SUPPORTING INFORMATION

Links Between Single-Site Heterogeneous and Homogeneous Catalysis. DFT Analysis of Pathways for Organozirconium Catalyst Chemisorptive Activation and Olefin Polymerization on γ-Alumina

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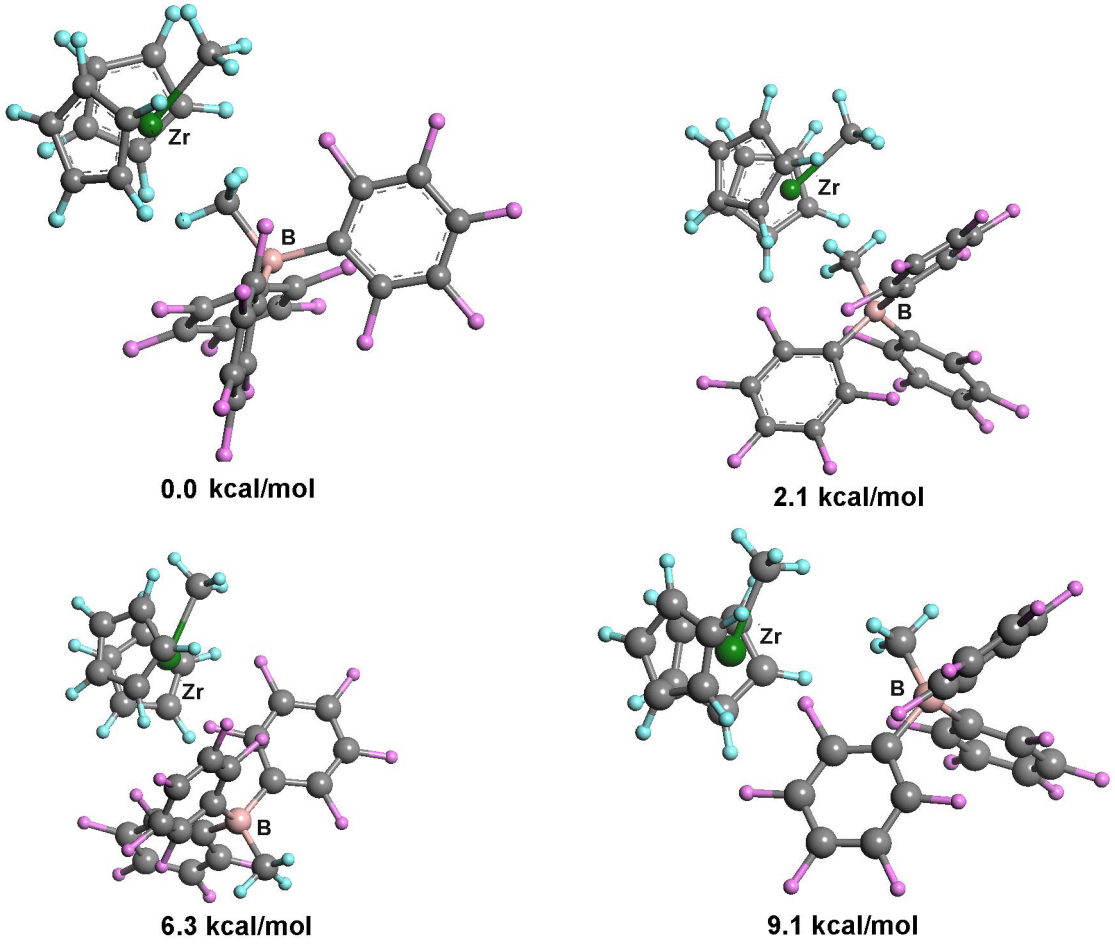

Figure S1. Possible cation - counteranion orientations in the homogeneous ion pair $Cp_2ZrCH_3^+H_3CB(C_6F_5)_3^-$ system. The energy scale refers to the most stable configuration.

Cartesian coordinates (Å) of optimized structures of key species investigated.

For all periodic calculations the lattice parameters are:
a = 16.826 Å; b = 16.136 Å; c = 50.000 Å;
$\alpha = \beta = \gamma = 90.00°$

Alumina (100) surface.

Al	1.176350	5.234075	0.229111
O	3.973576	7.522878	2.896063
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.309830	1.087695	2.475199
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.165919	2.839081	3.027007
Al	8.268006	3.298270	1.704362
Al	4.175445	1.087695	2.475199
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.319355	2.839081	3.027007
Al	4.308924	5.234075	0.229111
O	1.511698	7.522878	2.896063
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.949141	1.053944	2.713886
Al	6.949156	6.392276	1.639649
O	6.949259	7.457111	3.100296
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.742637	3.771177	2.481012
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949162	2.874832	2.976102
Al	1.176350	13.302075	0.229111
O	3.973814	15.590975	2.896048
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.309865	9.155621	2.475197
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.165870	10.906964	3.027019
Al	8.267993	11.366301	1.704330
Al	4.175411	9.155621	2.475198
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.319405	10.906964	3.027019
Al	4.308924	13.302075	0.229111
O	1.511461	15.590976	2.896048
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.949140	9.121949	2.713893
Al	6.949131	14.460329	1.639677
O	6.949382	15.525131	3.100318
O	6.949137	15.422509	0.120803

Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.742637	11.839086	2.481008
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.949148	10.942833	2.976095
Al	9.589350	5.234075	0.229111
O	12.386484	7.522909	2.896168
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.722853	1.087598	2.475253
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578845	2.838988	3.027011
Al	16.680960	3.298306	1.704311
Al	12.588422	1.087598	2.475253
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732429	2.838988	3.027011
Al	12.721924	5.234075	0.229111
O	9.924791	7.522910	2.896168
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.362133	1.053944	2.713886
Al	15.362120	6.392276	1.639649
O	15.362016	7.457111	3.100295
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.155637	3.771239	2.481145
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362112	2.874832	2.976102
Al	9.589350	13.302075	0.229111
O	12.386499	15.590863	2.896077
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.722880	9.155667	2.475242
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.578844	10.907042	3.027006
Al	16.680957	11.366316	1.704306
Al	12.588395	9.155666	2.475243
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.732432	10.907042	3.027005
Al	12.721924	13.302075	0.229111
O	9.924774	15.590862	2.896076
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.362135	9.121949	2.713893
Al	15.362144	14.460329	1.639677
O	15.361892	15.525132	3.100318
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837

Al	11.155638	11.839248	2.481035
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.362127	10.942833	2.976095

Zirconocenium precatalyst $Cp_2Zr(CH_3)_2$ system.

C	9.774452	8.563090	17.141600
C	9.249497	9.544078	16.244276
C	7.809731	9.375539	18.044120
C	8.034608	10.037325	16.797239
C	8.886356	8.468224	18.259656
H	10.712878	8.025618	17.018792
H	9.705732	9.861616	15.310231
H	6.965589	9.544706	18.709567
H	7.378421	10.778874	16.344079
H	9.026456	7.831082	19.130942
Zr	7.621237	7.526723	16.229568
C	5.392350	8.109118	16.405336
H	5.256420	9.180860	16.179864
H	4.960422	7.920236	17.405464
H	4.798015	7.531406	15.674793
C	7.079985	5.130395	15.368572
C	6.464119	5.248876	16.645321
C	8.754996	5.321747	16.944903
C	7.497070	5.384778	17.623743
C	8.495614	5.173804	15.549736
H	6.564359	5.019559	14.417672
H	5.396172	5.235168	16.847000
H	9.737712	5.363440	17.410367
H	7.346851	5.483072	18.697385
H	9.245152	5.098904	14.764106
C	7.923685	7.937218	13.973028
H	7.266859	7.281866	13.375356
H	7.660972	8.984211	13.738088
H	8.961410	7.769147	13.632960

Dioxo-bridged zirconocenium coordination on a μ_3-0 alumina surface site.

Al	1.176350	5.234075	0.229111
O	3.961759	7.510529	2.918763
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.307135	1.083653	2.471579
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.162633	2.833468	3.028920
Al	8.268006	3.298270	1.704362
Al	4.177873	1.082957	2.471093
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.320377	2.834675	3.028767
Al	4.308924	5.234075	0.229111
O	1.471130	7.468610	2.843290
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951297	1.051068	2.712415
Al	6.949156	6.392276	1.639649
O	6.937314	7.456024	3.102096
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741608	3.757933	2.456380
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.948528	2.873030	2.978749
Al	1.176350	13.302075	0.229111
O	3.995768	15.583991	2.878593
O	8.279908	13.177620	1.489022

O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.300841	9.099858	2.447577
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.099907	10.856418	3.072297
Al	8.267993	11.366301	1.704330
Al	4.193402	9.113233	2.454118
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.415535	10.840983	3.121230
Al	4.308924	13.302075	0.229111
O	1.501287	15.587988	2.882698
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.975839	9.122564	2.716362
Al	6.949131	14.460329	1.639677
O	6.945592	15.522868	3.105908
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.753138	11.792915	2.348405
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.918261	10.945745	2.976896
Al	9.589350	5.234075	0.229111
O	12.378242	7.568625	2.901000
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.725173	1.098584	2.473533
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578662	2.847536	3.029191
Al	16.680960	3.298306	1.704311
Al	12.584500	1.099997	2.473108
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.731492	2.846665	3.029328
Al	12.721924	5.234075	0.229111
O	9.934314	7.567250	2.900991
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.359537	1.049050	2.712109
Al	15.362120	6.392276	1.639649
O	15.369554	7.457114	3.107086
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.154683	3.770564	2.472500
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.361791	2.871535	2.979000
Al	9.589350	13.302075	0.229111
O	12.389513	15.610543	2.904591
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.750967	9.219669	2.474591
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.609016	10.926036	3.021273
Al	16.680957	11.366316	1.704306
Al	12.556471	9.221557	2.475885
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.711309	10.923483	3.019922

Al	12.721924	13.302075	0.229111
O	9.929051	15.610684	2.906524
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.330167	9.119256	2.706264
Al	15.362144	14.460329	1.639677
O	15.375908	15.519206	3.106982
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.155359	12.139128	3.116457
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.403745	10.940850	2.986259
C	0.724754	9.655909	6.700148
C	1.182664	8.754714	5.696828
C	2.883034	9.000759	7.231619
C	2.526461	8.377434	5.998439
C	1.780774	9.799212	7.660474
H	16.557249	10.094457	6.762091
H	0.602846	8.321850	4.882544
H	3.825558	8.878937	7.756541
H	3.135328	7.706324	5.393912
H	1.717746	10.349599	8.595240
Zr	2.628025	10.929614	5.569512
C	4.895719	10.626383	5.973302
C	11.155008	13.081741	4.841814
H	5.159400	9.590432	5.695547
H	5.197991	10.767945	7.023347
H	5.476081	11.318268	5.347833
H	12.037483	13.732333	4.937936
H	10.261596	13.717018	4.941175
H	11.160278	12.339210	5.661708
C	3.014780	13.451923	5.060538
C	3.576852	13.156726	6.340426
C	1.279210	12.874452	6.475407
C	2.511379	12.794302	7.215827
C	1.592103	13.305598	5.160443
H	3.553596	13.921370	4.233077
H	4.625670	13.256121	6.605806
H	0.276635	12.708290	6.864399
H	2.614063	12.575781	8.276169
H	0.880254	13.541527	4.373625

Oxo-bridged zirconocenium coordination on a μ_3-0 alumina surface site.

Al	1.176350	5.234075	0.229111
O	4.037454	7.461277	2.833725
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.305726	1.080541	2.475671
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.163895	2.835504	3.028452
Al	8.268006	3.298270	1.704362
Al	4.173860	1.085524	2.470228
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.320804	2.833760	3.028405
Al	4.308924	5.234075	0.229111
O	1.548357	7.546428	2.937447
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951224	1.049142	2.708833
Al	6.949156	6.392276	1.639649
O	6.951648	7.443958	3.115775
O	6.949137	7.354509	0.120803

Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.740543	3.759495	2.459802
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949037	2.870023	2.980547
Al	1.176350	13.302075	0.229111
O	3.999554	15.585175	2.878712
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.290746	9.146147	2.467404
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.166223	10.884062	3.125461
Al	8.267993	11.366301	1.704330
Al	4.189704	9.092712	2.439204
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.340036	10.895942	3.031696
Al	4.308924	13.302075	0.229111
O	1.517726	15.588953	2.903966
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.980963	9.098131	2.695390
Al	6.949131	14.460329	1.639677
O	6.939626	15.516977	3.107560
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.732613	11.803543	2.406878
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.887648	10.927816	2.998737
Al	9.589350	5.234075	0.229111
O	12.373199	7.565886	2.900511
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.728340	1.100916	2.472378
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578695	2.845340	3.029474
Al	16.680960	3.298306	1.704311
Al	12.587089	1.097138	2.473563
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.731297	2.848338	3.028784
Al	12.721924	5.234075	0.229111
O	9.927882	7.573233	2.903699
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.359479	1.055091	2.710003
Al	15.362120	6.392276	1.639649
O	15.371846	7.454013	3.100697
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.157151	3.769526	2.470397
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.361771	2.872888	2.977310
Al	9.589350	13.302075	0.229111
O	12.380142	15.610086	2.906356
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507

Al	14.043282	11.366301	1.704330
Al	9.758375	9.225802	2.477835
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.585722	10.922030	3.019211
Al	16.680957	11.366316	1.704306
Al	12.563340	9.217839	2.474128
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.686595	10.934007	3.017645
Al	12.721924	13.302075	0.229111
O	9.914637	15.610641	2.902366
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.339989	9.120647	2.712421
Al	15.362144	14.460329	1.639677
O	15.368061	15.527655	3.102131
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.153904	12.142663	3.109853
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.382119	10.939436	2.981047
C	2.993771	9.715815	6.619863
C	3.473213	8.838145	5.606231
C	5.138825	9.053899	7.186629
C	4.811814	8.460688	5.928657
C	4.022590	9.827447	7.616149
H	1.993806	10.140637	6.674441
H	2.904421	8.431399	4.769607
H	6.070077	8.917458	7.729274
H	5.428269	7.769924	5.353684
H	3.933807	10.349307	8.564498
Zr	4.903707	11.051282	5.593827
C	7.154566	10.739718	6.034021
C	11.132080	13.083297	4.835569
H	7.444423	9.712190	5.752267
H	7.437222	10.871497	7.090295
H	7.731048	11.449271	5.425264
H	12.029494	13.709706	4.953899
H	10.256388	13.745604	4.914501
H	11.104708	12.341024	5.654862
C	5.247376	13.586177	5.241207
C	5.814099	13.252167	6.500287
C	3.524046	12.921410	6.634562
C	4.756912	12.822042	7.363450
C	3.831773	13.394796	5.327742
H	5.775721	14.009613	4.392136
H	6.863716	13.341611	6.767891
H	2.527353	12.718254	7.022422
H	4.870359	12.549052	8.410228
H	3.113205	13.725168	4.578428

Dioxo-bridged zirconocenium coordination on a μ_2-0 alumina surface site.

Al	1.176350	5.234075	0.229111
O	3.978436	7.669837	3.112275
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.311406	1.078165	2.457465
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.171463	2.811917	3.023881
Al	8.268006	3.298270	1.704362
Al	4.169090	1.086954	2.459281
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000

O	1.289631	2.798933	3.027049
Al	4.308924	5.234075	0.229111
O	1.585376	7.660173	3.115357
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.945546	1.054423	2.711987
Al	6.949156	6.392276	1.639649
O	6.913957	7.437713	3.106682
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.722801	3.854994	2.790361
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949327	2.881796	2.980007
Al	1.176350	13.302075	0.229111
O	3.972261	15.590562	2.894992
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.292563	9.208107	2.468445
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.155411	10.955657	3.013243
Al	8.267993	11.366301	1.704330
Al	4.186388	9.230209	2.463308
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.329540	10.929464	3.039416
Al	4.308924	13.302075	0.229111
O	1.512756	15.582345	2.891739
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.980758	9.103302	2.703206
Al	6.949131	14.460329	1.639677
O	6.943499	15.526713	3.102124
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.731169	11.856183	2.447056
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.922139	10.920745	2.984462
Al	9.589350	5.234075	0.229111
O	12.378355	7.568884	2.897479
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.724543	1.098833	2.473834
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.577653	2.846421	3.029842
Al	16.680960	3.298306	1.704311
Al	12.587399	1.098168	2.473768
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.730519	2.848347	3.029493
Al	12.721924	5.234075	0.229111
O	9.924881	7.570633	2.897092
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.364989	1.056723	2.712664
Al	15.362120	6.392276	1.639649
O	15.395856	7.447218	3.091888
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428

Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.155670	3.767266	2.466882
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.356620	2.881050	2.978669
Al	9.589350	13.302075	0.229111
O	12.383372	15.610791	2.909767
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.755737	9.225573	2.475604
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.598465	10.926780	3.018047
Al	16.680957	11.366316	1.704306
Al	12.558060	9.222510	2.474531
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.709386	10.929510	3.018390
Al	12.721924	13.302075	0.229111
O	9.927549	15.611648	2.910401
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.329976	9.117064	2.717698
Al	15.362144	14.460329	1.639677
O	15.369706	15.528295	3.101297
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.156219	12.143271	3.120209
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.385976	10.933484	2.979229
C	4.935835	8.314286	6.520351
C	4.624903	9.401258	5.660803
C	2.857269	9.137562	7.117030
C	3.326996	9.893432	6.003104
C	3.841951	8.159247	7.430702
H	5.862725	7.746662	6.511592
H	5.300208	9.869050	4.949817
H	1.919430	9.292248	7.641250
H	2.822874	10.746421	5.558705
H	3.786658	7.441551	8.247226
Zr	2.901000	7.476575	5.114320
C	0.696385	7.774994	5.805024
C	11.155515	13.092842	4.843866
H	0.432034	8.840195	5.675634
H	0.516813	7.523927	6.863507
H	0.019155	7.185127	5.174194
H	12.047819	13.729052	4.936509
H	10.266799	13.734333	4.933739
H	11.152454	12.347880	5.660372
C	2.458577	5.157789	4.439785
C	1.929246	5.032501	5.778514
C	4.224121	5.217426	5.940418
C	3.003406	5.085513	6.682384
C	3.917980	5.319783	4.573912
H	1.818020	5.635332	3.682899
H	0.874087	4.937278	6.020101
H	5.229198	5.233812	6.356824
H	2.924502	5.013141	7.766080
H	4.644492	5.478947	3.784900

Oxo-bridged zirconocenium coordination on a μ_2-0 alumina surface site.

Al	1.176350	5.234075	0.229111
O	5.245642	8.837741	4.059832
O	8.279944	5.109620	1.489067

O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.301810	1.068740	2.476845
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.168218	2.831365	3.023339
Al	8.268006	3.298270	1.704362
Al	4.184038	1.072435	2.477432
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.315128	2.828130	3.026921
Al	4.308924	5.234075	0.229111
O	2.537080	7.915070	3.158329
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.953717	1.057241	2.715733
Al	6.949156	6.392276	1.639649
O	7.149469	7.395175	3.046513
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.739868	3.701235	2.412629
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.946642	2.882192	2.978797
Al	1.176350	13.302075	0.229111
O	3.969949	15.582678	2.903487
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.345995	9.158035	2.490820
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.106960	11.044845	3.023386
Al	8.267993	11.366301	1.704330
Al	4.138093	9.248200	2.739490
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.300588	10.889812	3.050503
Al	4.308924	13.302075	0.229111
O	1.506141	15.574875	2.891933
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.775170	9.105185	2.899280
Al	6.949131	14.460329	1.639677
O	6.943246	15.532153	3.103300
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.683473	11.871566	2.465210
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.935239	10.983742	2.965589
Al	9.589350	5.234075	0.229111
O	12.500590	7.552074	2.846671
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.725316	1.099207	2.474457
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.579795	2.850866	3.027516
Al	16.680960	3.298306	1.704311
Al	12.583768	1.101538	2.474100
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.730010	2.847279	3.031116

Al	12.721924	5.234075	0.229111
O	10.051395	7.584804	2.945195
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.356500	1.055164	2.714886
Al	15.362120	6.392276	1.639649
O	15.695557	7.485915	3.079037
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.152406	3.770609	2.470729
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.363180	2.880988	2.976160
Al	9.589350	13.302075	0.229111
O	12.388067	15.613445	2.908385
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.693671	9.206275	2.468420
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.609136	10.930838	3.018600
Al	16.680957	11.366316	1.704306
Al	12.536064	9.231591	2.475744
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.731668	10.918481	3.020720
Al	12.721924	13.302075	0.229111
O	9.933286	15.614177	2.913853
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.330852	9.136157	2.713586
Al	15.362144	14.460329	1.639677
O	15.372195	15.528303	3.101298
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.148360	12.129587	3.121347
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.380993	10.944074	2.977831
C	3.583795	6.467602	6.279781
C	4.490434	6.013641	5.268947
C	5.599733	5.948319	7.284048
C	5.732431	5.702020	5.881090
C	4.272358	6.400180	7.531586
H	2.544346	6.752360	6.125835
H	4.286730	5.967136	4.205877
H	6.372886	5.796650	8.033855
H	6.623527	5.346287	5.372318
H	3.849802	6.641982	8.505419
Zr	5.350221	8.287154	6.115824
C	7.642741	8.249135	6.324535
C	11.161406	13.089887	4.838866
H	8.048430	7.479513	5.649778
H	7.981104	8.027626	7.351658
H	8.079194	9.224797	6.044915
H	12.035515	13.753331	4.916779
H	10.256865	13.707501	4.947729
H	11.191634	12.348897	5.658915
C	5.307013	10.838750	6.501736
C	5.972859	10.282683	7.633392
C	3.769877	9.578969	7.687019
C	5.030033	9.492139	8.358535
C	3.944682	10.408285	6.540971
H	5.757135	11.465989	5.733422

H	7.013233	10.439888	7.902896
H	2.839783	9.112563	8.004792
H	5.229321	8.946698	9.280661
H	3.171211	10.678986	5.827533

Homogeneous cocatalyst $B(C_6F_5)_3$ system.

B	0.023745	-0.017210	0.011495
C	1.125595	-1.146151	0.001349
C	1.036860	-2.273919	-0.844896
C	2.005829	-3.284790	-0.873316
C	3.110356	-3.197385	-0.010536
C	3.234322	-2.104219	0.861765
C	2.261445	-1.096288	0.839293
C	-1.508624	-0.406488	-0.004419
C	-2.462792	0.298218	-0.773483
C	-3.829005	-0.007192	-0.766822
C	-4.296753	-1.050016	0.049737
C	-3.389876	-1.776826	0.838398
C	-2.027163	-1.455080	0.789276
C	0.449836	1.504499	0.028495
C	1.512675	1.995285	-0.763981
C	1.855405	3.352002	-0.830960
C	1.136949	4.280281	-0.061521
C	0.082526	3.841547	0.757174
C	-0.242247	2.479427	0.783738
F	-0.005379	-2.393972	-1.708210
F	1.895617	-4.332900	-1.719015
F	4.046627	-4.163544	-0.015739
F	4.291185	-2.029808	1.700763
F	2.421982	-0.063267	1.706465
F	-2.067323	1.306504	-1.593649
F	-4.700602	0.683249	-1.533983
F	-5.607993	-1.350553	0.077004
F	-3.840496	-2.773758	1.630660
F	-1.201286	-2.176198	1.591419
F	2.224647	1.149053	-1.552796
F	2.866435	3.774254	-1.620809
F	1.457281	5.586255	-0.105679
F	-0.596484	4.735288	1.508941
F	-1.260295	2.110703	1.603842

Homogeneous ion-pair $Cp_2ZrCH_3^+H_3CB(C_6F_5)_3^-$ system. Structure II.

C	10.027263	8.248909	21.139664
C	9.391883	9.354655	20.485698
C	8.132413	8.807799	22.340713
C	8.223512	9.694356	21.225186
C	9.256933	7.928605	22.299317
H	10.956261	7.772111	20.830212
H	9.751547	9.859788	19.593374
H	7.358224	8.822849	23.107351
H	7.531783	10.498343	20.989812
H	9.497516	7.161737	23.031476
Zr	7.832757	7.319228	20.276369
C	5.710584	8.188478	20.281324
H	5.759189	9.211614	19.871502
H	5.245883	8.251171	21.278564
H	5.050199	7.597834	19.627457
C	6.870632	5.031337	19.538413
C	6.324044	5.318330	20.821144
C	8.610726	5.019748	21.058100
C	7.400001	5.330360	21.763999
C	8.281584	4.841405	19.686285
H	6.311276	4.942671	18.608855
H	5.274914	5.478265	21.052593
H	9.601905	4.916944	21.495361
H	7.300070	5.479047	22.837329
H	8.979177	4.594045	18.888964
C	8.233616	7.755525	17.786232
B	8.731374	7.941226	16.159659
C	9.316023	6.419340	15.779719

C	10.442924	5.893421	16.448518
C	10.964553	4.611178	16.247540
C	10.331345	3.747923	15.344167
C	9.194637	4.200006	14.664904
C	8.712100	5.502767	14.893993
C	9.870459	9.174497	16.085826
C	9.575184	10.444723	16.622261
C	10.431002	11.554734	16.563525
C	11.674233	11.430667	15.929876
C	12.011216	10.200270	15.352728
C	11.122691	9.114833	15.438121
C	7.473266	8.445624	15.187449
C	6.139768	8.656664	15.571944
C	5.143659	9.173296	14.727174
C	5.458833	9.486926	13.399690
C	6.770910	9.282993	12.951809
C	7.731562	8.774466	13.838843
F	11.110527	6.658202	17.377028
F	12.061884	4.188278	16.929224
F	10.810833	2.499953	15.136478
F	8.562444	3.372630	13.796384
F	7.582505	5.822367	14.201774
F	8.364754	10.678076	17.235184
F	10.072303	12.741141	17.121452
F	12.522079	12.482634	15.860851
F	13.201571	10.068495	14.715836
F	11.538137	7.981973	14.810658
F	5.710700	8.359367	16.843975
F	3.877300	9.360752	15.181706
F	4.513003	9.977960	12.565853
F	7.092539	9.569904	11.665344
F	8.975390	8.574344	13.319877
H	9.170932	7.468686	18.310680
H	7.483344	6.952496	17.781642
H	7.825635	8.708996	18.151245

Ethylene insertion pathway for the homogeneous ion-paired $Cp_2ZrCH_3^+H_3CB(C_6F_5)_3^-$ catalyst system.

π-complex

C	10.063729	8.039583	20.991098
C	9.278485	9.079906	20.389152
C	8.280994	8.506946	22.386803
C	8.189642	9.373180	21.256693
C	9.457912	7.704081	22.236051
H	10.988679	7.620182	20.597392
H	9.505091	9.595431	19.456493
H	7.604435	8.501220	23.241470
H	7.430886	10.133418	21.100988
H	9.829203	6.979108	22.956888
Zr	7.838596	6.961593	20.421738
C	5.717596	7.833003	20.356249
H	5.716621	8.839372	19.908284
H	5.271653	7.935442	21.362467
H	5.041231	7.194250	19.764035
C	6.874268	4.655857	19.819620
C	6.331939	5.006106	21.089490
C	8.618045	4.715660	21.335322
C	7.410806	5.067297	22.026119
C	8.286010	4.458921	19.977764
H	6.309299	4.517759	18.898991
H	5.285019	5.188012	21.314427
H	9.607079	4.624699	21.779034
H	7.317664	5.282042	23.089535
H	8.981709	4.134615	19.206988
C	8.878031	6.973047	17.702990
C	7.609578	7.457745	17.685680
H	9.087590	5.915833	17.530301
H	9.741816	7.638928	17.759722
H	7.410647	8.528953	17.732457

H	6.752963	6.807995	17.493486
C	6.408254	13.145567	14.084443
B	6.557315	11.684932	14.882463
C	6.791681	12.075336	16.496669
C	7.849644	12.936021	16.871389
C	8.073106	13.401733	18.175007
C	7.211258	13.006994	19.207035
C	6.148880	12.151038	18.898189
C	5.962337	11.710983	17.575784
C	7.873961	10.866043	14.218762
C	7.951941	10.678917	12.819595
C	9.007804	10.023421	12.160988
C	10.062914	9.491786	12.912949
C	10.034968	9.633635	14.305039
C	8.964113	10.306929	14.912865
C	5.200994	10.709325	14.643860
C	3.915544	11.210704	14.340281
C	2.810652	10.403153	14.012339
C	2.941394	9.009646	14.011137
C	4.180865	8.452994	14.347370
C	5.253396	9.301532	14.663785
F	8.767186	13.338679	15.947757
F	9.124347	14.215619	18.460232
F	7.412244	13.425729	20.483387
F	5.316277	11.733921	19.898621
F	4.909337	10.849452	17.411046
F	6.943324	11.106416	12.009054
F	9.008806	9.883290	10.810686
F	11.090043	8.846811	12.306196
F	11.038369	9.095766	15.059840
F	9.013539	10.321821	16.287443
F	3.658468	12.546903	14.364180
F	1.609490	10.960380	13.711076
F	1.888621	8.213119	13.702991
F	4.323676	7.097770	14.388060
F	6.399237	8.647424	15.047421
H	7.395790	13.598453	13.902940
H	5.822011	13.868222	14.672674
H	5.912558	13.039593	13.110032

Insertion TS

C	10.089725073	8.073399667	21.046863367
C	9.300526963	9.009607122	20.307367471
C	8.209419159	8.566490055	22.297806709
C	8.143541592	9.319924672	21.076666729
C	9.424180535	7.816806736	22.287177294
H	11.047298152	7.663617199	20.732207485
H	9.554603562	9.439087712	19.340047561
H	7.488934521	8.622165540	23.122210588
H	7.362002913	10.035220098	20.811550957
H	9.796950677	7.188396947	23.094380558
Zr	7.925330360	6.849238277	20.423154147
C	5.900827547	7.556523994	19.252865797
H	5.462234347	8.430795851	18.742088462
H	5.732286893	7.796579668	20.355096138
H	5.311421001	6.666152509	19.003773510
C	6.975969010	4.467221290	20.141128905
C	6.415450625	4.958051141	21.358208755
C	8.697567611	4.721241596	21.660435211
C	7.477187082	5.119097470	22.297076247
C	8.385429076	4.310378592	20.332898103
H	6.429751342	4.228968030	19.230298912
H	5.361486447	5.138061015	21.558536923
H	9.679997290	4.670850710	22.129287972
H	7.370656345	5.458056965	23.327185992
H	9.090944293	3.905909647	19.605518518
C	8.760959725	6.670903438	18.217900891

C	7.616019946	7.421982157	17.823627763
H	8.791043746	5.643532515	17.836406771
H	9.707388290	7.198347656	18.017597935
H	7.677227479	8.494105333	17.774185830
H	6.911906213	6.983785016	17.121427491
C	6.083319704	13.428670644	14.462742412
B	6.227148327	11.958078547	15.229558488
C	6.448883239	12.300534639	16.865259525
C	7.468906173	13.199237281	17.271947393
C	7.671137206	13.633761061	18.586697808
C	6.845661989	13.144346690	19.608583758
C	5.820903963	12.252297310	19.271887169
C	5.649443236	11.857781688	17.934210536
C	7.549008954	11.160979366	14.554949999
C	7.621005261	10.986039044	13.154647649
C	8.699503965	10.386594684	12.479373671
C	9.793854903	9.915727699	13.212731156
C	9.773891703	10.037936052	14.606195400
C	8.666722088	10.635348433	15.231336211
C	4.866851278	10.990550434	14.962443733
C	3.587270285	11.500637071	14.654121225
C	2.482812013	10.699235387	14.313851340
C	2.606855349	9.305055882	14.302958084
C	3.846342722	8.742915613	14.634369671
C	4.918415528	9.584051099	14.961813391
F	8.361160040	13.681875436	16.360507725
F	8.682236427	14.488719981	18.896675679
F	7.029514968	13.531493339	20.897237207
F	5.021797423	11.745628636	20.260048454
F	4.630373484	10.958747425	17.740452915
F	6.586973353	11.379342500	12.356145626
F	8.697618566	10.268488352	11.125882972
F	10.855547952	9.348355027	12.586105676
F	10.820376827	9.563448523	15.343266891
F	8.734065392	10.644033082	16.610143683
F	3.332628743	12.838069583	14.689960459
F	1.280779130	11.262738799	14.018621401
F	1.552319371	8.513830660	13.983507601
F	3.983798483	7.384726488	14.661877695
F	6.066757268	8.925525629	15.342018617
H	7.068665837	13.890254480	14.292641118
H	5.490438335	14.142194592	15.056947005
H	5.593840417	13.336963643	13.483560353

Insertion γ-product

C	9.630429	7.804022	21.186694
C	9.110627	8.594420	20.116875
C	7.718788	8.862151	21.947133
C	7.921971	9.233105	20.577798
C	8.782747	7.998001	22.327785
H	10.548170	7.219305	21.164161
H	9.562337	8.709736	19.135499
H	6.906626	9.206753	22.587374
H	7.292454	9.917465	20.014982
H	8.930500	7.566162	23.316157
Zr	7.422606	6.759014	20.583606
C	5.452703	7.320960	18.597600
H	4.752070	8.038212	18.149011
H	5.453438	7.682382	19.661125
H	4.989581	6.325822	18.577781
C	6.394423	4.394045	20.505877
C	5.844167	5.048484	21.653299
C	8.118284	4.797317	21.986892
C	6.906983	5.297610	22.570682
C	7.796450	4.231232	20.714702

H	5.842950	4.060926	19.628684
H	4.795954	5.304269	21.807450
H	9.099910	4.789666	22.455994
H	6.806653	5.755863	23.552564
H	8.493545	3.749305	20.032528
C	7.915746	6.398505	18.388562
C	6.813802	7.361100	17.845328
H	7.700413	5.363095	18.084569
H	8.901465	6.668104	17.986027
H	7.172143	8.400613	17.825572
H	6.593371	7.102376	16.794961
C	3.462106	14.112983	21.741606
B	4.132664	12.753473	21.068154
C	5.492353	12.481902	22.026973
C	6.828357	12.710283	21.644330
C	7.935160	12.608690	22.507375
C	7.738827	12.256370	23.845959
C	6.430342	12.036217	24.294786
C	5.358942	12.164877	23.398396
C	4.534428	12.925364	19.439992
C	4.470452	14.123871	18.695799
C	4.786109	14.220764	17.326303
C	5.197985	13.085288	16.621419
C	5.279759	11.868399	17.307505
C	4.954056	11.828762	18.668659
C	3.018217	11.483124	21.092816
C	3.226509	10.171808	21.553996
C	2.265352	9.149473	21.537070
C	0.991476	9.407317	21.021774
C	0.724603	10.687242	20.520019
C	1.724945	11.675351	20.560487
F	7.150158	13.036617	20.352630
F	9.199592	12.817297	22.045713
F	8.793382	12.130707	24.693223
F	6.218952	11.689610	25.594303
F	4.124954	11.931896	23.933866
F	4.121347	15.303400	19.276286
F	4.704685	15.412837	16.680445
F	5.513501	13.156530	15.304367
F	5.695667	10.742685	16.650510
F	5.118665	10.592367	19.260642
F	4.458838	9.767095	22.020877
F	2.574837	7.893879	21.989501
F	0.045965	8.434603	20.991033
F	-0.495963	10.953497	19.986912
F	1.379868	12.864333	19.992190
H	4.213311	14.913892	21.832477
H	3.100156	13.892889	22.759241
H	2.614807	14.521702	21.174806

Insertion β-product

C	9.818364	7.798832	21.121191
C	9.280559	8.628673	20.090130
C	7.926864	8.838214	21.958018
C	8.107824	9.265476	20.603746
C	8.991146	7.946281	22.282025
H	10.731822	7.208518	21.059785
H	9.715246	8.780188	19.105103
H	7.132703	9.163863	22.627366
H	7.469677	9.968143	20.072632
H	9.153141	7.468030	23.246613
Zr	7.576878	6.805338	20.521369
C	5.667121	6.633224	17.126997
H	4.746023	7.232745	17.130500
H	5.419886	5.603772	17.424559
H	6.056254	6.602928	16.098117
C	6.209698	4.629605	20.422076
C	5.682399	5.409519	21.498643
C	7.861024	4.826681	22.022751
C	6.699319	5.528087	22.494300

C	7.548597	4.262087	20.746367
H	5.675886	4.345119	19.517418
H	4.678308	5.829956	21.560039
H	8.795407	4.693413	22.564151
H	6.597564	6.037276	23.449879
H	8.211212	3.649036	20.138962
C	7.991153	6.409147	18.306019
C	6.743599	7.249140	18.044497
H	7.868453	5.362049	18.002187
H	8.901470	6.828149	17.865372
H	6.167876	7.490341	19.021251
H	6.997503	8.263521	17.705956
C	3.463612	14.070562	21.738924
B	4.140091	12.717781	21.054072
C	5.501404	12.454669	22.010869
C	6.837605	12.702629	21.633380
C	7.942157	12.606358	22.499460
C	7.746667	12.245174	23.836019
C	6.438995	12.011133	24.280741
C	5.368390	12.131804	23.382856
C	4.533513	12.891293	19.423977
C	4.448252	14.088311	18.679117
C	4.760883	14.189548	17.309326
C	5.180496	13.057366	16.603748
C	5.275876	11.840758	17.288845
C	4.962033	11.796027	18.653182
C	3.033513	11.438840	21.079416
C	3.257949	10.126228	21.531542
C	2.301257	9.099523	21.513513
C	1.026011	9.347068	20.996408
C	0.748091	10.624682	20.495020
C	1.738330	11.622343	20.547117
F	7.159364	13.045706	20.346747
F	9.204512	12.832701	22.043643
F	8.800051	12.124432	24.684717
F	6.226962	11.657603	25.578213
F	4.135633	11.884313	23.912817
F	4.077731	15.260877	19.259938
F	4.665214	15.380574	16.664585
F	5.488284	13.132576	15.284780
F	5.700904	10.720828	16.628215
F	5.150528	10.564249	19.245508
F	4.494709	9.733393	21.993395
F	2.613767	7.846269	21.970163
F	0.088230	8.367594	20.964755
F	-0.474674	10.883307	19.964235
F	1.381165	12.812973	19.988385
H	4.207806	14.878837	21.824154
H	3.115205	13.844005	22.759666
H	2.607516	14.472625	21.181373

Ethylene enchainment pathway at the heterogeneous dioxo-bridged zirconocenium μ_3-O site.

π-complex

Al	1.176350	5.234075	0.229111
O	3.977928	7.522018	2.905236
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.308372	1.082495	2.474248
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.163398	2.834565	3.029357
Al	8.268006	3.298270	1.704362
Al	4.177032	1.082690	2.473957
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.321504	2.834902	3.029507
Al	4.308924	5.234075	0.229111
O	1.507737	7.521390	2.910984

O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951677	1.050996	2.710487
Al	6.949156	6.392276	1.639649
O	6.944775	7.451863	3.106839
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.742849	3.754106	2.450579
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949122	2.872539	2.980061
Al	1.176350	13.302075	0.229111
O	3.978186	15.589413	2.903131
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.299584	9.142363	2.459574
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.157952	10.904756	3.028951
Al	8.267993	11.366301	1.704330
Al	4.185019	9.144971	2.466772
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.335315	10.897241	3.031157
Al	4.308924	13.302075	0.229111
O	1.507975	15.589042	2.901996
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.969399	9.117257	2.704513
Al	6.949131	14.460329	1.639677
O	6.940292	15.524427	3.107197
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.745756	11.797915	2.381521
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.927134	10.936307	2.985321
Al	9.589350	5.234075	0.229111
O	12.376570	7.567147	2.904202
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.725846	1.098825	2.472971
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578775	2.847099	3.029814
Al	16.680960	3.298306	1.704311
Al	12.585607	1.098828	2.472833
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732528	2.847081	3.029836
Al	12.721924	5.234075	0.229111
O	9.937690	7.571070	2.905219
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.359719	1.050778	2.710516
Al	15.362120	6.392276	1.639649
O	15.366891	7.453381	3.105413
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.155552	3.767139	2.464591

O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362117	2.872842	2.980324
Al	9.589350	13.302075	0.229111
O	12.387264	15.612387	2.910864
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.751602	9.223040	2.474618
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.601265	10.923929	3.021902
Al	16.680957	11.366316	1.704306
Al	12.561126	9.218935	2.474495
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.712801	10.927041	3.020821
Al	12.721924	13.302075	0.229111
O	9.924210	15.612430	2.911214
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.338958	9.119234	2.705023
Al	15.362144	14.460329	1.639677
O	15.370711	15.524250	3.107356
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.157360	12.137652	3.111541
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.388423	10.937998	2.985529
C	2.410076	9.676377	5.957797
C	3.760585	9.588993	6.117819
H	1.954973	10.507883	5.417858
H	1.762940	8.830509	6.192106
H	4.227411	8.699387	6.542713
H	4.429274	10.368982	5.748272
C	0.861858	10.288861	9.519539
C	1.537929	9.115024	9.072208
C	2.897751	10.158526	10.615806
C	2.796078	9.038405	9.739423
C	1.699534	10.929388	10.487906
H	16.696305	10.613673	9.209931
H	1.145257	8.383411	8.370115
H	3.727995	10.374128	11.284908
H	3.544374	8.260041	9.612246
H	1.447034	11.820589	11.060193
Zr	2.917546	11.155282	8.270012
C	5.179970	10.886180	8.634865
C	11.159991	13.082084	4.837601
H	5.444706	9.830773	8.811384
H	5.503959	11.451125	9.529068
H	5.775680	11.256675	7.785035
H	12.049008	13.724319	4.931499
H	10.272656	13.725975	4.934306
H	11.160361	12.339593	5.658032
C	3.435625	13.133024	6.677564
C	3.891844	13.503541	7.975617
C	1.584080	13.299640	8.051110
C	2.754073	13.587915	8.834901
C	2.009332	13.021206	6.721914
H	4.063391	13.036360	5.792940
H	4.923404	13.708319	8.250164
H	0.552235	13.325734	8.396404
H	2.766984	13.901819	9.877834
H	1.352251	12.816183	5.877713

Insertion TS

Al	1.176350299	5.234075196	0.229111121

O	3.976386761	7.522278043	2.909893493
O	8.279943566	5.109619934	1.489066697
O	4.160379792	7.058908786	0.084507049
Al	5.630314839	3.298305565	1.704311452
Al	1.307726877	1.082156980	2.473622587
O	4.051770683	3.415890404	0.556335967
O	8.285938069	1.351566857	1.443000651
O	4.163376355	2.834829065	3.029585467
Al	8.268005601	3.298270256	1.704362144
Al	4.177244050	1.082073235	2.473553133
O	1.433503645	3.415890404	0.556335967
O	5.612410853	1.351574998	1.442999961
O	1.321490531	2.834744093	3.029539372
Al	4.308924029	5.234075196	0.229111121
O	1.511676372	7.524954528	2.913593167
O	5.618390615	5.109640648	1.489002166
O	1.324894536	7.058908786	0.084507049
Al	6.949137164	1.225769999	0.009444148
Al	6.951525112	1.049977745	2.709246576
Al	6.949156014	6.392276180	1.639649299
O	6.942634064	7.453433628	3.106131912
O	6.949137164	7.354508637	0.120802639
Al	2.742637313	7.151819943	1.460390342
Al	2.742637164	2.332601337	0.000000000
O	2.742637013	1.138213546	1.294012542
Al	2.742427848	3.753029125	2.446466016
O	2.742637264	5.289564588	1.533309110
O	6.949137164	3.103569407	0.223225080
O	6.948942391	2.872228699	2.980224773
Al	1.176350299	13.302075196	0.229111121
O	3.976796193	15.589935526	2.905219659
O	8.279907605	13.177619866	1.489021650
O	4.160379792	15.126908786	0.084507049
Al	5.630317443	11.366315731	1.704304642
Al	1.300889427	9.144576421	2.462401067
O	4.051770683	11.483890404	0.556335967
O	8.285924732	9.419561855	1.443037140
O	4.152014616	10.896281849	3.037941422
Al	8.267992577	11.366301130	1.704330004
Al	4.184436877	9.144437057	2.465471621
O	1.433503645	11.483890404	0.556335967
O	5.612364582	9.419559818	1.443013878
O	1.336246429	10.895469750	3.037560155
Al	4.308924029	13.302075196	0.229111121
O	1.506892349	15.589571053	2.905005256
O	5.618392812	13.177626445	1.489012429
O	1.324894536	15.126908786	0.084507049
Al	6.949137164	9.293769999	0.009444148
Al	6.969566123	9.119300762	2.705658966
Al	6.949131342	14.460329344	1.639676587
O	6.939746088	15.523837043	3.108408424
O	6.949137164	15.422508637	0.120802639
Al	2.742636897	15.219709386	1.461134276
Al	2.742637164	10.400601337	0.000000000
O	2.742637500	9.205981130	1.293822924
Al	2.744098368	11.800566135	2.399576682
O	2.742636431	13.357530466	1.533509586
O	6.949137164	11.171569407	0.223225080
O	6.928136075	10.938153294	2.983745174
Al	9.589350299	5.234075196	0.229111121
O	12.376828860	7.568748272	2.903916534
O	16.692887290	5.109641938	1.489004758
O	12.573379792	7.058908786	0.084507049

Al	14.043268490	3.298270665	1.704362281
Al	9.725625630	1.098235709	2.472056793
O	12.464770683	3.415890404	0.556335967
O	16.698863209	1.351575018	1.442999934
O	12.578784821	2.846159275	3.029645365
Al	16.680959550	3.298305505	1.704311173
Al	12.585973461	1.097691191	2.472437131
O	9.846503645	3.415890404	0.556335967
O	14.025336008	1.351566791	1.443000847
O	9.732680818	2.846526220	3.029547377
Al	12.721924029	5.234075196	0.229111121
O	9.934351393	7.568838471	2.904348689
O	14.031331841	5.109619873	1.489065963
O	9.737894536	7.058908786	0.084507049
Al	15.362137164	1.225769999	0.009444148
Al	15.359690096	1.049573840	2.708666913
Al	15.362120285	6.392275817	1.639649169
O	15.369187184	7.453635488	3.105634822
O	15.362137164	7.354508637	0.120802639
Al	11.155637456	7.151831933	1.460428379
Al	11.155637164	2.332601337	0.000000000
O	11.155636911	1.137919867	1.293822601
Al	11.155865990	3.764160840	2.459208465
O	11.155635990	5.289551426	1.533342776
O	15.362137164	3.103569407	0.223225080
O	15.362367367	2.871794609	2.980391647
Al	9.589350299	13.302075196	0.229111121
O	12.388604329	15.611898090	2.910515769
O	16.692882543	13.177626236	1.489013917
O	12.573379792	15.126908786	0.084507049
Al	14.043282200	11.366301275	1.704329925
Al	9.750678785	9.220357003	2.472889699
O	12.464770683	11.483890404	0.556335967
O	16.698910754	9.419558814	1.443013013
O	12.599660659	10.924300251	3.021121716
Al	16.680957299	11.366315546	1.704305506
Al	12.561156014	9.220346204	2.473462960
O	9.846503645	11.483890404	0.556335967
O	14.025350740	9.419562696	1.443038333
O	9.712300235	10.924584193	3.021058294
Al	12.721924029	13.302075196	0.229111121
O	9.923040302	15.612660066	2.910840897
O	14.031368382	13.177619336	1.489020106
O	9.737894536	15.126908786	0.084507049
Al	15.362137164	9.293769999	0.009444148
Al	15.341580327	9.119744082	2.706122178
Al	15.362144028	14.460329281	1.639676584
O	15.370854154	15.524813552	3.108461938
O	15.362137164	15.422508637	0.120802639
Al	11.155636872	15.219891639	1.460200573
Al	11.155637164	10.400601337	0.000000000
O	11.155637610	9.205963598	1.293836596
Al	11.156221512	12.136493758	3.107538169
O	11.155640063	13.357593389	1.533293904
O	15.362137164	11.171569407	0.223225080
O	15.383810467	10.938475593	2.983514710
C	0.915029816	10.424978515	7.517358831
C	1.829692717	9.791345287	6.658467374
H	0.431304414	11.336729935	7.163931229
H	0.328033400	9.817921597	8.207412304
H	2.001162271	8.717799194	6.730892955
H	2.047153548	10.243463027	5.693806564
C	2.292512872	10.429873191	11.134434800

C	1.947318367	9.297815454	10.334785409
C	4.246279289	9.519990082	10.299820356
C	3.151310587	8.746037599	9.803508822
C	3.718088965	10.560580328	11.118315302
H	1.598477795	11.055955353	11.692835051
H	0.945357763	8.896906779	10.201109178
H	5.300504429	9.328956168	10.103777937
H	3.227010185	7.855353659	9.182423901
H	4.299790095	11.302746107	11.661650968
Zr	2.925218651	11.081952782	8.746563277
C	4.083001046	10.067405590	6.994224806
C	11.156348822	13.080706198	4.833944211
H	4.253933938	8.990661419	6.896620591
H	4.891470865	10.448794743	7.682830685
H	4.239974875	10.567184943	6.033982252
H	12.054407889	13.709446500	4.937539032
H	10.278828352	13.739601260	4.921612350
H	11.139177234	12.337843388	5.654067279
C	2.899286084	13.206332818	7.288485316
C	4.168612230	13.170963487	7.934597760
C	2.542565748	13.454755514	9.558392493
C	3.954073677	13.311461755	9.341073432
C	1.894758105	13.388001391	8.290272860
H	2.727632438	13.161550613	6.215067852
H	5.132459388	13.079328198	7.437382385
H	2.051581804	13.623417104	10.516167959
H	4.728375459	13.377031509	10.103666787
H	0.830179025	13.516425817	8.106962781

Insertion γ-product

Al	1.176350	5.234075	0.229111
O	3.974610	7.522324	2.909632
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.307739	1.083142	2.473973
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.163569	2.835342	3.029953
Al	8.268006	3.298270	1.704362
Al	4.177258	1.083118	2.473612
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.321369	2.835417	3.030123
Al	4.308924	5.234075	0.229111
O	1.509064	7.522259	2.911368
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951737	1.050529	2.710103
Al	6.949156	6.392276	1.639649
O	6.942976	7.454143	3.107030
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.742544	3.754846	2.450043
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.948960	2.872581	2.980307
Al	1.176350	13.302075	0.229111
O	3.976650	15.590555	2.905614
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.301321	9.141839	2.459158
O	4.051771	11.483890	0.556336

O	8.285925	9.419562	1.443037
O	4.153041	10.897921	3.037942
Al	8.267993	11.366301	1.704330
Al	4.184506	9.145827	2.468980
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.333735	10.897544	3.029637
Al	4.308924	13.302075	0.229111
O	1.508649	15.590790	2.905929
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.969941	9.119337	2.704239
Al	6.949131	14.460329	1.639677
O	6.939177	15.523676	3.108266
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.747302	11.802902	2.400739
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.928105	10.937949	2.984915
Al	9.589350	5.234075	0.229111
O	12.375550	7.569191	2.904908
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.725860	1.098489	2.472454
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.579074	2.846314	3.029941
Al	16.680960	3.298306	1.704311
Al	12.585959	1.097791	2.473004
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732491	2.846748	3.029842
Al	12.721924	5.234075	0.229111
O	9.933710	7.569402	2.904412
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.359681	1.051498	2.709158
Al	15.362120	6.392276	1.639649
O	15.368590	7.453551	3.106277
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.155902	3.765737	2.462437
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362373	2.873083	2.980246
Al	9.589350	13.302075	0.229111
O	12.387921	15.611427	2.910660
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.751017	9.221499	2.472565
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.599304	10.924784	3.020760
Al	16.680957	11.366316	1.704306
Al	12.560861	9.221008	2.473859
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.711777	10.925064	3.021381
Al	12.721924	13.302075	0.229111
O	9.923007	15.612262	2.911020
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507

Al	15.362137	9.293770	0.009444
Al	15.341558	9.118648	2.705130
Al	15.362144	14.460329	1.639677
O	15.371518	15.524116	3.109325
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.156069	12.137534	3.109052
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.384417	10.936940	2.985191
C	0.951487	10.764066	8.835994
C	0.647607	10.996462	7.326259
H	0.392447	11.470810	9.463489
H	0.646054	9.748232	9.124372
H	16.527700	10.494737	7.055352
H	0.491006	12.062597	7.112242
C	4.080884	9.623037	10.574519
C	3.101899	8.793712	9.947298
C	4.872302	9.050565	8.477710
C	3.578748	8.458842	8.645166
C	5.187441	9.761468	9.673139
H	4.024915	10.018138	11.587774
H	2.168894	8.465097	10.396019
H	5.519428	8.943789	7.607652
H	3.073360	7.821115	7.921035
H	6.121244	10.279493	9.879867
Zr	3.222604	10.989351	8.636957
C	1.708867	10.433414	6.334251
C	11.156416	13.080089	4.836148
H	1.778601	9.337518	6.363560
H	2.755620	10.845922	6.399034
H	1.451746	10.725047	5.307238
H	12.057687	13.703155	4.944324
H	10.282385	13.743338	4.923360
H	11.133933	12.336100	5.654985
C	2.951128	13.431012	7.856826
C	4.350789	13.133482	7.778113
C	3.706829	13.030453	10.000641
C	4.818754	12.900570	9.103148
C	2.555086	13.380688	9.225970
H	2.314492	13.697097	7.014304
H	4.955841	13.135991	6.871327
H	3.745596	12.961895	11.087029
H	5.849792	12.700264	9.384651
H	1.562108	13.597609	9.612401

Insertion β-product

Al	1.176350	5.234075	0.229111
O	3.973964	7.525233	2.911119
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.308544	1.083776	2.473498
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.163742	2.835193	3.029681
Al	8.268006	3.298270	1.704362
Al	4.177432	1.083052	2.473600
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.321605	2.835834	3.029734
Al	4.308924	5.234075	0.229111
O	1.509998	7.523321	2.907691
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951704	1.050859	2.710375
Al	6.949156	6.392276	1.639649

O	6.943588	7.454207	3.106112
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.742942	3.755457	2.450801
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949024	2.872793	2.979965
Al	1.176350	13.302075	0.229111
O	3.977085	15.590559	2.905331
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.303101	9.148263	2.467123
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.155174	10.900751	3.037260
Al	8.267993	11.366301	1.704330
Al	4.182542	9.149741	2.469424
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.329443	10.899233	3.036759
Al	4.308924	13.302075	0.229111
O	1.508909	15.591618	2.906316
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.968008	9.119950	2.704753
Al	6.949131	14.460329	1.639677
O	6.940345	15.524039	3.107879
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.742213	11.809491	2.421162
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.928880	10.938281	2.984558
Al	9.589350	5.234075	0.229111
O	12.375702	7.569392	2.905019
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.725627	1.098536	2.472478
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578836	2.846801	3.029573
Al	16.680960	3.298306	1.704311
Al	12.585300	1.098238	2.472820
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732528	2.846753	3.029629
Al	12.721924	5.234075	0.229111
O	9.935489	7.568424	2.905016
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.359696	1.052023	2.705657
Al	15.362120	6.392276	1.639649
O	15.367335	7.452728	3.105600
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.155611	3.765965	2.462289
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362318	2.869431	2.979633
Al	9.589350	13.302075	0.229111
O	12.386234	15.611993	2.911472

O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.750191	9.220843	2.474731
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.599517	10.924771	3.020893
Al	16.680957	11.366316	1.704306
Al	12.560757	9.221267	2.473579
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.712572	10.925514	3.021393
Al	12.721924	13.302075	0.229111
O	9.923168	15.612165	2.910830
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.341826	9.117133	2.701486
Al	15.362144	14.460329	1.639677
O	15.369731	15.527091	3.102505
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.156365	12.137716	3.108788
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.382785	10.936015	2.984239
C	0.817712	10.987122	8.894144
C	0.769494	10.953803	7.371728
H	0.283513	11.843136	9.318594
H	0.456549	10.056440	9.347104
H	0.494043	11.933447	6.957193
H	1.825215	10.789185	6.908194
C	4.055882	9.550176	10.362816
C	2.945166	8.851734	9.790885
C	4.563349	9.098572	8.148021
C	3.253220	8.586434	8.422856
C	5.062159	9.683116	9.348804
H	4.156713	9.857745	11.403081
H	2.040727	8.543397	10.309545
H	5.095780	9.010720	7.202212
H	2.629191	8.042354	7.715694
H	6.044268	10.131260	9.478286
Zr	3.091692	11.123088	8.651857
C	16.740465	9.843131	6.727207
C	11.158642	13.080751	4.835417
H	15.720784	9.898963	7.133460
H	0.312727	8.840545	6.935454
H	16.686850	9.983575	5.640517
H	12.066386	13.693765	4.948133
H	10.291794	13.753621	4.919602
H	11.124808	12.336877	5.653784
C	2.923601	13.559995	7.877767
C	4.292145	13.179591	7.706298
C	3.800799	13.128500	9.971978
C	4.837391	12.922038	8.998111
C	2.624634	13.546295	9.271928
H	2.245861	13.855683	7.078615
H	4.830849	13.135363	6.760230
H	3.910280	13.054024	11.053006
H	5.871113	12.657922	9.208365
H	1.682143	13.835167	9.730479

Ethylene enchainment pathway at the heterogeneous oxo-bridged zirconocenium μ_3-O site.

π-complex

Al	1.176350	5.234075	0.229111
O	3.980309	7.530715	2.912221
O	8.279944	5.109620	1.489067

O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.307326	1.082608	2.474455
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.163868	2.835941	3.030003
Al	8.268006	3.298270	1.704362
Al	4.176567	1.083068	2.474235
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.321403	2.834545	3.029697
Al	4.308924	5.234075	0.229111
O	1.510350	7.519733	2.911026
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951898	1.048639	2.709764
Al	6.949156	6.392276	1.639649
O	6.947568	7.447385	3.109949
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741683	3.754191	2.449356
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949011	2.871941	2.981202
Al	1.176350	13.302075	0.229111
O	3.979957	15.589114	2.902251
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.299578	9.142862	2.469173
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.150969	10.908808	3.036421
Al	8.267993	11.366301	1.704330
Al	4.178349	9.152895	2.463100
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.327337	10.899561	3.029936
Al	4.308924	13.302075	0.229111
O	1.511295	15.589727	2.902743
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.966542	9.108440	2.694299
Al	6.949131	14.460329	1.639677
O	6.939441	15.521219	3.109450
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.730439	11.810061	2.407770
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.926586	10.934621	2.990683
Al	9.589350	5.234075	0.229111
O	12.375332	7.565058	2.901853
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.726735	1.099091	2.472071
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578788	2.844790	3.030277
Al	16.680960	3.298306	1.704311
Al	12.587237	1.096269	2.473452
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732381	2.847415	3.030012

Al	12.721924	5.234075	0.229111
O	9.932094	7.573760	2.910174
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.360325	1.051917	2.712134
Al	15.362120	6.392276	1.639649
O	15.366742	7.454967	3.102395
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.157055	3.765119	2.461343
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362393	2.874129	2.979391
Al	9.589350	13.302075	0.229111
O	12.385026	15.610547	2.911317
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.752900	9.223802	2.473520
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.591002	10.921262	3.021546
Al	16.680957	11.366316	1.704306
Al	12.563051	9.217515	2.475194
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.702877	10.927992	3.023884
Al	12.721924	13.302075	0.229111
O	9.918921	15.612856	2.911301
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.342970	9.122637	2.708910
Al	15.362144	14.460329	1.639677
O	15.370203	15.525124	3.105029
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.156787	12.139878	3.107611
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.378791	10.941017	2.980193
C	11.153514	13.078234	4.837895
H	12.092852	13.635623	4.977913
H	10.328448	13.804432	4.900632
H	11.058112	12.337415	5.653129
C	4.799986	9.244241	5.953476
C	6.149641	9.327970	6.117836
H	4.241349	10.049354	5.470107
H	4.262651	8.314887	6.150543
H	6.725365	8.478602	6.491295
H	6.711088	10.203726	5.783629
C	3.045832	10.070592	9.484187
C	3.699454	8.880979	9.051779
C	5.070349	9.909961	10.599631
C	4.954748	8.788606	9.727795
C	3.895340	10.710846	10.443838
H	2.061357	10.410367	9.168647
H	3.295786	8.155811	8.348780
H	5.901549	10.119578	11.268827
H	5.688622	7.993179	9.616397
H	3.664328	11.621090	10.995628
Zr	5.111801	10.891263	8.243589
C	7.352326	10.783349	8.756888
H	7.634317	9.739541	8.974928
H	7.609536	11.386419	9.647302
H	7.986118	11.146012	7.930355

C	5.376890	12.784954	6.517540
C	6.008792	13.230731	7.711996
C	3.742229	13.025864	8.136396
C	5.005769	13.356519	8.723855
C	3.971531	12.658879	6.781931
H	5.867479	12.636882	5.556750
H	7.064021	13.460712	7.829577
H	2.773379	13.066661	8.628490
H	5.165333	13.698490	9.745896
H	3.198552	12.390225	6.065292

Insertion TS

Al	1.176350	5.234075	0.229111
O	3.982716	7.528134	2.911464
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.307452	1.082493	2.473701
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.163850	2.835928	3.030089
Al	8.268006	3.298270	1.704362
Al	4.175972	1.082995	2.473285
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.321701	2.834595	3.030188
Al	4.308924	5.234075	0.229111
O	1.513031	7.517455	2.902253
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951474	1.047657	2.707829
Al	6.949156	6.392276	1.639649
O	6.942841	7.448783	3.116283
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741446	3.754368	2.448399
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949240	2.870941	2.981738
Al	1.176350	13.302075	0.229111
O	3.982997	15.589300	2.903490
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.299307	9.143723	2.472706
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.157348	10.907246	3.036924
Al	8.267993	11.366301	1.704330
Al	4.177793	9.150366	2.463528
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.332152	10.894922	3.034804
Al	4.308924	13.302075	0.229111
O	1.511490	15.590638	2.903039
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.969397	9.106154	2.687701
Al	6.949131	14.460329	1.639677
O	6.941224	15.520574	3.112263
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.735207	11.805309	2.408171
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225

O	6.925538	10.927244	2.996851
Al	9.589350	5.234075	0.229111
O	12.375037	7.567023	2.904014
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.726588	1.098859	2.471534
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578436	2.844404	3.030184
Al	16.680960	3.298306	1.704311
Al	12.587128	1.095413	2.472684
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732779	2.847302	3.030101
Al	12.721924	5.234075	0.229111
O	9.928092	7.572618	2.908375
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.360046	1.051234	2.710317
Al	15.362120	6.392276	1.639649
O	15.367632	7.454709	3.103802
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.157341	3.762579	2.456130
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362176	2.873296	2.980278
Al	9.589350	13.302075	0.229111
O	12.384948	15.610135	2.911819
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.753550	9.222447	2.472381
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.593277	10.922187	3.021467
Al	16.680957	11.366316	1.704306
Al	12.563446	9.217496	2.472747
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.704648	10.926304	3.026487
Al	12.721924	13.302075	0.229111
O	9.917597	15.612899	2.912092
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.343048	9.121584	2.707877
Al	15.362144	14.460329	1.639677
O	15.369166	15.525151	3.106364
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.157293	12.137081	3.102689
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.380304	10.939988	2.981411
C	11.149084	13.077660	4.833316
H	12.096602	13.618598	4.982972
H	10.337808	13.820758	4.880800
H	11.030609	12.341727	5.650483
C	4.016670	9.720983	6.801977
C	5.296901	9.630607	6.192416
H	3.295191	10.400510	6.343888
H	3.593720	8.807248	7.220568
H	5.804000	8.666419	6.161791
H	5.530952	10.311038	5.375769

C	4.085488	10.308043	10.661747
C	4.195152	9.106884	9.898496
C	6.331423	9.803780	10.446681
C	5.585110	8.803603	9.752949
C	5.409625	10.744122	10.998485
H	3.157380	10.783194	10.973576
H	3.364723	8.505658	9.538699
H	7.415969	9.840075	10.540487
H	6.000569	7.936966	9.243184
H	5.664181	11.610287	11.607826
Zr	5.185707	10.999754	8.472687
C	7.090528	10.346972	7.246236
H	7.566391	9.375312	7.412898
H	7.396857	11.007813	8.115249
H	7.490151	10.828811	6.349855
C	4.597680	12.917368	6.826916
C	5.830154	13.271090	7.439333
C	4.198308	13.232715	9.081065
C	5.595442	13.455212	8.841050
C	3.585806	12.886945	7.838657
H	4.453023	12.742562	5.763621
H	6.777123	13.411561	6.920919
H	3.687416	13.350923	10.033953
H	6.329574	13.783712	9.574085
H	2.528235	12.684016	7.679622

Insertion γ-product

Al	1.176350	5.234075	0.229111
O	3.979509	7.530041	2.914519
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.307070	1.082158	2.474009
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.164143	2.836495	3.029866
Al	8.268006	3.298270	1.704362
Al	4.175958	1.083985	2.473379
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.321637	2.834199	3.030189
Al	4.308924	5.234075	0.229111
O	1.509829	7.518503	2.904808
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951475	1.048440	2.708506
Al	6.949156	6.392276	1.639649
O	6.943814	7.451417	3.113977
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741163	3.754820	2.450047
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949151	2.871296	2.981339
Al	1.176350	13.302075	0.229111
O	3.981565	15.591179	2.906307
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.299143	9.142894	2.469767
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.154612	10.901518	3.025695
Al	8.267993	11.366301	1.704330
Al	4.180549	9.146464	2.452271
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014

O	1.334910	10.892667	3.036414
Al	4.308924	13.302075	0.229111
O	1.510724	15.589737	2.901477
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.969107	9.111534	2.693151
Al	6.949131	14.460329	1.639677
O	6.939652	15.521360	3.112400
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.734923	11.806868	2.406602
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.926667	10.932813	2.990488
Al	9.589350	5.234075	0.229111
O	12.374124	7.567453	2.904890
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.726719	1.099135	2.472057
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578686	2.844858	3.030085
Al	16.680960	3.298306	1.704311
Al	12.587129	1.096005	2.473223
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732629	2.847477	3.029985
Al	12.721924	5.234075	0.229111
O	9.930259	7.572185	2.909045
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.359900	1.051333	2.710076
Al	15.362120	6.392276	1.639649
O	15.365409	7.454611	3.103282
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.157275	3.764103	2.459433
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362176	2.872811	2.980242
Al	9.589350	13.302075	0.229111
O	12.384242	15.610391	2.912199
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.752761	9.221879	2.471960
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.594256	10.922722	3.021276
Al	16.680957	11.366316	1.704306
Al	12.563337	9.218222	2.472997
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.706182	10.924568	3.027128
Al	12.721924	13.302075	0.229111
O	9.919099	15.612739	2.912120
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.342947	9.121780	2.709033
Al	15.362144	14.460329	1.639677
O	15.369300	15.524898	3.105103
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201

Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.157079	12.136153	3.105221
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.381096	10.940106	2.981132
C	11.149422	13.069959	4.839496
H	12.085526	13.631986	4.983085
H	10.319659	13.790956	4.903176
H	11.057390	12.324462	5.651757
C	3.605125	9.710638	8.788388
C	3.052003	9.813246	7.332387
H	2.871731	10.096421	9.507578
H	3.811305	8.662282	9.042315
H	2.468900	8.902906	7.101722
H	2.352304	10.654556	7.238136
C	7.245349	10.162754	9.919628
C	6.513543	8.981082	9.578073
C	7.649326	9.701757	7.690643
C	6.751834	8.706327	8.198488
C	7.957511	10.596975	8.753324
H	7.301918	10.612485	10.908691
H	5.880478	8.407629	10.248812
H	8.069468	9.741321	6.686001
H	6.349080	7.865978	7.634291
H	8.650003	11.435059	8.693539
Zr	5.472205	10.918005	8.304442
C	4.098514	9.899472	6.175128
H	4.664517	8.969559	6.042597
H	4.819659	10.766369	6.154235
H	3.575348	10.107591	5.236367
C	3.862643	12.939212	8.149718
C	5.069700	13.321587	7.481582
C	5.553327	12.983169	9.718976
C	6.115318	13.351833	8.451618
C	4.154981	12.732489	9.529912
H	2.882613	12.859659	7.685569
H	5.170443	13.581719	6.426521
H	6.078647	12.971787	10.671265
H	7.148033	13.638360	8.263170
H	3.442269	12.470476	10.307505

Insertion β-product

Al	1.176350	5.234075	0.229111
O	3.978927	7.531195	2.917280
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.307642	1.082225	2.473793
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.164072	2.836183	3.029485
Al	8.268006	3.298270	1.704362
Al	4.176268	1.083725	2.473347
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.321663	2.834471	3.029494
Al	4.308924	5.234075	0.229111
O	1.514309	7.523538	2.908743
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.951522	1.048762	2.708678
Al	6.949156	6.392276	1.639649
O	6.942469	7.451701	3.112371
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741553	3.754413	2.449397

O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.949070	2.871473	2.980852
Al	1.176350	13.302075	0.229111
O	3.980773	15.590643	2.905358
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.300565	9.147842	2.469535
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.157126	10.903792	3.038474
Al	8.267993	11.366301	1.704330
Al	4.179710	9.153102	2.465963
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.329750	10.897810	3.034204
Al	4.308924	13.302075	0.229111
O	1.511440	15.589724	2.901995
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.967411	9.113440	2.696402
Al	6.949131	14.460329	1.639677
O	6.938680	15.521552	3.111624
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.738831	11.812005	2.425040
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.928553	10.932886	2.991509
Al	9.589350	5.234075	0.229111
O	12.373774	7.567368	2.903505
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.726528	1.099089	2.471745
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578600	2.844893	3.029659
Al	16.680960	3.298306	1.704311
Al	12.586635	1.096026	2.472882
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.732439	2.847246	3.029552
Al	12.721924	5.234075	0.229111
O	9.928702	7.572349	2.904141
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.360010	1.054313	2.707024
Al	15.362120	6.392276	1.639649
O	15.367671	7.454617	3.103039
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.156957	3.764999	2.460790
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362236	2.871016	2.978520
Al	9.589350	13.302075	0.229111
O	12.383695	15.610394	2.911714
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.751579	9.221478	2.468311
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013

O	12.594638	10.923194	3.020445
Al	16.680957	11.366316	1.704306
Al	12.562921	9.218647	2.473319
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.707595	10.922125	3.025197
Al	12.721924	13.302075	0.229111
O	9.918377	15.612556	2.911022
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.343253	9.121989	2.708519
Al	15.362144	14.460329	1.639677
O	15.368575	15.530133	3.104560
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.156241	12.135521	3.104108
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.380220	10.939963	2.980759
C	11.146190	13.072888	4.835719
H	12.081355	13.636907	4.977676
H	10.315608	13.793246	4.896541
H	11.055119	12.329839	5.650130
C	3.431841	9.882644	8.893590
C	3.186732	9.712680	7.400243
H	2.683131	10.507504	9.393811
H	3.534538	8.927899	9.419828
H	2.397672	10.389063	7.039896
H	4.091185	10.091163	6.769763
C	7.081642	9.842549	9.697415
C	6.372204	8.781013	9.051114
C	7.539836	9.961526	7.434268
C	6.644520	8.865180	7.648980
C	7.822166	10.555184	8.699625
H	7.111454	10.034807	10.769147
H	5.765299	8.028566	9.548036
H	7.959717	10.272025	6.477016
H	6.292580	8.176083	6.881686
H	8.495849	11.390729	8.880462
Zr	5.354437	10.970178	8.261587
C	2.936448	8.275959	6.897619
H	1.959240	7.938739	7.274645
H	3.700888	7.579550	7.270404
H	2.922222	8.212606	5.800531
C	3.896128	13.059258	7.981170
C	5.123387	13.330113	7.294931
C	5.589989	13.100200	9.553142
C	6.171292	13.358699	8.264417
C	4.180038	12.932766	9.375814
H	2.912366	13.003090	7.519437
H	5.236808	13.521006	6.227135
H	6.117073	13.098151	10.506136
H	7.215792	13.583913	8.059774
H	3.451342	12.767243	10.165481

Ethylene enchainment pathway at the heterogeneous dioxo-bridged zirconocenium μ_2-O site.

π-complex

Al	1.176350	5.234075	0.229111
O	4.069476	7.490350	2.810088
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.305496	1.079634	2.476009
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.162532	2.836383	3.028346

Al	8.268006	3.298270	1.704362
Al	4.179060	1.079454	2.475894
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.322762	2.835985	3.027163
Al	4.308924	5.234075	0.229111
O	1.539393	7.547274	2.932639
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.952640	1.051199	2.711005
Al	6.949156	6.392276	1.639649
O	6.964725	7.452739	3.115750
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.742289	3.730110	2.404274
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.947715	2.875065	2.982471
Al	1.176350	13.302075	0.229111
O	3.973946	15.587651	2.900728
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.298857	9.154023	2.458111
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.153898	10.890693	3.029235
Al	8.267993	11.366301	1.704330
Al	4.181744	9.145326	2.443763
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.328121	10.900445	3.031749
Al	4.308924	13.302075	0.229111
O	1.510189	15.587653	2.901833
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.970527	9.117418	2.699317
Al	6.949131	14.460329	1.639677
O	6.941145	15.525499	3.105879
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.742547	11.819445	2.439954
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.928279	10.934318	2.983816
Al	9.589350	5.234075	0.229111
O	12.377974	7.568167	2.902842
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.725946	1.098001	2.473631
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.579284	2.846785	3.030533
Al	16.680960	3.298306	1.704311
Al	12.585740	1.097722	2.473705
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.731608	2.847284	3.030555
Al	12.721924	5.234075	0.229111
O	9.941041	7.570255	2.907774
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.358755	1.051756	2.711550

Al	15.362120	6.392276	1.639649
O	15.373639	7.452514	3.108312
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.155796	3.764905	2.461087
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.363246	2.875243	2.981381
Al	9.589350	13.302075	0.229111
O	12.384832	15.611921	2.912381
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.750943	9.221842	2.475340
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.596964	10.924887	3.019098
Al	16.680957	11.366316	1.704306
Al	12.560373	9.221711	2.474593
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.710779	10.924770	3.021022
Al	12.721924	13.302075	0.229111
O	9.924911	15.611898	2.912003
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.340559	9.120395	2.708566
Al	15.362144	14.460329	1.639677
O	15.369219	15.525994	3.105318
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.154802	12.137636	3.116150
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.381439	10.937307	2.981232
C	3.945814	8.294538	5.385955
C	2.681794	8.781074	5.587450
H	4.115182	7.319381	4.939070
H	4.829915	8.905035	5.582776
H	2.503296	9.823336	5.859691
H	1.832894	8.188315	5.230597
C	4.763710	8.365477	9.077686
C	4.319697	9.527010	8.381354
C	2.714546	8.997744	9.952410
C	3.046794	9.904065	8.904108
C	3.770395	8.038633	10.059669
H	5.712136	7.853350	8.925150
H	4.864017	10.051128	7.599163
H	1.813384	9.032779	10.559889
H	2.446286	10.748327	8.572466
H	3.842926	7.244853	10.799903
Zr	2.691968	7.570206	7.840541
C	0.479389	8.163164	7.987941
C	11.151580	13.078714	4.842216
H	0.401371	9.262496	7.940347
H	16.800688	7.838055	8.912532
H	16.751679	7.734169	7.136302
H	12.039782	13.720526	4.941409
H	10.261703	13.718788	4.938373
H	11.151682	12.330323	5.656422
C	2.069767	5.469273	6.486271
C	1.416862	5.367375	7.747436
C	3.702074	5.220581	8.107017
C	2.424020	5.240085	8.756030
C	3.483258	5.360671	6.708718
H	1.573561	5.583758	5.523915

H	0.343452	5.364641	7.910450
H	4.667110	5.097601	8.594101
H	2.244222	5.108706	9.821064
H	4.257201	5.341918	5.942685

Insertion TS

Al	1.176350299	5.234075196	0.229111121
O	3.994075617	7.526821192	2.906678265
O	8.279943566	5.109619934	1.489066697
O	4.160379792	7.058908786	0.084507049
Al	5.630314839	3.298305565	1.704311452
Al	1.305719445	1.078072529	2.473852671
O	4.051770683	3.415890404	0.556335967
O	8.285938069	1.351566857	1.443000651
O	4.160935190	2.835193065	3.030830894
Al	8.268005601	3.298270256	1.704362144
Al	4.179091275	1.078708979	2.473786961
O	1.433503645	3.415890404	0.556335967
O	5.612410853	1.351574998	1.442999961
O	1.323781550	2.834014815	3.030234092
Al	4.308924029	5.234075196	0.229111121
O	1.511591346	7.532267884	2.920928713
O	5.618390615	5.109640648	1.489002166
O	1.324894536	7.058908786	0.084507049
Al	6.949137164	1.225769999	0.009444148
Al	6.952630907	1.049437336	2.708843291
Al	6.949156014	6.392276180	1.639649299
O	6.943457574	7.451480569	3.111840151
O	6.949137164	7.354508637	0.120802639
Al	2.742637313	7.151819943	1.460390342
Al	2.742637164	2.332601337	0.000000000
O	2.742637013	1.138213546	1.294012542
Al	2.741626520	3.730586643	2.403496417
O	2.742637264	5.289564588	1.533309110
O	6.949137164	3.103569407	0.223225080
O	6.947406478	2.873533303	2.982990050
Al	1.176350299	13.302075196	0.229111121
O	3.977638224	15.587805364	2.902405755
O	8.279907605	13.177619866	1.489021650
O	4.160379792	15.126908786	0.084507049
Al	5.630317443	11.366315731	1.704304642
Al	1.300983308	9.149201483	2.459925092
O	4.051770683	11.483890404	0.556335967
O	8.285924732	9.419561855	1.443037140
O	4.153020159	10.893059165	3.038477894
Al	8.267992577	11.366301130	1.704330004
Al	4.182358649	9.150002141	2.453501045
O	1.433503645	11.483890404	0.556335967
O	5.612364582	9.419559818	1.443013878
O	1.330919908	10.895056057	3.037732239
Al	4.308924029	13.302075196	0.229111121
O	1.508044096	15.587110628	2.901920997
O	5.618392812	13.177626445	1.489012429
O	1.324894536	15.126908786	0.084507049
Al	6.949137164	9.293769999	0.009444148
Al	6.969546646	9.117774148	2.703454214
Al	6.949131342	14.460329344	1.639676587
O	6.941245719	15.524736187	3.107276868
O	6.949137164	15.422508637	0.120802639
Al	2.742636897	15.219709386	1.461134276
Al	2.742637164	10.400601337	0.000000000
O	2.742637500	9.205981130	1.293822924
Al	2.741964227	11.817650217	2.438541023

O	2.742636431	13.357530466	1.533509586
O	6.949137164	11.171569407	0.223225080
O	6.928461196	10.935200898	2.983255266
Al	9.589350299	5.234075196	0.229111121
O	12.377310533	7.569498054	2.905475602
O	16.692887290	5.109641938	1.489004758
O	12.573379792	7.058908786	0.084507049
Al	14.043268490	3.298270665	1.704362281
Al	9.725724018	1.096873516	2.472552702
O	12.464770683	3.415890404	0.556335967
O	16.698863209	1.351575018	1.442999934
O	12.578956770	2.846363263	3.030413409
Al	16.680959550	3.298305505	1.704311173
Al	12.585688341	1.097035015	2.472481888
O	9.846503645	3.415890404	0.556335967
O	14.025336008	1.351566791	1.443000847
O	9.732059173	2.846460516	3.030380983
Al	12.721924029	5.234075196	0.229111121
O	9.933638497	7.569368510	2.905480495
O	14.031331841	5.109619873	1.489065963
O	9.737894536	7.058908786	0.084507049
Al	15.362137164	1.225769999	0.009444148
Al	15.358583097	1.049845684	2.709138390
Al	15.362120285	6.392275817	1.639649169
O	15.369487880	7.451903748	3.109983235
O	15.362137164	7.354508637	0.120802639
Al	11.155637456	7.151831933	1.460428379
Al	11.155637164	2.332601337	0.000000000
O	11.155636911	1.137919867	1.293822601
Al	11.155689496	3.761570997	2.453697509
O	11.155635990	5.289551426	1.533342776
O	15.362137164	3.103569407	0.223225080
O	15.363569631	2.873676426	2.982533294
Al	9.589350299	13.302075196	0.229111121
O	12.388080953	15.611728237	2.911368591
O	16.692882543	13.177626236	1.489013917
O	12.573379792	15.126908786	0.084507049
Al	14.043282200	11.366301275	1.704329925
Al	9.750819269	9.221241793	2.473267016
O	12.464770683	11.483890404	0.556335967
O	16.698910754	9.419558814	1.443013013
O	12.598094050	10.924829677	3.020722469
Al	16.680957299	11.366315546	1.704305506
Al	12.560758115	9.221472021	2.473516752
O	9.846503645	11.483890404	0.556335967
O	14.025350740	9.419562696	1.443038333
O	9.712109761	10.924303240	3.021100045
Al	12.721924029	13.302075196	0.229111121
O	9.923144383	15.611507561	2.911502329
O	14.031368382	13.177619336	1.489020106
O	9.737894536	15.126908786	0.084507049
Al	15.362137164	9.293769999	0.009444148
Al	15.342061353	9.118705178	2.704921353
Al	15.362144028	14.460329281	1.639676584
O	15.369989876	15.525019792	3.106948100
O	15.362137164	15.422508637	0.120802639
Al	11.155636872	15.219891639	1.460200573
Al	11.155637164	10.400601337	0.000000000
O	11.155637610	9.205963598	1.293836596
Al	11.155107123	12.137779070	3.110583206
O	11.155640063	13.357593389	1.533293904
O	15.362137164	11.171569407	0.223225080
O	15.382104485	10.936105879	2.982584252

C	4.957485498	7.384296748	7.073405225
C	4.100892537	7.790836648	6.013857317
H	5.361968534	6.371387650	7.024866491
H	5.649641925	8.127984558	7.474900956
H	4.035157710	8.856664029	5.793627734
H	3.915030216	7.155451781	5.145086502
C	3.675842864	9.125988566	10.183723675
C	3.985469465	9.759648790	8.942250755
C	1.685099968	9.586232849	9.102252383
C	2.757417862	10.031054733	8.266083364
C	2.249086789	9.029866121	10.287752355
H	4.395078752	8.813894068	10.938222990
H	4.978030965	10.033910488	8.594035998
H	0.623551923	9.690351873	8.881088284
H	2.649608618	10.544823436	7.314051842
H	1.696599445	8.628254138	11.135175867
Zr	2.941550743	7.473080198	8.385008358
C	1.924013468	7.658493035	6.305884187
C	11.152854603	13.080460024	4.837320763
H	1.735365830	8.590109387	5.768980842
H	1.151261730	7.631052573	7.143367173
H	1.717559437	6.812560583	5.644981280
H	12.024463603	13.746752360	4.924070577
H	10.248315568	13.698547045	4.947200988
H	11.180563803	12.336331322	5.655729986
C	2.989391057	4.915327873	8.043842966
C	1.664484482	5.229794076	8.462784828
C	3.103879318	5.721442986	10.207351591
C	1.729803148	5.748730281	9.793498688
C	3.879175057	5.207908458	9.126424180
H	3.273153309	4.487817533	7.083186479
H	0.757589956	5.091298260	7.875712173
H	3.481708316	6.010027107	11.186692375
H	0.880530905	6.045324745	10.406369835
H	4.951661637	5.027471862	9.139060020

Insertion γ-product

Al	1.176350	5.234075	0.229111
O	4.021281	7.532409	2.897030
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.304848	1.075957	2.474516
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.160861	2.837741	3.029787
Al	8.268006	3.298270	1.704362
Al	4.178827	1.080172	2.475456
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.323017	2.831830	3.030491
Al	4.308924	5.234075	0.229111
O	1.528668	7.537234	2.931703
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.952261	1.049192	2.709120
Al	6.949156	6.392276	1.639649
O	6.951214	7.449924	3.116104
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.739119	3.728676	2.401265
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225

O	6.947043	2.874204	2.983226
Al	1.176350	13.302075	0.229111
O	3.979589	15.590908	2.909244
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.299172	9.148890	2.467041
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.152260	10.898711	3.039552
Al	8.267993	11.366301	1.704330
Al	4.179940	9.160384	2.452277
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.328324	10.897416	3.036775
Al	4.308924	13.302075	0.229111
O	1.511223	15.585047	2.900238
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.969479	9.116261	2.701241
Al	6.949131	14.460329	1.639677
O	6.943710	15.524333	3.106623
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.738598	11.821830	2.443391
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.927604	10.933035	2.983440
Al	9.589350	5.234075	0.229111
O	12.377245	7.568859	2.904295
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.725679	1.097060	2.472830
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.579206	2.845933	3.030184
Al	16.680960	3.298306	1.704311
Al	12.585880	1.096583	2.472991
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.731665	2.846899	3.029949
Al	12.721924	5.234075	0.229111
O	9.934123	7.569159	2.905197
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.358247	1.051373	2.707594
Al	15.362120	6.392276	1.639649
O	15.369730	7.452303	3.108775
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.156163	3.762110	2.455091
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.363436	2.873318	2.981817
Al	9.589350	13.302075	0.229111
O	12.388223	15.610752	2.910586
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.750968	9.221179	2.473858
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.597421	10.924329	3.020306
Al	16.680957	11.366316	1.704306

Al	12.560672	9.221145	2.473573
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.710969	10.924408	3.020299
Al	12.721924	13.302075	0.229111
O	9.924839	15.611651	2.911887
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.341100	9.118981	2.704852
Al	15.362144	14.460329	1.639677
O	15.370888	15.525737	3.105746
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.154816	12.137396	3.111526
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.381344	10.936218	2.982299
C	5.219764	7.154042	7.938100
C	4.958947	7.328258	6.399329
H	5.559579	6.135583	8.168862
H	5.970633	7.870284	8.285192
H	5.132923	8.367991	6.099246
H	5.705968	6.724277	5.858089
C	2.847032	9.434663	9.710615
C	3.852119	9.785344	8.756145
C	1.819815	9.661764	7.653568
C	3.221312	9.912874	7.485831
C	1.587551	9.372618	9.028646
H	3.004980	9.300005	10.778850
H	4.900313	9.964741	8.977202
H	1.060534	9.727776	6.874399
H	3.701041	10.218519	6.558555
H	0.621621	9.171100	9.488660
Zr	3.004108	7.438772	8.171829
C	3.600917	6.849078	5.757824
C	11.152174	13.078412	4.838508
H	3.664397	7.067962	4.662411
H	2.641332	7.407319	5.975583
H	3.422911	5.772927	5.871710
H	12.022970	13.745633	4.925601
H	10.246732	13.694781	4.950176
H	11.181597	12.333289	5.655756
C	2.974870	4.891484	8.550769
C	1.648459	5.248521	8.156944
C	2.090490	6.243153	10.194738
C	1.099000	6.087498	9.170243
C	3.251152	5.501274	9.810155
H	3.653188	4.247642	7.994781
H	1.145391	4.930766	7.244310
H	1.960698	6.784012	11.130036
H	0.095768	6.509435	9.172798
H	4.169136	5.396831	10.384084

Insertion β-product

Al	1.176350	5.234075	0.229111
O	3.985017	7.534727	2.934583
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.305075	1.077256	2.475009
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.162286	2.837309	3.031057
Al	8.268006	3.298270	1.704362
Al	4.178472	1.079549	2.473873
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000

O	1.323747	2.834489	3.031252
Al	4.308924	5.234075	0.229111
O	1.511747	7.530759	2.923735
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.952529	1.049377	2.708441
Al	6.949156	6.392276	1.639649
O	6.940713	7.451236	3.111515
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741041	3.731437	2.404548
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.946651	2.875933	2.983579
Al	1.176350	13.302075	0.229111
O	3.979461	15.587697	2.904646
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.300850	9.148608	2.462690
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.154050	10.895466	3.037711
Al	8.267993	11.366301	1.704330
Al	4.180721	9.150756	2.457861
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.329245	10.894706	3.035852
Al	4.308924	13.302075	0.229111
O	1.510288	15.586264	2.900387
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.969413	9.117881	2.699738
Al	6.949131	14.460329	1.639677
O	6.942171	15.525091	3.106802
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.740109	11.822044	2.446540
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.928061	10.933631	2.983826
Al	9.589350	5.234075	0.229111
O	12.375701	7.569532	2.904054
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.726345	1.096558	2.473213
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578946	2.845783	3.030066
Al	16.680960	3.298306	1.704311
Al	12.586222	1.095940	2.473323
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.730818	2.847732	3.030285
Al	12.721924	5.234075	0.229111
O	9.927496	7.567517	2.904189
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.358510	1.052320	2.707287
Al	15.362120	6.392276	1.639649
O	15.371943	7.452753	3.110021
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428

Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.156344	3.761297	2.453514
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.363962	2.872011	2.980216
Al	9.589350	13.302075	0.229111
O	12.386910	15.610353	2.909855
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.751793	9.220666	2.474498
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.597451	10.925079	3.019793
Al	16.680957	11.366316	1.704306
Al	12.561558	9.221429	2.474947
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.711231	10.924081	3.020035
Al	12.721924	13.302075	0.229111
O	9.923255	15.610780	2.911098
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.341789	9.119533	2.704944
Al	15.362144	14.460329	1.639677
O	15.369892	15.529541	3.102388
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.155076	12.138228	3.111544
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.381890	10.936272	2.981223
C	5.436759	6.936410	7.973485
C	5.561168	6.691870	6.473110
H	5.676201	6.045110	8.565565
H	6.026637	7.788572	8.326172
H	4.529312	6.603914	5.951079
H	5.986969	7.555107	5.948157
C	3.061730	9.465575	8.886851
C	4.049086	9.718158	7.887285
C	2.015566	9.412014	6.822467
C	3.411367	9.666450	6.612248
C	1.799778	9.295574	8.228467
H	3.230543	9.456204	9.962793
H	5.094512	9.953090	8.066118
H	1.253227	9.341445	6.048554
H	3.889949	9.861907	5.654936
H	0.841317	9.139676	8.719210
Zr	3.223581	7.310489	7.537759
C	6.287188	5.402765	6.041616
C	11.142435	13.080909	4.836863
H	6.200220	5.239969	4.962606
H	5.896069	4.524799	6.574295
H	7.354025	5.502637	6.287979
H	11.972158	13.800395	4.906863
H	10.203993	13.641720	4.967262
H	11.232243	12.341168	5.653243
C	2.860368	4.773289	7.601416
C	1.638722	5.339593	7.116851
C	1.952655	6.053437	9.293633
C	1.077488	6.129260	8.159178
C	3.045892	5.198808	8.951683
H	3.506812	4.093237	7.051879
H	1.205845	5.202772	6.125410
H	1.783305	6.517121	10.265526
H	0.132637	6.664373	8.104712
H	3.855025	4.905882	9.614814

Ethylene enchainment pathway at the heterogeneous oxo-bridged zirconocenium μ_2-O site.

π-complex

Al	1.176350	5.234075	0.229111
O	5.273349	8.800641	4.022634
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.302395	1.069942	2.475335
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.165579	2.830575	3.028860
Al	8.268006	3.298270	1.704362
Al	4.184355	1.072011	2.475816
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.316779	2.829155	3.027474
Al	4.308924	5.234075	0.229111
O	2.485870	7.898890	3.162549
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.953735	1.055024	2.711905
Al	6.949156	6.392276	1.639649
O	7.246601	7.399613	3.047872
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741653	3.702764	2.403823
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.945831	2.877462	2.979864
Al	1.176350	13.302075	0.229111
O	3.967568	15.586486	2.908810
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.351210	9.164902	2.485042
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.106607	11.056526	3.031211
Al	8.267993	11.366301	1.704330
Al	4.150790	9.242765	2.782443
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.295001	10.895539	3.050453
Al	4.308924	13.302075	0.229111
O	1.500489	15.577314	2.895604
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.720682	9.094788	2.943817
Al	6.949131	14.460329	1.639677
O	6.943279	15.531822	3.108562
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.686632	11.864595	2.454926
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.942768	10.993382	2.963735
Al	9.589350	5.234075	0.229111
O	12.476285	7.565803	2.870254
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362

Al	9.724538	1.096999	2.473607
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.578963	2.850447	3.027956
Al	16.680960	3.298306	1.704311
Al	12.583736	1.099673	2.474508
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.730691	2.844429	3.032207
Al	12.721924	5.234075	0.229111
O	10.055639	7.576951	2.959266
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.356577	1.051939	2.710725
Al	15.362120	6.392276	1.639649
O	15.662892	7.480453	3.083037
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.150711	3.763960	2.458579
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.362468	2.877521	2.978976
Al	9.589350	13.302075	0.229111
O	12.390051	15.612540	2.911344
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.674537	9.194808	2.469004
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.618461	10.937779	3.021004
Al	16.680957	11.366316	1.704306
Al	12.530624	9.240922	2.473463
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.745491	10.905726	3.030236
Al	12.721924	13.302075	0.229111
O	9.932300	15.614413	2.918110
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.330540	9.134289	2.709246
Al	15.362144	14.460329	1.639677
O	15.369571	15.529662	3.105362
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.148447	12.126228	3.117107
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.379885	10.941830	2.979846
C	4.113166	11.008107	6.987525
C	5.306425	10.734879	6.394412
H	3.961479	11.899426	7.598980
H	3.219131	10.419042	6.750766
H	5.394304	9.940694	5.633263
H	6.167627	11.390482	6.556464
C	3.780261	7.157385	8.115857
C	4.370422	7.462838	6.851398
C	6.028382	6.609400	8.210580
C	5.753941	7.128124	6.911557
C	4.808601	6.622107	8.959137
H	2.726196	7.260716	8.371869
H	3.877859	7.844368	5.960156
H	6.991185	6.242222	8.560436
H	6.452364	7.227908	6.082623
H	4.674482	6.238842	9.968542

Zr	5.376172	9.036998	8.619037
C	7.643826	9.263950	8.378842
H	7.927799	8.960493	7.357534
H	8.261824	8.675449	9.077575
H	7.914139	10.325687	8.514910
C	5.251969	11.084154	10.186579
C	6.151686	10.169268	10.797804
C	4.040579	9.215907	10.803342
C	5.413607	8.995995	11.151602
C	3.940323	10.497367	10.200958
H	5.506936	12.077297	9.819124
H	7.214142	10.325643	10.959216
H	3.215493	8.531263	10.990502
H	5.816502	8.122609	11.660346
H	3.022803	10.968370	9.854374
C	11.159065	13.087568	4.834855
H	12.047486	13.730984	4.924159
H	10.269436	13.729438	4.926198
H	11.161036	12.349332	5.659491

Insertion TS

Al	1.176350	5.234075	0.229111
O	5.269710	8.827352	4.035403
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.302532	1.068730	2.474824
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.165727	2.831248	3.028743
Al	8.268006	3.298270	1.704362
Al	4.184029	1.071747	2.475007
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.318051	2.828824	3.028423
Al	4.308924	5.234075	0.229111
O	2.486594	7.896696	3.160718
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.953896	1.054389	2.711170
Al	6.949156	6.392276	1.639649
O	7.230207	7.400290	3.049231
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741742	3.700526	2.399640
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.945989	2.877006	2.980224
Al	1.176350	13.302075	0.229111
O	3.968388	15.586374	2.909113
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.350042	9.163464	2.484900
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.099529	11.058386	3.034652
Al	8.267993	11.366301	1.704330
Al	4.146788	9.243213	2.785085
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.290095	10.896336	3.046318
Al	4.308924	13.302075	0.229111
O	1.500732	15.576929	2.896351
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.715205	9.097665	2.944452

Al	6.949131	14.460329	1.639677
O	6.942273	15.531465	3.109193
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.680881	11.864093	2.452426
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.942345	10.995461	2.964832
Al	9.589350	5.234075	0.229111
O	12.483315	7.564569	2.869068
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.724852	1.096188	2.472576
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.579270	2.849736	3.028180
Al	16.680960	3.298306	1.704311
Al	12.584136	1.099199	2.473055
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.731704	2.843514	3.032132
Al	12.721924	5.234075	0.229111
O	10.057103	7.578274	2.961256
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.357011	1.051552	2.709546
Al	15.362120	6.392276	1.639649
O	15.667984	7.480828	3.084846
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.151036	3.762272	2.455143
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.363685	2.878351	2.979146
Al	9.589350	13.302075	0.229111
O	12.391396	15.613163	2.911616
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.673901	9.193245	2.468146
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.616162	10.936288	3.022093
Al	16.680957	11.366316	1.704306
Al	12.531117	9.239373	2.473125
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.743259	10.905410	3.031010
Al	12.721924	13.302075	0.229111
O	9.930664	15.613531	2.916953
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.330787	9.133634	2.708829
Al	15.362144	14.460329	1.639677
O	15.371041	15.526589	3.105732
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.147328	12.124296	3.114044
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.379451	10.941853	2.979686
C	3.401780	9.929399	7.529476

C	4.356370	10.536638	6.673062
H	2.867234	10.564050	8.239571
H	2.821901	9.102131	7.117070
H	4.577577	10.086567	5.699298
H	4.548533	11.606103	6.765290
C	4.727224	6.511657	8.776909
C	4.341781	6.905406	7.457122
C	6.640198	7.020986	7.579762
C	5.519960	7.238702	6.719506
C	6.158230	6.584955	8.853620
H	4.056415	6.165062	9.562077
H	3.330048	6.898425	7.056760
H	7.684906	7.151058	7.299100
H	5.545441	7.582063	5.677895
H	6.768969	6.301850	9.709354
Zr	5.329984	8.960392	8.610019
C	6.511776	10.327630	7.160202
H	6.754746	10.133468	6.113166
H	7.231016	9.686835	7.766640
H	6.720138	11.370780	7.415977
C	4.995527	10.988829	10.197323
C	6.352476	10.587996	10.341082
C	5.015036	8.877876	11.137445
C	6.371399	9.271691	10.903780
C	4.164938	9.935572	10.695717
H	4.652728	11.938933	9.791253
H	7.226421	11.177805	10.068795
H	4.689706	7.950611	11.603785
H	7.261640	8.703456	11.170449
H	3.077609	9.947884	10.752352
C	11.157296	13.082461	4.836123
H	12.033752	13.742650	4.919962
H	10.256100	13.706440	4.940504
H	11.180757	12.340537	5.657289

Insertion γ-product

Al	1.176350	5.234075	0.229111
O	5.262743	8.790721	4.011173
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.302623	1.068854	2.474775
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.165724	2.831408	3.028892
Al	8.268006	3.298270	1.704362
Al	4.183877	1.071927	2.475182
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.317934	2.828381	3.028544
Al	4.308924	5.234075	0.229111
O	2.480184	7.893635	3.158409
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507
Al	6.949137	1.225770	0.009444
Al	6.953887	1.054475	2.711499
Al	6.949156	6.392276	1.639649
O	7.249869	7.399877	3.047897
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741427	3.701566	2.401849
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.945900	2.877068	2.980021
Al	1.176350	13.302075	0.229111
O	3.969263	15.586102	2.908760
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507

Al	5.630317	11.366316	1.704305
Al	1.347066	9.159929	2.485733
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.099357	11.054019	3.037922
Al	8.267993	11.366301	1.704330
Al	4.146149	9.234779	2.771367
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.293063	10.894221	3.046304
Al	4.308924	13.302075	0.229111
O	1.501735	15.577157	2.896685
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.714269	9.091698	2.943651
Al	6.949131	14.460329	1.639677
O	6.942263	15.531134	3.109190
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.682136	11.856003	2.437494
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.938651	10.993409	2.967331
Al	9.589350	5.234075	0.229111
O	12.480986	7.564959	2.869873
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.724941	1.096486	2.472802
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.579242	2.849902	3.028200
Al	16.680960	3.298306	1.704311
Al	12.583946	1.099548	2.473015
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.731525	2.843624	3.032049
Al	12.721924	5.234075	0.229111
O	10.058481	7.579595	2.963967
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.356942	1.051867	2.710628
Al	15.362120	6.392276	1.639649
O	15.667206	7.481276	3.084179
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.150910	3.763164	2.457171
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225
O	15.363588	2.878606	2.978740
Al	9.589350	13.302075	0.229111
O	12.390154	15.613546	2.912068
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.673851	9.193797	2.467950
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.616151	10.936487	3.022332
Al	16.680957	11.366316	1.704306
Al	12.530930	9.239724	2.473229
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.742713	10.906046	3.031584
Al	12.721924	13.302075	0.229111

O	9.930194	15.613435	2.916786
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.330183	9.133927	2.709498
Al	15.362144	14.460329	1.639677
O	15.371044	15.526134	3.105823
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.147799	12.125072	3.114484
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.380101	10.942100	2.979935
C	3.283379	9.540914	8.231690
C	3.536249	10.027697	6.764268
H	2.880001	10.352159	8.854374
H	2.569603	8.707955	8.241237
H	3.473514	9.188710	6.060298
H	2.727099	10.729429	6.502960
C	5.487074	6.803569	8.978271
C	4.771418	6.927113	7.745720
C	6.974638	7.494509	7.352282
C	5.685183	7.371621	6.740773
C	6.859496	7.132094	8.724050
H	5.070981	6.460895	9.925256
H	3.721133	6.694955	7.593642
H	7.894002	7.778105	6.838977
H	5.467022	7.593533	5.689115
H	7.667302	7.092653	9.453994
Zr	5.508180	9.257686	8.441534
C	4.850053	10.819166	6.417486
H	4.841837	11.026173	5.338077
H	5.828408	10.258676	6.448272
H	4.953190	11.770598	6.953613
C	5.372871	11.437947	9.817612
C	6.731913	11.309484	9.398299
C	6.250742	9.564965	10.834261
C	7.278922	10.148775	10.025280
C	5.072639	10.365268	10.707434
H	4.681726	12.220261	9.511769
H	7.263481	11.979679	8.723933
H	6.360027	8.689866	11.471850
H	8.302489	9.793942	9.927409
H	4.124521	10.198534	11.214165
C	11.158223	13.083937	4.836448
H	12.039352	13.737667	4.922598
H	10.261928	13.715555	4.936497
H	11.174458	12.343288	5.659059

Insertion β-product

Al	1.176350	5.234075	0.229111
O	5.262440	8.791735	4.024702
O	8.279944	5.109620	1.489067
O	4.160380	7.058909	0.084507
Al	5.630315	3.298306	1.704311
Al	1.303137	1.068927	2.474908
O	4.051771	3.415890	0.556336
O	8.285938	1.351567	1.443001
O	4.165728	2.831391	3.028704
Al	8.268006	3.298270	1.704362
Al	4.184142	1.072029	2.475289
O	1.433504	3.415890	0.556336
O	5.612411	1.351575	1.443000
O	1.317933	2.828509	3.028201
Al	4.308924	5.234075	0.229111
O	2.475962	7.893977	3.159231
O	5.618391	5.109641	1.489002
O	1.324895	7.058909	0.084507

Al	6.949137	1.225770	0.009444
Al	6.953931	1.055206	2.712003
Al	6.949156	6.392276	1.639649
O	7.244810	7.403321	3.048185
O	6.949137	7.354509	0.120803
Al	2.742637	7.151820	1.460390
Al	2.742637	2.332601	0.000000
O	2.742637	1.138214	1.294013
Al	2.741548	3.702141	2.402673
O	2.742637	5.289565	1.533309
O	6.949137	3.103569	0.223225
O	6.945869	2.877552	2.979660
Al	1.176350	13.302075	0.229111
O	3.968162	15.586251	2.908958
O	8.279908	13.177620	1.489022
O	4.160380	15.126909	0.084507
Al	5.630317	11.366316	1.704305
Al	1.349146	9.162647	2.483793
O	4.051771	11.483890	0.556336
O	8.285925	9.419562	1.443037
O	4.101287	11.056088	3.031730
Al	8.267993	11.366301	1.704330
Al	4.147965	9.242403	2.784396
O	1.433504	11.483890	0.556336
O	5.612365	9.419560	1.443014
O	1.291035	10.896691	3.044199
Al	4.308924	13.302075	0.229111
O	1.502139	15.576825	2.896193
O	5.618393	13.177626	1.489012
O	1.324895	15.126909	0.084507
Al	6.949137	9.293770	0.009444
Al	6.711393	9.099581	2.954787
Al	6.949131	14.460329	1.639677
O	6.942770	15.532067	3.108245
O	6.949137	15.422509	0.120803
Al	2.742637	15.219709	1.461134
Al	2.742637	10.400601	0.000000
O	2.742638	9.205981	1.293823
Al	2.683892	11.857729	2.441794
O	2.742636	13.357530	1.533510
O	6.949137	11.171569	0.223225
O	6.941882	10.995363	2.963921
Al	9.589350	5.234075	0.229111
O	12.474632	7.566331	2.871601
O	16.692887	5.109642	1.489005
O	12.573380	7.058909	0.084507
Al	14.043268	3.298271	1.704362
Al	9.724737	1.096362	2.472867
O	12.464771	3.415890	0.556336
O	16.698863	1.351575	1.443000
O	12.579254	2.850181	3.027884
Al	16.680960	3.298306	1.704311
Al	12.583439	1.099730	2.473280
O	9.846504	3.415890	0.556336
O	14.025336	1.351567	1.443001
O	9.731434	2.843545	3.031924
Al	12.721924	5.234075	0.229111
O	10.051208	7.578587	2.959335
O	14.031332	5.109620	1.489066
O	9.737895	7.058909	0.084507
Al	15.362137	1.225770	0.009444
Al	15.357086	1.053965	2.707273
Al	15.362120	6.392276	1.639649
O	15.661472	7.480394	3.084448
O	15.362137	7.354509	0.120803
Al	11.155637	7.151832	1.460428
Al	11.155637	2.332601	0.000000
O	11.155637	1.137920	1.293823
Al	11.150698	3.764036	2.458696
O	11.155636	5.289551	1.533343
O	15.362137	3.103569	0.223225

O	15.363634	2.875768	2.977915
Al	9.589350	13.302075	0.229111
O	12.389584	15.613365	2.911439
O	16.692883	13.177626	1.489014
O	12.573380	15.126909	0.084507
Al	14.043282	11.366301	1.704330
Al	9.672403	9.193750	2.465667
O	12.464771	11.483890	0.556336
O	16.698911	9.419559	1.443013
O	12.617349	10.937334	3.021883
Al	16.680957	11.366316	1.704306
Al	12.530574	9.240718	2.473239
O	9.846504	11.483890	0.556336
O	14.025351	9.419563	1.443038
O	9.746078	10.902974	3.029446
Al	12.721924	13.302075	0.229111
O	9.931091	15.613306	2.916714
O	14.031368	13.177619	1.489020
O	9.737895	15.126909	0.084507
Al	15.362137	9.293770	0.009444
Al	15.330756	9.133909	2.709182
Al	15.362144	14.460329	1.639677
O	15.370855	15.530510	3.104785
O	15.362137	15.422509	0.120803
Al	11.155637	15.219892	1.460201
Al	11.155637	10.400601	0.000000
O	11.155638	9.205964	1.293837
Al	11.147106	12.124221	3.114250
O	11.155640	13.357593	1.533294
O	15.362137	11.171569	0.223225
O	15.379855	10.942034	2.979936
C	3.205495	9.427547	8.202454
C	3.572155	10.104866	6.888319
H	2.731029	10.103989	8.924660
H	2.600350	8.524908	8.073375
H	4.716221	10.288511	6.796029
H	3.420431	9.441409	6.028691
C	5.519594	6.669130	8.952057
C	4.804652	6.796880	7.717084
C	6.991547	7.435694	7.341842
C	5.709461	7.288551	6.723657
C	6.881153	7.047345	8.710411
H	5.113321	6.296116	9.892274
H	3.761459	6.539719	7.555175
H	7.903731	7.756483	6.839269
H	5.485638	7.530424	5.677551
H	7.687227	7.019551	9.443451
Zr	5.466934	9.130578	8.440200
C	2.970284	11.499161	6.626719
H	3.467236	11.988046	5.778566
H	3.047438	12.152996	7.507229
H	1.902542	11.386514	6.387967
C	5.418252	11.469438	9.523171
C	6.760539	11.244384	9.085433
C	6.270036	9.704069	10.743990
C	7.293612	10.159377	9.842911
C	5.115813	10.528715	10.550029
H	4.748299	12.243685	9.155662
H	7.290085	11.820095	8.325939
H	6.378245	8.918314	11.489467
H	8.299905	9.754451	9.758092
H	4.174272	10.447132	11.087647
C	11.156045	13.081045	4.837039
H	12.025233	13.750793	4.919025
H	10.248087	13.694042	4.948412
H	11.191769	12.337563	5.656095