

Energetic pathways and influence of the metallacyclobutane intermediates formed during isobutene / 2-butene cross-metathesis over $\text{WH}_3/\text{Al}_2\text{O}_3$ supported catalyst

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Dedicated to the memory of Yves Chauvin (1930-2015) in honor of his seminal contribution to the understanding of metallacyclobutanes

Evaluation of the ΔG associated to the metallacyclobutane formation and to the metathesis reaction

Considering the reaction (eq. 1):



In which Sur1 is the W-based catalyst supported on the alumina surface and Sur2 is the metallacyclobutane formed after the butene addition. In this case, the Gibbs free energy of reaction can be derived as (eq. 2):

$$\Delta G_{\text{reac}} = \Delta H_{\text{reac}} - T\Delta S_{\text{reac}} \quad (2)$$

ΔH_{reac} can be safely replaced by $\Delta E_{0K} + \text{ZPE}$ where ΔE_{0K} is the electronic energy computed as the result of the optimization procedure and ZPE represents the zero point energy computed with the frequency analysis. Moreover, ΔS_{reac} can be expressed by its components (eq. 3):

$$\Delta G_{\text{reac}} = (\Delta E_{0K} + \text{ZPE}) - T(S_{\text{Sur2}} - S_{\text{Sur1}} - S_{\text{butene}}) \quad (3)$$

We set $S_{\text{Sur2}} - S_{\text{Sur1}} = 0$ since the entropic variation on the surface can be neglected and we express S_{butene} with its translational (Tran), rotational (Rot) and vibrational (Vib) components (eq. 4):

$$\Delta G_{\text{reac}} = (\Delta E_{0K} + \text{ZPE}) - T[S(\text{trans})_{\text{butene}} + TS(\text{Rot})_{\text{butene}} + TS(\text{Vib})_{\text{butene}}]. \quad (4)$$

From a simplified molecular model calculation (Chart S1) it has been verified that ZPE and $TS(\text{Vib})_{\text{butene}}$ represent minority contributions on the overall energy evaluations.

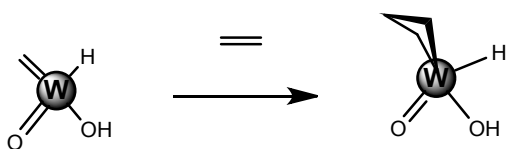


Chart S1. Molecular model adopted for the evaluation of the entropic contribution in the formation of metallacyclobutanes.

Moreover, it was seen that $ZPE \approx TS(\text{Vib})_{\text{butene}}$, then the eq. 4 can be simplified (eq. 5):

$$\Delta G_{\text{reac}} = \Delta E_{0\text{K}} - T[S(\text{trans})_{\text{butene}} + S(\text{Rot})_{\text{butene}}] \quad (5)$$

Similar considerations can be used to evaluate the Gibbs free energy of the overall metathesis reaction (eq. 6):






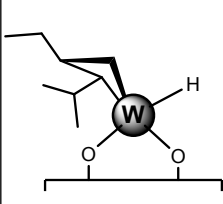
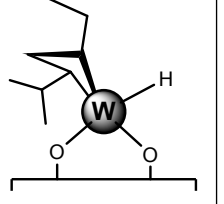
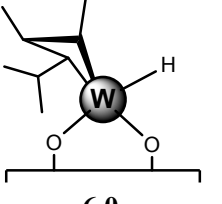
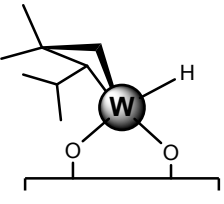
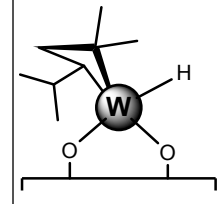
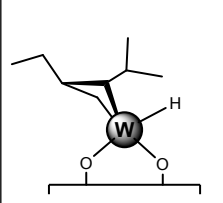
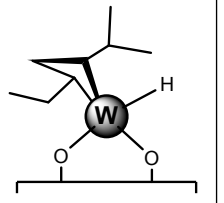
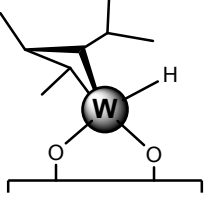
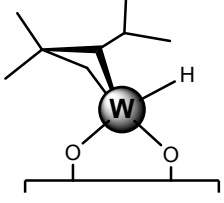
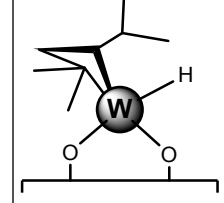
Where Sur1 and Sur3 represent the supported catalyst species before and after the reaction (**1**, **2a**, **2b**, **2c** or **2d**), respectively; mol1 represents the butene substrate (1-butene, *trans*-2-butene or isobutene) and mol2 represent the product of the metathesis (C2, C3, C5 or C6 alkenes). In this case, the equation (5) becomes (eq. 7):

$$\Delta G_{\text{reac}} = \Delta E_{0\text{K}} - T[S(\text{trans})_{\text{mol2}} + S(\text{Rot})_{\text{mol2}} - S(\text{trans})_{\text{mol1}} - S(\text{Rot})_{\text{mol1}}] \quad (7)$$

Or in a more contracted form (eq. 8):

$$\Delta G_{\text{reac}} = \Delta E_{0\text{K}} - T[\Delta S(\text{trans}) + \Delta S(\text{Rot})] \quad (8)$$

Table S1. All the butene insertions into supported species 1. Values refer to the metallacycle formation energy (kcal/mol)

					
	<i>(1,2) insertion</i>	<i>(2,1) insertion</i>	<i>(1,2) insertion</i>	<i>(2,1) insertion</i>	
Top Path	 4.2	 5.6	 6.0	 13.6	 8.7
Side Path	 3.8	 3.9	 8.4	 8.7	 16.2

Cartesian coordinates (Å) and associated energies (Hartree) of all the structures shows in the activation steps and in the investigated catalytic cycles.

Species 1. E: -2329.3570646885

Al	0.725219127	4.903298014	8.589493309
Al	4.875382030	6.972882891	7.212615812
O	3.415416046	7.191493343	11.207092703
O	7.711289259	4.853482497	9.762978595
O	3.405364286	6.845685286	8.454549006
O	7.782528083	5.007205837	7.123787946
Al	4.786047776	3.070425849	10.032169620
Al	0.663041230	0.965943814	11.342209431
O	7.629705505	0.808371044	7.279939859
O	3.511902482	3.061497679	8.644714790
O	7.571632117	1.126179230	10.080227444
O	3.508516226	2.883984583	11.349228069
Al	7.775791353	3.022960667	9.935889679
Al	3.510993528	0.974582630	11.336434183
O	4.993395794	0.729402913	7.213589769
O	0.619436065	3.070618853	8.640189324
O	4.996328670	1.133265320	10.084131025
O	0.688258857	2.840066260	11.284765447
Al	3.492182131	4.894828730	8.474550964
Al	7.760112081	7.115558309	7.221059953
O	0.765865304	7.189405571	11.288313757
O	4.844279639	4.931432360	9.931116725
O	0.776729890	6.851773813	8.474549458
O	4.913917157	5.084285155	7.274593983

Al	6.241502667	0.945641893	8.613728122
Al	6.286881518	0.833317150	11.439175314
Al	6.320158079	5.913620717	9.924564253
O	6.544769930	7.015520420	11.354927006
O	6.370731155	7.091642432	8.553026047
Al	2.076191559	7.020770646	9.909779625
Al	2.098513050	6.875537501	7.077763827
Al	2.047552819	2.052696544	8.573298707
O	2.187110685	0.954789038	7.126936869
O	2.102630749	0.876297759	9.928689764
Al	2.073499078	3.950443261	11.383441906
O	2.097444895	5.087494990	9.919689784
O	2.043908665	5.011831716	7.286786430
Al	6.228318166	3.929430475	7.194273394
O	6.261246292	2.858154336	8.656140951
O	6.300935781	2.912910037	11.276983065
H	1.917097540	1.379639780	6.298113558
H	4.109853559	1.141481913	7.279572156
H	7.337437678	1.402258154	6.543127427
H	6.275841039	7.680824634	5.358489568
H	3.578181291	6.201082721	5.335537714
H	0.621392459	7.610163897	5.215602538
H	5.881154755	2.437832679	5.413592518
H	8.284538858	4.724715473	6.333883336
O	6.322872830	6.946397491	5.989227981
O	3.507286892	7.022318584	5.851085532
O	0.627755319	6.947483587	5.919898382
O	6.606432807	2.978333051	5.765793745
Al	9.172125254	4.912863475	8.578414800
Al	13.303939833	7.051983151	7.310637103
O	11.683320822	7.260930320	11.435724058
O	16.119302400	4.908694038	9.837583244
O	11.826720419	6.931408713	8.557956687
O	16.118751474	5.062041942	7.190951367
Al	13.201013089	3.107212451	10.119666213
Al	9.073407974	1.033216321	11.340242678
O	15.977596048	0.890644209	7.432786266
O	11.931099306	3.121007419	8.736220835
O	15.949552363	1.130955657	10.170935165
O	11.908473530	2.906748237	11.437741603
Al	16.187198261	3.058071437	10.027415570
Al	11.892959129	1.026107089	11.448231166
O	13.249294107	0.792197041	7.508882750
O	9.117628996	3.064165546	8.638520405
O	13.394421343	1.188996127	10.239089491
O	9.047564045	2.899180294	11.283322030
Al	11.932931825	4.957947659	8.571821535
Al	16.155391894	7.134646285	7.295882222
O	13.246701518	4.931361118	9.999543675
O	9.179396764	6.863666948	8.480892404
O	13.321011660	5.165062828	7.355959668
Al	14.636904546	0.985282877	8.757804541
Al	14.691226068	0.889528932	11.576107315
Al	14.682086612	5.945694378	10.027939300
O	14.959220847	7.025003904	11.443133239
O	14.744579811	7.118005056	8.637289908
Al	10.507207634	7.093992512	9.958391107
Al	10.550176789	6.952995810	7.137866296
Al	10.567134767	2.020578755	8.562364874
O	10.346828073	0.876189967	7.191991482
O	10.515553005	0.885051246	10.009318278

Al	10.473978434	3.926940777	11.328538909
O	10.500318400	5.155838825	9.991319543
O	10.524132537	5.086194147	7.347904192
Al	14.582642936	3.972915023	7.342851921
O	14.654551402	2.901307454	8.791217668
O	14.725818859	2.985562149	11.380316681
H	9.365902435	0.993805714	7.073639137
H	13.373355627	1.365003304	6.727857678
H	15.714017216	1.432142824	6.658173445
H	14.645963113	7.783357194	5.467735644
H	12.095671657	6.234662817	5.479470627
H	9.078013163	6.663122818	5.103796802
H	14.363119971	3.114339748	5.119250891
H	16.603852332	4.895684723	6.355859680
O	14.729120176	7.026383685	6.066562778
O	11.983784772	7.086578325	5.935903188
O	9.116577237	7.174597618	5.922887393
O	14.646918104	2.831598000	5.999387595
Al	0.733590521	12.989895075	8.556967247
Al	4.870236409	14.988613064	7.071168879
O	3.505418659	15.252042876	11.052756747
O	7.695499796	12.981235682	9.755484207
O	3.409039128	14.866553179	8.322234618
O	7.724027444	12.994336059	7.051719862
Al	4.797121125	11.112607620	9.977000098
Al	0.724201351	9.150488297	11.447453000
O	7.640765058	8.940734198	7.373782082
O	3.504779244	11.045611467	8.564203746
O	7.625314933	9.270389256	10.162744088
O	3.520305748	10.932796443	11.271918636
Al	7.782134140	11.172658404	10.013411903
Al	3.549701406	9.067417092	11.374537752
O	4.995937524	8.858609660	7.357284461
O	0.617258808	11.175348065	8.713109559
O	5.060170408	9.188708703	10.156098292
O	0.711917757	11.045330866	11.373287495
Al	3.495044036	12.908285051	8.369598359
Al	7.701080885	15.088652116	7.137562445
O	0.794502455	15.238664634	11.129140491
O	4.826706332	12.916230325	9.766936882
O	0.776823016	14.922083595	8.381937441
O	4.899922585	13.075557412	7.122505535
Al	6.330359794	9.031082892	8.702684608
Al	6.330359429	8.959350458	11.528629649
Al	6.218365682	13.972598407	9.853661260
O	6.481573023	15.027194632	11.284634782
O	6.301811438	15.109807050	8.443485199
Al	2.162153724	15.086876244	9.809111105
Al	2.094691941	14.916760004	6.983427838
Al	1.992028155	10.091906384	8.602277915
O	2.110179267	8.950998196	7.192976132
O	2.044331488	8.951865590	10.006602642
Al	2.169949285	12.081009140	11.356321920
O	2.106162196	13.155108984	9.836300708
O	2.024792052	13.058152534	7.207012792
Al	6.204505740	11.910375462	7.186801006
O	6.283333912	10.918891602	8.701412237
O	6.305026784	11.065144837	11.290730647
H	2.399017374	9.350875676	6.357513907
H	4.180219982	9.330125078	7.609254912
H	7.398125067	9.548337232	6.633831566

H	6.348325647	14.257457019	5.255698711
H	3.515851520	14.173743682	5.261047963
H	0.570112639	15.653695015	5.077043854
H	5.718817881	10.279016896	5.652628207
H	8.283481174	12.770633513	6.279118055
O	6.317772390	15.019479784	5.851579370
O	3.493158539	15.011381961	5.753475123
O	0.618837303	15.084010511	5.855390155
O	6.464981955	10.892934128	5.768657514
Al	9.142504893	12.967243296	8.538036280
Al	13.257117752	15.073872843	7.220457403
O	11.840467893	15.264467178	11.274889613
O	16.134469092	13.068436817	9.904394544
O	11.776995698	14.919261621	8.469093497
O	16.129387856	13.078577146	7.184127807
Al	13.232111963	11.160799112	10.117354072
Al	9.080714768	9.186985794	11.394438107
O	16.118298748	8.948922271	7.521373115
O	11.965012538	11.079000007	8.706841775
O	16.026038432	9.275380939	10.254639725
O	11.927895935	10.973308937	11.423829499
Al	16.208013585	11.203696484	10.119181273
Al	11.977586260	9.100937326	11.448127375
O	13.467707837	8.936067472	7.436164222
O	9.050870292	11.139642322	8.646592849
O	13.471108190	9.212176912	10.252841269
O	9.105077689	11.047276717	11.352543057
Al	11.916913573	12.950066076	8.487147466
Al	16.137505179	15.223497348	7.236101487
O	9.127644483	15.249763564	11.198900778
O	13.236592652	12.979842883	9.918853126
O	9.123480227	14.861341153	8.394920011
O	13.323019868	13.156227671	7.275236584
Al	14.758586922	9.069270262	8.808846992
Al	14.753407754	8.932921028	11.629593707
Al	14.643392120	14.022769639	9.955793154
O	14.493873040	15.084775950	11.420517370
O	14.720057644	15.169386171	8.569148186
Al	10.521775583	15.096928727	9.870279212
Al	10.496414046	14.971700011	7.056546158
Al	10.470116438	10.119899330	8.647388686
O	10.529839212	8.961758572	7.268938098
O	10.511253387	9.027246088	10.076999811
Al	10.540863572	12.080514001	11.366753011
O	10.508012480	13.167037145	9.912288594
O	10.506684912	13.069416958	7.284192507
Al	14.621822852	11.983835647	7.313824611
O	14.715246072	10.980735440	8.818470290
O	14.720347551	11.124189806	11.419836802
H	9.946006959	9.249680430	6.546361127
H	12.654724021	9.457144974	7.567342785
H	15.958683172	9.610417017	6.810378326
H	14.725453658	14.452410077	5.346636077
H	11.956598394	14.230257428	5.392113470
H	9.048732330	15.584771815	5.114920299
H	14.240078016	10.319768496	5.791006075
H	16.663861153	12.828335724	6.399611929
O	14.719722737	15.166736765	6.000192895
O	11.919961469	15.083823227	5.857482803
O	9.052420641	14.940902461	5.838578380
O	14.952332310	10.971077240	5.918734834

O	7.716498756	9.118715045	12.720694094
H	7.880667835	8.373877937	13.335210132
H	14.654575717	11.742452720	12.164165762
O	13.326475824	9.026067427	12.795120620
O	10.507713719	9.034834403	12.717440687
O	-0.626004913	9.030597932	12.794503997
H	-0.587160219	9.778821190	13.407900105
O	2.415586985	13.234884593	12.650162463
O	10.587076566	13.313568304	12.651239183
H	7.487769798	14.962478579	11.322212523
H	13.498127279	15.002590951	11.541371387
H	3.345828429	14.593940922	11.774764652
H	11.531258700	14.711673532	12.035968078
O	1.873634188	5.002654708	12.792106111
H	7.548873087	6.946463709	11.480727451
H	4.139057516	6.552807127	11.087419656
H	15.967795416	6.952083065	11.500290312
O	7.701636514	0.967065850	12.639038049
H	7.780687604	0.313059481	13.346670232
O	-0.697711230	0.887268030	12.713351571
H	-0.619775768	0.109707056	13.286452094
H	6.341119462	3.454137878	12.081338867
O	4.901672985	0.817108039	12.641104072
O	2.097961770	0.882107043	12.563603136
H	14.817793005	3.594172105	12.131356429
O	13.258432755	0.892998957	12.787859020
O	10.439223796	0.962821192	12.642297886
O	2.171731162	9.114793692	12.641225740
O	4.911462912	8.946157775	12.704358060
H	2.172636465	8.324909469	13.203289118
H	4.858866455	9.666527659	13.349247830
H	13.178272297	8.222184892	13.332149881
H	10.495670126	9.627875253	13.484178702
H	13.245696152	1.630998268	13.414782194
H	10.379256948	1.706644212	13.260696589
H	2.092982697	1.623374879	13.189192921
H	4.807825249	-0.010106608	13.137454861
H	9.450675957	14.747121636	11.981910951
H	10.677174740	13.054858685	13.578266989
H	1.715635668	13.910302503	12.694281213
H	0.063800505	14.624961154	10.933138657
H	1.071757422	6.577661689	12.008400215
H	2.696281683	5.431611256	13.074935675
H	6.296773272	11.683302666	12.038718067
W	10.405074163	6.696494402	12.899872521
O	10.363773429	4.917640966	12.864468421
O	9.202504427	7.264827166	11.371035673
H	11.830370151	7.042735534	13.833094783
C	9.345292293	7.162741615	14.452337705
H	9.270658112	8.162335613	14.912064155
C	8.581753871	6.133567238	15.284961221
H	8.743936855	5.127771793	14.867656250
C	9.081149839	6.137722895	16.737920198
H	8.922578569	7.124806171	17.199510697
H	8.541117538	5.392483724	17.341603706
H	10.154830019	5.911899917	16.785591626
C	7.072112372	6.430420906	15.213460059
H	6.699879377	6.383765473	14.180076261
H	6.502677971	5.705717353	15.815555469
H	6.851322061	7.435796755	15.605930382

Species 2a. E: -2322.4692045853

Al	0.724976075	4.903254672	8.589460405
Al	4.875489679	6.972836359	7.212546561
O	3.415467576	7.190854219	11.207052825
O	7.711326461	4.853250429	9.762339699
O	3.405232507	6.845677979	8.454481495
O	7.782389837	5.006991007	7.123302477
Al	4.785904675	3.070181481	10.031872620
Al	0.662985573	0.965928942	11.342189362
O	7.629702510	0.808286369	7.279856756
O	3.511758619	3.061431766	8.644627533
O	7.570651452	1.125701907	10.079792860
O	3.508476264	2.884008644	11.349178003
Al	7.775602802	3.022604160	9.935352423
Al	3.510982556	0.974610475	11.336374037
O	4.993358577	0.729298520	7.213552637
O	0.619391966	3.070620817	8.640213345
O	4.996000660	1.133098190	10.084118948
O	0.688294771	2.840031107	11.284822145
Al	3.492116207	4.894757264	8.474502081
Al	7.760352817	7.116323498	7.220999256
O	0.765836519	7.189406589	11.288241869
O	4.844064758	4.931308524	9.930884294
O	0.776698700	6.851731505	8.474485447
O	4.913812692	5.084234859	7.274506712
Al	6.241450559	0.945281275	8.613907124
Al	6.286810343	0.833193095	11.439112984
Al	6.320185994	5.913284518	9.924309839
O	6.544671508	7.015554441	11.354436314
O	6.370540044	7.091706521	8.552816936
Al	2.075696414	7.020497884	9.909516870
Al	2.098456186	6.875427310	7.077669078
Al	2.047419114	2.052643383	8.573300168
O	2.187069707	0.954702656	7.126948815
O	2.102625193	0.876233123	9.928674722
Al	2.073354137	3.950293015	11.383265766
O	2.097386382	5.087483037	9.919645624
O	2.043809464	5.011805275	7.286763470
Al	6.227994187	3.929208139	7.194336611
O	6.260549906	2.857474275	8.655736881
O	6.300687332	2.912811739	11.276627315
H	1.917983875	1.379761261	6.297932698
H	4.109843409	1.141378970	7.279892846
H	7.337289722	1.402184799	6.543130204
H	6.276062709	7.680273273	5.357865810
H	3.578211972	6.200924536	5.335675669
H	0.621240435	7.610483486	5.215883656
H	5.881113335	2.437506409	5.413848477
H	8.283338351	4.724963331	6.332517135
O	6.322937889	6.946363830	5.989195268
O	3.507307116	7.022279227	5.851033594
O	0.627714309	6.947513218	5.919903032
O	6.606311946	2.978343410	5.765719154
Al	9.171726458	4.913214874	8.574441378
Al	13.303674048	7.052200243	7.310715637
O	11.684413319	7.259761600	11.438430662
O	16.119141512	4.908757321	9.837585847
O	11.826955470	6.931703825	8.557647459
O	16.118759538	5.061976351	7.190925519
Al	13.201830180	3.106275969	10.118864885
Al	9.073428530	1.033113180	11.339839103

O	15.977620874	0.890578625	7.432787951
O	11.930465573	3.120294962	8.735826119
O	15.949996521	1.130921431	10.170897631
O	11.909983421	2.904518531	11.435698694
Al	16.187197694	3.058150867	10.027569283
Al	11.893230037	1.025660238	11.447756148
O	13.249297376	0.792138858	7.508724476
O	9.117921217	3.063923307	8.637963832
O	13.395068513	1.186780480	10.238448284
O	9.047148510	2.897369607	11.281210521
Al	11.931808096	4.958097963	8.569557695
Al	16.155169504	7.134569361	7.295981882
O	13.246295536	4.930724181	9.999072847
O	9.178849101	6.863975053	8.480369984
O	13.321086568	5.165006456	7.355717868
Al	14.636990496	0.984788712	8.757950463
Al	14.691259443	0.889245800	11.575980561
Al	14.681138338	5.945394309	10.028126536
O	14.959223520	7.024916668	11.443098167
O	14.744452587	7.117951784	8.637342738
Al	10.507355800	7.091161555	9.960593619
Al	10.550197737	6.953479234	7.137627839
Al	10.567011436	2.019273211	8.560939364
O	10.346348388	0.875492661	7.191197445
O	10.515534657	0.884659299	10.008537927
Al	10.476652121	3.922278535	11.306215652
O	10.499562812	5.155683563	9.978937004
O	10.524191429	5.086679581	7.343734855
Al	14.582645599	3.972945072	7.342902468
O	14.654557364	2.901056161	8.791076177
O	14.725840370	2.985341185	11.379680431
H	9.365334755	0.993064806	7.073076710
H	13.373789404	1.364781855	6.727640946
H	15.713955584	1.432131443	6.658244712
H	14.645802478	7.783038892	5.467495625
H	12.095165736	6.234481859	5.480104143
H	9.078418400	6.660845355	5.104990425
H	14.362651638	3.114537228	5.119454758
H	16.603767167	4.895635556	6.355784609
O	14.729124306	7.026342753	6.066639571
O	11.984084417	7.087060125	5.935538433
O	9.116436766	7.174881461	5.922516971
O	14.646939750	2.831601521	5.999375129
Al	0.733544954	12.989711060	8.557038705
Al	4.870195109	14.988602899	7.071023874
O	3.505442997	15.252002956	11.052701907
O	7.695308719	12.981194919	9.755470698
O	3.409087718	14.866372579	8.322270649
O	7.723979287	12.994282968	7.051664293
Al	4.796941040	11.111921350	9.976836068
Al	0.723964933	9.150475562	11.447301579
O	7.640604300	8.941133649	7.373749871
O	3.504671357	11.045511945	8.564285972
O	7.624832781	9.270626995	10.162171066
O	3.520023265	10.929923410	11.271953930
Al	7.781595847	11.172879408	10.013263604
Al	3.549514687	9.065788499	11.373623193
O	4.995764792	8.858641069	7.357133759
O	0.617161976	11.175008807	8.713122396
O	5.060321832	9.188367690	10.155916540
O	0.711916038	11.045260392	11.373277249

Al	3.494951303	12.908217045	8.369621319
Al	7.701062225	15.088544378	7.137435210
O	0.794607066	15.238520716	11.129247725
O	4.826588937	12.915906702	9.767189221
O	0.776872535	14.922035140	8.382026186
O	4.899823039	13.075523554	7.122498767
Al	6.329992208	9.031072384	8.702290495
Al	6.330665081	8.955966808	11.528476108
Al	6.218153414	13.972592102	9.853457627
O	6.481365130	15.026799626	11.284617358
O	6.301711350	15.109363688	8.442941280
Al	2.162137574	15.086837069	9.809147817
Al	2.094664203	14.916696867	6.983505124
Al	1.991878791	10.091689520	8.602179030
O	2.110220643	8.950979406	7.192904444
O	2.044083607	8.951572009	10.006454104
Al	2.170430816	12.080173930	11.356175101
O	2.106242353	13.154892921	9.836394962
O	2.024753307	13.058062380	7.207017859
Al	6.204393066	11.910447119	7.186621046
O	6.282710125	10.919110486	8.701341818
O	6.305275104	11.064721991	11.291416821
H	2.398541485	9.350964596	6.357320020
H	4.179834603	9.329886959	7.608873651
H	7.398500698	9.548800879	6.633724407
H	6.348297757	14.257326426	5.255607924
H	3.515727712	14.173627062	5.261161953
H	0.570220761	15.654312868	5.077497547
H	5.719107019	10.278471389	5.653171008
H	8.283540541	12.770486039	6.279163801
O	6.317720104	15.019408580	5.851405920
O	3.493089329	15.011359471	5.753433750
O	0.618864047	15.083987275	5.855378439
O	6.464939212	10.892930082	5.768604684
Al	9.142518078	12.967195375	8.538024602
Al	13.257096629	15.073836684	7.220473346
O	11.840415865	15.264146186	11.274919694
O	16.134478858	13.068394083	9.904363050
O	11.776959904	14.919179062	8.468975503
O	16.129407077	13.078551323	7.184142493
Al	13.231888097	11.160642220	10.117224163
Al	9.081766307	9.185843538	11.388428641
O	16.118328020	8.948880536	7.521425856
O	11.964084317	11.079155752	8.706873854
O	16.025792732	9.275377073	10.254757066
O	11.927804463	10.973386062	11.423570593
Al	16.207765674	11.203666796	10.119269577
Al	11.977815236	9.100730333	11.448442353
O	13.467880407	8.936462901	7.436099940
O	9.050676703	11.139569288	8.646663842
O	13.470923158	9.212065317	10.252801777
O	9.105040397	11.046846326	11.352490371
Al	11.916846104	12.950059558	8.487193932
Al	16.137499588	15.223454014	7.236109264
O	9.127576224	15.249728863	11.198832139
O	13.236554280	12.979763367	9.918783464
O	9.123379165	14.861199387	8.394838049
O	13.323004068	13.156198187	7.275240287
Al	14.758533718	9.069074688	8.808916448
Al	14.753084941	8.932336128	11.629822097
Al	14.643335590	14.022755313	9.955883631

O	14.494006999	15.084493360	11.420807033
O	14.720152855	15.169223370	8.569088663
Al	10.521706469	15.096942130	9.870254216
Al	10.496345597	14.971376630	7.056389229
Al	10.469806722	10.119405958	8.646431751
O	10.530105674	8.961906690	7.268017990
O	10.511263353	9.025933720	10.075558725
Al	10.540857963	12.080585283	11.366403218
O	10.507895693	13.167103240	9.912199808
O	10.506625824	13.069366669	7.284127254
Al	14.621817458	11.983803230	7.313864323
O	14.715129666	10.980708143	8.818504722
O	14.720290395	11.124242477	11.419867902
H	9.949532533	9.250524417	6.543148859
H	12.654685352	9.457094890	7.567690590
H	15.958763042	9.610424449	6.810481836
H	14.725438433	14.452059448	5.346900448
H	11.956754766	14.230099990	5.392125351
H	9.048697317	15.584747295	5.114945828
H	14.240365009	10.319128698	5.792044925
H	16.663874510	12.828240778	6.399648967
O	14.719733110	15.166647623	6.000175533
O	11.919959857	15.083741606	5.857344300
O	9.052295593	14.940705662	5.838449667
O	14.952273723	10.971071237	5.918729900
O	7.718638202	9.115950434	12.722663952
H	7.901582237	8.357392336	13.313342476
H	14.654136302	11.742909715	12.163823139
O	13.326483273	9.025912057	12.795437822
O	10.507404779	9.034966908	12.711010591
O	-0.625997649	9.030616267	12.794570642
H	-0.587443891	9.779786910	13.406830105
O	2.415739665	13.234526631	12.649939460
O	10.586959663	13.313388542	12.651251978
H	7.487576818	14.962292063	11.322180721
H	13.498250268	15.002457121	11.541594203
H	3.346156968	14.593849936	11.774669540
H	11.531198585	14.711785421	12.036259491
O	1.873689336	5.002793444	12.791956073
H	7.549905520	6.946587394	11.476438745
H	4.139190240	6.552413030	11.085830114
H	15.967765748	6.952014845	11.499635731
O	7.701544598	0.967115495	12.638881866
H	7.781212219	0.313575848	13.346862017
O	-0.697661291	0.887213571	12.713337000
H	-0.619840660	0.109501473	13.286243983
H	6.339171089	3.455294921	12.080101361
O	4.901637498	0.817104485	12.641091878
O	2.097968021	0.882083076	12.563591010
H	14.815456291	3.594366317	12.130665531
O	13.258649594	0.892938501	12.787721505
O	10.439280754	0.963097843	12.642112276
O	2.171719263	9.114562072	12.641144517
O	4.911524653	8.946909347	12.705435164
H	2.171419821	8.324479287	13.202910457
H	4.856836126	9.677817184	13.338474186
H	13.175647902	8.220221922	13.329632038
H	10.467283652	9.639199204	13.467946057
H	13.244997756	1.631741741	13.413693913
H	10.380072059	1.711966488	13.254657491
H	2.093002830	1.623440927	13.189071863

H	4.807801924	-0.010004830	13.137596620
H	9.450645892	14.747185058	11.981874536
H	10.674127967	13.054115794	13.578415181
H	1.715855163	13.910159612	12.692680725
H	0.063840485	14.624924453	10.933103576
H	1.070720029	6.576930669	12.008113811
H	2.696222176	5.435680351	13.069227218
H	6.297270146	11.685163371	12.037559486
W	10.404477292	6.706748833	12.904306959
O	10.363234409	4.925854921	12.805254785
O	9.196956262	7.266530885	11.374976748
H	11.831186879	7.048427844	13.839557691
C	9.442894019	7.153054013	14.539435228
C	8.606410448	6.002893195	15.109466196
H	7.571773244	6.353109107	15.277533253
H	8.546687177	5.118736714	14.465638483
H	9.002898071	5.689136777	16.091252317
C	9.454417729	8.327307683	15.486057130
H	8.482516686	8.851127006	15.514474381
H	9.649815283	7.981297153	16.516057749
H	10.230822967	9.070776190	15.258730051

Species 2b. E: -2322.4678374438

Al	0.725345204	4.903344753	8.589584697
Al	4.875521067	6.972816360	7.212539886
O	3.415556612	7.191469986	11.207271086
O	7.711415237	4.853551635	9.762766713
O	3.405306818	6.845754798	8.454427208
O	7.782568128	5.007300863	7.123872696
Al	4.786136167	3.070263631	10.032238977
Al	0.663029208	0.965981162	11.342416400
O	7.629704195	0.808396862	7.279810680
O	3.512004248	3.061486294	8.644729656
O	7.571760136	1.126117837	10.080131138
O	3.508445633	2.883710213	11.349056660
Al	7.775716205	3.023002623	9.935639426
Al	3.511038098	0.974424500	11.336409838
O	4.993423793	0.729373812	7.213543624
O	0.619620336	3.070690001	8.640347037
O	4.996492091	1.133095683	10.084075927
O	0.688195635	2.839959517	11.284880159
Al	3.492358227	4.894862510	8.474752577
Al	7.759937126	7.115799800	7.221224355
O	0.765799017	7.189458149	11.288146437
O	4.844369999	4.931099298	9.930793798
O	0.776812598	6.851845178	8.474588497
O	4.914025974	5.084289290	7.274715901
Al	6.241580119	0.945621072	8.613687918
Al	6.286984251	0.833412630	11.439235567
Al	6.320216922	5.913611919	9.924757418
O	6.543653752	7.015662753	11.354460284
O	6.370610746	7.091645708	8.552935743
Al	2.076627829	7.020377865	9.909961566
Al	2.098443194	6.875467097	7.077594653
Al	2.047767470	2.052562572	8.573338814
O	2.187201066	0.954848588	7.126892990
O	2.102493346	0.876317748	9.928865827
Al	2.073428779	3.950175483	11.383476777
O	2.097433627	5.087377238	9.919745782
O	2.044025126	5.011907951	7.286929733
Al	6.228360591	3.929351175	7.194327213

O	6.262411815	2.858061033	8.656012260
O	6.300936032	2.912791652	11.276761966
H	1.911759025	1.378791650	6.299384852
H	4.110171333	1.142222603	7.278245226
H	7.336882085	1.401956174	6.542944126
H	6.275887933	7.680941348	5.358571562
H	3.578267519	6.200664699	5.335773204
H	0.620745522	7.608755791	5.214439117
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H	8.284004027	4.725089214	6.333511969
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O	3.507310319	7.022058922	5.851063683
O	0.627594473	6.947288752	5.919829594
O	6.606581713	2.978714042	5.765553356
Al	9.171991750	4.912957031	8.577955621
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O	11.683090667	7.260656410	11.435553673
O	16.119288800	4.908614495	9.837631912
O	11.826735571	6.931321170	8.557905254
O	16.118838567	5.062061851	7.190888434
Al	13.201184330	3.107258359	10.119431210
Al	9.073218279	1.033224669	11.340096825
O	15.977550436	0.890792577	7.432715338
O	11.931090507	3.120983965	8.736173963
O	15.949488491	1.130899480	10.170924893
O	11.908396919	2.906800657	11.437398670
Al	16.187206696	3.058044338	10.027441452
Al	11.892892936	1.025971690	11.448413642
O	13.249324297	0.792188744	7.508873400
O	9.117645015	3.064292992	8.638338495
O	13.394353907	1.189155510	10.239123682
O	9.047707201	2.899224425	11.283116577
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O	13.246796189	4.931350766	9.999447187
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O	13.321109705	5.165150434	7.356086350
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Al	14.682190000	5.945654890	10.027900436
O	14.959156074	7.025012065	11.443099537
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Al	10.550176289	6.953095778	7.137739497
Al	10.567045293	2.020572386	8.562449372
O	10.346785807	0.876155477	7.192040372
O	10.515597257	0.885113525	10.009386680
Al	10.473917898	3.927163340	11.329103912
O	10.500459552	5.155909040	9.991555103
O	10.524208058	5.086284744	7.347779941
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O	9.127662485	15.249790860	11.198957023
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H	6.340620816	3.454717705	12.080669707
O	4.901732619	0.817062662	12.641003834
O	2.097973575	0.882001791	12.563592007
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O	10.439139566	0.962750133	12.642224066
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O	9.202947687	7.265078103	11.371817020
H	11.835641302	7.035666490	13.825285192
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Species 2c. E: -2315.5821943830

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O	7.782636707	5.007241934	7.123820240
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Al	0.663133626	0.965913373	11.342307937
O	7.629752173	0.808346148	7.279957879
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O	0.776704220	6.851737105	8.474504130
O	4.913947441	5.084219076	7.274498918
Al	6.241898919	0.945995946	8.613823188
Al	6.287147216	0.833360045	11.439304990
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Al	2.047570248	2.052675147	8.573297769
O	2.187125057	0.954741189	7.126946956
O	2.102692297	0.876247405	9.928658967
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O	2.097474119	5.087469789	9.919651653
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Al	10.481078224	3.926788816	11.328267324
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Al	4.797270238	11.112152405	9.977030780
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O	10.508872547	9.035063444	12.715601085
O	-0.625959287	9.030464352	12.794482196
H	-0.586574490	9.777920221	13.408768731
O	2.415860990	13.234331349	12.649747244
O	10.586997094	13.313641487	12.652242599
H	7.487206431	14.962193575	11.322607692
H	13.498156152	15.002546087	11.541770753
H	3.346391651	14.593727466	11.774437929
H	11.532040883	14.713301573	12.039063400
O	1.873397904	5.002654395	12.791997072
H	7.540772515	6.938118401	11.494856103
H	4.138961530	6.551244077	11.092501816
H	15.967730717	6.951772474	11.500839431
O	7.701543655	0.967004578	12.638655764
H	7.780213714	0.317459168	13.350338412
O	-0.697660387	0.887333312	12.713326095
H	-0.619539732	0.110718545	13.287660691
H	6.341740951	3.454354650	12.080894544
O	4.901585416	0.817100453	12.640978665
O	2.097981046	0.882014437	12.563628555
H	14.818164539	3.593657230	12.132155559
O	13.258468062	0.893002193	12.788013792
O	10.439205806	0.962881255	12.642482217
O	2.171420562	9.114438802	12.641478827
O	4.911179960	8.946635458	12.704732572
H	2.171272837	8.325638974	13.205082606
H	4.857394394	9.669126458	13.347192325
H	13.181048738	8.223079374	13.333375326
H	10.492948037	9.616054895	13.491190714
H	13.245761060	1.629099615	13.417155357

H	10.378367937	1.705191159	13.262677310
H	2.093448283	1.622655456	13.189971991
H	4.807918039	-0.009077870	13.139042178
H	9.449480925	14.747467479	11.983289248
H	10.672608684	13.054886729	13.579698042
H	1.715842816	13.909773164	12.692732247
H	0.063904238	14.624696596	10.933478515
H	1.072342975	6.577740642	12.008598902
H	2.696286060	5.428529095	13.078580096
H	6.297132533	11.683554707	12.038593977
W	10.408281442	6.701902596	12.894462584
O	10.365090064	4.920972423	12.865676793
O	9.204861286	7.264304223	11.375951236
H	11.848733712	7.036348177	13.804591534
C	9.409799674	7.183110375	14.469570722
H	9.265049369	8.087884192	15.068090756
H	9.025794212	6.285160788	14.982484391

Ethylene. E: -13.725461527

C	8.119919958	7.976080242	7.330289458
C	7.881740831	8.033158755	8.642070039
H	7.961941353	8.969111722	9.197390154
H	7.594792441	7.148942418	9.213685910
H	8.406514777	8.862425204	6.761682873
H	8.040708718	7.042362270	6.771094321

Propylene. E: -20.615162586

C	7.872470114	8.518174448	7.957301831
C	7.634610389	8.584833720	9.271305362
H	7.717458884	9.523128317	9.820429489
H	7.347971615	7.699360273	9.843817677
C	7.783379026	7.275601541	7.125165329
H	8.747863577	7.053046054	6.641570881
H	7.492460505	6.404526203	7.727870052
H	7.048577011	7.393839772	6.313130897
H	8.156787259	9.433773833	7.427186824

1-butene. E: -27.4985808853

C	7.399015989	8.823762523	8.010904346
C	7.069445344	8.947993532	9.301236484
H	7.130108426	9.906507164	9.818356381
H	6.724953302	8.091412638	9.886886163
C	7.355754917	7.547727638	7.220679697
H	6.924744713	6.744864336	7.838870783
H	6.676422834	7.682986763	6.360967405
H	7.746584060	9.710558136	7.466438132
C	8.737055119	7.124988107	6.695863865
H	9.426126452	6.918998808	7.527205599
H	8.664958830	6.217879650	6.078707647
H	9.187378648	7.915481601	6.078120329

Trans-2butene. E: -27.503743849

C	8.150064364	7.949377570	7.358662271
C	7.848009144	8.053760203	8.659015687
H	7.495074803	7.158698882	9.185086215
C	8.048493493	6.694209311	6.545909106
H	9.025295671	6.411808978	6.121762591
H	7.684096419	5.851390163	7.149380588
H	7.364097148	6.823105592	5.692364871
H	8.502916128	8.844027779	6.831627774
C	7.951571373	9.307074939	9.474300616

H	6.978545854	9.582106942	9.911405931
H	8.646929278	9.178649161	10.319090474
H	8.304360751	10.154188436	8.870021932

Isobutene. E: -27.504923553

C	7.700306536	7.999161719	7.922018702
C	7.431305709	7.999336086	9.235357852
H	7.319164906	8.930136828	9.793859043
H	7.316518273	7.068669614	9.793564483
C	7.862565070	9.272378169	7.135631989
H	8.855670172	9.315273719	6.660317452
H	7.125377937	9.324491555	6.318075708
H	7.743024668	10.162846152	7.765478021
C	7.861011301	6.725726432	7.135683983
H	8.860072145	6.674852943	6.673604239
H	7.725659237	5.835379743	7.762600768
H	7.134418477	6.681144240	6.308234005

Isoamylene. E: -34.3839604574

C	7.985245518	8.848459167	8.510796228
C	7.563519232	9.094641022	9.754964797
H	7.748355479	10.050833421	10.245323566
H	7.015653741	8.342597912	10.327640062
C	7.776881296	7.564915081	7.753961129
H	7.236488290	6.864528502	8.413562268
H	8.532757158	9.629306984	7.968272467
C	9.127747698	6.933400215	7.376506263
H	9.732182864	6.721955568	8.268980490
H	8.980020175	5.991759583	6.828051306
H	9.706842358	7.609479106	6.729328801
C	6.920395428	7.808746677	6.499459298
H	7.417069085	8.517633427	5.819317998
H	6.761317167	6.871435293	5.946575065
H	5.938712708	8.225184930	6.762510481

4me-2pentene. E: -41.272710182

C	8.150729475	8.267008470	8.001871183
C	7.786559081	8.523729483	9.264193270
H	7.289105148	7.729323977	9.833923429
C	7.938738020	6.966460394	7.274686191
H	7.432871373	6.268661108	7.964139450
H	8.649548191	9.056888887	7.423513588
C	9.285077172	6.346563291	6.861713084
H	9.923085920	6.161279086	7.736544518
H	9.134545408	5.392833311	6.334702043
H	9.831396417	7.020133345	6.183413616
C	7.036586391	7.169954687	6.045004546
H	7.496779283	7.877448805	5.338024918
H	6.877809870	6.221156698	5.511533814
H	6.056101586	7.572960239	6.332951697
C	7.999968139	9.822421151	9.981780633
H	7.043993707	10.256690957	10.315046175
H	8.611136990	9.683347510	10.887579718
H	8.503477907	10.559523547	9.341329257

5me-3esene. E: -48.156345160

C	8.269623169	7.919169212	7.618627344
C	7.958233350	8.144186265	8.901014263
H	7.507006488	7.328516439	9.481234297
C	8.066964039	6.623414059	6.880313333
H	7.609602457	5.901469515	7.578778949

H	8.715542039	8.734011664	7.031656500
C	9.413011227	6.049262760	6.405217947
H	10.090506242	5.871353690	7.251438834
H	9.268626679	5.098337517	5.871423291
H	9.912088257	6.747192341	5.715295063
C	7.110531700	6.817864398	5.690995867
H	7.520084213	7.550456158	4.978407591
H	6.959256591	5.873147441	5.148273182
H	6.130575820	7.185578164	6.024650822
C	8.148512441	9.441854778	9.631200200
H	8.826793744	9.282172468	10.487583353
H	8.646921456	10.167847596	8.969732613
C	6.826269277	10.026638307	10.152365349
H	6.142124125	10.248764693	9.321436892
H	6.316637328	9.317894632	10.821565971
H	6.995428045	10.955613141	10.714983344

2,4me-2pentene. E: -48.1600820136

C	8.073303530	8.195532645	7.766283239
C	7.545931201	8.474948649	8.971837989
C	8.085041985	6.888945463	7.019274948
H	7.559810375	6.122267564	7.610041825
H	8.568796188	9.018087849	7.233611301
C	9.530339044	6.407746115	6.798977577
H	10.049400758	6.257469539	7.755509206
H	9.550312581	5.459652637	6.241195379
H	10.102442573	7.149005616	6.219765433
C	7.351624967	7.033942531	5.674168973
H	7.836340777	7.798926934	5.048142277
H	7.362468918	6.087239714	5.113930404
H	6.305770886	7.336116974	5.822287457
C	7.637386937	9.862260933	9.554809208
H	6.634264943	10.273989276	9.753855410
H	8.165181630	9.850338486	10.522581398
H	8.164745835	10.554136060	8.885262840
C	6.833367035	7.479191077	9.848910551
H	5.807109280	7.817996087	10.064655100
H	6.773537021	6.476914142	9.409411217
H	7.340625774	7.391610835	10.823473508

2pentene. E: -34.387302291

C	7.753903188	8.249081226	7.418429543
C	7.229014074	8.518356061	8.620629406
C	7.751514702	6.906086965	6.748001278
H	7.180773223	6.189562155	7.359622627
H	8.246643728	9.061067729	6.867778276
C	9.167883039	6.366724479	6.493083971
H	9.706507556	6.218473840	7.439531749
H	9.138171845	5.405269935	5.961159560
H	9.755398672	7.068793642	5.883446590
C	7.242896451	9.858913517	9.290757804
H	6.220395268	10.215986263	9.492632940
H	7.755079259	9.814529794	10.265148626
H	7.750370843	10.613143608	8.673372322
H	6.743647276	7.703272828	9.171280935
H	7.222610786	6.982523351	5.781706758

2me-2butene. E: -34.391109077

C	8.027556011	7.944479897	7.333665245
C	7.820488929	7.898834433	8.662421482

H	7.681216653	8.857411840	9.174816018
C	8.237488136	6.738472125	6.456850839
H	9.203207736	6.806683007	5.930197345
H	8.220357743	5.790991786	7.006989116
H	7.462513597	6.689673265	5.674359557
C	8.063861401	9.261230857	6.600650504
H	9.030648697	9.403255296	6.090217075
H	7.290901965	9.298562736	5.815440334
H	7.905971115	10.111621726	7.276841512
C	7.751940194	6.692457309	9.550284554
H	6.772829182	6.627848025	10.051752998
H	7.911304020	5.750298229	9.011583639
H	8.506470792	6.750181323	10.351000527

3esene. E: -41.2709007388

C	7.933999202	7.846738250	7.290008452
C	7.997565635	8.053993554	8.611574995
C	8.012994906	6.509515812	6.612746073
H	8.055653383	5.713387131	7.372659305
H	7.837214181	8.716602642	6.627341589
C	9.218691345	6.396845433	5.666355151
H	10.161333918	6.512651405	6.219158437
H	9.236873422	5.422704113	5.157505388
H	9.189432893	7.178406429	4.892974503
C	7.922407950	9.391330368	9.288964244
H	8.847691059	9.559057511	9.867501171
H	7.881154314	10.187537207	8.529093096
H	8.092323521	7.183589864	9.274403098
C	6.719579008	9.508231031	10.238355417
H	5.774683409	9.398730101	9.687906440
H	6.746818456	8.724528157	11.009661669
H	6.708024137	10.481134562	10.749756077
H	7.089549497	6.338896766	6.032251289

2me-2pentene. E: -41.2746891556

C	8.525210454	7.839399818	7.909278997
C	8.228163720	7.966230977	9.215691611
C	8.405812355	6.622725507	7.037622942
H	8.157871452	5.731924545	7.632099660
H	8.881140531	8.738195370	7.390765477
H	9.386917818	6.416843448	6.575507797
C	7.713557447	6.852787958	10.089499220
H	6.746303268	7.131314103	10.538413630
H	7.576323367	5.906947624	9.553114924
H	8.402535128	6.669277521	10.930053611
C	8.397604260	9.285483881	9.924769824
H	7.441367399	9.630390725	10.351456107
H	9.098607724	9.192721196	10.770556120
H	8.774481703	10.066986206	9.252236610
C	7.363569096	6.802689294	5.921230666
H	7.596290538	7.680649618	5.301038800
H	7.329504679	5.924449753	5.260832499
H	6.360502187	6.953727314	6.344152801

METALLACYCLOBUTANE

1-butene (1,2) insertion (side path) into species 1. E: -2356.8792225847

Al	0.723374900	4.903794537	8.589812169
Al	4.869801373	6.974143448	7.185940987
O	3.415714680	7.190956364	11.204474903

O	7.705114868	4.850506205	9.755115575
O	3.395677456	6.844989917	8.433329456
O	7.769016903	5.004776894	7.113601890
Al	4.782969183	3.069915622	10.030483402
Al	0.664465473	0.967763669	11.340258740
O	7.629586673	0.807693944	7.279951301
O	3.510388190	3.061394192	8.643397901
O	7.569559386	1.125267894	10.079712112
O	3.507845762	2.883055688	11.348883860
Al	7.769613479	3.022109869	9.932993685
Al	3.511052542	0.972952578	11.335333322
O	4.992660430	0.728304911	7.213007662
O	0.618682106	3.070841715	8.640498726
O	4.994989253	1.132382441	10.084594899
O	0.688538780	2.841121184	11.285042220
Al	3.489831128	4.895507545	8.468822230
Al	7.734608579	7.118900626	7.190517781
O	0.765853039	7.189590152	11.287112872
O	4.839581774	4.929694984	9.925741516
O	0.773611974	6.851249123	8.472969490
O	4.911571472	5.082638805	7.268697355
Al	6.239374408	0.941437609	8.614513671
Al	6.286011998	0.833821744	11.439641415
Al	6.312777192	5.913127066	9.889285161
O	6.552124593	7.026343523	11.293822136
O	6.325638488	7.085919408	8.502866470
Al	2.076632070	7.019812192	9.905438943
Al	2.093194116	6.872476595	7.072067609
Al	2.046553975	2.052481635	8.571323662
O	2.187252067	0.956063272	7.124961852
O	2.101880032	0.875499367	9.927128671
Al	2.074263878	3.951393242	11.382667164
O	2.096945877	5.088090536	9.918523646
O	2.038314635	5.008916630	7.284201812
Al	6.216224077	3.920546604	7.190942747
O	6.253308147	2.849724757	8.652113011
O	6.299687921	2.912870610	11.275435043
H	1.910271411	1.380561832	6.298230207
H	4.108616733	1.139937775	7.277537102
H	7.335692621	1.400649000	6.543207616
H	6.269101621	7.685252530	5.307732718
H	3.573423186	6.205852487	5.318402419
H	0.612072763	7.598534211	5.204937635
H	5.884930927	2.433791980	5.403541237
H	8.258362365	4.724693755	6.314301791
O	6.316882998	6.944903076	5.931396166
O	3.503528464	7.021042259	5.843361342
O	0.624614553	6.947144376	5.919348871
O	6.605174262	2.975885624	5.763377760
Al	9.149704885	4.907694715	8.540331012
Al	13.278172390	7.029178122	7.294266587
O	11.676832620	7.254482262	11.369995254
O	16.116961591	4.909022155	9.837623349
O	11.774670593	6.923572238	8.550496832
O	16.116491971	5.060672384	7.190630071
Al	13.203601022	3.108349463	10.113959368
Al	9.072226092	1.031386274	11.340555278
O	15.977755592	0.892159592	7.429535484
O	11.922781360	3.126324834	8.733930021
O	15.952182447	1.132012583	10.168547500
O	11.910001989	2.903579896	11.430258053

Al	16.187614624	3.058961009	10.027917681
Al	11.894977729	1.025478512	11.447429147
O	13.248147317	0.794336456	7.507667042
O	9.115928996	3.060450493	8.635819005
O	13.394771780	1.191088042	10.235553722
O	9.043397713	2.896469908	11.279710099
Al	11.908201396	4.962725931	8.556927273
Al	16.146761848	7.131525708	7.297274019
O	13.239111527	4.931647126	9.997627882
O	9.124616268	6.861473001	8.475258708
O	13.316238342	5.161108465	7.356791321
Al	14.638842581	0.983542206	8.755243812
Al	14.692445191	0.887129402	11.568479213
Al	14.675732890	5.944640032	10.027522372
O	14.958338837	7.024523581	11.442793488
O	14.733563705	7.112088302	8.635493121
Al	10.454159369	7.088349466	9.961157146
Al	10.519876261	6.949016127	7.136770128
Al	10.565102387	2.015212030	8.555088707
O	10.344148573	0.873017541	7.188377896
O	10.515315032	0.885218585	10.007302529
Al	10.474788634	3.905016384	11.239379584
O	10.452414081	5.151400583	9.931196662
O	10.508815824	5.082388821	7.299560935
Al	14.582179677	3.972545656	7.343136488
O	14.653612269	2.901388218	8.790128868
O	14.725881926	2.985909708	11.377668114
H	9.362522617	0.989967082	7.071236880
H	13.374358281	1.365953801	6.726010740
H	15.716742921	1.439298220	6.657938414
H	14.639028550	7.777877156	5.464161234
H	12.022830683	6.148432824	5.516099472
H	9.088100227	6.669368143	5.095211759
H	14.368014098	3.116235590	5.117800464
H	16.603874615	4.893693241	6.356961854
O	14.723531919	7.023059187	6.065230465
O	11.935710013	7.025777917	5.927633125
O	9.108600644	7.176778256	5.917334543
O	14.646553588	2.832138469	5.999178608
Al	0.732698184	12.981258586	8.529074280
Al	4.870128830	14.988250016	7.071398833
O	3.503862165	15.251349525	11.050678909
O	7.694449624	12.980635633	9.755614157
O	3.406735532	14.866194975	8.320009350
O	7.723216702	12.994796240	7.051249763
Al	4.794990729	11.114918785	9.975320475
Al	0.722704009	9.151052711	11.443519025
O	7.636182137	8.942241402	7.367893735
O	3.504566668	11.046877136	8.564080830
O	7.625855375	9.270109773	10.158532543
O	3.518601803	10.933755711	11.271535767
Al	7.782495077	11.170251447	10.014260119
Al	3.548308600	9.066733448	11.372239569
O	4.991373559	8.861946145	7.348212915
O	0.618346118	11.160063068	8.701596800
O	5.056967387	9.190323854	10.151314961
O	0.707120721	11.047964782	11.366649227
Al	3.495071169	12.908373718	8.369017649
Al	7.700478487	15.087866960	7.137507724
O	0.792329170	15.238584942	11.124548217
O	4.825085761	12.917809394	9.766606881

O	0.776602937	14.919721154	8.345394645
O	4.899700351	13.076435858	7.122032302
Al	6.319253847	9.032544558	8.692787918
Al	6.328976557	8.971270951	11.511319786
Al	6.217848837	13.971458045	9.855011507
O	6.480873487	15.027158719	11.284936676
O	6.301341044	15.108794271	8.444227683
Al	2.160912498	15.084423540	9.802722113
Al	2.095274133	14.914850732	6.973775537
Al	1.998775031	10.087114654	8.601051815
O	2.110135106	8.950556085	7.191355844
O	2.046971886	8.950878903	10.006191418
Al	2.167355505	12.082235241	11.351856814
O	2.102149467	13.155315696	9.830716551
O	2.029470225	13.053709640	7.201273257
Al	6.203452883	11.911195016	7.185797841
O	6.274428236	10.919932516	8.698449624
O	6.301977937	11.068469535	11.284562322
H	2.339895376	9.361465880	6.343232764
H	4.169305087	9.333453042	7.576974798
H	7.393113222	9.555656753	6.632026086
H	6.348825161	14.256988815	5.256426154
H	3.521666754	14.173323639	5.258638148
H	0.579639193	15.636448571	5.049855963
H	5.720120336	10.275567340	5.658503124
H	8.283527150	12.770594276	6.279426791
O	6.317667059	15.019718552	5.851382782
O	3.494849045	15.010840248	5.751127664
O	0.621033773	15.086736942	5.842780285
O	6.464662904	10.893105036	5.768118524
Al	9.139936728	12.967587259	8.538415556
Al	13.256353284	15.075685758	7.218163730
O	11.841068854	15.264597914	11.273550981
O	16.131062352	13.063243002	9.840038971
O	11.776672383	14.919517113	8.467779375
O	16.129689225	13.075463056	7.127597062
Al	13.223505563	11.157785402	10.102485342
Al	9.080029182	9.179108608	11.411869042
O	16.104553556	8.945897300	7.518842634
O	11.937709747	11.082373854	8.710409185
O	16.024400836	9.272211207	10.248229922
O	11.927487400	10.969290139	11.421507876
Al	16.209177343	11.195375584	10.095668623
Al	11.973537447	9.093002393	11.426281014
O	13.417029057	8.886693875	7.435761929
O	9.043478140	11.140892180	8.644192437
O	13.468597237	9.210448191	10.244563316
O	9.108029352	11.046320402	11.352037746
Al	11.911661622	12.949743615	8.485152291
Al	16.137812740	15.226517427	7.217245440
O	9.127948437	15.249905636	11.198951061
O	13.231864565	12.976689346	9.914917186
O	9.122824336	14.861667094	8.394631083
O	13.323193688	13.155772222	7.275445985
Al	14.735282195	9.058990273	8.795922303
Al	14.755744677	8.933660864	11.617107328
Al	14.642009509	14.012181995	9.923045039
O	14.492017060	15.087806926	11.364949699
O	14.720852760	15.170930366	8.558173880
Al	10.520618727	15.096693531	9.869528090
Al	10.495226507	14.970132507	7.055245697

Al	10.453510316	10.115379758	8.648903446
O	10.525015892	8.960976182	7.266576274
O	10.494891246	9.025222816	10.077113082
Al	10.541409763	12.079996940	11.363499881
O	10.506197215	13.169715473	9.911665639
O	10.504527524	13.070185078	7.282992891
Al	14.625272604	11.985828002	7.302057405
O	14.707965076	10.973793079	8.802112300
O	14.720664929	11.130428156	11.373887613
H	9.946913077	9.254108890	6.541222945
H	12.597932234	9.402952877	7.536675491
H	15.946089921	9.605923668	6.806058652
H	14.720642478	14.456692358	5.338939641
H	11.956302739	14.230479753	5.390320288
H	9.047331747	15.584746528	5.114717251
H	14.227840549	10.328858041	5.763620335
H	16.658350022	12.827472505	6.340380063
O	14.716833886	15.168085458	5.995410920
O	11.919462988	15.083785478	5.856061021
O	9.051447992	14.940370127	5.837906489
O	14.948347364	10.965309995	5.913584065
O	7.702369167	9.195809987	12.713033532
H	7.779824521	8.487582411	13.374052389
H	14.657560728	11.746515237	12.120570633
O	13.328075119	9.028625136	12.783487783
O	10.515615840	9.025771415	12.738354330
O	-0.627858199	9.031985125	12.791911200
H	-0.588192087	9.782645100	13.402426658
O	2.414863868	13.234286999	12.648349703
O	10.588015123	13.313288286	12.649470670
H	7.486718730	14.962096077	11.323339459
H	13.495827993	15.003019070	11.493384652
H	3.345343205	14.592354283	11.772027988
H	11.536312329	14.711294329	12.035944992
O	1.873471185	5.002888581	12.791862512
H	7.557712861	6.951308033	11.446589099
H	4.144294407	6.556843217	11.090296224
H	15.967274446	6.950743897	11.498018020
O	7.701471968	0.967246719	12.638752973
H	7.780945079	0.315824462	13.348641090
O	-0.698612510	0.886150252	12.710822568
H	-0.617660436	0.113714675	13.290218876
H	6.341003166	3.460746704	12.075180416
O	4.901139407	0.816646064	12.641201041
O	2.097600556	0.881567056	12.563024294
H	14.818016813	3.590805161	12.131618613
O	13.262792736	0.890779825	12.783097346
O	10.440158323	0.964362893	12.641611933
O	2.170702089	9.115400078	12.640062861
O	4.913987910	8.943780162	12.698222810
H	2.169319634	8.324774257	13.201077887
H	4.861673116	9.669416872	13.337607482
H	13.192419896	8.208944137	13.303192205
H	10.542772434	9.658517251	13.473153815
H	13.252194400	1.615358747	13.425851106
H	10.386246625	1.715943976	13.251759239
H	2.093982085	1.623745908	13.187582583
H	4.807814453	-0.010418789	13.137904901
H	9.451863817	14.745655050	11.980742256
H	10.668861253	13.055280531	13.577474156
H	1.715261809	13.909921344	12.693441847

H	0.051218210	14.641350078	10.921885789
H	1.073194128	6.578592451	12.007091498
H	2.696361486	5.429507012	13.077419655
H	6.301143257	11.676035654	12.040889202
W	10.524306112	6.671963200	12.934869606
O	10.449216077	4.926161132	12.728848736
O	9.202209425	7.264502494	11.440924193
H	12.082453801	7.005908185	13.530728003
C	8.748128784	6.907151714	14.207821926
H	8.635522370	7.918967897	14.636950751
C	10.767127504	6.542611974	15.143550601
C	9.322111880	6.056119970	15.345935069
C	11.971648356	5.783050450	15.746771471
H	12.877577794	6.251714373	15.324119071
C	12.029391009	4.291217631	15.387164120
H	12.120810229	4.134703206	14.304461677
H	12.890405611	3.815994644	15.880372537
H	11.123937472	3.765799878	15.728399109
C	12.051635904	5.958424441	17.275003731
H	13.004212442	5.564267337	17.660254135
H	11.983480522	7.018093743	17.560598800
H	11.241293538	5.421149426	17.786842353
H	7.803988551	6.569889260	13.752135437
H	10.814296210	7.584660202	15.514625626
H	9.248825562	4.989819228	15.071938307
C	8.650659063	6.251618738	16.716232877
H	9.155057189	5.627132181	17.469686171
H	8.802487718	7.299165789	17.030503506
C	7.155641977	5.921498922	16.697597385
H	6.985797696	4.877865368	16.391957929
H	6.612976727	6.563136667	15.988663484
H	6.699066717	6.057451681	17.688118381

1-butene (2,1) insertion (side path) into species 1. E: -2356.8789930070

Al	0.723681081	4.903185064	8.589808156
Al	4.871245095	6.974045321	7.184297860
O	3.415651379	7.192603702	11.204194464
O	7.699416716	4.857340401	9.761018498
O	3.397220196	6.845288336	8.432919722
O	7.775231359	5.005858285	7.117825354
Al	4.786187942	3.072783324	10.032176728
Al	0.664080956	0.966761027	11.342332411
O	7.629662995	0.808358461	7.279908959
O	3.511313799	3.062150242	8.644344724
O	7.573343592	1.127486888	10.080890789
O	3.508989996	2.884963745	11.349655892
Al	7.771410790	3.025385004	9.938381616
Al	3.511961399	0.974919818	11.336375024
O	4.993080293	0.729355547	7.213296644
O	0.618569612	3.070487945	8.640443914
O	4.995974857	1.133419337	10.084294894
O	0.688829088	2.840955001	11.284727492
Al	3.491204535	4.896162667	8.468763483
Al	7.738385775	7.117052455	7.193102079
O	0.766552526	7.189341821	11.287678734
O	4.841950553	4.933549871	9.928057711
O	0.774113036	6.850974057	8.473377884
O	4.912555480	5.082808093	7.268614965
Al	6.240561190	0.944941579	8.614524764
Al	6.286934258	0.839252658	11.440329053
Al	6.308655912	5.929088003	9.894833075

O	6.544418870	7.083717640	11.279953304
O	6.325745838	7.087401396	8.500294044
Al	2.077464044	7.020080456	9.905613584
Al	2.094469873	6.872563354	7.072491046
Al	2.047407501	2.053300899	8.573391294
O	2.186868062	0.954964451	7.126893914
O	2.102688028	0.876629758	9.928677551
Al	2.074677186	3.951719619	11.383460635
O	2.097053656	5.088262288	9.918776448
O	2.038849549	5.009107169	7.284459513
Al	6.221637634	3.924416356	7.191889179
O	6.256598715	2.855252442	8.654254044
O	6.300999917	2.912143025	11.275608248
H	1.921416110	1.381158837	6.297280261
H	4.109674563	1.141488464	7.280640656
H	7.336600484	1.402151993	6.543339336
H	6.271714472	7.686039960	5.308425072
H	3.572866048	6.206260573	5.317674646
H	0.614380826	7.600411190	5.206309693
H	5.884462941	2.435508778	5.407129761
H	8.272830766	4.718955113	6.326502265
O	6.318797910	6.944929412	5.931282117
O	3.503726129	7.021170649	5.843171298
O	0.625660890	6.947147178	5.919056699
O	6.606700926	2.976759629	5.764266773
Al	9.152696895	4.913549728	8.567982445
Al	13.292086681	7.052058141	7.310930795
O	11.668013781	7.257455785	11.369753521
O	16.116762218	4.908404809	9.837685806
O	11.782660144	6.930968950	8.554962595
O	16.116387376	5.060291991	7.191333044
Al	13.204614561	3.097166398	10.111943768
Al	9.073928944	1.032942559	11.340992422
O	15.977536166	0.890076371	7.433066618
O	11.925127857	3.124682047	8.737438172
O	15.951374060	1.130470124	10.170898739
O	11.917302689	2.893152981	11.428062424
Al	16.188149585	3.057496426	10.028399626
Al	11.895874726	1.016486067	11.446594915
O	13.249334164	0.792063286	7.508156093
O	9.114287048	3.063926095	8.639007752
O	13.396169906	1.150192065	10.235878476
O	9.053567954	2.902179679	11.284804549
Al	11.920184783	4.964720199	8.572437089
Al	16.151177383	7.132711680	7.296613749
O	13.241023526	4.929050673	9.999096964
O	9.127440091	6.862732582	8.480427234
O	13.316646484	5.166536658	7.358200420
Al	14.637901240	0.978061268	8.758739217
Al	14.692559628	0.880247373	11.575262613
Al	14.677018637	5.944637903	10.029638255
O	14.958160828	7.025554334	11.443445551
O	14.736227435	7.116385859	8.637947117
Al	10.459993342	7.091802223	9.963091875
Al	10.532569264	6.953479515	7.139931325
Al	10.562844448	2.019171803	8.560035630
O	10.345425013	0.875669558	7.190786661
O	10.515022258	0.884393543	10.008359361
Al	10.493123354	3.910885923	11.287915105
O	10.449465135	5.156874819	9.983958262
O	10.515080050	5.086795616	7.346631515

Al	14.578748506	3.973718624	7.343951070
O	14.651647250	2.898598612	8.791882553
O	14.723641332	2.982444005	11.373701546
H	9.364142660	0.992098087	7.072130658
H	13.377871110	1.362212763	6.725861502
H	15.713748671	1.432729231	6.659421243
H	14.643029669	7.782304511	5.468642396
H	12.085893384	6.232233015	5.482530841
H	9.083573849	6.666562787	5.097283607
H	14.363592329	3.114607397	5.119556878
H	16.602831161	4.891444990	6.357547493
O	14.726175796	7.025888143	6.068167856
O	11.975279575	7.084623290	5.938294055
O	9.114055335	7.174598804	5.918922122
O	14.646467909	2.832191726	6.000106268
Al	0.733598390	12.990882539	8.557282090
Al	4.869767088	14.989279440	7.070804514
O	3.505397206	15.252185860	11.052858537
O	7.692497044	12.981894769	9.755133659
O	3.408123892	14.867939288	8.322179951
O	7.722840730	12.995057697	7.050870226
Al	4.790029539	11.115608812	9.970928860
Al	0.724210636	9.149217910	11.446638784
O	7.636251935	8.941686450	7.368648416
O	3.502096616	11.048040639	8.563417614
O	7.624805894	9.276283737	10.157928611
O	3.519477871	10.936144860	11.272299847
Al	7.781214477	11.173662305	10.009519272
Al	3.548510832	9.067532681	11.371091210
O	4.990705723	8.862013467	7.347954730
O	0.616456033	11.176525519	8.712672567
O	5.054400298	9.194786920	10.150918361
O	0.711101692	11.044893553	11.372674501
Al	3.494120228	12.910131026	8.368997609
Al	7.700305407	15.088900058	7.137193323
O	0.794625957	15.238928348	11.129239855
O	4.825269658	12.918590138	9.766924506
O	0.776457582	14.922275605	8.381743067
O	4.898598987	13.077124237	7.121890178
Al	6.317761503	9.033456447	8.692904952
Al	6.326096904	8.998866148	11.513974797
Al	6.216558642	13.975054567	9.855243844
O	6.481389235	15.033076641	11.284150058
O	6.301422685	15.110348092	8.443115437
Al	2.162134419	15.087483326	9.809453042
Al	2.094426742	14.917995377	6.983336444
Al	1.991637810	10.092848190	8.602269727
O	2.109843595	8.952320934	7.193067725
O	2.044560751	8.951889008	10.005677147
Al	2.168375253	12.082262186	11.356524560
O	2.105650113	13.155669857	9.836289184
O	2.024265422	13.058918618	7.206583217
Al	6.202206655	11.912480294	7.184120248
O	6.267981449	10.922023714	8.697198583
O	6.302011275	11.068348460	11.287049069
H	2.340391019	9.363435185	6.345177936
H	4.166627567	9.330095231	7.576863118
H	7.395497106	9.555296869	6.632385516
H	6.348059574	14.258469379	5.254827228
H	3.515300330	14.173394956	5.261855666
H	0.570455399	15.656508183	5.078268630

H	5.720977337	10.273982789	5.660402036
H	8.283211491	12.770692080	6.279149742
O	6.317546300	15.020059137	5.851238186
O	3.492747724	15.011681771	5.753198488
O	0.618788169	15.084091426	5.854654194
O	6.464621109	10.893071375	5.767954121
Al	9.139749884	12.968813863	8.537473868
Al	13.255971277	15.073065153	7.220927754
O	11.839481115	15.259868282	11.276025257
O	16.133676832	13.068050248	9.903932908
O	11.776394413	14.918872311	8.468567974
O	16.129588364	13.078775022	7.183207212
Al	13.225234944	11.157207733	10.114373024
Al	9.076130138	9.193001517	11.406537966
O	16.116482593	8.948052980	7.521219644
O	11.938887853	11.075451417	8.712981498
O	16.024273916	9.275353959	10.253220328
O	11.924093820	10.967064750	11.424030821
Al	16.207029768	11.203687977	10.118151746
Al	11.969298601	9.087512881	11.434231942
O	13.461716571	8.933444155	7.436710318
O	9.042440287	11.142879464	8.643030770
O	13.468700303	9.213192684	10.248622453
O	9.104825369	11.051564388	11.351516527
Al	11.912035165	12.947661802	8.486739141
Al	16.137748991	15.222816996	7.235251435
O	9.127527650	15.250021846	11.198846607
O	13.234294672	12.976651761	9.917947785
O	9.122873079	14.861818923	8.394654158
O	13.321867936	13.154668926	7.275938689
Al	14.755658476	9.068063648	8.807092442
Al	14.752840399	8.937497153	11.626543878
Al	14.641478585	14.020555630	9.955775471
O	14.495181034	15.079876495	11.423300916
O	14.720614315	15.167349701	8.568525301
Al	10.520752002	15.096370488	9.869695367
Al	10.495850991	14.970976749	7.055982392
Al	10.449193884	10.113894603	8.646945553
O	10.524609945	8.960365859	7.267584227
O	10.458734607	9.024975697	10.075785346
Al	10.540142341	12.080595241	11.364602385
O	10.506521051	13.168481072	9.911622880
O	10.504990407	13.069849904	7.283437053
Al	14.622677185	11.984753464	7.312815470
O	14.712017911	10.980120015	8.816049373
O	14.719165870	11.123025064	11.417120513
H	9.954360716	9.252980692	6.536169485
H	12.648073482	9.453883617	7.568968959
H	15.951704802	9.607595400	6.809293324
H	14.725194625	14.453992056	5.344850360
H	11.956182880	14.230542421	5.391034527
H	9.048249422	15.584951764	5.114687744
H	14.236503121	10.325008532	5.784177273
H	16.665288973	12.828781362	6.399439805
O	14.719347756	15.166569212	6.000278293
O	11.919836292	15.083675030	5.857175846
O	9.052047892	14.940997353	5.838269185
O	14.952376664	10.970820980	5.918353560
O	7.709667028	9.194672191	12.719750845
H	7.803972337	8.453847658	13.345314187
H	14.652958605	11.740709855	12.161901790

O	13.324548458	9.026365276	12.789321718
O	10.501911448	9.027846871	12.730732345
O	-0.626664459	9.030725556	12.793988144
H	-0.585109053	9.780674688	13.405197792
O	2.415135332	13.235231404	12.650582186
O	10.587615652	13.313227795	12.650352902
H	7.487297105	14.967184479	11.321902522
H	13.499322516	14.999063987	11.543816489
H	3.345970391	14.594147209	11.774891071
H	11.527794137	14.706144430	12.035766246
O	1.873889783	5.002509473	12.792518655
H	7.543277157	6.994178959	11.444195319
H	4.141239647	6.553842407	11.098282833
H	15.966658140	6.951601493	11.501155469
O	7.702585055	0.968418060	12.639039450
H	7.780426800	0.318038736	13.349992959
O	-0.697515098	0.887178029	12.713056459
H	-0.616513519	0.113411044	13.290788696
H	6.346390786	3.461773406	12.075194473
O	4.901536504	0.817598636	12.641554142
O	2.098251917	0.882380772	12.563589434
H	14.800403038	3.589934681	12.127219249
O	13.260006460	0.892103487	12.787558628
O	10.440129223	0.962785850	12.641874348
O	2.172117051	9.114670333	12.640906604
O	4.913143369	8.948211844	12.702196266
H	2.173863610	8.321592437	13.198681788
H	4.846712414	9.668214579	13.346678183
H	13.184703839	8.208076249	13.309744700
H	10.529404074	9.646366675	13.477467104
H	13.246543019	1.629705090	13.414844365
H	10.385428620	1.710525351	13.255966882
H	2.093933707	1.623786480	13.189066754
H	4.809569071	-0.010424382	13.136810202
H	9.449319176	14.745903958	11.981342799
H	10.670948620	13.054545547	13.577996673
H	1.715992936	13.911394839	12.695772389
H	0.063319668	14.625938972	10.933630320
H	1.078026918	6.580695474	12.008121554
H	2.701439128	5.399165052	13.106126611
H	6.298064454	11.678956758	12.041096342
W	10.467349664	6.667842187	12.926717449
O	10.600890305	4.915848648	12.808111862
O	9.197029995	7.265357011	11.443012332
H	11.993823458	7.062375289	13.561469136
C	8.545871525	6.362245642	14.077089732
H	7.909997558	7.248873869	14.251097044
C	10.490028936	7.029832769	15.115579730
C	9.295732763	6.117285041	15.392153239
C	11.753227485	6.869165873	15.978980167
H	12.487633054	7.614541374	15.622502537
C	12.402606416	5.484838233	15.853493890
H	12.662336932	5.258131582	14.809896241
H	13.322083609	5.428981539	16.453546794
H	11.724826037	4.695694537	16.212120897
C	11.446006343	7.185436104	17.452345091
H	12.358664949	7.146620096	18.065505509
H	11.004911038	8.187302831	17.563411871
H	10.733468153	6.458385849	17.870187664
H	10.133092065	8.072247820	15.220052324
H	9.616956520	5.064763920	15.439040464

H	8.732042177	6.323153852	16.322331829
C	7.654971830	5.214413453	13.583013730
H	7.610217412	5.204947880	12.484671281
H	8.144056398	4.264369932	13.852032953
C	6.229704891	5.258871157	14.150918539
H	5.705302773	6.158940412	13.797819024
H	6.242291566	5.275774201	15.250635335
H	5.627749864	4.383794692	13.851658080

isobutene (1,2) insertion (side path) into species 1. E: -2356.877739202

Al	0.723161804	4.903130801	8.589541033
Al	4.871356408	6.973633251	7.186168835
O	3.415544966	7.189625062	11.204221519
O	7.705941417	4.851118590	9.754358346
O	3.396513399	6.844922572	8.434145239
O	7.771523486	5.004691489	7.113210061
Al	4.783822355	3.070407585	10.030727373
Al	0.663799593	0.966370426	11.342171993
O	7.629644990	0.807617114	7.279978463
O	3.510473080	3.061372354	8.643509108
O	7.571678185	1.126539213	10.080669859
O	3.508191431	2.884102973	11.349034125
Al	7.771749162	3.024498257	9.934211103
Al	3.511266843	0.974416548	11.336528777
O	4.993009104	0.728586620	7.213252861
O	0.618306694	3.070517710	8.640660626
O	4.995688067	1.132705827	10.084727674
O	0.688507929	2.840699058	11.285164823
Al	3.490288329	4.895603918	8.469077101
Al	7.738594956	7.120033224	7.192429448
O	0.765675170	7.189287541	11.287297043
O	4.839902835	4.930087635	9.925848985
O	0.773742975	6.850913475	8.473221019
O	4.911986354	5.082525379	7.268558699
Al	6.240063068	0.941906544	8.614742186
Al	6.286546693	0.833686451	11.440046908
Al	6.313991363	5.913395012	9.890298624
O	6.552170183	7.026026605	11.295400069
O	6.326870668	7.085580171	8.503652917
Al	2.075702926	7.019964567	9.904945363
Al	2.094381376	6.872671888	7.072543099
Al	2.046468814	2.052653432	8.572986997
O	2.187009326	0.954570932	7.126790770
O	2.102416640	0.876285055	9.928617697
Al	2.073731557	3.951380499	11.382836996
O	2.096723526	5.088047145	9.918498391
O	2.038632510	5.009028668	7.284404827
Al	6.217597452	3.921206248	7.191443244
O	6.254616712	2.850551384	8.652644528
O	6.300684895	2.913264807	11.275863439
H	1.924646237	1.380829861	6.296236337
H	4.109209147	1.139719358	7.281889974
H	7.335562464	1.400463845	6.543213007
H	6.270602806	7.686008884	5.309272433
H	3.573054285	6.206244538	5.318044521
H	0.614703259	7.601187026	5.206969403
H	5.885031000	2.434577493	5.403911279
H	8.259184975	4.724320701	6.312981852
O	6.318598461	6.945002841	5.932199908
O	3.503827412	7.021059685	5.843644372
O	0.625691454	6.947116243	5.919010662

O	6.605633358	2.976318347	5.763533811
Al	9.152774354	4.910160932	8.537123286
Al	13.291581084	7.054287488	7.309879573
O	11.681961052	7.257843138	11.366153089
O	16.116340922	4.908585509	9.837529348
O	11.779543157	6.929977253	8.549501269
O	16.116487562	5.060244902	7.191155860
Al	13.205457572	3.099008637	10.108143873
Al	9.073220208	1.032123799	11.340913026
O	15.977536116	0.890020286	7.433106828
O	11.923382913	3.125110842	8.731737510
O	15.951647188	1.130623625	10.170852729
O	11.915425416	2.891764313	11.419394755
Al	16.187900921	3.057966539	10.029099202
Al	11.895887030	1.016838163	11.445066175
O	13.249098220	0.792233070	7.508076098
O	9.117074642	3.061485081	8.635550650
O	13.396692551	1.149525039	10.234862214
O	9.049269565	2.901428607	11.282069196
Al	11.912642055	4.965159901	8.551909368
Al	16.150945140	7.133031581	7.296304407
O	13.239432106	4.929116550	9.997659474
O	9.127362399	6.861313587	8.474562323
O	13.317602823	5.166796666	7.356424316
Al	14.638060245	0.977576584	8.758899070
Al	14.692236891	0.881213501	11.574976261
Al	14.674960050	5.944134527	10.028359072
O	14.957448871	7.025075175	11.443221456
O	14.735894695	7.116974806	8.637695793
Al	10.446963113	7.088178256	9.963230582
Al	10.533847152	6.957327240	7.129126496
Al	10.564833942	2.014055121	8.554285900
O	10.343826636	0.872321000	7.187992847
O	10.514758294	0.884269245	10.006874100
Al	10.490135755	3.904341283	11.233957203
O	10.453437743	5.152469065	9.927795095
O	10.513790791	5.087551024	7.293419616
Al	14.579503686	3.973910689	7.343416912
O	14.651577947	2.898603955	8.791555135
O	14.723363099	2.982428782	11.374365448
H	9.362266292	0.989222936	7.070611189
H	13.378987434	1.361880071	6.725551960
H	15.713995388	1.432554492	6.659301144
H	14.642908307	7.780155547	5.466287563
H	12.086746705	6.236134206	5.478802508
H	9.084088831	6.663176959	5.097661009
H	14.360955775	3.114295181	5.120238178
H	16.602762974	4.892039989	6.357131763
O	14.726677235	7.025940418	6.068422150
O	11.981404768	7.090381690	5.932473315
O	9.112340913	7.176784631	5.915909899
O	14.646405219	2.832023943	6.000034158
Al	0.733962632	12.989381492	8.557271395
Al	4.869590917	14.988187020	7.071077852
O	3.505332467	15.252021629	11.052790561
O	7.693393622	12.980252128	9.755370961
O	3.408268433	14.866929370	8.322243165
O	7.722478943	12.994619395	7.051254033
Al	4.793188178	11.113116593	9.974841242
Al	0.724451968	9.148975156	11.446521599
O	7.636077843	8.942680125	7.368417462

O	3.502665735	11.047086554	8.564094911
O	7.623168570	9.269701757	10.159380171
O	3.517955706	10.924456501	11.271774220
Al	7.781315604	11.169794116	10.014960967
Al	3.548454231	9.062555901	11.371905063
O	4.990919560	8.861301285	7.348095083
O	0.616464599	11.173963362	8.712604297
O	5.056016518	9.188610185	10.150843305
O	0.711103076	11.044621794	11.372854828
Al	3.494615074	12.908610169	8.369654456
Al	7.700146890	15.087467069	7.137813823
O	0.794665511	15.238540320	11.129365648
O	4.824484639	12.917115210	9.767308343
O	0.776635607	14.921999742	8.381880655
O	4.898937913	13.076609178	7.122107497
Al	6.318120074	9.031826748	8.692841556
Al	6.326874478	8.970447893	11.510552717
Al	6.217032788	13.971248716	9.855449034
O	6.480956575	15.027669925	11.284901595
O	6.301486179	15.109078969	8.445119548
Al	2.162149319	15.086654907	9.809333988
Al	2.094464187	14.917157376	6.983476114
Al	1.992538764	10.091723186	8.602501802
O	2.109840782	8.951985402	7.192791336
O	2.043443038	8.950693591	10.005609902
Al	2.170937995	12.078381931	11.356389544
O	2.105872469	13.154662402	9.836629193
O	2.024382004	13.058361636	7.206815416
Al	6.201985253	11.910809642	7.185874419
O	6.267261992	10.918854392	8.698237618
O	6.300955085	11.068638404	11.284373119
H	2.346698028	9.362180017	6.346194568
H	4.167968430	9.330241836	7.579477544
H	7.394023422	9.556179981	6.632337322
H	6.348037802	14.257354848	5.256272674
H	3.515121500	14.173717698	5.261093585
H	0.570619663	15.657178513	5.078896560
H	5.720511262	10.274949167	5.658760690
H	8.282179527	12.770133315	6.279084255
O	6.317415053	15.019816725	5.851619825
O	3.492713158	15.011533373	5.753242873
O	0.618784482	15.084054298	5.854769448
O	6.464614257	10.893097080	5.768180043
Al	9.138991484	12.967076639	8.538023069
Al	13.255811071	15.072877643	7.220846953
O	11.839323069	15.260061706	11.275843015
O	16.133994989	13.067883666	9.903499448
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O	16.129752814	13.078675612	7.183173976
Al	13.226648150	11.158905501	10.112662833
Al	9.074769883	9.176351549	11.415108887
O	16.116853174	8.948149352	7.521116540
O	11.938297650	11.074916292	8.713098870
O	16.024619471	9.275197701	10.252842660
O	11.924588179	10.968801015	11.421989424
Al	16.207593664	11.203486463	10.117857542
Al	11.970917624	9.093588685	11.427007954
O	13.462250392	8.935643741	7.436768391
O	9.041793079	11.141563555	8.643962319
O	13.469253105	9.213978584	10.247134759
O	9.105798366	11.046507980	11.353022845

Al	11.911669092	12.947274944	8.486473003
Al	16.137878551	15.222600981	7.235408199
O	9.127593009	15.249894936	11.198681202
O	13.234383945	12.977399080	9.917652322
O	9.122717058	14.861064416	8.394672827
O	13.321802911	13.154625110	7.275941525
Al	14.756092937	9.068517071	8.806130240
Al	14.754130866	8.937404108	11.624712439
Al	14.641913619	14.020750719	9.955759469
O	14.495191586	15.080011287	11.423477237
O	14.720650945	15.167302935	8.568412892
Al	10.520325570	15.095598079	9.869300417
Al	10.495407797	14.969004595	7.055234878
Al	10.448349292	10.112277479	8.648317855
O	10.524391974	8.961408025	7.265986352
O	10.460010377	9.022291153	10.076653471
Al	10.538030478	12.079476964	11.363634116
O	10.506413777	13.168049262	9.911595072
O	10.504659767	13.069322031	7.283493994
Al	14.622766215	11.984870047	7.312163921
O	14.712233725	10.980468388	8.815433079
O	14.719602307	11.123596570	11.414665811
H	9.955354704	9.257959472	6.535142826
H	12.648845397	9.456328577	7.570009012
H	15.953091674	9.607813748	6.809135681
H	14.725259632	14.454503215	5.344509858
H	11.957163552	14.230758231	5.390034027
H	9.047412998	15.583995454	5.114680439
H	14.237366571	10.323742763	5.785346952
H	16.665286998	12.828838768	6.399225578
O	14.719322030	15.166737043	6.000318068
O	11.919826328	15.083439888	5.856918479
O	9.051303849	14.939942340	5.838151332
O	14.952376199	10.970855412	5.918120144
O	7.699148426	9.195820705	12.713763135
H	7.762041750	8.498041846	13.387123894
H	14.653374775	11.740706461	12.159896601
O	13.327829614	9.032714101	12.785635700
O	10.515095638	9.029894076	12.734234249
O	-0.626585246	9.030734352	12.794004517
H	-0.585363700	9.783555676	13.401762670
O	2.415760694	13.233974625	12.649473286
O	10.587367836	13.312941697	12.649667098
H	7.486820735	14.962636944	11.323254782
H	13.499224992	14.999291009	11.543340722
H	3.346885432	14.593423679	11.774504403
H	11.527825676	14.706654133	12.035813937
O	1.873536999	5.003049897	12.791928971
H	7.557093582	6.948164995	11.454134990
H	4.143907357	6.555781035	11.085946718
H	15.965830585	6.950584364	11.500329222
O	7.701998383	0.968087559	12.638125362
H	7.782238260	0.325578916	13.355839834
O	-0.697718698	0.887168498	12.713160350
H	-0.617105533	0.112045374	13.289160443
H	6.341259306	3.459313706	12.076985761
O	4.901513887	0.817227520	12.641344798
O	2.098041757	0.882223701	12.563698027
H	14.799037619	3.587835016	12.129941187
O	13.259432692	0.893253045	12.787460452
O	10.440089786	0.963792129	12.641412061

O	2.171582290	9.113876404	12.641101608
O	4.913765013	8.942959478	12.698908807
H	2.170271248	8.324376451	13.203735472
H	4.859597789	9.672282019	13.333979597
H	13.189382404	8.220978371	13.315800447
H	10.549374627	9.669380099	13.462924181
H	13.245735190	1.633668973	13.411667255
H	10.384664567	1.716735246	13.249432632
H	2.093774926	1.624047305	13.188669008
H	4.808050285	-0.009337136	13.138811952
H	9.449731778	14.745765082	11.981094389
H	10.664409785	13.055798291	13.578225593
H	1.716044702	13.909939741	12.690368021
H	0.063751160	14.625125145	10.933423858
H	1.071488562	6.577021899	12.006892955
H	2.696131461	5.434489261	13.071208297
H	6.300605517	11.676419576	12.040498209
W	10.549419256	6.672356089	12.941313037
O	10.582394219	4.925285879	12.718785600
O	9.202342536	7.256871545	11.452715674
H	12.049383469	7.132299551	13.553989640
C	8.824654606	6.980814750	14.263325386
H	8.788620934	8.024109276	14.618572518
C	10.837559104	6.347191508	15.126822601
C	9.326590135	6.138803535	15.450562511
C	11.846651846	5.239454737	15.514489564
H	11.452502307	4.293277948	15.106129214
C	11.943995318	5.092877329	17.043774475
H	10.974688291	4.858329275	17.500198264
H	12.645331612	4.288808144	17.314734762
H	12.311770641	6.025051274	17.499975028
C	13.260183388	5.423019440	14.937249530
H	13.937325347	4.651344449	15.334953108
H	13.278350772	5.361339766	13.841386742
H	13.683576965	6.400278151	15.219405582
C	8.879703365	6.731532939	16.799833310
H	7.780114343	6.758604576	16.859845605
H	9.249998160	6.148744176	17.655404175
H	9.249533546	7.761954445	16.910576000
C	8.829548673	4.688019097	15.361424094
H	9.267632476	4.062165925	16.152044080
H	7.737356885	4.667174547	15.493518534
H	9.055205492	4.222981252	14.393822348
H	7.845933459	6.681576333	13.847806207
H	11.151812450	7.288272323	15.612926376

isobutene (2,1) insertion (side path) into species 1. E: -2356.877822881

Al	0.723611711	4.902410313	8.588644254
Al	4.873261701	6.970268180	7.169174206
O	3.414718421	7.190760349	11.200068272
O	7.698698609	4.858533053	9.760391557
O	3.401701617	6.848569192	8.422590747
O	7.775395729	5.005628166	7.117530347
Al	4.786189281	3.073131629	10.031301808
Al	0.664073393	0.966738459	11.342261186
O	7.629811661	0.808369509	7.279922611
O	3.511283684	3.062404180	8.644191133
O	7.572670359	1.127643619	10.081328916
O	3.509159240	2.885514173	11.349348956
Al	7.771003554	3.026784859	9.938764065
Al	3.511835537	0.975166633	11.336321410

O	4.992964158	0.729480695	7.213171112
O	0.618637768	3.070428924	8.640501654
O	4.996213650	1.133210707	10.084626246
O	0.688879702	2.841329471	11.284674574
Al	3.493050008	4.897015710	8.466347919
Al	7.738842981	7.116545993	7.191184133
O	0.766546044	7.189488190	11.287072094
O	4.841879446	4.934575020	9.926718529
O	0.774547010	6.850728325	8.472457678
O	4.913484966	5.081198798	7.266348233
Al	6.240792547	0.944600002	8.614037124
Al	6.286661642	0.833425483	11.439294816
Al	6.308464703	5.931976453	9.888456144
O	6.546197263	7.082608251	11.274028703
O	6.320702789	7.091692911	8.491731211
Al	2.075418905	7.017529162	9.902953203
Al	2.095623263	6.871808953	7.069558375
Al	2.047495265	2.053285324	8.573345493
O	2.186800919	0.955088788	7.126815175
O	2.102723559	0.876768332	9.928733331
Al	2.074871729	3.951972114	11.383132832
O	2.097477815	5.088808287	9.917723104
O	2.039002252	5.008872466	7.284017891
Al	6.222653282	3.923081627	7.191274521
O	6.256169662	2.854235920	8.653650028
O	6.300189386	2.914500278	11.274251554
H	1.920901932	1.381142914	6.297270591
H	4.109687633	1.141818700	7.280683506
H	7.337121052	1.402205054	6.543229732
H	6.272872854	7.685485453	5.306375579
H	3.563982066	6.204437550	5.309835612
H	0.609491309	7.586199838	5.194301477
H	5.885537028	2.435127629	5.406079896
H	8.272783510	4.719266112	6.325854926
O	6.322283223	6.941969730	5.926230120
O	3.502122796	7.017862809	5.838551986
O	0.625406416	6.946879255	5.919281642
O	6.607616440	2.976205670	5.763740022
Al	9.152476992	4.913482297	8.567832872
Al	13.291361020	7.051859181	7.311404481
O	11.669323343	7.257704658	11.366431107
O	16.116774554	4.908505274	9.837178502
O	11.782022810	6.930883943	8.555123850
O	16.116113552	5.060023350	7.191375165
Al	13.204107894	3.097538335	10.112162721
Al	9.073495847	1.032852302	11.340597398
O	15.977510645	0.890052581	7.433065559
O	11.925186862	3.124871873	8.737446249
O	15.951358519	1.130451004	10.170965495
O	11.916487456	2.894148233	11.428643347
Al	16.187888067	3.057577315	10.028428941
Al	11.895351587	1.017260252	11.446739368
O	13.249332029	0.792049748	7.508107756
O	9.114015136	3.064010819	8.639058521
O	13.395849222	1.150768447	10.235882945
O	9.053274375	2.903701395	11.284881186
Al	11.919625917	4.965139453	8.572717021
Al	16.150576126	7.132906426	7.296839913
O	13.241059676	4.929084554	9.999079221
O	9.126441961	6.862582509	8.480743660
O	13.316501135	5.166519480	7.358162419

Al	14.637569840	0.978220359	8.758666106
Al	14.692471233	0.879447397	11.574820098
Al	14.676716800	5.944766622	10.029724436
O	14.957990667	7.025965316	11.443448469
O	14.736326799	7.116362935	8.638002393
Al	10.457228772	7.090130114	9.966543697
Al	10.532324946	6.953697906	7.140735737
Al	10.562724723	2.019655117	8.560488782
O	10.345700532	0.876023387	7.191054456
O	10.514872273	0.884589776	10.008691037
Al	10.492669595	3.914728437	11.290307278
O	10.449331160	5.156810752	9.983532575
O	10.514926364	5.086770861	7.346511637
Al	14.578139787	3.973524411	7.344127937
O	14.651689636	2.898583114	8.791864923
O	14.723629064	2.982599224	11.373603393
H	9.364390024	0.992326188	7.072593057
H	13.377886746	1.362197211	6.725811882
H	15.713655488	1.432535798	6.659327186
H	14.641183632	7.783771313	5.470318902
H	12.085078755	6.232161097	5.482656155
H	9.083979580	6.666021275	5.097308592
H	14.361767396	3.114245620	5.119948640
H	16.601817502	4.891651258	6.357110186
O	14.726077974	7.026046692	6.067999440
O	11.974991491	7.084703388	5.938261343
O	9.114699702	7.174349932	5.918732490
O	14.646723541	2.832273487	5.999981011
Al	0.733940554	12.990251754	8.557378865
Al	4.869503897	14.989779971	7.069819758
O	3.505440664	15.252367300	11.052870125
O	7.694379500	12.981534235	9.755092995
O	3.407737426	14.868693024	8.322086242
O	7.724908684	12.996902520	7.048948313
Al	4.791451713	11.113921552	9.956799782
Al	0.723722947	9.149283021	11.449308137
O	7.637382965	8.942086088	7.364302984
O	3.501507567	11.050641424	8.560977891
O	7.626783188	9.276735929	10.151928402
O	3.521408819	10.927445155	11.264064055
Al	7.783547875	11.172081506	10.005195981
Al	3.541581258	9.064514603	11.345655413
O	4.992989383	8.864406561	7.283650685
O	0.616828288	11.174630906	8.712254896
O	5.052337887	9.194153174	10.099491685
O	0.712354340	11.044463863	11.372570635
Al	3.493982698	12.911078256	8.367879648
Al	7.700959397	15.088886966	7.136365939
O	0.794723786	15.238862030	11.129369808
O	4.825191957	12.918074550	9.766307219
O	0.776426993	14.922299290	8.381919549
O	4.897839161	13.079246951	7.120847117
Al	6.305764719	9.041183530	8.663417594
Al	6.330912338	8.998702025	11.482474136
Al	6.217726558	13.972491134	9.852799821
O	6.480459470	15.028278705	11.283628013
O	6.301683515	15.109607036	8.441267160
Al	2.162270845	15.087223843	9.809580374
Al	2.094175970	14.918529087	6.983400645
Al	1.994445065	10.094365749	8.600992881
O	2.111191074	8.952869309	7.192939988

O	2.044908167	8.950924168	10.003490356
Al	2.172757851	12.078857099	11.354734828
O	2.105682551	13.155510703	9.836255865
O	2.023971494	13.059296659	7.206255897
Al	6.203950939	11.918696173	7.172109649
O	6.275511562	10.929921037	8.679288579
O	6.300834208	11.063507287	11.278919811
H	2.272060742	9.372943558	6.333260446
H	4.154549190	9.308703850	7.510010539
H	7.411995512	9.559061507	6.626057159
H	6.348371895	14.263314614	5.249411656
H	3.514928854	14.172981684	5.262670497
H	0.570110632	15.656428168	5.078215161
H	5.731705042	10.256111986	5.682124408
H	8.288621450	12.774372486	6.279045019
O	6.317757454	15.020895123	5.850787065
O	3.492296792	15.011976500	5.752871648
O	0.618638579	15.084093340	5.854651053
O	6.465105355	10.892643910	5.764238931
Al	9.140431999	12.969044964	8.537750274
Al	13.255878692	15.073151702	7.221174532
O	11.839562746	15.260089063	11.276295946
O	16.133940766	13.067704578	9.903602749
O	11.776524327	14.918967637	8.468750022
O	16.129591326	13.078624983	7.183373623
Al	13.225048880	11.157284462	10.114103392
Al	9.075578184	9.191674972	11.409915310
O	16.116239287	8.948320995	7.520667181
O	11.939091068	11.074847561	8.712806062
O	16.025222114	9.275343097	10.253358006
O	11.924167681	10.967085790	11.423113812
Al	16.207851437	11.203261901	10.118118699
Al	11.967889519	9.088451032	11.432414879
O	13.461749095	8.933168344	7.436691155
O	9.044157883	11.143333963	8.642025252
O	13.468862212	9.213401547	10.247943482
O	9.104270669	11.050899097	11.351374771
Al	11.911826169	12.947405335	8.487108891
Al	16.137785433	15.222795099	7.235490516
O	9.127610485	15.249924844	11.198610875
O	13.234461729	12.976657787	9.917928809
O	9.123211067	14.862164955	8.394572403
O	13.321866671	13.154628621	7.276043470
Al	14.755521825	9.068070756	8.807207002
Al	14.752734483	8.939090138	11.625547210
Al	14.641666789	14.020237156	9.955637824
O	14.495063165	15.079854879	11.423065634
O	14.720636780	15.167409153	8.568604102
Al	10.520737953	15.095992704	9.870185283
Al	10.496141560	14.971356340	7.056419639
Al	10.449205153	10.112942958	8.647561701
O	10.525329705	8.960183503	7.267501996
O	10.457032403	9.024086697	10.075976012
Al	10.539143121	12.079803087	11.365664355
O	10.506961707	13.168180598	9.911816239
O	10.505239091	13.070091229	7.283276337
Al	14.622630194	11.984856064	7.313143788
O	14.712363381	10.979987934	8.815888662
O	14.719460710	11.122884435	11.416783117
H	9.965397705	9.256147642	6.529732516
H	12.647950973	9.453207390	7.570069057

H	15.946395637	9.606838687	6.808718193
H	14.724991067	14.453999152	5.344895402
H	11.955915013	14.230284149	5.391746038
H	9.050400976	15.586950150	5.115212817
H	14.234724885	10.327384297	5.782183819
H	16.665024860	12.829810130	6.399089908
O	14.719368605	15.166487797	6.000406954
O	11.919962858	15.083735629	5.857339692
O	9.052949149	14.941912711	5.837846121
O	14.952462787	10.970685385	5.918404059
O	7.704644263	9.191122141	12.716176358
H	7.794685176	8.439982411	13.330560786
H	14.652827104	11.739986627	12.162024628
O	13.325286244	9.028195030	12.788786983
O	10.502677858	9.026087022	12.726265181
O	-0.627039570	9.030781375	12.794194542
H	-0.585194175	9.779182549	13.407252965
O	2.416158671	13.233574045	12.649115724
O	10.587614694	13.313145235	12.650485288
H	7.486309701	14.962873169	11.322899582
H	13.499016239	14.998962041	11.543239878
H	3.346868700	14.593977905	11.774744636
H	11.527942567	14.706590092	12.036327938
O	1.874053488	5.002858484	12.792154833
H	7.544608037	6.989494969	11.442071361
H	4.140626330	6.551992179	11.095330596
H	15.966314107	6.952071254	11.501175399
O	7.701662544	0.965823308	12.636883325
H	7.782213188	0.322754577	13.354044850
O	-0.697635133	0.887070795	12.712971586
H	-0.616194339	0.113392991	13.290802405
H	6.345077170	3.471849462	12.068292236
O	4.901992691	0.817675558	12.641472523
O	2.098291366	0.882489125	12.563616607
H	14.800844546	3.591443992	12.125964367
O	13.259931709	0.892042014	12.787428512
O	10.439599120	0.962557822	12.641832925
O	2.174498139	9.114462056	12.638120902
O	4.912249469	8.950836090	12.645999010
H	2.181048404	8.318167698	13.191305240
H	4.846122816	9.662606294	13.299588972
H	13.186764609	8.204925915	13.302092709
H	10.528964746	9.629239559	13.485917970
H	13.247673189	1.630834961	13.413129223
H	10.381377634	1.705465198	13.261308291
H	2.093867284	1.623729244	13.189298564
H	4.808397845	-0.008402238	13.139701065
H	9.449277478	14.745503313	11.981053698
H	10.662262796	13.052428710	13.578402935
H	1.715522567	13.908469460	12.690940798
H	0.063601196	14.625671610	10.933687686
H	1.077316379	6.580253754	12.007273883
H	2.699721705	5.406301678	13.102315085
H	6.289313111	11.668389840	12.037297860
W	10.485109236	6.677969612	12.939268921
O	10.599115361	4.921080684	12.811131094
O	9.198208292	7.262063377	11.452425043
H	12.021516469	7.084721041	13.519873728
C	8.601796948	6.453755832	14.201261158
H	8.069787623	7.396621567	14.417660514
C	10.678550012	6.978018298	15.162825245

C	9.422781074	6.163397023	15.462691343
H	9.694234248	5.100165948	15.508386991
C	11.938374127	6.365918068	15.782988460
H	11.815795503	6.284577799	16.878992801
H	12.132812716	5.355488965	15.395673301
H	12.835635308	6.972862068	15.590317690
C	10.529683586	8.422615305	15.637309809
H	9.601948930	8.894833247	15.280727705
H	10.492227544	8.445664594	16.741584306
H	11.388645845	9.043461580	15.333889971
H	8.932640708	6.406175794	16.429010007
C	7.539806412	5.390834185	13.787651714
H	7.548759072	5.302713466	12.688615555
C	6.124024151	5.818658397	14.211391352
H	5.375103565	5.066721215	13.910086640
H	6.066737138	5.917276065	15.306764898
H	5.830043180	6.773022114	13.757395724
C	7.829727754	3.991346639	14.347599430
H	7.107282705	3.253778385	13.970646747
H	8.823211355	3.628693299	14.058243348
H	7.757074028	3.981652090	15.444834043

2-butene insertion (top path) into species 1. E: -2356.8808140445

Al	0.723543647	4.902358542	8.588788816
Al	4.873282457	6.970205240	7.169115744
O	3.414832739	7.190520705	11.199978073
O	7.698955696	4.857833108	9.760206749
O	3.401553562	6.848619582	8.422562149
O	7.775507194	5.005620209	7.117627986
Al	4.786132896	3.072617717	10.030794215
Al	0.664069787	0.966736946	11.342210857
O	7.629821119	0.808358550	7.279780859
O	3.511230052	3.062335954	8.644007230
O	7.572471263	1.127760064	10.081250610
O	3.509295939	2.885487486	11.349379190
Al	7.771302416	3.026403745	9.938700225
Al	3.511735533	0.975085300	11.336367905
O	4.992861696	0.729409786	7.213049082
O	0.618600005	3.070349804	8.640467703
O	4.996018632	1.132959020	10.084364997
O	0.688980918	2.841186434	11.284558657
Al	3.492942374	4.896981778	8.466409808
Al	7.738828405	7.116485298	7.191238633
O	0.766695579	7.189427520	11.287183397
O	4.841775148	4.934105080	9.926687635
O	0.774455371	6.850543908	8.472370356
O	4.913486058	5.081200934	7.266364741
Al	6.240708946	0.944584235	8.613531970
Al	6.286164568	0.833157439	11.438667680
Al	6.308640134	5.930741368	9.888705979
O	6.547143759	7.077793360	11.276479992
O	6.320723825	7.091468986	8.492213501
Al	2.075493233	7.017448995	9.903025532
Al	2.095740190	6.871843306	7.069417518
Al	2.047480736	2.053227033	8.573317082
O	2.186851565	0.955056934	7.126814061
O	2.102717620	0.876713526	9.928737632
Al	2.074918089	3.951937533	11.383273867
O	2.097393030	5.088684759	9.917779844
O	2.038997692	5.008779822	7.284165829
Al	6.222695384	3.923070882	7.191215426

O	6.256064393	2.854012511	8.653493202
O	6.299892408	2.913957550	11.274719032
H	1.921040666	1.381158840	6.297266041
H	4.109535272	1.141693356	7.280436208
H	7.337224201	1.402300378	6.543107991
H	6.272591403	7.685570241	5.306613276
H	3.564144398	6.203882619	5.310493358
H	0.608188979	7.581355198	5.190499700
H	5.885464126	2.435397537	5.405863083
H	8.272927466	4.719274169	6.325959919
O	6.322282107	6.941891729	5.926246314
O	3.502070988	7.017775056	5.838505681
O	0.625345842	6.946661750	5.919386129
O	6.607627739	2.976249402	5.763687006
Al	9.152764619	4.913178895	8.568065496
Al	13.291518153	7.051706168	7.311398782
O	11.664422993	7.257498361	11.369470010
O	16.116940659	4.908493148	9.837537975
O	11.782246698	6.930930527	8.555067256
O	16.116091429	5.059914060	7.191359437
Al	13.204115940	3.097474517	10.112240137
Al	9.073963756	1.033166444	11.340222169
O	15.977526570	0.890095508	7.433105641
O	11.925262671	3.124860509	8.737378281
O	15.951357666	1.130499782	10.170892594
O	11.916745467	2.894216777	11.428775810
Al	16.187916429	3.057559591	10.028435338
Al	11.895246410	1.017448338	11.447314749
O	13.249353120	0.792008645	7.508152292
O	9.114020717	3.063807250	8.638921151
O	13.395918593	1.150774619	10.235981551
O	9.053986111	2.903611837	11.284509689
Al	11.920019330	4.964833599	8.572719410
Al	16.150481945	7.132819740	7.296855075
O	13.241017109	4.929089582	9.998966807
O	9.126741987	6.862493532	8.480284709
O	13.316557937	5.166536130	7.358150655
Al	14.637683114	0.978254175	8.758725313
Al	14.692448846	0.879979534	11.574968738
Al	14.676896476	5.944485821	10.030009304
O	14.958181623	7.025819557	11.443265234
O	14.736341297	7.116188452	8.638067667
Al	10.458343052	7.090675125	9.964583296
Al	10.532426195	6.953510571	7.140331396
Al	10.562801045	2.019697300	8.560549085
O	10.345784593	0.876011800	7.191018991
O	10.514896172	0.884613203	10.008662984
Al	10.493661223	3.915315196	11.292315484
O	10.449156982	5.157005801	9.984505770
O	10.515059368	5.086722770	7.346808592
Al	14.578255840	3.973422471	7.344076796
O	14.651668135	2.898585374	8.791872791
O	14.723585745	2.982518138	11.373590281
H	9.364489211	0.992344228	7.072521854
H	13.377830698	1.362179728	6.725873411
H	15.713604007	1.432444957	6.659308894
H	14.641428286	7.784508479	5.471070610
H	12.085617238	6.232431830	5.482284933
H	9.083751493	6.666784650	5.096843280
H	14.361838707	3.114120937	5.119875292
H	16.602228307	4.891528655	6.357349694

O	14.726145372	7.026045891	6.067855537
O	11.975264446	7.084711539	5.938308096
O	9.114626549	7.174505152	5.918649718
O	14.646402768	2.832171601	6.000034467
Al	0.733894729	12.989306850	8.557370414
Al	4.869497015	14.989620209	7.069656969
O	3.505367499	15.252272256	11.052820680
O	7.694383550	12.981933877	9.755132492
O	3.407774223	14.868240765	8.322066599
O	7.724942257	12.996837196	7.048921656
Al	4.791506188	11.113818918	9.957655732
Al	0.723645469	9.149244163	11.449488771
O	7.637156391	8.942111631	7.364372106
O	3.501740489	11.050614944	8.561088129
O	7.626398772	9.276746583	10.152194019
O	3.521298064	10.926838593	11.264228054
Al	7.782354506	11.172714626	10.004884073
Al	3.541845810	9.064066334	11.346541995
O	4.993020188	8.864256686	7.283564118
O	0.616687360	11.172903023	8.712155875
O	5.052748574	9.193562864	10.100294655
O	0.712350658	11.044435203	11.372556217
Al	3.494029787	12.910813793	8.367917291
Al	7.700930554	15.088893764	7.136071670
O	0.794705018	15.238809608	11.129364149
O	4.825219820	12.917977588	9.766233248
O	0.776418582	14.922100852	8.381934605
O	4.897873991	13.079118222	7.120795625
Al	6.305050637	9.041046779	8.663434957
Al	6.331168867	8.995898617	11.483675286
Al	6.217513132	13.972632646	9.852509126
O	6.480493367	15.028144363	11.283527586
O	6.301627648	15.109519237	8.440633345
Al	2.162081784	15.087044662	9.809456714
Al	2.094115244	14.918183749	6.983429167
Al	1.995102132	10.093865872	8.601452667
O	2.111414066	8.952708803	7.193337151
O	2.045361153	8.950625907	10.003698457
Al	2.172830703	12.078638361	11.354837551
O	2.105668200	13.155283566	9.836243730
O	2.023848761	13.059007191	7.206243796
Al	6.203947821	11.918512428	7.172243043
O	6.275995726	10.929812296	8.679742569
O	6.300651028	11.063647521	11.278786470
H	2.258288576	9.373985464	6.331989801
H	4.153766931	9.308899770	7.506324922
H	7.410958850	9.558765925	6.626032463
H	6.348328006	14.263449584	5.249006729
H	3.514863316	14.173228229	5.262164401
H	0.570088803	15.656493341	5.078373878
H	5.731112542	10.257165306	5.680462108
H	8.288517859	12.774328763	6.278913805
O	6.317729426	15.020829655	5.850626646
O	3.492209930	15.011923075	5.752855136
O	0.618624116	15.084057118	5.854734596
O	6.465125600	10.892707759	5.764244013
Al	9.140290101	12.969163326	8.537619589
Al	13.256003082	15.073046680	7.220998375
O	11.839535701	15.260235408	11.276133278
O	16.133973990	13.067400013	9.903463039
O	11.776589010	14.918934827	8.468670337

O	16.129590904	13.078467273	7.183547471
Al	13.225284970	11.157484503	10.114295640
Al	9.074741217	9.193547724	11.406422870
O	16.116180970	8.948231940	7.520597096
O	11.939477111	11.075272165	8.712673672
O	16.024755072	9.275151622	10.253710223
O	11.924468118	10.967016179	11.423260278
Al	16.207838111	11.202839854	10.118330409
Al	11.968895225	9.087145441	11.431436883
O	13.461869014	8.932918838	7.436731641
O	9.044139216	11.143410103	8.642167260
O	13.468852251	9.212959074	10.248084012
O	9.104344696	11.051527006	11.351012197
Al	11.912074348	12.947626120	8.486895935
Al	16.137828321	15.222776596	7.235693935
O	9.127470860	15.249875281	11.198529570
O	13.234554270	12.976787436	9.917893422
O	9.123165035	14.862257543	8.394538423
O	13.321894241	13.154599067	7.275907169
Al	14.755699936	9.067737754	8.807453091
Al	14.752541822	8.938082692	11.626569916
Al	14.641857130	14.020346089	9.955694353
O	14.495118371	15.079853474	11.423112656
O	14.720604418	15.167358294	8.568560040
Al	10.520870143	15.096284235	9.869999257
Al	10.496240101	14.971541106	7.056373401
Al	10.449549909	10.113599100	8.646842227
O	10.525324033	8.960251362	7.267301650
O	10.457690179	9.024695165	10.075164632
Al	10.539696320	12.080198997	11.364742536
O	10.506932347	13.168446921	9.911630283
O	10.505245242	13.070110518	7.283290409
Al	14.622576351	11.984713291	7.313258048
O	14.712284492	10.979892168	8.816082884
O	14.719269309	11.122715081	11.417269771
H	9.964050378	9.255666739	6.530300648
H	12.648087423	9.453088637	7.569433725
H	15.945407429	9.606585214	6.808716678
H	14.725149558	14.454134220	5.344743464
H	11.955901675	14.230412427	5.391384341
H	9.050444193	15.586582637	5.114837971
H	14.234456046	10.327985770	5.781081989
H	16.664850319	12.829785403	6.399098220
O	14.719418321	15.166496143	6.000396386
O	11.919937240	15.083732680	5.857201086
O	9.053015297	14.941904583	5.837791564
O	14.952453750	10.970714462	5.918384572
O	7.705447698	9.193115892	12.715643718
H	7.791715897	8.451083602	13.341167488
H	14.653259601	11.740105786	12.162329434
O	13.323796919	9.023391546	12.789361027
O	10.505015962	9.028754504	12.726176885
O	-0.626991518	9.030665410	12.794179318
H	-0.585382641	9.776991773	13.409710655
O	2.416195048	13.233502447	12.649049893
O	10.587821658	13.313200860	12.650190092
H	7.486425185	14.962800542	11.322157001
H	13.499062477	14.999163914	11.543097080
H	3.346609443	14.593915811	11.774695154
H	11.527788547	14.706143486	12.035661371
O	1.873971096	5.002555346	12.792292495

H	7.544033774	6.982007008	11.448179589
H	4.139421820	6.550181252	11.095596522
H	15.966501135	6.951778615	11.501347242
O	7.701400556	0.964593021	12.636654457
H	7.782983439	0.315940067	13.348839151
O	-0.697560437	0.887158500	12.713018272
H	-0.616342827	0.112937379	13.290154688
H	6.336449758	3.474497851	12.066983050
O	4.901994733	0.817386667	12.641417075
O	2.098317523	0.882541127	12.563595986
H	14.799582580	3.591289870	12.126164466
O	13.259869363	0.892104984	12.787584141
O	10.439411372	0.962507453	12.641733799
O	2.174464612	9.114299690	12.638264184
O	4.912646746	8.949474034	12.646388540
H	2.180284852	8.317875250	13.191309291
H	4.847531051	9.657884833	13.303523850
H	13.188258585	8.197766583	13.299406862
H	10.533302107	9.641156319	13.477868510
H	13.246995702	1.631514502	13.412627940
H	10.378156963	1.704238043	13.262490834
H	2.093691869	1.623763860	13.189292754
H	4.808233604	-0.008782407	13.139459467
H	9.449468346	14.746129483	11.981183095
H	10.670642475	13.054505762	13.577894742
H	1.715364298	13.908171705	12.691096008
H	0.063635207	14.625552642	10.933752183
H	1.078560512	6.580939215	12.007599252
H	2.700596835	5.398138586	13.109689867
H	6.288684754	11.668523873	12.037146426
W	10.465736776	6.678053691	12.936818619
O	10.599371790	4.922211748	12.814379454
O	9.196740441	7.264397155	11.446503772
H	12.023425357	6.994620733	13.542346049
C	8.570376276	6.381085063	14.161658750
H	7.972447331	7.298752036	14.317113279
C	10.508575666	7.186972067	15.095882136
C	9.374175126	6.235660565	15.462125106
H	9.792305276	5.216601069	15.521785346
C	11.776025533	7.108241579	15.938957312
H	11.554583202	7.263304268	17.009090380
H	12.257320510	6.124190848	15.839934946
H	12.515805561	7.866655975	15.643197340
C	7.589350074	5.242913040	13.761767257
H	7.643564146	5.119900560	12.665601583
C	6.131538519	5.589550277	14.118274012
H	5.439662035	4.791852834	13.796209611
H	6.016334035	5.698282770	15.207281798
H	5.808200198	6.521772007	13.638573922
C	7.956766567	3.888611992	14.384101134
H	7.318647802	3.084489188	13.994951550
H	8.991976701	3.605117520	14.158512328
H	7.834955958	3.911863442	15.476856940
H	10.093224093	8.211930808	15.147678058
C	8.639780218	6.531988385	16.776864619
H	7.829703114	5.811323313	16.961663118
H	9.323740209	6.495653286	17.638605312
H	8.191447347	7.537277474	16.740284990

1-butene (1,2) insertion (side path) into 2c species. E: -2343.1091575013

Al	0.723189332	4.903142600	8.589495507
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Al	4.871327127	6.973618644	7.185581742
O	3.415567753	7.189831561	11.204093980
O	7.705673671	4.851536252	9.755378382
O	3.396731160	6.844921018	8.433411515
O	7.772500884	5.004941638	7.114083667
Al	4.783844194	3.070207666	10.030249899
Al	0.663700601	0.966456645	11.342037611
O	7.629620003	0.807723876	7.279949024
O	3.510395052	3.061340989	8.643428666
O	7.571757787	1.126786059	10.080479840
O	3.508272417	2.884062125	11.348880913
Al	7.772798078	3.024629633	9.934545537
Al	3.511225621	0.974465367	11.336566633
O	4.992900506	0.728655887	7.213156130
O	0.618364835	3.070496815	8.640594614
O	4.995675430	1.132660904	10.084539206
O	0.688295409	2.840647079	11.284918502
Al	3.490289752	4.895545983	8.468758929
Al	7.738708692	7.118910924	7.192535587
O	0.765928330	7.189272579	11.287238745
O	4.839588178	4.929967510	9.925791202
O	0.773875589	6.850937313	8.473168553
O	4.912231969	5.082443916	7.268493094
Al	6.240197396	0.942485019	8.614266421
Al	6.286453793	0.834072127	11.439566130
Al	6.312998411	5.913150370	9.888929362
O	6.551228285	7.026158913	11.293885582
O	6.326838301	7.085497416	8.502900580
Al	2.076044002	7.019954491	9.904889350
Al	2.094397410	6.872564881	7.072318737
Al	2.046462396	2.052638801	8.572940621
O	2.186890397	0.954537513	7.126784776
O	2.102463134	0.876316674	9.928616924
Al	2.073814345	3.951247869	11.382692608
O	2.096775483	5.088061429	9.918466478
O	2.038613898	5.008963152	7.284289786
Al	6.218628984	3.921587181	7.191298644
O	6.254560539	2.851118749	8.652711292
O	6.300458037	2.913127739	11.275708643
H	1.924093471	1.380828899	6.296379532
H	4.109170578	1.139973495	7.281586666
H	7.336178342	1.400893184	6.543174634
H	6.270920206	7.686464244	5.309496587
H	3.572994744	6.206443829	5.317587010
H	0.614493401	7.601216168	5.206924163
H	5.885017161	2.434536867	5.404577313
H	8.262353837	4.723447907	6.315642020
O	6.318648403	6.944972272	5.931889799
O	3.503831661	7.021109132	5.843421410
O	0.625703023	6.947157592	5.918966237
O	6.605984100	2.976226004	5.763563708
Al	9.154058011	4.909369242	8.542876150
Al	13.291934080	7.053517417	7.309950587
O	11.675835548	7.256941293	11.369076385
O	16.116563400	4.908626727	9.837563426
O	11.779374879	6.929739812	8.550687274
O	16.116388315	5.060258839	7.191209803
Al	13.202609506	3.101198734	10.110711787
Al	9.073154918	1.032801921	11.340095038
O	15.977521734	0.890145653	7.433129656
O	11.924640049	3.124816424	8.732423070

O	15.950829512	1.130533048	10.170789439
O	11.912777105	2.898924364	11.427550972
Al	16.187380813	3.057873005	10.028307231
Al	11.894621495	1.019302808	11.446121315
O	13.249156060	0.792061706	7.508149585
O	9.116191682	3.061697220	8.635419277
O	13.395060774	1.154011536	10.236054058
O	9.048902424	2.901587730	11.282898962
Al	11.913821151	4.963909468	8.555903404
Al	16.151038232	7.132874506	7.296328180
O	13.239794850	4.929915095	9.997705195
O	9.128056514	6.861016648	8.475610999
O	13.317379433	5.166883606	7.356853094
Al	14.637465890	0.978959529	8.758575134
Al	14.692024977	0.881712618	11.574819893
Al	14.675550439	5.944293523	10.028781212
O	14.957993350	7.025555553	11.443031488
O	14.736040528	7.116885382	8.637695200
Al	10.449127865	7.088804563	9.961615371
Al	10.533783104	6.956459683	7.130170578
Al	10.564548773	2.016490066	8.557080124
O	10.344850097	0.873664812	7.189402297
O	10.515022028	0.884711415	10.007698108
Al	10.483435980	3.916592718	11.270155081
O	10.454769202	5.150947029	9.941730872
O	10.514008796	5.087338427	7.299111303
Al	14.579099164	3.973718475	7.343716327
O	14.651606173	2.898908185	8.791619232
O	14.723333346	2.982764825	11.373887448
H	9.363529610	0.990803653	7.071437426
H	13.377640755	1.362471453	6.725996555
H	15.714057253	1.432617048	6.659239067
H	14.642816893	7.781171783	5.467202838
H	12.087110578	6.235794246	5.479245049
H	9.083885429	6.664356141	5.097173800
H	14.361086779	3.114378586	5.120198469
H	16.602498458	4.891844631	6.357144435
O	14.726669950	7.026005702	6.068171625
O	11.980924588	7.089823809	5.933161233
O	9.112678924	7.176418369	5.916354670
O	14.646473126	2.832131691	6.000013590
Al	0.733887707	12.989282286	8.557269428
Al	4.869617286	14.988316140	7.070962066
O	3.505364338	15.251997012	11.052785856
O	7.693237201	12.980521826	9.755307305
O	3.408251212	14.867016332	8.322220395
O	7.722561796	12.994687206	7.051107909
Al	4.792952838	11.113240083	9.974635172
Al	0.724432448	9.149040655	11.446540931
O	7.636123918	8.942115154	7.368394985
O	3.502572540	11.047178227	8.564102090
O	7.623035200	9.270140825	10.158425491
O	3.518047124	10.925003896	11.271718957
Al	7.780700795	11.170413791	10.013954929
Al	3.548587288	9.062809716	11.372012300
O	4.990915846	8.861280714	7.347905498
O	0.616363935	11.173788103	8.712612170
O	5.056114259	9.188835592	10.150932263
O	0.711156071	11.044617302	11.372814495
Al	3.494503760	12.908649409	8.369575708
Al	7.700293724	15.087879315	7.137558044

O	0.794574481	15.238600273	11.129329116
O	4.824501049	12.917207566	9.767260658
O	0.776628578	14.921963635	8.381974007
O	4.898871311	13.076632143	7.122142454
Al	6.318121028	9.031967055	8.692517935
Al	6.327234130	8.971409727	11.510718144
Al	6.216821085	13.971650293	9.855062016
O	6.481208399	15.027871190	11.284718063
O	6.301460926	15.109184752	8.444465136
Al	2.162164068	15.086684691	9.809336500
Al	2.094416289	14.917170071	6.983528604
Al	1.992513688	10.091686648	8.602488128
O	2.109897734	8.952001447	7.192786856
O	2.043582119	8.950737378	10.005558290
Al	2.170844352	12.078542204	11.356412926
O	2.105790211	13.154722752	9.836632452
O	2.024316434	13.058311229	7.206761266
Al	6.202042125	11.911081108	7.185517608
O	6.267065071	10.919141555	8.697854319
O	6.301120967	11.068478332	11.284468363
H	2.345712437	9.362494318	6.346037957
H	4.167751675	9.329966016	7.579005243
H	7.394685941	9.555721764	6.632258971
H	6.348096346	14.257578955	5.255857702
H	3.515132341	14.173529566	5.261321894
H	0.570639229	15.657156332	5.078975837
H	5.720720422	10.274616751	5.659277570
H	8.282510924	12.770152784	6.279136369
O	6.317459240	15.019822594	5.851465044
O	3.492677618	15.011477716	5.753242159
O	0.618754045	15.083969610	5.854809660
O	6.464656554	10.893094015	5.768083038
Al	9.139102027	12.967479984	8.537969851
Al	13.255933517	15.073034444	7.220798769
O	11.839446389	15.260872182	11.275801879
O	16.133923423	13.067822275	9.903589828
O	11.776275115	14.918835770	8.468460354
O	16.129692421	13.078658055	7.183307695
Al	13.226476894	11.158902857	10.112995183
Al	9.074615386	9.180412400	11.412576355
O	16.116705410	8.948081941	7.521100223
O	11.938904739	11.075651277	8.712894090
O	16.024215006	9.275286740	10.253073867
O	11.924683377	10.968776250	11.422827293
Al	16.207487425	11.203357807	10.118047859
Al	11.971156323	9.093570280	11.428333725
O	13.462074720	8.934926328	7.436782142
O	9.041831442	11.141674705	8.643837880
O	13.468899819	9.213662199	10.247442396
O	9.105899645	11.047461395	11.352523925
Al	11.911777736	12.947680059	8.486424172
Al	16.137859492	15.222838786	7.235588090
O	9.127488142	15.249960702	11.198716581
O	13.234528119	12.977380028	9.917754051
O	9.122762300	14.861274500	8.394741143
O	13.321852926	13.154693302	7.275911973
Al	14.756168534	9.068288144	8.806368554
Al	14.753600830	8.937493187	11.625607603
Al	14.641947792	14.020847434	9.955627974
O	14.494914465	15.080508880	11.422933008
O	14.720518528	15.167592349	8.568535756

Al	10.520809339	15.095986823	9.869589443
Al	10.495511323	14.970152727	7.055684924
Al	10.449164080	10.113214691	8.648076038
O	10.524399069	8.961286306	7.266608288
O	10.462221084	9.023793858	10.076946990
Al	10.538563499	12.079902724	11.363919389
O	10.506464873	13.168275877	9.911649132
O	10.504683183	13.069585926	7.283554400
Al	14.622715266	11.984820176	7.312409514
O	14.712247446	10.980377064	8.815699273
O	14.719327260	11.123315785	11.415859001
H	9.954754257	9.257488155	6.536090688
H	12.648582546	9.455522735	7.569545065
H	15.952984942	9.607837264	6.809202049
H	14.725368617	14.454263293	5.344694647
H	11.956712732	14.230602449	5.390618243
H	9.047747785	15.584668286	5.114918151
H	14.237163940	10.323986814	5.785303896
H	16.665087773	12.828978542	6.399220708
O	14.719403974	15.166616299	6.000367726
O	11.919826582	15.083523192	5.857095577
O	9.051607525	14.940365523	5.838181892
O	14.952420783	10.970802212	5.918247520
O	7.700974449	9.195557711	12.712461944
H	7.779082541	8.484657900	13.370731926
H	14.653113036	11.740556651	12.160998233
O	13.325909054	9.029258119	12.787056164
O	10.513328408	9.027526167	12.737460147
O	-0.626537855	9.030842623	12.793999572
H	-0.585117780	9.782399722	13.403277408
O	2.415754433	13.234020173	12.649543796
O	10.587514836	13.313009482	12.649915480
H	7.487225668	14.962782260	11.322124117
H	13.498880834	14.999927872	11.542849789
H	3.346728979	14.593431336	11.774487798
H	11.528336125	14.707276997	12.035745590
O	1.873433503	5.002748601	12.791856634
H	7.555276153	6.948840610	11.450988217
H	4.143582239	6.555355022	11.087429411
H	15.966585646	6.951892492	11.498914922
O	7.701956665	0.967521617	12.638571541
H	7.781686661	0.316056705	13.348390914
O	-0.697771946	0.887182740	12.713085291
H	-0.617071914	0.111544124	13.288414372
H	6.339033467	3.460023965	12.076273540
O	4.901559003	0.817255876	12.641339078
O	2.098007176	0.882186958	12.563654783
H	14.801755162	3.591218054	12.126474699
O	13.259171601	0.892640765	12.787069109
O	10.439712139	0.963533325	12.641614239
O	2.171638404	9.113864754	12.641104360
O	4.913943350	8.942839924	12.698593702
H	2.170628323	8.323917269	13.203132442
H	4.860337311	9.670183133	13.335912512
H	13.184585179	8.209986002	13.306424408
H	10.541649408	9.658470583	13.473728478
H	13.247290151	1.628448886	13.416305620
H	10.382153209	1.716341114	13.249394302
H	2.093608184	1.623843124	13.188834680
H	4.807889261	-0.009561691	13.138350332
H	9.449972882	14.746133105	11.981155723

H	10.668244852	13.054876808	13.577902734
H	1.716018241	13.909943180	12.690693503
H	0.063641509	14.625247571	10.933288987
H	1.072623318	6.577344857	12.006791099
H	2.696524489	5.429237823	13.076956217
H	6.300163523	11.676626745	12.040314669
W	10.525644166	6.679372103	12.939958406
O	10.517158968	4.920552028	12.791038661
O	9.202889566	7.260004788	11.445943988
H	12.069137583	7.054071220	13.545001330
C	8.728498995	6.896702756	14.206931544
H	8.594908293	7.910142602	14.626263667
C	10.757640906	6.583361686	15.142210796
C	9.327676444	6.079697682	15.353607350
C	8.709469519	6.282009401	16.744264697
H	8.760920674	7.356776897	16.992086785
H	9.328067204	5.760587259	17.494280075
H	7.790342076	6.536680569	13.755874808
H	10.824305695	7.609073662	15.547806711
H	9.284860036	5.004259746	15.105097053
C	7.261849613	5.793961243	16.832934231
H	6.622148909	6.319517860	16.109079694
H	7.194538883	4.718354035	16.610617512
H	6.837199370	5.955619757	17.833674662
C	11.896070674	5.727492063	15.690708634
H	11.781644699	5.571190492	16.776855005
H	11.910364759	4.737049649	15.211979832
H	12.879780214	6.186986501	15.519852207

1-butene (2,1) insertion (side path) into 2c species. E: -2343.107270378

Al	0.723433148	4.902983611	8.589647970
Al	4.871102521	6.973635465	7.183474147
O	3.416308522	7.190352725	11.203857793
O	7.701560921	4.853051711	9.759229202
O	3.397486719	6.844980115	8.431840954
O	7.775091590	5.005553326	7.117394328
Al	4.785448873	3.070351303	10.031326367
Al	0.664142613	0.966671553	11.342207181
O	7.629668228	0.807985240	7.279964072
O	3.510562194	3.061392558	8.643964761
O	7.573627075	1.126855525	10.080974933
O	3.508841563	2.884139956	11.349520235
Al	7.772520952	3.022934768	9.937793368
Al	3.511817584	0.974459233	11.336593305
O	4.992882484	0.728835034	7.213195692
O	0.618473620	3.070452705	8.640439427
O	4.995894566	1.132620079	10.084349185
O	0.688803861	2.840824205	11.284695725
Al	3.490638763	4.895068550	8.468153709
Al	7.738776435	7.116339561	7.192871781
O	0.766616335	7.188998239	11.287766887
O	4.838910208	4.929958010	9.925549248
O	0.773992077	6.850835359	8.473316287
O	4.913091184	5.082367128	7.268605548
Al	6.240308997	0.943551479	8.614378278
Al	6.287078219	0.838430195	11.440488740
Al	6.307407082	5.916834234	9.885801587
O	6.544251834	7.038765764	11.285378870
O	6.325898672	7.085969994	8.500223167
Al	2.076917376	7.019268568	9.905320229
Al	2.094419563	6.872346458	7.072289170

Al	2.046873170	2.052684788	8.573186293
O	2.186904972	0.954510112	7.126880293
O	2.102586666	0.876273978	9.928688590
Al	2.074863712	3.951423519	11.383379107
O	2.096732204	5.088155931	9.918664533
O	2.038638177	5.008862898	7.284163234
Al	6.221513832	3.922755762	7.191243898
O	6.255585485	2.852272836	8.652951208
O	6.300900086	2.911597621	11.274598085
H	1.923308963	1.380732536	6.296700020
H	4.109449953	1.140827410	7.281257682
H	7.336372790	1.401447236	6.543313163
H	6.271875920	7.686256559	5.308601929
H	3.572542328	6.206461694	5.316678026
H	0.614179314	7.599985245	5.205890497
H	5.885238072	2.434798174	5.405955751
H	8.272333182	4.718807503	6.325760465
O	6.318857815	6.944805992	5.931080316
O	3.503634891	7.020885763	5.842948627
O	0.625600828	6.947149364	5.919019727
O	6.606935908	2.976440361	5.763550494
Al	9.153373410	4.911905731	8.567604630
Al	13.292082088	7.051904493	7.311096156
O	11.665417819	7.256690183	11.372868028
O	16.116637115	4.908337870	9.837559702
O	11.782585188	6.930862030	8.555180265
O	16.116330987	5.060228154	7.191260678
Al	13.204592119	3.097181997	10.111943350
Al	9.074262706	1.032623066	11.341334846
O	15.977554427	0.890005324	7.433073138
O	11.925367476	3.124466924	8.737375281
O	15.951414827	1.130362894	10.170803229
O	11.917402093	2.893146663	11.428170724
Al	16.188118744	3.057431724	10.028403521
Al	11.895795767	1.016513901	11.446097116
O	13.249317034	0.791988422	7.508076278
O	9.114723671	3.062872672	8.638415342
O	13.396182392	1.150172851	10.235756908
O	9.054992859	2.901859876	11.284566974
Al	11.920578804	4.964470658	8.572795147
Al	16.151039381	7.132628923	7.296601021
O	13.240943032	4.929121180	9.999144964
O	9.127468252	6.862279585	8.480302526
O	13.316575919	5.166513638	7.358095023
Al	14.637797481	0.978101178	8.758606167
Al	14.692729149	0.879756868	11.574888714
Al	14.677071884	5.944552072	10.029725092
O	14.958266822	7.025481645	11.443400955
O	14.736158510	7.116241468	8.637965538
Al	10.460047484	7.091074521	9.962975224
Al	10.532394111	6.953185488	7.139962149
Al	10.563297434	2.018793078	8.560196545
O	10.345574764	0.875333366	7.190787403
O	10.515096286	0.884158923	10.008405277
Al	10.493910855	3.912484204	11.290976729
O	10.449418347	5.156758665	9.984479866
O	10.515309015	5.086733163	7.346632797
Al	14.578643124	3.973633476	7.343910399
O	14.651722128	2.898561837	8.791787418
O	14.723605258	2.982418160	11.373449445
H	9.364357403	0.992117105	7.072161259

H	13.377890402	1.362054768	6.725723457
H	15.713908058	1.432552106	6.659321441
H	14.642936351	7.782565737	5.468901019
H	12.086074208	6.232373966	5.482404834
H	9.083823838	6.666853873	5.096897907
H	14.363547771	3.114648731	5.119522503
H	16.602846897	4.891273933	6.357548534
O	14.726129604	7.025873191	6.068075093
O	11.975118290	7.084561645	5.938468404
O	9.114092935	7.174407965	5.918824227
O	14.646383899	2.832165679	6.000067035
Al	0.733774942	12.988440118	8.557380755
Al	4.869633159	14.988790937	7.070967172
O	3.505419874	15.251898449	11.052682741
O	7.692259617	12.981489961	9.754920765
O	3.408292182	14.866795103	8.322269897
O	7.722705435	12.994835744	7.051011555
Al	4.791448101	11.113000170	9.973446965
Al	0.724172059	9.148713583	11.446734254
O	7.636250977	8.941135036	7.368757452
O	3.502571065	11.047339313	8.564001852
O	7.623524034	9.272151185	10.158685067
O	3.518116523	10.924821940	11.271835705
Al	7.778992771	11.173017897	10.010771259
Al	3.548359711	9.062411075	11.371708313
O	4.990676560	8.861504975	7.347350825
O	0.616159940	11.172096040	8.712612079
O	5.056144283	9.190425471	10.150815064
O	0.711219338	11.044420838	11.372730827
Al	3.494412065	12.909147845	8.369466253
Al	7.700325351	15.088573465	7.137547000
O	0.794695432	15.238585601	11.129422902
O	4.824815404	12.917096737	9.767645710
O	0.776664996	14.921811371	8.382042307
O	4.898766756	13.076679119	7.122003541
Al	6.317213601	9.032079443	8.691603312
Al	6.327733955	8.977404819	11.511214707
Al	6.216090266	13.973644258	9.855587780
O	6.481098044	15.030282919	11.284707434
O	6.301359430	15.109801082	8.444167338
Al	2.161967781	15.086785165	9.809440602
Al	2.094336306	14.917185099	6.983617792
Al	1.992775060	10.091217804	8.602733483
O	2.109994204	8.951981759	7.192829457
O	2.044547565	8.950456052	10.005714234
Al	2.170667309	12.078468544	11.356559117
O	2.105808634	13.154491609	9.836575331
O	2.024313313	13.058106984	7.206817654
Al	6.202292291	11.911799506	7.184863904
O	6.268234366	10.919849375	8.697669535
O	6.301959513	11.067002662	11.286188206
H	2.337309020	9.363962817	6.344510513
H	4.166428558	9.329563879	7.575760815
H	7.395838382	9.554894505	6.632498498
H	6.348183827	14.257759516	5.255724639
H	3.515287653	14.173548157	5.261456500
H	0.570586202	15.656846241	5.078844748
H	5.720939299	10.274142740	5.659826618
H	8.282890278	12.770491299	6.279152273
O	6.317499888	15.019909355	5.851432352
O	3.492635248	15.011532730	5.753305545

O	0.618792642	15.083844440	5.854804338
O	6.464553302	10.893115023	5.767990916
Al	9.139495639	12.968277281	8.537788775
Al	13.255970178	15.072921607	7.220930589
O	11.839439569	15.259820698	11.276087813
O	16.133949750	13.067420313	9.903457814
O	11.776349960	14.918732805	8.468620163
O	16.129622891	13.078408813	7.183540818
Al	13.225110776	11.157241050	10.114610596
Al	9.075769777	9.193018522	11.405485897
O	16.116430667	8.947820996	7.521265386
O	11.938756579	11.075547741	8.712980775
O	16.023600920	9.275118311	10.253558237
O	11.924147260	10.967211777	11.424035824
Al	16.206968630	11.202825228	10.118495337
Al	11.969297728	9.087430402	11.434084679
O	13.461687034	8.933294588	7.436730097
O	9.041762033	11.142186008	8.643576018
O	13.468392630	9.212840226	10.248718730
O	9.104368969	11.050964422	11.351221775
Al	11.912001366	12.947666929	8.486708524
Al	16.137999474	15.222631711	7.235632481
O	9.127582126	15.249846877	11.198887242
O	13.234384309	12.976609276	9.917854703
O	9.122819306	14.861626471	8.394720148
O	13.321838026	13.154656417	7.275904054
Al	14.755766406	9.067908471	8.807189300
Al	14.752544453	8.936922408	11.627029018
Al	14.641821272	14.020202601	9.955516555
O	14.495206662	15.079694463	11.423025069
O	14.720705165	15.167319061	8.568524922
Al	10.520560217	15.096194547	9.869756951
Al	10.495761033	14.970946651	7.056054750
Al	10.449190173	10.113931299	8.646786213
O	10.524766404	8.960413150	7.267479988
O	10.459413412	9.024612577	10.075594144
Al	10.539861876	12.080313749	11.364550432
O	10.506478076	13.168218853	9.911708952
O	10.504787172	13.069628700	7.283501574
Al	14.622421780	11.984494420	7.312941520
O	14.711848977	10.979992153	8.816191363
O	14.719101106	11.122967029	11.417510175
H	9.955866277	9.253423656	6.535199771
H	12.647852289	9.453434556	7.568991930
H	15.952219755	9.607686387	6.809584800
H	14.725363987	14.453850856	5.344912270
H	11.956156127	14.230462285	5.391024238
H	9.048018334	15.585009606	5.114942341
H	14.236852110	10.324539439	5.784361088
H	16.664686590	12.828709065	6.399245812
O	14.719408990	15.166327976	6.000453659
O	11.919826551	15.083572052	5.857207840
O	9.051925393	14.940823127	5.838316087
O	14.952350085	10.970803277	5.918378689
O	7.708668723	9.191277446	12.718996175
H	7.808407661	8.452325954	13.346251194
H	14.652590225	11.740796978	12.162154108
O	13.323969936	9.024414310	12.789656617
O	10.501856036	9.028148598	12.728913830
O	-0.626641880	9.030729284	12.793991210
H	-0.585062492	9.780316064	13.405618976

O	2.415825500	13.233964617	12.649536635
O	10.587373043	13.313122674	12.650273688
H	7.486971202	14.965048238	11.322313897
H	13.499272587	14.998784283	11.543270447
H	3.346555846	14.593591332	11.774556090
H	11.527835157	14.706374091	12.036023074
O	1.874032347	5.002329918	12.792421781
H	7.544004691	6.960539753	11.445642312
H	4.141747484	6.551569195	11.095952363
H	15.966759688	6.951610983	11.500888276
O	7.702564485	0.968487410	12.639093945
H	7.780465317	0.318664564	13.350558964
O	-0.697516311	0.887126327	12.713047227
H	-0.616262167	0.112812069	13.290052002
H	6.344642895	3.462533649	12.073430949
O	4.901646262	0.817291801	12.641565485
O	2.098198031	0.882264209	12.563604908
H	14.799723818	3.591190753	12.125993232
O	13.260133360	0.891970316	12.787362467
O	10.440210428	0.962644377	12.641949547
O	2.171931124	9.113743207	12.641289777
O	4.914857915	8.943722640	12.699681901
H	2.170727176	8.322817242	13.202098087
H	4.857596042	9.667352485	13.340891212
H	13.183093563	8.202913921	13.305145706
H	10.529427513	9.642933840	13.478705586
H	13.247200125	1.632153083	13.411480835
H	10.384500281	1.710706153	13.255485990
H	2.094005259	1.623867613	13.188849581
H	4.809548865	-0.010398278	13.137363371
H	9.449405552	14.745216082	11.981087479
H	10.668095433	13.054410101	13.578145050
H	1.715939441	13.909686041	12.691254010
H	0.063571495	14.625379484	10.933795410
H	1.077617693	6.580017945	12.008184395
H	2.701672346	5.400432138	13.104065880
H	6.299211249	11.677627125	12.040167201
W	10.459653919	6.671435437	12.927905649
O	10.600990819	4.917442571	12.812504013
O	9.196448755	7.265309141	11.441558403
H	11.988390090	7.046467262	13.578554928
C	8.526178241	6.338220552	14.060819133
H	7.873398372	7.215220817	14.221179444
C	10.433978654	7.088610187	15.109687699
C	9.281654589	6.126285425	15.376590923
H	10.033359187	8.115261007	15.198069039
H	9.658907625	5.091159192	15.429606212
C	11.672073032	6.941447306	15.984411159
H	12.144383982	5.958391953	15.840270482
H	12.430845509	7.705305197	15.759794277
H	8.712834601	6.306147594	16.310748880
C	7.654501807	5.173482391	13.575695597
H	8.152366145	4.232182047	13.858491386
H	7.617465062	5.152165604	12.477317011
H	11.412299027	7.028848777	17.054128050
C	6.224926712	5.208432712	14.133638431
H	5.632903988	4.325115087	13.838724084
H	6.229228706	5.234481516	15.233219011
H	5.694480749	6.100444270	13.769329787

isobutene (1,2) insertion (side path) into 2c species. E: -2343.108420107

Al	0.723172264	4.903220733	8.589587748
Al	4.871303145	6.973742375	7.185826404
O	3.415428868	7.189787588	11.204167797
O	7.705931177	4.851040375	9.754420830
O	3.396545508	6.844959888	8.433820934
O	7.771542243	5.004633355	7.113202994
Al	4.783621722	3.070357598	10.030861835
Al	0.663816714	0.966370888	11.342124406
O	7.629678708	0.807617082	7.279992124
O	3.510413262	3.061398574	8.643499919
O	7.570895765	1.126065994	10.080243171
O	3.508097878	2.884041681	11.349043239
Al	7.770804580	3.023899740	9.933445627
Al	3.511202252	0.974364817	11.336623732
O	4.992936727	0.728541256	7.213206635
O	0.618313478	3.070499164	8.640535504
O	4.995444196	1.132649918	10.084729811
O	0.688363433	2.840669090	11.285044746
Al	3.490273512	4.895671021	8.469003860
Al	7.738510916	7.120294789	7.192155081
O	0.765815118	7.189299062	11.287148703
O	4.839854322	4.929970546	9.925716870
O	0.773840489	6.850895242	8.473177901
O	4.911963463	5.082484320	7.268481039
Al	6.239837702	0.941519265	8.614816864
Al	6.286248943	0.833720125	11.440064386
Al	6.313807943	5.913320557	9.889631884
O	6.551390937	7.026097624	11.294260665
O	6.326832191	7.085640259	8.502916405
Al	2.075906751	7.019988172	9.904950525
Al	2.094402113	6.872643492	7.072410346
Al	2.046517016	2.052666972	8.572952063
O	2.186912366	0.954586192	7.126784298
O	2.102434780	0.876324834	9.928607668
Al	2.073767077	3.951290649	11.382733639
O	2.096746470	5.088055384	9.918496337
O	2.038602845	5.009017970	7.284346175
Al	6.217464558	3.921117093	7.191359929
O	6.254383996	2.850283373	8.652421639
O	6.300405282	2.913172425	11.275683761
H	1.924903191	1.380966015	6.296177891
H	4.109195459	1.139792076	7.281910115
H	7.335582419	1.400517243	6.543268664
H	6.270531601	7.685383553	5.308314768
H	3.572941945	6.206186069	5.318081238
H	0.614607361	7.601140068	5.206890526
H	5.885200154	2.434720584	5.403597884
H	8.258899393	4.724222612	6.312791482
O	6.318581998	6.944953498	5.931924330
O	3.503852505	7.021148399	5.843488631
O	0.625719099	6.947132153	5.918975972
O	6.605837214	2.976156406	5.763602594
Al	9.152578385	4.910026646	8.536990636
Al	13.291800431	7.054228915	7.309709324
O	11.678152791	7.258507781	11.366560411
O	16.116257108	4.908581922	9.837490783
O	11.779328787	6.930128918	8.549487495
O	16.116509379	5.060304307	7.191168347
Al	13.204908964	3.100099336	10.109202796
Al	9.072379676	1.031347154	11.340333624
O	15.977545589	0.890037651	7.433125781

O	11.923217051	3.124947158	8.732685569
O	15.951205643	1.130544416	10.170784633
O	11.913860224	2.895775765	11.423351250
Al	16.187820600	3.057902733	10.028491999
Al	11.895150812	1.017915801	11.445887657
O	13.249042837	0.792235968	7.508087237
O	9.117086045	3.061487447	8.635518061
O	13.395875652	1.151561183	10.235479805
O	9.046887317	2.899346278	11.280990609
Al	11.912881895	4.965169366	8.552562701
Al	16.151010323	7.132982237	7.296441753
O	13.239303472	4.929402447	9.997232893
O	9.127477680	6.861302962	8.474258951
O	13.317613293	5.166900997	7.356520775
Al	14.637905878	0.978049087	8.758733938
Al	14.692260223	0.881191146	11.574878153
Al	14.674729252	5.944303386	10.028855420
O	14.957864160	7.025584531	11.442973091
O	14.735927147	7.116899162	8.637620419
Al	10.446905222	7.089901439	9.961287614
Al	10.533912295	6.956868995	7.128682503
Al	10.564765491	2.013987178	8.554183482
O	10.343770556	0.872390086	7.187910960
O	10.514967014	0.884493608	10.007030707
Al	10.484439087	3.903361754	11.233708618
O	10.453687414	5.152604546	9.928772812
O	10.513826390	5.087362811	7.293775540
Al	14.579556075	3.973993038	7.343465986
O	14.651533186	2.898677427	8.791386432
O	14.723347534	2.982568925	11.373549329
H	9.362136434	0.989096998	7.070701110
H	13.379109147	1.362018437	6.725670661
H	15.714224814	1.432602966	6.659278033
H	14.643169516	7.780598362	5.466521323
H	12.087335263	6.236487508	5.478265256
H	9.083802042	6.663340132	5.097347107
H	14.360785782	3.114195464	5.120254732
H	16.602830150	4.892093272	6.357170759
O	14.726734127	7.026012609	6.068239658
O	11.981473954	7.090423987	5.932397444
O	9.112404591	7.176599476	5.915808543
O	14.646485300	2.832084788	6.000022129
Al	0.733894687	12.989399336	8.557303938
Al	4.869476099	14.988192245	7.070888942
O	3.505330548	15.251991131	11.052797047
O	7.693271759	12.980333548	9.755381673
O	3.408198094	14.867089486	8.322205079
O	7.722410638	12.994682799	7.051098998
Al	4.792740328	11.113517708	9.974571241
Al	0.724214314	9.149015325	11.446547701
O	7.636007617	8.942787832	7.368167876
O	3.502424398	11.047213590	8.564081315
O	7.622645249	9.270097262	10.158128585
O	3.517867914	10.925055848	11.271648913
Al	7.780681506	11.170094540	10.014456021
Al	3.548128350	9.062943424	11.372049384
O	4.990816805	8.861309921	7.347807826
O	0.616322569	11.174072052	8.712600499
O	5.055523288	9.188797038	10.150372896
O	0.711072117	11.044643944	11.372788857
Al	3.494442155	12.908713359	8.369613801

Al	7.700119459	15.087516609	7.137598707
O	0.794571707	15.238587511	11.129308289
O	4.824293372	12.917360031	9.767229954
O	0.776608020	14.921992453	8.381906159
O	4.898778637	13.076693827	7.122052416
Al	6.318038287	9.032138270	8.692448862
Al	6.326069532	8.971938387	11.508689226
Al	6.216836826	13.971346739	9.855280798
O	6.480686461	15.027515852	11.284851019
O	6.301406654	15.108886100	8.444637387
Al	2.162168799	15.086672954	9.809374643
Al	2.094423159	14.917143492	6.983511791
Al	1.992392237	10.091802264	8.602471565
O	2.109847709	8.952017100	7.192785580
O	2.043209812	8.950786902	10.005572460
Al	2.170726631	12.078580666	11.356445303
O	2.105759643	13.154757189	9.836610397
O	2.024320920	13.058345776	7.206751957
Al	6.201769903	11.911070970	7.185492859
O	6.266049303	10.919279207	8.697774891
O	6.300676924	11.068931455	11.283911903
H	2.346157748	9.362403103	6.346127555
H	4.167815848	9.330109164	7.579258481
H	7.394590089	9.556564243	6.632144271
H	6.348000380	14.257603542	5.255821526
H	3.515037457	14.173664984	5.261113535
H	0.570788258	15.657114176	5.078818232
H	5.721071068	10.273899944	5.660138440
H	8.282208430	12.770013280	6.279060289
O	6.317420086	15.019817781	5.851474289
O	3.492646697	15.011515194	5.753199853
O	0.618811104	15.084029899	5.854730387
O	6.464630995	10.893017818	5.768163511
Al	9.138952711	12.967238681	8.538047739
Al	13.255869874	15.072838495	7.220864187
O	11.839365696	15.260438032	11.275774532
O	16.133920287	13.067851225	9.903665473
O	11.776149545	14.918772270	8.468329313
O	16.129686676	13.078733118	7.183218235
Al	13.226364375	11.158791527	10.113046009
Al	9.074082559	9.177539784	11.414286512
O	16.116780027	8.948125828	7.521177743
O	11.938400287	11.075245312	8.713065934
O	16.023932045	9.275347314	10.253113598
O	11.924495177	10.968614510	11.422969252
Al	16.207365197	11.203389915	10.118073712
Al	11.970665292	9.093516827	11.427831296
O	13.462340372	8.935699342	7.436722712
O	9.041597735	11.141743454	8.643859760
O	13.468870263	9.214215553	10.247340224
O	9.105888483	11.046602231	11.353003134
Al	11.911721026	12.947312708	8.486479887
Al	16.137964761	15.222607402	7.235386492
O	9.127556448	15.249731388	11.198612778
O	13.234451035	12.977279646	9.917710534
O	9.122757595	14.861072041	8.394669672
O	13.321799616	13.154619974	7.275879800
Al	14.756169327	9.068427473	8.806461603
Al	14.753227837	8.937857950	11.625743817
Al	14.641908247	14.020704974	9.955684830
O	14.495108805	15.080173606	11.423160173

O	14.720604521	15.167443881	8.568462878
Al	10.520625515	15.095534710	9.869478779
Al	10.495387015	14.969095753	7.055237126
Al	10.448378609	10.112937392	8.647991036
O	10.524426580	8.961453791	7.266114581
O	10.459539040	9.023899760	10.076753915
Al	10.538002455	12.079551290	11.363965562
O	10.506436780	13.168031772	9.911611111
O	10.504630714	13.069415332	7.283547521
Al	14.622756781	11.984783532	7.312334970
O	14.712216340	10.980533374	8.815774361
O	14.719317428	11.123342298	11.416317380
H	9.955717849	9.258162092	6.535074503
H	12.648718429	9.456007287	7.569996929
H	15.953498125	9.607983534	6.809303833
H	14.725258577	14.454553099	5.344370319
H	11.957216278	14.230800855	5.390023230
H	9.047540797	15.584072706	5.114660751
H	14.237765083	10.323018904	5.786474077
H	16.665275894	12.828845545	6.399319183
O	14.719340156	15.166587300	6.000387266
O	11.919861411	15.083422663	5.857002128
O	9.051351322	14.939974287	5.838098013
O	14.952392527	10.970810279	5.918215068
O	7.697310319	9.196539842	12.711137499
H	7.756599337	8.490443527	13.376372787
H	14.653184240	11.740851392	12.161245420
O	13.325605228	9.028469927	12.787446502
O	10.515176683	9.026614204	12.739143949
O	-0.626588626	9.030773021	12.794002928
H	-0.585075727	9.782527409	13.403039169
O	2.415738658	13.234038365	12.649547043
O	10.587673255	13.312995096	12.649757824
H	7.486487600	14.962325512	11.323358970
H	13.499171202	14.999460647	11.543297428
H	3.346767728	14.593407697	11.774509904
H	11.528035782	14.706834075	12.035685760
O	1.873578070	5.002850615	12.791895686
H	7.555840279	6.948793321	11.452750062
H	4.144238617	6.556362936	11.086650291
H	15.966412167	6.952007676	11.498606436
O	7.701793124	0.967786776	12.638063048
H	7.781524903	0.324921177	13.355524428
O	-0.697734474	0.887164133	12.713072894
H	-0.616916864	0.112121776	13.289175437
H	6.342350822	3.459594610	12.076463599
O	4.901434532	0.817251314	12.641441096
O	2.097988818	0.882191185	12.563706824
H	14.799972443	3.591397996	12.126013452
O	13.259289040	0.892677509	12.786908977
O	10.439731944	0.963702358	12.641275857
O	2.171447121	9.113945250	12.641154189
O	4.913659775	8.942803960	12.697633949
H	2.170389704	8.324164032	13.203393968
H	4.860170687	9.669503951	13.335686132
H	13.185721382	8.206301990	13.302830468
H	10.547142667	9.664390307	13.469489678
H	13.246671044	1.628036496	13.416687440
H	10.381575069	1.715484236	13.250402642
H	2.093731555	1.623830631	13.188897202
H	4.807933009	-0.009237409	13.139031381

H	9.449789751	14.746076037	11.981272866
H	10.666163757	13.055616298	13.578143270
H	1.715972519	13.909899916	12.690991530
H	0.063663732	14.625122011	10.933504069
H	1.071672020	6.576928180	12.006644904
H	2.696195620	5.433988173	13.071574775
H	6.299810826	11.675821391	12.040723498
W	10.534953614	6.669365298	12.937338652
O	10.517355900	4.924281725	12.726384888
O	9.201718413	7.259854470	11.447929864
H	12.087246167	7.022942850	13.538598663
C	8.768663566	6.946501261	14.241618905
H	8.685770296	7.994992906	14.571392409
C	10.786219847	6.511914964	15.135172166
C	9.309254795	6.183144342	15.461968272
H	7.809845140	6.594888289	13.822747471
H	10.981832090	7.527675660	15.521764674
C	11.875987328	5.569163722	15.642913603
H	11.805960015	5.439290974	16.736430491
H	11.795672474	4.573764244	15.183451960
H	12.880291395	5.951896971	15.414430136
C	8.844617619	6.762831406	16.809420297
H	7.757955218	6.639575126	16.939472648
H	9.344184067	6.261145286	17.653200970
H	9.074280269	7.837341156	16.871158631
C	8.952308369	4.690031067	15.433457643
H	9.209671181	4.208876115	14.482801588
H	9.463341938	4.147782635	16.242304862
H	7.869610034	4.567131392	15.585724256

isobutene (2,1) insertion (top path) into 2c species. E: -2343.105615238

Al	0.722962413	4.903126016	8.589608035
Al	4.869979132	6.974302925	7.183806401
O	3.415743305	7.189883419	11.203674866
O	7.702528193	4.851885556	9.758706456
O	3.396098835	6.844888494	8.432203519
O	7.774258729	5.005371239	7.117344412
Al	4.784273199	3.070258502	10.030983523
Al	0.663962412	0.966572461	11.342198162
O	7.629601005	0.807874667	7.280189893
O	3.510447222	3.061286071	8.643532090
O	7.572838476	1.127176189	10.081644858
O	3.508247289	2.883974031	11.348815408
Al	7.771909694	3.023511722	9.938327701
Al	3.511433813	0.974398131	11.336761969
O	4.993033280	0.728734085	7.213401478
O	0.618317406	3.070482824	8.640521621
O	4.996201423	1.132968297	10.084811462
O	0.688351516	2.840763940	11.284882957
Al	3.489859702	4.895084742	8.467888082
Al	7.735450254	7.115632911	7.191551796
O	0.766051913	7.189237264	11.287406301
O	4.838722451	4.930094965	9.925817113
O	0.773443623	6.850779359	8.473139431
O	4.912666628	5.082408333	7.268608859
Al	6.240311078	0.943324471	8.614546100
Al	6.286608852	0.835353506	11.440865736
Al	6.309576352	5.913596017	9.883453042
O	6.548499730	7.034388977	11.281454262
O	6.325012177	7.085313225	8.499630879
Al	2.075707967	7.019790675	9.904744469

Al	2.093252064	6.872548570	7.072187516
Al	2.046552726	2.052637713	8.573041643
O	2.186944014	0.954483570	7.126862912
O	2.102511009	0.876247880	9.928611647
Al	2.074059268	3.951213001	11.382847043
O	2.096738795	5.088066258	9.918423947
O	2.038138816	5.008847859	7.284051381
Al	6.220700247	3.922431690	7.191017335
O	6.255059764	2.852384909	8.653400468
O	6.300872963	2.914077428	11.276867520
H	1.924650069	1.380787318	6.296313770
H	4.109347800	1.140179140	7.281729629
H	7.336364031	1.401146507	6.543391555
H	6.271633407	7.685103949	5.306889801
H	3.572418899	6.206954420	5.316506356
H	0.614065770	7.602386814	5.207954099
H	5.885221006	2.434275476	5.405801593
H	8.271182831	4.719135979	6.325348167
O	6.317381378	6.944645100	5.930597758
O	3.503297573	7.021119809	5.843100789
O	0.624697847	6.947233602	5.919031126
O	6.606636189	2.976184874	5.763573673
Al	9.152503158	4.910222053	8.567718280
Al	13.281593068	7.051430266	7.304818320
O	11.672386248	7.261286302	11.369503877
O	16.116372170	4.908616013	9.837569963
O	11.778181879	6.931074529	8.557885575
O	16.115600776	5.060330329	7.191188273
Al	13.203752142	3.098116032	10.112038311
Al	9.073855344	1.032212041	11.341655886
O	15.977527021	0.890034185	7.433183063
O	11.925015529	3.126376395	8.737409508
O	15.951168451	1.130456743	10.170770553
O	11.915987833	2.894362673	11.428524873
Al	16.187635304	3.057707686	10.028260396
Al	11.895498132	1.017231545	11.446262901
O	13.249206053	0.792097954	7.508205542
O	9.114743502	3.062123531	8.639041486
O	13.395845208	1.150991470	10.235847598
O	9.051626653	2.903186961	11.287260843
Al	11.918615512	4.967544592	8.574354514
Al	16.148243250	7.131774782	7.297042229
O	13.240883408	4.929488168	9.999260820
O	9.123784099	6.862216305	8.484623263
O	13.314802271	5.167576742	7.357481728
Al	14.637682190	0.978421689	8.758564072
Al	14.692533042	0.880016159	11.574748929
Al	14.676472990	5.945655518	10.028590742
O	14.957764025	7.026003561	11.443305706
O	14.734565686	7.116183466	8.637007817
Al	10.449300313	7.087597225	9.980374418
Al	10.522421039	6.955198537	7.150734634
Al	10.564142097	2.019218461	8.559896887
O	10.345771500	0.875511075	7.190846980
O	10.514897049	0.884610908	10.008632666
Al	10.490496453	3.914322808	11.292633448
O	10.447683109	5.157735312	9.986592949
O	10.513274138	5.086278418	7.348788962
Al	14.576936497	3.974365067	7.343818120
O	14.651393333	2.898918989	8.791705394
O	14.723458027	2.982569145	11.373605299

H	9.364502370	0.992169065	7.072690129
H	13.378063182	1.361998484	6.725755322
H	15.714293835	1.432972693	6.659574778
H	14.644593295	7.782103835	5.466315108
H	12.047287485	6.228832457	5.484653706
H	9.088276214	6.661733769	5.102268569
H	14.362806144	3.114589186	5.119745319
H	16.601771951	4.891117451	6.357324767
O	14.722565622	7.026019732	6.067032933
O	11.939908027	7.082963011	5.938083435
O	9.111340003	7.174712857	5.920934046
O	14.646317078	2.832424544	6.000203131
Al	0.733929083	12.988396441	8.557187699
Al	4.869857322	14.988376789	7.071371664
O	3.505324982	15.251942083	11.052613939
O	7.693727916	12.980334236	9.755918676
O	3.408471748	14.866529372	8.322251567
O	7.723006119	12.994911876	7.051280148
Al	4.793438728	11.112682663	9.973839126
Al	0.724297691	9.148894311	11.446431605
O	7.636369411	8.940267886	7.368948758
O	3.503153736	11.047074095	8.563935148
O	7.625709979	9.269721846	10.162379432
O	3.518449168	10.925375838	11.271415885
Al	7.782720426	11.169339777	10.013768478
Al	3.548657437	9.063026913	11.371494776
O	4.991021427	8.862076210	7.348190181
O	0.616294371	11.172074244	8.712349166
O	5.056601156	9.189989488	10.150415392
O	0.711041109	11.044495884	11.372548150
Al	3.494722672	12.908722637	8.369510113
Al	7.700473025	15.088230345	7.137999631
O	0.794546184	15.238601254	11.129317003
O	4.825293433	12.916593726	9.767278029
O	0.776688029	14.921801706	8.381912488
O	4.899399813	13.076255512	7.122356065
Al	6.319454601	9.031472859	8.693096480
Al	6.328981135	8.976315807	11.511008142
Al	6.217487252	13.971861491	9.855681333
O	6.481164861	15.028521913	11.284939993
O	6.301665928	15.109628323	8.445555265
Al	2.161894285	15.086622854	9.809347318
Al	2.094464635	14.916944696	6.983553892
Al	1.992938104	10.091126244	8.602359809
O	2.109809277	8.951951291	7.192545766
O	2.043945137	8.950626926	10.005535779
Al	2.170752722	12.078460770	11.356451479
O	2.105804515	13.154490537	9.836538418
O	2.024375416	13.058023624	7.206811376
Al	6.203367325	11.910895721	7.186091644
O	6.274507832	10.918649498	8.698965851
O	6.302438634	11.066753476	11.286547281
H	2.346511986	9.362343834	6.346002799
H	4.168323564	9.331460481	7.579382907
H	7.395928243	9.554441993	6.633082369
H	6.348220059	14.257221136	5.256730436
H	3.515570100	14.173732291	5.261078456
H	0.570708476	15.657033863	5.078943320
H	5.721095250	10.273949127	5.660625187
H	8.283298823	12.770602417	6.279475939
O	6.317583700	15.019882843	5.851819108

O	3.492849924	15.011420664	5.753412205
O	0.618790807	15.083924107	5.854831449
O	6.464690096	10.893038736	5.768363029
Al	9.139341969	12.967453302	8.538291421
Al	13.255778600	15.072869442	7.221231407
O	11.839499475	15.260042402	11.276096307
O	16.133823560	13.067210660	9.902956069
O	11.776271636	14.918651405	8.468791851
O	16.129697561	13.078411033	7.183256272
Al	13.224799207	11.156105355	10.113540941
Al	9.078622493	9.187119117	11.431839150
O	16.115282686	8.947361608	7.520986240
O	11.936417032	11.072988917	8.714618596
O	16.023795712	9.275097001	10.252731078
O	11.923285386	10.966833406	11.425514618
Al	16.207064070	11.202271970	10.117299318
Al	11.968526620	9.091833501	11.440360566
O	13.456550832	8.929521877	7.435318620
O	9.042062978	11.141879456	8.644408622
O	13.467700838	9.214075582	10.248508719
O	9.105921774	11.048583382	11.354918401
Al	11.911245730	12.946261260	8.486876847
Al	16.137907815	15.222678871	7.235577436
O	9.127586943	15.249774511	11.198873965
O	13.234010588	12.975790689	9.917875893
O	9.122942271	14.861372007	8.394969755
O	13.321653439	13.154298418	7.276203608
Al	14.752733561	9.066069121	8.805657213
Al	14.753683940	8.939106234	11.624431608
Al	14.641433508	14.019750496	9.955302121
O	14.495114527	15.079685709	11.422725373
O	14.720534173	15.167302501	8.568563254
Al	10.520636006	15.095901588	9.869746467
Al	10.495740828	14.970547349	7.056235406
Al	10.446380412	10.110614149	8.653411481
O	10.523097159	8.960496772	7.271791523
O	10.452030559	9.022183559	10.085417373
Al	10.539070443	12.080416192	11.366606279
O	10.506576605	13.167540426	9.912355936
O	10.504723154	13.069641404	7.283732514
Al	14.622642153	11.984607514	7.312544006
O	14.711411058	10.979236902	8.814881502
O	14.719167786	11.123178664	11.415998030
H	9.956448695	9.255305775	6.538558408
H	12.643115401	9.450747102	7.566777748
H	15.952136732	9.607475847	6.809322045
H	14.725138344	14.454400962	5.344516016
H	11.956256189	14.230517361	5.391106341
H	9.047990831	15.585089484	5.115219519
H	14.235859935	10.325957884	5.782246644
H	16.664818833	12.828976000	6.398908307
O	14.719318481	15.166509444	6.000449029
O	11.919830538	15.083563056	5.857394522
O	9.051934693	14.940781688	5.838475853
O	14.952312835	10.970676550	5.918213630
O	7.703846025	9.186911284	12.724415009
H	7.811294327	8.454675068	13.358286631
H	14.653856982	11.741043371	12.160719534
O	13.327696779	9.030014572	12.789262885
O	10.509672052	9.024015228	12.775556720
O	-0.626592010	9.030838841	12.793885231

H	-0.584894382	9.782577079	13.402946625
O	2.415770484	13.233980101	12.649478815
O	10.587532604	13.313424040	12.651126423
H	7.487070844	14.963449571	11.323046840
H	13.499180983	14.998926254	11.543156229
H	3.346745665	14.593579118	11.774505621
H	11.528101454	14.707011609	12.036413429
O	1.873444065	5.002754806	12.791864778
H	7.548594313	6.951136024	11.452249234
H	4.142674939	6.554394947	11.086160944
H	15.966163073	6.952158874	11.500578022
O	7.702233793	0.967626547	12.638788061
H	7.780623523	0.320742679	13.352855894
O	-0.697659611	0.887107047	12.713008336
H	-0.616486881	0.112858665	13.290110159
H	6.344687656	3.464743005	12.075643105
O	4.901385258	0.817224044	12.641434672
O	2.098038890	0.882195468	12.563680764
H	14.800888691	3.591334578	12.126014544
O	13.259988237	0.892008934	12.787332137
O	10.440095192	0.962648394	12.641935517
O	2.171938064	9.113817189	12.641036261
O	4.914980224	8.941801593	12.696131289
H	2.170476887	8.323364433	13.202416437
H	4.860977804	9.660606830	13.342858362
H	13.189684864	8.204496023	13.300545195
H	10.559326380	9.638196741	13.524939860
H	13.247731119	1.630759624	13.413108308
H	10.383576937	1.709456922	13.256920006
H	2.094174873	1.623596432	13.189167158
H	4.808155516	-0.009272025	13.139023622
H	9.449662826	14.745552381	11.981255680
H	10.663870149	13.054007045	13.579228116
H	1.715884152	13.909696324	12.691193626
H	0.063304524	14.625583424	10.933548445
H	1.073784402	6.577698654	12.006942624
H	2.697561292	5.423396459	13.082554395
H	6.298597940	11.676738242	12.041045754
W	10.528477098	6.676990783	12.960968147
O	10.593885344	4.919674380	12.809407507
O	9.203290426	7.263081647	11.502504719
H	12.080953293	7.071892830	13.504891947
C	8.691034656	6.592370756	14.287993718
H	8.284544029	7.572704885	14.599256661
C	10.843760638	6.822011550	15.176777871
C	9.528932534	6.107006002	15.472830736
H	9.669835240	5.016164562	15.401087608
C	12.073362980	6.062511108	15.683599134
H	11.995581761	5.916624921	16.776869885
H	12.157426742	5.068974791	15.220780023
H	13.010654198	6.602509830	15.483025978
H	9.096047819	6.307950873	16.476021264
C	10.847097788	8.242970213	15.738642673
H	10.889697663	8.209236341	16.842331117
H	11.723585238	8.814878973	15.394961069
H	9.937176053	8.802669041	15.474769993
C	7.544566844	5.639016768	13.937357886
H	7.936923770	4.695721742	13.525960187
H	6.980328220	5.384381726	14.852329867
H	6.828054355	6.052153315	13.220945829

1-butene (2,1) insertion (side path) into 2d species. E: -2336.221788550

Al	0.721991828	4.903396778	8.588025038
Al	4.868673466	6.973526625	7.182751472
O	3.414083964	7.191507492	11.203724931
O	7.699815594	4.852822758	9.759706773
O	3.391652595	6.845860669	8.430926740
O	7.773161778	5.005525028	7.117904687
Al	4.785213473	3.070319472	10.030768772
Al	0.665422818	0.968493034	11.340469999
O	7.629404973	0.808446478	7.279948528
O	3.510398716	3.061434519	8.643742363
O	7.574645224	1.127508703	10.081510883
O	3.508680364	2.883397342	11.349194184
Al	7.773412909	3.022785075	9.939541662
Al	3.512013728	0.973006217	11.335107832
O	4.992398156	0.728911854	7.212937076
O	0.618642758	3.070772749	8.640272014
O	4.995843064	1.132504133	10.084171551
O	0.689050648	2.841410608	11.284604669
Al	3.489277198	4.895022247	8.468407128
Al	7.734135563	7.115475170	7.191711890
O	0.762960611	7.190394025	11.286730950
O	4.837984661	4.930118596	9.925662905
O	0.771275966	6.852567395	8.471866595
O	4.912080391	5.082682409	7.268894120
Al	6.240075119	0.944466684	8.614062756
Al	6.287366971	0.839648712	11.440473985
Al	6.305889747	5.917447163	9.886050058
O	6.542892501	7.038827431	11.284946533
O	6.323247304	7.086251401	8.499594835
Al	2.074586577	7.019104997	9.904750051
Al	2.091502081	6.871996848	7.070895653
Al	2.046674072	2.052605555	8.571460220
O	2.187312963	0.955934013	7.125161634
O	2.101947554	0.875414083	9.927212744
Al	2.075313829	3.951710345	11.382927969
O	2.096105664	5.088554587	9.918316686
O	2.037631320	5.008811134	7.283867793
Al	6.220398482	3.922605640	7.191391534
O	6.254644360	2.852392759	8.653126288
O	6.300762702	2.911197450	11.274342066
H	1.918139544	1.382034726	6.296694511
H	4.108528813	1.140700882	7.278650456
H	7.336568214	1.402427296	6.543517139
H	6.270484776	7.685717995	5.307682014
H	3.572782583	6.205099144	5.317717727
H	0.607069459	7.585481736	5.193595197
H	5.884730133	2.433432982	5.407138787
H	8.271023414	4.719000892	6.326653424
O	6.317179742	6.944396139	5.930283517
O	3.502797910	7.020454615	5.842473762
O	0.622564332	6.949148927	5.921205028
O	6.606129777	2.976247356	5.763637108
Al	9.150499956	4.909108748	8.571874930
Al	13.278324526	7.022375823	7.293086156
O	11.620122004	7.259458218	11.426233260
O	16.117458853	4.908823936	9.837634425
O	11.774198035	6.924986056	8.561724085
O	16.115076556	5.061786800	7.191307563
Al	13.203038368	3.105197439	10.115746323
Al	9.074910884	1.034275426	11.342432053

O	15.977955547	0.891983751	7.429656180
O	11.925205284	3.127875642	8.738295834
O	15.952938478	1.131675976	10.168209022
O	11.914839034	2.900207203	11.433972314
Al	16.187880579	3.058393078	10.027780885
Al	11.896417338	1.024698246	11.447269223
O	13.248419638	0.794505234	7.507237974
O	9.113412646	3.062398964	8.639117089
O	13.395297885	1.189232712	10.234919023
O	9.057148598	2.904087313	11.287066559
Al	11.915376498	4.963312327	8.579645690
Al	16.140982602	7.138351167	7.300793258
O	13.240168795	4.932042421	10.000213140
O	9.123165013	6.861374378	8.482312849
O	13.314253127	5.160071385	7.358608586
Al	14.638629527	0.983624152	8.754578546
Al	14.694218126	0.883264317	11.566523638
Al	14.678247872	5.943763038	10.028183462
O	14.954921703	7.024507491	11.443085336
O	14.727718196	7.110030063	8.637341072
Al	10.455091238	7.087256444	9.975986990
Al	10.517970426	6.945905298	7.151773578
Al	10.563962442	2.021962374	8.562523257
O	10.346227157	0.877045545	7.191877144
O	10.515235814	0.885591949	10.009125639
Al	10.492001432	3.924059829	11.320567541
O	10.446950865	5.156377288	9.995949627
O	10.511350586	5.082211365	7.352849744
Al	14.581256874	3.972212686	7.343186558
O	14.653718964	2.901454542	8.790296084
O	14.726323927	2.986066567	11.376057190
H	9.365039391	0.994375888	7.073772672
H	13.373268694	1.366824456	6.725944142
H	15.717518729	1.439165185	6.657997811
H	14.635844887	7.784205965	5.471894705
H	12.018114064	6.146487242	5.517093289
H	9.090140966	6.670560314	5.097653555
H	14.370016126	3.116435846	5.116997016
H	16.600625600	4.899386425	6.355771747
O	14.721944317	7.021176141	6.062390137
O	11.929556957	7.022135492	5.931819743
O	9.110852114	7.175231469	5.921455283
O	14.646428104	2.832192745	5.999002274
Al	0.730700113	12.978550686	8.529967166
Al	4.869908026	14.989197874	7.071659633
O	3.503813835	15.251118811	11.050228146
O	7.687585968	12.981920804	9.753735951
O	3.405767981	14.865620117	8.320142492
O	7.722229816	12.995147641	7.051057109
Al	4.789628800	11.113391457	9.974861747
Al	0.713444379	9.149775505	11.442593911
O	7.635633053	8.940895106	7.369488306
O	3.501835797	11.047215666	8.564431889
O	7.619841567	9.272064202	10.157536465
O	3.514722103	10.926186008	11.271762014
Al	7.775058267	11.174800737	10.009647896
Al	3.544557747	9.063613382	11.374312215
O	4.989844872	8.860464735	7.345960674
O	0.609699918	11.154756596	8.701522185
O	5.053578923	9.190234195	10.151498771
O	0.702353624	11.045058841	11.363377758

Al	3.494439582	12.908662951	8.369223803
Al	7.700077899	15.089524441	7.137651419
O	0.792354302	15.238584165	11.124928786
O	4.823442063	12.917607707	9.767822474
O	0.776152366	14.918761360	8.347720453
O	4.898934016	13.077135260	7.122225232
Al	6.313504978	9.032245120	8.690925266
Al	6.322957083	8.974774760	11.511822284
Al	6.213518196	13.975536712	9.856151689
O	6.480995867	15.032260368	11.284744762
O	6.300514161	15.111298714	8.444637455
Al	2.159864910	15.084056372	9.802821988
Al	2.094496152	14.913838142	6.974218004
Al	1.996347955	10.088099510	8.602624458
O	2.107795587	8.951364344	7.193103237
O	2.038129238	8.950413598	10.005604791
Al	2.164616754	12.078850854	11.351817289
O	2.101073689	13.153770494	9.831025948
O	2.028426891	13.052239390	7.201951381
Al	6.201901828	11.911863672	7.184893490
O	6.260400945	10.918940005	8.697499971
O	6.300310672	11.067501675	11.285873349
H	2.292811802	9.369213101	6.337521563
H	4.163600503	9.329991646	7.563465189
H	7.396333006	9.554412837	6.632779067
H	6.349121876	14.256735836	5.257264571
H	3.522082899	14.174016198	5.258065249
H	0.580053067	15.643060366	5.055189262
H	5.721515639	10.273526870	5.660138634
H	8.284211726	12.770404538	6.280602295
O	6.317417454	15.019989688	5.851515649
O	3.494388798	15.010918370	5.751493752
O	0.620788182	15.086132468	5.843141895
O	6.464644803	10.893152623	5.768130301
Al	9.138077694	12.970641552	8.538425716
Al	13.256261889	15.076950181	7.216537241
O	11.841205319	15.265293680	11.273960301
O	16.128520820	13.060738906	9.839250347
O	11.775890285	14.921169081	8.467947734
O	16.127575035	13.073911018	7.128873042
Al	13.203574300	11.159337312	10.106306209
Al	9.062146270	9.193497339	11.400817478
O	16.051431960	8.949110343	7.517508377
O	11.920806476	11.108587796	8.716233755
O	15.981459192	9.274296432	10.246999954
O	11.917554782	10.969966956	11.430750664
Al	16.194300955	11.193062078	10.095104115
Al	11.944216570	9.092297133	11.455315946
O	13.400824155	8.880968312	7.433831805
O	9.038679739	11.143431916	8.643482321
O	13.420113256	9.207462427	10.249638633
O	9.100387274	11.052998217	11.348383931
Al	11.908587469	12.960731501	8.487023138
Al	16.137588138	15.226219368	7.218311956
O	9.126956997	15.251094898	11.199750991
O	13.228711203	12.980172818	9.917788535
O	9.121669260	14.864397178	8.394487356
O	13.321045367	13.158983749	7.274785557
Al	14.697048199	9.059333473	8.801265124
Al	14.735311910	8.932488403	11.618502810
Al	14.639741886	14.011661987	9.922738886

O	14.492348254	15.087508303	11.364922124
O	14.720873372	15.170964705	8.558244031
Al	10.517924389	15.100277890	9.870079341
Al	10.494175373	14.973515104	7.055130518
Al	10.448749617	10.120731704	8.652238926
O	10.527673097	8.961784642	7.270765328
O	10.453875237	9.023417879	10.078227706
Al	10.534218817	12.085347916	11.363550808
O	10.501192915	13.178227961	9.913052535
O	10.502170458	13.072968843	7.282539813
Al	14.616517360	11.986072777	7.303440939
O	14.659656948	10.973418588	8.802956563
O	14.713848778	11.129931602	11.375826296
H	9.961411605	9.255637993	6.536491202
H	12.564023199	9.371722447	7.510215697
H	15.905584729	9.613106653	6.805313843
H	14.721454079	14.457240446	5.338495684
H	11.953993909	14.229794548	5.392350946
H	9.045486818	15.587074272	5.114945474
H	14.220054496	10.341685716	5.749492722
H	16.653281963	12.824276662	6.340317230
O	14.717220309	15.168283565	5.995293711
O	11.919016845	15.084590439	5.855543901
O	9.051162685	14.942100422	5.837633627
O	14.947375466	10.966504290	5.914035258
O	7.702521652	9.192620140	12.718110551
H	7.806350013	8.452552664	13.343439205
H	14.644007816	11.747089036	12.121158803
O	13.318697653	9.027081382	12.791438435
O	10.445778800	9.034596044	12.738071942
O	-0.633455262	9.031237347	12.788464301
H	-0.592421239	9.782537724	13.398260478
O	2.414418674	13.232728458	12.647396141
O	10.586952023	13.314467926	12.651194236
H	7.486968364	14.966299100	11.321993191
H	13.496198531	15.002003055	11.493718587
H	3.346235597	14.591963789	11.771471577
H	11.535608614	14.710954697	12.035364461
O	1.873866197	5.002299820	12.792287693
H	7.545235669	6.962692094	11.443552140
H	4.140332162	6.553611015	11.096090754
H	15.963777260	6.955311784	11.499797665
O	7.702666957	0.968547768	12.639488877
H	7.780259105	0.316880754	13.349326877
O	-0.698152322	0.886170428	12.710331945
H	-0.616391890	0.115283362	13.291630976
H	6.343462730	3.461928659	12.073402143
O	4.901350984	0.817074874	12.641303220
O	2.098053540	0.881619789	12.562934152
H	14.817286529	3.593110704	12.128380235
O	13.267600294	0.889939724	12.782977054
O	10.440967918	0.962685728	12.642539022
O	2.166589663	9.114630453	12.639837791
O	4.912209999	8.944068452	12.700926222
H	2.162970965	8.324827955	13.202144347
H	4.858449234	9.667011981	13.343130148
H	13.180365847	8.217867809	13.325133144
H	10.442962281	9.661218063	13.478579912
H	13.262569146	1.627745054	13.410110425
H	10.383812973	1.705796159	13.261926227
H	2.094962036	1.623549941	13.187781883

H	4.810415858	-0.010754399	13.137079644
H	9.450797339	14.747690114	11.981980214
H	10.681608654	13.053515747	13.577094059
H	1.715542884	13.909293696	12.691137262
H	0.049839640	14.642920714	10.923812133
H	1.073558304	6.583358579	12.008829726
H	2.701307550	5.399337479	13.105744112
H	6.299370871	11.677973542	12.039960260
W	10.418567931	6.671389848	12.958595873
O	10.595322376	4.916210683	12.871037182
O	9.184553014	7.260638632	11.444400775
H	11.924923747	7.094637392	13.640196516
C	8.462630386	6.335146038	14.058575403
H	7.790609673	7.202192777	14.190205134
C	10.351758106	7.071554630	15.130091999
C	9.178583878	6.143788995	15.405132467
H	9.528171336	5.102846174	15.491763889
H	8.580441658	6.359676242	16.310955375
H	11.276649148	6.897367627	15.695044587
H	10.057160831	8.122779351	15.282748876
C	7.615880123	5.154225169	13.567058702
H	7.583377692	5.135830374	12.468536372
H	8.130798550	4.222346465	13.850555420
C	6.184429921	5.162922036	14.122369030
H	5.639146501	6.044634035	13.754922703
H	6.187981199	5.193478533	15.221831484
H	5.608713170	4.267505676	13.831560406

isobutene (2,1) insertion (top path) into 2d species. E: -2336.222459485

Al	0.723144568	4.903230914	8.589570348
Al	4.871258782	6.973779704	7.185838232
O	3.415473839	7.189929411	11.204141852
O	7.705816581	4.851264863	9.754508152
O	3.396681102	6.844917039	8.433592558
O	7.771838663	5.004721122	7.113410073
Al	4.783589062	3.070121653	10.030441164
Al	0.663762381	0.966398643	11.342117555
O	7.629618284	0.807646895	7.279924291
O	3.510326491	3.061373144	8.643478990
O	7.570789001	1.126174451	10.080080740
O	3.508180546	2.884017256	11.348923071
Al	7.771539618	3.024023213	9.933656358
Al	3.511175096	0.974383439	11.336575448
O	4.992866384	0.728550719	7.213064492
O	0.618321814	3.070496709	8.640592871
O	4.995391310	1.132573589	10.084564270
O	0.688367868	2.840697546	11.285025925
Al	3.490170388	4.895616362	8.468907923
Al	7.738578266	7.120016894	7.192194239
O	0.765816152	7.189314592	11.287212499
O	4.839664745	4.929911367	9.925706706
O	0.773844747	6.850927702	8.473225353
O	4.912071772	5.082503212	7.268499531
Al	6.239917986	0.941858596	8.614482365
Al	6.286247802	0.833715137	11.439693019
Al	6.313248329	5.913000556	9.888832736
O	6.551251015	7.026035126	11.293836375
O	6.326933054	7.085649140	8.502929041
Al	2.076079001	7.020067427	9.904958739
Al	2.094331933	6.872646570	7.072428646
Al	2.046441607	2.052611006	8.572973581

O	2.186979033	0.954605072	7.126763237
O	2.102466641	0.876334071	9.928641026
Al	2.073816109	3.951314671	11.382733518
O	2.096754158	5.088069382	9.918486276
O	2.038577259	5.008999787	7.284295607
Al	6.217792215	3.921205245	7.191254297
O	6.254261589	2.850554201	8.652395365
O	6.300241123	2.913103889	11.275446955
H	1.924251382	1.380887408	6.296330705
H	4.109124134	1.139836943	7.281639171
H	7.335900268	1.400648455	6.543132805
H	6.270475662	7.685879612	5.308803305
H	3.572940461	6.206191339	5.317995606
H	0.614663650	7.601695035	5.207329330
H	5.885165290	2.434490363	5.404013629
H	8.259935282	4.724184647	6.313497191
O	6.318599894	6.945017637	5.931903560
O	3.503849740	7.021076355	5.843512931
O	0.625721327	6.947182409	5.918966977
O	6.605879249	2.976164978	5.763517988
Al	9.153191144	4.909586688	8.538166644
Al	13.292034117	7.054101187	7.309722286
O	11.676324033	7.258316716	11.364332584
O	16.116385482	4.908552351	9.837504105
O	11.779739923	6.930085791	8.548887185
O	16.116478218	5.060301665	7.191204410
Al	13.204013601	3.100311670	10.109783082
Al	9.072621021	1.031845739	11.339753905
O	15.977455978	0.890036441	7.433108073
O	11.923694030	3.124759992	8.732337005
O	15.951210884	1.130509859	10.170737446
O	11.913454551	2.896213494	11.424046190
Al	16.187652311	3.057794651	10.028442189
Al	11.894957633	1.018243443	11.445531531
O	13.249091959	0.792115371	7.508082967
O	9.116723115	3.061466508	8.635127990
O	13.395799322	1.151967043	10.235477998
O	9.047243736	2.899539386	11.281008775
Al	11.913034280	4.964476600	8.553118590
Al	16.151044870	7.132989256	7.296377273
O	13.239381563	4.929600061	9.997311739
O	9.127891773	6.861409906	8.474210838
O	13.317558687	5.166879629	7.356564858
Al	14.637720621	0.978422217	8.758640372
Al	14.692183299	0.881174634	11.574726221
Al	14.675036509	5.944180198	10.028774744
O	14.957820446	7.025591972	11.443026406
O	14.735967801	7.116965374	8.637657584
Al	10.448355668	7.090119967	9.957684786
Al	10.534197556	6.956322569	7.127816224
Al	10.564678346	2.014717111	8.554990252
O	10.344107908	0.872686803	7.188290202
O	10.514934748	0.884435892	10.006957887
Al	10.483838663	3.907564302	11.243824336
O	10.453898956	5.152253467	9.930480557
O	10.513898368	5.087306039	7.294269595
Al	14.579386670	3.973857453	7.343595833
O	14.651553302	2.898736871	8.791472950
O	14.723317464	2.982628734	11.373618994
H	9.362596411	0.989601643	7.070854902
H	13.378448024	1.362061592	6.725710207

H	15.714097700	1.432599459	6.659266766
H	14.643202076	7.780671538	5.466569993
H	12.088085079	6.236593445	5.477790442
H	9.083202962	6.664426554	5.096562826
H	14.360976089	3.114256785	5.120202008
H	16.602749472	4.891917908	6.357222683
O	14.726792621	7.026030600	6.068193341
O	11.981688560	7.090361774	5.932101307
O	9.112409724	7.176507708	5.915738669
O	14.646482426	2.832092010	6.000014146
Al	0.733854739	12.989408936	8.557266032
Al	4.869510762	14.988207786	7.070778449
O	3.505296366	15.251984117	11.052781665
O	7.693111379	12.980462032	9.755228468
O	3.408235486	14.867005968	8.322212959
O	7.722465886	12.994670372	7.051072604
Al	4.792808423	11.113270021	9.974586971
Al	0.724414841	9.148995633	11.446616461
O	7.636000011	8.942663666	7.368252691
O	3.502500525	11.047160531	8.564077463
O	7.622891141	9.270335244	10.158273096
O	3.518049238	10.925626789	11.271658868
Al	7.780468063	11.170425485	10.013843763
Al	3.548598249	9.063197147	11.372206027
O	4.990841657	8.861311005	7.348003846
O	0.616360232	11.174100223	8.712615601
O	5.056067423	9.188902546	10.150932014
O	0.711089638	11.044650274	11.372822986
Al	3.494428160	12.908659784	8.369684185
Al	7.700233348	15.087641929	7.137471409
O	0.794617765	15.238611458	11.129311959
O	4.824458019	12.917227696	9.767291676
O	0.776594999	14.921967166	8.381927217
O	4.898797072	13.076652658	7.122154012
Al	6.318031971	9.032118166	8.692784718
Al	6.327541780	8.971364275	11.510740650
Al	6.216719109	13.971547429	9.854966273
O	6.480856213	15.027476204	11.284748994
O	6.301373315	15.108880311	8.444181051
Al	2.162119550	15.086715442	9.809344958
Al	2.094399067	14.917144903	6.983516463
Al	1.992363706	10.091748788	8.602472765
O	2.109801255	8.952004502	7.192772222
O	2.043428672	8.950817405	10.005587810
Al	2.170730767	12.078744027	11.356455311
O	2.105742351	13.154795203	9.836611255
O	2.024324147	13.058360925	7.206772397
Al	6.201903466	11.911125519	7.185469117
O	6.266455758	10.919270214	8.697799490
O	6.301280217	11.068298306	11.284670385
H	2.346751478	9.362335751	6.346263756
H	4.167951052	9.330311485	7.579385087
H	7.393931087	9.556217806	6.632216481
H	6.348096779	14.257663732	5.255614382
H	3.515051686	14.173630550	5.261157834
H	0.570671388	15.657208221	5.078955158
H	5.720526684	10.274911849	5.658843248
H	8.282357937	12.770027199	6.279102699
O	6.317427241	15.019780231	5.851373302
O	3.492610392	15.011500003	5.753205810
O	0.618782644	15.083987491	5.854764822

O	6.464600563	10.893147485	5.768033411
Al	9.139128917	12.967387737	8.538078548
Al	13.255942508	15.072882496	7.220848131
O	11.839373481	15.260470864	11.275834957
O	16.133916188	13.067858907	9.903602974
O	11.776203964	14.918747619	8.468358972
O	16.129674413	13.078669081	7.183238721
Al	13.226593828	11.159005599	10.112927310
Al	9.074990735	9.181878355	11.412945221
O	16.116813698	8.948143799	7.521159577
O	11.939070208	11.075675250	8.712718780
O	16.024178499	9.275351019	10.253057551
O	11.924656249	10.968822648	11.422704177
Al	16.207554312	11.203459868	10.118067878
Al	11.970607059	9.094571286	11.427839222
O	13.462391248	8.935474258	7.436721916
O	9.041731450	11.141750488	8.643760485
O	13.469005541	9.214011303	10.247217280
O	9.105622628	11.047742044	11.352569321
Al	11.911826193	12.947647339	8.486568092
Al	16.137889328	15.222673604	7.235502005
O	9.127530181	15.249814970	11.198663262
O	13.234559936	12.977433989	9.917729159
O	9.122749325	14.861082581	8.394699117
O	13.321795391	13.154665168	7.275878683
Al	14.756178221	9.068384225	8.806454517
Al	14.753493877	8.937931675	11.625464269
Al	14.641986287	14.020850919	9.955653713
O	14.495073004	15.080253847	11.423045390
O	14.720613943	15.167452685	8.568428599
Al	10.520689920	15.095529472	9.869562727
Al	10.495493473	14.969475556	7.055399216
Al	10.449113155	10.113600650	8.647499957
O	10.524352191	8.961464262	7.266063681
O	10.461286580	9.024618523	10.076422814
Al	10.538430537	12.079811588	11.364685582
O	10.506489631	13.168025864	9.911750814
O	10.504684685	13.069454197	7.283533002
Al	14.622736532	11.984805677	7.312395396
O	14.712309627	10.980510424	8.815763934
O	14.719295708	11.123309605	11.416334611
H	9.953967027	9.257681888	6.536102195
H	12.648955466	9.456104071	7.569647865
H	15.953013584	9.607869351	6.809221663
H	14.725351422	14.454290841	5.344596208
H	11.957077345	14.230692156	5.390264379
H	9.047756208	15.584235186	5.114694587
H	14.237284197	10.323721699	5.785628308
H	16.665210880	12.828876669	6.399280172
O	14.719364213	15.166569779	6.000341216
O	11.919835871	15.083431975	5.857027996
O	9.051464020	14.940094149	5.838100037
O	14.952383428	10.970788158	5.918239075
O	7.701922514	9.194304645	12.713461691
H	7.784330890	8.474868379	13.362344508
H	14.652892272	11.740836453	12.161245945
O	13.325811691	9.028833670	12.787063824
O	10.513329684	9.025591396	12.736674623
O	-0.626568106	9.030808800	12.793986858
H	-0.584974452	9.782552154	13.403031640
O	2.415743359	13.234117850	12.649585287

O	10.587531935	13.313077652	12.650100220
H	7.486755332	14.962273269	11.322679960
H	13.499115173	14.999534609	11.543156887
H	3.346634979	14.593439958	11.774508839
H	11.528216986	14.707054244	12.035949652
O	1.873452300	5.002831018	12.791858789
H	7.555174273	6.948450482	11.450824792
H	4.143864199	6.555906230	11.087465586
H	15.966422599	6.951949632	11.498849925
O	7.701828564	0.967544784	12.638325049
H	7.781630718	0.318476340	13.350298670
O	-0.697762043	0.887164873	12.713001949
H	-0.617017357	0.112374268	13.289428444
H	6.339580664	3.460252149	12.075783810
O	4.901462344	0.817228460	12.641376559
O	2.097975199	0.882211062	12.563703543
H	14.800900475	3.591139580	12.126229851
O	13.259347155	0.892659570	12.786805529
O	10.439724455	0.963769260	12.641229704
O	2.171610937	9.113995016	12.641127086
O	4.914004948	8.942915504	12.697772195
H	2.170817963	8.324379626	13.203604703
H	4.860995938	9.668082575	13.337550616
H	13.182688906	8.204687861	13.299092535
H	10.550440492	9.644722982	13.482880081
H	13.246950312	1.628560660	13.415952063
H	10.382263071	1.719595244	13.245337081
H	2.093805197	1.623890591	13.188854067
H	4.807791021	-0.009365188	13.138751461
H	9.449940205	14.746105481	11.981258902
H	10.667051320	13.054288439	13.578057375
H	1.715892736	13.909858542	12.691356187
H	0.063655599	14.625215949	10.933604597
H	1.072284391	6.577208409	12.006709451
H	2.696245779	5.431404188	13.074810127
H	6.299860677	11.676715188	12.040315716
W	10.527139100	6.677740416	12.929135260
O	10.517257415	4.924594765	12.737966342
O	9.202357901	7.261819374	11.444051807
H	12.070484426	7.055346048	13.532819449
C	8.724056800	6.858210121	14.200641606
H	8.532600441	7.861230607	14.612320380
C	10.793642510	6.571183243	15.147873757
C	9.359567751	6.054604826	15.336049236
H	7.804419330	6.454936840	13.749007585
H	9.310777782	4.974645072	15.133500610
C	11.883524334	5.583772434	15.571582417
H	11.807902936	5.391568623	16.657749644
H	11.784316902	4.621070350	15.051496615
H	12.893431606	5.970158582	15.369946696
H	8.931875767	6.222890353	16.344485444
C	11.004159686	7.908388455	15.857888776
H	10.995322178	7.762796840	16.953136648
H	11.970999646	8.360080685	15.589642385
H	10.215544323	8.640332818	15.628570664

2-butene insertion (top path) into 2d species. E: -2336.224178859

Al	0.723203635	4.903144639	8.589478586
Al	4.871352459	6.973676583	7.185712433
O	3.415460293	7.189843991	11.204150756
O	7.705716166	4.851435380	9.755407615

O	3.396662052	6.844925352	8.433585158
O	7.772540928	5.004907095	7.114147055
Al	4.783845881	3.070134171	10.030132072
Al	0.663681098	0.966406868	11.342070596
O	7.629604998	0.807734573	7.279979252
O	3.510395568	3.061320526	8.643370463
O	7.571759406	1.126767125	10.080492176
O	3.508271572	2.884029421	11.348861965
Al	7.772797003	3.024502503	9.934461063
Al	3.511212282	0.974470227	11.336527170
O	4.992898589	0.728613543	7.213148626
O	0.618337681	3.070458457	8.640553375
O	4.995651990	1.132631318	10.084552161
O	0.688275072	2.840644019	11.284964924
Al	3.490276967	4.895556388	8.468762250
Al	7.738719216	7.118875603	7.192595053
O	0.765817558	7.189312243	11.287194463
O	4.839687391	4.929957049	9.925752687
O	0.773845789	6.850892479	8.473163790
O	4.912232297	5.082479840	7.268551106
Al	6.240149023	0.942412712	8.614288053
Al	6.286472484	0.834016135	11.439574490
Al	6.313188045	5.913195418	9.889235316
O	6.551145504	7.026078195	11.294223242
O	6.326928829	7.085512903	8.503190867
Al	2.076042805	7.020045914	9.904833750
Al	2.094382652	6.872618120	7.072353874
Al	2.046477924	2.052637600	8.572902801
O	2.186866850	0.954547815	7.126771891
O	2.102455041	0.876328280	9.928592898
Al	2.073778761	3.951213057	11.382569943
O	2.096783067	5.088084752	9.918447463
O	2.038623555	5.008996395	7.284272401
Al	6.218618928	3.921627628	7.191302750
O	6.254500761	2.851051619	8.652664401
O	6.300432819	2.913087465	11.275602824
H	1.923996849	1.380797812	6.296371102
H	4.109148133	1.139912844	7.281484651
H	7.336181666	1.400915658	6.543203150
H	6.271012015	7.686096092	5.309245642
H	3.572965619	6.206301201	5.317829254
H	0.614581513	7.601385112	5.207043716
H	5.885038227	2.434528744	5.404603310
H	8.262640579	4.723155587	6.315946410
O	6.318647445	6.944936042	5.932026182
O	3.503843488	7.021105763	5.843466525
O	0.625724338	6.947173585	5.918942233
O	6.606007655	2.976216820	5.763591423
Al	9.154000765	4.909306568	8.543079792
Al	13.291911526	7.053567058	7.309970092
O	11.676051352	7.257288251	11.368140484
O	16.116512938	4.908607489	9.837502312
O	11.779314719	6.929793906	8.550674971
O	16.116424146	5.060242846	7.191214512
Al	13.202594898	3.101182643	10.110741807
Al	9.073145065	1.032759009	11.340162823
O	15.977508662	0.890139765	7.433094942
O	11.924635531	3.124906231	8.732458423
O	15.950785914	1.130515717	10.170784841
O	11.912736471	2.898992965	11.427636263
Al	16.187408937	3.057823502	10.028256874

Al	11.894557165	1.019354352	11.446095692
O	13.249138074	0.792067288	7.508137516
O	9.116215076	3.061657489	8.635440766
O	13.395023205	1.154335807	10.236008589
O	9.048846010	2.901572279	11.282924773
Al	11.913828578	4.963968755	8.556045099
Al	16.151036800	7.132865205	7.296310268
O	13.239756566	4.929925894	9.997734139
O	9.128065337	6.860999329	8.475720223
O	13.317353038	5.166899581	7.356862601
Al	14.637464725	0.979054008	8.758488057
Al	14.691987959	0.881732749	11.574814989
Al	14.675496107	5.944273291	10.028715571
O	14.957986326	7.025602256	11.442981220
O	14.736030783	7.116892441	8.637664589
Al	10.448621606	7.089047387	9.961345052
Al	10.533841116	6.956380505	7.130097712
Al	10.564596386	2.016518231	8.557111730
O	10.344876832	0.873652586	7.189392748
O	10.515041458	0.884734347	10.007748426
Al	10.483282466	3.916476462	11.270235147
O	10.454788350	5.150895186	9.942032350
O	10.513958121	5.087343935	7.299286997
Al	14.579073653	3.973759210	7.343702574
O	14.651619731	2.898934859	8.791626863
O	14.723359866	2.982785130	11.373929472
H	9.363560637	0.990777302	7.071438122
H	13.377609614	1.362468814	6.725971214
H	15.714072526	1.432615044	6.659200928
H	14.642976959	7.780834609	5.466847537
H	12.087372402	6.235920331	5.479099077
H	9.083758791	6.663460542	5.097701692
H	14.360996840	3.114337232	5.120191533
H	16.602551080	4.891784396	6.357168491
O	14.726672443	7.025987941	6.068212500
O	11.980876701	7.089835234	5.933141191
O	9.112644595	7.176458619	5.916322031
O	14.646424711	2.832139707	6.000011224
Al	0.733894410	12.989424417	8.557266963
Al	4.869611907	14.988270666	7.070941991
O	3.505327183	15.251993892	11.052784183
O	7.693307832	12.980539457	9.755292735
O	3.408249412	14.866990165	8.322225667
O	7.722561769	12.994720062	7.051128236
Al	4.793025754	11.113279945	9.974665366
Al	0.724422064	9.149041055	11.446489914
O	7.636131313	8.942077335	7.368427145
O	3.502604773	11.047175643	8.564104404
O	7.623045517	9.270077967	10.158589958
O	3.518016016	10.925272904	11.271638223
Al	7.780803582	11.170435361	10.014172716
Al	3.548550145	9.063066648	11.372238202
O	4.990941742	8.861307317	7.347986886
O	0.616383330	11.174092648	8.712595580
O	5.056087579	9.188852834	10.150918407
O	0.711108846	11.044652722	11.372796167
Al	3.494510212	12.908679650	8.369607826
Al	7.700318323	15.087939184	7.137626960
O	0.794558185	15.238608699	11.129317581
O	4.824531982	12.917216968	9.767239744
O	0.776618717	14.921989271	8.381952766

O	4.898911898	13.076624899	7.122166020
Al	6.318197209	9.031953906	8.692634228
Al	6.327212089	8.971484422	11.510725043
Al	6.216872129	13.971623145	9.855140424
O	6.481202658	15.027842858	11.284749041
O	6.301479611	15.109236927	8.444670722
Al	2.162144343	15.086708339	9.809322836
Al	2.094444632	14.917124490	6.983491829
Al	1.992457163	10.091785519	8.602464098
O	2.109888149	8.952023801	7.192796948
O	2.043382747	8.950802122	10.005542783
Al	2.170783975	12.078659546	11.356401699
O	2.105774780	13.154758560	9.836621889
O	2.024323556	13.058321246	7.206756396
Al	6.202099573	11.911043224	7.185570468
O	6.267475490	10.919125680	8.697919378
O	6.301125314	11.068460556	11.284509458
H	2.346026842	9.362431947	6.346102175
H	4.167874881	9.330084583	7.579242003
H	7.394560764	9.555613924	6.632271074
H	6.348138633	14.257467304	5.256020065
H	3.515158004	14.173605279	5.261201331
H	0.570629280	15.657071150	5.078891713
H	5.720648767	10.274759829	5.659052146
H	8.282461141	12.770231530	6.279106209
O	6.317463337	15.019803216	5.851511445
O	3.492690384	15.011485633	5.753234319
O	0.618784946	15.084002088	5.854807834
O	6.464664663	10.893087842	5.768085812
Al	9.139077228	12.967457391	8.537909056
Al	13.255928662	15.073017543	7.220824734
O	11.839461790	15.260887332	11.275785885
O	16.133909242	13.067860828	9.903635167
O	11.776252951	14.918833251	8.468472887
O	16.129680116	13.078668586	7.183277490
Al	13.226549239	11.158952903	10.112822734
Al	9.074450121	9.179897910	11.412881136
O	16.116734614	8.948099229	7.521094829
O	11.938789926	11.075485761	8.712921964
O	16.024126218	9.275311240	10.253044235
O	11.924670540	10.968753410	11.422744351
Al	16.207519669	11.203429598	10.118012016
Al	11.971193729	9.093970641	11.428211040
O	13.462095293	8.934950426	7.436753137
O	9.041843477	11.141737536	8.643919188
O	13.468914427	9.213784846	10.247362284
O	9.105911449	11.047356702	11.352574410
Al	11.911732529	12.947650341	8.486442903
Al	16.137854405	15.222817617	7.235546651
O	9.127524957	15.249932755	11.198730170
O	13.234495457	12.977405896	9.917761477
O	9.122790668	14.861300758	8.394753415
O	13.321827768	13.154676124	7.275920126
Al	14.756129388	9.068323011	8.806298800
Al	14.753650823	8.937435888	11.625486196
Al	14.641931319	14.020893504	9.955604850
O	14.494842796	15.080525471	11.422908084
O	14.720530568	15.167606119	8.568524709
Al	10.520753354	15.095959766	9.869562661
Al	10.495511853	14.970162246	7.055632243
Al	10.448948350	10.113171466	8.648048240

O	10.524397113	8.961269741	7.266554265
O	10.461117422	9.023800995	10.076918931
Al	10.538426664	12.079911160	11.363916846
O	10.506461733	13.168217217	9.911635545
O	10.504720406	13.069588390	7.283538506
Al	14.622726749	11.984845397	7.312323104
O	14.712203893	10.980403967	8.815655148
O	14.719335526	11.123391743	11.415875138
H	9.954756773	9.257429587	6.536009390
H	12.648578557	9.455534473	7.569439863
H	15.952978453	9.607817945	6.809166156
H	14.725348163	14.454305516	5.344598504
H	11.956698409	14.230566965	5.390654237
H	9.047662353	15.584423768	5.114731536
H	14.237197339	10.323965285	5.785176200
H	16.665184530	12.828978861	6.399263262
O	14.719384966	15.166564408	6.000369303
O	11.919841202	15.083500506	5.857112908
O	9.051573039	14.940343762	5.838191664
O	14.952413421	10.970790516	5.918226675
O	7.701005000	9.195340318	12.712784169
H	7.777435571	8.486273090	13.373127628
H	14.653119888	11.741088325	12.160646224
O	13.325956566	9.029253150	12.787068056
O	10.513805270	9.027599991	12.737312307
O	-0.626535016	9.030861045	12.793991105
H	-0.585215934	9.783057004	13.402508301
O	2.415739121	13.234067206	12.649550793
O	10.587623852	13.313011875	12.649899834
H	7.487203477	14.962739665	11.322209867
H	13.498757825	14.999941899	11.542704928
H	3.346595958	14.593475075	11.774514952
H	11.528362292	14.707397248	12.035801687
O	1.873569760	5.002761283	12.791836145
H	7.554748203	6.948154824	11.452899356
H	4.143888789	6.555952931	11.086799447
H	15.966613054	6.951982391	11.498742250
O	7.701937260	0.967490416	12.638503126
H	7.781533837	0.316385658	13.348671815
O	-0.697786358	0.887109889	12.713062006
H	-0.617226279	0.111786209	13.288818937
H	6.339020943	3.460246311	12.075951458
O	4.901537268	0.817221912	12.641335504
O	2.097983279	0.882194881	12.563672792
H	14.802177296	3.591268335	12.126457177
O	13.259129353	0.892755417	12.787123211
O	10.439733289	0.963503884	12.641568739
O	2.171591870	9.113963114	12.641116318
O	4.913894481	8.942827364	12.698012539
H	2.170395025	8.324288997	13.203509051
H	4.860445418	9.667946599	13.337806407
H	13.185325076	8.209453517	13.305801015
H	10.542460510	9.658832930	13.473315097
H	13.247155950	1.629690005	13.415082319
H	10.382074485	1.715833608	13.249919304
H	2.093665404	1.623895885	13.188789953
H	4.807968494	-0.009729312	13.138150446
H	9.450013668	14.745975932	11.981093557
H	10.667544256	13.055065740	13.578008844
H	1.715897152	13.909848234	12.691044100
H	0.063597216	14.625270431	10.933354960

H	1.071901041	6.576926098	12.006606043
H	2.696194130	5.433406465	13.072213558
H	6.299955073	11.676307612	12.040587204
W	10.527788546	6.679334587	12.939689674
O	10.516676212	4.920688069	12.791417824
O	9.203027579	7.259698565	11.446726258
H	12.074146368	7.049311227	13.539499397
C	8.738009500	6.903393374	14.219095252
H	8.612367896	7.920250940	14.631559106
C	10.771255770	6.585265387	15.141114756
C	9.340212622	6.088332993	15.364497906
H	7.791462457	6.543616913	13.783502821
H	10.844889798	7.611855884	15.543747314
C	11.909426078	5.726660118	15.685539244
H	11.796089693	5.568659740	16.771647907
H	11.921842829	4.737033519	15.204967799
H	12.893494252	6.185104003	15.514143048
H	9.294911391	5.013869652	15.117279146
C	8.736881848	6.302412530	16.755861306
H	7.686221508	5.977006407	16.790144922
H	9.289418179	5.742210649	17.525633540
H	8.769023667	7.369397459	17.026093262

1butene (1,2) insertion (top path) into 2b species. E: -2349.9941413027

Al	0.723624100	4.902283722	8.588771788
Al	4.873204533	6.970406328	7.169112421
O	3.414763287	7.190447048	11.199972668
O	7.698339520	4.858573952	9.760097613
O	3.401546611	6.848588799	8.422656157
O	7.775506726	5.005682028	7.117652466
Al	4.786361411	3.073083095	10.031766098
Al	0.664290979	0.966728728	11.342199093
O	7.629809884	0.808402637	7.279827905
O	3.511341305	3.062425100	8.644168666
O	7.573360184	1.127387493	10.080839446
O	3.509217138	2.885478849	11.349577685
Al	7.770949349	3.025864129	9.938434377
Al	3.512131244	0.974786693	11.336226970
O	4.993017847	0.729498963	7.213244258
O	0.618649899	3.070321043	8.640421189
O	4.995952523	1.133335469	10.084227321
O	0.688925534	2.841173287	11.284610087
Al	3.492942355	4.896903268	8.466387455
Al	7.738730292	7.116724361	7.191082578
O	0.766652990	7.189438008	11.287199007
O	4.841736072	4.934500813	9.926788621
O	0.774450317	6.850543658	8.472373772
O	4.913487229	5.081304133	7.266403562
Al	6.240782289	0.944358431	8.614370137
Al	6.286917252	0.838411368	11.440096609
Al	6.307601677	5.932392221	9.888505266
O	6.544696078	7.083020595	11.275803552
O	6.320694676	7.091733856	8.491803568
Al	2.075300570	7.017597494	9.902972007
Al	2.095745464	6.871857476	7.069454210
Al	2.047670519	2.053224224	8.573366202
O	2.186873818	0.955061338	7.126813871
O	2.102705482	0.876675915	9.928716836
Al	2.074877600	3.951819138	11.383141522
O	2.097358652	5.088687196	9.917767862
O	2.039004900	5.008814967	7.284111327

Al	6.222643916	3.923132866	7.191339392
O	6.256537771	2.854624007	8.653939657
O	6.301066893	2.912180651	11.275029447
H	1.921898754	1.381334240	6.297092131
H	4.109712662	1.141736009	7.280977930
H	7.336861338	1.402158969	6.543185627
H	6.272413966	7.685721273	5.306585605
H	3.564267230	6.203844477	5.310674238
H	0.608446664	7.581728926	5.190825647
H	5.885396551	2.435150749	5.406328733
H	8.272730063	4.719319970	6.325854471
O	6.322242276	6.941956812	5.926117843
O	3.502061866	7.017853842	5.838505203
O	0.625382437	6.946615062	5.919365948
O	6.607544449	2.976311740	5.763735319
Al	9.152531085	4.913594952	8.567882343
Al	13.291758406	7.051792283	7.311370271
O	11.667197585	7.256919469	11.371423655
O	16.116949984	4.908391788	9.837444174
O	11.782252892	6.930960529	8.555177788
O	16.116115347	5.059901280	7.191332256
Al	13.204562345	3.097095671	10.111880690
Al	9.073726550	1.032857119	11.340807275
O	15.977534696	0.890080925	7.433087963
O	11.925106601	3.124641224	8.737390940
O	15.951485463	1.130451483	10.170854219
O	11.917159157	2.893150922	11.428028825
Al	16.188058378	3.057435874	10.028408964
Al	11.895664543	1.016347966	11.446314687
O	13.249367603	0.792025640	7.508101408
O	9.114071109	3.064029268	8.639112344
O	13.396174412	1.150194305	10.235763257
O	9.053509392	2.902576792	11.284866167
Al	11.919970148	4.964613202	8.572600789
Al	16.150590501	7.132966942	7.296832436
O	13.240979924	4.928994685	9.998997654
O	9.126815041	6.862604798	8.480206632
O	13.316558134	5.166550125	7.358219783
Al	14.637830432	0.978033859	8.758641174
Al	14.692671848	0.879645367	11.574974559
Al	14.677011002	5.944383063	10.029821116
O	14.958323095	7.025521719	11.443191144
O	14.736285889	7.116101816	8.637992909
Al	10.459396143	7.091909181	9.963609739
Al	10.532373849	6.953435135	7.140023539
Al	10.562647178	2.019294484	8.560201272
O	10.345547567	0.875888614	7.190810909
O	10.515031252	0.884435201	10.008341054
Al	10.493253259	3.911485510	11.288901278
O	10.449227305	5.156849277	9.984257206
O	10.515111613	5.086761498	7.346735504
Al	14.578343930	3.973460548	7.344010720
O	14.651681517	2.898530640	8.791790580
O	14.723637280	2.982479256	11.373385034
H	9.364186259	0.992066592	7.072332527
H	13.377902910	1.362070241	6.725741772
H	15.713649931	1.432452258	6.659292255
H	14.641479580	7.784370266	5.470870363
H	12.085832288	6.232318090	5.482515040
H	9.083570893	6.667384224	5.096430446
H	14.362211647	3.114171802	5.119729833

H	16.602332811	4.891507410	6.357365552
O	14.726207252	7.026029652	6.067813403
O	11.975354270	7.084669259	5.938407745
O	9.114615001	7.174500222	5.918596627
O	14.646452113	2.832217419	5.999989907
Al	0.733923122	12.989314328	8.557335645
Al	4.869552683	14.989745897	7.069901569
O	3.505333478	15.252159427	11.052688947
O	7.694190329	12.982182599	9.755284122
O	3.407722207	14.868360344	8.322071847
O	7.724976637	12.996877407	7.048964517
Al	4.791457166	11.114094303	9.957682174
Al	0.723550965	9.149504137	11.449327907
O	7.637186754	8.942314848	7.364259282
O	3.501725538	11.050717767	8.561185496
O	7.626433471	9.277035666	10.152030871
O	3.521224533	10.927347426	11.264339961
Al	7.782299431	11.172895308	10.004775365
Al	3.542012581	9.064332103	11.346537603
O	4.993117976	8.864364448	7.283656928
O	0.616668712	11.172936985	8.712234339
O	5.052408561	9.194191278	10.100194786
O	0.712281504	11.044504376	11.372535125
Al	3.494093622	12.911008309	8.367995165
Al	7.700762386	15.088954968	7.136314789
O	0.794709037	15.238798404	11.129361814
O	4.825389234	12.918318890	9.766396350
O	0.776379025	14.922128327	8.381918983
O	4.897801238	13.079168280	7.120794300
Al	6.305348564	9.041456709	8.663903784
Al	6.330234203	8.997445491	11.484957513
Al	6.217512463	13.973834521	9.853887018
O	6.481013606	15.031832276	11.283628470
O	6.301576995	15.109499159	8.440942312
Al	2.162058453	15.087067753	9.809394290
Al	2.094121946	14.918214532	6.983411113
Al	1.995086479	10.093947814	8.601394933
O	2.111354369	8.952726783	7.193273068
O	2.045156957	8.950688262	10.003648195
Al	2.172669226	12.078824192	11.354841559
O	2.105641629	13.155299919	9.836232876
O	2.023867868	13.059034724	7.206244408
Al	6.203950849	11.918759893	7.172346103
O	6.276247609	10.930419868	8.679901350
O	6.300577605	11.063808228	11.278990244
H	2.260463774	9.373779006	6.332201607
H	4.154216801	9.309345699	7.507051478
H	7.410184377	9.558833973	6.625988935
H	6.348228253	14.263283591	5.249345159
H	3.515025586	14.173163382	5.262397446
H	0.570141080	15.656755741	5.078476561
H	5.730641527	10.257963185	5.679685832
H	8.288525315	12.774435281	6.278918962
O	6.317726556	15.020872992	5.850711587
O	3.492253251	15.011963170	5.752903712
O	0.618616920	15.084106250	5.854683314
O	6.465146458	10.892786812	5.764296924
Al	9.140182747	12.969192718	8.537602356
Al	13.256025063	15.072990937	7.220939409
O	11.839523859	15.259862225	11.276027417
O	16.134030353	13.067442997	9.903403941

O	11.776631499	14.918915697	8.468575614
O	16.129605428	13.078471278	7.183502979
Al	13.225281149	11.157158119	10.114589332
Al	9.074637213	9.194191930	11.406980842
O	16.116156884	8.948245883	7.520686001
O	11.939647299	11.075365901	8.712772168
O	16.024652112	9.275066634	10.253760679
O	11.923924954	10.967161718	11.423774058
Al	16.207639804	11.202878810	10.118400349
Al	11.968851603	9.087849627	11.434608926
O	13.461801711	8.932941543	7.436823761
O	9.044279203	11.143367390	8.642185407
O	13.468696847	9.213035166	10.248456020
O	9.104478916	11.051878987	11.350832490
Al	11.912116561	12.947661637	8.486929963
Al	16.137856327	15.222750967	7.235649522
O	9.127576071	15.249998954	11.198758411
O	13.234490952	12.976663061	9.917914017
O	9.123193626	14.862246863	8.394527301
O	13.321911894	13.154605653	7.275882112
Al	14.755590730	9.067851055	8.807720882
Al	14.752287866	8.937146130	11.626844934
Al	14.641874359	14.020186337	9.955647820
O	14.495189512	15.079746737	11.423047367
O	14.720629522	15.167296569	8.568552639
Al	10.520655641	15.096322798	9.869696276
Al	10.496200532	14.971365193	7.056209468
Al	10.449894364	10.113725253	8.647346720
O	10.525157305	8.960234668	7.267711199
O	10.459146861	9.024669486	10.076102909
Al	10.539525797	12.080593895	11.364545597
O	10.506883035	13.168643504	9.911567276
O	10.505247988	13.070098981	7.283302938
Al	14.622563986	11.984675862	7.313259067
O	14.712223382	10.979851568	8.816036530
O	14.719315754	11.122978242	11.416958764
H	9.961915816	9.255326958	6.532050716
H	12.648109898	9.453269744	7.569473660
H	15.945483318	9.606618201	6.808806250
H	14.725249061	14.454042843	5.344840796
H	11.955977278	14.230445332	5.391262640
H	9.050166189	15.586541673	5.114929356
H	14.234416425	10.328102254	5.780842111
H	16.664876430	12.829714935	6.399084236
O	14.719423875	15.166550616	6.000337563
O	11.919946482	15.083738577	5.857124924
O	9.052883347	14.941814610	5.837842917
O	14.952428246	10.970758349	5.918348886
O	7.705766372	9.194503881	12.715018924
H	7.796594222	8.450647639	13.337465633
H	14.653269382	11.740202317	12.162144343
O	13.324079500	9.026242910	12.788888702
O	10.500391684	9.027735887	12.731162643
O	-0.626938524	9.030639209	12.794174172
H	-0.585961719	9.777491094	13.409113993
O	2.416119944	13.233568982	12.649137311
O	10.587656673	13.313326667	12.650256152
H	7.486823127	14.965866108	11.321871155
H	13.499195867	14.998868002	11.543179175
H	3.346516141	14.593820130	11.774557095
H	11.527754343	14.706012628	12.035709736

O	1.873967734	5.002609967	12.792204806
H	7.542823133	6.991803262	11.442139322
H	4.139388303	6.550487027	11.093368146
H	15.966746670	6.951704048	11.500842247
O	7.702501273	0.968313996	12.638950879
H	7.780520410	0.317423533	13.349440613
O	-0.697495450	0.887170124	12.713009309
H	-0.616042717	0.113088496	13.290288424
H	6.346183863	3.462764541	12.074008015
O	4.901570304	0.817350058	12.641428605
O	2.098330360	0.882506038	12.563517214
H	14.799678223	3.591171145	12.125999575
O	13.260095523	0.891952998	12.787347702
O	10.440025303	0.962823915	12.641795598
O	2.174415167	9.114252096	12.638182918
O	4.912099570	8.949478818	12.647083614
H	2.179821731	8.317377904	13.190557811
H	4.845379695	9.658965387	13.302902427
H	13.180287327	8.208352547	13.309124732
H	10.526647806	9.644870193	13.478997263
H	13.246956911	1.631576228	13.412132914
H	10.384158644	1.710927429	13.255302609
H	2.094132086	1.623927673	13.188959213
H	4.809288960	-0.010621037	13.136717129
H	9.449233802	14.745540819	11.981131051
H	10.669444024	13.054547087	13.578006129
H	1.715431591	13.908420307	12.690947019
H	0.063641976	14.625575487	10.933653466
H	1.078729315	6.580994928	12.007543659
H	2.701803442	5.396007154	13.109080809
H	6.288597613	11.668657473	12.037371733
W	10.466867577	6.670451694	12.929456132
O	10.599925335	4.918117256	12.809703658
O	9.197484407	7.264350052	11.443777050
H	11.996194637	7.059957379	13.574154362
C	8.539923815	6.373530803	14.088563955
H	7.912064656	7.267182327	14.264877279
C	10.489006082	7.012539428	15.106779880
C	9.281635579	6.139673469	15.417239129
H	9.607033643	5.083769718	15.447582127
C	8.518784414	6.446142827	16.715584014
H	8.162579685	7.490355733	16.666051433
H	7.616865797	5.814374976	16.766687041
C	9.362848293	6.243548507	17.976149593
H	9.709592264	5.202062189	18.054856391
H	10.254008453	6.887377880	17.965648852
H	8.793583186	6.475261758	18.887465611
H	10.246545739	8.073090344	15.297371581
H	11.426150662	6.785534967	15.630931484
C	7.641394570	5.232433991	13.583559920
H	7.660717386	5.189601751	12.484756531
H	8.092856335	4.279826246	13.906018381
C	6.181692748	5.314685175	14.055153250
H	5.704998126	6.228078983	13.671996248
H	6.113895589	5.324678779	15.151706664
H	5.579209174	4.457134910	13.708041718

isobutene (1,2) insertion (top path) into 2b species. E: -2349.994999687

Al	0.723301571	4.903196892	8.589870786
Al	4.871090984	6.973661065	7.183543482
O	3.416438663	7.190309323	11.203922647

O	7.704305897	4.853539540	9.756199309
O	3.397479230	6.845049752	8.432215326
O	7.772726388	5.005097757	7.114470680
Al	4.785872709	3.070377899	10.031390826
Al	0.664273867	0.966574556	11.342203152
O	7.629707024	0.807856389	7.280041058
O	3.510931608	3.061358089	8.643788959
O	7.575561193	1.127887577	10.081393903
O	3.509186080	2.884233038	11.349485366
Al	7.774717505	3.025220406	9.937219067
Al	3.511983374	0.974343768	11.336666710
O	4.993059086	0.728948077	7.213340864
O	0.618553121	3.070547043	8.640490745
O	4.996354354	1.132744320	10.084361059
O	0.689372386	2.840878422	11.284948191
Al	3.490483800	4.895184523	8.468706436
Al	7.738994857	7.119510643	7.191559599
O	0.766688455	7.189107840	11.287593445
O	4.839406449	4.930069378	9.925643359
O	0.774109786	6.850951345	8.473260665
O	4.912604363	5.082417025	7.268502785
Al	6.240707109	0.943483194	8.614681292
Al	6.287764427	0.838951613	11.440444141
Al	6.309317977	5.915758373	9.884558641
O	6.544691550	7.037400540	11.285351562
O	6.326325874	7.086261987	8.499513366
Al	2.076978721	7.019485138	9.905314287
Al	2.094492130	6.872508900	7.072358978
Al	2.046937204	2.052746862	8.573224437
O	2.186943353	0.954573695	7.126897317
O	2.102808718	0.876346392	9.928725584
Al	2.075126866	3.951482641	11.383523173
O	2.096971233	5.088092605	9.918652050
O	2.038646369	5.008959704	7.284326932
Al	6.218848828	3.921215892	7.191254559
O	6.256521170	2.852005701	8.652909645
O	6.301876078	2.911829826	11.274079588
H	1.922450014	1.380654291	6.296923271
H	4.109485497	1.140640134	7.281362039
H	7.336369521	1.401081986	6.543279510
H	6.271160724	7.684762870	5.306516235
H	3.572301249	6.206485536	5.316714580
H	0.614049024	7.599568773	5.205558840
H	5.885638184	2.434574497	5.404047104
H	8.263336729	4.722516488	6.316868833
O	6.318761378	6.944936962	5.930867351
O	3.503724784	7.020954111	5.842939728
O	0.625751619	6.947132443	5.919041269
O	6.606396870	2.976274383	5.763421035
Al	9.153669495	4.910473929	8.543855153
Al	13.293042236	7.054179332	7.308790855
O	11.671334869	7.256556835	11.366425671
O	16.116442551	4.908470923	9.837368441
O	11.780939634	6.929578707	8.548118144
O	16.116680881	5.060531363	7.190975067
Al	13.209728300	3.097539120	10.093321985
Al	9.075640125	1.033854736	11.340876857
O	15.977905249	0.889660418	7.432718581
O	11.925322811	3.126726048	8.722792663
O	15.953094681	1.130668422	10.170205855
O	11.913079872	2.886885661	11.377331997

Al	16.189081064	3.057769971	10.029189915
Al	11.896292026	1.016724588	11.436701509
O	13.249630126	0.791415695	7.507760879
O	9.116232188	3.062720627	8.636249082
O	13.399220201	1.145783470	10.231935956
O	9.060150812	2.905430122	11.283980675
Al	11.915453328	4.963286245	8.552396566
Al	16.151248232	7.133234546	7.296805569
O	13.239924871	4.929334355	9.995748520
O	9.128988510	6.861389152	8.475691470
O	13.318138122	5.167426232	7.355643021
Al	14.639376267	0.974997099	8.758347459
Al	14.692700619	0.881925751	11.573547752
Al	14.674977426	5.944286735	10.028860280
O	14.958178843	7.025336347	11.442887778
O	14.736118837	7.116927522	8.637444760
Al	10.460883338	7.091101043	9.955880599
Al	10.533932426	6.956252450	7.128400190
Al	10.565075636	2.017314488	8.556487555
O	10.344480514	0.873556271	7.189279477
O	10.514419707	0.882993936	10.005923838
Al	10.500367687	3.916331368	11.265302690
O	10.452789286	5.153601788	9.945135736
O	10.513663440	5.087801633	7.299673119
Al	14.579898223	3.974347949	7.341475988
O	14.652728957	2.898120794	8.789312717
O	14.723084673	2.981943484	11.370708937
H	9.363066912	0.990409277	7.071901323
H	13.377383245	1.361904980	6.725634492
H	15.713055736	1.431798252	6.659058097
H	14.644185291	7.781835974	5.467004518
H	12.088294456	6.237132639	5.476760461
H	9.082839923	6.663877144	5.096862634
H	14.361541481	3.112725089	5.118998027
H	16.603805726	4.892683382	6.357349534
O	14.727048414	7.026282508	6.067634006
O	11.981176082	7.090127547	5.932305870
O	9.112624000	7.176355145	5.915785646
O	14.646604965	2.831893136	5.999351363
Al	0.733781932	12.988795928	8.557451695
Al	4.869621245	14.988857724	7.071248431
O	3.505406021	15.251928647	11.052766251
O	7.692304346	12.981293657	9.755061808
O	3.408269127	14.866920299	8.322298023
O	7.722596652	12.994806669	7.051121376
Al	4.791888793	11.113393328	9.973807893
Al	0.724152130	9.148783547	11.446868753
O	7.636035363	8.942424895	7.368513400
O	3.502634182	11.047404626	8.564074037
O	7.623902197	9.271258618	10.159420205
O	3.518247058	10.925300172	11.271873606
Al	7.779682385	11.172681218	10.011947326
Al	3.548252705	9.062658172	11.371579349
O	4.990575257	8.861539234	7.347396849
O	0.616267371	11.172830879	8.712670478
O	5.056205456	9.190266653	10.150896019
O	0.711304223	11.044481347	11.372766876
Al	3.494297230	12.909075642	8.369536622
Al	7.700222338	15.088180438	7.137846950
O	0.794803504	15.238530268	11.129444182
O	4.824952101	12.917265275	9.767510165

O	0.776647140	14.921871435	8.381888502
O	4.898872492	13.076783789	7.122214784
Al	6.316767097	9.032237149	8.691721577
Al	6.327416359	8.976146084	11.511174329
Al	6.216364556	13.973779426	9.856358890
O	6.481746564	15.031456122	11.284751930
O	6.301488216	15.110227015	8.445219679
Al	2.161967620	15.086803014	9.809418125
Al	2.094369234	14.917233772	6.983559420
Al	1.992692508	10.091507466	8.602833773
O	2.110101643	8.952050225	7.192965328
O	2.044786479	8.950534417	10.005730358
Al	2.170591004	12.078707531	11.356599300
O	2.105834992	13.154637199	9.836599693
O	2.024291049	13.058209017	7.206768651
Al	6.202166871	11.911656841	7.185320755
O	6.268399682	10.919564977	8.698065273
O	6.301809519	11.067298237	11.285843220
H	2.336592369	9.364080458	6.344451971
H	4.166011932	9.329147831	7.575615341
H	7.395228070	9.556509311	6.632525723
H	6.347914643	14.257798748	5.256023519
H	3.515354013	14.173477791	5.261572639
H	0.570608509	15.656785622	5.078593746
H	5.720826648	10.274492151	5.659630865
H	8.282530060	12.770813257	6.278964920
O	6.317454318	15.019947240	5.851748927
O	3.492738018	15.011496006	5.753358152
O	0.618869956	15.083866207	5.854606783
O	6.464709972	10.893078969	5.768270958
Al	9.139311402	12.967888411	8.537645958
Al	13.255782691	15.072680514	7.220556235
O	11.839292651	15.259925695	11.275099542
O	16.133967304	13.067580102	9.903511590
O	11.776246160	14.918615066	8.468257110
O	16.129719120	13.078478164	7.183285226
Al	13.225383853	11.157130257	10.114519488
Al	9.076807013	9.190526635	11.406910318
O	16.116670958	8.948183858	7.521159406
O	11.938590283	11.075216481	8.712993207
O	16.024153650	9.275171091	10.253468575
O	11.923651737	10.966724966	11.423752714
Al	16.206996884	11.203107786	10.118574916
Al	11.969539622	9.086950516	11.433237676
O	13.462375370	8.935312552	7.436798354
O	9.041653310	11.142007760	8.643566226
O	13.468733888	9.213380282	10.248161627
O	9.104774897	11.050587303	11.351261466
Al	11.912031282	12.947662358	8.486679193
Al	16.138049133	15.221906508	7.235073577
O	9.127612731	15.250069045	11.199036248
O	13.234228064	12.976543568	9.917910535
O	9.122638677	14.861052477	8.394706101
O	13.321814312	13.154550339	7.275907442
Al	14.756115489	9.068249474	8.807323199
Al	14.752726398	8.936482606	11.626604160
Al	14.641586002	14.020266264	9.956106240
O	14.495782936	15.079703120	11.423569198
O	14.721028949	15.166713576	8.568258322
Al	10.519611968	15.095563935	9.869058947
Al	10.495641196	14.970531938	7.055566423

Al	10.448956589	10.113917869	8.646525557
O	10.524608276	8.961250424	7.265700122
O	10.458213450	9.023698478	10.074915816
Al	10.539857241	12.080559987	11.364422632
O	10.506305966	13.168020213	9.911554254
O	10.504770371	13.069502809	7.283482453
Al	14.622587982	11.984577311	7.312899196
O	14.712037790	10.980224830	8.816138419
O	14.719204882	11.123208119	11.417021004
H	9.957334119	9.257718015	6.533466654
H	12.649047992	9.456100404	7.569739940
H	15.952285334	9.608033587	6.809486773
H	14.725189601	14.454220302	5.344334082
H	11.956298177	14.230585871	5.390226269
H	9.047595001	15.584466524	5.114893406
H	14.237137534	10.324121677	5.785187805
H	16.664982964	12.828398457	6.399241640
O	14.719397522	15.166422648	6.000184320
O	11.919801286	15.083476893	5.856789141
O	9.051467112	14.940282522	5.838265814
O	14.952413181	10.970848342	5.918345377
O	7.708077976	9.195460563	12.717321641
H	7.804157632	8.474365042	13.364271825
H	14.652856485	11.740630847	12.162003650
O	13.324392593	9.027322829	12.788189556
O	10.499513111	9.027452345	12.730242191
O	-0.626623030	9.030654252	12.793973548
H	-0.585611452	9.780809570	13.404961979
O	2.415829953	13.234068656	12.649571545
O	10.587538251	13.313087479	12.650334071
H	7.487762964	14.966152885	11.322447576
H	13.500085391	14.999242025	11.544462315
H	3.346464163	14.593650591	11.774670895
H	11.527411431	14.708653375	12.036280354
O	1.874177051	5.002527608	12.792392917
H	7.543840960	6.959050876	11.448060190
H	4.142293548	6.552044780	11.095423429
H	15.966582253	6.951053753	11.499702843
O	7.703387623	0.969014042	12.638605880
H	7.782397086	0.322497599	13.352887571
O	-0.697778407	0.887127256	12.712918011
H	-0.617512968	0.110942892	13.287588935
H	6.343264723	3.462141754	12.073558238
O	4.901900361	0.817379769	12.641529789
O	2.098289720	0.882229613	12.563646588
H	14.794825091	3.593213060	12.121586271
O	13.258103291	0.893932732	12.783288831
O	10.441857338	0.964409745	12.640259581
O	2.172013637	9.113802790	12.641247817
O	4.915008308	8.943517078	12.699792610
H	2.171007340	8.323086780	13.202325927
H	4.858383373	9.668100398	13.340049740
H	13.180396996	8.211301781	13.311214351
H	10.532283970	9.651752989	13.471857441
H	13.245940666	1.625830619	13.416918686
H	10.384373606	1.711641780	13.254827108
H	2.093832437	1.623602341	13.189140658
H	4.810178883	-0.010505277	13.137070217
H	9.449530210	14.745915385	11.981461320
H	10.669908810	13.054782077	13.578164062
H	1.715959186	13.909783309	12.691567575

H	0.063515094	14.625538441	10.933695675
H	1.077087943	6.579912148	12.007997588
H	2.701499667	5.403399821	13.101388618
H	6.300158156	11.677184917	12.040397770
W	10.480235332	6.659260497	12.925429161
O	10.670030356	4.914679066	12.798044420
O	9.200981615	7.260438414	11.445360531
H	11.988984186	7.093062593	13.586949448
C	8.552655337	6.339179581	14.066457744
H	7.877185979	7.210223531	14.115297757
C	10.482169661	6.993783791	15.102055937
C	9.199214955	6.252120997	15.481856153
C	7.703408303	5.161278463	13.567104818
H	8.202956119	4.217059334	13.827322650
H	7.679422690	5.164376766	12.468267930
C	6.264175350	5.166381707	14.104147498
H	5.675660595	4.299651005	13.755912818
H	6.247188882	5.133870467	15.202604113
H	5.737489078	6.075862416	13.779722425
H	11.396188003	6.672144845	15.624146045
H	10.380472619	8.079140356	15.270120247
C	9.515311696	4.819927125	15.932735648
H	10.091646229	4.845222253	16.869533382
H	8.598193681	4.242405052	16.118578358
H	10.112919710	4.280326386	15.185119723
C	8.390512421	6.956592557	16.582551653
H	7.445103105	6.433215980	16.791569027
H	8.965716830	7.007610356	17.520854051
H	8.144849106	7.987474459	16.283748862

2butene insertion (top path) into 2b species. E: -2349.996076330

Al	0.723506686	4.903416957	8.590013425
Al	4.871256844	6.974225681	7.184283543
O	3.415685984	7.192937107	11.204231548
O	7.702635332	4.858429904	9.758242671
O	3.397084454	6.845503391	8.433056920
O	7.773147788	5.005588845	7.114671334
Al	4.784799699	3.073638509	10.030445068
Al	0.664204392	0.967059924	11.342481044
O	7.629755678	0.808628934	7.279762376
O	3.511030697	3.062581694	8.643766806
O	7.575892602	1.131595429	10.079602703
O	3.509104591	2.885976783	11.349653298
Al	7.774506003	3.028003304	9.934823630
Al	3.512289719	0.975433861	11.336730945
O	4.993173267	0.730047566	7.213344940
O	0.618596566	3.070630582	8.640504968
O	4.995464497	1.136278751	10.083519554
O	0.689019791	2.841253700	11.284944028
Al	3.490711485	4.896829197	8.468820206
Al	7.738517801	7.120540919	7.191735502
O	0.766633369	7.189538827	11.287557340
O	4.842613820	4.934076352	9.927935292
O	0.774111008	6.851166092	8.473391949
O	4.911918000	5.083193128	7.268389360
Al	6.241160426	0.945994399	8.615333075
Al	6.286784579	0.859080195	11.441767497
Al	6.310878056	5.928576367	9.893661477
O	6.544731944	7.084122415	11.279169924
O	6.326085391	7.087945823	8.499498180
Al	2.077481713	7.020448177	9.905792539

Al	2.094393247	6.872769043	7.072551964
Al	2.047286133	2.053294066	8.573352700
O	2.186701525	0.955142091	7.126741016
O	2.102785655	0.876875628	9.928748050
Al	2.074636458	3.952117784	11.383742449
O	2.097127286	5.088389107	9.918734106
O	2.038675670	5.009232028	7.284407879
Al	6.219171958	3.923908914	7.191011156
O	6.257165229	2.858068998	8.654080440
O	6.301134994	2.912971847	11.275876974
H	1.918892841	1.381105373	6.297758943
H	4.109851526	1.142391676	7.279942250
H	7.336828694	1.402088270	6.542981259
H	6.270792451	7.685036303	5.306773459
H	3.572473207	6.206048623	5.318000479
H	0.614084070	7.599432320	5.205391019
H	5.884651540	2.434724813	5.406074344
H	8.265028483	4.722835503	6.317909744
O	6.318769365	6.945117088	5.930997068
O	3.503677233	7.021162953	5.843222228
O	0.625767191	6.947229376	5.919087490
O	6.606003279	2.976676897	5.763934772
Al	9.153424635	4.911915668	8.544202572
Al	13.292978902	7.053956383	7.308928221
O	11.664027772	7.255391168	11.367159122
O	16.116574031	4.908540706	9.837435020
O	11.780693508	6.929821736	8.548072499
O	16.116642703	5.060690219	7.191064877
Al	13.208140467	3.099018613	10.094701343
Al	9.074619587	1.035295368	11.339842629
O	15.977775419	0.889862505	7.432684402
O	11.925402148	3.126909864	8.722925834
O	15.952618383	1.130692688	10.170283514
O	11.910196316	2.891583701	11.379947598
Al	16.188762628	3.057816509	10.028925885
Al	11.895283575	1.018596679	11.437316308
O	13.249557278	0.791475005	7.507842291
O	9.115948846	3.063988604	8.635965173
O	13.398303163	1.147397323	10.232545243
O	9.054376653	2.905021148	11.283380310
Al	11.914722576	4.963513833	8.553147281
Al	16.151344038	7.133199785	7.296770294
O	13.240017975	4.929996461	9.995810937
O	9.128911497	6.861965393	8.475335106
O	13.317948151	5.167528184	7.355796529
Al	14.639001071	0.975765444	8.758362315
Al	14.692453628	0.882255071	11.573560376
Al	14.675346325	5.944314239	10.028678493
O	14.958055740	7.025559351	11.442855583
O	14.736248183	7.117106808	8.637484220
Al	10.458370382	7.091509194	9.953926646
Al	10.534066428	6.956081842	7.127658989
Al	10.564746062	2.018217636	8.556668026
O	10.344445980	0.873975302	7.189538400
O	10.514397716	0.883528373	10.005921205
Al	10.491985946	3.918805660	11.269149699
O	10.452413185	5.153649337	9.944103829
O	10.513486231	5.088055934	7.299354726
Al	14.579605197	3.974436208	7.341673298
O	14.652591912	2.898354502	8.789548528
O	14.722883449	2.982162699	11.371055410

H	9.362984558	0.990733598	7.072062063
H	13.376796159	1.362302759	6.725890358
H	15.712792269	1.432095431	6.659114555
H	14.644000592	7.781623028	5.466838645
H	12.088797413	6.237309469	5.476522586
H	9.081958030	6.664637702	5.096528362
H	14.361577938	3.112843011	5.119087769
H	16.603792757	4.892593809	6.357512808
O	14.727053931	7.026318580	6.067753730
O	11.981440856	7.090258318	5.932114010
O	9.112528987	7.176453060	5.915829981
O	14.646592153	2.831957986	5.999442647
Al	0.733573368	12.992197040	8.557356624
Al	4.869830849	14.990108363	7.071123520
O	3.505632992	15.252412922	11.053134157
O	7.686977511	12.983941588	9.756637357
O	3.407785694	14.869345380	8.322331689
O	7.722650986	12.995232418	7.051523896
Al	4.790057118	11.118034959	9.971411639
Al	0.724106968	9.149350707	11.446743881
O	7.635840632	8.943402111	7.368553363
O	3.502236325	11.048880273	8.563742879
O	7.624619856	9.276661944	10.157703767
O	3.519830364	10.939524976	11.272609526
Al	7.779652533	11.175183173	10.010274227
Al	3.548373994	9.069109715	11.370525138
O	4.990372443	8.862056426	7.347813640
O	0.616724776	11.178897757	8.712784327
O	5.054055878	9.195149597	10.151141475
O	0.711066383	11.045086224	11.372682917
Al	3.494214595	12.911347847	8.369421904
Al	7.699776987	15.089155487	7.137455381
O	0.794612799	15.239069388	11.129275572
O	4.826334868	12.921692967	9.768482839
O	0.776337668	14.922512681	8.381620936
O	4.898104426	13.077737485	7.122078794
Al	6.316507737	9.034245013	8.692849604
Al	6.326088944	8.998800522	11.513488682
Al	6.214445467	13.985830668	9.862344238
O	6.479849781	15.072528436	11.278090822
O	6.301046722	15.112723975	8.443170249
Al	2.162178809	15.088185466	9.809563832
Al	2.094521262	14.918515367	6.983169923
Al	1.991452762	10.094084789	8.602349389
O	2.109876547	8.952646135	7.193393409
O	2.044634476	8.952478612	10.005607595
Al	2.167565572	12.083503830	11.356531466
O	2.105665315	13.156278027	9.836268893
O	2.024401271	13.059446634	7.206611446
Al	6.201671357	11.913515869	7.185070031
O	6.265437499	10.922749927	8.697967614
O	6.301751060	11.068378068	11.287683172
H	2.336579525	9.364169127	6.344655160
H	4.165634085	9.329531156	7.575582827
H	7.394883412	9.557452688	6.632523792
H	6.347863291	14.258512149	5.255034834
H	3.515680900	14.172981911	5.262806710
H	0.570352433	15.656084008	5.077717130
H	5.720597601	10.274862370	5.660713814
H	8.283348756	12.770764601	6.280063701
O	6.317448979	15.020174837	5.851344771

O	3.492852348	15.011805274	5.753231489
O	0.618837440	15.084156062	5.854451671
O	6.464581215	10.893485207	5.768606433
Al	9.138092766	12.969956316	8.538437273
Al	13.255722692	15.072838208	7.220599754
O	11.839140093	15.260549262	11.275200511
O	16.133485387	13.068384673	9.904273628
O	11.776191454	14.918700459	8.468367246
O	16.129563228	13.078974681	7.183029031
Al	13.225200922	11.157388622	10.114310800
Al	9.075768804	9.193149112	11.405346089
O	16.116818132	8.948498087	7.521120109
O	11.938482570	11.075659949	8.712892886
O	16.024506736	9.275584092	10.253115735
O	11.924012788	10.966755683	11.423740702
Al	16.207028246	11.204267340	10.118143236
Al	11.969010151	9.086880113	11.432403018
O	13.462402209	8.935258860	7.436812771
O	9.041395205	11.143879053	8.643612226
O	13.468531367	9.212861243	10.248268714
O	9.104632976	11.051613334	11.351369313
Al	11.911625297	12.947920114	8.486534209
Al	16.137758079	15.222343242	7.234705617
O	9.126690136	15.250822947	11.198617757
O	13.234093489	12.976645465	9.917918599
O	9.122421577	14.861751024	8.394826654
O	13.321758008	13.154600191	7.275878546
Al	14.756197882	9.068244672	8.807108819
Al	14.752895195	8.937108474	11.626376269
Al	14.641139437	14.020808466	9.956274413
O	14.495362023	15.080082245	11.423755215
O	14.720838641	15.166934283	8.568294715
Al	10.520024612	15.096299158	9.869358491
Al	10.495537346	14.970790153	7.055583726
Al	10.448487769	10.114879998	8.645998437
O	10.524463832	8.961585697	7.265628180
O	10.458589769	9.024879367	10.074392150
Al	10.540221485	12.080721962	11.364864843
O	10.505809416	13.168525045	9.911770138
O	10.504350149	13.069778871	7.283638089
Al	14.622745405	11.984864500	7.312826312
O	14.712043533	10.980294363	8.816231992
O	14.719044337	11.122909747	11.417222471
H	9.957375159	9.257874164	6.533160803
H	12.648931451	9.455812816	7.569780965
H	15.951569145	9.607843514	6.809096473
H	14.725142285	14.454066081	5.344498686
H	11.956181650	14.230469766	5.390579975
H	9.047808711	15.584864354	5.114962871
H	14.236834030	10.324546519	5.785006377
H	16.665666944	12.828537936	6.399668815
O	14.719313234	15.166483447	6.000113170
O	11.919771741	15.083507278	5.856883310
O	9.051483002	14.940598756	5.838277035
O	14.952436330	10.970867587	5.918377053
O	7.709815450	9.193834834	12.719904531
H	7.803402637	8.452980561	13.345733798
H	14.652645910	11.740621845	12.161975075
O	13.323813217	9.024276757	12.788808269
O	10.502531516	9.026890157	12.728905866
O	-0.626712578	9.030778676	12.793885889

H	-0.585183740	9.780454768	13.405418221
O	2.414967687	13.235663631	12.650937384
O	10.587475760	13.313244696	12.650517897
H	7.485493745	14.997794315	11.317934350
H	13.499550341	14.999922056	11.544461968
H	3.344400049	14.595046975	11.775453312
H	11.526950298	14.709531512	12.036444657
O	1.873971510	5.002874392	12.792571952
H	7.542973472	6.993155257	11.444792578
H	4.141662695	6.554951917	11.095711698
H	15.966432023	6.951198322	11.500129211
O	7.704361875	0.971270194	12.639677836
H	7.777655506	0.315711108	13.346217241
O	-0.697945826	0.887215423	12.712990924
H	-0.617516263	0.110821670	13.287347724
H	6.345985541	3.463816535	12.074808462
O	4.900393528	0.821850202	12.642392936
O	2.098144751	0.882356924	12.563416419
H	14.796502832	3.593358536	12.121824232
O	13.257776685	0.894358332	12.783387297
O	10.441538181	0.964878496	12.639978023
O	2.172316221	9.114926366	12.640708544
O	4.913145191	8.948368012	12.701694569
H	2.175014841	8.321432818	13.197906314
H	4.847243766	9.666279681	13.348503045
H	13.184333623	8.202486090	13.304127522
H	10.530874803	9.641343680	13.478898814
H	13.246407448	1.626279528	13.416979584
H	10.382385863	1.714867113	13.251044798
H	2.094603748	1.622721860	13.190085247
H	4.816223119	-0.012214149	13.128766971
H	9.446166064	14.745052148	11.980919521
H	10.669316538	13.054229273	13.578205685
H	1.715763080	13.911621877	12.697709320
H	0.063279734	14.626207815	10.933301300
H	1.077531626	6.580567453	12.007976415
H	2.701379816	5.402168944	13.103349320
H	6.298224379	11.676940923	12.043282085
W	10.465495277	6.669666070	12.924529386
O	10.601131616	4.915532582	12.802289650
O	9.196882524	7.264315093	11.440501890
H	11.998301677	7.043548415	13.561245023
C	8.542839246	6.353740620	14.077787827
H	7.915051870	7.245323588	14.265885257
C	10.471893066	7.058555716	15.107091252
C	9.303918581	6.115760078	15.389195585
C	7.641954824	5.215074027	13.575832017
H	8.092765907	4.260374063	13.892997300
H	7.654998913	5.175289343	12.476696068
C	6.185872259	5.302630961	14.057607078
H	5.576479844	4.448459914	13.714634722
H	6.126762053	5.313055731	15.154658408
H	5.710747630	6.218687050	13.678873317
H	10.086880209	8.090283151	15.220636250
H	9.684972486	5.077923221	15.383933331
C	11.725937536	6.880695442	15.955473164
H	11.493862848	6.952267959	17.032163216
H	12.185593869	5.896641267	15.781348827
H	12.487285246	7.641273315	15.729886189
C	8.545842351	6.344464042	16.703100475
H	7.728665498	5.619677900	16.831645365

H	9.213517940	6.252265654	17.573385149
H	8.107126381	7.354382852	16.718119053

Ibutene (1,2) insertion (side path) into 2a species. E: -2349.9948435518

Al	0.723481537	4.903187766	8.589295771
Al	4.871336500	6.973607541	7.185389818
O	3.415451640	7.190025670	11.204091212
O	7.703160185	4.851125213	9.758171773
O	3.396876883	6.844859854	8.433090749
O	7.774665695	5.005367993	7.116928962
Al	4.783702981	3.070035045	10.029960303
Al	0.663621081	0.966372739	11.342065034
O	7.629623715	0.807820829	7.280013680
O	3.510323947	3.061315352	8.643400113
O	7.571324058	1.126268496	10.080625989
O	3.508261451	2.884024088	11.348887467
Al	7.771667647	3.022752168	9.935569406
Al	3.511109520	0.974499197	11.336581076
O	4.992842455	0.728636364	7.213034254
O	0.618536762	3.070558882	8.640516545
O	4.995550170	1.132598847	10.084534771
O	0.688260663	2.840639336	11.284817853
Al	3.490581769	4.895422068	8.468283418
Al	7.738432760	7.116348400	7.193691144
O	0.765901758	7.189314525	11.287325640
O	4.839123687	4.929799082	9.925828859
O	0.773962184	6.850986005	8.473226031
O	4.912695349	5.082348175	7.268468293
Al	6.240008697	0.942651074	8.613982576
Al	6.286183191	0.833621213	11.439592418
Al	6.311130695	5.914010360	9.889715871
O	6.551050797	7.026470034	11.293948664
O	6.326344890	7.085135876	8.503212140
Al	2.076173918	7.019956312	9.904786215
Al	2.094402086	6.872676742	7.072332011
Al	2.046542010	2.052658783	8.572871692
O	2.186926924	0.954547589	7.126754483
O	2.102414684	0.876339614	9.928583358
Al	2.073906800	3.951236108	11.382475947
O	2.096814797	5.088137436	9.918435426
O	2.038671827	5.008995514	7.284154616
Al	6.221097827	3.922917245	7.191288662
O	6.254462876	2.851375496	8.652903883
O	6.300150559	2.912878903	11.275866159
H	1.924852511	1.380909225	6.296163726
H	4.109171174	1.140078241	7.281407300
H	7.336666239	1.401387800	6.543312631
H	6.271700573	7.686963696	5.310291381
H	3.573014110	6.206639819	5.317305353
H	0.615059909	7.602665483	5.207938670
H	5.884894486	2.434271803	5.406658649
H	8.270467894	4.720040832	6.323873571
O	6.318664044	6.944835354	5.931971450
O	3.503797284	7.021141806	5.843384997
O	0.625673428	6.947339438	5.918844967
O	6.606605977	2.976281261	5.763711817
Al	9.153352593	4.911578904	8.564738373
Al	13.291120499	7.052499827	7.311342510
O	11.675442609	7.257873307	11.372259767
O	16.117164603	4.909062306	9.837778152
O	11.780876548	6.931470523	8.556458590

O	16.116476495	5.061257978	7.191150068
Al	13.202397757	3.106213036	10.115073848
Al	9.072758627	1.032124628	11.340390769
O	15.977463059	0.890550289	7.432973081
O	11.925076539	3.128125069	8.736761761
O	15.950082846	1.131002189	10.170670194
O	11.912076940	2.900890218	11.432011593
Al	16.187412650	3.058326820	10.027747260
Al	11.894068985	1.023701219	11.446068467
O	13.248977864	0.792734338	7.508813073
O	9.115214394	3.062313115	8.637953411
O	13.395477050	1.184727459	10.237141745
O	9.047275241	2.900195085	11.284520235
Al	11.918087788	4.967183177	8.571909424
Al	16.150951378	7.132840351	7.296160016
O	13.241262913	4.932209962	9.999369934
O	9.126270925	6.862320292	8.480161933
O	13.316329723	5.167220216	7.358316456
Al	14.637349522	0.983997323	8.757849189
Al	14.691748054	0.888331821	11.575098288
Al	14.678053730	5.945893452	10.029075663
O	14.958178179	7.026067067	11.443509043
O	14.736431030	7.117151974	8.637812540
Al	10.449506444	7.089460918	9.969052395
Al	10.532024140	6.954687231	7.141213583
Al	10.565258771	2.020126067	8.559020184
O	10.345911950	0.875466401	7.190768424
O	10.515159719	0.885274618	10.008147672
Al	10.480935027	3.914247167	11.286213280
O	10.451121243	5.156118328	9.978425053
O	10.514734766	5.087347339	7.343991170
Al	14.578435684	3.974894292	7.343183663
O	14.653091029	2.901478838	8.790855670
O	14.725439032	2.985515934	11.378330559
H	9.364558315	0.992276389	7.073187818
H	13.375898860	1.363609756	6.726733714
H	15.715024845	1.433390681	6.658979431
H	14.642629900	7.782366044	5.468617788
H	12.084469929	6.231819723	5.484320612
H	9.085024342	6.665949789	5.097867111
H	14.363307123	3.114135483	5.119253498
H	16.602708002	4.892749225	6.357172376
O	14.725960846	7.026034540	6.068222995
O	11.974763907	7.085036236	5.938795268
O	9.113939203	7.174735443	5.919062925
O	14.646429117	2.832391592	5.999954180
Al	0.733893420	12.989385082	8.557207758
Al	4.869652075	14.988288028	7.070842479
O	3.505290992	15.252020631	11.052797948
O	7.693145276	12.980547722	9.755225992
O	3.408221319	14.866999014	8.322220409
O	7.722643611	12.994757479	7.051104984
Al	4.792942658	11.113217092	9.974441550
Al	0.724480287	9.149105714	11.446474310
O	7.636224552	8.941065479	7.368455658
O	3.502508112	11.047132531	8.564078153
O	7.623009692	9.270430032	10.158230234
O	3.518093310	10.925511740	11.271679141
Al	7.780629066	11.170496828	10.013709855
Al	3.548708696	9.063172037	11.372180859
O	4.991002941	8.861320239	7.347994932

O	0.616367847	11.174035597	8.712620267
O	5.056114261	9.188934712	10.150994369
O	0.711097752	11.044706935	11.372802587
Al	3.494518408	12.908686514	8.369567653
Al	7.700432830	15.088152075	7.137489602
O	0.794359990	15.238713849	11.129267189
O	4.824467117	12.917227094	9.767238803
O	0.776534425	14.922019079	8.382038318
O	4.898904305	13.076645124	7.122157207
Al	6.318654449	9.031864435	8.692634886
Al	6.327613017	8.972276808	11.510784473
Al	6.216750511	13.971643873	9.854784398
O	6.481025830	15.027480821	11.284753485
O	6.301444924	15.109253504	8.444279985
Al	2.162131934	15.086702809	9.809320059
Al	2.094395500	14.917164966	6.983490999
Al	1.992401674	10.091712979	8.602380808
O	2.109770479	8.952032285	7.192659793
O	2.043502206	8.950800192	10.005582583
Al	2.170778772	12.078736876	11.356360243
O	2.105722379	13.154788370	9.836622305
O	2.024316019	13.058375357	7.206779719
Al	6.202126898	11.911072228	7.185339558
O	6.266606879	10.919229620	8.697708460
O	6.301234685	11.068421765	11.284662073
H	2.349973211	9.361889895	6.346829750
H	4.168406782	9.330344091	7.580365356
H	7.394746294	9.554252097	6.632098055
H	6.348262628	14.257461063	5.255935799
H	3.515119360	14.173606697	5.261221660
H	0.570584849	15.656963847	5.078982538
H	5.720698207	10.274423865	5.659568852
H	8.282777689	12.769983181	6.279333747
O	6.317524953	15.019810927	5.851406115
O	3.492646318	15.011512627	5.753216039
O	0.618671385	15.084016891	5.854992729
O	6.464570823	10.893041570	5.768001760
Al	9.139298790	12.967534543	8.538087509
Al	13.256154847	15.073371070	7.221171663
O	11.840252862	15.263647496	11.274718958
O	16.133721532	13.067902421	9.903708970
O	11.776494125	14.919072470	8.468759797
O	16.129587126	13.078670148	7.183520041
Al	13.226012807	11.158670150	10.113096775
Al	9.074862839	9.182787133	11.414107607
O	16.116607021	8.948076558	7.521127779
O	11.938788025	11.075740535	8.713046180
O	16.024162139	9.275391343	10.253047205
O	11.924770317	10.968788635	11.423347188
Al	16.207475035	11.203391582	10.117967434
Al	11.970421348	9.094104030	11.430113641
O	13.461504163	8.933962450	7.436582212
O	9.041867394	11.141733664	8.643847102
O	13.468778789	9.213495473	10.247580731
O	9.105721664	11.048070552	11.352437437
Al	11.911684737	12.947660073	8.486633830
Al	16.137666292	15.223440155	7.235976834
O	9.127648492	15.249809831	11.198790311
O	13.234592479	12.977409068	9.917861486
O	9.122896920	14.861555998	8.394822225
O	13.321835384	13.154772664	7.275960970

Al	14.755677513	9.068383565	8.806302651
Al	14.753436534	8.938853081	11.625509735
Al	14.641833416	14.021194885	9.954948466
O	14.493776284	15.083838144	11.419672934
O	14.719901908	15.168815072	8.568902851
Al	10.520605163	15.096541453	9.869474390
Al	10.495657443	14.970790675	7.056028063
Al	10.449048555	10.113054337	8.648974625
O	10.524368885	8.960582650	7.268360727
O	10.462624816	9.024500676	10.078386945
Al	10.538639289	12.079982202	11.364772462
O	10.506575170	13.168483519	9.911859345
O	10.504779752	13.069820119	7.283635581
Al	14.622590010	11.984810931	7.312424030
O	14.712123762	10.980320837	8.815728287
O	14.719262893	11.123106054	11.416412583
H	9.952924431	9.253746967	6.538074180
H	12.647680948	9.454141657	7.568997533
H	15.953446497	9.608004051	6.809287051
H	14.725339995	14.453891698	5.345261031
H	11.956559096	14.230512685	5.391419721
H	9.047946823	15.585390958	5.115236817
H	14.237060857	10.324132965	5.785063428
H	16.664997224	12.829317080	6.399335719
O	14.719400664	15.166642945	6.000489560
O	11.919914662	15.083691363	5.857458270
O	9.051985097	14.940850891	5.838294929
O	14.952349196	10.970840697	5.918228006
O	7.701373275	9.195171978	12.713060359
H	7.785363434	8.473194693	13.359166938
H	14.652714289	11.740500855	12.161398623
O	13.326059661	9.028608844	12.787926835
O	10.512353780	9.026559348	12.738954058
O	-0.626530054	9.030903585	12.794050796
H	-0.584641386	9.782452803	13.403316602
O	2.415733693	13.234077055	12.649563044
O	10.587695805	13.313367611	12.650037668
H	7.486959977	14.962191329	11.322234556
H	13.498117029	15.002088129	11.541413863
H	3.346592556	14.593486749	11.774529632
H	11.530621692	14.710923524	12.035834797
O	1.873365111	5.002632505	12.791847738
H	7.555020400	6.949270733	11.451074629
H	4.143258276	6.555153543	11.088696122
H	15.966797397	6.952918838	11.500382628
O	7.701651557	0.967135759	12.638941154
H	7.780385870	0.313927135	13.347330383
O	-0.697763336	0.887342174	12.713087904
H	-0.619215536	0.110199371	13.286664792
H	6.339230026	3.459639206	12.076485338
O	4.901469861	0.817201209	12.641371154
O	2.097953478	0.882177741	12.563653868
H	14.816004574	3.593913703	12.129660452
O	13.259018665	0.892832897	12.787142322
O	10.439644797	0.963188969	12.641771752
O	2.171640216	9.113989671	12.641120250
O	4.913984598	8.942843668	12.698325563
H	2.170683625	8.323957008	13.203023469
H	4.860746633	9.668816446	13.337198303
H	13.183768168	8.202896405	13.297513276
H	10.549264602	9.644410292	13.486211885

H	13.246489263	1.631804885	13.412853691
H	10.380501616	1.711738528	13.254460186
H	2.093488930	1.623644694	13.189039416
H	4.807567961	-0.009432959	13.138636183
H	9.450558331	14.745578644	11.980910386
H	10.668110882	13.054225917	13.577839672
H	1.715873551	13.909823244	12.691210185
H	0.063181364	14.625757418	10.932975284
H	1.072975280	6.577454133	12.006771538
H	2.696465317	5.428597894	13.077659106
H	6.300034775	11.676879418	12.040275604
W	10.521129096	6.682057181	12.941941149
O	10.517850033	4.921900497	12.798653565
O	9.202291843	7.262789463	11.447193756
H	12.063651490	7.057215633	13.548783589
C	8.706617383	6.851475802	14.189355502
H	8.500276829	7.853667331	14.602080138
C	10.759882900	6.633836122	15.171104908
C	9.331110081	6.075530200	15.350136437
H	9.356153077	5.001699056	15.095875646
C	11.864166692	5.677768462	15.632284245
H	11.775642481	5.501350615	16.719761020
H	11.797173097	4.704791287	15.126352345
H	12.868338818	6.084417911	15.443008011
C	10.961775938	8.000231799	15.829534617
H	10.159024864	8.714481315	15.592767958
H	10.991686107	7.907419457	16.928610026
H	11.915623976	8.448348276	15.513120981
C	8.650459985	6.207732762	16.721824160
H	9.285906655	5.733594613	17.489248015
H	8.578508792	7.273967939	16.991733525
H	7.795792102	6.438828890	13.729255670
C	7.255959823	5.577199558	16.742439846
H	6.593423170	6.058746098	16.008774019
H	7.302646899	4.506960978	16.490587890
H	6.782630997	5.668157163	17.730161162

isobutene (1,2) insertion (side path) into 2a species. E: -2349.991627485

Al	0.724730792	4.903604323	8.589793659
Al	4.875229386	6.973107771	7.213875612
O	3.415306358	7.190813979	11.206923596
O	7.713973669	4.853333320	9.758614261
O	3.405037242	6.845725285	8.455043153
O	7.781020309	5.006122526	7.120336308
Al	4.786894111	3.071591018	10.033173739
Al	0.663765275	0.966168077	11.342200962
O	7.629779682	0.807937879	7.279913453
O	3.512575666	3.061729587	8.645041232
O	7.573491313	1.126963023	10.081164485
O	3.508763344	2.884341577	11.349338123
Al	7.775334141	3.025487186	9.935179847
Al	3.511395740	0.974629886	11.336480793
O	4.993728930	0.729346404	7.214096185
O	0.619201634	3.070631467	8.640201488
O	4.996985409	1.133517873	10.084463940
O	0.688757238	2.840365951	11.285100350
Al	3.492491885	4.895552394	8.475596257
Al	7.758527490	7.120649314	7.218950526
O	0.765594995	7.189392602	11.288224518
O	4.847492298	4.932504812	9.931422082
O	0.776429054	6.851610510	8.474529449

O	4.913266282	5.084187792	7.274567149
Al	6.241863125	0.944406328	8.614807739
Al	6.287351512	0.832586701	11.439789816
Al	6.325850478	5.916567477	9.928733067
O	6.550434298	7.020450591	11.356549367
O	6.370915890	7.092114815	8.552621051
Al	2.075704100	7.020550328	9.909737787
Al	2.098246266	6.875482978	7.077755759
Al	2.047807235	2.053003885	8.573447544
O	2.187180988	0.955065895	7.126993212
O	2.102885699	0.876415996	9.928714715
Al	2.073735182	3.950735428	11.383840255
O	2.097454317	5.087409023	9.919794523
O	2.043902344	5.011828449	7.287143630
Al	6.224860760	3.927623160	7.195299651
O	6.264303167	2.856059673	8.655923124
O	6.302056865	2.913200362	11.277170232
H	1.918796972	1.380383349	6.297875332
H	4.110069629	1.141077336	7.280679059
H	7.335635784	1.400895033	6.543127029
H	6.274255592	7.678148469	5.355620333
H	3.578109569	6.200708184	5.336416560
H	0.620979405	7.610125574	5.215891146
H	5.881329834	2.440337815	5.409377469
H	8.272683150	4.729308902	6.321479958
O	6.322335901	6.946240116	5.989177341
O	3.507333404	7.022331336	5.851368560
O	0.627536411	6.947356119	5.920099716
O	6.606018184	2.978628679	5.765990910
Al	9.169612399	4.908800282	8.544712382
Al	13.300875717	7.054076313	7.309367283
O	11.685258075	7.259236166	11.368680130
O	16.117611994	4.908552062	9.837252105
O	11.819488497	6.929009415	8.546914891
O	16.118819709	5.061016759	7.190893824
Al	13.207668570	3.097080953	10.108582690
Al	9.074318672	1.032111004	11.341040761
O	15.977728724	0.889866216	7.432713603
O	11.926978088	3.118988953	8.731800739
O	15.952298323	1.130415642	10.170728414
O	11.917993329	2.889653990	11.421463223
Al	16.188368312	3.057856276	10.028402759
Al	11.896720166	1.015508335	11.445511343
O	13.249331202	0.791692694	7.507763449
O	9.120088714	3.062011426	8.636640973
O	13.397364441	1.148151489	10.235052940
O	9.053555627	2.903013607	11.282424226
Al	11.926441222	4.961193985	8.550344766
Al	16.154277799	7.134359921	7.296143621
O	13.243533859	4.926852037	9.997494863
O	9.176577137	6.863098148	8.478347252
O	13.322354396	5.164535013	7.353689569
Al	14.638456552	0.977089084	8.758554104
Al	14.692899446	0.880414939	11.574843845
Al	14.676323326	5.944652699	10.027824253
O	14.957807749	7.025856150	11.442877589
O	14.742366399	7.118044186	8.637104305
Al	10.476637207	7.090373904	9.959083494
Al	10.552009458	6.955784870	7.127040332
Al	10.567126873	2.012121995	8.554426139
O	10.343716666	0.871969765	7.187670783

O	10.514995650	0.883844800	10.007316843
Al	10.497680426	3.903880624	11.236667515
O	10.494511606	5.150839793	9.928881365
O	10.520880693	5.086268870	7.293800937
Al	14.583765569	3.972433242	7.342571121
O	14.652920677	2.897717444	8.791085915
O	14.723910728	2.981806741	11.373365765
H	9.362222150	0.989122292	7.070504190
H	13.378143313	1.362447194	6.725892219
H	15.713078022	1.431466923	6.658557399
H	14.645788669	7.780612252	5.465084147
H	12.095127741	6.239747530	5.471565951
H	9.078613073	6.653966234	5.108524809
H	14.361579571	3.114319921	5.119908424
H	16.604165821	4.895307718	6.355785339
O	14.729096538	7.026284422	6.067143441
O	11.987395468	7.091715082	5.928789211
O	9.114558094	7.176841774	5.920588100
O	14.647014802	2.831160084	5.999398985
Al	0.733829422	12.990334732	8.557025089
Al	4.870109818	14.988581500	7.071815375
O	3.505502506	15.252144218	11.052737496
O	7.695603524	12.980670559	9.756039827
O	3.408767989	14.866996448	8.322219629
O	7.723326435	12.994532114	7.051628795
Al	4.796137739	11.113662779	9.975948746
Al	0.724682452	9.150129206	11.446997251
O	7.640363299	8.942771047	7.372701002
O	3.504322975	11.045825831	8.563979318
O	7.627369352	9.268343400	10.162225678
O	3.519267726	10.928224342	11.271549503
Al	7.785312435	11.170282412	10.015815278
Al	3.549449861	9.064665428	11.373964833
O	4.995805568	8.858574554	7.357074332
O	0.617268816	11.176032824	8.712793972
O	5.058872113	9.189112568	10.154052265
O	0.711595585	11.045213124	11.373103171
Al	3.494916586	12.908563386	8.369472796
Al	7.700426353	15.087607836	7.138237034
O	0.794993876	15.238486354	11.129300804
O	4.825739122	12.916782264	9.766718856
O	0.776838070	14.922105185	8.381765597
O	4.899909832	13.075713755	7.122571970
Al	6.331005382	9.031512806	8.702209850
Al	6.328436378	8.975313234	11.519483557
Al	6.218630239	13.971258784	9.855215686
O	6.481581818	15.027526019	11.284953781
O	6.301928359	15.109916979	8.445949587
Al	2.162315333	15.086801663	9.809254386
Al	2.094777251	14.916947917	6.983321425
Al	1.991758891	10.091888355	8.602045201
O	2.109970145	8.950988600	7.192897551
O	2.043593090	8.951507682	10.006283597
Al	2.170695798	12.079630420	11.356335044
O	2.106174401	13.154932060	9.836420597
O	2.024770384	13.058354930	7.206904104
Al	6.204223729	11.909922428	7.187451844
O	6.281350387	10.918449963	8.701212015
O	6.302358959	11.068759387	11.285543000
H	2.401592283	9.350201392	6.358077850
H	4.180779866	9.330732045	7.609991759

H	7.398235303	9.551318508	6.633177853
H	6.347843701	14.256846963	5.257165292
H	3.516104330	14.173924514	5.261050501
H	0.570621607	15.654954591	5.077357427
H	5.719141196	10.278673238	5.652950160
H	8.282713278	12.770985710	6.278944303
O	6.317523293	15.019650460	5.852087310
O	3.493258439	15.011495470	5.753575853
O	0.619055001	15.084045154	5.854830300
O	6.464997904	10.893044857	5.768708430
Al	9.140702764	12.966812398	8.538023500
Al	13.256311770	15.073049216	7.220087831
O	11.839352522	15.259678886	11.275986545
O	16.134503296	13.068316240	9.904028094
O	11.776234639	14.919058459	8.468300552
O	16.129689029	13.078857605	7.183207500
Al	13.228937442	11.161098896	10.113942452
Al	9.083613417	9.176564417	11.414506441
O	16.118280521	8.948913003	7.521209353
O	11.947232897	11.081810845	8.710676476
O	16.026783549	9.275823339	10.252983762
O	11.926819139	10.970619398	11.424237776
Al	16.208181068	11.204139721	10.118152406
Al	11.975823381	9.096252612	11.427577156
O	13.466812672	8.938253854	7.435406710
O	9.046157023	11.140314001	8.644985140
O	13.471959485	9.215570067	10.247160151
O	9.108301425	11.045529619	11.352567317
Al	11.913859561	12.950000154	8.486710534
Al	16.137928169	15.222278046	7.235051240
O	9.127588109	15.249784010	11.198952862
O	13.235581836	12.979155282	9.918434022
O	9.123017924	14.861062608	8.394727397
O	13.322316823	13.155600553	7.275555073
Al	14.757806246	9.069586402	8.806391918
Al	14.754931440	8.938891552	11.624630687
Al	14.642972447	14.021571605	9.956000644
O	14.495772650	15.080013839	11.423888726
O	14.721000582	15.167424065	8.568323884
Al	10.520347003	15.095164743	9.869626159
Al	10.495557181	14.969049892	7.054984526
Al	10.459386384	10.116718393	8.647729630
O	10.528662802	8.962228196	7.267013540
O	10.500806085	9.026532288	10.077246139
Al	10.540429726	12.079918406	11.365174578
O	10.507004379	13.168044535	9.912000225
O	10.505317718	13.069632063	7.283604436
Al	14.622273731	11.984570626	7.312415764
O	14.713943463	10.981464772	8.816675081
O	14.720144168	11.123828216	11.417631082
H	9.956850808	9.256108573	6.537294271
H	12.651038718	9.454763991	7.567769161
H	15.959336453	9.610003708	6.809665293
H	14.725209369	14.453740473	5.344877686
H	11.957285658	14.230785092	5.389758334
H	9.047038874	15.583190814	5.114156132
H	14.240623501	10.318488074	5.792902214
H	16.664938429	12.827942093	6.399403757
O	14.719513253	15.166602541	6.000027242
O	11.919820086	15.083449672	5.856670218
O	9.051088810	14.939795263	5.838205086

O	14.952347562	10.970937008	5.918388552
O	7.703639165	9.196955289	12.714436773
H	7.764625174	8.480934732	13.369337115
H	14.654764036	11.741082233	12.162840317
O	13.327491821	9.028731757	12.787416024
O	10.515811805	9.025200999	12.739055370
O	-0.626251618	9.030872405	12.794109230
H	-0.585696932	9.781645388	13.404391226
O	2.415800459	13.234396963	12.649778049
O	10.587304512	13.313222226	12.650451748
H	7.487635945	14.962548894	11.323567387
H	13.500041131	14.998552692	11.544054855
H	3.346478031	14.593880992	11.774693848
H	11.527967016	14.705908658	12.035832922
O	1.873502472	5.002983327	12.792239451
H	7.556724921	6.950317413	11.498627070
H	4.140883490	6.554275733	11.086802585
H	15.966066810	6.951976219	11.499556011
O	7.702366079	0.968277572	12.637973419
H	7.783440341	0.326634116	13.356382972
O	-0.697462597	0.887023393	12.713208419
H	-0.617004820	0.112129978	13.289562070
H	6.341580139	3.454101507	12.081841556
O	4.901817814	0.817267382	12.641127985
O	2.098153275	0.882190093	12.563649132
H	14.797748133	3.591997590	12.124949050
O	13.260091396	0.892184879	12.787207162
O	10.440181774	0.963267925	12.641466302
O	2.171621266	9.114458252	12.641307197
O	4.912390762	8.947064173	12.703681220
H	2.171519136	8.325003883	13.203978969
H	4.853061958	9.675697216	13.339091633
H	13.186597125	8.198674310	13.290469077
H	10.559884505	9.650371102	13.479868934
H	13.246809180	1.630130848	13.413944636
H	10.383062676	1.713704964	13.252234480
H	2.093496860	1.623332522	13.189403796
H	4.808005131	-0.009068903	13.138933376
H	9.449879389	14.746017485	11.981564134
H	10.669341996	13.054707692	13.578284146
H	1.715839593	13.909942000	12.692439866
H	0.064295883	14.624652354	10.933717859
H	1.070794868	6.577340975	12.008302607
H	2.695951982	5.434008328	13.072606122
H	6.301650014	11.676791866	12.041542673
W	10.546088068	6.670634016	12.938094639
O	10.586121886	4.925381423	12.728845390
O	9.215206552	7.260508685	11.446358091
H	12.090595744	7.037602814	13.540865064
C	8.751194858	6.865039092	14.211478821
H	7.816655584	6.462464968	13.785616986
H	8.598643428	7.906515141	14.536010303
C	10.790609058	6.596312889	15.176225674
C	9.311536131	6.153976251	15.454081502
C	11.873561948	5.605799518	15.619833204
H	11.821629761	5.455942278	16.713735083
H	11.771120985	4.624507100	15.140106822
H	12.878923874	5.983954115	15.385157635
C	11.111417999	7.966426973	15.786162130
H	10.359316785	8.733200392	15.547556673
H	11.164185551	7.905477532	16.886301659

H	12.084846519	8.333653167	15.431110370
C	8.701987007	6.655980811	16.779151140
H	7.642061109	6.365127928	16.834674953
H	9.213887542	6.217488357	17.650183268
H	8.749843213	7.748688900	16.871549148
C	9.076686499	4.634128155	15.416325526
H	9.446968689	4.161073231	14.501141451
H	9.552773235	4.141440540	16.276294534
H	7.996798196	4.433483621	15.476953834

2butene insertion (side path) into 2a species. E: -2349.992449045

Al	0.723316023	4.903186816	8.589336560
Al	4.870965218	6.974235990	7.183839801
O	3.415694471	7.190114481	11.203819802
O	7.702589093	4.851809381	9.758445340
O	3.396854418	6.844979275	8.432366656
O	7.774811627	5.005426851	7.117095143
Al	4.784155253	3.070236462	10.030901022
Al	0.663705370	0.966469251	11.342129996
O	7.629643515	0.807873292	7.280164035
O	3.510459776	3.061298844	8.643513395
O	7.571753137	1.126649259	10.081087597
O	3.508174279	2.884020958	11.348922046
Al	7.771247930	3.023203680	9.936790187
Al	3.511387388	0.974500777	11.336818942
O	4.992980126	0.728687413	7.213305731
O	0.618502583	3.070563820	8.640455035
O	4.995877877	1.132902618	10.084751900
O	0.688231664	2.840672340	11.284747136
Al	3.490291461	4.895082946	8.467970858
Al	7.737985143	7.115845106	7.192707956
O	0.766078740	7.189354989	11.287341579
O	4.838692776	4.929977808	9.925764964
O	0.773957935	6.851009994	8.473185227
O	4.912830209	5.082405117	7.268465167
Al	6.240114430	0.942988672	8.614415381
Al	6.286360619	0.835444970	11.440602598
Al	6.309703565	5.913478159	9.883677016
O	6.548202917	7.034361812	11.280897605
O	6.325597973	7.085252764	8.499647850
Al	2.076265112	7.019937918	9.904626739
Al	2.094159965	6.872580872	7.072197915
Al	2.046608418	2.052685574	8.573012101
O	2.186980209	0.954504068	7.126852814
O	2.102436324	0.876303079	9.928627662
Al	2.073995074	3.951183602	11.382632495
O	2.096815121	5.088145698	9.918374004
O	2.038584484	5.008997314	7.284057804
Al	6.221093190	3.922714498	7.190962591
O	6.254748532	2.852127091	8.653135792
O	6.300378444	2.913948319	11.276626005
H	1.925349446	1.380912111	6.296141079
H	4.109262308	1.140062378	7.281662674
H	7.336533176	1.401144467	6.543305561
H	6.272312384	7.685051070	5.307098931
H	3.572656034	6.206736422	5.316810043
H	0.614722674	7.601356705	5.206866137
H	5.885085298	2.434270467	5.406303958
H	8.271198998	4.719514754	6.324640502
O	6.318562848	6.944808556	5.930988312
O	3.503693783	7.021146235	5.843094720

O	0.625619766	6.947274736	5.918876559
O	6.606737975	2.976221374	5.763548175
Al	9.153230452	4.911384780	8.566650815
Al	13.290378354	7.052862617	7.311808630
O	11.668997754	7.260415876	11.371014915
O	16.116993637	4.909157560	9.837797130
O	11.779939798	6.931496429	8.557781969
O	16.116439443	5.061324107	7.191197634
Al	13.202172576	3.106637111	10.115226723
Al	9.072868114	1.032133859	11.340924342
O	15.977434837	0.890535070	7.433039792
O	11.924657752	3.129434398	8.737284434
O	15.949999468	1.131030294	10.170654310
O	11.912174320	2.901192435	11.432432394
Al	16.187372084	3.058338848	10.027680612
Al	11.894036058	1.023946634	11.446140929
O	13.248926496	0.792707643	7.508914744
O	9.114932225	3.062561607	8.638557363
O	13.395337585	1.185629539	10.237202265
O	9.047982987	2.901306997	11.285798656
Al	11.918876468	4.968709282	8.572920092
Al	16.150625567	7.132910499	7.296253000
O	13.241146260	4.932450986	9.999569093
O	9.125247934	6.862359770	8.483568382
O	13.316202870	5.167329405	7.358307040
Al	14.637300795	0.984214457	8.757850331
Al	14.691800835	0.888445911	11.574996760
Al	14.677918072	5.946262957	10.029426767
O	14.958005800	7.026436033	11.443622423
O	14.736272731	7.117232929	8.637878772
Al	10.447290943	7.087542350	9.980000656
Al	10.531901459	6.955687877	7.144922692
Al	10.565165204	2.020809379	8.559743776
O	10.346145050	0.875831131	7.191164062
O	10.515223740	0.885430470	10.008393956
Al	10.481895175	3.916206594	11.293310441
O	10.447739972	5.158017936	9.985653266
O	10.514394187	5.087461870	7.346665019
Al	14.578383183	3.975067738	7.343167390
O	14.653031907	2.901561485	8.790824146
O	14.725487271	2.985666415	11.378438327
H	9.364824791	0.992693907	7.073415483
H	13.375731196	1.363467807	6.726739982
H	15.715084536	1.433467588	6.659061035
H	14.642321933	7.782477139	5.468916900
H	12.082593424	6.230916180	5.486577967
H	9.087340340	6.663556686	5.100321834
H	14.363366914	3.114206002	5.119268751
H	16.602626934	4.892865184	6.357192098
O	14.725674925	7.026071567	6.068405486
O	11.973106101	7.084504081	5.940396702
O	9.114183780	7.174644094	5.920173927
O	14.646369861	2.832425799	5.999997161
Al	0.733983177	12.989361444	8.557153637
Al	4.869928946	14.988290015	7.071147443
O	3.505326699	15.252013337	11.052771027
O	7.693928999	12.980316041	9.755857020
O	3.408428564	14.866780560	8.322258346
O	7.723037198	12.994918518	7.051250850
Al	4.793626426	11.113027678	9.973690917
Al	0.724684238	9.149036473	11.446519451

O	7.636578062	8.940711491	7.368543071
O	3.503135461	11.047204188	8.563912154
O	7.625458709	9.269977691	10.162076728
O	3.518683134	10.926764945	11.271425315
Al	7.782726638	11.169286948	10.013827490
Al	3.548877297	9.063814625	11.371389390
O	4.991098647	8.861957749	7.348196340
O	0.616474932	11.173955899	8.712581938
O	5.056480431	9.190124814	10.150533668
O	0.711146632	11.044686489	11.372728661
Al	3.494729709	12.908860504	8.369484245
Al	7.700568748	15.088249771	7.137733178
O	0.794299562	15.238763895	11.129235214
O	4.825287722	12.916794988	9.767130671
O	0.776617373	14.922029179	8.382050002
O	4.899334005	13.076259406	7.122304611
Al	6.319398702	9.031370586	8.693275591
Al	6.329198913	8.975872662	11.510989215
Al	6.217629612	13.971818761	9.855347891
O	6.480979151	15.028157125	11.284880346
O	6.301639632	15.109257040	8.444842123
Al	2.162072696	15.086800944	9.809464275
Al	2.094474202	14.917210187	6.983527274
Al	1.992621485	10.091856931	8.602294028
O	2.109884950	8.952133728	7.192724256
O	2.043866916	8.950964758	10.005521926
Al	2.170726883	12.079054097	11.356408205
O	2.105794674	13.154817198	9.836575512
O	2.024374257	13.058285566	7.206791553
Al	6.203321404	11.910947051	7.186023510
O	6.274024917	10.918761254	8.698815872
O	6.302387285	11.067004649	11.286394392
H	2.346512091	9.362522600	6.346140821
H	4.168039228	9.330626416	7.579480471
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H	6.348239110	14.257411847	5.256237142
H	3.515385015	14.173661416	5.261161886
H	0.570585243	15.656902260	5.079011948
H	5.720433472	10.274935289	5.659662490
H	8.283425493	12.770378637	6.279584691
O	6.317597569	15.019849699	5.851601237
O	3.492825292	15.011438716	5.753355190
O	0.618722198	15.083981752	5.855037658
O	6.464713796	10.893009626	5.768308406
Al	9.139535861	12.967475489	8.538351210
Al	13.256060007	15.073257370	7.221474537
O	11.840336448	15.263670617	11.274795032
O	16.133571086	13.067840658	9.903658252
O	11.776473423	14.918870798	8.469058245
O	16.129600039	13.078598371	7.183600069
Al	13.224651217	11.156163591	10.114057875
Al	9.078048748	9.186477677	11.431307877
O	16.116449559	8.948096404	7.521117981
O	11.936779147	11.072975267	8.714571579
O	16.024239070	9.275513653	10.252926078
O	11.923373344	10.966608643	11.425666990
Al	16.207333726	11.203308648	10.117875265
Al	11.967666273	9.090856924	11.439316530
O	13.461158900	8.934274484	7.436698610
O	9.042330386	11.141775195	8.644282784
O	13.467816446	9.213653651	10.248581825

O	9.105992411	11.048505020	11.354877437
Al	11.911354854	12.946300569	8.486890156
Al	16.137643272	15.223514851	7.236055567
O	9.127796134	15.249877996	11.198758935
O	13.234080013	12.975948529	9.918009024
O	9.123030994	14.861543814	8.394966340
O	13.321749108	13.154392453	7.276302902
Al	14.755072856	9.068252694	8.806385763
Al	14.753561421	8.940176165	11.624534283
Al	14.641238686	14.020487777	9.954761653
O	14.493659547	15.083805078	11.419002106
O	14.719777913	15.168672006	8.568875801
Al	10.520749425	15.096470026	9.869712381
Al	10.495754534	14.970897191	7.056399142
Al	10.446799500	10.110240462	8.652873702
O	10.523772706	8.960181402	7.270257150
O	10.452221044	9.022516382	10.085047827
Al	10.539070549	12.080395358	11.366599157
O	10.506786240	13.167747884	9.912403449
O	10.504814143	13.069748923	7.283771290
Al	14.622756842	11.984634082	7.312636736
O	14.711864837	10.980148961	8.815963638
O	14.719142603	11.122871582	11.417115233
H	9.948388737	9.253166499	6.542981532
H	12.647788705	9.455068840	7.570083124
H	15.952511141	9.607760034	6.809177023
H	14.725173283	14.453955200	5.345238782
H	11.956241054	14.230585244	5.391470383
H	9.048075061	15.585560917	5.115439939
H	14.236485373	10.325122861	5.783843520
H	16.664718941	12.829467784	6.399153020
O	14.719371286	15.166551337	6.000634411
O	11.919931301	15.083671406	5.857693443
O	9.052058281	14.940933069	5.838413990
O	14.952401372	10.970829817	5.918306273
O	7.703553523	9.187681938	12.723979438
H	7.812796900	8.460689311	13.363425266
H	14.653409473	11.740360685	12.162095128
O	13.326969156	9.027777376	12.789656694
O	10.510311426	9.023443794	12.774658491
O	-0.626596096	9.030914679	12.793921665
H	-0.584231629	9.782035493	13.403696265
O	2.415665013	13.234174011	12.649645668
O	10.587790818	13.313653377	12.650881262
H	7.486798882	14.963048299	11.323088630
H	13.498032396	15.002197340	11.541194838
H	3.346630749	14.593678770	11.774663710
H	11.530758879	14.711669962	12.036425115
O	1.873364428	5.002628558	12.791842683
H	7.548681864	6.951363392	11.451692304
H	4.143126395	6.555189223	11.086495356
H	15.966448576	6.953020184	11.501412387
O	7.701949238	0.967406740	12.638855564
H	7.779988626	0.318194025	13.350888713
O	-0.697795374	0.887328928	12.713058663
H	-0.619184239	0.110384987	13.286889731
H	6.343416103	3.464669965	12.075287187
O	4.901400480	0.817219412	12.641481422
O	2.097990801	0.882152524	12.563634425
H	14.816850854	3.594157262	12.129606907
O	13.259092261	0.892758111	12.787010132

O	10.439738625	0.963176910	12.641853224
O	2.172066981	9.113950270	12.641035126
O	4.914931009	8.941670645	12.696123779
H	2.171410438	8.323352557	13.202196990
H	4.861786870	9.659682942	13.343778963
H	13.191844091	8.197439800	13.293876107
H	10.559061544	9.637847939	13.523935895
H	13.246544933	1.631463721	13.412979673
H	10.380675643	1.709744854	13.256966823
H	2.093833856	1.623485598	13.189189167
H	4.808162733	-0.009661928	13.138431461
H	9.450487653	14.745821959	11.981066522
H	10.664157818	13.054218407	13.578966474
H	1.715854949	13.909929232	12.691710992
H	0.062853814	14.626193180	10.932810912
H	1.073961373	6.577828940	12.006813496
H	2.697393617	5.423803551	13.082002752
H	6.298728398	11.676971289	12.040908045
W	10.520591197	6.679352309	12.965016858
O	10.528394602	4.920690218	12.811733667
O	9.200684194	7.264724905	11.500465761
H	12.090009011	7.030884326	13.494103596
C	8.703053125	6.642238627	14.313637118
H	8.330242261	7.634035149	14.637436709
C	10.861981494	6.832531455	15.178986822
C	9.532515947	6.134979733	15.499048288
H	9.689181476	5.050545932	15.355428301
C	7.527530862	5.722178062	13.964678522
H	7.891736588	4.784044536	13.517463946
H	6.973571045	5.453286980	14.880996068
H	6.803993874	6.166007736	13.274636814
C	12.082120996	6.047553109	15.674728237
H	12.020679968	5.909643932	16.769750716
H	12.138474649	5.050078982	15.215985688
H	13.027853922	6.565828544	15.457467345
C	10.930512172	8.265162333	15.710776765
H	10.025824518	8.848210348	15.480480166
H	11.037321520	8.267308618	16.809095815
H	11.803496903	8.797495815	15.302305244
C	8.924648242	6.332413018	16.895254568
H	7.982450313	5.773700901	16.992094601
H	9.602103561	5.975956222	17.686109120
H	8.704926999	7.392309251	17.089038382