10.1071/CH17573_AC

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Supplementary Material

Mechanism for Three-Component Ni-Catalyzed Carbonyl–Ene Reaction for CO_2 Transformation: What Practical Lessons Do We Learned from DFT Modelling?

Bun Chan,* Ying Luo, Masanari Kimura

Graduate School of Engineering, Nagasaki University, Bunkyo 1-14, Nagasaki 852-8521, Japan

*Email: bun.chan@nagasaki-u.ac.jp

Optimized geometries and, where available, zero-point vibrational energies (kJ mol^{-1}) and M06L/6-311+G(3df,2p) single-point energies (hartree) for each species

Me_2CO

764.8, -2281.47851

C	0.000000	0.000000	0.185842
C	-0.000000	1.294151	-0.618291
H	-0.885851	1.342095	-1.277551
H	0.885851	1.342095	-1.277551
H	-0.000000	2.157619	0.062328
C	-0.000000	-1.294151	-0.618291
H	-0.885851	-1.342095	-1.277551
H	-0.000000	-2.157619	0.062328
H	0.885851	-1.342095	-1.277551
O	0.000000	0.000000	1.411248

$AlMe_3$

945.9, -2132.45586

Al	0.000000	0.000000	0.027941
C	0.000000	1.981265	-0.004573
H	-0.893155	2.416448	0.477987
H	0.000000	2.348986	-1.049615
H	0.893155	2.416448	0.477987
C	1.715826	-0.990633	-0.004573
H	1.646128	-1.981719	0.477987
H	2.539283	-0.434729	0.477987
H	2.034281	-1.174493	-1.049615
C	-1.715826	-0.990633	-0.004573
H	-2.539283	-0.434729	0.477987
H	-1.646128	-1.981719	0.477987
H	-2.034281	-1.174493	-1.049615

Me_2CO–$AlMe_3$

1014.1, -2642.77884

C	1.761136	-0.188492	-0.000080
O	0.641041	-0.735134	-0.000188
Al	-1.266349	0.015784	-0.000004
C	2.997323	-1.043023	0.000098
H	3.616595	-0.803510	-0.883972
H	3.616320	-0.803521	0.884363
H	2.736980	-2.110464	0.000049
C	1.906070	1.308580	-0.000020
H	1.381763	1.718624	-0.881258
H	1.382543	1.718467	0.881761
H	2.956219	1.635357	-0.000416
C	-1.278020	1.056062	1.715537
H	-0.815488	2.060020	1.667299
H	-2.329740	1.223352	2.019875
H	-0.804908	0.513446	2.556061
C	-1.278790	1.053950	-1.716794
H	-0.806906	0.509860	-2.557046
H	-2.330710	1.221585	-2.020289
H	-0.815523	2.057658	-1.670418
C	-2.271494	-1.701924	0.001348
H	-2.051698	-2.322250	0.890365
H	-3.365113	-1.530924	0.002411
H	-2.053470	-2.322732	-0.887765

$Ni(COD)_2$

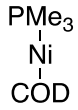
1013.6, -2642.78086

Ni	0.000245	-0.000151	0.000017
C	-1.291433	1.461980	-0.706989
C	-1.454660	0.286585	-1.463999
C	-2.597218	-0.717504	-1.339745
H	-3.510906	-0.218821	-0.973991
H	-2.850106	-1.100214	-2.344660
C	-2.209572	-1.898742	-0.420455
H	-3.115889	-2.403391	-0.022977
H	-0.964842	0.283508	-2.444496
H	-1.679637	-2.661648	-1.020767
C	-1.291506	-1.462233	0.706561
H	-0.719525	-2.274213	1.176628
C	-1.453789	-0.286815	1.463947
H	-0.964357	-0.285408	2.444656
C	-2.595839	0.718102	1.340964
H	-2.846633	1.101656	2.346074
H	-3.510562	0.219753	0.977266
C	-2.209371	1.898702	0.420146
H	-3.116259	2.402302	0.022682
H	-1.679670	2.662564	1.019424
H	-0.718951	2.273536	-1.177185
C	1.291347	1.461790	0.707677
H	0.719208	2.273003	1.178906
C	1.454302	-0.285874	-1.464200
H	0.964727	-0.282655	-2.444839
C	1.454561	0.285810	1.464073
H	0.965079	0.282589	2.444745
C	1.291725	-1.461859	-0.707755
H	0.719437	-2.273362	-1.178297
C	2.208550	1.899476	-0.419581
H	3.114811	2.404475	-0.022465
H	1.677779	2.662388	-1.019161
C	2.596357	0.719024	-1.339958
H	3.510717	0.220786	-0.975320
H	2.848159	1.102626	-2.344803
C	2.596878	-0.718640	1.339497
H	2.849447	-1.102007	2.344248
H	3.510823	-0.220034	0.974300
C	2.209112	-1.899263	0.419464
H	3.115344	-2.404413	0.022464
H	1.678294	-2.662025	1.019210

PMe_3

516.3, -2162.55880

P	0.000009	-0.000106	0.611549
C	-0.037545	1.641742	-0.283195
H	-0.940277	2.202721	0.012395
H	0.838758	2.243284	0.012155
H	-0.035092	1.527495	-1.382629
C	-1.403234	-0.853299	-0.283294
H	-1.437666	-1.915639	0.012083
H	-2.362245	-0.395245	0.012490
H	-1.305985	-0.793799	-1.382768
C	1.440770	-0.788285	-0.283300
H	2.377908	-0.287178	0.012786
H	1.523438	-1.848051	0.011767
H	1.341083	-0.732941	-1.382771



799.4, -2524.81879

Ni	0.121148	0.309383	-0.277518
P	-1.986990	0.094510	-0.035993
C	1.474806	1.376480	0.825730
C	0.945376	0.249385	1.496779
C	1.609432	-1.130626	1.525180
H	2.706663	-1.010965	1.543745
H	1.346320	-1.642189	2.468038
C	1.200396	-2.067899	0.329976
H	1.994540	-2.833481	0.201871
H	0.238411	0.446811	2.315102
H	0.290189	-2.629854	0.612767
C	0.911227	-1.351314	-0.984050
H	0.314938	-1.925070	-1.706620
C	1.669325	-0.245548	-1.440806
H	1.487042	0.054125	-2.485919
C	3.001542	0.221932	-0.860581
H	3.690559	0.498157	-1.680343
H	3.498178	-0.606781	-0.326430
C	2.798878	1.436934	0.079516
H	3.659898	1.542208	0.775614
H	2.794263	2.358793	-0.532092
H	1.090933	2.353774	1.156695
C	-2.892371	1.385079	-1.029228
H	-2.641803	1.279487	-2.097727
H	-3.986588	1.291897	-0.911911
H	-2.585462	2.391669	-0.700421
C	-2.868526	-1.447963	-0.596144
H	-2.624697	-1.638313	-1.654499
H	-2.506609	-2.307563	-0.006930
H	-3.965676	-1.378002	-0.485206
C	-2.782983	0.329722	1.632252
H	-2.480091	1.306921	2.044106
H	-3.885943	0.284638	1.587238
H	-2.424981	-0.453709	2.321574

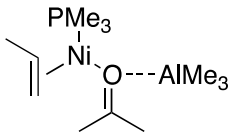
COD

797.2, -2524.80501

C	-1.199224	-1.252777	-0.495656
C	0.038478	-1.705813	-0.212151
C	1.106144	-1.091000	0.668453
H	0.683508	-0.704517	1.609188
H	1.811927	-1.887011	0.968429
C	1.928039	0.016220	-0.030680
H	2.756760	0.322847	0.642358
H	0.337122	-2.639186	-0.709597
H	2.432295	-0.426573	-0.913220
C	1.199208	1.252788	-0.495671
H	1.797648	1.875175	-1.177068
C	-0.038494	1.705808	-0.212144
H	-0.337197	2.639142	-0.709626
C	-1.106117	1.090977	0.668499
H	-1.811870	1.886983	0.968554
H	-0.683441	0.704421	1.609182
C	-1.928036	-0.016188	-0.030690
H	-2.756806	-0.322811	0.642289
H	-2.432229	0.426641	-0.913250
H	-1.797701	-1.875193	-1.176997

1016.8, -2642.76748

C	-1.288928	-0.220297	0.000027
H	-2.256636	0.291537	-0.000202
H	-1.312509	-1.316792	-0.000071
C	-0.130307	0.456949	0.000117
H	-0.159828	1.556247	-0.000128
C	1.236889	-0.164286	0.000051
H	1.182058	-1.265968	0.000757
H	1.819802	0.149758	-0.886470
H	1.821194	0.151021	0.884943



1027.6, -2642.81488

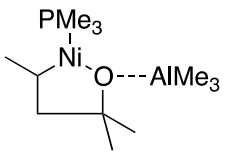
C	-0.457324	2.643112	0.063135
C	-1.754819	2.179139	-0.332461
Ni	-0.621132	0.709419	0.148680
H	-2.023715	2.222791	-1.400688
H	-2.613102	2.355391	0.334356
H	-0.378859	3.089792	1.069131
O	1.068286	0.034397	0.632163
C	1.547677	-0.029185	1.830267
C	2.913965	-0.571077	2.094003
H	3.579586	-0.422869	1.229785
H	2.870875	-1.660958	2.293266
H	3.352353	-0.093358	2.986069
C	0.647820	0.417597	2.930699
H	-0.209868	-0.280855	3.021175
H	0.204519	1.396856	2.659100
H	1.159941	0.481172	3.903494
P	-2.102265	-0.826725	-0.008019
Al	2.033743	-0.729988	-1.083836
C	3.618585	0.482848	-1.245420
H	4.537367	0.130752	-0.739596
H	3.421498	1.509152	-0.882516
H	3.879110	0.584941	-2.316889
C	2.331312	-2.633401	-0.536834
H	1.529519	-3.038842	0.109905
H	3.289609	-2.814181	-0.015913
H	2.344061	-3.274828	-1.439638
C	0.663560	-0.503498	-2.519390
H	0.226312	0.505888	-2.620245
H	-0.172065	-1.223445	-2.451430
H	1.169179	-0.714675	-3.485024
C	0.520860	3.237307	-0.932392
H	0.369349	4.331535	-1.029083
H	1.574174	3.080635	-0.637900
H	0.394595	2.801063	-1.938601
C	-3.426898	-0.753881	1.291961
H	-2.986182	-0.953040	2.283040
H	-3.866619	0.256755	1.310931
H	-4.227731	-1.491046	1.103955
C	-1.639607	-2.623948	0.076629
H	-1.136798	-2.830727	1.036437

H	-2.521403	-3.283676	-0.012383
H	-0.929672	-2.860161	-0.732405
C	-3.120279	-0.797526	-1.556075
H	-2.463797	-0.939950	-2.429486
H	-3.894984	-1.584372	-1.551457
H	-3.605634	0.187140	-1.652305

Coupling TS

275.8, -362.20838

C	-0.128559	2.412567	-0.639683
C	1.220962	2.065977	0.036068
Ni	0.576683	0.391827	-0.283415
H	0.009232	2.480220	-1.733080
O	-1.264626	0.103626	-0.554250
C	-1.487361	1.517346	-0.374309
C	-2.048788	1.812663	1.023900
H	-1.380527	1.445838	1.818302
H	-3.015120	1.295550	1.142864
H	-2.212276	2.895618	1.165438
C	-2.473047	1.968672	-1.461271
H	-2.081925	1.719956	-2.461418
H	-2.663700	3.055439	-1.409663
H	-3.425079	1.430815	-1.322913
P	2.298173	-0.710876	-0.135032
Al	-2.155365	-1.439854	0.233739
C	-1.747022	-1.441401	2.208677
H	-2.374083	-0.755943	2.809858
H	-0.691487	-1.189603	2.441603
H	-1.913544	-2.455400	2.624633
C	-4.098943	-1.262880	-0.238003
H	-4.268230	-1.173750	-1.328464
H	-4.613775	-0.404954	0.237735
H	-4.654459	-2.164639	0.087640
C	-1.166338	-2.900087	-0.739764
H	-0.205468	-3.171219	-0.257555
H	-0.946829	-2.638526	-1.793363
H	-1.761053	-3.833997	-0.769632
C	3.944555	0.134076	-0.156660
H	4.062922	0.691647	-1.100140
H	4.020338	0.846966	0.680008
H	4.764300	-0.599973	-0.072887
C	2.489259	-1.939199	-1.503886
H	2.586122	-1.406209	-2.463646
H	3.386511	-2.563630	-1.345809
H	1.596286	-2.583178	-1.549404
C	2.390643	-1.742082	1.395402
H	1.496587	-2.382958	1.455604
H	3.297382	-2.372431	1.395192
H	2.404428	-1.087201	2.281604
H	-0.447770	3.415118	-0.293153
H	2.054717	2.405149	-0.604354
C	1.436010	2.505060	1.475933
H	2.417501	2.166277	1.851561
H	1.423437	3.611031	1.549166
H	0.664388	2.120793	2.162348



1019.1, -2642.78106

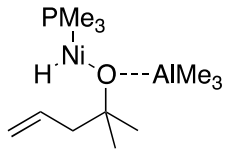
C	0.325853	1.936207	0.139925
C	-1.101973	2.449101	-0.147908
Ni	0.294223	0.086839	-0.438914
H	-1.198583	2.669775	-1.229175
H	-1.294785	3.402757	0.387645
H	0.494249	1.972728	1.235840
O	-1.594099	0.193669	-0.428372
C	-2.145379	1.385151	0.200311
C	-2.296910	1.179639	1.715171
H	-2.995302	0.351254	1.927965
H	-2.699714	2.091272	2.190524
H	-1.330226	0.938880	2.187012
C	-3.508964	1.654917	-0.445846
H	-4.205977	0.823950	-0.241132
H	-3.400412	1.752513	-1.538832
H	-3.956297	2.584358	-0.052208
P	2.296617	-0.276725	0.104214
Al	-1.449911	-1.624470	-0.003092
C	-0.913276	-2.123415	1.861085
H	-1.790021	-2.140983	2.536477
H	-0.159453	-1.464722	2.331009
H	-0.498374	-3.151023	1.871681
C	0.027051	-1.691532	-1.568790
H	0.755220	-1.084074	-2.146997
H	-0.819716	-1.811556	-2.272038
H	0.496678	-2.681611	-1.432048
C	-2.969780	-2.687981	-0.720833
H	-3.830624	-2.685702	-0.025604
H	-2.691942	-3.749637	-0.866198
H	-3.336199	-2.311468	-1.693230
C	1.339429	2.863840	-0.537644
H	1.140871	3.924146	-0.273993
H	2.383968	2.656499	-0.247135
H	1.283346	2.797072	-1.640277
C	2.864917	0.498191	1.686360
H	2.826669	1.596278	1.628108
H	2.190633	0.172611	2.495720
H	3.894725	0.185406	1.930288
C	2.654708	-2.056111	0.480499
H	3.683025	-2.172201	0.864631
H	1.939661	-2.420204	1.235145
H	2.542018	-2.670128	-0.426357
C	3.668629	0.114993	-1.083665
H	4.656431	-0.133977	-0.657706
H	3.519390	-0.474154	-2.003987
H	3.649057	1.182062	-1.353541

Hydrogen abstraction TS

216.7, -193.19552

C	-0.021495	-2.033791	-0.910963
C	-0.957616	-2.428367	0.223512
Ni	0.329983	-0.124066	-0.850453
H	-0.329596	-2.772627	1.066419
H	-1.579080	-3.298959	-0.071526

O	-1.052082	-0.080830	0.652852
C	-1.856313	-1.272940	0.740513
C	-3.174246	-1.139521	-0.044798
H	-3.781196	-0.317079	0.368438
H	-3.761342	-2.071868	0.031638
H	-3.010938	-0.926360	-1.111566
C	-2.186052	-1.486012	2.228212
H	-2.813902	-0.660455	2.604861
H	-1.257826	-1.512354	2.823175
H	-2.731935	-2.433382	2.384961
P	2.205772	-0.074483	0.288826
Al	-1.159803	1.668032	0.132706
C	-0.386194	2.813831	1.564930
H	0.609667	2.489551	1.919068
H	-1.045781	2.819902	2.453692
H	-0.285408	3.868933	1.245998
C	0.175034	1.821757	-1.640298
H	1.226905	1.930072	-1.955512
H	-0.002410	2.829080	-1.189418
H	-0.449461	1.805046	-2.549263
C	3.498563	-1.309076	-0.212768
H	3.092283	-2.330620	-0.129252
H	3.774744	-1.137389	-1.266544
H	4.406672	-1.236315	0.411667
C	3.206823	1.486866	0.243152
H	4.125233	1.407037	0.851043
H	3.490039	1.707723	-0.799749
H	2.598113	2.326195	0.616231
C	2.087038	-0.398605	2.110089
H	3.069379	-0.337493	2.610648
H	1.396133	0.329987	2.563001
H	1.664582	-1.404606	2.269344
C	-0.450650	-1.419930	-2.157377
H	0.029493	-1.794586	-3.073955
H	-1.501577	-1.167668	-2.340612
H	0.678637	-0.302069	-2.256632
H	0.842886	-2.707934	-1.006227
C	-2.870295	2.247848	-0.699330
H	-3.168646	1.642269	-1.574198
H	-3.714830	2.221317	0.014716
H	-2.790447	3.295607	-1.047408



576.4, -2331.59574

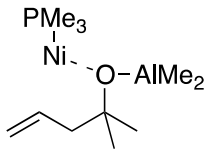
C	3.517352	1.859208	0.887876
C	2.284957	1.022265	0.682506
Ni	-0.742492	-0.017314	-0.540800
H	1.385493	1.665309	0.673462
H	2.168029	0.318855	1.531300
H	4.457169	1.314101	1.057940
O	1.051297	-0.619183	-0.651508
C	2.265743	0.170250	-0.619889
C	2.276111	1.059256	-1.866417
H	3.166684	1.709030	-1.879849
H	2.270405	0.436878	-2.777156
H	1.375296	1.697019	-1.875573
C	3.434119	-0.826864	-0.653518
H	4.402214	-0.300853	-0.710473
H	3.342944	-1.482738	-1.534861
H	3.439468	-1.463925	0.248869
P	-2.546997	0.831961	0.018258
Al	0.344935	-1.957271	0.457409
C	0.022382	-1.506835	2.379953
H	-0.118154	-0.430972	2.589836
H	0.846182	-1.861728	3.028529
H	-0.892340	-2.025263	2.730362
C	1.157455	-3.744709	0.147911
H	2.056885	-3.897455	0.773564
H	0.453703	-4.557261	0.412839
H	1.459764	-3.906437	-0.902841
C	-1.358817	-1.933004	-0.913367
H	-1.836422	-1.363251	-1.740540
H	-2.172510	-2.448527	-0.374850
H	-0.765824	-2.701211	-1.447381
H	-0.452057	1.435101	-0.638199
C	3.544421	3.202429	0.885277
H	4.471545	3.762779	1.044742
H	2.633701	3.792871	0.728234
C	-3.269138	2.072356	-1.146850
H	-2.540497	2.884009	-1.300245
H	-3.462044	1.596380	-2.122335
H	-4.213528	2.493524	-0.759965
C	-2.436354	1.791094	1.593712
H	-2.113840	1.123162	2.408763
H	-1.681709	2.585255	1.480386
H	-3.409379	2.241338	1.857651
C	-3.991641	-0.277893	0.351257
H	-3.729681	-0.991163	1.149561
H	-4.874469	0.304874	0.666172
H	-4.246382	-0.851646	-0.554381

Hydrogen–methyl coupling TS

1013.3, -2642.78099

C	-1.582117	3.406611	-0.824501
C	-1.226332	1.947024	-0.765462
Ni	0.517101	-1.003760	-0.197773
H	-0.152373	1.805953	-0.988654
H	-1.791063	1.390331	-1.539813
H	-2.647460	3.654833	-0.711653
O	-1.075686	-0.133801	0.449492
C	-1.511525	1.234815	0.588577
C	-0.720931	1.870660	1.737423
H	-0.961398	2.941708	1.842589
H	-0.947959	1.355551	2.685903
H	0.361924	1.776538	1.547587
C	-3.013153	1.213526	0.906189
H	-3.407928	2.232424	1.061630
H	-3.195245	0.634857	1.828096
H	-3.577438	0.744550	0.080774
P	2.407214	0.063998	0.130139
Al	-1.704981	-1.799024	0.028858
C	-2.857616	-1.868724	-1.589049
H	-2.608765	-1.085305	-2.328001
H	-3.926799	-1.747188	-1.331235
H	-2.769406	-2.842092	-2.106595
C	-2.021243	-3.004690	1.572999
H	-3.066368	-2.942942	1.931781

H	-1.841434	-4.060121	1.296894
H	-1.361247	-2.771123	2.426440
C	0.618538	-2.426243	-1.537968
H	1.618606	-2.566430	-1.996126
H	-0.008278	-1.922639	-2.309221
H	0.194787	-3.439230	-1.414639
H	1.272328	-2.223732	-0.137754
C	-0.704553	4.406659	-1.011005
H	-1.020903	5.454071	-1.051049
H	0.366945	4.212364	-1.142038
C	3.017683	0.025626	1.883350
H	2.331042	0.588152	2.537005
H	3.028047	-1.022066	2.227529
H	4.034369	0.446281	1.981969
C	2.746533	1.830821	-0.350491
H	2.576988	1.942300	-1.435076
H	2.056543	2.512583	0.173238
H	3.784478	2.133759	-0.122535
C	3.834822	-0.763553	-0.723107
H	3.682425	-0.735814	-1.815304
H	4.798605	-0.279042	-0.486617
H	3.879533	-1.820677	-0.412375



1009.2, -2642.74112

C	-1.127023	-2.135873	0.184309
C	-2.353652	-1.392078	0.682675
Ni	0.151685	-0.670489	-0.076843
H	-2.156068	-0.988933	1.694587
H	-3.234699	-2.059917	0.769665
H	-1.269371	-2.739078	-0.725153
O	-1.395368	0.424026	-0.574704
C	-2.674942	-0.207535	-0.263245
C	-3.262214	-0.683122	-1.599664
H	-4.237135	-1.179348	-1.450597
H	-3.407533	0.177497	-2.273658
H	-2.579882	-1.391666	-2.097456
C	-3.597693	0.822486	0.396663
H	-4.574609	0.372540	0.645938
H	-3.778124	1.672227	-0.284484
H	-3.148900	1.208333	1.327988
P	2.199532	-0.238641	-0.127672
Al	-0.244850	1.634546	0.181338
C	-0.486307	2.126604	2.096788
H	-0.778509	1.276785	2.739078
H	-1.264390	2.906490	2.207049
H	0.443923	2.549122	2.520053
C	0.303775	3.016366	-1.135756
H	-0.397410	3.872287	-1.105692
H	1.309871	3.431514	-0.940399
H	0.294421	2.627645	-2.169238
C	0.046498	-2.346933	0.946881
H	0.717607	-3.170025	0.668693
H	0.054003	-2.107274	2.021465
C	3.011356	0.929722	1.069574
H	2.657816	1.960462	0.899305
H	2.740481	0.641130	2.098543
H	4.110974	0.911981	0.969317
C	2.875479	0.350291	-1.754694
H	2.586619	-0.364065	-2.543611
H	2.447966	1.332913	-2.008111
H	3.977000	0.425134	-1.728716
C	3.282511	-1.732777	0.130246
H	3.022438	-2.508134	-0.609303
H	4.352393	-1.480140	0.022658
H	3.110204	-2.148399	1.136353

CH_4

206.5, -117.92452

C	0.000000	0.000000	0.000000
H	0.635016	0.635016	0.635016
H	-0.635016	-0.635016	0.635016
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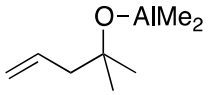


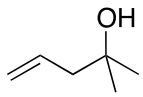
1021.1, -2642.76971

C	0.168205	1.465626	1.115815
C	1.406673	1.283656	0.301643
H	2.301192	1.557079	0.890436
H	1.366950	1.933576	-0.590273
H	0.181203	1.085812	2.147073
O	0.355147	-0.597055	-0.827717
C	1.556785	-0.209280	-0.204086
C	2.677526	-0.250717	-1.257148
H	2.797647	-1.283181	-1.625910
H	3.642919	0.087392	-0.841187
H	2.415459	0.389727	-2.115847
C	1.908353	-1.148797	0.968059
H	1.984982	-2.182924	0.592693
H	1.128184	-1.135408	1.747562
H	2.872369	-0.876817	1.434131
C	-0.997916	1.964733	0.629539
H	-1.890145	2.058047	1.259011
H	-1.052432	2.407684	-0.372141
Al	-1.300564	-0.422709	-0.227309
C	-2.604255	0.095784	-1.625696
H	-3.496845	0.591527	-1.202744
H	-2.167207	0.771212	-2.381666
H	-2.965973	-0.799874	-2.165219
C	-1.922715	-1.429753	1.364180
H	-2.859357	-1.004297	1.770776
H	-2.152955	-2.474807	1.082305
H	-1.195766	-1.480609	2.193906

H_2O

1010.3, -2642.73726

O	0.000000	-0.000000	0.121876
H	-0.000000	0.763518	-0.487505
H	0.000000	-0.763518	-0.487505



438.5, -311.12502

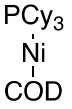
C	-1.690628	0.405637	-0.457150
C	-0.407774	-0.191872	-0.967336
H	-0.126687	0.263834	-1.935166
H	-0.539594	-1.276372	-1.132154
H	-1.825081	1.488022	-0.591810
O	0.445177	-0.667809	1.275304
C	0.778902	-0.021292	0.038740
C	2.013457	-0.757975	-0.489909
H	2.837035	-0.684258	0.240019
H	2.353112	-0.325534	-1.446221
H	1.786013	-1.826077	-0.643395
C	1.098044	1.464720	0.290661
H	1.933208	1.548045	1.005803
H	0.229235	1.989891	0.724792
H	1.382135	1.986563	-0.640872
H	-0.446281	-0.328752	1.516222
C	-2.634951	-0.285748	0.208685
H	-3.536614	0.195541	0.601729
H	-2.550197	-1.369256	0.356470

$AlMe_2OH$

Al	0.000786	0.041531	-0.000082
C	-1.738032	-0.898081	-0.000045
H	-1.821436	-1.561726	-0.880583
H	-1.828540	-1.547809	0.890160
H	-2.613775	-0.226523	-0.008680
C	1.748107	-0.861520	0.000066
H	1.875415	-1.504316	-0.889953
H	2.575112	-0.131654	0.008138
H	1.869047	-1.517275	0.881444
O	0.079252	1.779274	0.000127
H	-0.760510	2.272811	-0.000601

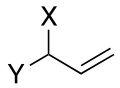
Hydrogen–oxygen coupling TS

C	-1.322935	-2.657352	0.285143
C	0.053212	-2.550854	0.608243
C	1.156870	-2.569010	-0.432772
Ni	-0.714828	-0.790712	0.273512
H	0.709706	-2.587121	-1.445647
H	1.784483	-3.479954	-0.353838
H	0.363777	-2.701927	1.652725
H	0.018163	-0.158843	-0.860328
O	1.179969	-0.154429	-0.124122
C	2.074990	-1.328192	-0.317952
C	2.967036	-1.399455	0.926987
H	3.581832	-0.490698	1.015265
H	3.642449	-2.270206	0.860411
H	2.359116	-1.496195	1.841360
C	2.890907	-1.119949	-1.595583
H	3.529634	-0.226855	-1.512349
H	2.222281	-0.993364	-2.464511
H	3.538724	-1.994065	-1.783634
P	-2.410389	0.440724	-0.125237
Al	1.614901	1.788708	0.169094
C	0.779608	2.063635	1.975293
H	-0.136206	1.460890	2.138021
H	0.495806	3.118998	2.153920
H	1.482333	1.786395	2.784351
C	0.718942	2.585028	-1.444761
H	0.582839	3.678747	-1.332501
H	-0.278520	2.174255	-1.692288
H	1.345426	2.443354	-2.346404
C	3.594356	2.111213	0.157598
H	4.154265	1.676860	1.006714
H	3.724693	3.209659	0.246961
H	4.125858	1.825105	-0.769204
C	-2.897927	0.589152	-1.904152
H	-3.027877	-0.418755	-2.331780
H	-3.841393	1.150808	-2.017586
H	-2.103246	1.104066	-2.467630
C	-2.475766	2.189192	0.476824
H	-1.617120	2.754894	0.084726
H	-3.416843	2.680633	0.173033
H	-2.406889	2.191425	1.576709
C	-3.969030	-0.230509	0.624956
H	-3.858559	-0.275150	1.721322
H	-4.840038	0.403458	0.382193
H	-4.152411	-1.252715	0.256504
H	-1.632910	-2.947388	-0.729829
H	-2.033395	-2.952402	1.069348

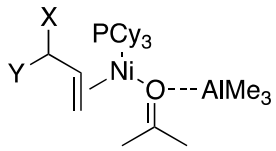


Ni	-1.563767	-0.397353	-0.024689
P	0.501673	0.244249	-0.072579
C	1.115196	-0.767623	-1.544278
C	2.881816	-1.763376	-3.066404
C	0.593209	-2.857665	-2.904968
C	2.099820	-3.086949	-3.115226
C	0.326283	-2.096108	-1.596800
C	2.622600	-0.999960	-1.752427
H	2.575141	-1.127681	-3.921234
H	0.191236	-2.271345	-3.755580
H	2.478658	-3.761447	-2.321160
H	0.601826	-2.732629	-0.735478
H	3.032253	-1.589855	-0.910206
H	0.757060	-0.166575	-2.405085
H	3.964816	-1.951169	-3.187690
H	0.052502	-3.821938	-2.902782
H	2.278780	-3.602874	-4.076450
H	-0.761837	-1.880506	-1.486466
H	3.166232	-0.037107	-1.758394
C	1.038320	2.009608	-0.489699
C	0.788460	3.959517	-2.123224
C	0.889605	4.422516	0.359414
C	0.304328	4.872401	-0.987114
C	0.566261	2.945836	0.645385
C	0.469171	2.479135	-1.844048
H	1.884332	4.079170	-2.241886
H	1.989742	4.559501	0.342994
H	-0.802231	4.833922	-0.934323
H	-0.529598	2.824965	0.762244
H	-0.627916	2.327068	-1.843652
H	2.145170	2.053289	-0.548140
H	0.334746	4.263625	-3.084775

H	0.506962	5.056752	1.180566
H	0.574090	5.924150	-1.195311
H	1.015729	2.645668	1.609761
H	0.869760	1.862646	-2.668945
C	1.584046	-0.134932	1.446027
C	2.184847	-1.922184	3.159169
C	3.672817	0.110351	2.877934
C	3.622333	-1.383884	3.233138
C	3.031984	0.396981	1.504911
C	1.552399	-1.640594	1.785236
H	1.571301	-1.439286	3.946124
H	3.130756	0.686562	3.654731
H	4.257977	-1.948559	2.521483
H	3.640114	-0.081031	0.713967
H	2.114076	-2.204223	1.014497
H	1.013001	0.380081	2.249623
H	2.167259	-3.007748	3.369378
H	4.716856	0.475262	2.889444
H	4.049000	-1.555021	4.238636
H	3.062223	1.483744	1.310195
H	0.513156	-2.015099	1.752587
C	-2.401368	-1.912097	1.095724
C	-2.216782	-0.718671	1.824927
C	-3.313109	0.314582	2.082368
H	-4.289294	-0.194587	2.165728
H	-3.138068	0.793587	3.062082
C	-3.388902	1.433248	0.988398
H	-4.417485	1.851896	0.975039
H	-1.384088	-0.700242	2.542805
H	-2.729383	2.269500	1.286645
C	-2.965943	0.977325	-0.399702
H	-2.664944	1.785024	-1.080085
C	-3.348729	-0.267415	-0.950837
H	-3.190045	-0.378173	-2.036242
C	-4.382630	-1.214911	-0.350044
H	-5.006590	-1.646037	-1.154589
H	-5.080079	-0.656985	0.299102
C	-3.697691	-2.359369	0.442207
H	-4.402922	-2.794200	1.183922
H	-3.456405	-3.181886	-0.257444
H	-1.683550	-2.722616	1.293938



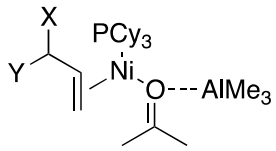
C	5.550582	1.056871	0.270098
H	6.601812	1.074080	-0.035715
H	5.196552	1.913050	0.857134
C	4.734793	0.040806	-0.051250
H	5.132269	-0.800993	-0.639885
C	3.277921	-0.066666	0.325331
H	3.004975	0.826964	0.920668
C	3.027863	-1.320710	1.183244
H	3.626011	-1.287924	2.109218
H	3.311081	-2.236782	0.632185
H	1.963012	-1.407866	1.457580
C	2.394655	-0.062264	-0.960115
H	2.638573	-0.960610	-1.559302
H	2.685950	0.812726	-1.569858
C	0.906997	-0.018220	-0.683041
C	-1.903542	0.082232	-0.109449
C	0.101864	-1.170048	-0.767039
C	0.278018	1.182503	-0.309335
C	-1.094571	1.232158	-0.028496
C	-1.268288	-1.119689	-0.486975
H	0.557140	-2.122808	-1.062991
H	0.871862	2.102468	-0.242456
H	-1.534532	2.193022	0.252869
H	-1.854291	-2.042001	-0.569572
C	-3.414757	0.096253	0.187209
C	-3.717531	-0.873525	1.355817
H	-3.186014	-0.564543	2.272606
H	-3.410141	-1.906677	1.120923
H	-4.800801	-0.885861	1.573899
C	-3.922106	1.497365	0.580818
H	-3.425902	1.872544	1.493031
H	-5.006210	1.455930	0.784829
H	-3.763456	2.233596	-0.226578
C	-4.190285	-0.362869	-1.071980
H	-3.899366	-1.380238	-1.383996
H	-4.001022	0.316456	-1.921170
H	-5.277169	-0.369713	-0.872447



Isomer for *E*-product formation

C	-0.823316	-0.571585	1.869175
C	0.478304	-1.147178	2.040500
Ni	0.447917	0.026853	0.522185
H	0.610953	-2.211076	1.792945
H	1.110281	-0.835499	2.885280
O	-0.578361	1.341437	-0.424597
C	-1.532221	1.081447	-1.256108
C	-2.430532	2.131553	-1.825447
H	-3.464160	1.958034	-1.464520
H	-2.464381	2.035309	-2.927022
H	-2.130892	3.153252	-1.561447
C	-1.753910	-0.341416	-1.636299
H	-1.999888	-0.931648	-0.733031
H	-0.819178	-0.769995	-2.043656
H	-2.565816	-0.452841	-2.372256
P	2.392794	-0.536593	-0.270621
C	3.759767	-0.526792	1.038488
C	6.181207	-0.913210	1.704653
C	4.666071	0.499950	3.171894
C	6.106206	0.267028	2.686729
C	3.696027	0.683256	1.991258
C	5.201193	-0.733217	0.528751
H	5.933633	-1.851584	2.240954
H	4.339308	-0.368760	3.778750
H	6.469594	1.183139	2.179137
H	3.959746	1.611783	1.452523
H	5.512159	0.150143	-0.062273
H	3.487188	-1.406077	1.656585
H	7.212014	-1.033034	1.322210
H	4.620984	1.382345	3.836285
H	6.781663	0.095241	3.544971
H	2.661563	0.819560	2.349477

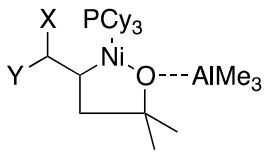
H	5.266467	-1.601028	-0.153669
C	2.462180	-2.349274	-0.897449
C	2.939894	-4.819792	-0.447876
C	1.127124	-4.192959	-2.083726
C	1.585992	-5.225292	-1.045377
C	1.100548	-2.772176	-1.493705
C	2.905181	-3.398847	0.146981
H	3.714708	-4.860832	-1.239912
H	1.819348	-4.214008	-2.949703
H	0.832791	-5.287888	-0.234683
H	0.336051	-2.710554	-0.694051
H	2.205556	-3.383659	1.004997
H	3.213844	-2.355536	-1.714877
H	3.251569	-5.539031	0.332043
H	0.126571	-4.453169	-2.476356
H	1.647375	-6.231925	-1.498138
H	0.787487	-2.058101	-2.274545
H	3.903596	-3.161382	0.550320
C	3.182592	0.337115	-1.756080
C	2.935482	0.918270	-4.232750
C	4.088959	2.540939	-2.675990
C	3.223385	2.396737	-3.935927
C	3.458813	1.825347	-1.466858
C	2.311646	0.198621	-3.021973
H	3.882812	0.408975	-4.502135
H	5.093196	2.112518	-2.870755
H	2.267832	2.934959	-3.781554
H	2.508263	2.324574	-1.199221
H	1.309522	0.624839	-2.812463
H	4.150694	-0.170538	-1.950031
H	2.268242	0.820141	-5.109438
H	4.243834	3.608745	-2.435164
H	3.718336	2.873193	-4.802233
H	4.123684	1.932697	-0.592622
H	2.160624	-0.864962	-3.277450
H	-1.560350	-1.223351	1.371190
C	-1.496519	0.400326	2.844321
H	-1.750260	1.345541	2.323716
C	-0.627581	0.760042	4.056613
H	-1.141951	1.494649	4.701025
H	0.334693	1.203568	3.749371
H	-0.406626	-0.134263	4.666895
Al	-0.199578	3.373116	0.171500
C	1.274533	3.355911	1.502934
H	2.259866	3.052610	1.114694
H	1.074449	2.769608	2.416499
H	1.378260	4.410929	1.834418
C	0.292318	4.144227	-1.618013
H	0.363972	3.390914	-2.425577
H	1.281158	4.638255	-1.564718
H	-0.423015	4.913545	-1.967125
C	-1.969954	3.896332	0.960878
H	-2.730244	3.093700	0.961869
H	-2.424244	4.759161	0.436072
H	-1.837220	4.203525	2.015483
C	-2.854155	-0.194324	3.335568
H	-3.261612	0.481017	4.112692
H	-2.657807	-1.166442	3.826031
C	-3.882677	-0.368810	2.239416
C	-5.784093	-0.666006	0.102960
C	-4.199128	-1.630641	1.707047
C	-4.547491	0.746084	1.687445
C	-5.471736	0.600107	0.647568
C	-5.126218	-1.777009	0.662111
H	-3.714604	-2.522519	2.122470
H	-4.339907	1.746813	2.084877
H	-5.970504	1.496624	0.261136
H	-5.335825	-2.783781	0.289454
C	-6.809316	-0.783550	-1.040354
C	-6.318312	0.036663	-2.258675
H	-7.047960	-0.025705	-3.086213
H	-5.350487	-0.347697	-2.627748
H	-6.186513	1.103282	-2.008246
C	-7.015811	-2.241666	-1.494924
H	-7.754066	-2.274876	-2.314979
H	-7.398996	-2.875653	-0.676425
H	-6.080013	-2.691748	-1.870509
C	-8.174681	-0.226070	-0.568281
H	-8.919643	-0.293161	-1.381697
H	-8.102798	0.831876	-0.264296
H	-8.555733	-0.798599	0.294903



Isomer for *Z*-product formation

C	1.098074	2.161775	-1.818019
C	1.342375	1.070939	-2.868347
H	1.692507	1.505596	-3.822568
H	0.418774	0.502858	-3.071288
H	2.112518	0.355599	-2.529028
C	0.601383	1.645802	-0.468678
C	-0.178449	2.515313	0.346463
Ni	-1.252553	1.024894	-0.278662
H	-0.458662	3.506922	-0.040229
H	-0.096618	2.476158	1.442897
H	1.325493	0.978306	0.017066
H	0.331383	2.856427	-2.220605
O	-2.934752	1.977612	-0.521565
C	-3.420817	2.085783	-1.718784
C	-4.477541	3.083121	-2.067017
H	-4.462242	3.944239	-1.382471
H	-5.484864	2.626044	-2.001202
H	-4.345020	3.435341	-3.104686
C	-2.857730	1.178360	-2.751695
H	-2.603327	0.211421	-2.260001
H	-1.899574	1.568421	-3.152330
H	-3.544030	1.032498	-3.603660
P	-1.076654	-1.145085	-0.043516
C	-2.686306	-2.145274	-0.194453
C	-4.038557	-4.290337	0.057276
C	-5.225393	-2.053823	0.003356
C	-5.245355	-3.484977	0.562490
C	-3.899682	-1.343485	0.326113
C	-2.705337	-3.581687	0.370040
H	-4.125869	-4.426854	-1.039637
H	-5.360860	-2.091221	-1.096934
H	-5.217397	-3.442672	1.669767
H	-3.822963	-1.206767	1.421143

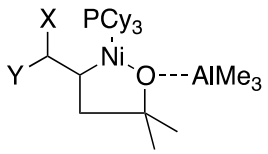
H	-2.564128	-3.552799	1.467630
H	-2.816711	-2.220170	-1.294917
H	-4.036301	-5.303990	0.499512
H	-6.071969	-1.467077	0.405296
H	-6.188191	-3.994558	0.291354
H	-3.888032	-0.326648	-0.101129
H	-1.869049	-4.176118	-0.036880
C	0.125664	-2.021345	-1.235319
C	1.855379	-3.784578	-1.836212
C	0.533852	-2.652601	-3.675312
C	1.244250	-3.941964	-3.236431
C	-0.505944	-2.202442	-2.632849
C	0.803040	-3.340530	-0.800726
H	2.665733	-3.029092	-1.872575
H	1.283239	-1.848543	-3.811542
H	0.512254	-4.774520	-3.221831
H	-1.302771	-2.970413	-2.579115
H	0.045865	-4.141130	-0.697970
H	0.925715	-1.261223	-1.335549
H	2.323758	-4.731736	-1.510148
H	0.043526	-2.796542	-4.656093
H	2.023331	-4.221686	-3.969112
H	-0.994218	-1.267039	-2.963696
H	1.287258	-3.236789	0.185122
C	-0.371093	-1.636473	1.642184
C	1.651907	-1.503278	3.186961
C	-0.667868	-1.772821	4.164251
C	0.740276	-1.200025	4.385516
C	-1.283016	-1.291013	2.836141
C	1.021664	-1.010196	1.872652
H	1.827289	-2.596362	3.123277
H	-0.614471	-2.880550	4.159269
H	0.667982	-0.101938	4.515884
H	-1.435772	-0.196920	2.875871
H	0.904494	0.089101	1.922706
H	-0.257935	-2.739283	1.612301
H	2.644204	-1.033681	3.322564
H	-1.332935	-1.494577	5.002355
H	1.178200	-1.600499	5.318304
H	-2.282463	-1.742095	2.715781
H	1.704297	-1.212112	1.027522
Al	-3.839568	2.949353	1.137320
C	-3.325032	4.866900	0.871321
H	-3.936353	5.442531	0.151233
H	-2.267942	4.992034	0.571525
H	-3.429608	5.388920	1.843050
C	-5.760055	2.423368	0.890456
H	-5.888141	1.409253	0.462948
H	-6.365825	3.114190	0.275893
H	-6.242806	2.390092	1.886859
C	-3.031670	2.066006	2.729620
H	-3.460182	2.550686	3.630576
H	-1.934914	2.150863	2.821587
H	-3.297441	0.996190	2.801456
C	2.381411	3.040791	-1.613206
H	2.101473	3.891687	-0.966868
H	2.669302	3.459334	-2.596849
C	3.563811	2.315574	-1.007478
C	5.749207	0.859089	0.158241
C	3.727284	2.231388	0.390900
C	4.528211	1.675162	-1.805161
C	5.595006	0.961697	-1.236747
C	4.789964	1.519916	0.956377
H	3.002716	2.732298	1.042986
H	4.448700	1.737302	-2.897221
H	6.316606	0.483322	-1.905189
H	4.873571	1.483766	2.048629
C	6.895351	0.074051	0.822639
C	6.298643	-1.052904	1.701845
H	5.709009	-1.758625	1.090897
H	5.634405	-0.651632	2.486392
H	7.104971	-1.620544	2.200794
C	7.729665	1.028451	1.711673
H	7.116179	1.494727	2.501029
H	8.175133	1.839070	1.109352
H	8.549705	0.475810	2.204977
C	7.840210	-0.570773	-0.210139
H	7.309508	-1.288364	-0.860218
H	8.640812	-1.123315	0.311859
H	8.322674	0.186056	-0.853142



Isomer for *E*-product formation

C	-0.248304	2.620510	0.495636
C	0.178669	3.583976	-0.616168
Ni	0.686981	0.967225	0.310018
H	0.389604	4.581019	-0.187979
H	-0.602810	3.720198	-1.384867
O	2.067529	2.102784	-0.282409
C	1.464104	3.005610	-1.274924
C	2.481562	4.077756	-1.680048
H	2.025967	4.763168	-2.416319
H	3.371287	3.618227	-2.141662
H	2.806407	4.674193	-0.813910
C	1.103641	2.184701	-2.523265
H	1.994412	1.662926	-2.913074
H	0.715281	2.846321	-3.317879
H	0.330557	1.428480	-2.299155
H	0.106432	2.995876	1.473322
C	-1.668178	2.070665	0.668071
H	-2.243935	2.612701	1.447198
C	-1.348320	0.647620	1.167588
H	-2.229862	-0.021209	1.160920
H	-0.920703	0.618898	2.183636
H	-0.710438	0.069169	0.389965
P	1.672869	-1.070303	-0.035722
C	3.218374	-0.917619	-1.124408
C	5.635320	-0.129155	-1.203406
C	4.778610	-1.732923	-2.958938
C	6.001634	-1.283465	-2.146586
C	3.588663	-2.098765	-2.049648
C	4.449230	-0.494481	-0.294137
H	5.368688	0.765788	-1.798592
H	4.471043	-0.913275	-3.639067
H	6.824396	-0.987312	-2.822909
H	3.862645	-2.983027	-1.442067
H	4.755317	-1.332483	0.363780

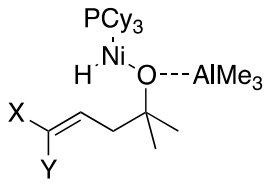
H	2.956798	-0.049285	-1.760988
H	6.501491	0.161215	-0.582273
H	5.032248	-2.595808	-3.602471
H	6.376714	-2.139855	-1.550466
H	2.737188	-2.404476	-2.681830
H	4.204286	0.359816	0.358425
C	2.220559	-2.021896	1.497883
C	1.768073	-2.492298	3.959021
C	3.158076	-4.115948	2.602361
C	2.156222	-3.964853	3.756821
C	2.618937	-3.499781	1.296897
C	1.218849	-1.863722	2.666052
H	2.658117	-1.917455	4.283024
H	4.106244	-3.611126	2.874975
H	1.246044	-4.556318	3.530054
H	1.742248	-4.085951	0.959219
H	0.251308	-2.337379	2.412132
H	3.132185	-1.470209	1.801711
H	1.021018	-2.395602	4.768124
H	3.405064	-5.181177	2.438183
H	2.578446	-4.383705	4.688501
H	3.380856	-3.590573	0.502873
H	1.017370	-0.791172	2.833944
C	0.599236	-2.261844	-1.031599
C	-1.391917	-3.834364	-1.170512
C	-0.637284	-2.574351	-3.238428
C	-1.829913	-3.200851	-2.499699
C	0.126485	-1.586751	-2.339011
C	-0.621235	-2.837935	-0.282688
H	-0.740077	-4.706216	-1.379246
H	0.054940	-3.376659	-3.564048
H	-2.584262	-2.414158	-2.295607
H	-0.538283	-0.738165	-2.078363
H	-1.302128	-2.017268	0.015080
H	1.250490	-3.117389	-1.300297
H	-2.268640	-4.223513	-0.620888
H	-0.977230	-2.062053	-4.157104
H	-2.328943	-3.952150	-3.138624
H	0.974809	-1.145996	-2.891755
H	-0.311878	-3.342923	0.647550
Al	3.097675	2.857919	1.242821
C	2.840852	1.531823	2.738555
H	1.798168	1.440283	3.101561
H	3.417579	1.933903	3.597599
H	3.225433	0.509604	2.572239
C	2.365527	4.632015	1.869241
H	1.313814	4.633142	2.214340
H	2.476623	5.491867	1.182021
H	2.969747	4.889401	2.764284
C	4.997185	3.016713	0.592830
H	5.126472	2.852634	-0.492973
H	5.679230	2.308518	1.101902
H	5.387506	4.031417	0.803779
C	-2.538919	2.053346	-0.607837
H	-2.001423	1.509381	-1.409299
H	-2.652997	3.094944	-0.960530
C	-3.908331	1.442581	-0.397830
C	-6.496018	0.281007	0.047026
C	-4.230072	0.161849	-0.885574
C	-4.907783	2.130713	0.313298
C	-6.170848	1.563334	0.531097
C	-5.491592	-0.404162	-0.668229
H	-3.479875	-0.396848	-1.459526
H	-4.698431	3.135266	0.700760
H	-6.913234	2.143553	1.086065
H	-5.695295	-1.402293	-1.072135
C	-7.873892	-0.372683	0.261424
C	-7.696833	-1.702334	1.034968
H	-8.676112	-2.191227	1.186071
H	-7.245045	-1.525180	2.026420
H	-7.048685	-2.410173	0.490838
C	-8.523614	-0.663680	-1.113772
H	-9.509597	-1.143644	-0.978224
H	-7.902394	-1.339124	-1.726131
H	-8.671204	0.268794	-1.685619
C	-8.831142	0.528562	1.065665
H	-9.800926	0.017529	1.195153
H	-9.025959	1.484990	0.549678
H	-8.436296	0.752657	2.072096



Isomer for *Z*-product formation

C	-0.129209	0.491233	3.100927
C	-0.821757	0.814629	4.447764
H	-0.565706	0.063871	5.217455
H	-1.921493	0.839414	4.350513
H	-0.503536	1.801424	4.828419
C	-0.661139	1.429289	1.987784
C	-0.311486	2.915877	2.267930
Ni	-0.033654	0.959335	0.226807
H	0.639955	2.982029	2.825278
H	-1.082952	3.395543	2.901649
H	-1.764003	1.338697	1.991535
H	-0.398679	-0.544696	2.824584
O	0.592589	2.728728	0.134543
C	-0.124546	3.683317	0.958824
C	-1.468795	4.056020	0.312102
H	-1.312287	4.506984	-0.681302
H	-2.014483	4.779861	0.943273
H	-2.102346	3.161088	0.186218
C	0.751247	4.931990	1.120718
H	0.905394	5.431927	0.148483
H	1.739249	4.658334	1.527270
H	0.277919	5.657752	1.804925
P	-1.484461	-0.647920	-0.195011
C	-2.889252	0.332086	-1.047613
C	-3.420486	1.936437	-2.952526
C	-5.296523	0.770443	-1.715111
C	-4.843502	1.368367	-3.055343
C	-4.299846	-0.285954	-1.196551
C	-2.427390	0.892573	-2.411086
H	-3.421224	2.814161	-2.276079
H	-5.388622	1.579899	-0.963329
H	-4.865475	0.576288	-3.830682
H	-4.275708	-1.125100	-1.916087
H	-2.348748	0.061261	-3.139890
H	-2.991483	1.199325	-0.362176

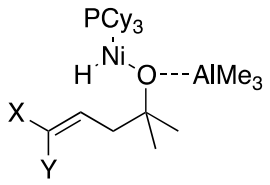
H	-3.074744	2.302651	-3.936253
H	-6.300213	0.316552	-1.811960
H	-5.550352	2.151095	-3.386370
H	-4.672966	-0.699322	-0.244740
H	-1.422661	1.342242	-2.328610
C	-0.906630	-1.891207	-1.511066
C	0.941348	-3.400506	-2.377690
C	-1.427346	-3.711963	-3.211286
C	-0.094026	-4.406824	-2.901341
C	-1.953938	-2.916224	-2.000640
C	0.412010	-2.620362	-1.160745
H	1.199935	-2.682544	-3.181590
H	-1.288325	-3.017467	-4.063824
H	-0.261458	-5.189345	-2.133979
H	-2.196179	-3.623660	-1.183410
H	0.244486	-3.331076	-0.331047
H	-0.674985	-1.223572	-2.364934
H	1.880107	-3.918155	-2.108965
H	-2.186544	-4.450623	-3.528924
H	0.287614	-4.924968	-3.800148
H	-2.897772	-2.419165	-2.277306
H	1.178305	-1.912767	-0.806428
C	-2.483396	-1.719470	1.012054
C	-2.629703	-3.756249	2.530832
C	-4.238359	-1.829364	2.847870
C	-3.467662	-2.961757	3.542986
C	-3.281525	-0.915058	2.061693
C	-1.694381	-2.851903	1.703552
H	-3.310838	-4.292039	1.839101
H	-4.988866	-2.262819	2.156029
H	-2.798154	-2.524682	4.310572
H	-2.582597	-0.449627	2.774462
H	-0.913105	-2.423695	2.359291
H	-3.224427	-2.211720	0.348654
H	-2.034188	-4.532957	3.045129
H	-4.801203	-1.232368	3.588870
H	-4.162936	-3.634290	4.077825
H	-3.845177	-0.088896	1.593896
H	-1.168779	-3.471046	0.959409
Al	1.301081	2.791573	-1.602912
C	0.144351	3.727022	-2.945306
H	0.214524	4.827017	-2.836570
H	-0.930962	3.473969	-2.935514
H	0.510852	3.504450	-3.967452
C	1.289209	0.737442	-1.677807
H	2.382367	0.564195	-1.705915
H	0.855153	0.339542	-2.610344
H	1.013252	-0.010311	-0.881426
C	3.165534	3.514437	-1.566543
H	3.191522	4.620188	-1.527777
H	3.724089	3.225580	-2.479218
H	3.755457	3.150356	-0.704662
C	1.403489	0.496559	3.351091
H	1.574022	-0.122842	4.253681
H	1.723221	1.515630	3.635450
C	2.322348	-0.012643	2.260022
C	4.279279	-1.000733	0.401561
C	2.449346	-1.391684	1.992057
C	3.183185	0.856501	1.567354
C	4.138982	0.375008	0.661053
C	3.401193	-1.871357	1.085383
H	1.810616	-2.105690	2.527134
H	3.108525	1.935510	1.741710
H	4.784174	1.099134	0.156757
H	3.473696	-2.953200	0.924614
C	5.344806	-1.564899	-0.556778
C	4.658361	-2.388856	-1.672517
H	3.957183	-1.762458	-2.251286
H	4.089638	-3.240091	-1.260743
H	5.413103	-2.796207	-2.369419
C	6.177592	-0.453064	-1.224961
H	5.548083	0.231571	-1.819951
H	6.918997	-0.904258	-1.907269
H	6.731783	0.147416	-0.482713
C	6.307659	-2.483311	0.235729
H	5.772662	-3.322966	0.711527
H	6.824369	-1.919284	1.031525
H	7.074127	-2.908953	-0.437100



Isomer for *E*-product formation

C	-1.400321	2.896624	-0.703988
C	-0.300714	3.008700	-1.722060
Ni	2.173636	1.201245	-0.035848
H	-0.650658	3.525378	-2.634625
H	0.023152	1.997286	-2.041744
O	1.573578	2.989522	-0.117111
C	0.976644	3.731788	-1.208291
C	0.648780	5.139410	-0.694987
H	0.243312	5.758574	-1.514020
H	1.554850	5.626307	-0.299381
H	-0.108686	5.102783	0.106256
C	2.012430	3.796743	-2.338737
H	2.931304	4.296241	-1.989315
H	1.620280	4.351172	-3.209163
H	2.275673	2.773746	-2.659600
H	-1.050867	2.690948	0.316531
C	-2.736062	3.004216	-0.888073
C	-3.406808	3.237030	-2.218796
H	-4.112920	4.087711	-2.164588
H	-4.005039	2.353880	-2.514219
H	-2.690482	3.439546	-3.030186
P	2.193651	-0.900918	-0.135017
C	0.437432	-1.476155	-0.590957
C	-1.390597	-1.425118	-2.352508
C	-1.503453	-3.107889	-0.462447
C	-1.868745	-2.821135	-1.926335
C	-0.000729	-2.902344	-0.183531
C	0.113712	-1.245055	-2.081758
H	-1.953142	-0.651603	-1.793720
H	-2.084998	-2.429460	0.192666
H	-2.961069	-2.915698	-2.070494
H	0.580259	-3.654105	-0.751785
H	0.677589	-1.973970	-2.698063
H	-0.192272	-0.766260	-0.014237
H	-1.600791	-1.256728	-3.424873

H	-1.792884	-4.138888	-0.186350
H	-1.395881	-3.583378	-2.578151
H	0.192943	-3.096163	0.885071
H	0.440289	-0.237388	-2.394517
C	3.301428	-1.544389	-1.511896
C	5.485262	-1.221878	-2.786004
C	4.334168	-3.474962	-2.814974
C	5.684543	-2.744086	-2.841824
C	3.493581	-3.073980	-1.587292
C	4.656807	-0.801267	-1.558561
H	4.962800	-0.889500	-3.705444
H	3.768651	-3.228107	-3.735850
H	6.292297	-3.066193	-1.972343
H	4.000064	-3.435320	-0.671535
H	5.238523	-1.004162	-0.639212
H	2.744524	-1.225661	-2.416603
H	6.460729	-0.702082	-2.774165
H	4.484279	-4.570376	-2.823076
H	6.255222	-3.026106	-3.745487
H	2.515374	-3.585076	-1.626590
H	4.476416	0.289757	-1.578253
C	2.576473	-1.888100	1.418855
C	4.296315	-2.632040	3.142601
C	1.908609	-2.204142	3.860438
C	3.384767	-2.151307	4.281560
C	1.663139	-1.407800	2.567032
C	4.059982	-1.835268	1.845504
H	4.100187	-3.706060	2.949269
H	1.610911	-3.260896	3.703965
H	3.650727	-1.108359	4.545834
H	1.850701	-0.333701	2.749755
H	4.368601	-0.785424	2.000790
H	2.331063	-2.945617	1.191013
H	5.359284	-2.555185	3.436513
H	1.260858	-1.811544	4.665610
H	3.550473	-2.758755	5.190106
H	0.599815	-1.479685	2.276384
H	4.705342	-2.239359	1.046932
Al	1.536926	2.836413	1.749072
C	2.059857	4.523457	2.676195
H	3.000315	4.964043	2.296197
H	2.174222	4.384239	3.767243
H	1.271876	5.290628	2.544739
C	3.355467	1.720993	1.587442
H	3.973437	1.070657	0.934207
H	3.414764	1.254481	2.588693
H	3.900042	2.681025	1.629666
C	-0.029812	1.938688	2.623690
H	-0.427439	1.062258	2.077180
H	-0.873329	2.639476	2.777615
H	0.263551	1.582556	3.630434
C	-3.676156	2.861113	0.304977
H	-4.393213	3.706227	0.300580
H	-3.089032	2.943155	1.236741
C	-4.456054	1.554808	0.324722
C	-5.889266	-0.931863	0.342345
C	-5.713737	1.431696	-0.295607
C	-3.932283	0.414917	0.958231
C	-4.635712	-0.798952	0.971236
C	-6.409491	0.217488	-0.289254
H	-6.162004	2.306685	-0.781693
H	-2.960949	0.481423	1.464347
H	-4.191622	-1.650508	1.493345
H	-7.388368	0.170843	-0.780041
C	-6.698929	-2.243422	0.335768
C	-6.979426	-2.665991	-1.126785
H	-7.567843	-3.601083	-1.150590
H	-6.036278	-2.839007	-1.673948
H	-7.549372	-1.896267	-1.674125
C	-8.043546	-2.015238	1.066491
H	-8.645515	-2.942037	1.064498
H	-8.641380	-1.223665	0.583080
H	-7.875340	-1.716020	2.115494
C	-5.961379	-3.402234	1.037408
H	-6.573729	-4.319398	0.984485
H	-5.778587	-3.187297	2.104722
H	-4.990807	-3.621624	0.558241
H	1.787502	0.897702	-1.421228



Isomer for *Z*-product formation

C	2.954712	3.411283	0.700171
C	4.191266	4.244875	0.941396
H	4.335960	4.438441	2.022067
H	4.138081	5.217016	0.424177
H	5.100574	3.718710	0.595853
C	1.933058	3.878293	-0.056808
C	0.639731	3.187359	-0.395661
Ni	-2.114864	1.108899	0.133941
H	0.691538	2.105655	-0.185827
H	0.446649	3.281533	-1.482769
H	2.048657	4.890843	-0.471424
O	-1.776286	2.970866	-0.070572
C	-0.621663	3.735223	0.338177
C	-0.495666	3.589716	1.858185
H	0.398133	4.111758	2.237731
H	-1.390985	4.003906	2.352295
H	-0.424520	2.519260	2.118197
C	-0.892039	5.198012	-0.044548
H	-0.068176	5.850442	0.291943
H	-1.827046	5.545926	0.424808
H	-0.996404	5.307819	-1.138261
P	-2.120356	-0.990855	0.213546
C	-3.682505	-1.768173	-0.518301
C	-5.139725	-1.923632	-2.592058
C	-5.413012	-3.608891	-0.712491
C	-5.525423	-3.365788	-2.225854
C	-4.016190	-3.235991	-0.176011
C	-3.746158	-1.560540	-2.047966
H	-5.887999	-1.222626	-2.170863
H	-6.174374	-2.999814	-0.185294
H	-4.849620	-4.066600	-2.756095
H	-3.267247	-3.908077	-0.636571
H	-2.998405	-2.214075	-2.539145
H	-4.482890	-1.140882	-0.075271
H	-5.162732	-1.784843	-3.688423

H	-5.635769	-4.665249	-0.473469
H	-6.549127	-3.592881	-2.575551
H	-3.979451	-3.415200	0.913184
H	-3.481860	-0.521877	-2.314587
C	-0.703502	-1.824325	-0.716313
C	1.616599	-1.617851	-1.735500
C	0.691117	-3.906398	-1.176619
C	1.958610	-3.046623	-1.288341
C	-0.352930	-3.256377	-0.248591
C	0.573857	-0.963131	-0.812469
H	1.215420	-1.643677	-2.769041
H	0.247844	-4.037937	-2.184163
H	2.464904	-3.006939	-0.303143
H	0.060150	-3.218441	0.777492
H	1.010160	-0.821579	0.195523
H	-1.104900	-1.898642	-1.747291
H	2.528109	-0.995019	-1.761243
H	0.936660	-4.919266	-0.806787
H	2.675787	-3.510180	-1.991285
H	-1.253410	-3.892494	-0.200009
H	0.319720	0.044986	-1.183260
C	-2.083307	-1.647521	1.972189
C	-0.824778	-1.824902	4.174432
C	-3.357077	-1.726612	4.179405
C	-2.073761	-1.370992	4.945760
C	-3.333794	-1.169393	2.744769
C	-0.807846	-1.253009	2.745414
H	-0.803964	-2.932427	4.127571
H	-3.465373	-2.829259	4.138279
H	-2.030471	-0.273196	5.090704
H	-3.325751	-0.060459	2.778804
H	-0.744230	-0.148868	2.791529
H	-2.113916	-2.753987	1.904981
H	0.092118	-1.516747	4.709754
H	-4.245823	-1.344215	4.714172
H	-2.090563	-1.822130	5.954738
H	-4.261489	-1.457138	2.217596
H	0.097952	-1.591928	2.212445
Al	-2.752645	2.732864	-1.656424
C	-1.774951	1.858545	-3.169845
H	-1.127854	1.008927	-2.884507
H	-1.136371	2.585087	-3.709094
H	-2.497504	1.473762	-3.916895
C	-3.807066	4.334348	-2.195934
H	-3.213791	5.035179	-2.812920
H	-4.679543	4.041719	-2.812018
H	-4.198077	4.907380	-1.335180
C	-4.072022	1.587441	-0.427563
H	-3.980432	1.062763	0.556710
H	-4.748965	0.980312	-1.048380
H	-4.582556	2.532554	-0.164698
C	2.963591	2.043250	1.356787
H	3.170837	2.165373	2.438844
H	1.960284	1.582934	1.296841
C	3.986637	1.069194	0.782252
C	5.833378	-0.842978	-0.297720
C	4.298198	1.049815	-0.587406
C	4.623755	0.122846	1.606754
C	5.520195	-0.812002	1.078470
C	5.203768	0.115680	-1.114331
H	3.827160	1.783718	-1.251588
H	4.411305	0.117481	2.683014
H	5.991190	-1.529854	1.759607
H	5.415615	0.145986	-2.186989
C	6.825385	-1.888313	-0.840423
C	7.024607	-1.771030	-2.364212
H	7.435783	-0.787191	-2.650437
H	7.737566	-2.541373	-2.706133
H	6.079561	-1.923680	-2.914460
C	8.200964	-1.696715	-0.155678
H	8.131561	-1.805664	0.939976
H	8.611067	-0.694309	-0.368700
H	8.921982	-2.448722	-0.524155
C	6.293977	-3.309491	-0.530698
H	5.313841	-3.477480	-1.010747
H	6.997725	-4.073554	-0.907702
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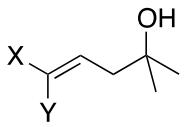
H	-0.845808	0.810562	0.809926



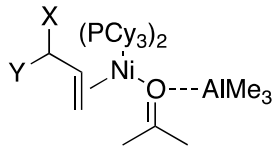
C	1.943662	1.660217	-0.034722
C	1.880382	1.803929	1.468165
H	2.048449	2.857660	1.764948
H	2.611729	1.169326	1.989070
H	0.875511	1.531787	1.838438
C	2.969230	1.086505	-0.711840
C	4.196995	0.441611	-0.122579
H	4.448137	0.892097	0.853581
H	5.062530	0.616640	-0.789143
H	2.891911	1.061814	-1.808368
O	2.923423	-1.342046	0.972357
C	4.040813	-1.097585	0.100673
C	3.834538	-1.841953	-1.231567
H	3.699936	-2.919364	-1.039024
H	4.696717	-1.712421	-1.910103
H	2.933436	-1.474951	-1.754666
C	5.263741	-1.644785	0.842350
H	5.140845	-2.724201	1.033006
H	5.380808	-1.136043	1.813909
H	6.183078	-1.495562	0.251200
C	0.755714	2.236665	-0.790617
H	0.981991	2.244451	-1.873226
H	0.603877	3.292034	-0.489747
C	-0.537020	1.470521	-0.544267
C	-2.954676	0.001178	-0.079346
C	-0.659922	0.124204	-0.940715
C	-1.639651	2.063516	0.088676
C	-2.824144	1.344506	0.316251
C	-1.839834	-0.589637	-0.715388
H	0.185438	-0.369770	-1.435746
H	-1.577043	3.110635	0.408902
H	-3.654639	1.853346	0.813528
H	-1.892365	-1.633601	-1.044046
C	-4.235449	-0.822036	0.151000
C	-3.903670	-2.052742	1.030298
H	-3.516000	-1.740871	2.015569
H	-3.144432	-2.700422	0.560173
H	-4.810620	-2.662147	1.194736

C	-5.336078	-0.007252	0.858066
H	-5.012520	0.342102	1.854223
H	-6.230671	-0.637873	1.001309
H	-5.640963	0.872797	0.265039
C	-4.789352	-1.302006	-1.213095
H	-4.059059	-1.925908	-1.755693
H	-5.045073	-0.444212	-1.859036
H	-5.703053	-1.905485	-1.064964
H	2.162987	-0.874644	0.559217

$Ni(PCy_3)_2(COD)$

Ni	0.029270	-1.362077	-0.258256
P	-1.796889	0.004649	-0.022938
C	-2.814932	-0.190707	1.587580
C	-4.692009	-1.261245	2.891314
C	-2.582564	-0.580044	4.126066
C	-4.110247	-0.436467	4.069947
C	-1.924416	-0.009985	2.843525
C	-3.653838	-1.472133	1.761554
H	-5.034194	-2.249607	3.250201
H	-2.169987	-0.073148	5.017136
H	-4.361959	0.634307	3.944976
H	-0.949740	-0.500578	2.674562
H	-2.991560	-2.309419	2.029005
H	-3.542560	0.640965	1.561874
H	-5.587037	-0.751630	2.487089
H	-2.325043	-1.650582	4.238506
H	-4.571138	-0.748933	5.023896
H	-1.703561	1.063547	2.992184
H	-4.171032	-1.771502	0.834240
C	-1.589969	1.934934	0.024423
C	-1.019149	4.032031	-1.324741
C	-2.138981	4.261749	0.923109
C	-1.967540	4.882853	-0.469198
C	-2.581332	2.785271	0.855685
C	-1.489027	2.566534	-1.379735
H	0.002325	4.081476	-0.895938
H	-1.175394	4.320106	1.469666
H	-1.597137	5.921427	-0.388677
H	-3.590485	2.728957	0.402957
H	-2.491053	2.556194	-1.846821
H	-0.596043	2.052188	0.497601
H	-0.947143	4.441962	-2.349861
H	-2.869981	4.840209	1.518382
H	-2.955858	4.937737	-0.968250
H	-2.677112	2.413052	1.888017
H	-0.831494	1.968776	-2.031442
C	-3.190030	-0.306634	-1.299583
C	-5.634534	-0.340429	-1.981749
C	-3.818120	-0.766310	-3.711849
C	-5.244299	-0.245355	-3.465808
C	-2.817316	-0.056690	-2.782434
C	-4.586196	0.311450	-1.055513
H	-6.625042	0.123365	-1.816001
H	-3.780482	-1.859435	-3.531040
H	-5.295238	0.815202	-3.784873
H	-2.865780	1.023865	-2.999770
H	-4.546820	1.400253	-1.256804
H	-3.298542	-1.406923	-1.190340
H	-5.738207	-1.407665	-1.699612
H	-3.532608	-0.611936	-4.769041
H	-5.973628	-0.794727	-4.089374
H	-1.779823	-0.361005	-3.001484
H	-4.912793	0.199207	-0.008097
P	1.787041	0.041366	0.052752
C	3.519938	-0.760119	0.133460
C	5.117760	-2.301522	-1.110026
C	6.077755	-0.566040	0.456229
C	6.013411	-2.063672	0.131036
C	4.682337	-0.017831	0.860519
C	4.030058	-1.210341	-1.253865
H	4.644087	-3.298625	-1.041058
H	6.455824	-0.023121	-0.431454
H	7.023998	-2.476650	-0.036458
H	4.562707	-0.125238	1.952136
H	3.205705	-1.570330	-1.886371
H	3.306963	-1.684130	0.705070
H	5.736258	-2.314451	-2.026771
H	6.801753	-0.365868	1.266671
H	5.603021	-2.603203	1.006158
H	4.656561	1.062686	0.652846
H	4.459155	-0.339551	-1.780818
C	1.981863	1.472694	-1.209306
C	3.213224	3.449361	-2.264837
C	1.584854	2.125404	-3.664205
C	2.883692	2.944085	-3.675738
C	1.636208	0.980392	-2.635705
C	3.296459	2.288342	-1.253605
H	2.430230	4.164120	-1.939538
H	0.739622	2.800791	-3.425350
H	3.716448	2.307544	-4.036960
H	2.396154	0.246346	-2.963315
H	4.132862	1.631064	-1.553573
H	1.175409	2.169723	-0.904634
H	4.167295	4.009151	-2.265204
H	1.378312	1.711104	-4.668765
H	2.803471	3.789633	-4.383749
H	0.674733	0.435658	-2.611002
H	3.555725	2.690759	-0.262042
C	1.602875	0.934415	1.745958
C	1.497504	0.596572	4.287626
C	1.881194	2.903963	3.344922
C	2.196209	1.946476	4.502250
C	2.285968	2.298868	1.986495
C	1.858071	-0.031278	2.927348
H	0.401878	0.748185	4.342077
H	0.793543	3.122636	3.338170
H	3.292629	1.791345	4.558190
H	3.385575	2.190149	1.965155
H	2.920165	-0.334944	2.952765
H	0.512438	1.126529	1.760477
H	1.755880	-0.108932	5.099193
H	2.394794	3.872872	3.488625
H	1.891436	2.390040	5.468094
H	2.016667	3.008236	1.183746
H	1.271172	-0.954945	2.782236
C	0.865593	-2.938173	0.802400
C	-0.524643	-2.902353	1.035020
C	-1.476217	-3.896561	0.389421
H	-1.303262	-4.916310	0.796908
H	-2.510971	-3.638483	0.665437
C	-1.361240	-3.911065	-1.156727

H	-0.754523	-4.777639	-1.483178
H	-0.850131	-2.509754	2.007363
H	-2.362187	-4.067314	-1.599057
C	-0.756824	-2.626333	-1.714089
H	-1.415670	-2.062370	-2.376386
C	0.627435	-2.495629	-1.935210
H	0.954505	-1.840432	-2.752641
C	1.564448	-3.638976	-1.584463
H	2.593915	-3.386411	-1.880064
H	1.302344	-4.533747	-2.188494
C	1.528528	-4.000733	-0.070915
H	1.002208	-4.964913	0.071301
H	2.559418	-4.170588	0.290249
H	1.504433	-2.550994	1.605592



Isomer 1

C	1.419824	-0.979634	-2.368081
C	1.629459	-2.197942	-1.453634
H	1.632343	-3.135721	-2.043151
H	0.827752	-2.266153	-0.697871
H	2.593454	-2.156860	-0.920470
C	1.198112	0.361825	-1.661668
C	0.315646	1.292065	-2.289273
Ni	-0.466938	0.667038	-0.623522
H	-0.111409	1.057299	-3.272704
H	0.528404	2.370605	-2.178487
H	2.099074	0.754250	-1.172564
H	0.504553	-1.181596	-2.960294
O	-1.164261	-4.359621	-0.096416
C	-1.146878	-4.744894	-1.282260
C	-0.833973	-6.168161	-1.654845
H	-1.206346	-6.862319	-0.886775
H	0.266565	-6.275359	-1.700581
H	-1.239573	-6.427685	-2.645847
C	-1.431583	-3.758234	-2.381394
H	-1.327198	-2.724028	-2.011560
H	-2.468876	-3.899747	-2.741303
H	-0.767863	-3.929558	-3.247629
P	-2.661013	0.776103	-0.841655
C	-3.428575	-0.023082	-2.405814
C	-5.498196	-0.575208	-3.799183
C	-3.206685	-0.734764	-4.845430
C	-4.689355	-0.425267	-5.095313
C	-2.607848	0.111368	-3.704393
C	-4.912302	0.306326	-2.680137
H	-5.484896	-1.636630	-3.476960
H	-3.106452	-1.809151	-4.584161
H	-4.788918	0.614893	-5.465581
H	-2.546694	1.169696	-4.019476
H	-4.998188	1.362988	-2.995843
H	-3.381607	-1.098230	-2.148499
H	-6.559150	-0.312965	-3.969499
H	-2.617364	-0.584652	-5.769235
H	-5.094145	-1.081382	-5.888009
H	-1.575978	-0.226271	-3.520269
H	-5.517200	0.202006	-1.762594
C	-3.581271	-0.244728	0.531315
C	-5.419503	-0.627116	2.279852
C	-4.195281	-2.599261	1.320051
C	-5.540137	-2.096763	1.859388
C	-3.712553	-1.734512	0.143202
C	-4.906274	0.270602	1.134807
H	-4.717591	-0.559061	3.134236
H	-3.440858	-2.573815	2.127891
H	-6.315866	-2.194889	1.072853
H	-4.443511	-1.850813	-0.680555
H	-5.687032	0.331105	0.352337
H	-2.824810	-0.221559	1.339794
H	-6.390116	-0.239447	2.642015
H	-4.270585	-3.654809	0.997821
H	-5.874232	-2.716132	2.711978
H	-2.738337	-2.113824	-0.216135
H	-4.771593	1.291987	1.529666
C	-3.243448	2.607132	-0.829623
C	-2.690282	4.850140	-1.918099
C	-4.783539	4.601392	-0.519651
C	-4.130043	5.336888	-1.698495
C	-4.714670	3.068536	-0.686896
C	-2.624826	3.319319	-2.057746
H	-2.061309	5.159801	-1.058835
H	-4.269191	4.885835	0.420651
H	-4.721205	5.144743	-2.616579
H	-5.290199	2.786437	-1.586404
H	-3.182822	3.019020	-2.966756
H	-2.702310	2.988141	0.060770
H	-2.252642	5.327722	-2.814733
H	-5.838252	4.914804	-0.406035
H	-4.150990	6.430290	-1.534625
H	-5.216753	2.593100	0.166440
H	-1.583398	2.990609	-2.204638
P	0.394097	0.905303	1.418625
C	1.661895	-0.457868	1.929055
C	4.173269	-1.110740	1.942162
C	2.566443	-2.202465	3.557188
C	3.626062	-2.445992	2.457043
C	1.843982	-0.834998	3.414506
C	3.062043	-0.267234	1.267978
H	4.994629	-1.265592	1.219253
H	1.820659	-3.016056	3.539400
H	4.438596	-3.087222	2.842984
H	2.436220	-0.052881	3.925482
H	3.376492	0.787989	1.286924
H	1.193128	-1.339661	1.450776
H	4.609541	-0.551943	2.793948
H	3.046946	-2.238243	4.552860
H	3.174763	-3.000831	1.612276
H	0.875893	-0.896029	3.938882
H	2.998577	-0.538049	0.205296
C	1.417324	2.495833	1.203081
C	1.448287	4.823660	0.191794
C	3.322480	4.068182	1.742670
C	2.515786	5.264043	1.207717
C	2.392217	2.974235	2.303947
C	0.557292	3.701815	0.756486
H	1.943958	4.455185	-0.728965
H	3.938219	3.639094	0.926248

H	2.014496	5.765260	2.060182
H	1.822979	3.399842	3.148942
H	-0.005221	4.093171	1.626586
H	2.039074	2.222855	0.324980
H	0.826786	5.687691	-0.110122
H	4.028243	4.404131	2.525275
H	3.190475	6.015213	0.756612
H	2.986011	2.143118	2.720473
H	-0.196467	3.392487	0.009004
C	-0.664567	1.176046	2.988626
C	-0.986036	1.620887	5.474603
C	-2.916627	1.974397	3.874947
C	-2.279775	2.404317	5.205354
C	-1.913051	2.039653	2.708877
C	-0.015299	1.727046	4.282045
H	-1.227633	0.554416	5.656508
H	-3.286298	0.934218	3.971156
H	-2.041747	3.486188	5.161399
H	-1.601440	3.092120	2.564577
H	0.220403	2.796929	4.129726
H	-1.020463	0.142142	3.198189
H	-0.496012	1.993009	6.393795
H	-3.799877	2.602285	3.651065
H	-2.997151	2.273682	6.036544
H	-2.395367	1.733510	1.768625
H	0.933749	1.228324	4.522201
Al	-0.740890	-5.285655	1.689747
C	-2.147467	-6.711444	1.776118
H	-2.035988	-7.555927	1.070117
H	-3.167326	-6.304018	1.637549
H	-2.134430	-7.160090	2.788815
C	-0.992652	-3.753328	2.949220
H	-0.256055	-3.783698	3.774914
H	-1.991346	-3.754429	3.423753
H	-0.868983	-2.771995	2.449447
C	1.152035	-5.845478	1.343273
H	1.656992	-6.080504	2.300208
H	1.754982	-5.045857	0.870727
H	1.255983	-6.748775	0.712765
C	2.567857	-0.862802	-3.429368
H	2.271350	-0.081135	-4.151889
H	2.623480	-1.818095	-3.987710
C	3.932327	-0.533715	-2.864796
C	6.478415	0.109987	-1.696346
C	4.348297	0.803942	-2.699364
C	4.828109	-1.537465	-2.455878
C	6.071027	-1.224425	-1.883008
C	5.586044	1.115407	-2.127925
H	3.683393	1.612335	-3.024520
H	4.552857	-2.590443	-2.590875
H	6.728194	-2.045902	-1.583446
H	5.862989	2.170449	-2.019871
C	7.824545	0.496873	-1.056645
C	8.656329	-0.735481	-0.650906
H	8.906082	-1.366788	-1.521665
H	8.127970	-1.361522	0.089537
H	9.606239	-0.408597	-0.193064
C	8.655047	1.331676	-2.061518
H	8.869469	0.750176	-2.975074
H	9.618596	1.629965	-1.609829
H	8.127255	2.251532	-2.365473
C	7.560029	1.341131	0.215037
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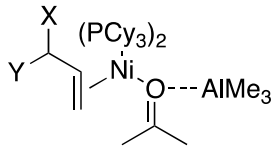

Isomer 2

C	0.950322	-0.106270	-1.442552
C	1.473588	-0.601345	-0.204707
Ni	-0.464725	-0.677901	-0.216842
H	1.882564	0.132759	0.503764
H	2.031208	-1.547916	-0.196202
O	0.118490	4.891313	1.174167
C	-0.878741	5.520040	1.581429
C	-0.794476	6.979452	1.935547
H	-1.751003	7.387398	2.293524
H	-0.451931	7.542392	1.049236
H	-0.012573	7.117186	2.703068
C	-2.193162	4.806465	1.723721
H	-2.965207	5.322416	1.123442
H	-2.531722	4.861213	2.775120
H	-2.107976	3.756710	1.409801
P	-0.518040	-1.520305	1.804175
C	-1.967947	-2.197086	2.844915
C	-4.112676	-1.696693	4.135548
C	-3.794710	-3.966179	3.059940
C	-4.811327	-2.891233	3.468629
C	-2.675051	-3.389821	2.173886
C	-2.983379	-1.115187	3.262201
H	-3.681840	-2.026146	5.102654
H	-3.340847	-4.402058	3.973050
H	-5.354057	-2.543132	2.568582
H	-3.090498	-3.074662	1.197449
H	-3.411155	-0.639567	2.360683
H	-1.498774	-2.571351	3.778597
H	-4.847474	-0.905052	4.375416
H	-4.300851	-4.798171	2.535548
H	-5.572747	-3.317752	4.147801
H	-1.947954	-4.187799	1.947808
H	-2.479124	-0.310422	3.825921
C	0.702281	-2.977120	1.932625
C	1.924971	-4.760393	3.264698
C	1.778941	-4.945118	0.737390
C	1.863928	-5.717840	2.063681
C	0.604853	-3.949348	0.736944
C	0.744454	-3.768990	3.256084
H	2.875969	-4.191662	3.231237
H	2.723850	-4.387653	0.577247
H	0.969681	-6.365820	2.163845
H	-0.346485	-4.513587	0.776946
H	-0.195193	-4.340875	3.383721
H	1.677285	-2.461506	1.826234
H	1.932822	-5.330580	4.212507
H	1.681307	-5.646681	-0.111884
H	2.740794	-6.391407	2.064058
H	0.587005	-3.377014	-0.206320

H	0.816727	-3.091503	4.126975
C	0.151651	-0.293648	3.116496
C	2.028506	0.669808	4.532810
C	0.067144	2.136527	3.889405
C	1.567825	2.100368	4.216117
C	-0.285108	1.147326	2.764268
C	1.668571	-0.315081	3.402749
H	1.548064	0.331038	5.473275
H	-0.514190	1.879081	4.798633
H	2.135620	2.482713	3.345125
H	0.223327	1.454243	1.829172
H	2.229340	-0.040028	2.490934
H	-0.350682	-0.576926	4.065340
H	3.119342	0.648226	4.712898
H	-0.233686	3.161122	3.600690
H	1.797396	2.775585	5.061399
H	-1.368708	1.179427	2.544840
H	2.006027	-1.326259	3.687625
H	0.945096	0.996497	-1.521711
C	1.263531	-0.747117	-2.795611
H	0.449641	-0.484594	-3.505888
C	1.357056	-2.278298	-2.786545
H	2.168297	-2.636552	-2.130154
H	1.561664	-2.663588	-3.802267
H	0.412217	-2.728051	-2.436557
P	-2.208165	-0.096449	-1.431178
C	-2.609819	-1.442914	-2.706102
C	-2.521245	-3.956862	-3.120058
C	-3.872835	-2.460905	-4.661043
C	-3.747260	-3.862190	-4.042673
C	-3.881287	-1.359820	-3.581265
C	-2.529681	-2.845542	-2.056984
H	-1.597429	-3.868568	-3.726529
H	-3.020751	-2.285536	-5.348302
H	-3.695420	-4.630309	-4.836304
H	-4.777721	-1.497461	-2.947233
H	-3.400338	-2.989389	-1.387945
H	-1.732058	-1.354014	-3.383518
H	-2.482386	-4.948335	-2.631655
H	-4.790111	-2.391844	-5.275269
H	-4.661181	-4.079635	-3.453841
H	-3.986398	-0.372107	-4.057496
H	-1.635423	-2.905499	-1.408731
C	-3.849192	0.467178	-0.629601
C	-5.993929	1.850242	-0.555705
C	-5.852129	-0.292299	0.769737
C	-6.781508	0.656574	-0.000449
C	-4.654373	-0.732816	-0.090619
C	-4.798907	1.397930	-1.417659
H	-5.617402	2.462403	0.289450
H	-5.482198	0.220197	1.680711
H	-7.248815	0.106425	-0.841704
H	-5.038611	-1.325859	-0.941437
H	-5.179142	0.870761	-2.313049
H	-3.481359	1.037169	0.251353
H	-6.654617	2.509245	-1.149618
H	-6.413669	-1.179857	1.116379
H	-7.608143	1.001895	0.647555
H	-3.991504	-1.403266	0.480914
H	-4.267360	2.291094	-1.780509
C	-1.686736	1.395816	-2.492865
C	-1.676657	2.921027	-4.527327
C	-0.772386	3.773863	-2.328542
C	-1.517749	4.148007	-3.617890
C	-1.472905	2.625580	-1.580916
C	-2.403181	1.763578	-3.811627
H	-0.671647	2.576847	-4.844350
H	0.259466	3.460356	-2.584249
H	-2.521094	4.546664	-3.362310
H	-2.444199	2.990781	-1.193096
H	-3.455181	2.052125	-3.642032
H	-0.675677	1.074419	-2.799704
H	-2.222562	3.188396	-5.451281
H	-0.669594	4.652244	-1.664940
H	-0.984515	4.956658	-4.150783
H	-0.872255	2.327017	-0.700032
H	-2.418887	0.888516	-4.484604
Al	2.065993	5.435685	0.830272
C	1.845688	6.894320	-0.528499
H	1.117637	6.642944	-1.323441
H	2.813725	7.044793	-1.045305
H	1.564410	7.884227	-0.122113
C	2.746156	3.693546	0.138912
H	2.671955	2.878153	0.883519
H	3.811540	3.757721	-0.155534
H	2.189333	3.362380	-0.758635
C	2.654294	5.961244	2.673841
H	2.353776	5.230276	3.448332
H	2.319498	6.959862	3.012940
H	3.761229	5.991042	2.698711
C	2.545636	-0.106105	-3.431950
H	2.386480	0.987760	-3.481967
H	2.618057	-0.463056	-4.477930
C	3.850120	-0.390857	-2.720686
C	6.311228	-0.961727	-1.354544
C	4.312010	0.424654	-1.672033
C	4.651619	-1.492515	-3.080788
C	5.848860	-1.772265	-2.413228
C	5.513856	0.144765	-1.005392
H	3.725210	1.298631	-1.367016
H	4.332647	-2.140886	-3.906024
H	6.437739	-2.639997	-2.732374
H	5.825704	0.814902	-0.199011
C	7.634753	-1.302183	-0.643940
C	7.532861	-2.715549	-0.019621
H	8.478326	-2.983024	0.486727
H	7.329778	-3.485844	-0.782875
H	6.719460	-2.758404	0.725589
C	7.970451	-0.303157	0.480524
H	8.922614	-0.589248	0.960921
H	7.191929	-0.290257	1.263254
H	8.087064	0.724542	0.094473
C	8.793448	-1.280379	-1.670759
H	9.749824	-1.535396	-1.178703
H	8.896894	-0.279997	-2.125732
H	8.630867	-2.005005	-2.486595