

SUPPORTING INFORMATION

FOR

Al-Alkenyl-Induced Formation of Long-Chain Branched Polyethylene via Coordinative Tandem Insertion and Chain-Transfer Polymerization Using $(n\text{BuCp})_2\text{ZrCl}_2/\text{MAO}$ Systems: An Experimental and Theoretical Study

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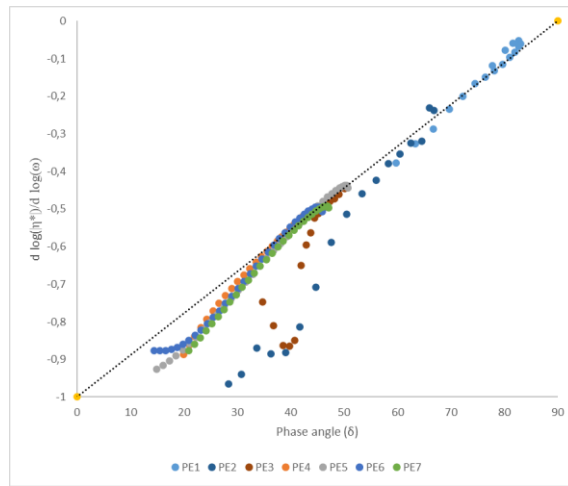


Figure S1. $d \log|\eta^*|/d \log \omega$ vs. δ plot of the data series for entries **PE1-PE3**.

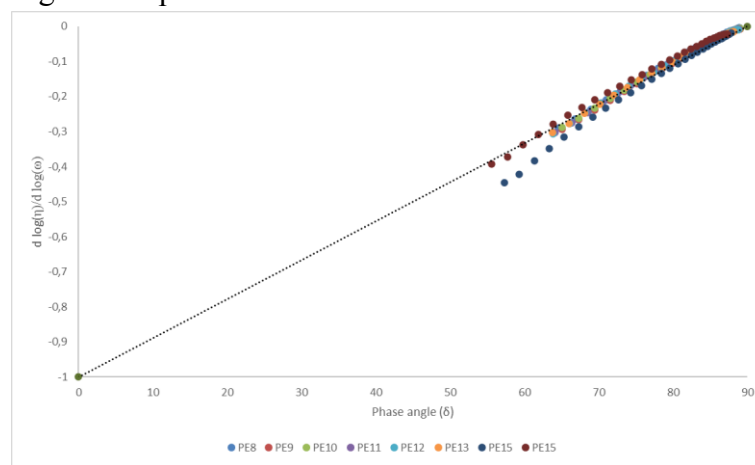


Figure S2. $d \log|\eta^*|/d \log \omega$ vs. δ plot of the data series for entries **PE4-PE11**.

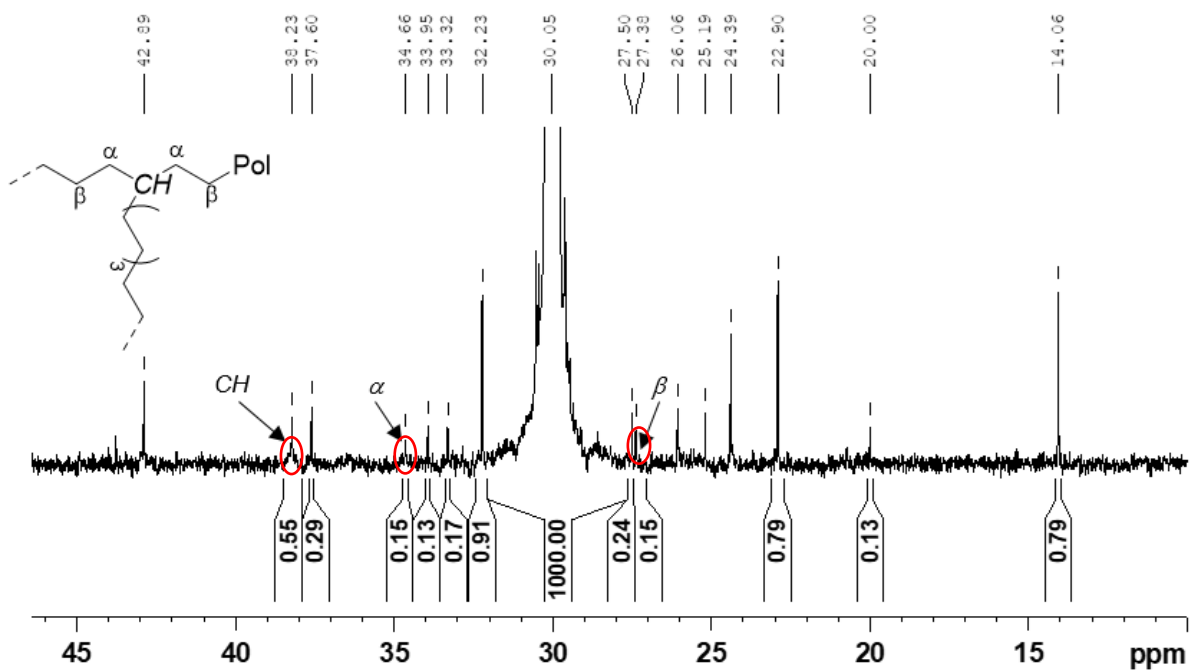


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (500 MHz, 1,2,4-trichlorobenzene/ C_6D_6 5:1, 135 °C) of **PE2**, synthesised with MAO/**Zr-1** 5,000 (Table 1, entry 2).

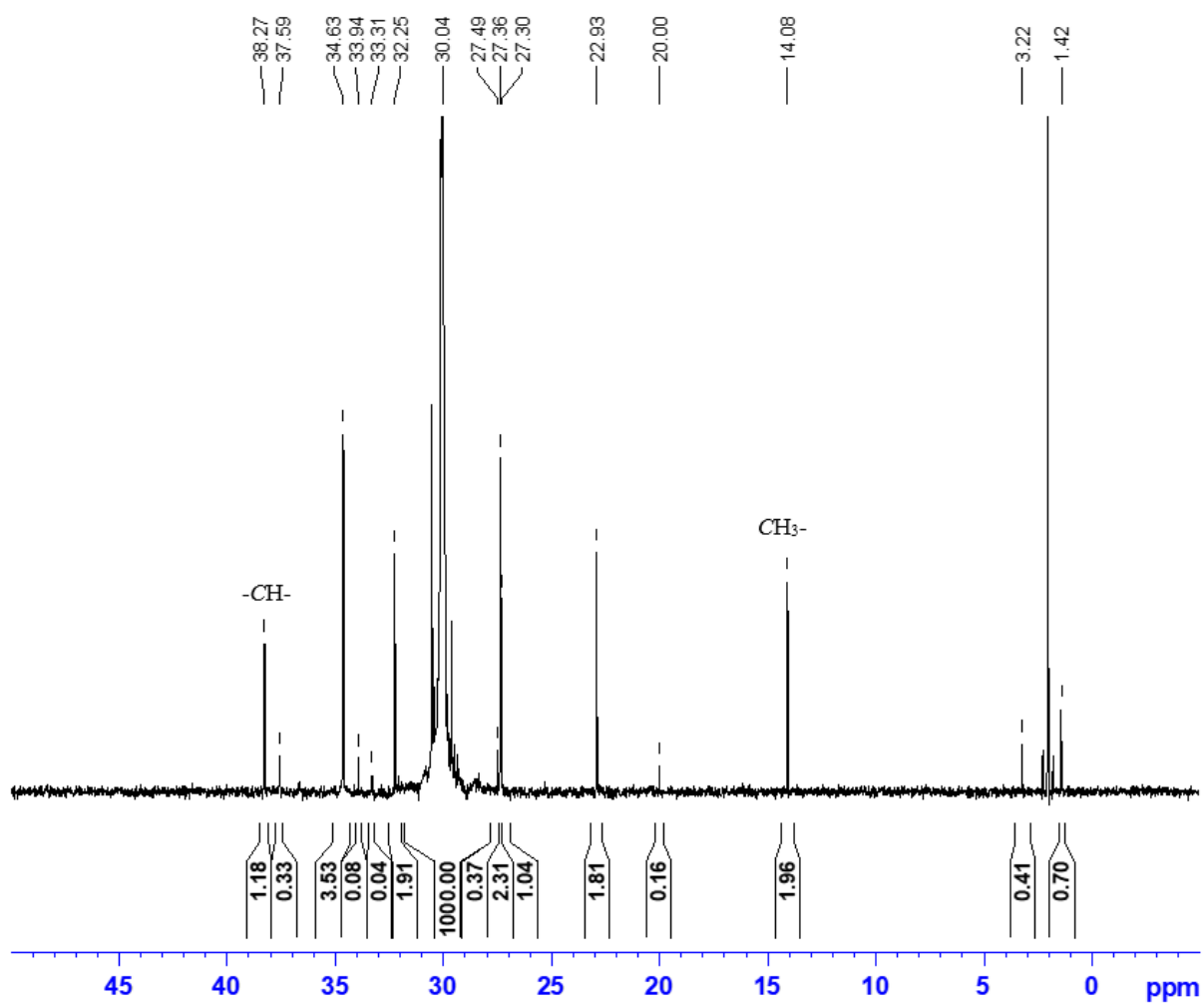


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (500 MHz, 1,2,4-trichlorobenzene/ C_6D_6 5:1, 135 °C) of **PE3**, synthesised with MAO/**Al-1**/**Zr-1** 4,500/500/1 (Table 1, entry 3).

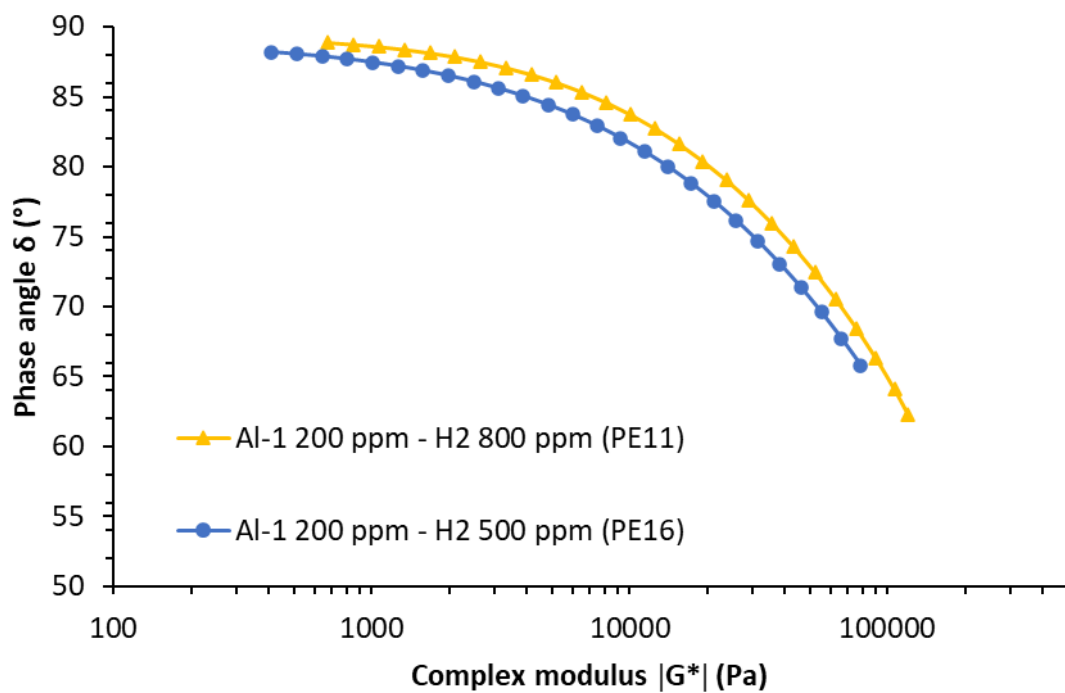


Figure S6. Effect of the concentration of H₂ on the formation of LCB with the supp-Zr-1/Al-1 system: comparison of the vGP plots of two PE samples. For **PE11**: M_w 56 kDa, M_w/M_n 2.6; for **PE16**: M_w 72 kDa, M_w/M_n 2.5.

Computational details. All calculations were carried out with the Gaussian 09 suite of programs [1]. Zirconium atoms were treated with the very small core Stuttgart–Dresden effective core potential associated with its adapted basis sets and additional *f* and *g* polarization functions [2]. Carbon and hydrogen atoms were described with a 6-31G(d,p) double- ζ basis set [3]. Silicon atoms have been treated with the small core Stuttgart–Dresden effective core potential associated with its adapted basis set and additional *d* polarization functions [4]. Calculations were carried out at the DFT level of theory with the hybrid functional B3PW91 [5]. Solvation energies were evaluated by a self-consistent reaction field (SCRF) approach based on accurate numerical solutions of the Poisson-Boltzmann equation by using the SMD solvation model [6]. Toluene was used as solvent. All geometries were optimized without any symmetry restriction and the nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. Enthalpies were obtained at $T = 298\text{ K}$ within the harmonic approximation and are given in $\text{kcal}\cdot\text{mol}^{-1}$.

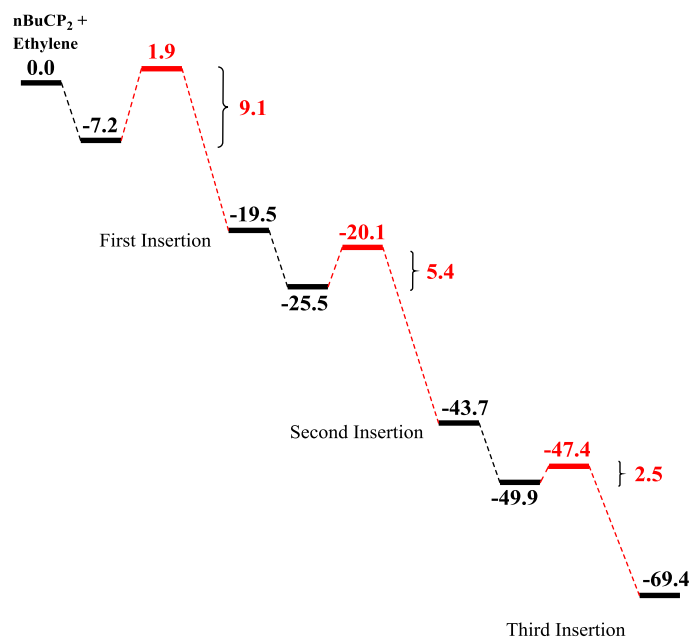


Figure S7. The first three insertions of ethylene onto the $[(n\text{BuCp})_2\text{ZrMe}]^+$ catalyst.

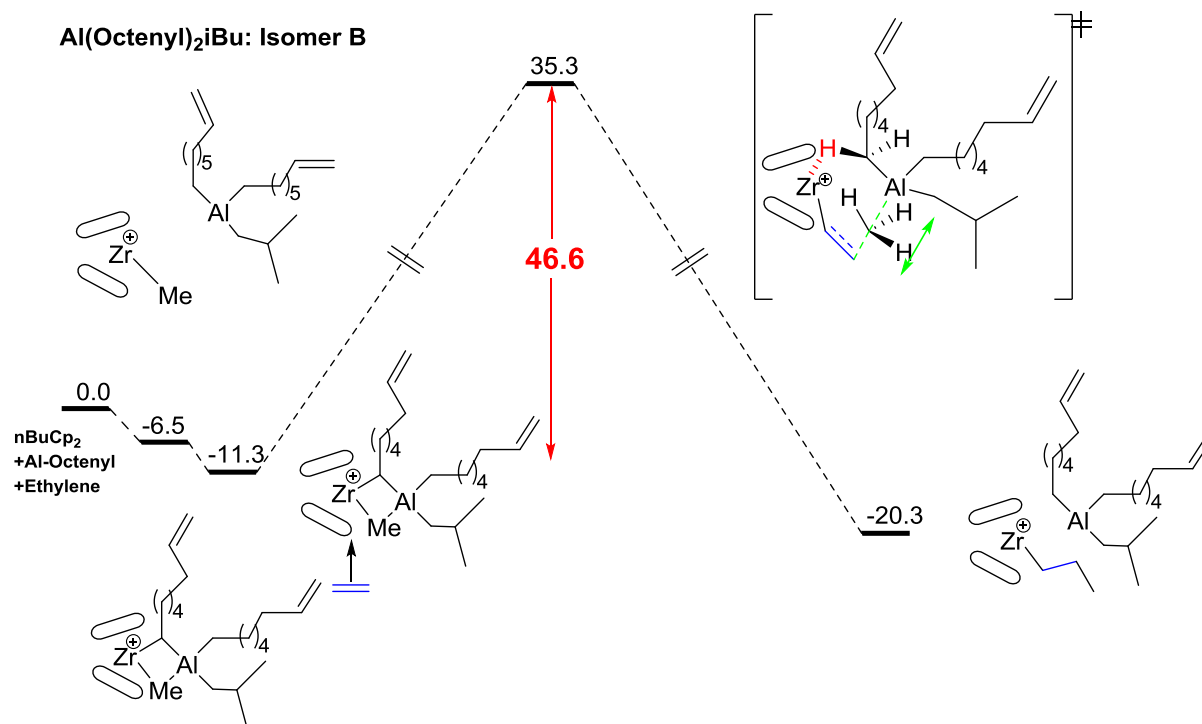


Figure S8. The first insertion of ethylene whereby the transition state is accessed through a nucleophilic attack of the methyl group towards the ethylene monomer being inserted. This is a less kinetically viable pathway in comparison to insertion of ethylene.

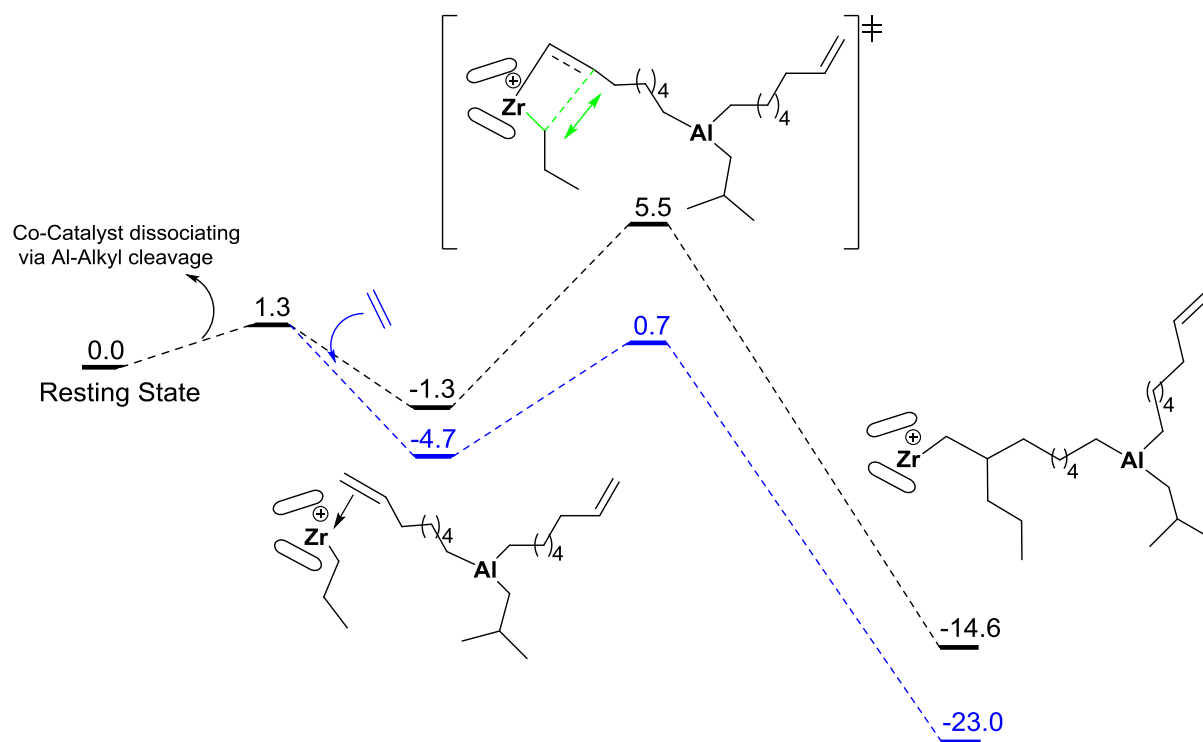


Figure S9. The comparison between the second insertion of ethylene and a vinyl coordination/insertion. It is assumed that, from a re-coordination of the co-catalyst, a dissociation has occurred and thus kinetically the coordination and insertion of ethylene becomes favourable over a vinyl coordination. A branched product is also less likely in comparison.

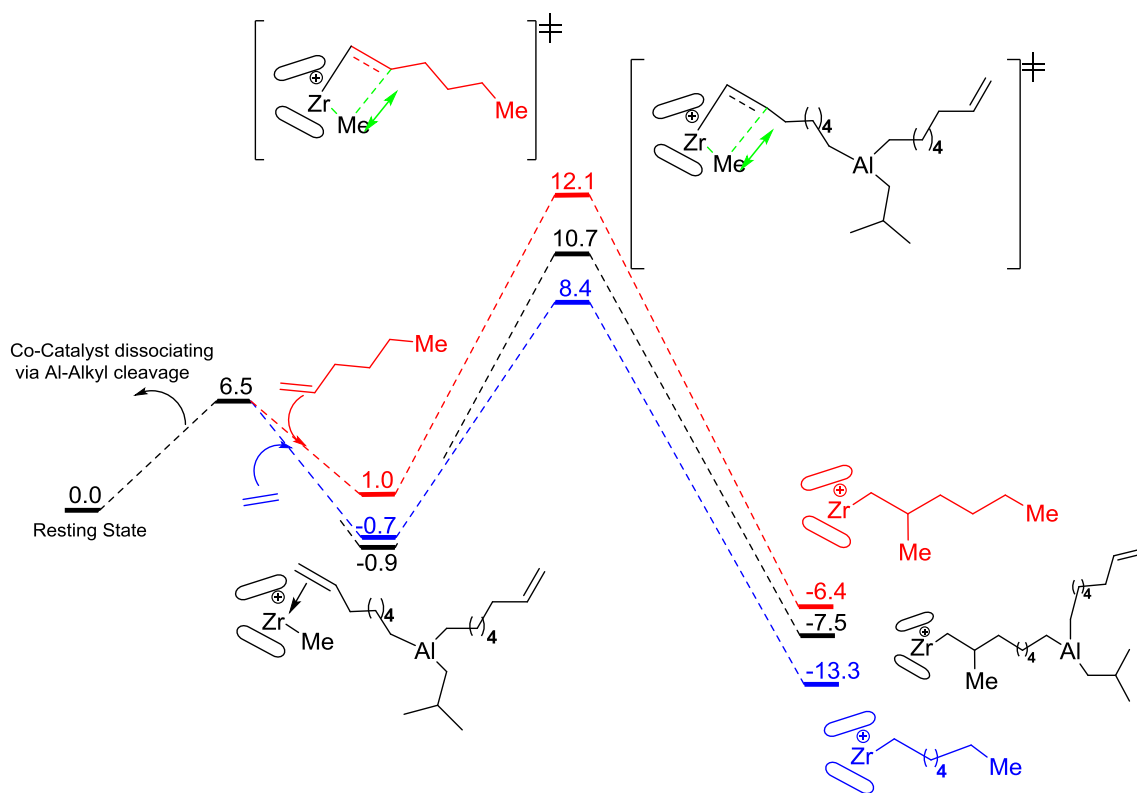


Figure S10. A comparison between the vinyl coordination/insertion from the co-catalyst, an ethylene coordination/insertion and 1-Hexene coordination and insertion. It is interesting to note a competitive environment for the coordination of each moiety kinetically and the subsequent insertion products favour insertion of ethylene.

Cartesian Coordinates:

! Active Catalyst !

scf done: -788.279190

C	-2.785866	-1.274946	-1.586067
C	-3.692563	-0.862218	-2.603017
C	-4.825683	-0.272623	-1.990365
C	-4.594266	-0.299203	-0.579096
C	-3.354305	-0.942057	-0.331596
Zr	-2.819433	1.255828	-1.472650
C	-0.544975	1.664582	-2.586706
C	-0.988886	2.919446	-2.084388
C	-2.161436	3.304300	-2.785649
C	-2.463211	2.283813	-3.726726
C	-1.474037	1.272074	-3.594160
C	-1.659748	1.418506	0.458564
H	-2.921177	-1.145350	0.638271
H	-3.284379	2.283576	-4.434017
H	-1.843313	-1.785739	-1.743526
C	-6.059429	0.245233	-2.678623
H	-5.818327	0.519512	-3.712855
H	-6.414962	1.158941	-2.182594
C	-7.211359	-0.775502	-2.689382
H	-7.436853	-1.077464	-1.658415
H	-6.883403	-1.682017	-3.214000
C	-8.472935	-0.220179	-3.351344
H	-8.237424	0.090617	-4.378408
H	-8.787864	0.689183	-2.821134
C	-9.624730	-1.219957	-3.373776
H	-10.512440	-0.790022	-3.848964
H	-9.358365	-2.125182	-3.930997
H	-9.908453	-1.526397	-2.360575
C	0.731015	0.959096	-2.227445
H	0.599643	-0.125226	-2.328430
H	0.980727	1.155270	-1.178709
C	1.903549	1.402725	-3.120546
H	2.055645	2.483970	-3.004899
H	1.638016	1.239465	-4.173336
C	3.201801	0.662054	-2.799276
H	3.042212	-0.418240	-2.920169
H	3.456626	0.817051	-1.742089
C	4.369126	1.104941	-3.676189
H	5.282696	0.554865	-3.428246
H	4.158537	0.933213	-4.738031
H	4.581915	2.172522	-3.549465
H	-2.717514	4.224347	-2.638642
H	-0.492665	3.496556	-1.314963
H	-1.400393	0.373896	-4.194529
H	-3.557052	-0.999035	-3.668981
H	-5.282680	0.060959	0.178723
H	-2.316717	1.189349	1.310536
H	-0.825691	0.706513	0.513144
H	-1.239594	2.418832	0.617683

! Ethylene Monomer !

scf done: -78.561376

C	0.138668	-0.266277	0.093858
C	0.146459	-0.030817	1.403036
H	1.024180	-0.116972	-0.519947
H	-0.753581	-0.616591	-0.420920
H	1.038964	0.321087	1.916159
H	-0.739091	-0.179595	2.016819

! Co-Catalyst !

scf done: -787.383539

C	1.553379	2.500668	-0.654374
Al	2.459252	1.336368	0.693350
C	1.822557	-0.530919	1.000676
C	0.313505	-0.818090	0.916509
C	-0.457553	-0.041728	1.986675
C	4.151922	1.824739	1.629842
C	4.884953	3.117255	1.250131
C	6.220859	3.310331	1.975407
C	6.939160	4.608268	1.602939
C	8.279698	4.792391	2.315127
C	8.986496	6.103405	1.940603
C	10.283001	6.301490	2.668035
C	11.478606	6.434921	2.092871
C	0.013388	-2.316991	1.023082
H	0.528675	-2.882022	0.237899
H	0.348640	-2.715199	1.989282
H	-1.060087	-2.525160	0.932737
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H	-1.535865	-0.232205	1.932075
H	12.383538	6.571388	2.679950
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H	10.217542	6.325208	3.757898
H	9.161611	6.134386	0.857589
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H	8.122228	4.762814	3.402505
H	8.941914	3.948309	2.080238
H	7.100733	4.634806	0.515560
H	6.286652	5.463382	1.832162
H	6.046826	3.286945	3.061011
H	6.875634	2.454313	1.756596
H	5.068201	3.142196	0.166147
H	4.243251	3.984011	1.460658
H	3.947776	1.819598	2.713543
H	4.826772	0.963379	1.485956
H	2.351910	-1.157035	0.260938
H	2.207098	-0.875372	1.974281
H	-0.050014	-0.479575	-0.065632
H	0.525408	2.136248	-0.797608
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H	2.054655	2.294183	-1.615351

H	1.038714	4.527915	-1.251370	C	5.898380	-3.468363	5.176363
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H	-0.201950	4.002047	0.871661	C	10.081546	-4.643985	6.795169
H	1.326715	3.941152	1.738354	C	10.459649	-6.043763	7.179813
C	0.022855	6.313996	2.401840	C	11.612779	-6.639870	6.876551
H	1.766069	6.337499	1.129138	C	3.339499	-6.004184	9.296074
H	0.242883	6.395288	0.257523	H	2.784443	1.052440	3.592584
C	-0.057488	7.832773	2.613425	H	4.374468	-4.389601	7.426819
H	-0.993621	5.895907	2.389123	H	2.691055	-3.931781	7.519527
H	0.528638	5.858903	3.263957	H	4.750352	-6.624492	4.216493
C	-0.805348	8.213082	3.856693	H	3.759342	-5.959918	2.944153
H	0.953742	8.258101	2.645703	H	1.117840	-4.940936	3.979037
H	-0.557488	8.280378	1.741056	H	0.933911	-4.095597	5.531870
C	-0.303219	8.907871	4.878059	H	0.616474	-3.309237	4.032316
H	-1.842218	7.874350	3.909797	H	2.809885	-7.957407	5.073427
H	-0.900272	9.147089	5.754718	H	1.757828	-7.243943	3.868241
H	0.724716	9.266966	4.874643	H	2.260246	-10.296262	4.094008
! Isomer A !				H	1.222206	-9.523639	2.906828
scf done: -1575.677914				H	0.804288	-1.795142	6.227896
C	2.614685	0.282438	4.335376	H	4.189778	-1.020716	1.111236
C	1.353543	-0.286828	4.676120	H	4.018242	-3.711394	1.203508
C	1.565597	-1.208200	5.731596	H	3.674589	-6.826449	7.353244
C	2.953252	-1.225333	6.023728	H	3.130942	-6.966264	9.779078
C	3.606161	-0.271325	5.186991	H	4.391323	-5.760770	9.484514
Zr	2.645544	-2.149789	3.671126	H	2.728876	-5.242667	9.797757
C	1.329623	-4.006256	4.514288	H	1.353020	-7.423758	8.012886
Al	3.310885	-4.706752	5.114562	H	0.893058	-5.718365	8.003955
C	3.719467	-6.309178	3.988816	H	1.340338	-6.528899	6.492732
C	2.801810	-7.537994	4.058587	H	-0.820969	-2.906100	2.294030
C	3.184230	-8.637922	3.062128	H	-0.721465	-1.148301	2.221789
C	2.255873	-9.852952	3.088114	H	-0.691612	-1.249003	-0.279044
C	2.629307	-10.922398	2.060269	H	-0.771180	-3.003622	-0.215639
C	1.681061	-12.130070	2.067523	H	-2.980516	-2.868087	0.962736
C	2.061230	-13.175598	1.061111	H	-2.902648	-1.113794	0.918952
C	1.301165	-13.571641	0.039740	H	-4.348216	-1.983726	-0.924079
C	5.030611	0.192277	5.293439	H	-2.936624	-1.165043	-1.602082
C	5.175715	1.322288	6.329738	H	-3.001715	-2.931973	-1.564265
C	6.615836	1.816498	6.469212	H	1.709686	-0.027675	1.456687
C	6.762345	2.917491	7.515234	H	1.451574	-4.363617	1.616930
C	1.074700	-2.158830	1.630454	H	3.429654	-1.815302	6.796610
C	1.845932	-3.357414	1.548943	H	0.398681	-0.027273	4.235617
C	3.198886	-3.015161	1.326704	H	5.382231	0.551403	4.318512
C	3.289923	-1.599467	1.285494	H	5.679729	-0.639699	5.584821
C	1.982583	-1.075599	1.473856	H	4.523943	2.159064	6.046928
C	-0.424509	-2.069172	1.705296	H	4.813821	0.964055	7.302460
C	-1.077022	-2.090513	0.311558	H	7.266061	0.971412	6.733103
C	-2.603118	-2.020161	0.374980	H	6.970501	2.184529	5.496873
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C	3.366715	-4.701721	7.114726	H	6.147026	3.789703	7.266596
C	3.035697	-6.046638	7.795272	H	6.455558	2.569066	8.508015
C	1.579335	-6.451817	7.560507	H	5.003559	-3.849419	3.265180
C	4.733676	-3.305005	4.176710	H	4.807979	-2.222991	3.879984
				H	3.193824	-8.211671	2.048044

H	4.215953	-8.960083	3.262867	C	3.502765	-7.622985	4.442099
H	2.633852	-10.480397	1.054805	C	3.244495	-8.588891	3.280723
H	3.656354	-11.266567	2.246063	H	3.534030	1.107152	3.912224
H	1.686920	-12.575799	3.073399	H	4.642126	-6.134223	3.376875
H	0.652684	-11.795649	1.879533	H	2.917789	-5.969780	3.180102
H	3.048524	-13.624387	1.188793	H	1.312621	-4.802147	4.855938
H	1.636860	-14.330813	-0.662344	H	1.334809	-3.632099	6.182179
H	0.310221	-13.153671	-0.130497	H	0.913085	-3.194141	4.539269
H	5.970317	-4.519272	5.487098	C	4.705074	-8.095729	5.261366
H	5.696799	-2.900755	6.092740	H	2.618829	-7.657469	5.098821
H	7.447767	-3.640547	3.681878	H	0.535187	-1.185201	6.078586
H	7.163535	-1.999452	4.238357	H	4.974087	-1.386475	1.805122
H	9.295968	-2.656577	5.080550	H	4.394882	-4.006930	2.128397
H	8.216039	-2.586592	6.460459	H	-0.369849	-2.377207	2.442680
H	8.002802	-5.091015	6.424364	H	0.008530	-0.708917	2.022697
H	9.015276	-5.158314	4.989246	H	0.318572	-1.393657	-0.374354
H	10.922217	-4.161609	6.280598	H	-0.051765	-3.057680	0.053701
H	9.892788	-4.056646	7.706312	H	-2.328659	-2.332842	0.855709
H	9.710317	-6.601435	7.745239	H	-1.959793	-0.680646	0.385941
H	11.825562	-7.661135	7.182225	H	-3.316076	-1.814768	-1.378016
H	12.392126	-6.127018	6.315271	H	-1.719079	-1.415418	-2.019411
! Isomer B !				H	-2.090581	-3.077193	-1.542780
scf done: -1575.679577				H	2.651261	-0.045210	1.649164
C	3.693443	-0.091822	5.789104	H	1.724890	-4.255693	2.197371
C	3.064216	0.447779	4.632547	H	2.872996	-1.411806	7.388112
C	1.691496	0.072048	4.643564	H	0.942270	0.380681	3.925162
C	1.476637	-0.742125	5.779381	H	5.783961	0.181227	5.396885
C	2.712244	-0.859936	6.470955	H	5.425170	-0.575287	6.945988
Zr	2.955566	-2.020210	4.161037	H	4.850998	2.351571	6.240153
C	5.004311	-3.066347	4.962013	H	4.507505	1.603196	7.792056
C	6.223726	-3.938079	4.585260	H	6.949408	1.124765	8.108125
C	7.558554	-3.200757	4.747795	H	7.298558	1.843017	6.543773
C	8.793066	-4.070930	4.486184	H	7.754804	3.474303	8.375428
C	8.922406	-4.591677	3.053398	H	6.432118	4.067765	7.365601
C	10.220258	-5.378893	2.821472	H	6.085984	3.345599	8.942099
C	10.324483	-5.939328	1.433913	H	5.133355	-2.167037	4.304327
C	11.292880	-5.660394	0.561172	H	5.158893	-2.682530	5.977499
C	5.092323	0.201900	6.248879	H	6.116611	-4.305404	3.560110
C	5.194361	1.574858	6.936167	H	6.251660	-4.835456	5.221629
C	6.614495	1.896628	7.401990	H	7.574540	-2.331800	4.073178
C	6.727489	3.270086	8.056769	H	7.617640	-2.798767	5.767729
C	2.757132	-1.111369	1.808064	H	9.686348	-3.481666	4.731783
C	1.682159	-2.038857	1.924022	H	8.791360	-4.920037	5.184178
C	2.271551	-3.327146	2.092581	H	8.069450	-5.238291	2.807485
C	3.680632	-3.197386	2.061450	H	8.884860	-3.748827	2.349031
C	3.984011	-1.818900	1.892210	H	11.086098	-4.737710	3.028953
C	0.216661	-1.751802	1.757861	H	10.261770	-6.204739	3.547649
C	-0.264004	-2.013729	0.319453	H	9.529335	-6.626464	1.136910
C	-1.755548	-1.730992	0.137140	H	11.311672	-6.102734	-0.431665
C	-2.246520	-2.025297	-1.277206	H	12.109776	-4.984932	0.809830
Al	3.604776	-4.717626	5.307291	H	3.100322	-9.616860	3.634136
C	3.802806	-5.121830	7.254852	H	2.350688	-8.306124	2.712251
C	1.631171	-3.787352	5.141080	H	4.091377	-8.594332	2.582718
C	3.693085	-6.177094	3.932877	H	4.559547	-9.116023	5.633444
				H	5.616332	-8.097421	4.649331

H	4.888850	-7.454244	6.129582	C	3.696523	-8.455403	3.278231
H	4.812525	-5.537491	7.395844	C	2.736406	-9.646026	3.300294
C	3.579332	-4.012702	8.287515	C	3.156743	-10.793406	2.380908
H	3.127078	-5.963948	7.473285	C	2.182455	-11.979949	2.414948
C	3.778111	-4.447961	9.743360	C	2.627007	-13.128597	1.558621
H	4.265680	-3.175714	8.087776	C	1.943233	-13.638779	0.534098
H	2.563972	-3.601010	8.184772	C	6.968399	-3.602845	4.022421
C	3.590163	-3.304465	10.742002	H	3.042105	1.157225	4.098730
H	3.078787	-5.262813	9.977043	H	4.372478	-5.350485	7.801968
H	4.786106	-4.871362	9.856844	H	3.289653	-3.985203	7.893529
C	3.815594	-3.707616	12.199319	H	5.220636	-6.446068	4.491571
H	4.280962	-2.486310	10.487709	H	4.337849	-5.744038	3.160662
H	2.576867	-2.889946	10.634582	H	1.539839	-4.997526	4.555330
C	3.643186	-2.535789	13.176741	H	1.185954	-3.888954	5.891350
H	3.120336	-4.511562	12.474430	H	0.945750	-3.451205	4.220986
H	4.825582	-4.126446	12.308948	H	3.172564	-7.702210	5.224288
C	3.930847	-2.907841	14.600984	H	2.250649	-6.999309	3.913350
H	4.324444	-1.726236	12.872603	H	2.649390	-10.022419	4.329665
H	2.625280	-2.132674	13.098505	H	1.729486	-9.305851	3.017204
C	3.065022	-2.818803	15.610768	H	-0.043110	-1.574224	5.501194
H	4.936204	-3.284340	14.800470	H	4.889082	-0.921795	2.028505
H	3.336870	-3.106249	16.623357	H	4.875474	-3.608910	2.306145
H	2.051207	-2.449691	15.464340	H	-0.119448	-3.137665	2.090115
! IsomerC !				H	-0.116996	-1.390710	1.859528
scf done: -1575.672194				H	0.586026	-1.717010	-0.532451
C	2.934386	-0.097031	5.946182	H	0.565851	-3.458524	-0.297171
C	2.511661	0.416376	4.686008	H	-1.882354	-3.348892	0.270008
C	1.225980	-0.118240	4.386567	H	-1.858520	-1.609711	0.023031
C	0.877005	-1.008339	5.427359	H	-2.737195	-2.763705	-2.005880
C	1.932961	-1.005879	6.378695	H	-1.211800	-1.960362	-2.395027
Zr	2.826558	-2.022799	4.166625	H	-1.251660	-3.710450	-2.145088
C	4.884474	-2.777757	5.330296	H	2.356802	-0.123214	1.646675
C	6.399465	-3.161307	5.368214	H	2.337629	-4.446198	2.119163
C	6.726218	-4.178886	6.463021	H	1.956488	-1.575534	7.299933
C	4.146321	0.341768	6.716379	H	0.617550	0.126396	3.525682
C	3.898816	1.656032	7.478360	H	4.998076	0.479414	6.038155
C	5.122841	2.110173	8.274193	H	4.433545	-0.434469	7.434920
C	4.897235	3.424518	9.015412	H	3.610805	2.438788	6.764440
C	2.678586	-1.142783	1.817891	H	3.044326	1.525485	8.155056
C	1.829534	-2.285834	1.844047	H	5.399062	1.326723	8.992852
C	2.671706	-3.418147	2.061454	H	5.978191	2.215529	7.592626
C	4.010703	-2.978890	2.159748	H	5.790557	3.722705	9.573793
C	4.015716	-1.563794	2.020512	H	4.654565	4.238261	8.322535
C	0.360030	-2.322713	1.533250	H	4.072303	3.343487	9.732372
C	0.095562	-2.522250	0.030116	H	4.909892	-1.932837	4.585540
C	-1.395346	-2.550120	-0.305707	H	4.669507	-2.305103	6.296663
C	-1.663207	-2.757496	-1.793423	H	3.786767	-8.075690	2.249985
Al	3.696073	-4.620148	5.433275	H	4.702882	-8.790226	3.566809
C	3.431345	-4.956461	7.392207	H	3.242363	-10.429548	1.348102
C	2.288165	-5.898553	7.802126	H	4.159724	-11.140349	2.666144
C	2.112496	-6.033286	9.318552	H	2.087462	-12.323965	3.456076
C	1.652951	-3.960521	4.905717	H	1.183042	-11.650370	2.102606
C	4.218323	-6.101395	4.193576	H	3.597427	-13.560878	1.810776
C	3.267101	-7.310551	4.201898	H	2.325519	-14.473672	-0.047835
				H	0.971215	-13.244777	0.241705

H	6.919447	-2.232525	5.646626
H	8.044860	-3.783693	4.112641
H	6.510985	-4.532826	3.669380
H	6.836712	-2.835198	3.251603
H	7.812064	-4.283860	6.557715
H	6.338104	-3.870359	7.438675
H	6.328945	-5.174558	6.233772
H	1.334725	-5.554643	7.375125
H	2.456050	-6.897715	7.376573
C	0.921907	-6.904824	9.721721
H	3.034619	-6.442821	9.754498
H	1.991712	-5.030972	9.755282
C	0.732785	-7.022918	11.234467
H	0.005217	-6.491627	9.275755
H	1.040749	-7.909163	9.290609
C	-0.492809	-7.861777	11.624998
H	1.633548	-7.464360	11.683092
H	0.633787	-6.021032	11.673603
C	-0.655413	-8.007484	13.108994
H	-1.399783	-7.415219	11.197464
H	-0.392103	-8.859888	11.172655
C	-1.708270	-7.590385	13.812640
H	0.172060	-8.489182	13.633739
H	-1.764176	-7.723003	14.890225
H	-2.557795	-7.104065	13.335648

! First Ethylene Insertion to the Catalyst -
Adduct !

scf done: -866.854795

C	1.310603	-0.037709	-1.518908
C	2.216529	0.652842	-0.663121
C	1.619261	1.906163	-0.364704
C	0.395978	2.014425	-1.078368
C	0.200374	0.810277	-1.793334
Zr	-0.003302	0.157529	0.600163
C	-0.766553	-1.910939	1.838845
C	-0.280608	-2.324702	0.575072
C	-1.173428	-1.838748	-0.420267
C	-2.221039	-1.124868	0.217202
C	-1.943851	-1.149762	1.618596
C	-3.424968	-0.517032	-0.448899
C	-4.504793	-1.557164	-0.795631
C	-5.731596	-0.927347	-1.456457
C	-6.802850	-1.949591	-1.825424
C	3.583578	0.186088	-0.258671
C	4.678242	0.645273	-1.237055
C	6.065493	0.152570	-0.822619
C	7.172606	0.617144	-1.763758
C	1.513422	-0.064215	2.264522
H	-0.321491	-2.140639	2.797063
H	-0.627001	0.583102	-2.453941
H	0.602591	-2.926938	0.397476
H	-3.127742	-0.002664	-1.372320
H	-3.865053	0.243731	0.207968
H	-4.805135	-2.085248	0.118422

H	-4.073448	-2.314982	-1.462634
H	-5.418723	-0.384215	-2.358981
H	-6.160390	-0.174866	-0.780488
H	-7.666000	-1.466723	-2.295102
H	-6.418041	-2.695030	-2.530801
H	-7.165220	-2.486727	-0.941516
H	3.595541	-0.909010	-0.198961
H	3.822826	0.558954	0.743117
H	4.677390	1.741881	-1.293315
H	4.443531	0.283597	-2.246834
H	6.059822	-0.945156	-0.776432
H	6.281762	0.498958	0.197239
H	8.150807	0.249497	-1.436789
H	7.008730	0.254860	-2.785045
H	7.228417	1.710948	-1.805531
H	-0.267144	2.871374	-1.083848
H	2.051190	2.668399	0.273639
H	1.481221	-1.016391	-1.951856
H	-1.088413	-2.013025	-1.485860
H	-2.569086	-0.709390	2.387278
H	1.030697	-0.244113	3.233824
H	2.172516	-0.924906	2.084667
H	2.156950	0.818386	2.365858
C	-0.902324	2.044796	2.776876
C	-1.488212	2.663165	1.737497
H	-2.496323	2.409555	1.414032
H	-1.006777	3.494775	1.230341
H	0.072981	2.354916	3.142952
H	-1.413697	1.269547	3.342679

! First Ethylene Insertion to the Catalyst -
Transition State !

scf done: -866.662967

C	-1.469089	0.965443	-3.602803
C	-0.528207	1.436590	-2.648934
C	-0.990228	2.713503	-2.211756
C	-2.168739	3.042656	-2.930157
C	-2.475840	1.955763	-3.783776
Zr	-2.794894	1.073874	-1.440880
C	-3.448393	-1.060228	-0.231289
C	-2.961940	-1.413984	-1.516241
C	-3.901691	-0.942798	-2.477352
C	-4.973034	-0.300314	-1.794946
C	-4.670352	-0.368269	-0.405276
C	-6.215420	0.286877	-2.405703
C	-7.292290	-0.761430	-2.732703
C	-8.564385	-0.122387	-3.292037
C	-9.641005	-1.139500	-3.658006
C	0.788067	0.798074	-2.303831
C	1.937857	1.439048	-3.102660
C	3.291442	0.773491	-2.856783
C	4.426765	1.460269	-3.610914
C	-1.681865	1.379366	0.564954
H	-2.976119	-1.296480	0.713681
H	-3.308468	1.899625	-4.475132

H	-2.061848	-1.978261	-1.730206
H	-5.963584	0.828920	-3.326097
H	-6.640287	1.025657	-1.714902
H	-7.531414	-1.331730	-1.825627
H	-6.889608	-1.483321	-3.455372
H	-8.309754	0.474747	-4.178653
H	-8.965390	0.585320	-2.553386
H	-10.540386	-0.643601	-4.037503
H	-9.292637	-1.829999	-4.434529
H	-9.936995	-1.739953	-2.790171
H	0.747203	-0.276233	-2.521278
H	0.999263	0.900207	-1.232199
H	1.999774	2.504436	-2.843943
H	1.697869	1.397134	-4.173128
H	3.236817	-0.281907	-3.156124
H	3.511412	0.776357	-1.780470
H	5.382989	0.955978	-3.437770
H	4.245156	1.461134	-4.691835
H	4.541344	2.503621	-3.295155
H	-2.718134	3.971571	-2.856734
H	-0.486589	3.353664	-1.497490
H	-1.396639	0.028531	-4.142007
H	-3.833355	-1.081261	-3.549758
H	-5.293173	0.023540	0.390185
H	-1.927711	0.870663	1.496391
H	-1.150942	0.614766	-0.069270
H	-0.946452	2.161219	0.750165
C	-3.427709	2.694923	0.589427
C	-4.246401	2.788673	-0.547280
H	-5.232781	2.335896	-0.512083
H	-4.154171	3.670502	-1.171942
H	-2.729637	3.495089	0.809602
H	-3.780391	2.145392	1.456155

! First Ethylene Insertion to the Catalyst - Product !

scf done: -866.879949

C	1.305058	-0.020054	-1.779647
C	2.183767	0.658452	-0.896253
C	1.553099	1.887242	-0.538992
C	0.320135	1.984134	-1.230311
C	0.154090	0.795794	-1.987241
Zr	0.029210	0.072587	0.377556
C	-0.722244	-1.923449	1.671640
C	-0.272728	-2.399981	0.411558
C	-1.168901	-1.924394	-0.579604
C	-2.194348	-1.165783	0.055765
C	-1.900469	-1.157983	1.449814
C	-3.379490	-0.531984	-0.617012
C	-4.557797	-1.503851	-0.803039
C	-5.734410	-0.851063	-1.530220
C	-6.919309	-1.792972	-1.721737
C	3.532466	0.178680	-0.431347
C	4.689605	0.678880	-1.314242
C	6.048337	0.175497	-0.825742

C	7.210031	0.661728	-1.686530
C	1.046066	0.916086	3.291361
H	-0.267163	-2.127569	2.634045
H	-0.671824	0.572366	-2.651318
H	0.593411	-3.027868	0.234781
H	-3.083788	-0.149729	-1.602249
H	-3.716000	0.331723	-0.031666
H	-4.883793	-1.870445	0.178836
H	-4.217563	-2.382941	-1.365721
H	-5.394957	-0.486309	-2.509567
H	-6.058628	0.036335	-0.969959
H	-7.741037	-1.292922	-2.244784
H	-6.640496	-2.673294	-2.312087
H	-7.307458	-2.148433	-0.760561
H	3.550284	-0.918970	-0.418187
H	3.713878	0.512870	0.598425
H	4.683450	1.776380	-1.329239
H	4.522174	0.352378	-2.348549
H	6.041222	-0.923116	-0.806060
H	6.202550	0.498716	0.212957
H	8.166690	0.288493	-1.306771
H	7.110807	0.320081	-2.723014
H	7.265417	1.756101	-1.701763
H	-0.377068	2.811199	-1.177225
H	1.964726	2.634856	0.128845
H	1.493042	-0.981992	-2.241736
H	-1.107305	-2.132405	-1.641004
H	-2.498979	-0.677153	2.212383
H	1.308346	0.571398	4.296970
H	1.293932	0.054834	2.632069
H	1.726553	1.733501	3.030342
C	-0.421845	1.337708	3.182321
C	-0.821954	1.716453	1.743966
H	-1.908407	1.853582	1.667409
H	-0.371346	2.682516	1.483431
H	-0.586863	2.180977	3.866999
H	-1.053087	0.522743	3.556335

! Second Ethylene Insertion to the Catalyst - Adduct !

scf done: -945.451884

C	-0.760314	-1.011848	-1.516395
C	-0.501987	-1.955913	-0.481704
C	0.890806	-2.240204	-0.468581
C	1.489417	-1.421986	-1.468858
C	0.475547	-0.684709	-2.127948
Zr	0.456051	0.270437	0.210069
C	-0.770567	2.444689	0.638180
C	-0.247504	2.018437	1.882339
C	-0.921282	0.822083	2.249663
C	-1.851327	0.515605	1.228948
C	-1.776977	1.524867	0.224546
C	-2.736741	1.738648	-0.912667
C	-3.781085	2.815456	-0.565661
C	-4.800964	3.041942	-1.681112

C	-5.816595	4.128789	-1.339417	C	-0.264300	-1.120170	-0.851426
C	1.558168	-3.322042	0.331611	Zr	0.099946	-0.013060	1.390264
C	1.465415	-4.680126	-0.389418	C	-0.888996	2.258497	2.022915
C	2.099296	-5.824033	0.401182	C	-0.473368	1.666130	3.236833
C	1.987102	-7.166765	-0.315294	C	-1.271633	0.514381	3.456542
C	2.270685	-0.347797	2.611370	C	-2.187380	0.410193	2.378355
C	3.182914	-0.155962	1.643951	C	-1.958168	1.487994	1.474728
C	1.777066	1.793875	-0.892118	C	-2.770616	1.839624	0.257831
C	2.369460	3.008803	-0.165463	C	-3.886415	2.855104	0.555518
C	3.484626	3.693116	-0.961177	C	-4.697136	3.213432	-0.690773
H	0.520121	2.524211	2.455147	C	-5.805399	4.224589	-0.413710
H	-1.734190	-0.653318	-1.819213	C	1.545200	-3.495394	1.431527
H	-0.761333	0.248019	3.155232	C	1.567645	-4.859547	0.719189
H	-3.256571	0.801535	-1.142886	C	2.486619	-5.865335	1.413231
H	-2.198967	2.040378	-1.820190	C	2.506545	-7.226772	0.725099
H	-3.264781	3.758671	-0.344168	C	1.795743	-0.564763	3.061450
H	-4.301646	2.526286	0.356985	C	2.592535	0.292470	2.314426
H	-5.327227	2.100748	-1.890247	C	1.731345	1.339174	0.418089
H	-4.273878	3.310795	-2.606699	C	2.259688	2.753712	0.657006
H	-6.536368	4.270297	-2.152162	C	3.773016	2.885775	0.489269
H	-6.384327	3.876886	-0.436229	H	0.313189	2.030980	3.885667
H	-5.325835	5.092830	-1.162601	H	-2.365591	-1.272349	-0.119546
H	1.082835	-3.414504	1.316608	H	-1.214162	-0.153880	4.307288
H	2.614023	-3.079429	0.502662	H	-3.219762	0.932113	-0.162239
H	1.947524	-4.597001	-1.372086	H	-2.116208	2.254467	-0.519854
H	0.409167	-4.907746	-0.583682	H	-3.444232	3.764791	0.982476
H	1.619549	-5.893494	1.387158	H	-4.552777	2.444549	1.325401
H	3.156965	-5.595657	0.590319	H	-5.133771	2.298752	-1.114736
H	2.441925	-7.970464	0.272656	H	-4.021151	3.613132	-1.459388
H	0.940159	-7.438432	-0.492752	H	-6.365092	4.458354	-1.325314
H	2.491318	-7.143621	-1.288020	H	-6.520800	3.842529	0.323458
H	0.620474	-0.001144	-2.954287	H	-5.400159	5.165649	-0.024628
H	2.544996	-1.399357	-1.713368	H	1.230995	-3.649483	2.471365
H	-1.247874	-2.433632	0.142385	H	2.567188	-3.096499	1.459013
H	-2.540774	-0.319851	1.226579	H	1.888909	-4.720446	-0.321280
H	-0.496407	3.346071	0.107656	H	0.546655	-5.260581	0.676577
H	2.774140	2.725807	0.817602	H	2.166478	-5.987452	2.457111
H	1.587865	3.748291	0.044072	H	3.506665	-5.459076	1.452122
H	3.882779	4.563243	-0.426414	H	3.169541	-7.925154	1.246121
H	4.319274	3.007452	-1.149037	H	1.507296	-7.676220	0.699781
H	3.118544	4.038929	-1.934648	H	2.859197	-7.147060	-0.309540
H	1.854598	-1.332579	2.817035	H	-0.355821	-0.478256	-1.720015
H	1.988201	0.453109	3.288823	H	1.917409	-1.601353	-0.815593
H	3.659059	0.809159	1.493897	H	-1.327497	-2.877241	1.782226
H	3.532030	-0.976490	1.021745	H	-2.954144	-0.347760	2.272783
H	1.273600	2.133713	-1.810746	H	-0.484814	3.164352	1.587532
H	2.606909	1.161936	-1.254194	H	1.963374	3.120183	1.648657
! Second Ethylene Insertion to the Catalyst - Transition State !				H	1.779118	3.433360	-0.060233
scf done: -945.423236				H	4.088743	3.920975	0.652845
C	-1.320886	-1.529855	-0.004035	H	4.329009	2.260598	1.195023
C	-0.769520	-2.372337	1.001576	H	4.082623	2.601540	-0.522560
C	0.624636	-2.519539	0.757799	H	1.952785	-1.635098	2.984698
C	0.938018	-1.699199	-0.363218	H	1.375579	-0.214049	3.998723
				H	2.765356	1.306789	2.656292
				H	3.336558	-0.109777	1.634933

H 0.738091 1.430673 -0.123884
H 2.369680 0.801478 -0.287903

! Second Ethylene Insertion to the Catalyst -
Product !

scf done: -945.484002

C -0.959192 -1.530393 -1.828550
C -0.789852 -2.361116 -0.684801
C 0.603366 -2.571852 -0.471417
C 1.286319 -1.839513 -1.482073
C 0.331083 -1.215018 -2.323478
Zr 0.055167 -0.091735 -0.075365
C -0.854991 1.863172 1.271615
C -0.594259 0.805679 2.180754
C -1.471955 -0.261156 1.856873
C -2.295413 0.160595 0.772781
C -1.926438 1.479986 0.408966
C -2.552720 2.326625 -0.666354
C -3.851131 3.017239 -0.213652
C -4.456935 3.890384 -1.313102
C -5.761338 4.561678 -0.893984
C 1.226715 -3.491863 0.537212
C 1.576114 -4.858751 -0.078344
C 2.207511 -5.821392 0.927362
C 2.568073 -7.169573 0.309864
C 2.086034 -0.034546 0.964569
C 2.579094 1.396769 0.669569
C 2.290889 1.846085 -0.770576
C 2.619016 3.313691 -1.072988
C 4.094429 3.657159 -0.876330
H 0.132520 0.815391 2.981382
H -1.904711 -1.230322 -2.263698
H -1.543723 -1.208884 2.377282
H -2.778418 1.711493 -1.547460
H -1.838345 3.093719 -0.991275
H -3.646637 3.627485 0.675318
H -4.576133 2.252926 0.094745
H -4.632355 3.277217 -2.207981
H -3.728382 4.658134 -1.607675
H -6.162085 5.184673 -1.700166
H -6.527749 3.821739 -0.636884
H -5.616457 5.205675 -0.019381
H 0.537794 -3.638196 1.377861
H 2.137153 -3.037233 0.945517
H 2.262544 -4.705880 -0.921664
H 0.667232 -5.308935 -0.498900
H 1.514788 -5.975300 1.765880
H 3.108205 -5.360291 1.355206
H 3.009895 -7.841497 1.052831
H 1.684273 -7.669730 -0.102639
H 3.293206 -7.056018 -0.504225
H 0.551734 -0.605229 -3.193215
H 2.361547 -1.790582 -1.601818
H -1.586914 -2.810608 -0.104810
H -3.082839 -0.423498 0.311964

H -0.356875 2.825790 1.259569
H 2.006997 3.958549 -0.428723
H 2.328318 3.539151 -2.106206
H 4.284721 4.695085 -1.166793
H 4.406101 3.550235 0.167043
H 4.741699 3.019023 -1.488609
H 2.775045 -0.759549 0.518522
H 2.086873 -0.228844 2.042327
H 2.112421 2.113367 1.358492
H 3.659763 1.471078 0.846655
H 1.190654 1.743980 -0.995596
H 2.806931 1.189421 -1.482162

! Third Ethylene Insertion to the Catalyst -
Adduct !

scf done: -1024.055865

C -0.747004 -2.750553 0.425574
C 0.381586 -2.488269 -0.411992
C -0.079923 -1.677882 -1.480089
C -1.468307 -1.428498 -1.301507
C -1.880861 -2.111632 -0.125806
Zr -0.393378 -0.185219 0.558781
C -0.942561 1.707656 2.183877
C -1.995432 0.759930 2.290479
C -2.698535 0.753867 1.061518
C -2.083932 1.686900 0.178904
C -0.989965 2.268577 0.886049
C -2.596490 2.112288 -1.169252
C -3.544001 3.320397 -1.068002
C -4.090126 3.762848 -2.425564
C -5.009977 4.976280 -2.326623
C 1.754178 -3.079160 -0.270486
C 1.861966 -4.464907 -0.932312
C 3.253712 -5.081551 -0.793506
C 3.359142 -6.456801 -1.446436
C 0.939950 -1.269013 2.975614
C 1.839404 -0.463897 2.382069
C 1.383959 0.791482 -0.495266
C 2.309139 1.923741 -0.036818
C 3.161742 2.490576 -1.182205
C 4.149191 3.590159 -0.774900
C 5.308302 3.108900 0.095305
H -0.233569 1.964294 2.961904
H -2.887015 -2.152112 0.270869
H -2.239368 0.167806 3.165145
H -3.128356 1.279534 -1.645669
H -1.756992 2.370848 -1.826556
H -3.011541 4.155902 -0.595064
H -4.377643 3.068351 -0.399334
H -4.633275 2.927766 -2.888803
H -3.251510 3.992397 -3.096811
H -5.389386 5.268721 -3.311104
H -5.875951 4.770662 -1.686880
H -4.485779 5.841518 -1.904857
H 2.016217 -3.174368 0.791207

H	2.494037	-2.407452	-0.722674
H	1.600803	-4.375933	-1.994896
H	1.115718	-5.136190	-0.487145
H	3.511554	-5.160313	0.271788
H	3.996393	-4.405735	-1.238840
H	4.363778	-6.876115	-1.330284
H	2.651947	-7.165881	-1.001046
H	3.144381	-6.406638	-2.520002
H	-2.108902	-0.870497	-1.973684
H	0.526903	-1.314178	-2.299793
H	-0.740617	-3.363532	1.319800
H	-3.577602	0.163732	0.834486
H	-0.341363	3.043650	0.500964
H	3.607500	4.393480	-0.256002
H	4.558093	4.044249	-1.686390
H	6.008221	3.924418	0.306054
H	4.969649	2.718497	1.061549
H	5.873171	2.312750	-0.404456
H	2.014543	-0.020646	-0.884780
H	0.815949	1.137054	-1.387273
H	1.747893	2.750947	0.417644
H	2.975589	1.548459	0.750227
H	2.485841	2.885681	-1.953575
H	3.715332	1.668215	-1.658689
H	0.223912	-0.885546	3.699280
H	0.952647	-2.343967	2.819315
H	1.884986	0.598552	2.605814
H	2.607678	-0.858252	1.722514

! Third Ethylene Insertion to the Catalyst -
Transition State !

scf done: -1023.496218

C	-0.995119	-3.162241	0.842951
C	0.135870	-2.914692	0.005337
C	-0.320790	-2.113146	-1.070813
C	-1.710220	-1.866144	-0.911163
C	-2.130308	-2.540192	0.268180
Zr	-0.674879	-0.633150	1.002732
C	-1.366720	1.132710	2.730353
C	-2.454556	0.232626	2.605399
C	-2.981851	0.371618	1.294300
C	-2.225782	1.353316	0.595861
C	-1.216134	1.810848	1.496723
C	-2.531021	1.913295	-0.766618
C	-3.531832	3.080163	-0.706186
C	-3.864389	3.646290	-2.086798
C	-4.856687	4.804245	-2.031941
C	1.510510	-3.497233	0.159833
C	1.654710	-4.868955	-0.522404
C	3.055586	-5.460063	-0.361002
C	3.210655	-6.820071	-1.035280
C	0.613278	-1.408619	2.989369
C	1.605821	-0.624736	2.432768
C	1.320980	0.271055	0.252302
C	2.179930	1.505091	0.464820

C	2.572541	2.192705	-0.852553
C	3.389164	3.477722	-0.673150
C	4.776261	3.275501	-0.068034
H	-0.761660	1.283921	3.615877
H	-3.140654	-2.584033	0.654389
H	-2.830932	-0.428928	3.377010
H	-2.943265	1.126048	-1.409646
H	-1.606287	2.260151	-1.244528
H	-3.120739	3.874724	-0.069778
H	-4.452998	2.738221	-0.216107
H	-4.272337	2.845370	-2.718701
H	-2.938660	3.979748	-2.575631
H	-5.080230	5.182840	-3.034627
H	-5.805118	4.496625	-1.576819
H	-4.463562	5.640866	-1.443247
H	1.753271	-3.607789	1.224008
H	2.252754	-2.811191	-0.267190
H	1.415952	-4.767857	-1.589296
H	0.911628	-5.560666	-0.104344
H	3.288697	-5.552279	0.708822
H	3.794408	-4.759969	-0.774886
H	4.222806	-7.215765	-0.902184
H	2.511473	-7.554504	-0.619403
H	3.020347	-6.755943	-2.112731
H	-2.344857	-1.316071	-1.595203
H	0.292968	-1.750373	-1.887286
H	-0.995349	-3.774389	1.736968
H	-3.842185	-0.153297	0.898035
H	-0.493552	2.587437	1.280976
H	2.817976	4.184549	-0.055353
H	3.495639	3.954659	-1.655253
H	5.324725	4.222290	-0.026835
H	4.732442	2.886136	0.955052
H	5.373620	2.576736	-0.665582
H	1.885609	-0.498097	-0.282320
H	0.473193	0.559868	-0.443339
H	1.670720	2.233619	1.108692
H	3.091381	1.208160	0.997958
H	1.657703	2.433346	-1.412000
H	3.135609	1.484907	-1.477028
H	0.005303	-1.018270	3.800388
H	0.679543	-2.488713	2.914749
H	1.749775	0.398482	2.763249
H	2.450270	-1.082766	1.928887

! Third Ethylene Insertion to the Catalyst -
Product !

scf done: -1024.091077

C	-0.733105	-3.037926	0.512376
C	0.202311	-2.619578	-0.474964
C	-0.534147	-1.911473	-1.472633
C	-1.905136	-1.912437	-1.111531
C	-2.030671	-2.609585	0.121554
Zr	-0.831663	-0.505235	0.653114
C	-1.610416	1.126839	2.420135

H	1.650645	-5.964743	2.178931
H	2.638982	-6.699006	3.403532
H	5.627392	-6.725442	1.217855
H	5.560689	-5.405008	0.082948
H	-1.153384	-0.634455	-0.981585
H	-1.376432	0.032204	0.652198
H	3.379465	-7.537477	0.414275
C	3.083777	-6.006809	-1.046996
H	-3.696561	2.330907	1.652746
H	0.292870	1.569036	-2.954284
H	-1.579373	-0.306237	-3.411831
H	-4.754985	3.590408	-3.725926
H	-3.535040	4.815729	-3.394388
H	-2.678608	4.587925	-5.743544
H	-3.896958	3.364654	-6.069420
H	-5.707315	5.041688	-5.580870
H	-4.485852	6.263861	-5.263492
H	-5.376253	6.503176	-7.580843
H	-3.665262	6.065954	-7.644993
H	-4.902873	4.844038	-7.963432
H	-0.871736	3.979200	-3.209109
H	-3.899275	0.949869	-3.941675
H	-1.012213	2.298984	1.653590
H	-4.505726	4.121019	-0.208792
H	0.404627	4.524378	-1.242258
H	0.916135	3.351359	-0.033294
H	0.054750	6.234048	0.552542
H	0.539824	5.064054	1.771092
H	2.803115	4.884975	0.704647
H	2.321687	6.044232	-0.524389
H	3.650247	7.164692	1.267330
H	2.004053	7.806944	1.256056
H	2.489717	6.639334	2.492057
H	4.125858	-2.738513	3.386672
H	5.628366	-3.609837	3.536505
H	5.989827	-1.532509	2.230210
H	4.034340	-2.733964	0.204256
H	3.692479	-1.347829	1.230549
H	-0.019688	0.550933	-0.346966
H	-5.492055	1.444316	-0.041239
H	-5.523480	1.282243	-1.885477
H	-4.044325	-0.562861	0.113925
H	-4.086901	-0.738398	-1.728463
H	5.593662	-0.097107	0.166166
H	5.936718	-1.483846	-0.854214
H	3.658120	-1.299518	-1.885301
H	3.304393	0.087535	-0.864161
H	5.180839	1.368904	-1.919702
H	5.591565	-0.040006	-2.892377
H	3.339939	0.121731	-4.069893
H	2.801945	2.433996	-4.591187
H	3.922286	3.025706	-3.239117
H	-0.272757	-5.742319	3.849256
H	0.721065	-6.480295	5.092421
H	0.460711	-4.428517	6.521962

H	-0.532229	-3.686881	5.278385
H	-2.207061	-5.549226	5.509747
H	-1.219693	-6.280971	6.762982
H	-1.495424	-4.237209	8.194852
H	-2.449521	-3.483117	6.920728
H	-4.215656	-5.313018	7.190837
H	-4.574540	-5.855343	9.533369
H	-2.903650	-5.187911	9.969516
H	2.422266	-6.599099	-1.690090
H	2.443462	-5.380901	-0.410536
H	3.661299	-5.336063	-1.696340
H	4.181382	-8.437630	-1.766573
H	5.478622	-7.231470	-1.795659
H	5.467858	-8.488069	-0.551700

! First Ethylene Insertion once the co-catalyst has dissociated - Transition State !

scf done: -1654.197002

C	0.594902	-1.956595	1.392952
C	1.899297	-2.380732	1.748991
C	2.693115	-1.221039	1.955671
C	1.867692	-0.089008	1.729310
C	0.561815	-0.533606	1.372954
Zr	0.999558	-1.210065	3.819860
Al	7.097541	-8.444643	6.985055
C	7.953516	-6.784928	7.694309
C	8.621588	-5.865511	6.661921
C	7.640542	-5.307256	5.629616
C	8.285252	-4.376941	4.601743
C	7.300696	-3.818215	3.574113
C	7.962610	-2.884426	2.550643
C	7.019688	-2.390330	1.495059
C	6.763521	-1.108521	1.221921
C	-0.589547	0.327689	0.935371
C	-0.632482	0.514805	-0.591046
C	-1.813324	1.371473	-1.047934
C	-1.866680	1.550042	-2.562289
C	0.371152	-0.325059	6.128863
C	1.785433	-0.286505	6.071850
C	2.182083	0.660812	5.085634
C	0.980940	1.203828	4.535262
C	-0.130318	0.602510	5.178018
C	3.583934	1.131292	4.813737
C	3.996495	2.288178	5.740042
C	5.418310	2.781848	5.470852
C	5.829628	3.935644	6.380425
C	7.979726	-9.493084	5.536643
C	7.062585	-10.315757	4.613028
C	7.866443	-11.227685	3.680728
C	1.593639	-3.250039	4.803188
C	5.439613	-9.173234	7.823234
C	4.750650	-8.321710	8.898230
C	3.501579	-8.975501	9.496973
C	2.806083	-8.127196	10.563032
C	1.561474	-8.791425	11.152486

C	0.862963	-7.934543	12.218363
C	-0.383955	-8.570039	12.758289
C	-0.597328	-8.887997	14.035364
C	-1.203990	-2.153590	3.962667
C	-0.548957	-3.324877	4.382656
H	4.471196	-7.343463	8.479090
H	5.457192	-8.100138	9.710975
H	9.419040	-6.408999	6.136309
H	0.931532	1.980023	3.781315
H	4.720566	-9.414075	7.023893
H	5.702565	-10.157064	8.247764
H	8.686285	-10.174312	6.041811
H	8.620221	-8.836891	4.927415
H	1.765858	-4.217049	4.331277
H	1.527067	-3.373472	5.884416
H	6.428106	-10.961217	5.239290
C	6.135689	-9.408925	3.800133
H	-0.221966	-0.948835	6.786422
H	3.746332	-1.203915	2.211626
H	2.238250	-3.406233	1.823357
H	-1.536876	-0.117373	1.264923
H	-0.521140	1.312544	1.413679
H	0.308566	0.971767	-0.924518
H	-0.683936	-0.470320	-1.072870
H	-2.749238	0.913354	-0.699388
H	-1.756730	2.356209	-0.564077
H	-2.722037	2.165540	-2.859524
H	-0.961249	2.039237	-2.939002
H	-1.959679	0.586004	-3.075375
H	2.185853	0.945002	1.777227
H	-0.235556	-2.606754	1.145719
H	2.461167	-0.869050	6.687565
H	-1.173010	0.824713	4.987431
H	3.671939	1.460491	3.771563
H	4.290258	0.302073	4.943980
H	3.287963	3.117952	5.617359
H	3.910002	1.961445	6.784754
H	6.122313	1.947763	5.596616
H	5.500794	3.095920	4.421120
H	6.851316	4.265296	6.165446
H	5.169866	4.801200	6.251648
H	5.792210	3.645547	7.436649
H	7.219331	-6.214350	8.281518
H	8.706400	-7.110931	8.431303
H	9.118296	-5.021700	7.164433
H	7.155323	-6.145582	5.102267
H	6.833905	-4.771855	6.152813
H	2.541224	-2.669085	4.617815
H	-1.764087	-1.590603	4.702715
H	-1.601882	-2.124243	2.952623
H	-0.633777	-3.646411	5.414864
H	-0.385373	-4.123670	3.667060
H	8.774351	-3.543889	5.126001
H	9.086181	-4.916440	4.077144
H	6.814301	-4.649912	3.044593

H	6.499281	-3.272150	4.092458
H	8.424455	-2.032658	3.065654
H	8.780778	-3.432995	2.060251
H	6.527386	-3.162271	0.899461
H	6.093756	-0.820825	0.414981
H	7.244745	-0.300480	1.770769
H	2.790984	-9.199759	8.687860
H	3.779485	-9.947306	9.929244
H	3.516668	-7.905236	11.372036
H	2.527603	-7.154279	10.130972
H	0.850432	-9.016296	10.344774
H	1.834526	-9.758875	11.594112
H	1.558217	-7.726811	13.041625
H	0.607145	-6.961097	11.772082
H	-1.162097	-8.789880	12.024249
H	-1.524129	-9.353669	14.361235
H	0.147375	-8.693078	14.805292
H	5.468182	-9.988454	3.151653
H	5.501556	-8.787811	4.447471
H	6.714965	-8.733177	3.157538
H	7.213617	-11.837923	3.044332
H	8.516829	-10.638140	3.021862
H	8.507453	-11.910108	4.250081

! First Ethylene Insertion once the co-catalyst has dissociated - Product !

scf done: -1654.271926

C	-2.981337	3.906116	0.428741
C	-2.355034	3.004680	1.325191
C	-0.950806	3.132837	1.160086
C	-0.688967	4.099131	0.152842
C	-1.962109	4.562938	-0.307920
Zr	-1.890670	2.168221	-1.032917
C	-2.584992	2.607465	-3.474289
C	-2.348438	1.210079	-3.359352
C	-0.975932	0.998407	-3.073280
C	-0.347428	2.268408	-2.979388
C	-1.340760	3.255875	-3.227379
C	-3.869495	3.266551	-3.887947
C	-3.977726	3.406856	-5.416664
C	-5.276389	4.079257	-5.861899
C	-5.376417	4.228501	-7.377221
C	0.652505	4.659457	-0.228458
C	1.043811	5.857012	0.655015
C	2.391339	6.467264	0.268161
C	2.777664	7.654255	1.145574
C	-3.916730	1.196002	-0.791130
C	-3.219133	-0.082491	-0.347416
C	3.798556	2.545853	-3.606700
C	4.009368	1.248918	-3.367814
C	4.889184	0.693926	-2.288167
C	4.151520	-0.238053	-1.315880
C	5.073053	-0.868723	-0.271561
C	4.352108	-1.797845	0.705615
C	5.273564	-2.442575	1.742692

C	-0.088205	2.620062	-0.716058	H	0.417310	0.349222	-7.906435
C	0.963238	2.634538	-1.679296	H	0.234996	-1.184163	-9.865897
C	0.370587	2.354237	-2.938159	H	1.688353	-1.574532	-8.939270
C	-1.029537	2.189001	-2.755516	H	0.249020	-2.592517	-8.799037
Zr	0.037681	0.230102	-1.626594	H	2.540208	0.195440	-3.625047
Al	-0.374345	-0.811996	3.004925	H	-1.025373	-2.274090	-3.351477
C	-0.093407	-2.548282	3.931845	H	0.029398	2.822490	0.342824
C	-1.083299	-3.020353	5.011258	H	-1.754712	1.993161	-3.536120
C	2.396883	3.014885	-1.435370	H	3.063994	2.399449	-2.052074
C	2.666165	4.498722	-1.745049	H	2.661255	2.820212	-0.389293
C	4.118725	4.897515	-1.486310	H	2.407375	4.701595	-2.792552
C	4.395633	6.367085	-1.789628	H	1.997729	5.120717	-1.135596
C	0.782704	-2.165613	-2.045832	H	4.371102	4.686188	-0.438086
C	1.951749	-1.366821	-2.147211	H	4.781650	4.266050	-2.093760
C	1.805352	-0.516544	-3.268890	H	5.441970	6.622164	-1.592085
C	0.551033	-0.797630	-3.893916	H	4.189748	6.604921	-2.839531
C	-0.070814	-1.819090	-3.122734	H	3.773216	7.025862	-1.173248
C	0.072301	-0.294294	-5.227170	H	1.070222	-1.291041	0.874951
C	0.578012	-1.172701	-6.384945	H	0.641133	0.467679	0.966716
C	0.091401	-0.688398	-7.750914	H	2.566163	-0.901980	2.923087
C	0.593057	-1.556929	-8.900731	H	2.267246	0.818443	2.768891
C	-1.987489	-2.442118	0.495890	H	3.652273	-0.964141	0.705471
C	-1.382531	0.764353	3.692361	H	3.285484	0.740936	0.453963
C	-2.803274	0.632708	4.262205	H	5.592611	0.581648	1.093434
C	-3.867228	0.373985	3.195644	H	4.725889	1.344893	2.414325
C	-5.292376	0.293654	3.744627	H	4.732144	-0.821712	3.679303
C	-6.345814	0.057269	2.661756	H	5.527392	-1.615710	2.328269
C	-7.778349	-0.010007	3.210799	H	7.508670	-0.096907	2.595863
C	-8.797573	-0.289563	2.146166	H	6.687795	0.727126	3.919260
C	-9.805964	0.516380	1.812693	H	6.733701	-1.442021	5.271280
C	0.974943	-0.420200	1.541670	H	8.844513	-2.617296	4.985551
C	2.341772	-0.114413	2.191529	H	9.142619	-1.738810	3.382888
C	3.526215	-0.003844	1.226546	H	-2.169833	-2.667992	-1.628682
C	4.854441	0.390441	1.883922	H	-3.596113	-2.032789	-0.847366
C	5.427009	-0.652257	2.846562	H	-2.468926	0.133516	-0.402869
C	6.794305	-0.245616	3.415745	H	-2.664383	-0.196002	-2.095443
C	7.345087	-1.246789	4.387860	H	-2.373573	-3.435180	0.745989
C	8.497658	-1.901244	4.244814	H	-0.893774	-2.502974	0.523210
C	-2.498849	-1.960707	-0.858241	H	-2.324218	-1.761002	1.292045
C	-2.096070	-0.522275	-1.208079	H	-2.840279	-0.168450	5.012088
H	0.895441	2.316351	-3.883988	H	-3.070835	1.554258	4.799566
H	-0.716102	1.141839	4.489417	H	-5.350752	-0.510376	4.491579
H	-1.368168	1.558420	2.930206	H	-5.525259	1.223998	4.281460
H	0.906808	-2.441846	4.388095	H	-6.289919	0.858327	1.912035
H	0.039332	-3.343259	3.180822	H	-6.119127	-0.877165	2.128513
H	-2.293042	2.330093	-0.923614	H	-7.824727	-0.802614	3.972709
H	2.802549	-1.394919	-1.476369	H	-8.024578	0.929572	3.721375
H	0.587328	-2.926640	-1.300752	H	-8.677717	-1.232846	1.608991
H	-3.817496	1.172457	2.440009	H	-10.509913	0.255005	1.026455
H	-3.633249	-0.561712	2.664140	H	-9.970149	1.466368	2.318619
H	-1.024284	-0.276270	-5.244919	C	-0.521935	-4.209090	5.798129
H	0.409759	0.735478	-5.388919	H	-1.238016	-2.196592	5.724022
H	1.675884	-1.191647	-6.370109	C	-2.443006	-3.378128	4.410548
H	0.249889	-2.207760	-6.222915	H	-1.215030	-4.538774	6.581199
H	-1.007035	-0.668169	-7.758092	H	-0.339639	-5.064778	5.135563

H 0.428698 -3.956927 6.281402
H -3.157615 -3.679798 5.184456
H -2.885877 -2.534581 3.867524
H -2.351488 -4.214198 3.705723

! Ethylene Insertion after Chain Transfer -
Adduct !

scf done: -1140.724396

C -3.572587 0.013722 1.254070
C -2.861721 1.051135 0.579830
C -2.429165 1.967588 1.579092
C -2.879698 1.513623 2.842007
C -3.585054 0.294467 2.640581
Zr -1.176825 -0.222002 2.051572
C 0.582020 -2.060059 1.610212
C 0.173410 -1.523487 0.363219
C -1.195083 -1.840942 0.183079
C -1.623095 -2.589956 1.317688
C -0.518191 -2.749987 2.193316
C -0.491726 -3.595558 3.434958
C -0.077453 -5.049399 3.142352
C -0.050730 -5.915015 4.402426
C 0.357025 -7.358895 4.124902
C -2.747937 1.243758 -0.905369
C -3.866159 2.145055 -1.458271
C -3.791822 2.310560 -2.976352
C -4.887127 3.216623 -3.530596
C -1.125594 -0.437327 5.142661
C 0.104476 -0.186422 4.662651
C 0.466466 1.275988 1.523570
C 1.960963 0.962737 1.654054
C 2.841528 2.212341 1.501340
C 4.345375 1.975514 1.681049
C 4.988222 1.090270 0.611721
C 6.512532 0.979102 0.764188
C 7.134458 0.060767 -0.245923
C 8.030209 0.419952 -1.165727
H -2.727268 2.018695 3.788006
H -1.792651 -1.609672 -0.688483
H -4.066894 -0.303062 3.406171
H -2.794380 0.274021 -1.414071
H -1.775832 1.686436 -1.153968
H -3.808423 3.129216 -0.975278
H -4.840631 1.722008 -1.180540
H -3.859430 1.322641 -3.452357
H -2.807688 2.714521 -3.250409
H -4.812681 3.308666 -4.619090
H -5.884521 2.824677 -3.300752
H -4.823422 4.226200 -3.108983
H -1.483697 -3.602067 3.904197
H 0.208328 -3.174937 4.166817
H 0.913038 -5.053947 2.669276
H -0.771843 -5.480880 2.409960
H -1.042382 -5.899267 4.874968
H 0.642718 -5.473420 5.131400

H 0.367745 -7.951087 5.045715
H -0.336279 -7.843361 3.428058
H 1.359671 -7.413987 3.685789
H 0.796496 -0.977350 -0.332241
H 1.577150 -1.987396 2.031753
H -2.608297 -3.017119 1.463582
H -4.052397 -0.830163 0.773912
H -1.877518 2.879997 1.393161
H 4.531526 1.540865 2.674291
H 4.850981 2.950608 1.681499
H 4.553211 0.082289 0.643417
H 4.758803 1.491773 -0.384645
H 0.268539 1.698064 0.526046
H 0.223492 2.103006 2.217127
H 2.180572 0.507875 2.631691
H 2.259476 0.220334 0.904956
H 2.513636 2.962992 2.233760
H 2.659179 2.657586 0.512525
H -1.776652 0.362606 5.484972
H -1.493887 -1.453730 5.265055
H 0.492761 0.828697 4.613316
H 0.789838 -0.990342 4.408788
H 6.965377 1.975599 0.686682
H 6.738338 0.610804 1.776332
H 6.802964 -0.979313 -0.212271
H 8.439476 -0.295652 -1.874531
H 8.393047 1.443679 -1.241033

! Ethylene Insertion After Chain Transfer -
Transition State !

scf done: -1140.303391

C -3.855234 0.412502 1.279670
C -3.038734 1.311911 0.530500
C -2.432016 2.188080 1.476926
C -2.853170 1.827585 2.776052
C -3.733574 0.719716 2.656783
Zr -1.460157 -0.145862 1.939624
C 0.136896 -1.953790 1.066891
C -0.749765 -1.594972 0.010714
C -2.047924 -2.028901 0.370697
C -1.964280 -2.642113 1.649880
C -0.602977 -2.639409 2.066352
C -0.023482 -3.385763 3.232628
C 0.548420 -4.749772 2.804848
C 1.161647 -5.527827 3.968992
C 1.724415 -6.881579 3.545780
C -2.981829 1.436361 -0.966791
C -4.060075 2.390853 -1.508153
C -4.021846 2.529688 -3.029875
C -5.088834 3.479699 -3.566033
C -1.329318 -0.490595 4.358168
C -0.089520 0.121869 4.224245
C 0.483299 1.126377 2.200939
C 1.986512 0.939666 2.299416
C 2.762257 1.909333 1.393266

C	4.284910	1.850131	1.557391	C	-2.946686	1.452695	-0.994872
C	4.922835	0.519674	1.154434	C	-2.215435	2.283659	-0.098123
C	6.457384	0.556425	1.203692	C	-2.607512	1.984612	1.234858
C	7.084330	-0.760314	0.852217	C	-3.565543	0.944398	1.179057
C	7.899051	-0.972725	-0.181439	Zr	-1.395759	-0.073009	0.390457
H	-2.565442	2.320314	3.696541	C	0.186245	-1.944828	-0.290159
H	-2.942043	-1.927344	-0.229959	C	-0.565634	-1.573249	-1.440206
H	-4.251510	0.221813	3.467093	C	-1.912802	-1.934834	-1.214713
H	-3.112866	0.450666	-1.429620	C	-1.991901	-2.505446	0.085295
H	-1.994606	1.802350	-1.275409	C	-0.685228	-2.555150	0.652719
H	-3.931937	3.377752	-1.044392	C	-0.298634	-3.310316	1.888843
H	-5.048557	2.030042	-1.194355	C	0.048156	-4.775599	1.568289
H	-4.148877	1.539574	-3.488807	C	0.417009	-5.583245	2.812664
H	-3.028098	2.883342	-3.337451	C	0.763746	-7.034940	2.495413
H	-5.040790	3.556247	-4.657177	C	-2.942338	1.551041	-2.494660
H	-6.096544	3.137884	-3.303531	C	-3.923238	2.622074	-3.004021
H	-4.966496	4.489638	-3.158217	C	-3.895059	2.777699	-4.524572
H	-0.794576	-3.552297	3.994054	C	-4.860773	3.846256	-5.028876
H	0.774099	-2.799312	3.705744	C	-0.560893	-0.031212	2.517526
H	1.306167	-4.594476	2.025571	C	0.963855	0.143939	2.385434
H	-0.250538	-5.344202	2.342761	C	1.368093	1.185795	1.335135
H	0.402036	-5.674040	4.748920	C	2.879529	1.340437	1.163088
H	1.958619	-4.926718	4.427930	C	3.282540	2.377152	0.113731
H	2.155878	-7.416350	4.398172	C	4.789156	2.648324	0.035945
H	0.945533	-7.521096	3.115049	C	5.635903	1.444737	-0.382162
H	2.513238	-6.770127	2.792824	C	7.123709	1.790482	-0.543925
H	-0.474361	-1.101138	-0.914149	C	7.967364	0.596391	-0.879966
H	1.209814	-1.807411	1.069240	C	8.676314	0.446297	-1.999010
H	-2.785516	-3.100622	2.189502	H	-2.249439	2.476300	2.129085
H	-4.484847	-0.363221	0.862041	H	-2.735601	-1.802745	-1.905322
H	-1.764763	3.005459	1.229195	H	-4.062577	0.487648	2.027142
H	4.547462	2.081859	2.599467	H	-3.205826	0.583114	-2.936867
H	4.725670	2.651587	0.950154	H	-1.933993	1.799128	-2.850885
H	4.565800	-0.285812	1.810334	H	-3.682073	3.583300	-2.531762
H	4.606853	0.252803	0.136366	H	-4.938423	2.363747	-2.675188
H	0.197198	1.036069	1.105311	H	-4.135022	1.814235	-4.994410
H	0.211615	2.146591	2.486588	H	-2.873864	3.027905	-4.843785
H	2.295945	1.117611	3.338455	H	-4.818626	3.936482	-6.119162
H	2.263808	-0.093228	2.062883	H	-5.895987	3.610438	-4.757313
H	2.423355	2.932463	1.603740	H	-4.624158	4.829707	-4.606911
H	2.503239	1.710324	0.343353	H	-1.124477	-3.287216	2.609856
H	-2.144902	0.058844	4.815509	H	0.560756	-2.833964	2.373034
H	-1.376164	-1.570821	4.452215	H	0.879813	-4.801581	0.851609
H	0.064354	1.138348	4.571373	H	-0.805771	-5.247325	1.064176
H	0.808080	-0.481424	4.135172	H	-0.418378	-5.553107	3.525479
H	6.829293	1.336009	0.527082	H	1.266717	-5.104378	3.318006
H	6.768593	0.847046	2.218373	H	1.018186	-7.590610	3.403820
H	6.831942	-1.598387	1.505459	H	-0.076650	-7.551341	2.017325
H	8.320557	-1.953981	-0.384589	H	1.621376	-7.102923	1.816341
H	8.182300	-0.169813	-0.860013	H	-0.169275	-1.115053	-2.340079
				H	1.258093	-1.832929	-0.173766
				H	-2.888563	-2.908829	0.543605
				H	-4.471698	-0.122068	-0.563428
				H	-1.507822	3.052800	-0.391009
				H	5.139471	3.017457	1.010233
! Ethylene Insertion After Chain Transfer - Product !							
scf done: -1140.755780							
C	-3.771643	0.615862	-0.189868				

H	4.958519	3.467143	-0.675750	C	-7.679449	1.806899	12.164280
H	5.537549	0.639921	0.358307	C	-7.184642	2.017496	13.384325
H	5.259115	1.038575	-1.331253	C	1.780657	-2.407256	-1.038539
H	0.956130	0.912498	0.328565	C	-5.575130	4.818621	1.654809
H	0.927010	2.159927	1.586693	C	-5.809170	6.341737	1.649671
H	3.297905	1.625473	2.138594	C	-7.034057	6.742522	2.472579
H	3.313862	0.362520	0.919811	C	-4.565688	7.096067	2.125021
H	2.767644	3.322606	0.333582	H	3.861001	-2.517405	-6.373410
H	2.922815	2.054631	-0.875273	H	5.635962	-3.989612	-4.271208
H	-0.979706	0.807555	3.084414	H	5.086588	-1.859659	-0.523529
H	-0.792567	-0.932972	3.098050	H	0.237998	-1.661349	-4.134004
H	1.404619	0.441469	3.347855	H	2.751493	-0.820469	-0.049367
H	1.436467	-0.811864	2.124974	H	1.113919	0.793287	-1.047209
H	7.244205	2.558447	-1.318444	H	-0.059009	-0.512284	-1.290867
H	7.483049	2.234398	0.396447	H	0.945882	0.499019	1.433157
H	7.979280	-0.203535	-0.136658	H	-0.214275	-0.804090	1.202159
H	9.267585	-0.446632	-2.185885	H	-0.608946	2.100653	0.299204
H	8.697680	1.216154	-2.768554	H	-1.757164	0.800792	0.017126
				H	5.846879	-0.071954	-2.388290
				H	1.064854	-4.142214	-3.464860
				H	6.167053	-1.390886	-4.709739
				H	3.302769	-4.668441	-4.849653
				H	2.169047	0.655565	-3.573602
				H	3.584087	0.827501	-2.511855
				H	3.794756	0.757137	-4.256500
				H	0.857957	-2.792347	-1.463663
				H	2.567255	-3.127611	-0.809656
				H	-1.998678	0.476905	2.499631
				H	-0.872110	1.795209	2.780248
				H	-2.417584	3.370858	1.596026
				H	-3.529838	2.055492	1.286535
				H	-3.813026	1.729367	3.795578
				H	-2.731110	3.058604	4.087223
				H	-7.097688	4.222608	4.846253
				H	-5.795647	5.197400	5.462875
				H	-6.007477	2.146710	5.815603
				H	-4.689519	3.124843	6.423826
				H	-6.295055	4.408505	7.854416
				H	-7.624510	3.448765	7.228685
				H	-6.571000	1.369810	8.170846
				H	-5.239783	2.328089	8.798178
				H	-6.845486	3.616467	10.239853
				H	-8.178218	2.667820	9.602368
				H	-7.121976	0.581000	10.512148
				H	-5.800983	1.533711	11.183752
				H	-6.491357	4.311739	1.308059
				H	-4.812101	4.568867	0.902797
				H	-6.001748	6.654751	0.611046
				H	-7.230719	7.818485	2.396913
				H	-7.933801	6.217641	2.131624
				H	-6.897163	6.509506	3.535553
				H	-4.696348	8.182362	2.055315
				H	-4.344241	6.867586	3.178756
				H	-3.681280	6.830225	1.534298
				H	-8.762727	1.815075	12.027099
! First Vinyl coordinaiton/insertion - Adduct !							
scf done: -1575.678217							
C	5.271256	-2.071336	-1.570883				
C	5.684675	-1.129451	-2.545923				
C	5.850872	-1.824490	-3.768412				
C	5.565219	-3.197584	-3.536161				
C	5.212304	-3.366138	-2.173188				
Zr	3.389714	-1.919129	-3.274852				
C	3.209586	0.343260	-3.423914				
C	4.960965	-4.673892	-1.474910				
C	6.261691	-5.308421	-0.950410				
C	6.021459	-6.626233	-0.213750				
C	7.309092	-7.255969	0.309001				
C	1.126154	-2.159019	-4.506324				
C	1.558848	-3.468570	-4.154559				
C	2.741025	-3.743750	-4.874990				
C	3.039100	-2.601163	-5.671496				
C	2.013573	-1.628431	-5.479630				
C	1.823216	-0.370812	-6.273996				
C	1.091066	-0.631405	-7.602069				
C	0.857935	0.649542	-8.403718				
C	0.169839	0.399018	-9.742497				
C	1.846334	-1.142204	-0.567937				
C	0.735654	-0.148605	-0.629074				
C	0.150480	0.136111	0.769070				
C	-0.987528	1.156950	0.716602				
C	-1.631841	1.423737	2.077912				
C	-2.791146	2.424517	2.012912				
C	-3.472315	2.683891	3.361930				
Al	-5.025874	3.942495	3.369619				
C	-6.021805	4.189131	5.078121				
C	-5.761718	3.154219	6.182164				
C	-6.552111	3.411355	7.468899				
C	-6.312481	2.365870	8.559035				
C	-7.105792	2.627496	9.839818				
C	-6.867325	1.568479	10.926031				

H	-7.831188	2.191234	14.240949	C	-12.127524	4.346950	10.240690
H	-6.112406	2.021959	13.573808	C	-12.577929	4.692155	11.660512
H	1.252557	0.356102	-5.685352	C	-12.033849	3.721755	12.719168
H	2.794532	0.090332	-6.487430	C	-12.496769	4.048823	14.107830
H	1.673906	-1.341891	-8.203204	C	-11.702770	4.353534	15.134740
H	0.128679	-1.119091	-7.397665	C	-4.653107	0.331725	0.464273
H	0.254583	1.345659	-7.805302	C	-12.773153	6.624052	3.239274
H	1.820643	1.150751	-8.574949	C	-12.972978	8.150992	3.298362
H	0.010136	1.334836	-10.288075	C	-14.069078	8.551939	4.286252
H	0.769626	-0.257573	-10.383330	C	-11.660705	8.869456	3.620934
H	-0.809056	-0.075192	-9.607611	H	-2.330365	-0.341234	-4.351067
H	4.277553	-4.529155	-0.628579	H	-0.563731	-1.148162	-2.360553
H	4.471849	-5.378321	-2.159245	H	-1.787170	0.230232	1.573765
H	6.945525	-5.473882	-1.793089	H	-6.134343	0.855417	-2.626255
H	6.763457	-4.597437	-0.281081	H	-3.877380	2.186655	1.161135
H	5.332401	-6.452611	0.624461	H	-5.714014	3.583949	0.171179
H	5.514048	-7.331599	-0.885961	H	-6.576190	2.122900	-0.331195
H	7.106985	-8.193468	0.837245	H	-5.936004	2.861303	2.580517
H	8.005102	-7.480764	-0.507074	H	-6.903744	1.489004	2.058941
H	7.824072	-6.587554	1.008422	H	-7.590827	4.433333	1.534289
! First Vinyl coordinaiton/insertion - Transition State !				H	-8.583318	3.066598	1.048576
scf done: -1575.658267				H	-1.065906	2.378522	0.137935
C	-1.461740	0.215896	0.541407	H	-5.549536	-1.610118	-1.706973
C	-1.079248	1.355314	-0.215058	H	-0.301223	1.523795	-2.307699
C	-0.673428	0.906459	-1.498159	H	-3.186166	-2.345282	-2.767815
C	-0.820860	-0.504620	-1.527830	H	-4.645590	3.050961	-1.723215
C	-1.287519	-0.949043	-0.256175	H	-3.372079	3.529385	-0.566202
Zr	-3.152638	0.495269	-1.389689	H	-2.940068	2.663568	-2.012275
C	-3.734552	2.733876	-1.217259	H	-5.587321	-0.146799	0.181943
C	-1.431123	-2.390756	0.164335	H	-4.062361	-0.207657	1.200553
C	-1.945612	-2.621912	1.585086	H	-8.898372	2.428585	3.451789
C	-2.017914	-4.106140	1.947624	H	-7.852276	3.748733	3.948134
C	-2.509831	-4.351626	3.370603	H	-9.450380	5.392042	2.925815
C	-5.241300	0.286647	-2.856444	H	-10.510672	4.076323	2.468729
C	-4.933405	-1.014031	-2.367721	H	-10.795187	3.447884	4.901284
C	-3.692350	-1.400988	-2.924977	H	-9.704541	4.716287	5.369779
C	-3.236268	-0.338361	-3.756559	H	-13.772123	5.977326	6.675895
C	-4.212162	0.696824	-3.747102	H	-12.409027	7.007663	6.998246
C	-4.196112	1.934810	-4.597989	H	-12.473489	3.973726	7.504543
C	-4.886930	1.717879	-5.956017	H	-11.065940	4.981015	7.764917
C	-4.861289	2.969928	-6.833144	H	-12.343111	6.340464	9.439246
C	-5.539757	2.764087	-8.184176	H	-13.749709	5.319603	9.193894
C	-4.641554	1.743312	0.525190	H	-12.452816	3.325537	9.994598
C	-5.917117	2.542309	0.437826	H	-11.028345	4.330487	10.205080
C	-6.632433	2.520620	1.802010	H	-12.256357	5.711880	11.911388
C	-7.877119	3.410503	1.817395	H	-13.676154	4.699657	11.704671
C	-8.575483	3.443213	3.178232	H	-12.359950	2.702844	12.460073
C	-9.780832	4.388025	3.229449	H	-10.936612	3.715926	12.687392
C	-10.454408	4.454083	4.605311	H	-13.740099	6.141425	3.021425
Al	-11.986528	5.715794	4.840919	H	-12.132888	6.377659	2.379143
C	-12.671188	5.979736	6.695683	H	-13.293806	8.494478	2.301880
C	-12.165369	4.997699	7.762108	H	-14.244555	9.634055	4.270800
C	-12.650240	5.316793	9.179748	H	-15.019490	8.059963	4.049665
				H	-13.802030	8.276682	5.313794
				H	-11.772224	9.959632	3.587231

H	-11.309574	8.615482	4.632717	C	-11.449566	4.787158	7.918993
H	-10.867376	8.595961	2.915401	C	-12.080063	4.606848	9.303585
H	-13.577563	4.040592	14.263167	C	-11.256299	3.732335	10.250320
H	-12.104183	4.587349	16.117699	C	-11.892028	3.562290	11.630724
H	-10.619021	4.377474	15.032131	C	-11.059573	2.687317	12.579509
H	-4.694175	2.758667	-4.073487	C	-11.715384	2.483335	13.912965
H	-3.160133	2.250676	-4.774573	C	-11.207677	2.852971	15.089153
H	-4.397229	0.888206	-6.482450	C	-4.889208	1.449858	-0.345180
H	-5.925907	1.405858	-5.786855	C	-12.478899	6.958858	3.688998
H	-5.349876	3.796828	-6.299874	C	-13.368365	8.165818	4.034980
H	-3.819459	3.280819	-6.990401	C	-14.598072	7.763262	4.850294
H	-5.502656	3.675651	-8.789496	C	-12.570080	9.257857	4.750621
H	-5.054159	1.966445	-8.757896	H	-2.174524	-1.422982	-3.882994
H	-6.594254	2.490274	-8.064592	H	-0.946953	-1.736926	-1.225753
H	-2.067348	-2.931781	-0.548687	H	-2.529786	1.252376	1.507199
H	-0.438938	-2.853759	0.069628	H	-5.862684	0.830007	-3.396481
H	-1.289235	-2.108395	2.299892	H	-3.707395	3.191849	0.162232
H	-2.942949	-2.175490	1.702484	H	-5.417822	4.915113	-0.353648
H	-2.677853	-4.622074	1.236718	H	-6.548732	3.658791	-0.843797
H	-1.024197	-4.556290	1.821599	H	-5.392115	4.005766	1.973898
H	-2.550213	-5.421909	3.597137	H	-6.485712	2.715060	1.493172
H	-1.847582	-3.883875	4.108158	H	-7.156986	5.700567	1.411863
H	-3.516213	-3.944398	3.523700	H	-8.217993	4.414746	0.860370
! First Vinyl coordinaiton/insertion - Product !				H	-1.106439	2.529912	-0.377645
scf done: -1575.693045				H	-5.922857	-1.215901	-1.663881
C	-2.032386	0.783886	0.668507	H	-0.127082	0.676038	-2.082612
C	-1.272552	1.460020	-0.324782	H	-3.638524	-2.621786	-1.962536
C	-0.756610	0.486986	-1.220282	H	-4.868420	3.121537	-2.683369
C	-1.194857	-0.784833	-0.771955	H	-3.766483	4.337646	-2.022757
C	-1.971786	-0.617469	0.412181	H	-3.163488	2.757076	-2.311753
Zr	-3.233088	0.478313	-1.552838	H	-5.876592	1.254042	-0.780238
C	-4.074478	3.289153	-1.949296	H	-4.944144	1.185570	0.714082
C	-2.476669	-1.736194	1.283001	H	-8.159974	3.408070	3.184290
C	-3.837845	-1.524636	1.949951	H	-7.193325	4.768297	3.728756
C	-4.219557	-2.675777	2.881791	H	-9.053557	6.332657	3.093488
C	-5.595733	-2.498837	3.515767	H	-10.002250	4.973116	2.533707
C	-5.082916	0.089450	-3.266630	H	-9.927511	3.994734	4.894708
C	-5.117899	-0.990795	-2.351742	H	-9.052943	5.395183	5.434274
C	-3.908358	-1.718780	-2.496191	H	-13.287090	5.234995	6.857953
C	-3.138122	-1.088285	-3.517089	H	-12.454499	6.647194	7.437650
C	-3.872722	0.019823	-4.017889	H	-11.293948	3.795535	7.469574
C	-3.480764	0.903209	-5.169834	H	-10.443698	5.213998	8.041835
C	-4.029490	0.381361	-6.510213	H	-12.230916	5.595917	9.759627
C	-3.628586	1.259419	-7.695581	H	-13.083906	4.173429	9.186913
C	-4.180800	0.748737	-9.023170	H	-11.107873	2.742168	9.795155
C	-4.537253	2.946563	-0.515641	H	-10.252269	4.166049	10.364484
C	-5.717054	3.874940	-0.157152	H	-12.041089	4.547551	12.092367
C	-6.211339	3.756998	1.283730	H	-12.893724	3.123849	11.519621
C	-7.420401	4.646849	1.581057	H	-10.900451	1.708126	12.102744
C	-7.963425	4.474622	3.000936	H	-10.066109	3.132248	12.719505
C	-9.246196	5.265906	3.276770	H	-13.077588	6.214524	3.135782
C	-9.802065	5.072073	4.693254	H	-11.705396	7.273550	2.971877
Al	-11.537944	5.953780	5.140599	H	-13.735746	8.600404	3.091476
C	-12.278529	5.665089	6.970502	H	-15.260952	8.619381	5.022470
				H	-15.182750	6.991341	4.336364

H	-14.313706	7.365643	5.831916	C	-3.326823	2.029564	1.881577
H	-13.179120	10.149950	4.938615	C	-3.938867	2.399608	3.238036
H	-12.202492	8.906312	5.725488	Al	-5.643211	3.443860	3.235730
H	-11.700166	9.570809	4.161096	C	-6.347160	4.165296	1.505818
H	-12.694532	2.000319	13.891500	C	-6.688571	5.667127	1.443165
H	-11.741042	2.680904	16.020865	C	-5.489320	6.526848	1.849280
H	-10.237296	3.340894	15.165986	C	-6.585854	3.687135	4.976062
H	-3.853694	1.922570	-5.009604	C	-6.163413	2.759077	6.124371
H	-2.387060	0.969405	-5.235707	C	-6.899926	3.027593	7.440600
H	-3.669971	-0.643233	-6.670268	C	-6.484478	2.097811	8.581830
H	-5.123654	0.318925	-6.449097	C	-7.223564	2.371503	9.892327
H	-3.979687	2.285950	-7.523400	C	-6.800518	1.434878	11.033341
H	-2.532861	1.315902	-7.750931	C	-7.556680	1.680409	12.305237
H	-3.873139	1.391133	-9.854621	C	-7.012851	2.034585	13.469976
H	-3.825789	-0.265140	-9.239831	C	-7.915118	6.013057	2.287947
H	-5.276478	0.721174	-9.015487	H	3.737539	-3.074214	-5.944142
H	-2.488943	-2.664424	0.699130	H	5.397179	-4.182076	-3.896215
H	-1.722533	-1.893962	2.067606	H	5.531867	-1.322812	-0.626669
H	-3.829863	-0.587122	2.521135	H	0.390123	-1.069324	-4.038418
H	-4.614759	-1.410419	1.181103	H	2.643743	-0.252769	-0.056588
H	-4.191754	-3.620734	2.322072	H	0.558910	0.469330	-1.254841
H	-3.460224	-2.766501	3.669868	H	-0.183273	-1.115001	-0.963421
H	-5.831527	-3.327643	4.190928	H	0.665211	0.856782	1.235510
H	-5.651515	-1.572572	4.099176	H	-0.137565	-0.685581	1.492430
H	-6.384836	-2.460128	2.755572	H	-1.308310	1.717654	-0.011271
				H	-2.117088	0.164632	0.150447
				H	6.053739	0.004844	-2.907865
				H	0.693093	-3.469042	-2.861912
				H	5.941637	-1.758552	-4.935574
				H	2.773264	-4.713181	-4.035300
				H	2.160371	0.682558	-3.480681
				C	3.708400	1.534797	-2.253551
				H	3.729868	0.685181	-4.237179
				H	1.410251	-3.022545	-0.579842
				H	3.142234	-2.620112	-0.048852
				H	-2.130659	0.398294	2.632551
				H	-1.268524	1.923172	2.515453
				H	-3.173793	2.934867	1.277221
				H	-4.033586	1.410214	1.310507
				H	-4.095331	1.486686	3.834200
				H	-3.207836	2.980958	3.825868
				H	-7.669487	3.596752	4.802731
				H	-6.447746	4.736154	5.287577
				H	-6.329393	1.710141	5.837696
				H	-5.081375	2.847998	6.298805
				H	-6.729559	4.071858	7.739798
				H	-7.982441	2.936140	7.270460
				H	-6.655544	1.053728	8.281406
				H	-5.401669	2.190152	8.750459
				H	-7.054002	3.411490	10.201599
				H	-8.306065	2.275811	9.727716
				H	-6.964924	0.395397	10.711040
				H	-5.723653	1.537664	11.219100
				H	-7.240512	3.579884	1.233036
				H	-5.605075	3.929924	0.728668

! Second Vinyl Coordination/Insertion - Adduct !

scf done: -1654.275277

C	2.127004	-1.667611	-5.301890
C	1.153876	-1.799770	-4.276117
C	1.312315	-3.067427	-3.654582
C	2.410998	-3.718533	-4.263253
C	2.924539	-2.847266	-5.265319
Zr	3.430667	-1.789189	-3.037475
C	3.225121	0.494915	-3.273110
C	2.206721	-0.573649	-6.325615
C	1.262075	-0.834487	-7.512151
C	1.343113	0.252929	-8.584007
C	0.385949	0.011122	-9.747396
C	5.540032	-1.750280	-1.623312
C	5.821756	-1.047005	-2.821188
C	5.760226	-1.976565	-3.890164
C	5.477550	-3.257676	-3.337666
C	5.361526	-3.134914	-1.930629
C	5.227665	-4.270434	-0.954766
C	6.579064	-4.960045	-0.693125
C	6.472348	-6.111680	0.306804
C	7.812856	-6.790560	0.572444
C	1.861945	-0.955463	-0.349777
C	2.168273	-2.268982	-0.378102
C	0.502990	-0.368307	-0.547224
C	-0.054156	0.155386	0.792239
C	-1.411543	0.844639	0.648433
C	-1.993900	1.282359	1.993750

H	-6.931034	5.922289	0.399305	C	-0.323975	-2.234937	1.807715
H	-8.180324	7.072547	2.192322	C	-0.588463	-3.292473	2.879467
H	-8.788210	5.424485	1.983781	C	0.692410	-3.885082	3.459124
H	-7.736315	5.813504	3.351648	C	-4.395033	2.161445	0.591251
H	-5.696656	7.597129	1.733293	C	-4.331481	0.758814	0.806447
H	-5.226790	6.366360	2.906418	C	-5.737662	2.842932	0.483517
H	-4.603023	6.294678	1.247229	C	-6.359072	3.004589	1.882910
H	-8.640715	1.562957	12.244745	C	-7.703200	3.734091	1.845221
H	-7.619492	2.203053	14.356332	C	-8.339746	3.891070	3.227526
H	-5.937927	2.166955	13.582425	C	-9.669075	4.652959	3.213004
H	1.950512	0.388587	-5.868222	C	-10.311321	4.796987	4.598063
H	3.235221	-0.486049	-6.697245	Al	-12.017753	5.823246	4.752225
H	1.498934	-1.809636	-7.957890	C	-12.798565	6.738901	3.151531
H	0.231406	-0.908537	-7.140718	C	-12.995773	8.266023	3.231852
H	1.126457	1.228493	-8.127732	C	-11.682017	8.979449	3.559376
H	2.372933	0.314538	-8.961479	C	-12.896080	5.847192	6.542686
H	0.463992	0.803801	-10.498753	C	-12.417878	4.791320	7.550422
H	0.596472	-0.940697	-10.248615	C	-13.089167	4.891768	8.923759
H	-0.655655	-0.018465	-9.407349	C	-12.607782	3.838064	9.922593
H	4.833328	-3.904226	0.000090	C	-13.272400	3.947517	11.295348
H	4.514516	-5.016223	-1.329280	C	-12.785796	2.883399	12.289984
H	6.983471	-5.331996	-1.643446	C	-13.469648	2.969974	13.621993
H	7.295482	-4.215099	-0.323238	C	-12.861820	3.191239	14.787931
H	6.059626	-5.734788	1.252700	C	-14.086908	8.655342	4.229897
H	5.752810	-6.852527	-0.067889	H	-2.778254	-0.766642	-4.099912
H	7.707913	-7.609047	1.292042	H	-1.161684	-1.827654	-1.683726
H	8.237384	-7.210932	-0.346336	H	-1.233380	1.303379	1.328052
H	8.543972	-6.083560	0.981010	H	-6.233665	1.077816	-2.216205
H	3.125761	1.448676	-1.327025	H	-3.616033	2.753944	1.066920
H	4.751227	1.355977	-1.962421	H	-5.651053	3.833183	0.024873
C	3.588147	2.974082	-2.762141	H	-6.409117	2.245016	-0.143815
H	3.922706	3.696265	-2.008137	H	-5.663163	3.557684	2.528449
H	4.196443	3.126995	-3.661278	H	-6.485730	2.015715	2.341703
H	2.551541	3.219755	-3.020929	H	-7.564913	4.726303	1.392733
				H	-8.394388	3.190999	1.184925
				H	-0.501533	2.418393	-1.004765
				H	-5.756180	-1.258094	-0.962747
				H	-0.471691	0.482746	-2.879193
				H	-3.611480	-2.392700	-2.118235
				H	-4.583996	3.132524	-1.802121
				C	-2.946996	4.201031	-0.864225
				H	-2.984982	2.540397	-2.214629
				H	-5.271934	0.214288	0.777760
				H	-3.628127	0.406113	1.555899
				H	-8.499003	2.897973	3.671513
				H	-7.637698	4.411060	3.895130
				H	-9.500340	5.645240	2.770653
				H	-10.363199	4.141563	2.530390
				H	-10.478980	3.799250	5.034514
				H	-9.593350	5.271683	5.288573
				H	-13.985647	5.767736	6.405666
				H	-12.749816	6.851738	6.974123
				H	-12.592961	3.783119	7.146933
				H	-11.329086	4.868217	7.683661
				H	-12.911140	5.895033	9.337125
! Second Vinyl Coordination/Insertion - Transtion State !							
scf done: -1654.210316							
C	-4.474711	0.548696	-3.483869				
C	-5.425189	0.391405	-2.436946				
C	-5.174408	-0.838389	-1.772555				
C	-4.043353	-1.434925	-2.379607				
C	-3.602984	-0.573454	-3.424224				
Zr	-3.165453	0.612086	-1.244585				
C	-3.612580	2.921884	-1.348315				
C	-4.475855	1.619173	-4.537856				
C	-5.311709	1.214587	-5.764647				
C	-5.345095	2.298339	-6.842586				
C	-6.159437	1.892438	-8.067469				
C	-1.141321	0.787901	0.379174				
C	-0.757008	1.377782	-0.848784				
C	-0.754639	0.362596	-1.840409				
C	-1.117113	-0.856587	-1.206471				
C	-1.350846	-0.605659	0.173443				
C	-1.620012	-1.642469	1.227204				

H	-14.178325	4.806744	8.798882	C	2.520889	-1.827319	-8.332750
H	-12.791378	2.835128	9.510197	C	2.907416	-0.946035	-9.520350
H	-11.517487	3.921019	10.040500	C	2.396963	-1.491334	-10.850861
H	-13.085639	4.943769	11.718054	C	4.559789	-1.273223	-1.195255
H	-14.362371	3.864743	11.181120	C	5.401434	-0.839844	-2.254328
H	-12.968100	1.889037	11.854785	C	5.772349	-1.982891	-3.009549
H	-11.700102	2.970609	12.425740	C	5.153892	-3.114328	-2.413030
H	-13.766709	6.262815	2.927326	C	4.407954	-2.684563	-1.276141
H	-12.155507	6.505008	2.290178	C	3.699032	-3.565379	-0.288112
H	-13.320462	8.623227	2.241515	C	4.645788	-4.081480	0.809724
H	-14.264082	9.737273	4.226102	C	3.941171	-4.989052	1.818455
H	-15.037790	8.163795	3.994919	C	4.878795	-5.508015	2.904415
H	-13.813666	8.370921	5.253709	C	1.823572	0.622199	-1.925487
H	-11.792072	10.070006	3.535280	C	1.641703	-0.912284	-2.023204
H	-11.329877	8.717246	4.568995	C	0.526318	1.347179	-1.519596
H	-10.889186	8.710400	2.851811	C	-0.079708	0.940489	-0.175666
H	-14.554903	2.849432	13.608202	C	-1.314056	1.779988	0.162238
H	-13.417566	3.249037	15.720622	C	-1.970549	1.450962	1.503751
H	-11.782701	3.320550	14.853982	C	-3.191978	2.331256	1.791374
H	-4.877022	2.551529	-4.123025	C	-3.877058	2.069545	3.138283
H	-3.448945	1.831626	-4.861223	Al	-5.465744	3.215960	3.543137
H	-4.904561	0.286384	-6.186695	C	-6.279643	4.247516	2.032319
H	-6.335391	0.982884	-5.442398	C	-6.665482	5.723063	2.248275
H	-5.759606	3.222165	-6.416113	C	-5.463304	6.548521	2.712121
H	-4.317498	2.537490	-7.149172	C	-6.223371	3.213092	5.387171
H	-6.163440	2.685769	-8.822125	C	-5.624007	2.216186	6.388846
H	-5.750289	0.991270	-8.538359	C	-6.262741	2.281179	7.779675
H	-7.202193	1.682056	-7.803456	C	-5.665170	1.292099	8.781278
H	-2.205931	-1.206628	2.045574	C	-6.306130	1.367511	10.167482
H	-2.225098	-2.455193	0.806008	C	-5.699348	0.375353	11.170135
H	0.268868	-2.673855	0.994562	C	-6.356942	0.428566	12.517155
H	0.284969	-1.425029	2.230454	C	-5.745693	0.732394	13.662546
H	-1.185313	-2.848242	3.687801	C	-7.842587	5.879117	3.211711
H	-1.203203	-4.096228	2.451614	H	4.366760	-3.600639	-5.718706
H	0.471518	-4.637495	4.223216	H	5.270972	-4.141542	-2.736212
H	1.295443	-4.369678	2.682731	H	4.126133	-0.642453	-0.430485
H	1.314205	-3.112724	3.926154	H	0.660466	-1.381323	-5.207231
H	-3.605926	4.689966	-0.136352	H	2.581265	0.845698	-1.160167
H	-2.018271	3.971504	-0.328854	H	0.720099	2.427156	-1.487795
C	-2.654194	5.188549	-1.995944	H	-0.220923	1.194398	-2.313375
H	-2.208013	6.107236	-1.601126	H	0.672307	1.059959	0.617990
H	-1.953156	4.770328	-2.727691	H	-0.352089	-0.122860	-0.187211
H	-3.568680	5.466985	-2.530967	H	-1.034621	2.843578	0.154775
				H	-2.056825	1.661000	-0.640115
				H	5.721193	0.179890	-2.436572
				H	0.628578	-3.439606	-3.482228
				H	6.427922	-1.998334	-3.872641
				H	2.919219	-4.822252	-3.801778
				H	1.631665	0.960312	-4.064039
				C	2.690836	2.682299	-3.302984
				H	3.313622	0.696009	-3.542210
				H	0.666688	-1.120311	-2.482770
Zr	3.302056	-1.715524	-3.373665	H	1.617972	-1.371240	-1.028516
C	2.349208	1.187583	-3.262866	H	-2.271430	0.393395	1.521868
C	3.036409	-1.279384	-6.989299	H	-1.236975	1.572614	2.313849

! Second Vinyl Coordination/Insertion -
Product !
scf done: -1654.299941

C	2.656755	-2.169344	-5.838377
C	1.448319	-2.115132	-5.082834
C	1.426074	-3.203313	-4.174917
C	2.640509	-3.918448	-4.329231
C	3.401159	-3.275840	-5.348836
Zr	3.302056	-1.715524	-3.373665
C	2.349208	1.187583	-3.262866
C	3.036409	-1.279384	-6.989299

H	-2.879831	3.384493	1.733158	scf done: -1732.882324		
H	-3.916173	2.198335	0.974710	C	4.873534	-3.703078 -1.926263
H	-4.193241	1.014437	3.196331	C	5.208249	-2.343147 -1.658391
H	-3.150200	2.180132	3.958500	C	5.702726	-1.749138 -2.848254
H	-7.309918	3.048485	5.304686	C	5.625441	-2.719131 -3.877858
H	-6.136541	4.234391	5.792889	C	5.106091	-3.917429 -3.309805
H	-5.722217	1.190705	6.003540	Zr	3.277261	-2.168197 -3.316330
H	-4.542867	2.389945	6.488351	C	3.372781	0.121798 -3.136773
H	-6.162281	3.303524	8.172043	C	3.908815	0.869634 -1.911327
H	-7.343300	2.099684	7.686591	C	3.771770	2.394272 -2.029617
H	-5.767770	0.269510	8.389591	C	4.519431	-4.754217 -0.912434
H	-4.584403	1.474285	8.871486	C	5.762092	-5.551381 -0.474433
H	-6.204456	2.385874	10.565834	C	5.445782	-6.614370 0.577460
H	-7.385785	1.180925	10.080671	C	6.680055	-7.394714 1.020574
H	-5.798925	-0.641026	10.759679	C	2.145527	-1.388609 -5.545876
H	-4.623626	0.565785	11.276034	C	1.103190	-1.893125 -4.722223
H	-7.168938	3.686495	1.698555	C	1.301829	-3.288988 -4.537591
H	-5.574589	4.180057	1.190736	C	2.493252	-3.653058 -5.201326
H	-6.986233	6.137307	1.278806	C	3.028094	-2.478204 -5.803031
H	-8.147499	6.928381	3.302470	C	2.210528	-0.030380 -6.177386
H	-8.715206	5.310638	2.869897	C	1.433553	0.024032 -7.504607
H	-7.588859	5.522856	4.217341	C	1.496788	1.400192 -8.167772
H	-5.708851	7.613478	2.799639	C	0.727946	1.463338 -9.484439
H	-5.111461	6.217764	3.700861	C	1.456359	-1.579458 -0.598774
H	-4.622790	6.459484	2.013770	C	0.342502	-0.589913 -0.684375
H	-7.426307	0.207773	12.533001	C	-0.329999	-0.387856 0.688393
H	-6.283035	0.760427	14.607304	C	-1.529821	0.557846 0.617810
H	-4.682155	0.962983	13.698366	C	-2.224504	0.751043 1.966956
H	2.629172	-0.271627	-6.840593	C	-3.487236	1.615537 1.884365
H	4.128301	-1.179436	-7.043238	C	-4.195459	1.816764 3.229658
H	2.915298	-2.840903	-8.480630	Al	-5.926866	2.816084 3.208586
H	1.428722	-1.924972	-8.283758	C	-6.803436	3.210127 4.955925
H	2.514036	0.067752	-9.365048	C	-5.984604	2.900901 6.217430
H	4.000940	-0.848066	-9.558916	C	-6.724145	3.207650 7.523396
H	2.691429	-0.845204	-11.684174	C	-5.924365	2.867058 8.781713
H	2.795676	-2.492131	-11.051734	C	-6.663423	3.193738 10.079945
H	1.303358	-1.563103	-10.859492	C	-5.861321	2.836521 11.339832
H	2.876016	-3.009584	0.175917	C	-6.604131	3.128699 12.609724
H	3.251855	-4.424250	-0.803892	C	-6.206376	3.979260 13.556354
H	5.477155	-4.625708	0.342473	C	1.436641	-2.813689 -1.144032
H	5.092106	-3.224817	1.331551	C	-6.692390	3.217801 1.405897
H	3.109971	-4.440670	2.282245	C	-7.813051	4.255990 1.231767
H	3.488935	-5.838381	1.288282	C	-9.094222	3.843332 1.958101
H	4.348889	-6.155941	3.610159	C	-7.357810	5.649484 1.669344
H	5.702499	-6.090394	2.475780	H	3.902768	-2.437152 -6.440780
H	5.319762	-4.685288	3.478546	H	4.972390	-4.857315 -3.830759
H	1.769543	3.261497	-3.180696	H	5.151596	-1.860812 -0.689183
H	3.328311	2.927875	-2.443606	H	0.266771	-1.314671 -4.347150
C	3.379583	3.106106	-4.596459	H	2.311439	-1.293195 0.016307
H	3.587071	4.180574	-4.598272	H	0.730736	0.376674 -1.031037
H	4.338987	2.591000	-4.733586	H	-0.404890	-0.929180 -1.411287
H	2.756159	2.892381	-5.472619	H	0.408034	-0.001613 1.403674
				H	-0.655891	-1.362981 1.072563
				H	-1.205823	1.533166 0.227978
				H	-2.254608	0.163515 -0.108738

! Third Vinyl Coordination/Insertion - Adduct
!

H	6.081745	-0.742321	-2.951686
H	0.653933	-3.957004	-3.982200
H	5.956578	-2.591833	-4.900378
H	2.906526	-4.650694	-5.270829
H	2.321239	0.417500	-3.293413
H	3.895535	0.483311	-4.036789
H	0.563280	-3.167825	-1.686442
H	2.201254	-3.548457	-0.900586
H	-2.492067	-0.231282	2.382148
H	-1.521606	1.201130	2.682279
H	-3.220300	2.591628	1.454345
H	-4.176723	1.155863	1.161573
H	-4.399387	0.833898	3.688091
H	-3.512797	2.306819	3.941751
H	-7.748215	2.641971	4.985723
H	-7.123017	4.263607	4.969643
H	-5.686982	1.842253	6.218997
H	-5.043740	3.469846	6.203001
H	-6.995539	4.273138	7.539304
H	-7.674685	2.654917	7.535016
H	-5.666699	1.797832	8.770527
H	-4.967588	3.408822	8.763565
H	-6.910749	4.263467	10.104730
H	-7.623480	2.658917	10.097428
H	-5.613857	1.764642	11.304413
H	-4.906630	3.378083	11.338424
H	-7.031261	2.246224	1.005575
H	-5.840460	3.488517	0.762102
H	-8.056589	4.319135	0.158999
H	-9.909770	4.550155	1.765094
H	-9.434831	2.852175	1.635546
H	-8.942607	3.806295	3.043895
H	-8.130931	6.404423	1.484301
H	-7.130403	5.673238	2.743719
H	-6.455140	5.963003	1.131654
H	-7.549556	2.598309	12.741412
H	-6.795242	4.152302	14.453752
H	-5.272975	4.533297	13.469942
H	1.804020	0.722382	-5.492511
H	3.256078	0.243542	-6.364027
H	1.833388	-0.733990	-8.191098
H	0.385820	-0.249029	-7.321610
H	1.101498	2.155356	-7.474663
H	2.547225	1.668972	-8.344505
H	0.796906	2.457770	-9.937582
H	1.120129	0.742415	-10.211058
H	-0.335217	1.240075	-9.338556
H	4.073643	-4.286622	-0.026021
H	3.776423	-5.451549	-1.320586
H	6.213536	-6.025383	-1.355517
H	6.512511	-4.853387	-0.080935
H	4.983291	-6.135165	1.451101
H	4.696036	-7.310854	0.177556
H	6.422551	-8.150332	1.769841
H	7.150294	-7.912897	0.176985

H	7.433354	-6.733501	1.463720
H	3.381777	0.547887	-1.001573
H	4.966695	0.634230	-1.736418
C	4.284624	3.158468	-0.808043
H	4.314717	2.731293	-2.924286
H	2.716825	2.651656	-2.203174
C	4.157701	4.672973	-0.949617
H	3.734741	2.828687	0.084639
H	5.336810	2.895775	-0.630657
H	4.532299	5.191173	-0.060499
H	4.726801	5.041880	-1.810744
H	3.113564	4.975213	-1.091891

! Third Vinyl Coordination/Insertion -
Transition State !

scf done: -1732.853748

C	-1.402480	-1.046074	-0.033072
C	-1.129521	0.268277	0.446338
C	-0.631841	1.051397	-0.621599
C	-0.611613	0.240311	-1.787269
C	-1.079603	-1.049412	-1.419217
Zr	-3.041063	0.529987	-1.271899
C	-3.288953	2.860834	-1.078132
C	-2.600973	4.029826	-0.390759
C	-2.178923	5.140838	-1.362326
C	-1.813408	-2.235678	0.787561
C	-0.606475	-2.985995	1.377407
C	-1.016956	-4.200200	2.211251
C	0.175682	-4.957444	2.787884
C	-4.354519	0.823890	-3.513160
C	-5.306098	0.554315	-2.492738
C	-5.092717	-0.763235	-2.001678
C	-3.981643	-1.302501	-2.690186
C	-3.510147	-0.316958	-3.602789
C	-4.299010	2.042498	-4.389827
C	-5.153913	1.894531	-5.660617
C	-5.086429	3.131310	-6.556844
C	-5.943255	3.007006	-7.813244
C	-4.245468	1.915894	0.725515
C	-5.536855	2.689282	0.621903
C	-6.228797	2.751506	1.996435
C	-7.520820	3.569788	1.955817
C	-8.247468	3.625861	3.301082
C	-9.528052	4.467096	3.268096
C	-10.266463	4.531423	4.610698
Al	-11.958293	5.593257	4.680949
C	-12.883798	5.741834	6.441296
C	-12.157658	5.136492	7.651311
C	-12.949670	5.235673	8.958692
C	-12.233366	4.625301	10.164271
C	-13.041462	4.712964	11.459363
C	-12.322890	4.095197	12.667715
C	-13.151161	4.127362	13.917806
C	-12.824270	4.758894	15.045663
C	-4.272678	0.500911	0.767239

C	0.173101	0.943167	0.350242	H	-7.293324	1.340434	7.825388
C	-1.029544	1.821886	0.703481	H	-5.121912	0.825022	8.984611
C	-1.799611	1.376718	1.947977	H	-4.849619	2.541597	9.236727
C	-3.089566	2.174719	2.168134	H	-6.952783	2.671655	10.611464
C	-3.885132	1.775596	3.417851	H	-7.219132	0.954648	10.360476
Al	-5.686068	2.619326	3.624070	H	-5.039921	0.455100	11.501889
C	-6.599779	2.521884	5.393702	H	-4.784071	2.175678	11.780952
C	-5.723881	2.181371	6.607869	H	-6.713584	2.516071	1.310404
C	-6.505019	2.100976	7.923264	H	-5.659465	3.892590	1.429633
C	-5.639627	1.782321	9.143152	H	-7.946363	4.624752	0.983459
C	-6.433097	1.717882	10.448934	H	-9.821394	4.258106	2.541807
C	-5.561982	1.408527	11.674961	H	-9.176996	2.706044	1.993776
C	-6.352280	1.312972	12.946321	H	-8.789083	3.304858	3.613881
C	-6.183354	2.086619	14.019095	H	-8.238015	6.288891	2.788599
C	1.525964	-0.886043	-1.790860	H	-7.173684	5.361768	3.852254
C	-6.482055	3.381923	1.954983	H	-6.525119	6.114310	2.385595
C	-7.702852	4.315318	2.012755	H	-7.129859	0.546494	12.966936
C	-8.939050	3.607821	2.570423	H	-6.794281	1.969148	14.910741
C	-7.393797	5.589489	2.800632	H	-5.423227	2.865649	14.046975
H	3.743281	-3.591514	-5.796849	H	2.706162	0.160070	-6.401038
H	4.620651	-4.692789	-3.025760	H	4.060333	-0.939310	-6.666162
H	3.819740	-1.621683	-0.052849	H	2.737659	-2.167284	-8.392708
H	0.574496	-0.740633	-4.929764	H	1.373803	-1.091007	-8.126714
H	2.797385	0.465422	-0.667019	H	2.770496	0.866590	-8.840565
H	1.265515	2.440148	-0.728459	H	4.144580	-0.198668	-9.091336
H	0.136866	1.529996	-1.719487	H	2.998613	0.289879	-11.257489
H	0.882502	0.925852	1.190100	H	2.872126	-1.433045	-10.886067
H	-0.172414	-0.089837	0.213688	H	1.483436	-0.368548	-10.630697
H	-0.698001	2.861947	0.834368	H	2.130962	-3.871331	-0.141537
H	-1.717435	1.832342	-0.154786	H	2.577820	-5.164665	-1.252603
H	5.659106	-0.654960	-1.765088	H	4.598535	-5.663757	0.154038
H	0.063851	-2.982781	-3.538203	H	4.146385	-4.373844	1.258932
H	6.146051	-2.559349	-3.618709	H	1.980001	-5.560153	1.745956
H	2.020108	-4.756773	-4.081709	H	2.449417	-6.854743	0.655580
H	1.890536	1.407068	-3.430128	H	2.927624	-7.488755	3.021265
H	3.382527	0.509080	-3.185167	H	4.444175	-7.367478	2.121893
H	0.565225	-0.805365	-2.314425	H	3.961261	-6.068834	3.220346
H	1.329564	-1.461040	-0.878239	H	2.813996	3.244775	-1.998299
H	-2.053274	0.309864	1.861124	H	4.240951	2.280566	-1.660211
H	-1.156492	1.464276	2.835136	C	4.909499	4.347061	-3.432099
H	-2.839376	3.244677	2.215878	H	4.831118	2.299591	-4.101477
H	-3.717860	2.063099	1.272605	H	3.375247	3.223833	-4.449289
H	-4.049391	0.683507	3.413802	C	5.573851	4.900558	-4.688963
H	-3.284008	1.956199	4.321679	H	4.221206	5.097183	-3.020504
H	-7.404267	1.772178	5.302751	H	5.670726	4.176474	-2.658703
H	-7.132284	3.467502	5.575947	H	6.114071	5.829323	-4.478623
H	-5.206404	1.225596	6.441051	H	6.295066	4.188792	-5.108077
H	-4.927433	2.931974	6.716608	H	4.834724	5.119244	-5.468517
H	-7.026882	3.054949	8.086832				

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