Supplementary Material (ESI) for Dalton Transactions

Supplementary informations : **Can 1,3 butadiene be catalytically hydrophosphinated in the presence of Cp_2EuH ? A DFT Investigation**

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				E	Free Gibbs Energy
	H2			-1.1775165	-1.178857
1	0.000000	0.000000	0.128253		
1	0.000000	0.000000	0.871747		
	PH3			-8.3567828	-8.354119
15	-0.162581	-0.286543	0.038401		
1	0.047583	0.074815	1.410523		
1	1.197088	0.002524	-0.317718		
1	-0.606915	1.032232	-0.312206		
	butene			-155.9382784	-155.879349
6	1.539182	-0.492493	0.079092		
6	0.725668	0.553352	-0.105590		
6	-0.725668	0.553352	0.105589		
6	-1.539182	-0.492493	-0.079092		
1	2.604674	-0.422117	-0.116904		
1	1.167434	-1.446033	0.444890		
1	1.160325	1.502998	-0.418475		
1	-1.160325	1.502999	0.418475		
1	-2.604674	-0.422117	0.116903		
1	-1.167435	-1.446033	-0.444890		

1-First step :

1.1/ P-H activation on Cp2EuH with P in alpha position

Cp2EuH + PH3 -> add1 -> [TS-H-PH3] -> add2 ->Cp2EuPH2 + H2

	Cp2EuH			-422.9294464	-422.799137
63	0.392440	-0.599562	-0.003663		
1	-0.515856	-2.456930	0.066705		
6	1.477442	-0.551054	2.501455		
6	1.627127	0.772096	2.008623		
6	0.335049	1.345625	1.902364		
6	-0.609667	0.375178	2.325000		
6	0.096165	-0.796232	2.700923		
6	1.396193	0.465087	-2.315636		
6	0.743878	-0.732371	-2.713940		
6	-0.647836	-0.560835	-2.524622		
6	-0.858515	0.741200	-1.998985		
6	0.404313	1.377568	-1.878312		
1	2.282604	-1.241929	2.727923		
1	2.564841	1.275159	1.799830		
1	0.112232	2.358748	1.589007		
1	-1.683010	0.516452	2.388050		
1	-0.341620	-1.710176	3.080187		
1	2.459566	0.667797	-2.385546		
1	1.221786	-1.615931	-3.122060		
1	-1.412988	-1.293768	-2.745726		
1	-1.820592	1.192033	-1.781601		
1	0.577178	2.393083	-1.542474		
	add1(b)			-431.304128	-431.151434
6	-2.152278	-1.659445	-0.488960		
6	-1.849112	-1.740791	0.895231		
6	-2.154207	-0.489065	1.483328		
6	-2.654493	0.362954	0.463211		
6	-2.656609	-0.361042	-0.754957		
63	-0.006274	-0.024465	-0.157208		
15	0.004550	2.971328	-0.232711		
6	2.620617	-0.275029	-0.890279		
6	2.659823	0.335362	0.388303		
6	2.207806	-0.611715	1.344878		
6	1.891788	-1.809132	0.656683		
6	2.140678	-1.598620	-0.724303		
1	2.162248	-0.464069	2.418314		
1	1.552854	-2.733262	1.109816		
1	2.022337	-2.334760	-1.511689		
1	2.917903	0.181712	-1.825252		
1	3.024588	1.332890	0.604913		
1	-2.069127	-0.243384	2.536259		
1	-3.020966	1.373544	0.601602		
1	-2.995746	0.007279	-1.714431		
1	-2.058239	-2.464940	-1.208894		

1	-1.480846	-2.616400	1.416551
1	-1.081973	3.492011	-0.988109
1	0.041676	4.034233	0.739670
1	1.052640	3.475732	-1.050987
1	-0.064432	1.009903	-1.971780

[TS-H-PH3] -431.2938446 -431.142020

6	1.963402	-1.906477	-0.011958
6	1.781920	-1.466810	-1.350727
6	2.233643	-0.127306	-1.435106
6	2.697803	0.260184	-0.150161
6	2.537513	-0.842488	0.727098
63	-0.001474	-0.044024	0.122212
15	0.173817	2.813434	0.966721
6	-2.604983	-0.541182	0.773647
6	-2.651199	0.573911	-0.101327
6	-2.258872	0.136670	-1.394209
6	-1.965304	-1.246551	-1.317119
6	-2.172625	-1.663915	0.025028
1	-2.227804	0.745282	-2.291116
1	-1.670621	-1.882406	-2.143506
1	-2.063179	-2.674814	0.401092
1	-2.864720	-0.538581	1.824314
1	-2.982130	1.572874	0.158089
1	2.257608	0.481377	-2.332183
1	3.147847	1.213462	0.101757
1	2.814813	-0.870982	1.772882
1	1.743430	-2.897913	0.367500
1	1.399993	-2.063312	-2.170716
1	1.279297	3.324772	1.707806
1	-0.850793	3.449739	1.727015
1	0.105979	1.518351	1.868472
1	0.028124	0.137953	2.217410

add2 (f) -431.3136417 -431.157495

6	-2.007151	-1.629606	-0.804666
6	-1.848647	-1.784027	0.596847
6	-2.273938	-0.582979	1.219739
6	-2.699766	0.314259	0.206070
6	-2.536614	-0.334804	-1.043518
63	-0.000017	0.070748	-0.105130
15	-0.000002	2.827723	0.605700
6	2.536761	-0.334006	-1.043552
6	2.699886	0.313718	0.206466
6	2.273936	-0.583950	1.219436
6	1.848555	-1.784475	0.595805
6	2.007163	-1.629069	-0.805565
1	2.303406	-0.395368	2.286848
1	1.501233	-2.677637	1.101201
1	1.809380	-2.386600	-1.555487

1	2.808390	0.075287	-2.010066
1	3.106085	1.304643	0.364194
1	-2.303365	-0.393783	2.287044
1	-3.105829	1.305347	0.363119
1	-2.808189	0.073907	-2.010294
1	-1.809479	-2.387627	-1.554122
1	-1.501397	-2.676889	1.102821
1	-1.059269	3.408355	-0.167596
1	1.059219	3.408351	-0.167662
1	-0.000123	1.645028	-2.065007
1	-0.000068	1.033681	-2.519698

Cp2EuPH2 -430.1332677 -429.995748

6	0.421344	1.373507	-1.843946
6	1.324232	0.374630	-2.287882
6	0.562083	-0.741775	-2.725057
6	-0.807395	-0.436578	-2.545255
6	-0.895953	0.869724	-1.993369
63	0.200315	-0.629016	-0.018182
6	0.039984	-0.790762	2.700507
6	1.420426	-0.636987	2.422729
6	1.625457	0.668627	1.904208
6	0.368262	1.324145	1.863985
6	-0.610852	0.421386	2.351218
15	-0.985871	-3.220886	0.041565
1	2.190253	-1.377937	2.608408
1	2.579841	1.107497	1.635501
1	0.193269	2.346361	1.550397
1	-1.666864	0.633725	2.477453
1	-0.431164	-1.668056	3.125337
1	2.403305	0.471218	-2.339896
1	0.955832	-1.658847	-3.147363
1	-1.640338	-1.080112	-2.800940
1	-1.811433	1.410156	-1.779007
1	0.689790	2.359061	-1.483146
1	-0.291184	-3.734550	-1.108317
1	-0.067686	-3.798734	0.985598

1.2/ 1,2 butadiene insertion on Cp2EuH

Cp2EuH + 1,2 -> add3 -> [TS-H-1,2] -> Cp2Eu1,2

add3 -578.878764 -578.666205

6	-0.065510	2.398371	-1.117426
6	-1.225272	2.325192	-0.301107
6	-0.820540	2.420664	1.051555
6	0.591762	2.546103	1.073892
6	1.056629	2.540899	-0.265984
63	0.166546	0.008782	0.218019

6	-1.431207	-1.236047	-2.204830
6	-2.123007	-1.488376	-1.073865
6	-3.314347	-0.772649	-0.645604
6	-3.901029	-0.982079	0.542025
6	2.783451	-0.593468	-0.273872
6	2.576475	-0.858355	1.104704
6	1.743165	-1.999326	1.214123
6	1.419635	-2.427779	-0.095246
6	2.065323	-1.559883	-1.016920
1	-0.769985	-0.523829	1.976272
1	-1.471023	2.400828	1.915879
1	1.203118	2.658590	1.961704
1	2.086438	2.656548	-0.581652
1	-0.043200	2.397885	-2.201714
1	-2.248180	2.254168	-0.651567
1	3.010944	-0.308088	1.931162
1	1.412050	-2.457844	2.136121
1	0.830189	-3.302142	-0.348994
1	2.060200	-1.650519	-2.097521
1	3.409149	0.188961	-0.685776
1	-1.747780	-0.460268	-2.898372
1	-0.569393	-1.833377	-2.485528
1	-1.779271	-2.288684	-0.412676
1	-3.724755	-0.038767	-1.337928
1	-3.494985	-1.692329	1.256702
1	-4.789086	-0.433979	0.840021

[TS-H-1,2] -578.8736179 -578.662506

6	0.274321	2.578792	-1.078901
6	-1.057420	2.372962	-0.632626
6	-1.039563	2.286597	0.781490
6	0.304409	2.435255	1.209558
6	1.114862	2.623718	0.060957
63	0.268089	0.032421	-0.063460
6	-1.614755	-1.142961	-1.530790
6	-2.262390	-1.439911	-0.346243
6	-3.484248	-0.742229	0.068206
6	-4.394061	-1.260729	0.898530
6	2.912071	-0.622355	-0.133602
6	2.492556	-0.873604	1.199171
6	1.624873	-1.995198	1.183154
6	1.501891	-2.431481	-0.159245
6	2.298155	-1.585630	-0.972295
1	-1.214208	-0.775334	1.141134
1	-1.900000	2.149886	1.424032
1	0.646414	2.442793	2.238205
1	2.184069	2.799189	0.057475
1	0.587244	2.729348	-2.106570
1	-1.939566	2.340849	-1.261391
1	2.814144	-0.329570	2.079829
1	1.155809	-2.451418	2.045687

1	0.932042	-3.288988	-0.497673
1	2.448137	-1.684973	-2.042084
1	3.610255	0.144412	-0.448075
1	-1.962719	-0.319930	-2.152226
1	-0.963719	-1.878525	-1.997534
1	-2.089663	-2.407254	0.118488
1	-3.662098	0.229294	-0.391220
1	-4.247174	-2.228633	1.371466
1	-5.312754	-0.733005	1.134260

Cp2Eu1,2	-578.9005543	-578.686722

6	0.310110	2.629694	-1.147106
6	-0.996480	2.452004	-0.627408
6	-0.895512	2.369613	0.784264
6	0.473350	2.502867	1.137057
6	1.217932	2.667294	-0.057414
63	0.307506	0.084975	-0.136828
6	-1.588152	-0.943836	-1.258472
6	-2.180050	-1.289651	0.108510
6	-3.624790	-0.929110	0.294289
6	-4.582433	-1.769324	0.686329
6	2.909183	-0.745829	-0.037787
6	2.402471	-0.963623	1.268575
6	1.451449	-2.013987	1.199071
6	1.371821	-2.447420	-0.149798
6	2.270553	-1.662994	-0.912310
1	-1.642519	-0.749883	0.964911
1	-1.724552	2.273793	1.476586
1	0.874287	2.522295	2.144072
1	2.287791	2.827012	-0.123147
1	0.565164	2.761360	-2.193121
1	-1.911302	2.415645	-1.204950
1	2.717646	-0.445697	2.167062
1	0.917386	-2.445385	2.038540
1	0.754003	-3.252733	-0.526662
1	2.461650	-1.769520	-1.974530
1	3.680239	-0.034776	-0.310738
1	-2.234315	-0.243869	-1.799904
1	-1.464267	-1.841175	-1.869850
1	-2.021942	-2.344605	0.360218
1	-3.883572	0.102133	0.049466
1	-4.366107	-2.807588	0.929289
1	-5.619149	-1.454584	0.766147

1.3/ 1,4 butadiene insertion on Cp2EuH

Cp2EuH + 1,4 -> (add4 -> [TS-H-1,4]) -> Cp2Eu1,4

Cp2Eu1,4	-578.9414972	-578.723790

6	0.435249	0.639497	-1.851810
6	0.486881	-0.670714	-2.392957
6	-0.843317	-1.134471	-2.544809
6	-1.717896	-0.114338	-2.097155
6	-0.928663	0.983763	-1.669895
63	-0.432060	-0.951367	0.190252
6	-0.831956	-0.628305	2.887444
6	0.555269	-0.878309	2.751998
6	1.137586	0.227962	2.080567
6	0.109735	1.164692	1.806989
6	-1.109395	0.631861	2.298185
6	0.435567	-3.524040	0.085429
1	1.086437	-1.744543	3.127008
1	2.191404	0.357926	1.859873
1	0.237248	2.128496	1.329278
1	-2.075533	1.123660	2.270152
1	-1.551262	-1.272979	3.377060
1	1.384447	-1.206589	-2.680529
1	-1.140990	-2.090260	-2.959485
1	-2.801289	-0.152502	-2.114239
1	-1.302177	1.933768	-1.306128
1	1.285700	1.280983	-1.651759
1	0.342049	-3.465925	-1.003887
6	1.744973	-4.060166	0.602028
6	-0.745281	-3.552747	0.820320
1	1.937734	-5.083959	0.251030
1	2.602417	-3.455896	0.281561
1	1.754846	-4.086317	1.697203
6	-1.989191	-3.035178	0.404036
1	-0.641319	-3.780878	1.884851
1	-2.835643	-3.101806	1.080931
1	-2.245715	-3.083076	-0.655598

2-Second step

2.1/ butadiene insertion on Cp2EuPH2

2.1.a/ 1,2 insertion

Cp2EuPH2 + 1,2 -> add5 -> [TS-PH2-1,2] -> Cp2Eu1,2-PH2

add5	-586.0820387	-585.863985

15	-1.103603	-0.732862	2.437622
6	-2.603002	-0.586401	-1.275008
6	-1.595223	-0.907315	-2.116583
1	-1.626040	-1.993858	1.975301
1	-2.306166	-0.005635	2.125516
1	-1.119476	-1.882652	-2.077193

1	-1.300847	-0.242641	-2.926993
1	-2.892497	-1.296881	-0.500882
6	-3.379992	0.640844	-1.344204
1	-3.117225	1.350031	-2.127928
6	-4.401818	0.903508	-0.517303
1	-4.681977	0.212810	0.273797
1	-4.984245	1.815155	-0.605070
1	0.382295	-3.457127	-0.472477
1	1.608326	-2.048724	-2.425874
6	1.134957	-2.689370	-0.332918
6	1.776331	-1.945497	-1.359428
6	2.726289	-1.090340	-0.750954
1	3.400747	-0.417821	-1.266997
1	3.294257	-0.820356	1.394169
6	2.668818	-1.300872	0.651054
6	1.691221	-2.296293	0.907052
1	1.427876	-2.694021	1.878838
63	0.333865	-0.076095	0.053565
6	1.333475	2.276720	-0.869304
6	0.452717	2.374845	1.248259
1	0.363628	2.395340	2.327500
1	2.653055	2.156350	0.929187
6	1.656351	2.236505	0.512084
6	-0.613457	2.495171	0.325924
1	-0.622964	2.548772	-1.908062
6	-0.069977	2.438771	-0.981950
1	-1.658196	2.626422	0.578129
1	2.039874	2.240065	-1.690248

[TS-PH2-1,2] -586.0596929 -585.839144

15	1.569430	1.187285	1.454060
6	-0.352805	2.390521	0.974008
6	-1.288334	1.765953	0.047006
1	1.542894	1.570130	2.823623
1	2.486721	2.171014	0.995119
1	-2.263221	1.551109	0.485023
1	-1.359655	2.259937	-0.922499
1	-0.670677	2.380879	2.016941
6	0.259137	3.678954	0.576879
1	0.577155	3.746832	-0.464176
6	0.372475	4.747658	1.371105
1	0.054193	4.723193	2.410925
1	0.780220	5.684933	1.005043
1	-1.797863	-0.376996	2.803815
1	-3.299097	-1.125270	0.702426
6	-1.546727	-1.148260	2.085016
6	-2.338356	-1.542856	0.979449
6	-1.669780	-2.605135	0.319491
1	-2.036988	-3.152397	-0.540901
1	0.252344	-3.646436	0.787386
6	-0.464989	-2.868990	1.022752

6	-0.391818	-1.970797	2.115177
1	0.396113	-1.936779	2.858342
63	-0.099151	-0.436648	-0.156917
6	-0.043418	-1.131214	-2.786410
6	2.020124	-0.673736	-1.896816
1	3.010399	-0.794523	-1.473457
1	1.312872	-2.778601	-2.116792
6	1.126643	-1.717350	-2.232275
6	1.404737	0.558811	-2.239883
1	-0.566386	1.001341	-3.190319
6	0.135109	0.274605	-2.799571
1	1.851366	1.541208	-2.138948
1	-0.897332	-1.669042	-3.182227

Cp2Eu1,2-PH2 -586.0718927 -585.850500

15	-2.070578	-0.027015	1.527668
6	-2.617292	-0.726921	-0.140613
6	-1.714757	0.048864	-1.121718
1	-2.808346	-0.737782	2.527056
1	-2.852583	1.167088	1.569047
1	-1.756985	-0.432254	-2.108975
1	-2.129108	1.060446	-1.257422
1	-2.308064	-1.780193	-0.100269
6	-4.093395	-0.652711	-0.372087
1	-4.496870	0.357378	-0.464846
6	-4.909234	-1.700923	-0.506990
1	-4.542436	-2.722702	-0.431738
1	-5.970017	-1.577057	-0.705388
1	-0.203727	-2.849574	-1.373187
1	2.102509	-1.796739	-2.270043
6	0.608023	-2.482806	-0.757685
6	1.820780	-1.919560	-1.230185
6	2.629980	-1.610230	-0.106159
1	3.630500	-1.195901	-0.137126
1	2.270387	-1.878404	2.079942
6	1.910973	-1.963410	1.060314
6	0.661252	-2.505893	0.656925
1	-0.094524	-2.915709	1.317067
63	0.548076	0.164470	-0.019599
6	2.010756	2.161464	-1.157495
6	1.512314	2.513673	1.052775
1	1.602377	2.590576	2.130840
1	3.510310	1.727702	0.442309
6	2.517495	2.061531	0.165006
6	0.385881	2.900357	0.279991
1	0.047459	2.905449	-1.924383
6	0.695617	2.688808	-1.084183
1	-0.536791	3.317684	0.665476
1	2.555425	1.930145	-2.066030

2.1.b/ 1,4 insertion

Cp2EuPH2 + 1,4 -> add6 -> [TS-PH2-1,4] -> Cp2Eu1,4-PH2

	add6			-586.0818729	-585.865221
6	-1.918319	-2.125101	0.313885		
6	-2.136392	-1.345545	1.481634		
6	-2.798443	-0.156027	1.093731		
6	-2.976270	-0.192492	-0.313013		
6	-2.441131	-1.415599	-0.792641		
63	-0.307221	0.094249	0.034043		
6	0.191852	2.726530	-0.472357		
6	1.429167	2.232118	0.006547		
6	1.270191	1.912927	1.378413		
6	-0.067369	2.202203	1.747336		
6	-0.734343	2.706737	0.600977		
6	3.386109	-1.060386	0.157782		
6	4.010338	-1.082274	-1.028886		
6	2.184274	-1.834553	0.430017		
6	1.509412	-1.817614	1.600578		
1	-1.891568	-1.631269	2.498617		
1	-3.129104	0.633091	1.757888		
1	-3.473824	0.561380	-0.912145		
1	-2.446443	-1.754788	-1.820381		
1	-1.471029	-3.111926	0.275779		
1	-0.006596	3.068030	-1.480763		
1	-1.759974	3.053962	0.563239		
1	-0.492769	2.100608	2.738882		
1	2.048149	1.556007	2.043631		
1	2.339044	2.133984	-0.572199		
1	0.662573	-2.474249	1.772968		
1	1.846645	-1.212162	2.439225		
1	1.835485	-2.477994	-0.378779		
1	3.783486	-0.459615	0.974894		
1	3.620340	-1.661489	-1.861985		
1	4.916896	-0.511075	-1.202777		
15	0.476566	-0.571599	-2.650335		
1	-0.740167	-0.322878	-3.367757		
1	1.110797	0.641162	-3.082068		
	[TS-PH2-1,4]			-586.0680759	-585.845854
6	-1.902263	-2.086594	-0.137636		
6	-2.206052	-1.536384	1.133531		
6	-2.788228	-0.261543	0.932036		
6	-2.847401	-0.024261	-0.467349		
6	-2.306969	-1.155995	-1.125988		
63	-0.218641	0.070690	0.152027		
6	0.027522	2.739084	-0.354209		
6	1.320213	2.361220	0.089943		
6	1.229593	2.025755	1.462064		
6	-0.120346	2.189999	1.867262		

6	-0.859250	2.643802	0.745628
6	2.799160	-0.986236	-0.178642
6	3.171222	-1.208913	-1.499495
6	1.966997	-1.861002	0.568749
6	1.396500	-1.594045	1.793832
1	-2.048084	-2.018291	2.091336
1	-3.158481	0.398779	1.706912
1	-3.275410	0.847602	-0.947820
1	-2.226895	-1.292337	-2.197056
1	-1.468515	-3.062120	-0.323469
1	-0.227644	3.068824	-1.354570
1	-1.913066	2.892880	0.737318
1	-0.507422	2.049348	2.870035
1	2.054561	1.737987	2.103291
1	2.218816	2.355237	-0.514488
1	0.819668	-2.352716	2.311340
1	1.720875	-0.736323	2.381078
1	1.698656	-2.802690	0.083490
1	3.081599	-0.041561	0.283337
1	3.100261	-2.200562	-1.934334
1	3.875638	-0.542873	-1.984172
15	1.047283	-0.528758	-2.512596
1	0.727816	-1.924050	-2.425838
1	0.308582	-0.368546	-3.753495

Cp2Eu1,4-PH2 -586.1009997 -585.877143

6	-0.489980	2.657333	-0.198594
6	0.481912	2.662691	0.831131
6	1.727084	2.303877	0.261178
6	1.528026	2.093980	-1.130455
6	0.160441	2.311968	-1.412965
63	0.273099	0.013922	0.100850
6	1.811402	-1.600455	-1.478228
6	0.802151	-2.471936	-0.996704
6	0.999463	-2.646445	0.394585
6	2.134130	-1.886725	0.775641
6	2.637610	-1.243038	-0.382204
6	-2.227606	-0.718965	1.059273
6	-3.294341	-0.261431	0.101234
6	-1.626329	0.094863	2.012517
6	-0.412708	-0.167053	2.672083
1	0.309147	2.911798	1.870597
1	2.674431	2.248135	0.784820
1	2.294963	1.840999	-1.852487
1	-0.303471	2.252621	-2.390342
1	-1.533097	2.931022	-0.091406
1	1.951706	-1.295145	-2.508685
1	3.518750	-0.614357	-0.428163
1	2.560446	-1.833878	1.770327
1	0.409309	-3.278886	1.047302
1	0.038432	-2.952727	-1.596514

1	-0.064537	0.525908	3.431184
1	-0.098674	-1.201995	2.806595
1	-2.004322	1.119241	2.078680
1	-2.004051	-1.787765	1.068180
1	-3.508292	0.804207	0.237066
1	-4.240216	-0.811374	0.149623
15	-2.432807	-0.453021	-1.560933
1	-3.338990	0.104138	-2.528051
1	-2.762209	-1.815687	-1.839223

2.2/ Activation P-H from PH3 on Cp2Eu1,2

2.2.a/ with P in alpha position

Cp2Eu1,2 + PH2-H -> add7 -> [TS-1,2-PH2-H] -> add8 -> Cp2EuPH2 + but1-ène

add7 -587.2726452 -587.034115

6	2.672296	-0.695484	-1.168764
6	2.522403	-1.527975	-0.030291
6	1.448812	-2.420915	-0.273612
6	0.939606	-2.143955	-1.567779
6	1.695253	-1.079031	-2.120829
63	0.255253	0.056914	-0.087312
15	1.291742	0.418053	2.685315
6	0.498530	2.802809	-0.147182
6	0.405399	2.402816	-1.502003
6	-0.905255	1.908257	-1.724212
6	-1.628502	2.022999	-0.506278
6	-0.763489	2.570243	0.465575
6	-1.313050	-0.970579	1.537450
6	-2.082225	-1.582891	0.363822
6	-3.576972	-1.468131	0.447474
6	-4.368822	-0.848954	-0.429917
1	0.140060	-2.680832	-2.065412
1	1.570063	-0.655950	-3.110681
1	3.428889	0.068585	-1.305852
1	3.158187	-1.522350	0.847563
1	1.106136	-3.202273	0.393277
1	-1.303354	1.565397	-2.672680
1	-2.663273	1.742810	-0.348936
1	-1.028004	2.800807	1.490648
1	1.361236	3.262030	0.322400
1	1.190868	2.480129	-2.244358
1	-1.034131	-1.737522	2.265649
1	-1.923115	-0.212879	2.043913
1	-1.810365	-1.139066	-0.640926
1	-1.799516	-2.638460	0.254723
1	-4.016314	-1.924920	1.335215
1	-5.444175	-0.791204	-0.288072
1	-3.968715	-0.381159	-1.327825
1	0.370020	1.002016	3.602583

1	2.451915	1.087339	3.201620
1	1.492609	-0.794140	3.407349

[TS-1,2-PH2-H] -587.2577031 -587.019750

6	2.688989	-0.674286	-1.103025
6	2.495018	-1.547098	-0.002572
6	1.414952	-2.412349	-0.311581
6	0.945711	-2.077570	-1.607027
6	1.732525	-1.004251	-2.096686
63	0.286522	0.076508	-0.057397
15	1.353080	0.396474	2.721696
6	0.595504	2.784244	-0.266157
6	0.274539	2.341759	-1.571896
6	-1.071269	1.890186	-1.563649
6	-1.586248	2.071467	-0.252578
6	-0.556860	2.618537	0.548016
6	-1.422740	-1.025496	1.508255
6	-2.084582	-1.566676	0.229035
6	-3.585723	-1.516137	0.259964
6	-4.360898	-0.829217	-0.580357
1	0.152069	-2.580330	-2.147850
1	1.642920	-0.543553	-3.073375
1	3.457599	0.085426	-1.185380
1	3.096288	-1.574412	0.898210
1	1.042776	-3.213439	0.315426
1	-1.625973	1.531785	-2.423537
1	-2.594312	1.843437	0.071990
1	-0.642066	2.897036	1.591680
1	1.542365	3.205849	0.050517
1	0.932591	2.365746	-2.432334
1	-1.288906	-1.836807	2.229023
1	-2.063032	-0.264859	1.970185
1	-1.791684	-1.022126	-0.708768
1	-1.749240	-2.597229	0.057608
1	-4.043355	-2.080875	1.072823
1	-5.442311	-0.821031	-0.480570
1	-3.942030	-0.252413	-1.402764
1	0.017426	-0.367592	2.105686
1	0.467236	0.949464	3.698866
1	1.611057	-0.809858	3.444702

add8 -587.3074164 -587.071555

6	2.162724	-0.858195	-1.800939
6	2.174825	-1.730939	-0.681566
6	0.901298	-2.341022	-0.590730
6	0.102553	-1.856196	-1.659881
6	0.882752	-0.941700	-2.409391
63	0.496130	0.315825	-0.034167
15	1.785684	0.013295	2.494171
6	0.861604	2.943475	0.589465

6	1.322702	2.787271	-0.743919
6	0.197809	2.535713	-1.571663
6	-0.955259	2.522400	-0.749170
6	-0.543229	2.773266	0.586725
6	-2.304697	-0.598632	1.109042
6	-2.989802	-1.947165	1.363133
6	-4.239916	-2.114497	0.550181
6	-4.442317	-3.077279	-0.349163
1	-0.909538	-2.167978	-1.893434
1	0.570435	-0.426034	-3.309499
1	3.000975	-0.272401	-2.160003
1	3.013176	-1.907122	-0.019227
1	0.603854	-3.075383	0.148613
1	0.214522	2.409149	-2.647294
1	-1.976777	2.393129	-1.089674
1	-1.192140	2.856121	1.451000
1	1.474849	3.166746	1.453346
1	2.348054	2.894170	-1.078910
1	-2.957322	0.244500	1.354367
1	-2.065571	-0.512888	0.036016
1	-2.293673	-2.765381	1.147771
1	-3.231039	-2.012593	2.432723
1	-5.024151	-1.375241	0.722471
1	-5.369040	-3.147369	-0.911207
1	-3.690845	-3.838683	-0.548089
1	-1.404437	-0.508080	1.738769
1	0.776525	0.675783	3.278953
1	1.284415	-1.305823	2.780541

but-1-ène -157.1703003 -157.088946

6	0.176778	0.103075	-0.000545
1	0.229463	0.035577	1.090860
1	1.146681	0.453924	-0.366911
1	0.022014	-0.909421	-0.389505
6	-0.949255	1.044482	-0.442304
6	-1.080304	1.131482	-1.934524
1	-1.897963	0.685121	-0.017943
1	-0.784026	2.046793	-0.029053
6	-0.962288	2.246063	-2.655627
1	-1.277847	0.188693	-2.448744
1	-1.063564	2.241439	-3.737308
1	-0.762200	3.207882	-2.187560

2.2.b/ with P in beta position

Cp2Eu1,2 + H-PH2 -> add9 -> [TS-1,2-H-PH2] -> add10 -> Cp2EuH + 4-PH2-but-1-ene

add9 -587.2585802 -587.035503

6	0.625581	-0.495985	2.827157
6	-0.686114	-0.039735	2.536408

6	-0.587068	1.286461	2.035929
6	0.780050	1.641992	2.003637
6	1.532600	0.538707	2.489515
63	0.498075	-0.317701	0.097306
15	-6.513921	0.942191	-0.485044
6	0.307612	-2.012842	-2.049641
6	-0.659289	-2.472403	-1.120839
6	0.024687	-3.007956	0.000944
6	1.416568	-2.872738	-0.230915
6	1.590702	-2.257755	-1.498477
6	0.096847	1.430925	-1.548278
6	1.604099	1.542398	-1.790491
6	2.162034	2.934485	-1.744982
6	3.049557	3.397737	-0.863397
1	-5.584410	1.031307	0.605062
1	-5.475762	1.054922	-1.469179
1	-6.466344	-0.492081	-0.499183
1	-0.446326	1.228898	-2.474859
1	-0.295887	2.349881	-1.100105
1	1.867870	1.067594	-2.744818
1	2.229515	0.955561	-1.040657
1	1.755707	3.607378	-2.500798
1	3.386776	4.429948	-0.880186
1	3.476039	2.757502	-0.092722
1	-1.604645	-0.583753	2.727015
1	0.884815	-1.457084	3.255386
1	2.607607	0.513904	2.632492
1	1.181201	2.592942	1.674113
1	-1.414338	1.923333	1.746170
1	0.102426	-1.576188	-3.018695
1	2.539808	-2.055453	-1.982375
1	2.207307	-3.220395	0.424323
1	-0.433987	-3.470779	0.866891
1	-1.734479	-2.454901	-1.261895

[TS-1,2-H-PH2] -587.2099108 -586.969196

6	2.301021	1.917486	-0.074740
6	1.885042	1.929676	1.279579
6	0.570567	2.461283	1.329064
6	0.171834	2.767420	0.007189
6	1.238381	2.423344	-0.865440
63	0.362095	0.019770	0.067226
15	-1.228976	-1.373486	2.424969
6	0.412164	-2.569059	-0.825896
6	1.576147	-2.416576	-0.032519
6	2.451645	-1.526958	-0.702165
6	1.829351	-1.127285	-1.913616
6	0.571521	-1.777050	-1.990505
6	-2.112487	0.017706	0.932652
6	-2.573425	-0.414758	-0.462766
6	-3.688245	0.441391	-0.995697

6	-3.625612	1.196963	-2.092474
1	0.209343	-0.616417	2.081146
1	-2.210600	-2.228511	1.737184
1	-0.323999	-2.512234	2.449218
1	-2.967596	-0.008627	1.610818
1	-1.793976	1.075627	0.952866
1	-2.892555	-1.465590	-0.400265
1	-1.770602	-0.409367	-1.232324
1	-4.602123	0.434477	-0.400645
1	-4.465648	1.804958	-2.414595
1	-2.732903	1.231055	-2.714985
1	2.478604	1.625382	2.133426
1	3.269671	1.600432	-0.440699
1	1.261162	2.581087	-1.937711
1	-0.770522	3.215195	-0.287975
1	-0.015154	2.616822	2.227112
1	-0.436619	-3.198984	-0.590774
1	-0.125423	-1.713139	-2.818985
1	2.259101	-0.477893	-2.666924
1	3.438355	-1.231969	-0.365790
1	1.766738	-2.907010	0.914146

	add10	-587.2550525	-587.024367

6	-3.053980	2.432622	0.696554
6	-2.546311	2.610723	-0.616485
6	-1.161482	2.301739	-0.601537
6	-0.817494	1.923228	0.719725
6	-1.985262	2.003874	1.523360
63	-2.442877	-0.070934	-0.196601
15	7.453993	-2.551962	0.186945
6	-3.415227	-2.567248	0.340758
6	-3.870996	-2.263534	-0.964972
6	-4.816121	-1.209862	-0.859808
6	-4.950809	-0.871447	0.511723
6	-4.081351	-1.708614	1.254951
6	8.096504	-0.870314	-0.375606
6	7.659190	0.345726	0.450125
6	8.241287	1.628162	-0.071937
6	7.534141	2.655126	-0.542911
1	-1.254918	-0.643972	-1.789895
1	7.749016	-2.388462	1.584460
1	6.082659	-2.159568	0.363629
1	9.190111	-0.953260	-0.394180
1	7.783758	-0.753885	-1.419630
1	7.973980	0.195799	1.492448
1	6.564768	0.411719	0.460284
1	9.330811	1.694005	-0.066815
1	8.013021	3.556449	-0.915011
1	6.446547	2.632939	-0.569640
1	-3.108682	2.965529	-1.473314
1	-4.069496	2.628003	1.020152

1	-2.041045	1.822811	2.591160
1	0.176131	1.655554	1.062760
1	-0.486532	2.353147	-1.445738
1	-2.706160	-3.346697	0.597717
1	-3.985146	-1.725679	2.335028
1	-5.626953	-0.131238	0.922940
1	-5.374457	-0.772678	-1.680392
1	-3.558573	-2.753302	-1.877926

4-PH2-but-1-ene -164.3232008 -164.237493

15	0.021523	0.391803	0.010449
6	0.086994	0.039124	1.871317
1	1.430667	0.609824	-0.157310
1	-0.253402	1.799193	0.086456
6	-1.299340	-0.211467	2.486164
1	0.600968	0.846355	2.399687
6	-2.202573	0.987088	2.462973
1	-1.170509	-0.546222	3.523047
6	-2.660067	1.616863	3.544803
1	-2.495199	1.354032	1.477957
1	-3.312589	2.482120	3.469776
1	-2.401496	1.285279	4.548565
1	0.695928	-0.866073	1.974110
1	-1.780473	-1.038824	1.944882

2.3/ Activation P-H from PH3 on Cp2Eu1,4

2.3.a/ with P in alpha position

Cp2Eu1,4 + PH2-H -> add11 -> [TS-14-PH2-H] -> add12 -> Cp2EuPH2 + but2ène

add1 -587.2969413 -587.058005

6	0.490565	2.760482	0.171905
6	1.764677	2.164112	0.029700
6	1.850587	1.611161	-1.275226
6	0.628327	1.876840	-1.940293
6	-0.216270	2.579759	-1.045048
63	-0.011660	0.036731	-0.026622
6	0.459286	-1.789332	-1.992721
6	0.623471	-2.530591	-0.797361
6	-0.644097	-2.646711	-0.171078
6	-1.594289	-1.986002	-0.987779
6	-0.913799	-1.449864	-2.109355
6	-1.865393	-0.097036	1.949496
6	-2.414672	0.819461	1.063881
6	-3.779522	0.661174	0.449288
6	-0.595033	-0.006683	2.559458
1	-2.658881	-1.920789	-0.802998
1	-1.369872	-0.916699	-2.935420
1	1.237802	-1.553780	-2.708099

1	1.549001	-2.976781	-0.452848
1	-0.854116	-3.185305	0.744996
1	0.390305	1.610161	-2.963046
1	-1.208519	2.954016	-1.267488
1	0.131942	3.292792	1.044953
1	2.555661	2.172562	0.771022
1	2.713659	1.111827	-1.698793
1	-2.025457	1.839376	1.096569
1	-3.811406	0.993732	-0.594961
1	-4.106342	-0.384169	0.471882
1	-4.537299	1.247905	0.987778
1	-0.308911	-0.781137	3.264989
1	-0.201692	0.985108	2.791872
1	-2.368929	-1.065650	2.013932
15	2.974943	-0.961567	1.342969
1	1.632683	-0.710783	1.867496
1	3.549270	-0.201381	2.413851
1	3.038503	-2.202199	2.057743

[TS-1,4-PH2-H] -587.2905724 -587.050211

6	0.457115	-0.344996	-2.731508
6	-0.043903	0.975423	-2.647170
6	0.922853	1.771957	-1.980907
6	2.027620	0.943101	-1.665135
6	1.738701	-0.366992	-2.121751
63	0.016351	0.086928	-0.034223
6	1.013418	1.871356	1.749177
6	-0.304868	1.633921	2.207273
6	-0.370916	0.300582	2.686428
6	0.912283	-0.280434	2.537076
6	1.767767	0.685447	1.952965
6	-0.974464	-2.408003	0.503401
6	0.240769	-2.743514	-0.041304
6	1.313733	-3.499332	0.688909
6	-2.036495	-1.686657	-0.152302
1	1.200196	-1.279442	2.839810
1	2.823672	0.558300	1.744810
1	1.389725	2.805562	1.349856
1	-1.109596	2.358583	2.221320
1	-1.238469	-0.171494	3.132052
1	2.944109	1.260553	-1.182507
1	2.402820	-1.221206	-2.061284
1	-0.032684	-1.180020	-3.218869
1	-0.983712	1.328764	-3.054158
1	0.840470	2.833466	-1.780504
1	0.351218	-2.675278	-1.124870
1	2.307973	-3.062217	0.541219
1	1.117769	-3.531637	1.765250
1	1.372076	-4.537740	0.335745
1	-3.003593	-1.748872	0.343556
1	-2.119132	-1.845905	-1.230541

1	-1.091782	-2.573613	1.576765
15	-2.596702	1.582513	-0.341563
1	-2.230357	-0.074716	-0.169164
1	-3.468401	1.101319	-1.373145
1	-3.533584	1.330264	0.713220

add12 -587.3212031 -587.080698

6	-1.229827	-2.433337	0.159215
6	-2.330441	-1.592234	-0.126925
6	-2.174436	-1.105681	-1.450147
6	-0.984825	-1.661247	-1.986660
6	-0.397732	-2.477703	-0.991740
63	-0.189004	0.111409	-0.081246
6	-0.010218	1.819959	-2.160228
6	-0.140025	2.670617	-1.035103
6	1.050234	2.574724	-0.274379
6	1.920855	1.673297	-0.935259
6	1.265405	1.200088	-2.098702
6	1.977142	-0.576575	2.020411
6	2.198054	-1.621973	1.200228
6	3.234604	-1.678855	0.119991
6	1.057590	-0.593007	3.204792
1	2.932384	1.428938	-0.633427
1	1.684436	0.531246	-2.841135
1	-0.740472	1.695316	-2.950699
1	-0.995298	3.291944	-0.801461
1	1.264851	3.122429	0.635565
1	-0.607273	-1.508393	-2.990415
1	0.496969	-3.077606	-1.111214
1	-1.077267	-2.984732	1.080133
1	-3.154935	-1.369417	0.537914
1	-2.866424	-0.453558	-1.969853
1	1.641680	-2.542603	1.382562
1	2.802236	-1.942379	-0.851808
1	3.768959	-0.731574	0.015762
1	3.969889	-2.458348	0.355197
1	1.628023	-0.405875	4.122762
1	0.550467	-1.556529	3.309376
1	2.564337	0.332104	1.871590
15	-2.097042	1.439031	1.596703
1	0.292356	0.191889	3.148802
1	-2.243709	0.426949	2.610825
1	-1.166582	2.217541	2.374483

but-2-ene -157.1762665 -157.095432

6	-0.008172	0.094655	0.036692
1	0.409309	-0.204017	1.006736
1	0.824983	0.357966	-0.622170
6	-0.852498	-0.993414	-0.551097
1	-0.596684	1.003274	0.217081

6	-0.636616	-1.585621	-1.728141
1	-1.708793	-1.315082	0.045323
6	-1.480866	-2.673757	-2.315880
1	0.219678	-1.263941	-2.324554
1	-1.898210	-2.375297	-3.286044
1	-0.892308	-3.582405	-2.496009
1	-2.314093	-2.936972	-1.657075

2.3.b/ with P in beta position

Cp2Eu1,4 + H-PH2 -> add13 -> [TS-1,4-H-PH2] -> add14 -> Cp2EuH + 1-PH2-but-2-ène

add13 -587.298297 -587.071136

6	1.068308	-1.420246	-0.550691
6	1.900099	-0.300587	-0.808763
6	2.688696	-0.064228	0.346192
6	2.334181	-1.029086	1.322249
6	1.335588	-1.869463	0.765258
63	0.154794	0.589907	1.079302
6	-2.199717	0.049672	0.093708
6	-2.069328	-0.931150	1.098472
6	-1.817184	-0.689785	2.445029
6	-1.645658	-1.785363	3.464418
6	1.122538	3.141902	1.047096
6	1.276635	2.707093	2.388339
6	-0.015510	2.596755	2.963291
6	-0.965486	2.962867	1.978216
6	-0.264195	3.297626	0.794148
15	-1.335292	-3.368677	-7.851440
1	2.217933	2.533564	2.896896
1	3.445488	0.703246	0.454911
1	-0.235585	2.323316	3.989140
1	2.783990	-1.136321	2.303217
1	-2.039359	3.008086	2.115480
1	-0.708396	3.647528	-0.130952
1	0.371077	-1.868303	-1.247780
1	1.925158	3.354828	0.350866
1	1.957488	0.249076	-1.741804
1	0.883782	-2.726072	1.250269
1	-1.551645	-3.943431	-9.148095
1	-0.154989	-2.675139	-8.280992
1	-2.180787	-2.244166	-8.133408
1	-2.378687	-0.270157	-0.928422
1	-2.643611	1.011063	0.357432
1	-1.919890	-1.960474	0.760477
1	-2.118893	0.285418	2.840611
1	-2.573791	-1.979097	4.020768
1	-0.879541	-1.547319	4.212483
1	-1.353143	-2.726230	2.985382

[TS-1,4-H-PH2] -587.226777 -586.984757

6	2.643403	1.869326	-4.219333
6	1.436319	2.519361	-4.582588
6	1.172468	2.227269	-5.944794
6	2.224799	1.413913	-6.429663
6	3.130806	1.188817	-5.359475
63	3.331268	3.882854	-5.956241
6	6.066752	3.077146	-5.694480
6	5.561421	2.745741	-7.056726
6	5.433656	3.588919	-8.110545
6	5.053541	3.160109	-9.494909
6	1.385664	5.766157	-6.097091
6	1.625997	5.398505	-7.445783
6	2.906922	5.888228	-7.807200
6	3.461754	6.543810	-6.681568
6	2.522535	6.466638	-5.622966
15	5.932042	4.824099	-4.395051
1	0.932679	4.882852	-8.099521
1	0.307165	2.552600	-6.509160
1	3.358684	5.818255	-8.789337
1	2.293863	0.989981	-7.425199
1	4.423242	7.039991	-6.641178
1	2.644455	6.889834	-4.633094
1	3.099343	1.878028	-3.237396
1	0.480744	5.567697	-5.535715
1	0.805412	3.101553	-3.921477
1	4.014319	0.562627	-5.393286
1	6.787405	5.419485	-5.434401
1	5.229677	6.090657	-4.322697
1	4.338374	4.282509	-4.107545
1	5.891512	2.248487	-5.003306
1	7.139103	3.278054	-5.733431
1	5.262586	1.707550	-7.222973
1	5.735974	4.630204	-7.982424
1	5.919060	3.234552	-10.165822
1	4.271204	3.795538	-9.923097
1	4.705569	2.122892	-9.513868

	add14	-587.2719574	-587.035198

6	2.286141	2.030798	-4.096051
6	1.118156	2.482436	-4.759493
6	1.167377	2.022865	-6.102424
6	2.368200	1.289782	-6.265883
6	3.060921	1.300355	-5.027979
63	3.099454	3.926523	-5.894033
6	6.747498	3.196126	-5.836844
6	5.823818	2.788611	-6.950452
6	5.361408	3.540817	-7.966418
6	4.539854	3.015628	-9.108321
6	1.128779	5.634145	-6.692561
6	2.132074	5.786483	-7.679455
6	3.250020	6.419105	-7.072385

6	2.936445	6.656553	-5.712075
6	1.629180	6.163787	-5.475373
15	7.506223	4.919811	-5.780452
1	2.034140	5.528057	-8.728052
1	0.398509	2.163581	-6.852973
1	4.160041	6.724338	-7.576098
1	2.675283	0.769199	-7.166143
1	3.576762	7.131835	-4.981007
1	1.095008	6.211285	-4.533604
1	2.543831	2.212083	-3.060950
1	0.142534	5.213222	-6.846967
1	0.308800	3.045831	-4.310366
1	4.000603	0.804033	-4.815320
1	7.826202	5.030295	-7.178185
1	6.283637	5.659043	-5.907916
1	4.262377	4.350233	-4.242557
1	6.229610	3.090064	-4.872964
1	7.584372	2.485924	-5.804895
1	5.541991	1.732153	-6.938802
1	5.663992	4.586349	-8.023629
1	5.102981	3.107350	-10.045243
1	3.615888	3.588632	-9.251925
1	4.278840	1.962260	-8.974152

1-PH2-but-2-ène	-164.3316474	-164.246369

6	0.022023	-0.518147	0.031685
6	0.026446	-0.039157	1.449591
6	-1.021483	0.494219	2.084816
6	-1.004706	0.984312	3.497444
15	-1.273376	2.868469	3.544799
1	0.766044	0.018126	-0.570881
1	0.279851	-1.582996	-0.029631
1	-0.956458	-0.379212	-0.437713
1	0.967775	-0.144487	1.992769
1	-1.964140	0.607324	1.546298
1	-1.838475	0.556339	4.067555
1	-0.074995	0.713241	4.003611
1	-1.011700	3.043868	4.947704
1	0.063581	3.231653	3.170511

3-Third Step

3.1/Activation P-H of PH3 on Cp2Eu1,2-PH2

3.1.a/ Activation beta

Cp2Eu1,2-PH2 + PH3 -> add15 -> [TS-1,2PH2-PH3] -> add16 -> Cp2EuH + 3,4-PH2-but-1-ene

add16 -594.4292794 -594.201997

6	2.858610	-1.630278	-1.215149
6	2.828613	-1.041730	-2.506310
6	1.628149	-1.440075	-3.140033
6	0.920246	-2.285329	-2.244201
6	1.682057	-2.407536	-1.058652
63	0.876946	0.220610	-1.068623
6	-0.643537	-0.536627	0.751420
6	2.212834	2.533177	-1.659363
6	0.887344	2.962439	-1.399140
6	0.625867	2.768460	-0.018934
6	1.787022	2.219571	0.574158
6	2.769014	2.071047	-0.438719
15	-3.050181	-0.298365	6.753757
1	3.599720	-0.414336	-2.937087
1	0.210342	3.408162	-2.119712
1	1.327631	-1.186018	-4.150697
1	-0.290046	3.023380	0.500367
1	-0.013976	-2.793888	-2.452538
1	1.422541	-3.004013	-0.193317
1	3.781796	1.712097	-0.297909
1	3.664965	-1.543714	-0.495774
1	2.724996	2.584405	-2.613132
1	1.909582	1.976107	1.622915
1	-3.963717	-1.222720	7.361868
1	-1.902323	-0.986674	7.270959
1	-3.020822	-1.029715	5.520456
6	-1.881648	-0.825719	-0.121257
15	-3.447376	-1.100609	0.939208
6	-2.059842	0.286190	-1.105536
6	-1.890778	0.203663	-2.440589
1	-0.869878	0.271588	1.461148
1	-0.384222	-1.425394	1.338624
1	-3.556565	0.259437	1.388436
1	-4.465399	-0.921254	-0.067819
1	-1.743055	-1.769299	-0.666730
1	-2.273522	1.264345	-0.668246
1	-2.015098	1.072789	-3.081675
1	-1.716561	-0.750933	-2.933180

[TS-1,2PH2-PH2-H] -594.3687917 -594.121806

6	2.502520	1.855390	0.849628
6	1.430158	2.756592	0.628354
6	1.075878	2.680216	-0.741271
6	1.914549	1.722149	-1.363296
6	2.799973	1.217176	-0.379985
63	0.384589	0.239908	0.383846
6	-0.841293	-1.904984	-1.098909
6	0.202453	0.712196	3.062254
6	-1.142187	0.543608	2.651519

6	-1.323523	-0.821885	2.304788
6	-0.089724	-1.487857	2.482265
6	0.858190	-0.537195	2.942272
15	1.313222	-2.065641	-1.594887
1	0.994731	3.424185	1.361975
1	-1.912665	1.306491	2.668369
1	0.333891	3.295013	-1.234711
1	-2.256897	-1.282069	2.002154
1	1.905748	1.443540	-2.409782
1	3.576236	0.480075	-0.544738
1	1.890229	-0.744425	3.199062
1	3.024391	1.703131	1.786457
1	0.646452	1.632021	3.420615
1	0.100107	-2.540757	2.313094
1	0.775583	-1.528918	-2.856734
1	2.529298	-1.295658	-1.843034
1	1.555620	-1.521810	-0.097758
6	-1.755074	-0.982554	-1.899326
15	-3.295850	-1.938686	-2.503734
6	-2.147240	0.229044	-1.115217
6	-1.837410	1.501242	-1.423653
1	-1.157985	-1.993505	-0.049369
1	-0.886454	-2.924942	-1.491448
1	-3.941922	-2.023764	-1.222688
1	-4.093980	-0.810511	-2.907594
1	-1.239411	-0.683787	-2.826206
1	-2.741621	0.038103	-0.218873
1	-2.184534	2.334256	-0.817934
1	-1.290116	1.745212	-2.330388

add15 -594.4209381 -594.178228

6	3.165140	-1.305049	0.612472
6	3.331170	-1.128867	-0.785069
6	2.288986	-1.828002	-1.440234
6	1.485575	-2.446718	-0.446080
6	2.028489	-2.127130	0.822351
63	1.078085	0.258026	-0.124986
6	-3.023686	-0.753346	1.471003
6	2.385657	2.338777	-1.297743
6	1.021280	2.642221	-1.528225
6	0.423560	2.949841	-0.278118
6	1.417199	2.842784	0.723405
6	2.629577	2.460595	0.095622
15	-2.047264	-2.223088	2.144077
1	4.129338	-0.577294	-1.267064
1	0.538158	2.695475	-2.498057
1	2.160828	-1.919587	-2.513330
1	-0.601009	3.265353	-0.118913
1	0.634678	-3.092823	-0.628702
1	1.651395	-2.457521	1.781352
1	3.586240	2.325732	0.586808

1	3.816945	-0.914884	1.385791
1	3.122296	2.099670	-2.055470
1	1.273667	3.023921	1.780726
1	-2.833762	-3.228615	1.475068
1	-1.023337	-2.239219	1.143681
1	0.064322	0.195928	1.685114
6	-3.144438	-0.649655	-0.059505
15	-4.834662	0.159067	-0.466344
6	-2.063848	0.138673	-0.716268
6	-1.318759	-0.262267	-1.764066
1	-2.543906	0.142695	1.877229
1	-4.013822	-0.831793	1.936292
1	-4.498241	1.475143	0.000964
1	-4.565566	0.496979	-1.835895
1	-3.204969	-1.648975	-0.505541
1	-1.928064	1.151341	-0.329740
1	-0.679219	0.444644	-2.298583
1	-1.422705	-1.252896	-2.198557

3,4-PH2-but-1-ene -171.477727 -171.387693

C	0.028355	0.186095	-0.114452
C	-0.054490	-0.024641	1.405199
P	1.630143	-0.017135	2.282075
H	-0.638474	0.784827	1.860460
H	-0.584795	-0.959482	1.607363
C	-1.337850	0.257656	-0.721647
P	1.089658	1.723197	-0.534131
H	0.577602	-0.653560	-0.560098
H	0.572426	1.893219	-1.861906
H	0.183627	2.690876	0.021767
C	-1.799428	-0.555703	-1.673221
H	-1.983303	1.047127	-0.332384
H	-2.801559	-0.446356	-2.077171
H	-1.188972	-1.354984	-2.088027
H	1.178624	-0.712815	3.455583
H	2.130565	-1.220220	1.676354

3.1.b/ Activation alpha

Cp2Eu1,2-PH2 + H-PH2 -> add17 -> [TS-1,2-PH2-H-PH2] -> add18 -> Cp2EuPH2 + CH3-CH(PH2)-CH=CH2

add17 -594.4293521 -594.199174

6	0.630934	-2.205741	2.036594
6	1.389137	-1.007023	2.081696
6	0.539274	0.033889	2.535166
6	-0.745166	-0.518234	2.754351
6	-0.689989	-1.903453	2.443909
63	-0.342606	-0.638737	0.019033
6	-0.299615	1.831136	-0.281568

6	-1.746911	2.108814	0.170395
15	-2.273345	3.909203	-0.197206
6	0.933607	-0.798244	-2.404685
6	1.335386	-1.943639	-1.670679
6	0.212964	-2.804596	-1.552847
6	-0.881739	-2.185352	-2.203827
6	-0.435291	-0.944909	-2.728768
6	-2.659222	1.115532	-0.475494
6	-3.336821	0.129970	0.146756
1	-1.604772	0.012276	3.147644
1	-1.501619	-2.614981	2.550054
1	1.004385	-3.183963	1.758696
1	2.445142	-0.912792	1.855147
1	0.827795	1.063695	2.702828
1	0.204608	-3.778331	-1.077483
1	-1.873627	-2.608042	-2.321668
1	-1.027739	-0.247657	-3.309345
1	1.566248	0.036261	-2.681134
1	2.335695	-2.149579	-1.307754
1	-0.177631	2.124046	-1.333952
1	0.400720	2.432009	0.310279
1	-1.824046	2.011848	1.262322
1	-2.703899	1.168515	-1.565741
1	-3.957416	-0.567815	-0.409869
1	-3.361806	0.054412	1.232084
1	-2.295497	3.763514	-1.626150
1	-3.706543	3.774747	-0.093590
15	5.809511	1.868617	-0.110332
1	5.003335	2.980921	-0.523221
1	6.515238	2.650688	0.863471
1	6.793852	2.114454	-1.124643

[TS-1,2-PH2-H-PH2] -594.4178296 -594.172689

6	-2.229847	1.777690	-1.159476
6	-2.143129	2.139499	0.206222
6	-0.848037	2.677302	0.435766
6	-0.136807	2.638140	-0.784160
6	-0.987298	2.072300	-1.772434
63	-0.480994	-0.008349	-0.064879
6	1.847331	-0.078443	1.284747
6	2.700099	0.289777	0.059307
15	4.554671	-0.029352	0.424334
6	-1.628273	-2.388762	0.677830
6	-2.543732	-1.777740	-0.216138
6	-1.965731	-1.794018	-1.511167
6	-0.692634	-2.406466	-1.413166
6	-0.480462	-2.771088	-0.059515
6	2.236931	-0.461149	-1.147039
6	1.809281	0.078990	-2.301490
1	0.866131	3.015825	-0.944040
1	-0.753401	1.948732	-2.823304
1	-3.100391	1.362465	-1.652450

1	-2.934254	2.052979	0.940913
1	-0.481627	3.076685	1.373769
1	-2.430271	-1.433499	-2.421222
1	-0.018663	-2.601087	-2.238952
1	0.383238	-3.292464	0.335613
1	-1.797707	-2.567735	1.732481
1	-3.527359	-1.402982	0.040362
1	2.022737	-1.130959	1.553175
1	2.181894	0.520842	2.139755
1	2.638056	1.368401	-0.133589
1	2.231993	-1.548131	-1.042547
1	1.484210	-0.541288	-3.132095
1	1.832912	1.151944	-2.470636
1	4.459409	-1.462804	0.405446
1	5.061014	0.022957	-0.923867
15	-1.020511	0.135656	2.922130
1	0.363163	0.091867	2.009146
1	-0.398233	1.214622	3.628411
1	-0.418786	-0.891117	3.718311

	add18	-594.4726012	-594.226734

6	2.641595	-1.548457	-1.301064
6	3.012333	-1.575648	0.068092
6	2.032781	-2.320172	0.774638
6	1.050016	-2.737143	-0.153869
6	1.426959	-2.262116	-1.438258
63	0.823182	0.006084	-0.001950
6	-3.593659	0.236556	1.563070
6	-3.526164	-0.454266	0.197756
15	-5.244814	-0.307107	-0.630676
6	1.661093	2.544332	0.557213
6	2.503690	2.065464	-0.477313
6	1.729241	1.960152	-1.662399
6	0.409180	2.375853	-1.356086
6	0.366146	2.730407	0.016112
6	-2.481272	0.100046	-0.705930
6	-1.643727	-0.622973	-1.474942
1	0.184066	-3.348378	0.073726
1	0.907149	-2.455494	-2.369940
1	3.204307	-1.088606	-2.104431
1	3.910194	-1.144141	0.494690
1	2.045516	-2.540731	1.834391
1	2.095583	1.665835	-2.638773
1	-0.408686	2.460116	-2.063576
1	-0.494278	3.109783	0.554299
1	1.957190	2.742676	1.579725
1	3.563071	1.856179	-0.389346
1	-3.773893	1.311907	1.453945
1	-4.403523	-0.179022	2.169899
1	-3.372378	-1.531874	0.330511
1	-2.445262	1.189450	-0.769906

1	-1.010834	-0.139196	-2.220226
1	-1.674348	-1.709348	-1.484783
1	-5.147223	1.090033	-0.952003
1	-4.850958	-0.710942	-1.950139
15	0.447090	0.042466	2.831644
1	-2.653069	0.107574	2.106788
1	-0.454942	-1.077767	2.917644
1	-0.601565	1.026044	2.893691

CH3-CH(PH2)-CH=CH2 -164.3259911 -164.240144

6	0.029275	0.066554	-0.045154
6	-0.051073	-0.230936	1.457171
1	0.945480	-0.341676	1.896665
1	-0.565447	0.575202	1.992497
1	-0.609297	-1.155865	1.635514
6	-1.319199	0.243015	-0.665772
15	1.158281	1.584956	-0.301870
1	0.556295	-0.755000	-0.546816
1	0.815442	1.827154	-1.673845
1	0.220179	2.563264	0.177420
6	-1.784643	-0.445153	-1.709818
1	-1.950957	1.003988	-0.203419
1	-2.774766	-0.261678	-2.116543
1	-1.188835	-1.212695	-2.199267

3.2/Activation P-H of PH3 on Cp2Eu1,4-PH2

3.2.a/ Activation beta

Cp2Eu1,4-PH2 + PH3 -> add19 -> [TS-1,4PH2-PH3] -> add20 -> Cp2EuH + 1,4-diPH2-but-2-ene

add19 -594.4579398 -594.223272

6	-1.909027	-0.230305	2.218620
6	-0.817977	0.127530	3.051345
6	0.132194	-0.922383	2.999539
6	-0.366628	-1.924642	2.131760
6	-1.629546	-1.497717	1.649602
63	0.137444	0.249862	0.491446
6	0.054466	-1.513394	-1.510500
6	-1.479755	2.137339	-0.610339
6	-0.880201	2.776355	0.508900
6	0.490448	2.965167	0.220706
6	0.742735	2.445256	-1.077097
6	-0.477960	1.945827	-1.592200
15	-4.211872	-2.579837	-5.119460
1	-0.742903	1.025660	3.653178
1	-1.390133	3.088691	1.412162
1	1.060286	-0.966282	3.556942
1	1.214440	3.448891	0.865678
1	0.113492	-2.869812	1.907414

1	-2.281617	-2.056122	0.988818
1	-0.626084	1.506511	-2.570718
1	-2.813348	0.347977	2.071197
1	-2.529453	1.888511	-0.714684
1	1.689130	2.482199	-1.604058
1	-3.959529	-3.991652	-5.158415
1	-5.602096	-2.767006	-4.817276
1	-3.852739	-2.485171	-3.733639
6	1.386162	-1.061460	-1.507788
6	2.296950	-1.213382	-0.469027
6	3.559358	-0.407086	-0.321092
15	3.225971	0.550313	1.264372
1	-0.545726	-1.373872	-2.403805
1	-0.209087	-2.379192	-0.903010
1	1.654765	-0.335466	-2.281170
1	2.157144	-2.037471	0.233681
1	3.651994	0.324249	-1.131441
1	4.487062	-0.987148	-0.274145
1	3.722317	-0.392621	2.216907
1	4.324299	1.468027	1.397016

[TS-1,4PH2-PH2-H] -594.3782943 -594.131668

6	-2.133475	-0.016745	2.201283
6	-0.808008	0.024435	2.704590
6	-0.187239	-1.211172	2.390654
6	-1.120910	-2.007874	1.684515
6	-2.323930	-1.268561	1.565231
63	-0.567602	0.105004	-0.007091
6	0.687319	-1.086404	-2.259964
6	-1.892838	2.425417	-0.448658
6	-0.864125	2.761412	0.467419
6	0.375643	2.667728	-0.209875
6	0.109724	2.288596	-1.552183
6	-1.290022	2.140311	-1.700365
15	-1.177702	-2.206410	-2.107760
1	-0.365492	0.834160	3.272418
1	-1.003506	3.057492	1.499833
1	0.809545	-1.512442	2.689577
1	1.350578	2.885374	0.210123
1	-0.956841	-3.014080	1.319890
1	-3.235211	-1.610479	1.089528
1	-1.812857	1.875738	-2.610959
1	-2.878208	0.762778	2.307052
1	-2.956499	2.422528	-0.241382
1	0.845899	2.183912	-2.340403
1	-0.260147	-3.299152	-1.745204
1	-2.088324	-2.705474	-1.093229
1	-1.810291	-0.749793	-1.523202
6	1.737785	-0.690328	-1.276728
6	2.108220	-1.381429	-0.172269
6	3.280484	-1.077591	0.714465

15	3.963856	0.684242	0.582051
1	0.443388	-0.255314	-2.927636
1	1.049085	-1.918066	-2.868213
1	2.260613	0.248562	-1.480493
1	1.594417	-2.321825	0.040570
1	4.077350	-1.803893	0.513285
1	3.004461	-1.217052	1.766059
1	5.099468	0.447764	1.425592
1	4.727396	0.499739	-0.619504

add20 -594.4260925 -594.184613

6	-2.492022	-0.337520	2.117210
6	-1.356621	0.139725	2.822149
6	-0.314962	-0.804498	2.659357
6	-0.809152	-1.868207	1.857838
6	-2.156209	-1.582134	1.528555
63	-0.725468	0.322156	0.176553
6	0.782342	-1.392047	-2.823030
6	-1.712385	2.834625	0.312033
6	-0.345066	2.973270	0.669957
6	0.431912	2.743100	-0.492458
6	-0.452938	2.455830	-1.562932
6	-1.776851	2.517949	-1.067724
15	0.280779	-3.191370	-2.575513
1	-1.305825	1.049850	3.407555
1	0.032589	3.259175	1.644683
1	0.663078	-0.754812	3.125287
1	1.510548	2.832471	-0.561998
1	-0.270527	-2.771060	1.593400
1	-2.814528	-2.202475	0.935351
1	-2.677258	2.350761	-1.644238
1	-3.459751	0.147618	2.065580
1	-2.559214	2.983104	0.971557
1	-0.173170	2.259284	-2.591217
1	1.522165	-3.657277	-2.019328
1	-0.342379	-3.033475	-1.293353
1	-1.882017	-0.539688	-1.297772
6	1.548655	-0.643117	-1.770890
6	1.914094	-1.070255	-0.546074
6	2.796945	-0.306097	0.392724
15	4.572845	-1.010285	0.327581
1	-0.159010	-0.865221	-3.032219
1	1.357433	-1.355970	-3.757970
1	1.876919	0.354540	-2.074851
1	1.640603	-2.079437	-0.238007
1	2.433221	-0.357897	1.422674
1	2.875390	0.746042	0.101157
1	4.999321	-0.478534	1.592728
1	4.249576	-2.286856	0.901376

1,4-diPH2-but-2-ene -171.486834 -171.396945

C	0.395357	-0.461684	0.088455
C	0.045736	-0.478860	1.541203
P	1.277177	1.166962	-0.357364
H	1.113896	-1.256251	-0.147009
H	-0.488242	-0.607134	-0.537550
C	-1.201287	-0.479380	2.025659
H	0.884203	-0.473499	2.240017
C	-1.550926	-0.463801	3.478415
H	-2.039758	-0.473857	1.326843
P	-2.434148	1.163666	3.925704
H	-2.268681	-1.259309	3.713200
H	-0.667156	-0.608993	4.104226
H	-2.452246	0.958553	5.348369
H	-1.253263	1.976766	3.978694
H	1.294564	0.963675	-1.780300
H	0.095621	1.979205	-0.408563

3.2.b/ Activation alpha

Cp2Eu1,4-PH2 + H-PH2 -> add21 -> [TS-1,4PH2-H-PH2] -> add22 -> Cp2EuPH2 + CH3-CH-CH-CH2-PH2

add21 -594.4533193 - 594.210830

6	1.510542	2.554410	0.162155
6	2.081901	1.980448	-1.004444
6	1.056533	1.858394	-1.974238
6	-0.148160	2.342356	-1.405068
6	0.136347	2.777470	-0.084908
63	0.428504	0.017268	-0.059756
6	1.897191	-1.734393	-1.532687
6	1.779695	-2.376327	-0.275319
6	0.424569	-2.748373	-0.092849
6	-0.296304	-2.345352	-1.244504
6	0.611080	-1.716304	-2.133046
6	-1.723137	-0.516209	1.515314
6	-2.264611	0.158640	0.424186
6	-3.371716	-0.411090	-0.415023
15	-5.066430	0.230596	0.183095
6	-0.697614	-0.044257	2.354888
1	-1.349355	-2.516010	-1.429745
1	0.373900	-1.331734	-3.117980
1	2.813038	-1.360249	-1.973721
1	2.595794	-2.591710	0.404491
1	0.022264	-3.286258	0.756872
1	-1.106204	2.414463	-1.906393
1	-0.566822	3.234882	0.601041
1	2.044027	2.823802	1.066668
1	3.125276	1.722933	-1.141150
1	1.178526	1.485697	-2.984137
1	-2.179264	1.247434	0.416922
1	-3.294166	-0.096186	-1.461976

1	-3.361122	-1.504491	-0.396653
1	-1.968246	-1.578884	1.593276
1	-0.378837	-0.667915	3.184466
1	-0.618041	1.030144	2.530786
1	-5.891495	-0.657930	-0.593066
1	-5.143936	-0.596858	1.353508
15	3.211365	-0.043822	2.010884
1	1.773534	-0.125869	2.245395
1	3.345561	0.938492	3.045731
1	3.437871	-1.149710	2.893836

[TS-1,4PH2-H-PH2] -594.4460438 -594.202473

6	-0.897415	0.876201	-2.740451
6	-0.165473	2.019734	-2.328816
6	1.176591	1.622271	-2.108305
6	1.271713	0.232440	-2.369302
6	-0.011999	-0.227059	-2.763845
63	-0.248467	0.462857	-0.094509
6	0.370938	2.709046	1.286197
6	-0.763578	2.199650	1.962498
6	-0.385793	0.995232	2.610257
6	0.986787	0.769457	2.343952
6	1.455447	1.822441	1.520857
6	-0.361359	-2.114444	0.848625
6	0.839337	-2.135552	0.176460
6	2.152758	-2.438730	0.830271
15	2.672900	-4.236436	0.455168
6	-1.653973	-1.843813	0.277438
1	1.585298	-0.047103	2.728004
1	2.473393	1.954479	1.173317
1	0.412653	3.631255	0.719506
1	-1.738181	2.669867	2.005933
1	-1.023889	0.384981	3.238479
1	2.177592	-0.361128	-2.328760
1	-0.260958	-1.234982	-3.075041
1	-1.942107	0.862351	-3.026977
1	-0.559796	3.024252	-2.233216
1	1.993291	2.272036	-1.817349
1	0.819005	-2.193952	-0.913029
1	2.958809	-1.812594	0.431499
1	2.106551	-2.279063	1.910440
1	-0.313034	-2.163642	1.938905
1	-2.499033	-2.126796	0.902300
1	-1.787480	-2.155791	-0.761427
1	3.776251	-4.293755	1.375994
1	1.767572	-4.856690	1.380134
15	-3.216492	1.048036	-0.136365
1	-2.325791	-0.390560	0.145138
1	-4.001943	0.183377	-0.967492
1	-3.894771	0.678189	1.070668

add22 -594.4756653 -594.230352

6	1.821665	2.455772	-0.126122
6	1.962994	1.897722	-1.422525
6	0.678420	1.849380	-2.024034
6	-0.256073	2.365457	-1.095122
6	0.450250	2.735232	0.080237
63	0.659022	-0.016502	-0.042506
6	1.448360	-1.650108	-2.046370
6	2.079263	-2.183642	-0.895682
6	1.077917	-2.747980	-0.067374
6	-0.171801	-2.566008	-0.707793
6	0.052790	-1.878985	-1.929219
6	-1.832877	-0.389467	1.808304
6	-2.366343	0.366559	0.827152
6	-3.060694	-0.158140	-0.389900
15	-4.926661	0.229809	-0.266693
6	-1.314088	0.137970	3.111720
1	-1.125577	-2.940579	-0.353945
1	-0.696656	-1.631116	-2.671906
1	1.946927	-1.178226	-2.884226
1	3.141577	-2.170740	-0.685626
1	1.247769	-3.251345	0.876351
1	-1.314922	2.511512	-1.275150
1	0.023735	3.195971	0.963926
1	2.625017	2.646261	0.573903
1	2.896285	1.599770	-1.885643
1	0.458188	1.511039	-3.029372
1	-2.396325	1.448288	0.967548
1	-2.721169	0.358551	-1.294988
1	-2.899122	-1.229411	-0.522651
1	-1.848810	-1.475451	1.693640
1	-1.936192	-0.237842	3.933803
1	-1.334495	1.230985	3.143823
1	-5.308556	-0.521492	-1.429219
1	-5.246423	-0.844033	0.629591
15	2.637792	-0.152906	2.014642
1	-0.288893	-0.193755	3.310654
1	2.118889	0.878434	2.875047
1	2.054700	-1.223277	2.783423

1-PH2-but-2-ene -164.331655 -164.246327

6	0.006533	0.150113	-0.109712
6	-0.147703	0.262085	1.374727
1	1.045337	-0.069595	-0.386772
1	-0.628279	-0.639827	-0.522060
1	-0.256996	1.091571	-0.608161
6	-0.953026	-0.497067	2.123920
1	0.454885	1.027883	1.867371
6	-1.112773	-0.368839	3.605090
1	-1.562349	-1.260995	1.637532

15	-2.884923	0.180951	4.033433
1	-0.982982	-1.341287	4.095950
1	-0.380390	0.323493	4.027507
1	-2.662023	0.396306	5.437163
1	-2.705856	1.568236	3.713011

4-Shift and P-H activation step on Cp2Eu1,4-PH2

4.1/Shift

Cp2Eu1,4-PH2 -> [TS shift] -> Cp2EuPH-CH2-CH2-CH=CH2

[TS shift] -586.0489515 -585.826315

C	-0.835922	-2.407365	-1.241061
C	-0.825023	-2.749236	0.134116
C	-1.939157	-2.123332	0.750825
C	-2.632616	-1.388760	-0.241960
C	-1.949091	-1.563454	-1.474413
Eu	-0.296444	-0.052153	0.057125
C	-1.835444	2.164982	0.381820
C	-0.602065	2.525788	0.975663
C	0.369907	2.618394	-0.051078
C	-0.266857	2.327942	-1.285815
C	-1.627703	2.046443	-1.019758
P	2.591573	-0.173955	-1.687007
C	3.374919	0.000129	0.066508
H	4.385647	-0.410960	0.132538
C	2.329666	-0.718320	0.927077
H	-0.115896	-3.410564	0.617839
H	-2.231852	-2.219397	1.789615
H	-3.547489	-0.826905	-0.096101
H	-2.247724	-1.153908	-2.432186
H	-0.128767	-2.747627	-1.987543
H	-0.439493	2.721474	2.028848
H	1.404024	2.917237	0.072503
H	0.205136	2.340601	-2.260890
H	-2.386576	1.815487	-1.757531
H	-2.780433	2.045617	0.898763
H	3.428960	1.065669	0.312012
H	2.981624	-1.549863	-1.846735
H	1.682065	-0.838356	-0.350523
H	2.498024	-1.789007	1.059290
C	1.647977	-0.038681	1.992779
C	0.543252	-0.490018	2.687228

H	1.908232	1.014851	2.120587
H	0.085341	0.133575	3.447615
H	0.276126	-1.544602	2.692020

Cp2EuPH-CH2-CH2-CH=CH2 -586.1096715 -585.883394

C	-1.566410	-2.022636	-1.410413
C	-1.594852	-2.381095	-0.041889
C	-2.499107	-1.511726	0.623132
C	-3.029336	-0.614780	-0.336433
C	-2.449304	-0.926785	-1.593248
Eu	-0.410204	0.103305	-0.141401
C	-1.313931	2.620216	0.384920
C	-0.005036	2.613256	0.928681
C	0.917658	2.524331	-0.145137
C	0.179459	2.482756	-1.352416
C	-1.198936	2.540984	-1.027868
P	1.970393	-0.968345	-1.348472
C	3.303270	-0.828776	0.012258
H	4.170831	-1.424377	-0.290711
C	2.861985	-1.258293	1.416401
H	-1.044534	-3.198446	0.408655
H	-2.774986	-1.557216	1.671047
H	-3.770770	0.153090	-0.150575
H	-2.677401	-0.444322	-2.536728
H	-0.985195	-2.510201	-2.183279
H	0.244969	2.712559	1.979499
H	1.997944	2.526350	-0.066144
H	0.600328	2.426053	-2.349225
H	-2.020418	2.558941	-1.734074
H	-2.237455	2.717785	0.943758
H	3.640644	0.215311	0.027829
H	1.662543	-2.352982	-1.091436
H	2.527855	-2.302123	1.402266
H	3.717273	-1.207158	2.111937
C	1.784008	-0.383617	1.978627
C	0.605398	-0.790495	2.484522
H	2.011903	0.684270	1.998153
H	-0.082331	-0.087599	2.955890
H	0.338714	-1.843827	2.525773

4.2/Activation P-H of PH3 on shift product Cp2EuPH-CH2-CH2-CH=CH2

Cp2EuPH-CH2-CH2-CH=CH2 + PH3 -> add23 -> [TS Cp2EuPH-CH2-CH2-CH=CH2 PH3] -> add24 -> CP2EuPH2 + PH2-CH2-CH2-CH=CH

add23 -594.470825 -594.225669

C	-2.466084	-1.948177	-1.000486
C	-1.442625	-1.829047	-1.977242

C	-0.235687	-2.309566	-1.408654
C	-0.508544	-2.713671	-0.078298
C	-1.888970	-2.494631	0.171982
Eu	-0.809983	0.020539	-0.099127
C	-2.757477	1.840990	-0.666317
C	-1.779071	1.988951	-1.684642
C	-0.616125	2.550443	-1.097789
C	-0.869065	2.737413	0.283678
C	-2.195506	2.304565	0.548590
P	-1.027730	-0.186909	2.899400
P	1.860890	0.213546	0.425752
C	3.247097	-1.044620	0.617036
H	3.605689	-1.033576	1.652894
C	4.429285	-0.872601	-0.352665
H	2.553530	1.434330	0.679242
H	2.781325	-2.023253	0.456683
H	-2.421507	-2.754167	1.079863
H	-3.512210	-1.703377	-1.142171
H	-1.572196	-1.480359	-2.995207
H	0.723227	-2.369313	-1.908208
H	0.202545	-3.152565	0.611254
H	-1.915609	1.760676	-2.735281
H	-3.769620	1.478559	-0.803719
H	-0.182679	3.170698	1.001024
H	0.301643	2.802263	-1.614446
H	-2.709702	2.369331	1.500810
H	-0.468400	0.884591	3.652333
H	-2.217788	-0.323989	3.690754
H	-0.304836	-1.235515	3.537547
H	5.070389	-1.764618	-0.267082
H	4.058990	-0.841097	-1.383730
C	5.263466	0.341772	-0.074290
C	5.493382	1.333597	-0.934730
H	5.707137	0.393495	0.922317
H	6.113678	2.186231	-0.672203
H	5.066120	1.326810	-1.934958

[TS Cp2EuPH-CH2-CH2-CH=CH2 PH3] -594.4543917 -594.212220

C	2.704685	2.003393	-0.416618
C	1.872849	2.013239	-1.568795
C	0.583213	2.448637	-1.172827
C	0.613794	2.696928	0.222178
C	1.926015	2.426228	0.688664
Eu	0.936848	-0.016048	-0.038770
C	2.715809	-2.015733	0.443467
C	2.839758	-1.724077	-0.938985
C	1.642547	-2.131490	-1.581526
C	0.781440	-2.681824	-0.597542
C	1.445303	-2.610541	0.653369
P	-0.089714	-0.059626	2.722041
P	-1.874033	-0.254628	-0.521967

C	-3.086554	1.044289	0.113348
H	-3.116839	1.023153	1.209821
C	-4.507219	0.916505	-0.460778
H	-2.490531	-1.439085	-0.016120
H	-2.662417	2.012006	-0.176182
H	2.276496	2.546620	1.707024
H	3.759450	1.755580	-0.395497
H	2.183514	1.779248	-2.580586
H	-0.268644	2.587639	-1.827721
H	-0.208865	3.067755	0.821997
H	3.709168	-1.296152	-1.424030
H	3.473291	-1.849101	1.200845
H	-0.195331	-3.113316	-0.778712
H	1.435297	-2.068104	-2.643656
H	1.066669	-2.982313	1.597887
H	-0.985469	-0.183640	1.202003
H	-0.870905	-1.181796	3.133459
H	-1.053048	0.931628	3.084452
H	-5.069435	1.816783	-0.167872
H	-4.467508	0.908805	-1.556175
C	-5.246817	-0.292464	0.030421
C	-5.758327	-1.249278	-0.744062
H	-5.363624	-0.369336	1.113383
H	-6.291907	-2.098243	-0.325818
H	-5.662571	-1.215420	-1.827063

add24 -594.4785929 -594.233224

C	-3.013036	-0.975022	-1.138389
C	-2.019871	-1.008065	-2.151357
C	-1.036672	-1.952034	-1.767789
C	-1.427475	-2.509578	-0.521201
C	-2.648481	-1.909351	-0.133965
Eu	-0.827310	0.131890	0.022511
C	-0.884249	2.379466	-1.524241
C	0.493961	2.107408	-1.338905
C	0.806684	2.341259	0.026459
C	-0.377893	2.750785	0.684972
C	-1.424415	2.770232	-0.272861
P	-1.500883	-0.021822	2.802969
P	1.740468	-1.225824	0.965442
C	3.126075	-1.999115	-0.047774
H	3.807083	-2.525242	0.628562
C	3.892988	-0.987402	-0.910676
H	2.492660	-0.509401	1.940263
H	2.650537	-2.753123	-0.684253
H	-3.213518	-2.134820	0.761825
H	-3.917706	-0.377737	-1.153399
H	-2.028823	-0.436625	-3.071614
H	-0.168625	-2.237142	-2.352022
H	-0.906656	-3.289610	0.021643
H	1.193244	1.822298	-2.117209

H	-1.423234	2.328521	-2.462562
H	-0.467237	3.021969	1.729287
H	1.787914	2.256086	0.477884
H	-2.449815	3.068862	-0.086292
H	1.415526	-2.340409	1.792099
H	-0.287880	0.500632	3.372746
H	-1.152498	-1.395162	3.050487
H	4.576796	-1.557948	-1.556126
H	3.204714	-0.457377	-1.580623
C	4.690816	0.001975	-0.111175
C	4.633497	1.326804	-0.249922
H	5.376044	-0.425359	0.623412
H	5.252945	1.989236	0.347650
H	3.974092	1.797371	-0.975904

PH2-CH2-CH2-CH=CH -164.324158 -164.238313

H	2.757234	2.026917	-0.365236
H	1.728302	2.039041	-1.904387
C	1.794541	2.216987	-0.834756
C	0.749081	2.650347	-0.130261
H	-0.199215	2.825243	-0.642340
H	0.532106	3.984205	1.517581
C	0.754980	2.920644	1.346014
H	1.758897	2.739567	1.748932
C	-0.276231	2.087062	2.121079
H	-1.286704	2.269069	1.742871
H	-0.265974	2.378497	3.177115
P	0.130335	0.237276	2.083242
H	-0.439435	-0.059706	0.800962
H	-1.043826	-0.194075	2.790225