.265934
C	2.073859	-0.135395	1.068104
C	1.537452	1.174123	1.030186
Ti	0.002126	-0.259150	-0.085581
C	-0.006832	-1.890276	1.403545
C	-2.084607	0.306544	-1.110821
C	-2.358331	-0.596936	-0.060281
C	-2.004472	0.029762	1.165390
C	-1.499701	1.314405	0.865873
C	-1.526180	1.479546	-0.547792
O	0.120169	-1.444829	-1.549722
H	1.119108	2.538901	-0.691549
H	1.233730	1.759682	1.889728
H	2.252453	-0.721494	1.959616
H	2.657042	-1.524400	-0.582295
H	1.988144	0.489874	-2.209802
H	-2.209874	0.119858	-2.171326
H	-1.224063	2.361912	-1.097889
H	-1.149831	2.045036	1.584573
H	-2.101065	-0.404378	2.152111
H	-2.734805	-1.608547	-0.164466
H	0.857209	-2.526854	1.187196
H	0.037321	-1.564371	2.449615
H	-0.917871	-2.481154	1.256870
H	-0.724602	-1.863364	-1.796801

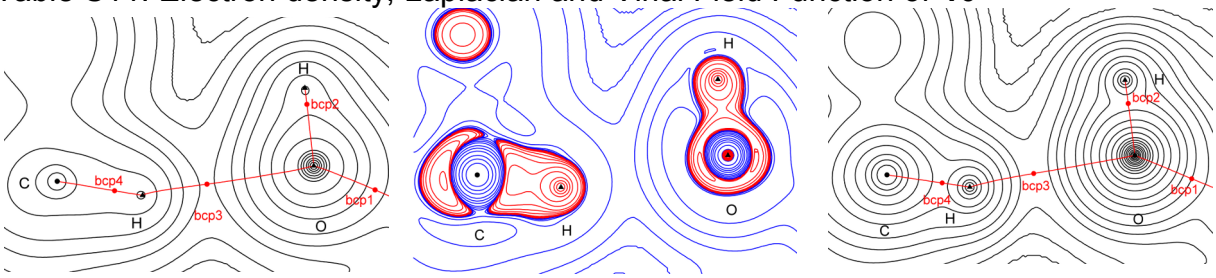
Cartesian coordinates (in Å) of compound {[$Cp_2TiMe(OH)$](CH_2Cl_2)} (**10**) (B3LYP/ECP11)

C	1.347380	1.821160	-1.279298
C	2.565510	1.831951	-0.555263
C	2.261926	2.104809	0.798563
C	0.861183	2.249597	0.912755
C	0.295919	2.076185	-0.371445
Ti	1.271335	-0.053808	0.268963
O	-0.370225	-0.255443	1.168169
C	2.498413	-1.163637	-1.497823
C	2.669520	-1.957275	-0.346864
C	1.404364	-2.494469	0.006162
C	0.458087	-2.038856	-0.933461
C	1.121713	-1.194611	-1.850943
C	2.457535	-0.406075	2.058194
Cl	-3.837233	-1.427578	0.493457
C	-3.445194	0.320475	0.648784
Cl	-3.707259	1.227229	-0.878602
H	3.274892	-0.626391	-2.019461
H	0.664992	-0.700480	-2.693999
H	-0.601299	-2.248294	-0.930648
H	1.205404	-3.129381	0.856732
H	3.596215	-2.124193	0.178675
H	3.552735	1.671992	-0.961332
H	1.240959	1.655279	-2.339820
H	-0.756062	2.094029	-0.612525
H	0.313105	2.401646	1.829178
H	2.976238	2.183333	1.601431
H	2.293595	-1.429324	2.405197
H	3.532397	-0.258904	1.917242
H	2.107787	0.278527	2.834124
H	-0.627792	-1.158880	1.375739
H	-4.109889	0.738163	1.396156
H	-2.392621	0.390618	0.912075



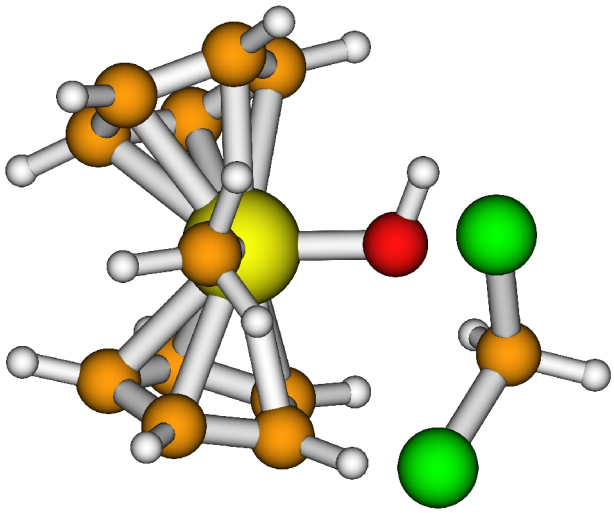
	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.1189	0.1212
$\nabla^2\rho(\mathbf{r})$	-0.1446	-0.1310
bcp2, $\rho(\mathbf{r})$	0.3634	0.3815
$\nabla^2\rho(\mathbf{r})$	0.6032	0.3024
bcp3, $\rho(\mathbf{r})$	0.0184	0.0185
$\nabla^2\rho(\mathbf{r})$	-0.0152	-0.0152
bcp4, $\rho(\mathbf{r})$	0.2927	0.2927
$\nabla^2\rho(\mathbf{r})$	0.2645	0.2628

Table S11: Electron density, Laplacian and Virial Field Function of **10**



Plane through H-O-H

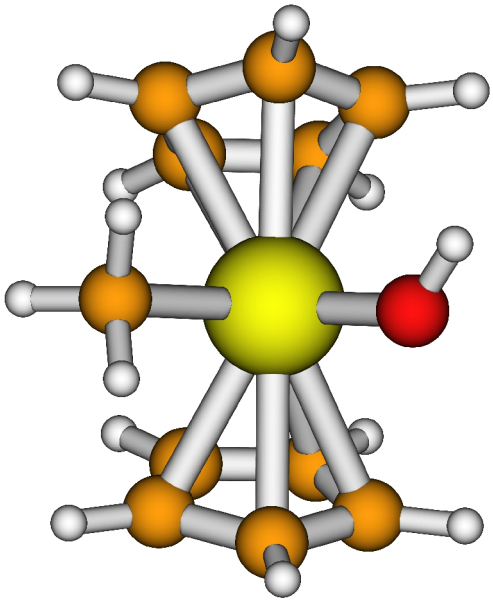
Cartesian coordinates (in Å) of compound {[$Cp_2TiMe(OH)$](CH_2Cl_2)} (**10-MP2**) (MP2/ECP11)



C	2.370859	-1.903587	0.618386
C	2.038565	-1.998171	-0.762656
C	0.628349	-2.112294	-0.866486
C	0.089204	-2.080578	0.445809
C	1.163701	-1.953779	1.362925
Ti	1.110935	0.027502	0.072651
O	-0.207729	0.484106	1.354332
C	3.241291	0.781143	-0.656602
C	2.276024	1.604239	-1.283423
C	1.605368	2.344421	-0.267257
C	2.166461	1.984601	0.979850
C	3.155064	0.992754	0.751407
C	-0.190210	0.369661	-1.682924
C	-3.242914	0.068884	0.711680
Cl	-3.397313	1.654659	-0.061551
Cl	-3.594228	-1.274606	-0.390676
H	3.915075	0.096378	-1.153080
H	3.761611	0.519162	1.511294
H	1.856716	2.343081	1.953231
H	0.780116	3.026784	-0.426087
H	2.071027	1.654777	-2.343454
H	2.733563	-1.975836	-1.591693
H	3.368338	-1.808451	1.025469
H	1.070088	-1.837954	2.434738
H	-0.962684	-2.079778	0.693022
H	0.063698	-2.200607	-1.783010
H	-0.439923	1.434985	-1.734713
H	0.260817	0.064647	-2.635065
H	-1.114439	-0.196260	-1.532378
H	-0.301502	1.436521	1.468213
H	-3.958756	0.022990	1.528323
H	-2.215129	-0.022338	1.060080

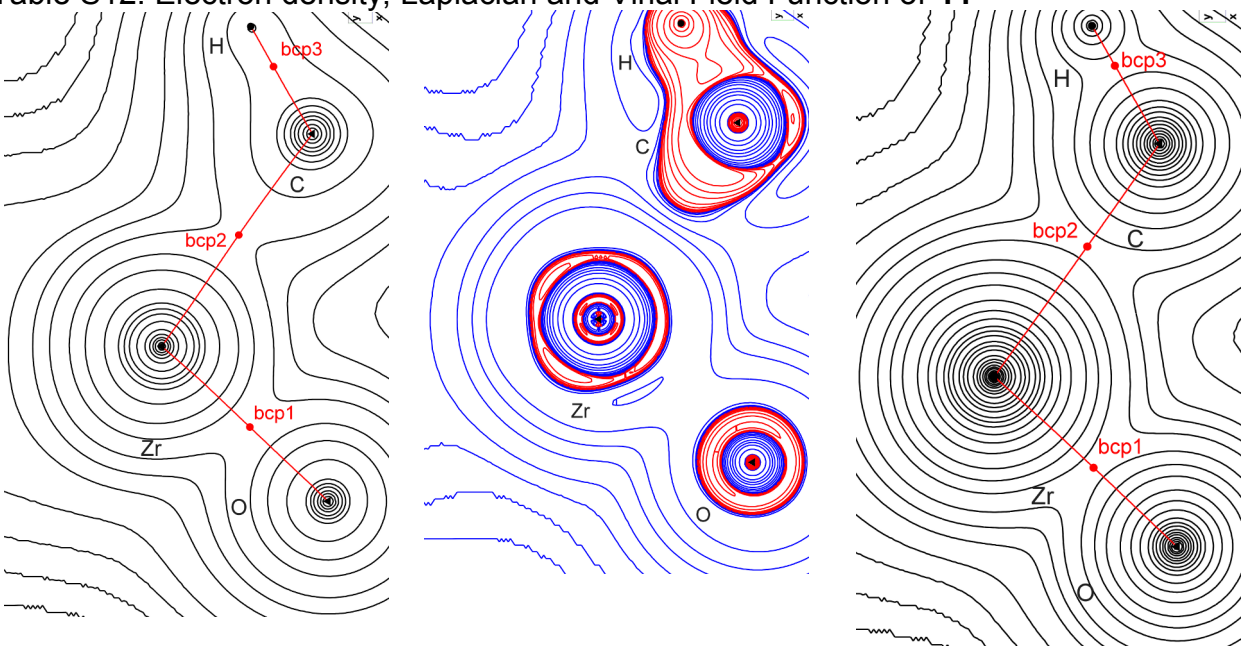
Cartesian coordinates (in Å) of compound [$Cp_2ZrMe(OH)$] (**11**)
(B3LYP/ECP11)

C	1.662570	1.658260	-0.349722
C	1.670067	1.304293	1.027556
C	2.249371	0.020358	1.144971
C	2.597358	-0.424151	-0.155280
C	2.247058	0.592752	-1.074761
Zr	-0.000311	-0.286845	-0.118994
O	-0.061676	-1.409180	-1.783032
C	-1.684783	1.641401	-0.370251
C	-2.247061	0.556855	-1.087385
C	-2.585427	-0.453080	-0.160175
C	-2.254432	0.012441	1.139286
C	-1.701417	1.306867	1.011864
C	0.013391	-2.005486	1.409842
H	1.319049	1.919041	1.842794
H	1.312040	2.590652	-0.765614
H	2.388150	0.562022	-2.145190
H	3.054539	-1.372526	-0.396680
H	2.397561	-0.528257	2.061642
H	-2.353949	0.490625	-2.159371
H	-1.348133	2.575822	-0.793922
H	-1.367638	1.937561	1.822440
H	-2.401566	-0.527166	2.061747
H	-3.001099	-1.419459	-0.402512
H	0.901289	-2.629073	1.256395
H	0.008204	-1.689313	2.458825
H	-0.867322	-2.635971	1.247652
H	0.664552	-1.789777	-2.279871



	Electron Density	Virial Field Function
bcp3, $\rho(\mathbf{r})$	0.1084	0.1092
$\nabla^2\rho(\mathbf{r})$	-0.1225	-0.1168
bcp3, $\rho(\mathbf{r})$	0.0883	0.0923
$\nabla^2\rho(\mathbf{r})$	-0.0148	-0.0024
bcp3, $\rho(\mathbf{r})$	0.2635	0.2647
$\nabla^2\rho(\mathbf{r})$	0.2074	0.2124

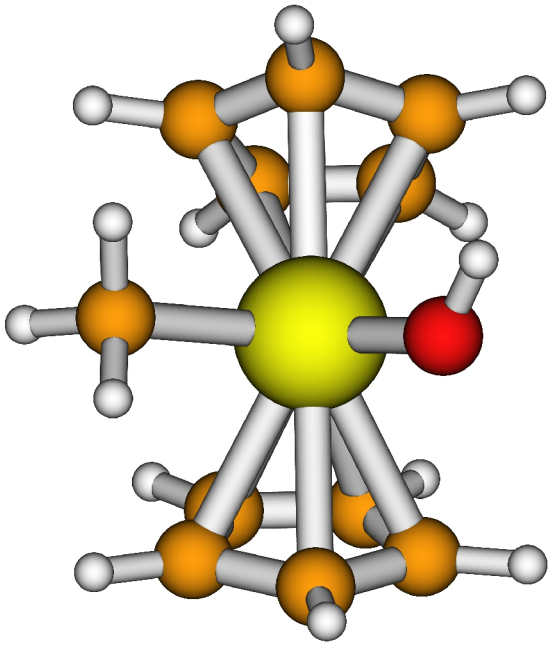
Table S12: Electron density, Laplacian and Virial Field Function of **11**



Plane through O-Zr-C

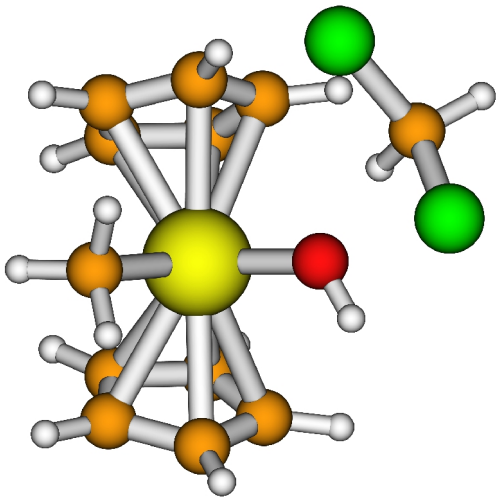
Cartesian coordinates (in Å) of compound [$Cp_2ZrMe(OH)$] (**11-MP2**)
(MP2/ECP11)

C	-1.623959	1.525809	-0.721268
C	-2.170712	0.304958	-1.204894
C	-2.547669	-0.481281	-0.085324
C	-2.245984	0.255082	1.093602
C	-1.674271	1.494939	0.701903
Zr	0.003389	-0.307602	-0.010764
C	0.056052	-1.380305	2.029476
C	1.602594	1.634981	0.435806
C	2.176434	0.516608	1.091989
C	2.569868	-0.421850	0.096123
C	2.254232	0.125280	-1.173722
C	1.636839	1.389258	-0.968967
O	-0.098342	-1.939246	-1.216180
H	1.217876	2.525936	0.915024
H	1.300983	2.064835	-1.744962
H	2.430440	-0.342177	-2.134373
H	3.025807	-1.386450	0.281644
H	2.287168	0.391713	2.160622
H	-2.250085	0.006742	-2.242502
H	-1.263398	2.347175	-1.327301
H	-1.348622	2.282684	1.369333
H	-2.418820	-0.071231	2.109937
H	-2.952821	-1.484215	-0.125230
H	0.975136	-1.974451	2.116480
H	0.010820	-0.703651	2.892375
H	-0.796759	-2.068333	2.093720
H	0.642716	-2.470577	-1.518935



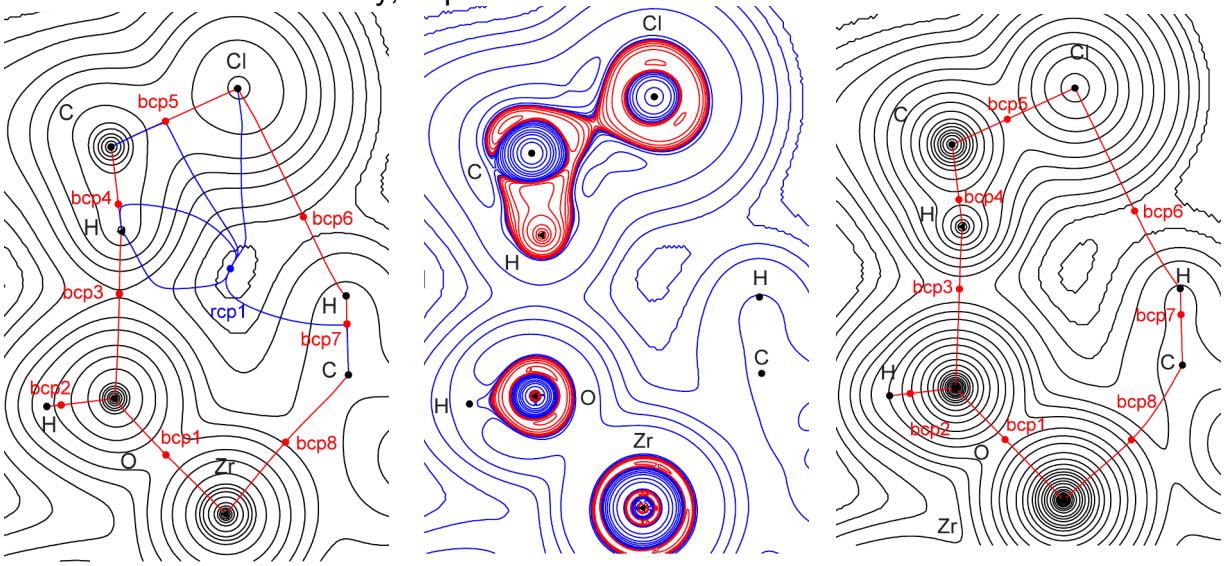
Cartesian coordinates (in Å) of compound {[$Cp_2ZrMe(OH)$](CH_2Cl_2)}$^+$ (**12**)
(B3LYP/ECP11)

C	-3.174157	-0.975298	-1.100899
C	-2.257007	-2.052358	-1.066220
C	-2.072238	-2.428969	0.285585
C	-2.893625	-1.598999	1.088965
C	-3.572181	-0.698529	0.236310
Zr	-1.096118	-0.031050	0.073402
C	-0.520786	-0.165920	2.294126
C	-2.121770	2.331631	0.004958
C	-0.963410	2.447628	0.807111
C	0.167810	2.224295	-0.020129
C	-0.291836	1.983375	-1.334383
C	-1.707147	2.032452	-1.322404
O	0.605443	-0.838867	-0.694077
Cl	4.403791	-1.758629	-0.187221
C	3.719237	-0.166821	-0.661991
Cl	4.169677	1.151190	0.473169
H	-3.140503	2.468019	0.335986
H	-2.353377	1.913243	-2.179168
H	0.326179	1.759075	-2.190588
H	1.198631	2.225933	0.301663
H	-0.940818	2.670173	1.862341
H	-1.775610	-2.497383	-1.924823
H	-3.538511	-0.481192	-1.988758
H	-4.288296	0.048723	0.543707
H	-2.982667	-1.646273	2.162675
H	-1.426351	-3.215857	0.646950
H	0.417096	0.374627	2.458838
H	-1.264726	0.240112	2.988360
H	-0.352748	-1.213965	2.565489
H	2.635381	-0.261529	-0.665447
H	4.130059	0.086597	-1.632796
H	0.731141	-1.785832	-0.795205



	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.1033	0.1043
$\nabla^2\rho(\mathbf{r})$	-0.1139	-0.1077
bcp2, $\rho(\mathbf{r})$	0.3625	0.3806
$\nabla^2\rho(\mathbf{r})$	0.6028	0.3010
bcp3, $\rho(\mathbf{r})$	0.0195	0.0197
$\nabla^2\rho(\mathbf{r})$	-0.0162	-0.0161
bcp4, $\rho(\mathbf{r})$	0.2924	0.2924
$\nabla^2\rho(\mathbf{r})$	0.2643	0.2623
bcp5, $\rho(\mathbf{r})$	0.1787	0.1790
$\nabla^2\rho(\mathbf{r})$	0.0529	0.0488
bcp6, $\rho(\mathbf{r})$	0.0037	0.0037
$\nabla^2\rho(\mathbf{r})$	-0.0027	-0.0028
bcp7, $\rho(\mathbf{r})$	0.2827	0.2831
$\nabla^2\rho(\mathbf{r})$	0.2444	0.2482
bcp8, $\rho(\mathbf{r})$	0.0383	0.0365
$\nabla^2\rho(\mathbf{r})$	-0.0306	-0.0338

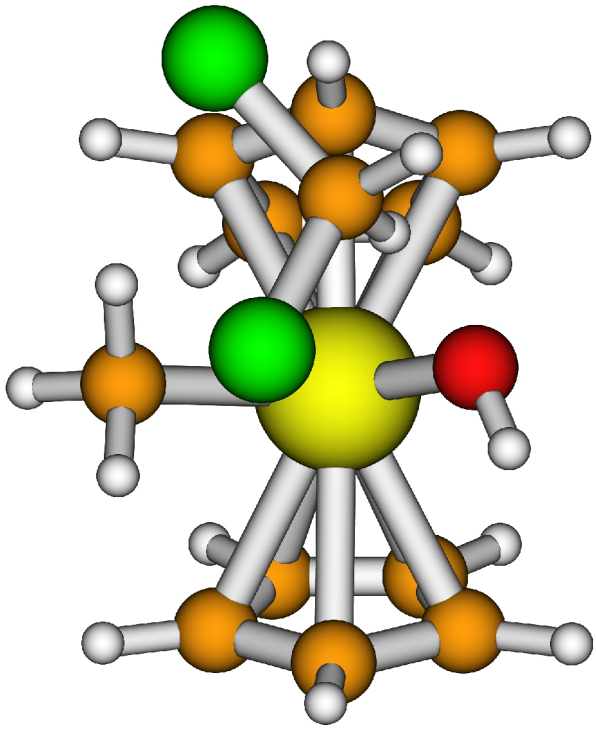
Table S13: Electron density, Laplacian and Virial Field Function of **12**



Plane through Zr-O-H

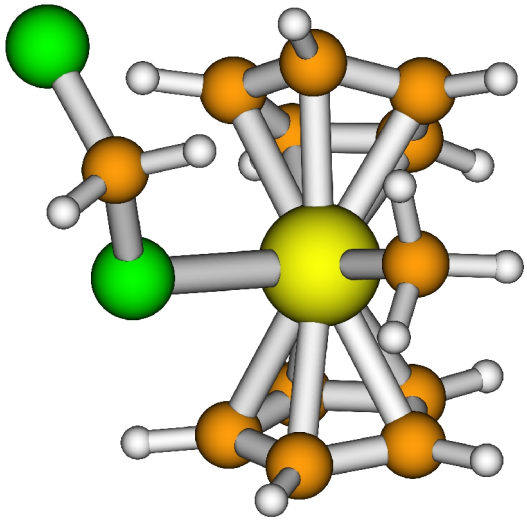
Cartesian coordinates (in Å) of compound {[$Cp_2ZrMe(OH)$](CH_2Cl_2)}$^+$ (**12-MP2**) (MP2/ECP11)

C	-2.022386	2.085635	-1.033565
C	-1.976705	2.243931	0.383530
C	-0.614620	2.343548	0.769685
C	0.183226	2.247029	-0.405462
C	-0.685388	2.102424	-1.517451
Zr	-0.942853	-0.032070	-0.134046
O	0.481874	-0.675940	-1.461443
C	-3.241127	-0.951841	-0.711271
C	-2.329947	-1.997472	-1.021253
C	-1.744260	-2.445743	0.192013
C	-2.311847	-1.696392	1.259979
C	-3.233555	-0.772105	0.703784
C	0.254493	-0.300785	1.811138
C	3.453714	-0.204055	-0.456935
Cl	3.786793	1.210543	0.559152
Cl	3.582596	-1.733020	0.426953
H	-2.831223	2.298119	1.045808
H	-2.917518	2.009999	-1.637629
H	-0.379102	1.976655	-2.548030
H	1.264947	2.256601	-0.433735
H	-0.244628	2.467275	1.778322
H	-2.112725	-2.371636	-2.014052
H	-3.861603	-0.418484	-1.419668
H	-3.841508	-0.069186	1.258451
H	-2.073815	-1.806524	2.309052
H	-0.992209	-3.218748	0.292924
H	1.189427	0.268985	1.750326
H	-0.283639	0.033781	2.707395
H	0.513958	-1.358547	1.946692
H	2.437797	-0.135061	-0.842177
H	4.190140	-0.216143	-1.256276
H	0.595589	-1.602784	-1.693464



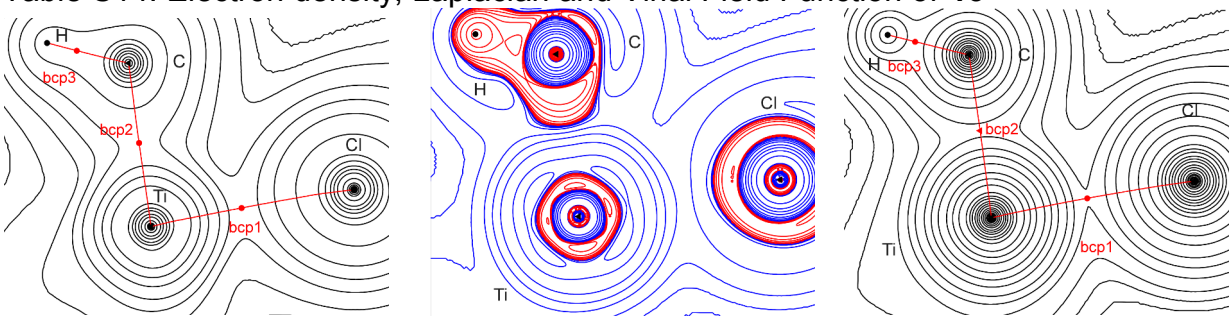
Cartesian coordinates (in Å) of compound $[Cp_2TiMe(CH_2Cl_2)]^+$ (**13**)
(B3LYP/ECP11)

C	1.660054	-1.639683	-1.260533
C	1.752324	-2.111382	0.078354
C	2.646231	-1.274674	0.776730
C	3.089403	-0.266053	-0.117502
C	2.492802	-0.510955	-1.384830
Ti	0.780617	0.089491	0.168558
C	-0.729602	1.934569	0.451400
C	0.516568	2.308972	1.001355
C	1.465987	2.332808	-0.049583
C	0.791491	1.998620	-1.257500
C	-0.560240	1.755074	-0.945530
C	0.437895	-0.268630	2.253159
Cl	-1.351173	-1.461158	-0.327914
C	-2.924116	-1.026348	0.533169
Cl	-3.897218	0.148042	-0.344170
H	1.226488	1.969225	-2.243738
H	2.501136	2.623637	0.039601
H	1.068047	-2.078632	-2.051743
H	1.233745	-2.965296	0.487792
H	2.940514	-1.380677	1.808718
H	2.663045	0.053631	-2.287484
H	0.711189	2.535176	2.037999
H	-1.655573	1.835068	0.996570
H	-1.330587	1.473096	-1.648108
H	3.814037	0.501393	0.106616
H	0.407712	-1.342705	2.449003
H	1.231936	0.159638	2.873024
H	-2.640245	-0.640828	1.505745
H	-3.453831	-1.970652	0.595796
H	-0.501300	0.188186	2.575235



	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.0277	0.0290
$\nabla^2\rho(\mathbf{r})$	-0.0284	-0.0209
bcp2, $\rho(\mathbf{r})$	0.0969	0.0982
$\nabla^2\rho(\mathbf{r})$	-0.0229	-0.0121
bcp3, $\rho(\mathbf{r})$	0.2656	0.2664
$\nabla^2\rho(\mathbf{r})$	0.2117	0.2167

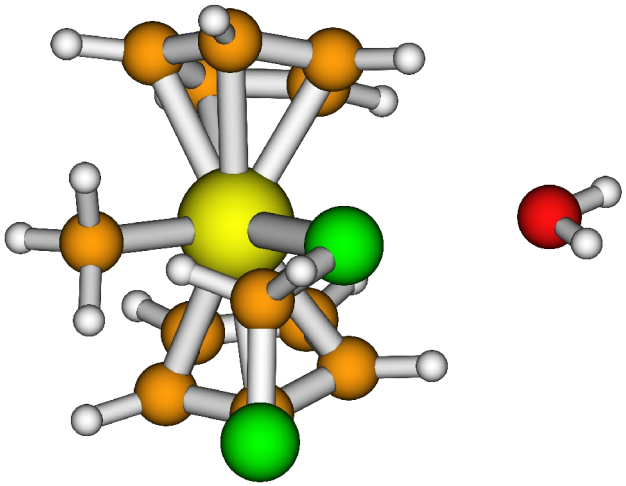
Table S14: Electron density, Laplacian and Virial Field Function of **13**



Plane through Cl-Ti-C

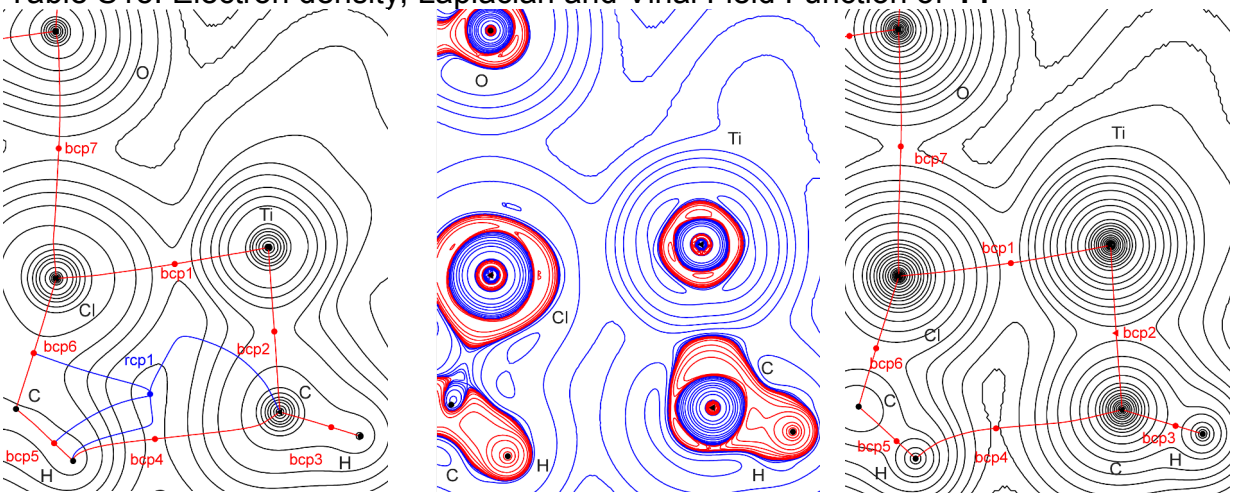
Cartesian coordinates (in Å) of compound $[Cp_2TiMe(CH_2Cl_2)]^+[H_2O]$ (**14**) (B3LYP/ECP11)

Ti	0.764644	-0.313581	-0.244753
C	2.227466	0.339799	-2.019908
C	1.386810	1.443584	-1.758342
C	1.652550	1.900304	-0.441384
C	2.650907	1.075435	0.112974
C	2.998948	0.093888	-0.856057
H	3.759245	-0.664480	-0.748607
H	3.084565	1.185674	1.093580
H	1.157624	2.709784	0.075453
H	0.663125	1.864232	-2.439788
H	2.268341	-0.225046	-2.938124
C	-0.503120	-1.684534	1.225830
C	0.314119	-2.543871	0.460713
C	1.666048	-2.244347	0.766016
C	1.673097	-1.232260	1.764500
C	0.339500	-0.870645	2.032371
H	0.025275	-0.074390	2.692604
H	2.549497	-0.813490	2.232270
H	2.532126	-2.745025	0.359787
H	-0.025406	-3.295509	-0.233318
H	-1.581642	-1.655175	1.206282
C	-0.208600	-1.184309	-1.948462
H	-0.397473	-0.427422	-2.714020
H	0.424263	-1.952610	-2.405371
H	-1.146411	-1.668919	-1.665375
Cl	-1.510961	1.278872	-0.022559
C	-2.961479	0.673608	-0.970813
Cl	-3.920864	-0.519313	-0.092849
H	-2.576394	0.238436	-1.884905
H	-3.558984	1.561660	-1.144469
O	0.117648	2.454588	2.482598
H	0.727898	2.893715	3.085523
H	-0.745472	2.818209	2.709545



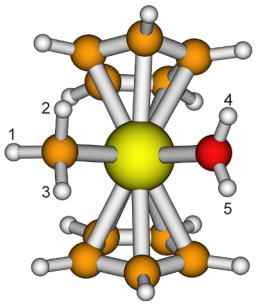
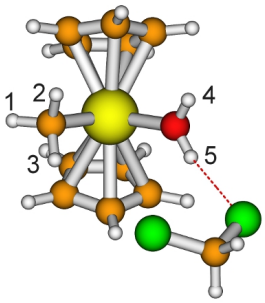
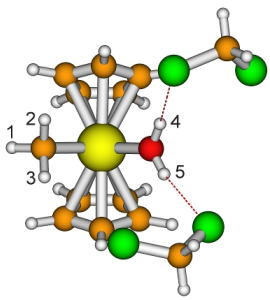
	Electron Density	Virial Field Function
bcp1, $\rho(\mathbf{r})$	0.0220	0.0233
$\nabla^2\rho(\mathbf{r})$	-0.0221	-0.0159
bcp2, $\rho(\mathbf{r})$	0.0959	0.0974
$\nabla^2\rho(\mathbf{r})$	-0.0239	-0.0126
bcp3, $\rho(\mathbf{r})$	0.2651	0.2660
$\nabla^2\rho(\mathbf{r})$	0.2107	0.2157
bcp4, $\rho(\mathbf{r})$	0.0071	0.0071
$\nabla^2\rho(\mathbf{r})$	-0.0065	-0.0066
bcp5, $\rho(\mathbf{r})$	0.2933	0.2932
$\nabla^2\rho(\mathbf{r})$	0.2632	0.2641
bcp6, $\rho(\mathbf{r})$	0.1631	0.1638
$\nabla^2\rho(\mathbf{r})$	0.0409	0.0359
bcp7, $\rho(\mathbf{r})$	0.0064	0.0064
$\nabla^2\rho(\mathbf{r})$	-0.0067	-0.0067

Table S15: Electron density, Laplacian and Virial Field Function of **14**



Plane through Cl-Ti-C

Table S16: Selected bond distances, angles, chemical shifts and CH coupling constants of **5**, **6** and **13**. Bond distances are in Å, angles in °, chemical shifts in ppm relative to TMS and coupling constants in Hz. Values in parenthesis are at the MP2/ECP11 level of theory.

	 **5**	 **6**	 **7**
d(Zr-C)	2.27 (2.28)	2.27 (2.28)	2.27 (2.28)
d(C-H1)	1.09 (1.10)	1.09 (1.07)	1.09 (1.10)
d(C-H2)	1.10 (1.10)	1.10 (1.10)	1.10 (1.10)
d(C-H3)	1.10 (1.10)	1.10 (1.10)	1.10 (1.10)
d(Zr-O)	2.29 (2.35)	2.27 (2.31)	2.26 (2.27)
d(O-H4)	0.97 (0.97)	0.96 (0.97)	0.97 (0.97)
d(O-H5)	0.97 (0.97)	0.98 (0.98)	0.97 ((0.97)
d(H4-Cl)			2.32 (2.22)
d(H5-Cl)		2.28 (2.20)	2.32 (2.21)
∠(Zr-C-H1)	114.9 (114.5)	115.0 (114.5)	115.3 (114.7)
∠(Zr-C-H2)	109.9 (109.7)	109.8 (109.3)	109.6 (109.1)
∠(Zr-C-H3)	109.9 (109.7)	109.6 (109.7)	109.3 (109.6)
∠(H4-O-H5)	108.0 (106.5)	107.5 (106.7)	107.2 (106.8)
δ(CH_3)	1.36	1.19	1.05
δ(CH_3)	49.1	46.6	44.5
$^1J_{CH1}$	123.8	123.4	123.3
$^1J_{CH2}$	118.5	118.2	118.1
$^1J_{CH3}$	118.5	118.7	118.4
δ(OH_2)	2.68	3.89	4.89
δ(C_5H_5)	6.33	6.28	6.28
δ(C_5H_5)	115.6	103.9	114.2