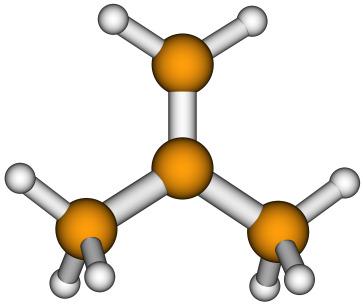
Electronic Supplementary Information
Cartesian Coordinates for Isobutene



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000356	1.459496	-0.000007
2	1	0	0.925154	2.031392	-0.000081
3	1	0	-0.924161	2.031886	0.000211
4	6	0	-0.000006	0.122891	-0.000056
5	6	0	-1.278289	-0.678646	0.000011
6	1	0	-2.163247	-0.034946	0.000848
7	1	0	-1.333099	-1.334027	-0.880450
8	1	0	-1.332334	-1.335340	0.879528
9	6	0	1.277980	-0.679200	0.000011
10	1	0	1.332496	-1.334512	0.880531
11	1	0	1.331778	-1.335899	-0.879507
12	1	0	2.163172	-0.035801	-0.000832

Bader Analysis of Isobutene

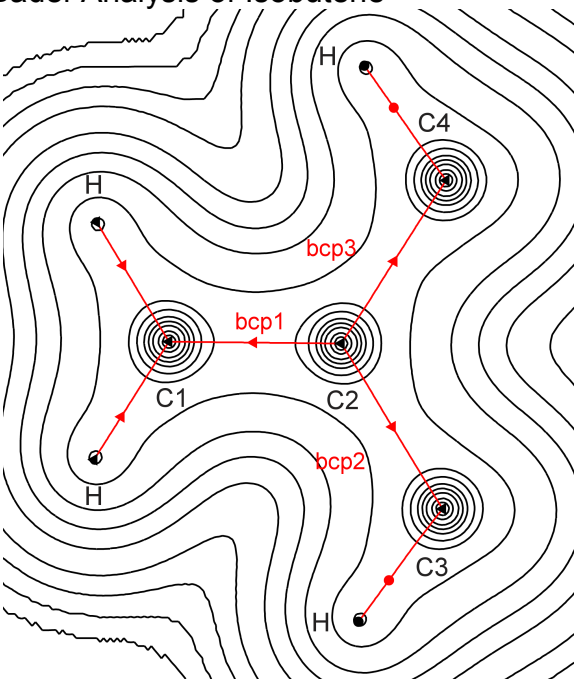
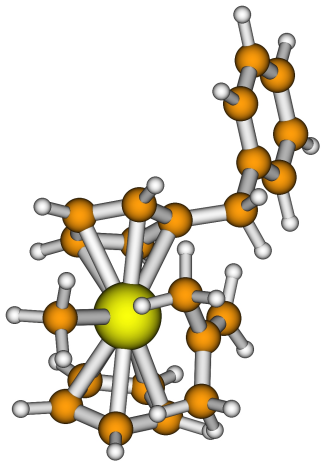


Figure S1: Electron Density Plot of isobutene

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.3438	0.24695
bcp2	0.2547	0.15073
bcp3	0.2547	0.15071

Cartesian Coordinates for **6**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.286634	-0.050130	-0.260231
2	6	0	-5.657282	0.790965	0.661486
3	6	0	-4.299028	1.079056	0.532578
4	6	0	-3.552438	0.530470	-0.519036
5	6	0	-4.190990	-0.308219	-1.439330
6	6	0	-5.551559	-0.597977	-1.311819
7	6	0	-2.065654	0.836268	-0.653288
8	6	0	-1.247174	0.170604	0.435501
9	6	0	-0.592017	0.816726	1.529575
10	6	0	-0.075469	-0.172089	2.406001
11	6	0	-0.360261	-1.440375	1.837071
12	6	0	-1.083235	-1.225550	0.625314
13	40	0	1.283529	-0.398754	0.276377
14	6	0	2.811272	0.218400	1.845927
15	6	0	3.351797	-1.361013	-0.938131
16	6	0	2.292555	-1.378246	-1.883976
17	6	0	1.296959	-2.274959	-1.417997
18	6	0	1.753881	-2.827183	-0.185253
19	6	0	3.024867	-2.264695	0.104622
20	1	0	-0.549823	1.887666	1.692945
21	1	0	4.263335	-0.782353	-1.009473
22	1	0	-0.129787	-2.401449	2.279325
23	1	0	0.381402	-2.536565	-1.932974
24	1	0	-1.492380	-1.998098	-0.013633
25	1	0	1.245003	-3.584043	0.397067
26	1	0	0.438596	0.007542	3.339917
27	1	0	2.260304	-0.827861	-2.816609
28	1	0	-1.728794	0.509984	-1.645763
29	1	0	-1.905685	1.921001	-0.607669
30	1	0	-3.818870	1.739634	1.251496
31	1	0	-3.627624	-0.727536	-2.270778
32	1	0	-6.225902	1.226749	1.477982
33	1	0	-6.035588	-1.245329	-2.037491
34	1	0	-7.345200	-0.271601	-0.161200
35	1	0	3.639904	-2.488406	0.966191
36	1	0	2.503751	1.142647	2.353055
37	1	0	2.955392	-0.538702	2.628613
38	1	0	3.794477	0.382156	1.383706
39	6	0	1.333943	1.852433	-1.169826
40	1	0	1.304357	1.288211	-2.101897
41	1	0	0.384609	2.216281	-0.787194
42	6	0	2.493278	2.456792	-0.775975
43	6	0	3.801333	2.217142	-1.473502
44	1	0	4.139791	3.159209	-1.925057
45	1	0	4.581064	1.924143	-0.760040
46	1	0	3.730731	1.467875	-2.265300

47	6	0	2.515004	3.470378	0.331903
48	1	0	3.286036	3.230084	1.072509
49	1	0	2.780940	4.449853	-0.087849
50	1	0	1.549909	3.566301	0.835338

Bader Analysis of **6**

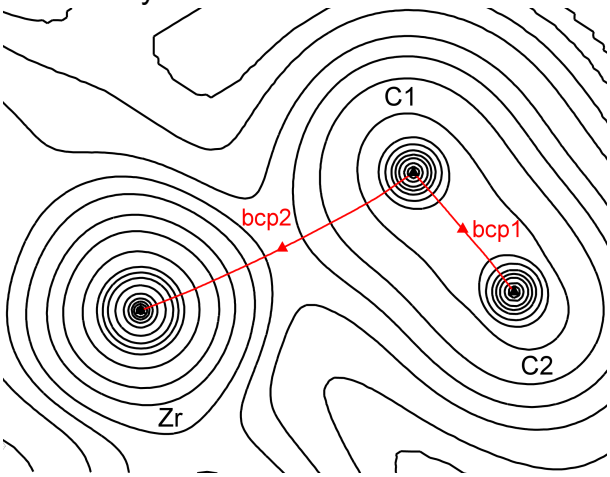


*Figure S2: Electron Density Plot of **6**, view along the Zr-C1-C2 plane*

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.3291	0.23457
bcp2	0.0315	-0.01862

NBO Analysis of **6**

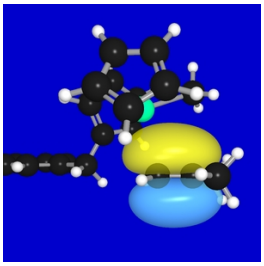


Figure S3: C1($sp^{62.51}$)-C2($sp^{99.99}$) orbital

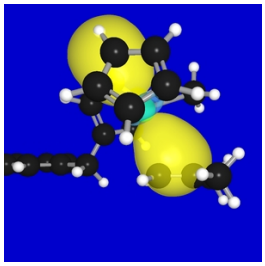


Figure S4: empty Zr($sd^{20.37}$) orbital

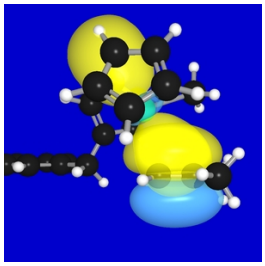
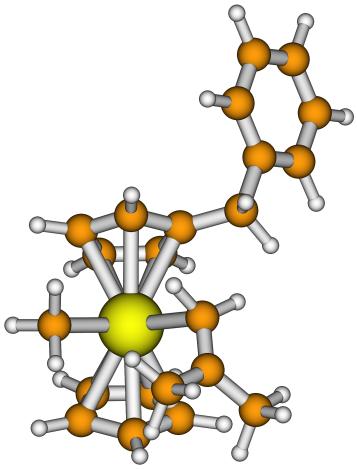


Figure S5: C1-C2 -> Zr

Cartesian Coordinates for **7**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.339403	0.140456	0.317484
2	6	0	5.712343	0.260537	-0.925451
3	6	0	4.348194	0.541020	-0.997012
4	6	0	3.593299	0.705027	0.172246
5	6	0	4.229578	0.585382	1.412791
6	6	0	5.595856	0.304861	1.486570
7	6	0	2.100552	1.006279	0.094990
8	6	0	1.304592	-0.197055	-0.365575
9	6	0	0.819762	-0.444062	-1.684430
10	6	0	0.301440	-1.764224	-1.744868
11	6	0	0.415831	-2.330635	-0.449341
12	6	0	1.023519	-1.359605	0.402011
13	40	0	-1.286257	-0.524978	-0.204521
14	6	0	-2.482801	-0.764368	-2.126460
15	6	0	-3.477178	-0.296614	1.110890
16	6	0	-2.427998	-0.226570	2.074385
17	6	0	-1.774397	-1.479762	2.101983
18	6	0	-2.413082	-2.327656	1.148840
19	6	0	-3.478539	-1.598951	0.555644
20	1	0	0.885842	0.245906	-2.518046
21	1	0	-4.180785	0.489825	0.872193
22	1	0	0.147926	-3.341128	-0.169289
23	1	0	-0.951603	-1.755552	2.748424
24	1	0	1.305095	-1.511070	1.436640
25	1	0	-2.175302	-3.367070	0.963003
26	1	0	-0.103727	-2.249824	-2.622035
27	1	0	-2.184234	0.628014	2.693868
28	1	0	1.759067	1.332479	1.085720
29	1	0	1.928203	1.841024	-0.595929
30	1	0	3.870854	0.640330	-1.969626
31	1	0	3.659244	0.724471	2.329134
32	1	0	6.286973	0.141347	-1.839507
33	1	0	6.077676	0.221256	2.456517
34	1	0	7.402476	-0.074565	0.372785
35	1	0	-4.168531	-1.974434	-0.187267
36	1	0	-1.942782	-0.320263	-2.974214
37	1	0	-2.695673	-1.806684	-2.398427
38	1	0	-3.453023	-0.257551	-2.030141
39	6	0	-1.169412	2.071815	-0.515223
40	1	0	-0.317868	2.172964	0.158327
41	1	0	-0.945482	1.880694	-1.565242
42	6	0	-2.368240	2.625298	-0.170455
43	6	0	-2.606802	3.205287	1.194037
44	1	0	-2.748609	4.290012	1.095669
45	1	0	-3.530378	2.818559	1.641124
46	1	0	-1.772090	3.034666	1.878458

47	6	0	-3.480921	2.783662	-1.165914
48	1	0	-4.434331	2.421567	-0.763007
49	1	0	-3.623265	3.853993	-1.368705
50	1	0	-3.275416	2.279443	-2.112464

Bader Analysis of **7**

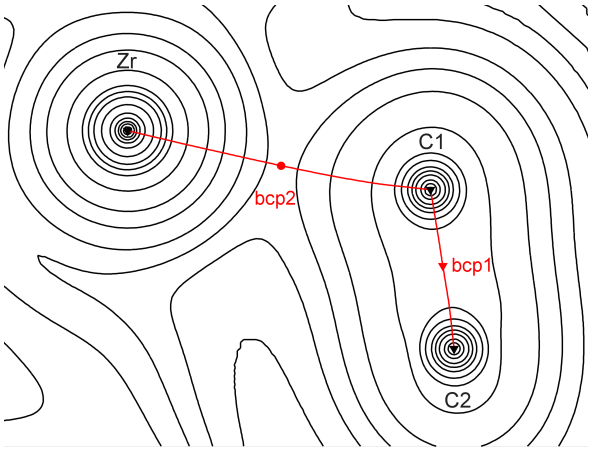
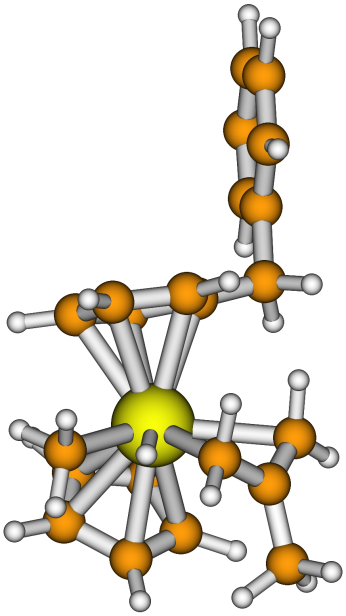


*Figure S6: Electron Density Plot of **7**, view along the Zr-C1-C2 plane*

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.3305	0.23689
bcp2	0.0348	-0.02124

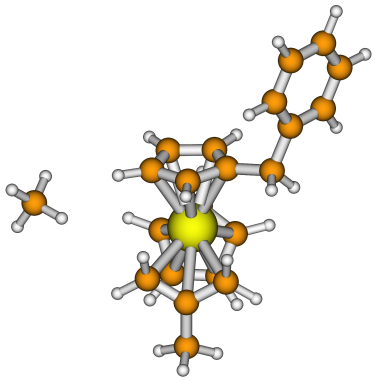
Cartesian Coordinates for **TS7-8**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.389954	-1.116782	-0.976962
2	6	0	2.369433	-0.971726	-1.953479
3	6	0	1.302288	-1.836607	-1.610775
4	6	0	1.686289	-2.559507	-0.439075
5	6	0	2.972480	-2.117987	-0.055601
6	40	0	1.362566	-0.155313	0.273969
7	6	0	2.546507	2.128506	0.691458
8	6	0	2.351443	2.116722	-0.754907
9	6	0	3.571128	2.196682	-1.638561
10	6	0	-1.219693	0.202913	0.308975
11	6	0	-0.680069	0.978326	1.382671
12	6	0	-0.117372	0.104068	2.343902
13	6	0	-0.263307	-1.222416	1.861421
14	6	0	-0.945252	-1.156914	0.613663
15	6	0	-2.093833	0.699777	-0.823903
16	6	0	-3.565761	0.396145	-0.569174
17	6	0	-4.289173	1.127986	0.382153
18	6	0	-5.630821	0.838554	0.629402
19	6	0	-6.267652	-0.187465	-0.073402
20	6	0	-5.556728	-0.918193	-1.026066
21	6	0	-4.212832	-0.627006	-1.271361
22	6	0	2.903575	-0.234423	2.289678
23	6	0	1.088177	1.953687	-1.285100
24	1	0	-0.752291	2.055884	1.476691
25	1	0	2.395161	-0.316194	-2.812642
26	1	0	0.042355	-2.125527	2.375129
27	1	0	1.110037	-3.336107	0.046463
28	1	0	-1.262166	-2.005390	0.020797
29	1	0	3.548120	-2.490038	0.780707
30	1	0	0.337516	0.394524	3.281309
31	1	0	0.386525	-1.969766	-2.172714
32	1	0	-1.790010	0.236154	-1.769867
33	1	0	-1.957701	1.781331	-0.943770
34	1	0	-3.805054	1.934472	0.929201
35	1	0	-3.670075	-1.192300	-2.026578
36	1	0	-6.180701	1.417513	1.365890
37	1	0	-6.047465	-1.710443	-1.584187
38	1	0	-7.313362	-0.410645	0.116583
39	1	0	4.349409	-0.617055	-0.971862
40	1	0	2.784706	0.442698	3.142264
41	1	0	2.513655	-1.208206	2.595458
42	1	0	3.970346	-0.340176	2.071301
43	1	0	0.949107	1.869771	-2.358876
44	1	0	0.214353	2.254614	-0.720804
45	1	0	3.829427	3.259678	-1.739481
46	1	0	4.443588	1.700567	-1.204355

47	1	0	3.392546	1.810337	-2.645036
48	1	0	3.540895	2.448545	1.011239
49	1	0	1.769642	2.639925	1.263501
50	1	0	2.666117	0.922315	1.365133

Cartesian Coordinates for **8**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.355784	0.387850	0.293540
2	6	0	-5.737608	0.662863	-0.929238
3	6	0	-4.441607	0.211021	-1.175897
4	6	0	-3.747259	-0.521885	-0.203824
5	6	0	-4.374681	-0.795563	1.016849
6	6	0	-5.672800	-0.343682	1.265672
7	6	0	-2.325382	-1.001793	-0.467880
8	6	0	-1.332934	0.143690	-0.461445
9	6	0	-0.625826	0.664833	-1.579207
10	6	0	0.112507	1.810904	-1.170565
11	6	0	-0.123394	2.002471	0.214616
12	6	0	-0.997092	0.964453	0.656728
13	40	0	1.180978	-0.125615	0.082508
14	6	0	3.896344	4.081742	-0.642819
15	6	0	3.386908	-0.378513	1.317455
16	6	0	2.577244	-1.473411	1.725489
17	6	0	1.469947	-0.953075	2.452885
18	6	0	1.606401	0.459398	2.508578
19	6	0	2.779239	0.818264	1.790269
20	1	0	-0.672426	0.269446	-2.587293
21	1	0	4.320558	-0.440687	0.775669
22	1	0	0.261859	2.813026	0.820552
23	1	0	0.683751	-1.535624	2.919806
24	1	0	-1.413048	0.865799	1.652013
25	1	0	0.938897	1.142820	3.016666
26	1	0	0.723954	2.439167	-1.807029
27	1	0	2.782294	-2.521048	1.553480
28	1	0	-2.057924	-1.746961	0.292294
29	1	0	-2.271930	-1.511398	-1.437648
30	1	0	-3.971237	0.424157	-2.133555
31	1	0	-3.854141	-1.379250	1.773815
32	1	0	-6.267362	1.224676	-1.693183
33	1	0	-6.150244	-0.570158	2.214719
34	1	0	-7.366380	0.737072	0.483656
35	1	0	3.165411	1.822485	1.660354
36	1	0	3.700515	4.757741	-1.478922
37	1	0	3.385211	4.454328	0.249932
38	1	0	4.972325	4.040360	-0.455483
39	6	0	1.157185	-2.198684	-1.264776
40	1	0	1.070724	-3.206513	-0.865034
41	1	0	0.308757	-1.885969	-1.870591
42	6	0	2.439424	-1.695983	-1.580590
43	6	0	3.665234	-2.529046	-1.305715
44	1	0	3.913378	-3.048585	-2.241166
45	1	0	4.537449	-1.927485	-1.036010
46	1	0	3.496605	-3.299882	-0.548869

47	6	0	2.575588	-0.339551	-1.954827
48	1	0	3.573968	0.072461	-2.082383
49	1	0	1.828050	0.097398	-2.612840
50	1	0	3.531957	3.079423	-0.895078

Bader analysis of **8**

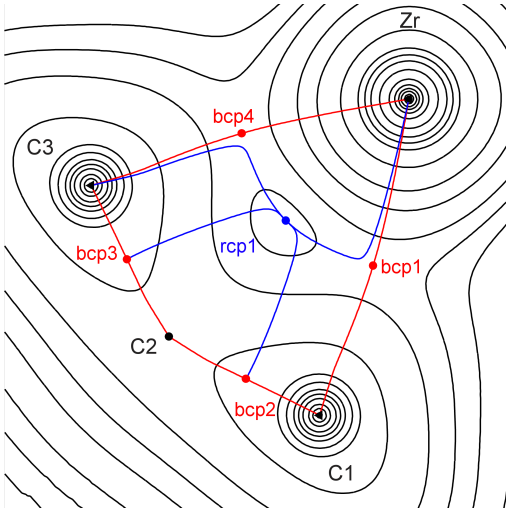


*Figure S7: Electron Density Plot of **8**, with Zr, C1 and C3 in plane and C2 below plane*

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.0565	-0.02090
bcp2	0.3011	0.19716
bcp3	0.3009	0.19723
bcp4	0.0560	-0.02062
rcp1	0.0353	-0.03959

NBO Analysis of **8**

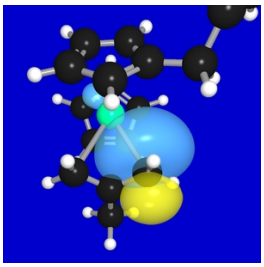


Figure S8: Zr-C1 bond, 16.41% Zr($sd^{3.52}$) and 83.59% C1($sp^{9.68}$)

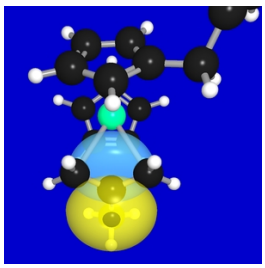


Figure S9: empty C2(p) orbital

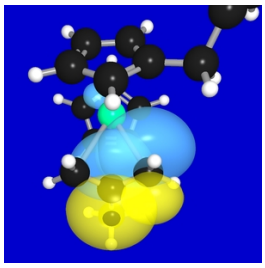


Figure S10: Zr-C1 -> C2, 548.97 kJ/mol

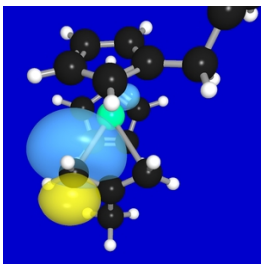


Figure S11: Zr-C3 bond, 16.67% Zr($sd^{3.50}$) and 83.33% C3($sp^{9.50}$)

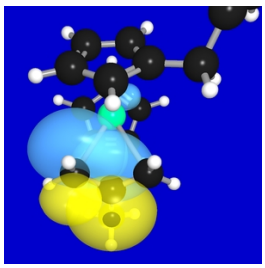
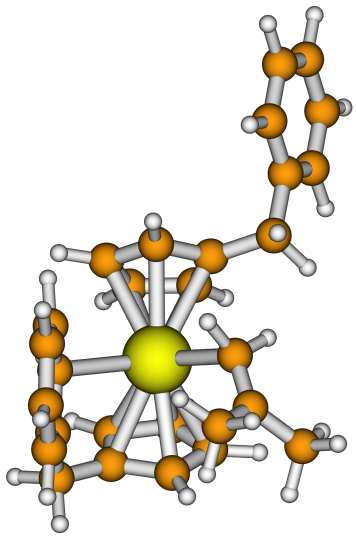


Figure S12: ZrC3 -> C2, 557.47 kJ/mol

Cartesian Coordinates for **9**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.837499	3.145019	-1.156819
2	6	0	-4.057952	2.756623	-0.587762
3	6	0	-4.440140	1.409411	-0.540221
4	6	0	-3.616041	0.423516	-1.082085
5	6	0	-2.366003	0.812073	-1.639997
6	6	0	-2.000223	2.177047	-1.704684
7	6	0	-3.980093	-1.050959	-1.068173
8	6	0	-2.844309	-1.823173	-0.442250
9	6	0	-2.498572	-1.811715	0.936157
10	6	0	-1.313673	-2.585789	1.111681
11	6	0	-0.913164	-3.065608	-0.158613
12	6	0	-1.835549	-2.569625	-1.124897
13	40	0	-0.632033	-0.563936	-0.242005
14	6	0	1.931568	-0.037598	-0.178965
15	6	0	1.314668	0.893798	-1.066778
16	6	0	0.804174	0.183009	-2.191330
17	6	0	1.025074	-1.198733	-1.975360
18	6	0	1.687796	-1.338280	-0.715693
19	6	0	2.821990	0.291639	0.997819
20	6	0	4.270073	0.400098	0.527174
21	6	0	5.103415	-0.726016	0.533944
22	6	0	6.423149	-0.627567	0.092076
23	6	0	6.918538	0.596400	-0.363489
24	6	0	6.093140	1.723657	-0.370439
25	6	0	4.773506	1.625468	0.071086
26	6	0	-0.419395	0.796240	1.883561
27	6	0	-1.423034	0.753738	2.823902
28	6	0	-1.398461	-0.231297	3.950996
29	6	0	-2.536056	1.753228	2.832109
30	1	0	1.336899	1.971875	-0.956538
31	1	0	-3.080586	-1.350471	1.723144
32	1	0	0.796569	-1.999719	-2.667222
33	1	0	-0.079969	-3.727112	-0.356351
34	1	0	2.071053	-2.264253	-0.304191
35	1	0	-1.830897	-2.802425	-2.183673
36	1	0	0.360688	0.623063	-3.077091
37	1	0	-0.832077	-2.815229	2.055027
38	1	0	2.743341	-0.489788	1.763749
39	1	0	-4.904438	-1.212722	-0.505321
40	1	0	2.511725	1.238863	1.453012
41	1	0	-4.165075	-1.409209	-2.088016
42	1	0	4.732093	-1.678613	0.906949
43	1	0	-5.401874	1.136810	-0.114790
44	1	0	4.143672	2.512931	0.082397
45	1	0	-1.868893	0.109001	-2.325558
46	1	0	7.066520	-1.501934	0.114048

47	1	0	-4.731336	3.513762	-0.195533
48	1	0	6.479746	2.680321	-0.708458
49	1	0	-1.089834	2.474316	-2.216235
50	1	0	7.947243	0.674101	-0.701658
51	1	0	-2.569922	4.195447	-1.211531
52	1	0	-3.510487	1.266447	2.958950
53	1	0	-2.412287	2.403003	3.710807
54	1	0	-2.550498	2.384177	1.941395
55	1	0	-1.256945	0.322844	4.890215
56	1	0	-2.358835	-0.750130	4.059343
57	1	0	-0.589464	-0.961019	3.869293
58	1	0	-0.299391	1.710156	1.294186
59	1	0	0.502981	0.255325	2.112150

Bader Analysis of **9**

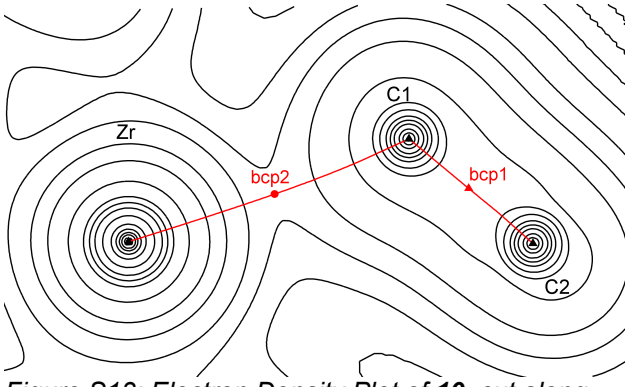
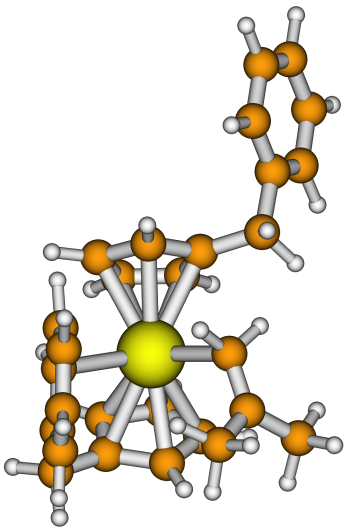


*Figure S13: Electron Density Plot of **10**, cut along the Zr-C1-C2 plane*

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.3247	0.23111
bcp2	0.0438	-0.02317

Cartesian Coordinates for **10**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.669813	3.267287	0.189871
2	6	0	-3.891106	2.727981	0.558718
3	6	0	-4.313173	1.499549	0.075649
4	6	0	-3.524395	0.795649	-0.807753
5	6	0	-2.283136	1.336373	-1.177502
6	6	0	-1.873721	2.583960	-0.702874
7	6	0	-3.899887	-0.543546	-1.356430
8	6	0	-2.781384	-1.478664	-1.054905
9	6	0	-2.444331	-1.950118	0.223290
10	6	0	-1.262659	-2.715258	0.119067
11	6	0	-0.856186	-2.700938	-1.218349
12	6	0	-1.772772	-1.909734	-1.941342
13	40	0	-0.626197	-0.383564	-0.407769
14	6	0	1.854274	0.119507	-0.142306
15	6	0	1.230741	1.273979	-0.650998
16	6	0	0.750111	0.989189	-1.945679
17	6	0	1.004386	-0.359483	-2.215851
18	6	0	1.656324	-0.906616	-1.086940
19	6	0	2.709539	0.037294	1.072264
20	6	0	4.142935	0.216004	0.664846
21	6	0	4.943788	-0.886112	0.429784
22	6	0	6.251979	-0.719727	0.024214
23	6	0	6.763388	0.550294	-0.151149
24	6	0	5.966816	1.654051	0.082709
25	6	0	4.659651	1.486792	0.488093
26	6	0	-0.429415	0.157775	1.969290
27	6	0	-1.407380	-0.454124	2.689555
28	6	0	-1.184882	-1.767289	3.322171
29	6	0	-2.692537	0.209558	2.970944
30	1	0	1.223205	2.241087	-0.166689
31	1	0	-3.038362	-1.806175	1.113404
32	1	0	0.793117	-0.876251	-3.140494
33	1	0	-0.009268	-3.227775	-1.631306
34	1	0	2.061776	-1.905822	-1.011397
35	1	0	-1.759580	-1.740213	-3.009617
36	1	0	0.295548	1.695616	-2.627149
37	1	0	-0.776569	-3.251229	0.922515
38	1	0	2.592669	-0.933158	1.564033
39	1	0	-4.829620	-0.899095	-0.910444
40	1	0	2.427198	0.814193	1.787669
41	1	0	-4.069410	-0.483948	-2.434342
42	1	0	4.552687	-1.885605	0.588396
43	1	0	-5.279387	1.106488	0.367596
44	1	0	4.042423	2.356467	0.687716
45	1	0	-1.796214	0.929444	-2.077265
46	1	0	6.878909	-1.585131	-0.144341

47	1	0	-4.537993	3.283835	1.226576
48	1	0	6.370348	2.650116	-0.041351
49	1	0	-0.956370	3.030871	-1.065191
50	1	0	7.791111	0.681379	-0.462230
51	1	0	-2.370393	4.239217	0.558307
52	1	0	-3.539033	-0.476224	2.892070
53	1	0	-2.673358	0.534584	4.017924
54	1	0	-2.861774	1.087110	2.349485
55	1	0	-1.212678	-1.632785	4.409066
56	1	0	-1.993026	-2.468519	3.096724
57	1	0	-0.224073	-2.210416	3.065007
58	1	0	-0.519026	1.226930	1.756794
59	1	0	0.582083	-0.234236	2.058988

Bader Analysis of **10**

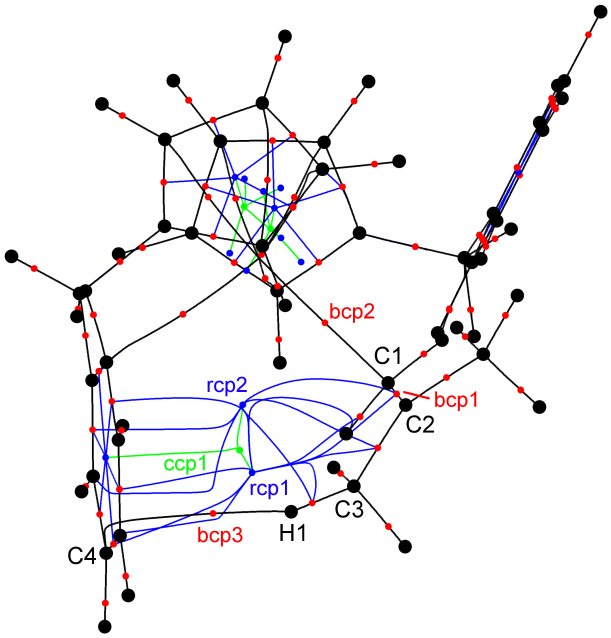


*Figure S14: Molecular representation of **10**. Atoms are drawn in black, bond critical points in red and bonding paths in black, ring critical points and paths in blue and cage critical points and paths in green. View from the top of the molecule*

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.3363	0.25629
bcp2	0.0527	-0.02662
bcp3	0.0089	-0.00696
rcp1	0.0025	-0.00209
rcp2	0.0030	-0.00233
ccp1	0.0024	-0.00230

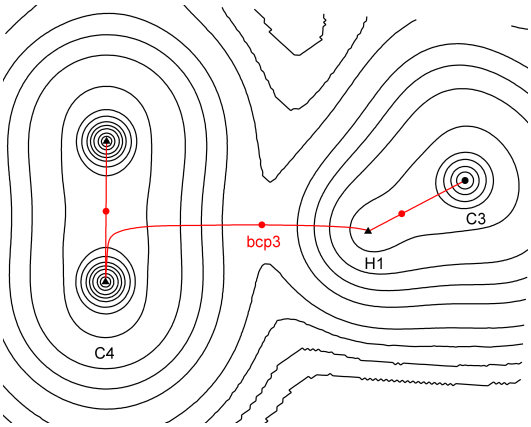


Figure S15: Electron Density Map of Me-arene interaction

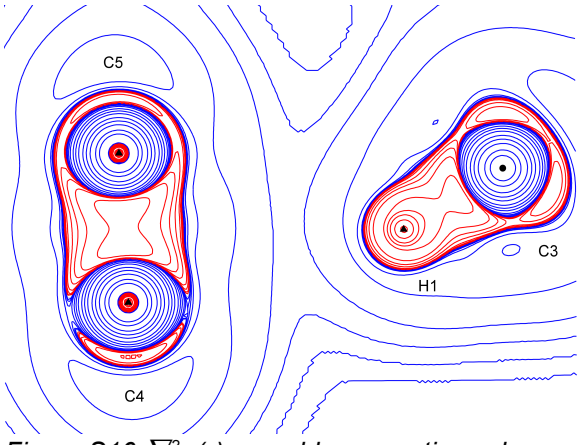
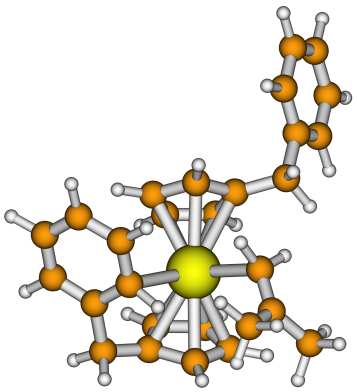


Figure S16: $\nabla^2\rho(\boldsymbol{r})$ map: blue: negative values; red: positive values; standard values used

Cartesian Coordinates for **11**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.314390	-3.089635	1.980090
2	6	0	2.238997	-1.703144	2.080710
3	6	0	2.734023	-0.889358	1.035757
4	6	0	3.362934	-1.474795	-0.100007
5	6	0	3.398832	-2.871285	-0.193527
6	6	0	2.894870	-3.666885	0.841764
7	6	0	3.983224	-0.576198	-1.161692
8	6	0	2.923193	0.375387	-1.659625
9	6	0	2.652186	1.683213	-1.170194
10	6	0	1.470365	2.166139	-1.805877
11	6	0	0.992765	1.153295	-2.671291
12	6	0	1.873262	0.035527	-2.564396
13	40	0	0.757455	0.207518	-0.354428
14	6	0	-1.787197	-0.169829	0.042562
15	6	0	-1.061496	-1.142373	0.792154
16	6	0	-0.377099	-2.004116	-0.115607
17	6	0	-0.628201	-1.541660	-1.429770
18	6	0	-1.461946	-0.385984	-1.331968
19	6	0	-2.822005	0.800766	0.567357
20	6	0	-4.222333	0.242174	0.332359
21	6	0	-4.976052	0.666840	-0.769441
22	6	0	-6.252649	0.148551	-0.991305
23	6	0	-6.783249	-0.801271	-0.115571
24	6	0	-6.036694	-1.227982	0.985873
25	6	0	-4.760706	-0.710382	1.207973
26	6	0	0.311169	1.881039	1.528957
27	6	0	1.233909	2.883564	1.718053
28	6	0	1.094020	4.218184	1.054066
29	6	0	2.377824	2.732352	2.673269
30	1	0	-1.101370	-1.263566	1.868528
31	1	0	3.281097	2.239627	-0.485762
32	1	0	-0.293987	-2.009584	-2.346574
33	1	0	0.146877	1.234703	-3.341369
34	1	0	-1.893872	0.154350	-2.165237
35	1	0	1.811628	-0.877696	-3.143097
36	1	0	0.218015	-2.867454	0.153879
37	1	0	1.036938	3.151175	-1.686225
38	1	0	-2.733964	1.767428	0.056337
39	1	0	4.830790	-0.022443	-0.741497
40	1	0	-2.659669	0.974435	1.637477
41	1	0	4.373825	-1.177626	-1.987566
42	1	0	-4.579248	1.423825	-1.443439
43	1	0	2.909203	0.171259	1.241167
44	1	0	-4.193706	-1.035594	2.078007
45	1	0	3.875760	-3.341451	-1.048978
46	1	0	-6.835974	0.494863	-1.839123

47	1	0	1.838784	-1.244011	2.980673
48	1	0	-6.451920	-1.955536	1.676663
49	1	0	2.977726	-4.747727	0.770039
50	1	0	-7.778663	-1.200203	-0.284780
51	1	0	1.953726	-3.719256	2.787445
52	1	0	3.330403	3.020997	2.211629
53	1	0	2.232323	3.433448	3.507479
54	1	0	2.459468	1.727720	3.095645
55	1	0	0.927836	4.977068	1.831938
56	1	0	2.019628	4.516910	0.546265
57	1	0	0.254723	4.266359	0.356654
58	1	0	0.271403	1.067042	2.257689
59	1	0	-0.643988	2.147424	1.069191

Bader Analysis of **11**

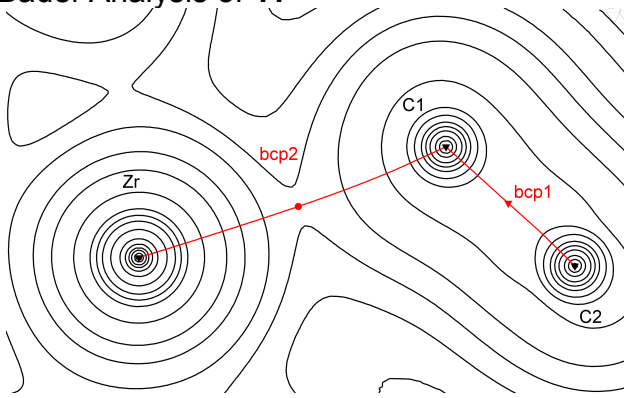
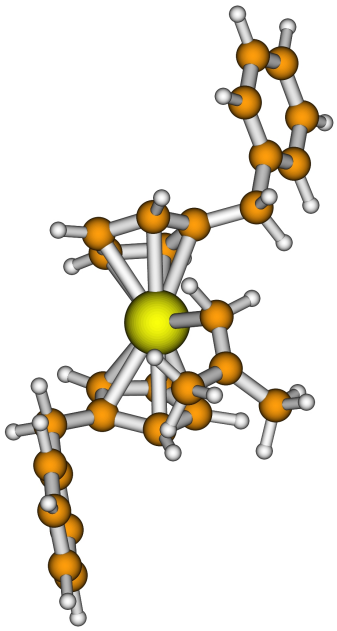


*Figure S17: Electron Density Map of **11**, Zr, C1 and C2 in plane*

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.3248	0.23097
bcp2	0.0417	-0.0223

Cartesian Coordinates for **12**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.920681	0.390280	-0.055919
2	6	0	-6.462269	-0.604188	0.813094
3	6	0	-5.239635	-1.233104	0.576593
4	6	0	-4.459249	-0.872315	-0.533173
5	6	0	-4.927565	0.122050	-1.401903
6	6	0	-6.154315	0.750121	-1.166354
7	6	0	-3.145854	-1.582079	-0.807054
8	6	0	-2.126063	-1.457540	0.310668
9	6	0	-2.037277	-0.405143	1.274819
10	6	0	-0.948875	-0.682388	2.153180
11	6	0	-0.333843	-1.888030	1.724833
12	6	0	-1.055570	-2.360093	0.583054
13	40	0	0.055171	-0.253753	-0.096789
14	6	0	2.548341	0.063896	-0.467647
15	6	0	1.898894	0.277051	-1.719091
16	6	0	1.307133	-0.953484	-2.145700
17	6	0	1.563840	-1.929200	-1.151059
18	6	0	2.287876	-1.296928	-0.094399
19	6	0	3.414818	1.046819	0.290517
20	6	0	4.871896	0.601688	0.216279
21	6	0	5.505366	0.057662	1.341139
22	6	0	6.837742	-0.350694	1.267371
23	6	0	7.541776	-0.226731	0.066743
24	6	0	6.913216	0.312409	-1.059619
25	6	0	5.582154	0.720555	-0.987989
26	6	0	-0.205369	2.247647	-0.208292
27	6	0	-1.392884	2.723407	0.311834
28	6	0	-1.526538	3.098872	1.754105
29	6	0	-2.577217	2.973359	-0.565702
30	1	0	1.926418	1.196518	-2.292464
31	1	0	-2.750671	0.400796	1.374732
32	1	0	1.297201	-2.976918	-1.202824
33	1	0	0.481532	-2.400777	2.219623
34	1	0	2.701982	-1.794789	0.774224
35	1	0	-0.879225	-3.295908	0.066901
36	1	0	0.792570	-1.121677	-3.086958
37	1	0	-0.660737	-0.094990	3.018915
38	1	0	3.112873	1.101852	1.344688
39	1	0	-3.308158	-2.654050	-0.984789
40	1	0	3.290668	2.048457	-0.137859
41	1	0	-2.725369	-1.204258	-1.755481
42	1	0	4.970009	-0.020569	2.285364
43	1	0	-4.905976	-2.023403	1.245904
44	1	0	5.105566	1.152795	-1.865373
45	1	0	-4.354036	0.381840	-2.290306
46	1	0	7.328388	-0.753823	2.148026



47	1	0	-7.064289	-0.901395	1.666470
48	1	0	7.461997	0.421608	-1.990005
49	1	0	-6.517519	1.503765	-1.858839
50	1	0	8.579103	-0.541948	0.010650
51	1	0	-7.877983	0.869985	0.123305
52	1	0	-3.451213	2.396132	-0.235845
53	1	0	-2.867036	4.029797	-0.477725
54	1	0	-2.381947	2.756847	-1.618780
55	1	0	-1.540798	4.197750	1.812360
56	1	0	-2.480490	2.768149	2.180073
57	1	0	-0.696544	2.748664	2.373169
58	1	0	-0.058260	2.322354	-1.288280
59	1	0	0.706033	2.373941	0.390722

Bader Analysis of **12**

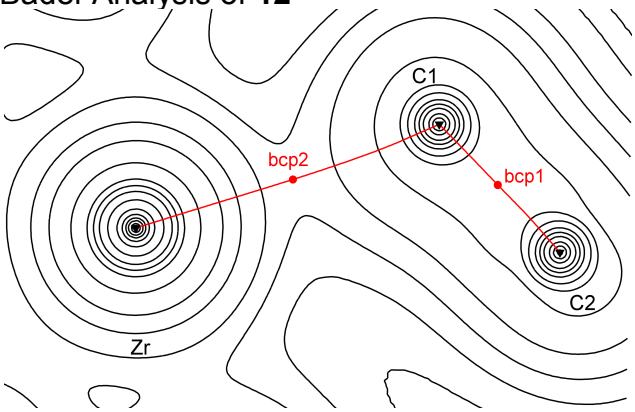


*Figure S18: Electron Density Map of **12**, Zr, C1 and C2 in plane*

	$\rho(\boldsymbol{r})$	$\nabla^2\rho(\boldsymbol{r})$
bcp1	0.3220	0.22757
bcp2	0.0464	-0.02409