

Supplementary data for the article:

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Methane Activations by Titanium Neopentylidene Complexes: electronic resilience and steric control

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Supporting Information

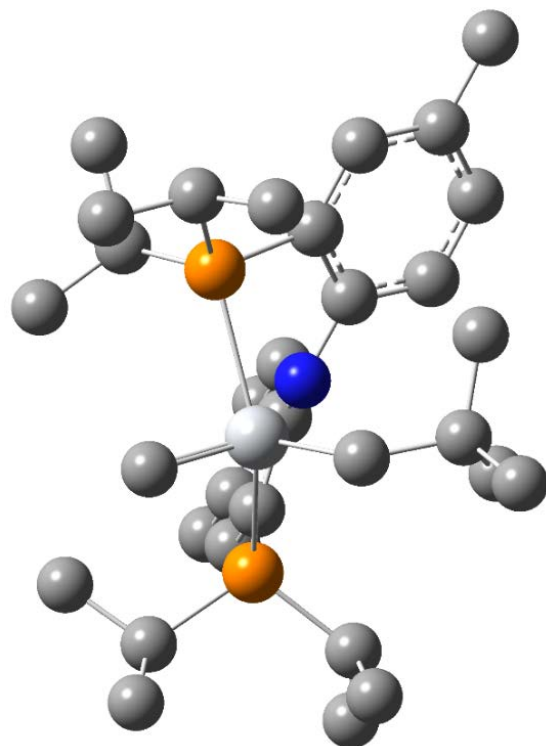
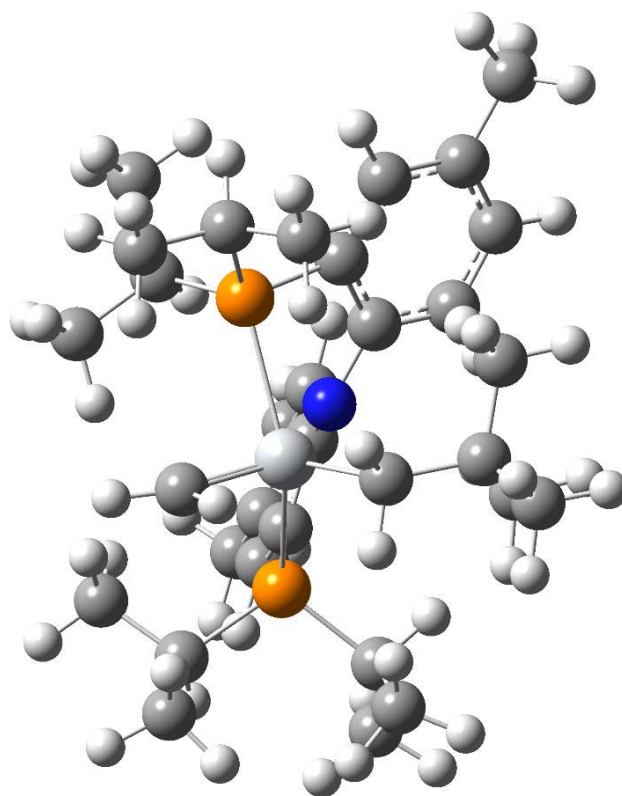


Figure S1. Geometry of the methyldene product isomer 7 with and without H atoms.

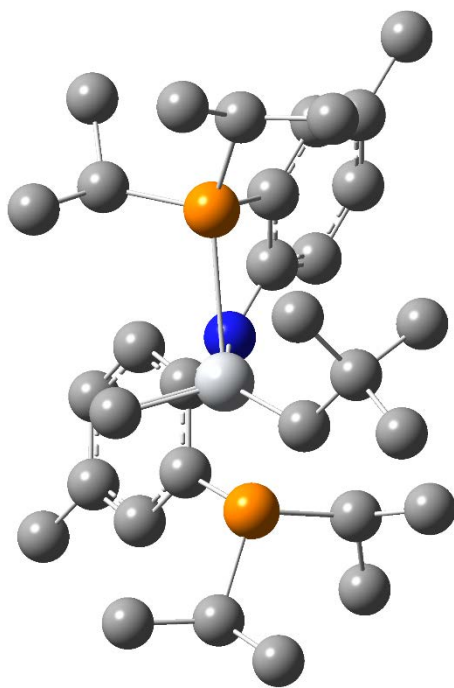
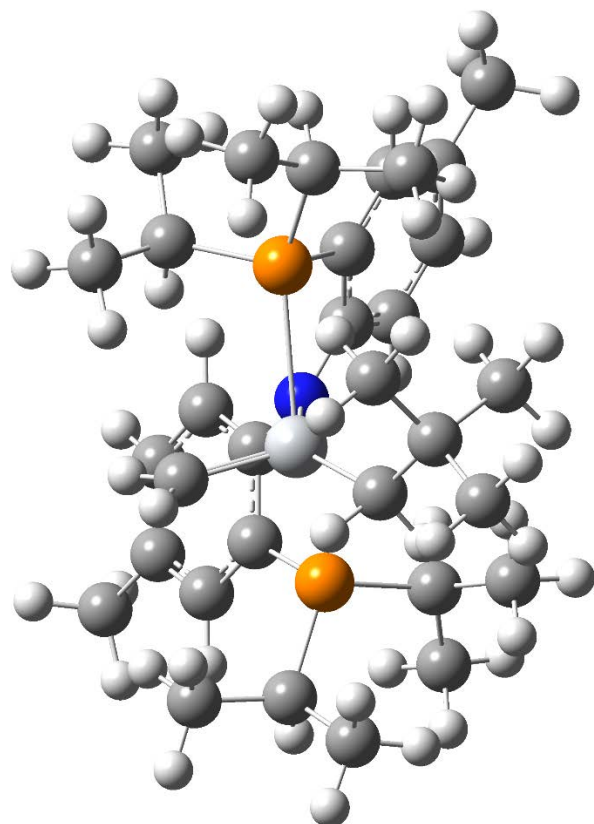


Figure S2. Geometry of the methylidene product isomer 7' with and without H atoms.

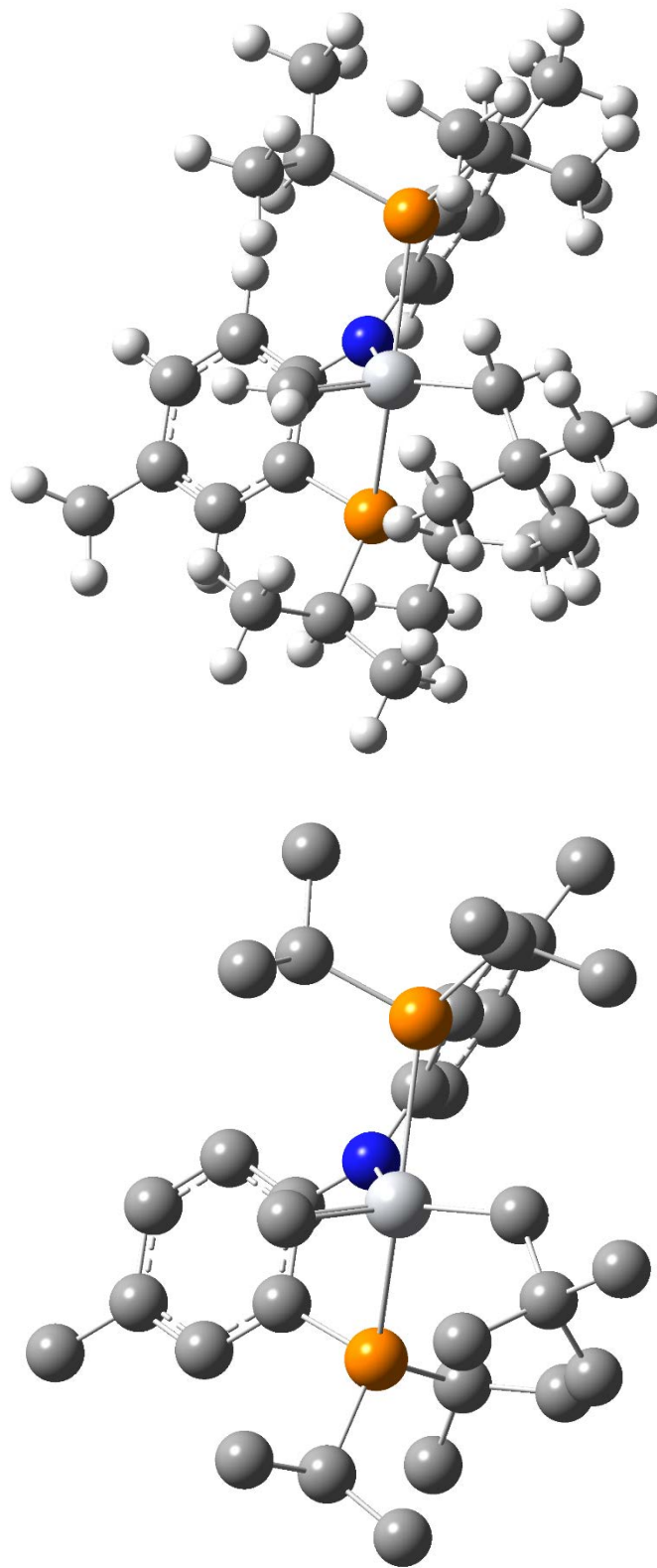


Figure S3. Geometry of the methylidene product isomer 7'' with and without H atoms.

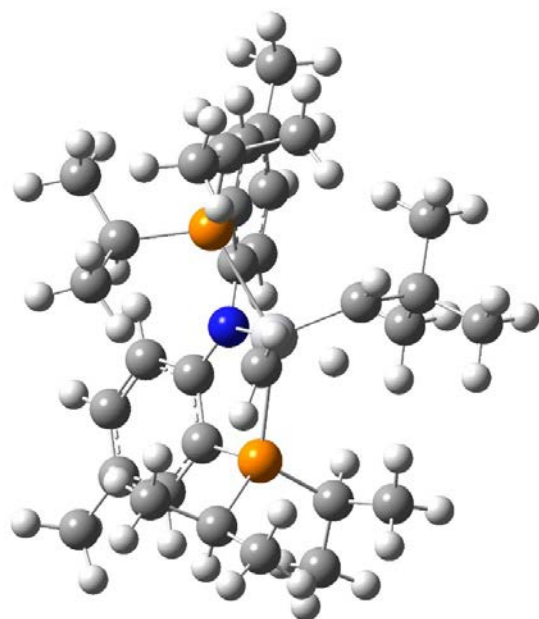


Figure S4. Geometry of the transition state 6-7.

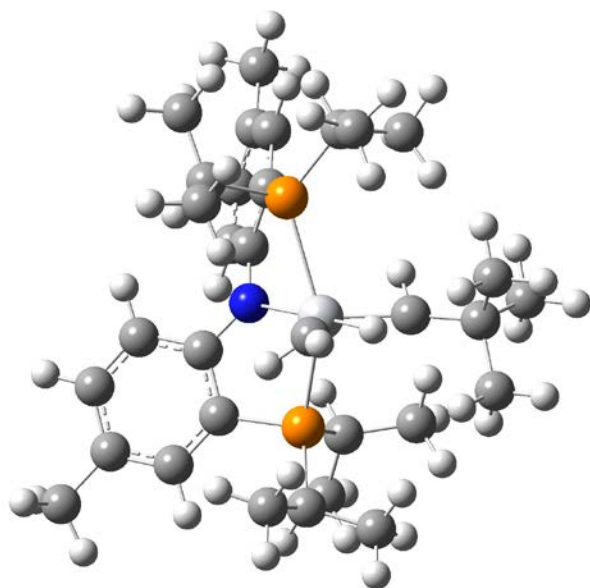


Figure S5. Geometry of the transition state 6'-7'

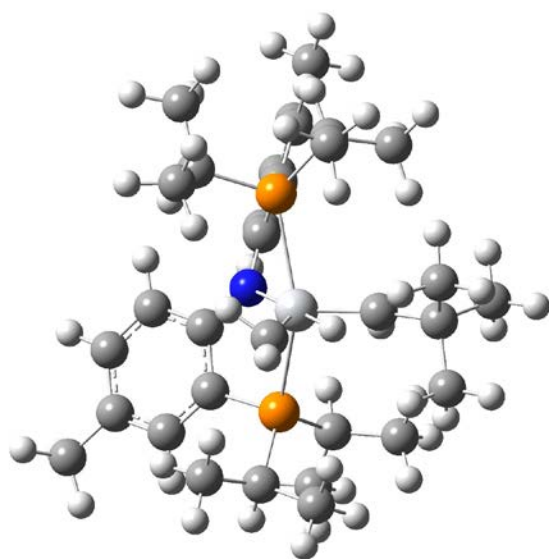


Figure S6. Geometry of the transition state 6'-7''

Computational details

Coordinates and energies (Hartree):

Original complex

1

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6

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6'

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7'

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H -0.728858 1.947126 -2.852788

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H 0.996229 2.663746 1.213457

7"

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C -1.993157 1.778684 2.889769
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C 3.059310 -1.945582 1.422657
C 2.072316 -1.339496 0.639631
C 0.708442 -1.572159 0.917884
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C 0.388428 -2.422308 1.992862
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H -1.007143 0.083341 -2.902722
H -0.648715 3.174916 0.776250

MODIFICATIONS ON THE AROMATIC RINGS

(Substituent on the phenyl rings in *para* position to nitrogen atom of the PNP ligand)

CF3

1

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5-6-TS

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H 2.342170 3.495292 -3.416032
H -4.347851 -1.152809 0.582335
H -2.450094 -3.154608 -2.714815
H -0.274402 -2.197645 -2.066130
H -4.236648 -0.046799 2.536830
H -0.550046 -1.439687 2.446412
H 0.121347 -0.818662 4.757478
H -0.979283 0.573223 4.732366
H 0.398277 0.503686 3.608352
H -2.961660 -1.261897 4.354916
H -1.739668 -2.545967 4.307638
H -2.836546 -2.326370 2.929856
H -3.140163 0.971635 4.518140
H -4.493635 1.991492 4.002800
H -2.830204 2.475515 3.613005
H -5.291396 2.049011 1.659115
H -4.414785 1.217210 0.353656
H -3.692774 2.638358 1.125235
H -2.154927 4.808753 -3.019623
H -0.598138 4.734624 -2.157536
H -2.120260 4.848203 -1.240239
H -3.752072 2.908790 -1.225606
H -3.731020 2.765889 -2.999086

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H -1.121635 1.175885 -3.327230
H -0.030383 2.577192 -3.427634
C -0.039599 3.667055 1.506080
H -0.602288 3.309522 0.331405
H 1.053923 3.789095 1.558862
H -0.398732 3.257183 2.467398
H -0.469870 4.676115 1.414950
F 6.159117 -2.360678 -0.719323
F 5.209686 -4.295965 -0.607690
F 5.690907 -3.224792 1.191584
F -5.525179 -1.841338 -2.313339
F -4.782839 -3.858402 -2.247036
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6

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C -1.292545 1.061717 0.015071
C -2.523817 0.371050 -0.138591
C -2.557238 3.137938 0.239127
C -3.764217 2.446736 0.079569
C -3.732016 1.067318 -0.098575
N -0.108688 0.350758 0.031469
P -2.402717 -1.442253 -0.341775
C -3.830935 -2.079793 0.665173
C -4.034736 -3.584561 0.486385
C -3.628475 -1.713613 2.136794
C -2.786181 -1.737979 -2.140938
C -4.208277 -1.383463 -2.567126
C -2.382397 -3.147440 -2.578469
C -5.057013 3.204284 0.103059
C 3.489446 1.207268 0.123759
C 2.255978 0.649106 0.447615
C 1.095275 0.981974 -0.291862
C 3.601542 2.097367 -0.941892
C 2.464762 2.426670 -1.687134
C 1.231678 1.880303 -1.368346
C 4.927164 2.686203 -1.326136
P 1.939739 -0.569751 1.766450
C 3.575516 -1.243234 2.310265
C 1.284453 0.532368 3.125826
C 0.384425 -0.219036 4.107182
C 2.361696 1.370023 3.810091
C 3.399195 -2.110751 3.559665
C 4.225298 -2.040086 1.179402
Ti 0.091205 -1.737313 0.402944

C 0.979886 -2.427431 -1.029848
C 1.625582 -2.382796 -2.400717
C 1.601369 -3.770220 -3.062180
C 3.085837 -1.913078 -2.279267
C 0.866334 -1.385148 -3.289847
C -0.292309 -3.278486 1.848756
H -0.426933 3.023488 0.365833
H -2.564058 4.218185 0.403339
H -4.674911 0.527247 -0.200385
H -4.733854 -1.564840 0.296069
H -4.363258 -3.842676 -0.529875
H -4.813029 -3.938902 1.180351
H -3.114741 -4.149059 0.702748
H -2.764140 -2.247483 2.558211
H -4.516951 -2.000264 2.721072
H -3.470959 -0.634191 2.281379
H -2.088146 -1.028288 -2.617511
H -4.317943 -1.525825 -3.653946
H -4.460979 -0.335962 -2.349518
H -4.955335 -2.029024 -2.078640
H -3.101171 -3.907074 -2.237814
H -1.390057 -3.415068 -2.186979
H -2.345404 -3.203419 -3.677881
H 4.379050 0.948263 0.700267
H 2.547337 3.110113 -2.535280
H 0.357028 2.133491 -1.969768
H 4.219578 -0.384358 2.565319
H 0.636280 1.214803 2.551184
H -0.046469 0.485463 4.836174
H 0.925130 -0.992414 4.673071
H -0.450260 -0.710092 3.585397
H 3.028373 0.756809 4.436160
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H 2.980698 1.914127 3.079845
H 3.051817 -1.535038 4.428877
H 4.363228 -2.566861 3.833597
H 2.681499 -2.927612 3.382924
H 5.197279 -2.436987 1.512216
H 4.400080 -1.429530 0.283702
H 3.590549 -2.888933 0.882240
H 2.047536 -3.737725 -4.070363
H 0.571124 -4.146340 -3.163114
H 2.170189 -4.502599 -2.466704
H 3.676223 -2.609121 -1.664500
H 3.563011 -1.852633 -3.272219
H 3.139384 -0.915926 -1.816016
H 1.373483 -1.252659 -4.260195
H 0.799910 -0.401074 -2.802782
H -0.156076 -1.736569 -3.491724
H 1.014010 -3.424704 -0.510220
H 0.662380 -3.803746 2.048012
H -0.674922 -2.931429 2.825150

H -0.991168 -4.045772 1.466257
F 4.880792 4.025530 -1.383242
F 5.897935 2.362856 -0.463468
F 5.326657 2.271261 -2.537692
F -5.146892 4.075108 -0.914939
F -5.195382 3.927275 1.225468
F -6.123066 2.398630 0.021949

6'

E: -3431.56251423 H: -3430.778518 G: -3430.913311
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C 1.334397 -1.197629 0.005242
C 2.539588 -0.462602 -0.159231
C 2.676775 -3.162247 0.530246
C 3.853654 -2.426909 0.374285
C 3.772129 -1.076873 0.024784
N 0.129554 -0.530627 -0.129213
P 2.265362 1.270168 -0.673231
C 3.857100 2.149931 -0.310548
C 3.851611 3.558013 -0.909423
C 4.132028 2.190065 1.194291
C 2.156912 1.050084 -2.530316
C 3.479194 0.640849 -3.174567
C 1.500017 2.224477 -3.252527
C 5.191459 -3.050544 0.633498
C -3.405962 -1.592746 -0.251661
C -2.237358 -0.940850 0.133558
C -1.010881 -1.224422 -0.516955
C -3.391351 -2.523680 -1.289716
C -2.187964 -2.806434 -1.942638
C -1.016709 -2.169417 -1.563034
C -4.674005 -3.164763 -1.731935
P -2.095357 0.257126 1.507038
C -3.795405 0.962610 1.735064
C -1.750497 -0.877236 2.953537
C -1.054329 -0.155518 4.107935
C -2.960837 -1.685790 3.412245
C -3.795482 1.939949 2.912799
C -4.280303 1.640089 0.453162
Ti -0.049980 1.524251 0.524926
C -0.919273 2.760888 -0.512472
C -1.309142 4.202645 -0.785316
C -0.046875 5.017777 -1.127211
C -1.940390 4.818388 0.476455
C -2.300729 4.300383 -1.954916
C 0.702462 2.519262 2.220513
H 0.532937 -3.155602 0.486116
H 2.727212 -4.217395 0.806369
H 4.694506 -0.507828 -0.112154

H 4.656987 1.569665 -0.800991
H 3.842773 3.543604 -2.008357
H 4.757848 4.099830 -0.596433
H 2.979389 4.138927 -0.570908
H 3.408100 2.834398 1.712958
H 5.137672 2.600809 1.376016
H 4.090284 1.194704 1.660203
H 1.458668 0.197855 -2.592508
H 3.312569 0.361233 -4.226897
H 3.938150 -0.225046 -2.674245
H 4.206504 1.468210 -3.170566
H 2.137008 3.121501 -3.256327
H 0.541377 2.490542 -2.787734
H 1.308867 1.953997 -4.303155
H -4.346337 -1.383998 0.263552
H -2.168910 -3.529145 -2.760580
H -0.084388 -2.396463 -2.083434
H -4.470301 0.123673 1.974187
H -1.016066 -1.572233 2.510923
H -0.765836 -0.882688 4.883428
H -1.702935 0.594158 4.585638
H -0.141795 0.356584 3.772576
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H -3.571363 1.443990 3.868226
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H -5.265810 2.101240 0.623676
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H 0.673005 4.982014 -0.294930
H -1.258896 4.727086 1.336382
H -2.159872 5.888930 0.326113
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H -3.218690 3.726798 -1.750279
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H 1.186077 3.466304 1.917925
H -0.149303 2.782364 2.876664
H 1.427284 1.935770 2.816810
H -1.214696 2.012892 -1.294442
F 6.143135 -2.547471 -0.167323
F 5.613110 -2.845021 1.893131
F 5.177114 -4.376181 0.448241
F -4.470297 -4.343472 -2.331264
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6'-7'-TS

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C 2.730161 -3.202643 0.748865
C 3.889890 -2.464436 0.506267
C 3.774692 -1.137520 0.083924
N 0.118961 -0.653314 0.004882
P 2.220295 1.156913 -0.660442
C 3.793887 2.074616 -0.306838
C 3.772822 3.468556 -0.933987
C 4.041778 2.161483 1.200459
C 2.102667 0.908426 -2.509463
C 3.426487 0.515678 -3.160591
C 1.413152 2.063621 -3.233471
C 5.255977 -3.050729 0.691695
C -3.422738 -1.657307 -0.267660
C -2.268764 -0.991160 0.129450
C -0.998822 -1.369824 -0.383570
C -3.362744 -2.707996 -1.184575
C -2.121542 -3.089967 -1.700452
C -0.962726 -2.437407 -1.309155
C -4.631036 -3.368050 -1.633050
P -2.183701 0.357042 1.355692
C -3.868426 1.133874 1.373725
C -1.978229 -0.605342 2.947113
C -1.544449 0.247890 4.139087
C -3.176139 -1.490344 3.284459
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Ti -0.043471 1.531389 0.527079
C -0.660953 3.053692 -0.358724
C -0.997229 4.470444 -0.773325
C 0.298934 5.293674 -0.809727
C -1.966765 5.108981 0.239648
C -1.646703 4.475238 -2.165078
C 0.402303 2.474597 2.082945
H 0.587375 -3.225390 0.782462
H 2.805046 -4.235567 1.093137
H 4.682595 -0.559196 -0.106541
H 4.611145 1.496515 -0.770371
H 3.736890 3.434759 -2.031934
H 4.684788 4.018194 -0.652547
H 2.907354 4.048562 -0.579955
H 3.270767 2.778299 1.687219
H 5.019713 2.631101 1.390533
H 4.046893 1.175175 1.687731

H 1.420994 0.041688 -2.554375
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 H 3.901690 -0.339313 -2.656445
 H 4.141045 1.354097 -3.167101
 H 2.039964 2.967382 -3.269783
 H 0.468287 2.329595 -2.740808
 H 1.194472 1.774736 -4.273805
 H -4.391501 -1.366230 0.145741
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 H -1.890793 5.502864 -2.480017
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 H -0.975055 4.041886 -2.921639
 H -0.137019 3.157817 0.972124
 H 0.492898 3.246708 2.853321
 H 1.234839 1.721565 2.139237
 H -1.420310 2.279921 -0.687041
 F 5.980796 -2.362998 1.590418
 F 5.969171 -3.033286 -0.447666
 F 5.217473 -4.320285 1.109170
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6'-7"-TS

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 C 2.548370 -0.490760 -0.102173

C 2.793626 -3.170189 0.634725
C 3.944063 -2.407433 0.407771
C 3.806126 -1.069317 0.040730
N 0.141655 -0.641599 -0.005505
P 2.244091 1.233978 -0.611649
C 3.739643 2.193647 -0.068992
C 3.574569 3.668978 -0.440144
C 3.993098 2.040440 1.431626
C 2.318375 1.080232 -2.478526
C 3.676319 0.637834 -3.018376
C 1.796524 2.308129 -3.226347
C 5.306946 -2.988971 0.627123
C -3.387662 -1.682662 -0.283257
C -2.240443 -1.003030 0.116107
C -0.967963 -1.362662 -0.400436
C -3.318058 -2.721183 -1.210645
C -2.072654 -3.078600 -1.738565
C -0.922875 -2.414336 -1.346524
C -4.553210 -3.482591 -1.584373
P -2.190323 0.333814 1.355238
C -3.880797 1.096638 1.357465
C -1.996604 -0.639147 2.942831
C -1.666892 0.227529 4.160484
C -3.148096 -1.598072 3.235302
C -3.937059 2.218244 2.398764
C -4.232932 1.616626 -0.036634
Ti -0.069760 1.542336 0.486958
C -0.845221 2.982717 -0.414603
C -1.302048 4.353824 -0.868181
C -0.075466 5.260261 -1.088684
C -2.193124 4.984240 0.212203
C -2.084464 4.240040 -2.185098
C 0.533380 2.619131 1.896597
H 0.654443 -3.225049 0.681920
H 2.884944 -4.215333 0.937646
H 4.703750 -0.473776 -0.140426
H 4.603298 1.782588 -0.618549
H 3.529639 3.830215 -1.526008
H 4.427731 4.250933 -0.057734
H 2.655820 4.081377 0.005640
H 3.140701 2.428279 2.008688
H 4.891550 2.611896 1.713785
H 4.154469 0.995610 1.731998
H 1.594698 0.261047 -2.638315
H 3.600870 0.426414 -4.096945
H 4.044230 -0.276824 -2.531645
H 4.436976 1.425616 -2.896417
H 2.512484 3.142803 -3.198295
H 0.841300 2.670461 -2.822567
H 1.634950 2.056557 -4.286312
H -4.358991 -1.405075 0.132203
H -2.005542 -3.877106 -2.480502

H 0.034708 -2.697835 -1.786283
 H -4.601202 0.310634 1.640523
 H -1.097477 -1.234234 2.702861
 H -1.246998 -0.399958 4.962063
 H -2.563859 0.715462 4.568960
 H -0.936157 1.016177 3.932206
 H -4.074133 -1.054285 3.482128
 H -2.901084 -2.227958 4.104834
 H -3.357216 -2.271931 2.391889
 H -3.898135 1.834835 3.427460
 H -4.877172 2.782346 2.295029
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 H -4.316507 0.812146 -0.780758
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 H -0.378303 6.260701 -1.440657
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 H -2.475234 6.012742 -0.065650
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 H -2.968993 3.595134 -2.073773
 H -1.456470 3.813617 -2.984076
 H -0.199462 3.189711 0.828266
 H 0.816608 3.474026 2.517888
 H 0.372275 1.686270 2.498412
 H -0.446329 2.343813 -1.260421
 F 5.753651 -2.785409 1.878958
 F 6.222935 -2.447367 -0.190158
 F 5.330724 -4.312906 0.427071
 F -4.492394 -3.967247 -2.831498
 F -4.761671 -4.537892 -0.777071
 F -5.656725 -2.725085 -1.505829

7'

E: -3431.55465078 H: -3430.770605 G: -3430.902746
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 C 1.118770 -1.313480 0.217538
 C 2.371822 -0.724381 -0.079155
 C 2.288025 -3.294518 1.007858
 C 3.521408 -2.701692 0.714925
 C 3.553056 -1.419103 0.173257
 N -0.034435 -0.565378 0.012633
 P 2.255457 0.925562 -0.867458
 C 3.953536 1.657940 -0.695372
 C 4.113252 2.937481 -1.518735
 C 4.300937 1.907035 0.772992
 C 2.039401 0.397429 -2.653206

C 3.306242 -0.167490 -3.289829
C 1.361228 1.451591 -3.526616
C 4.785286 -3.462119 0.989257
C -3.641953 -1.270077 -0.316568
C -2.441854 -0.696602 0.099158
C -1.208176 -1.191156 -0.386147
C -3.647444 -2.339332 -1.209592
C -2.431922 -2.839267 -1.690308
C -1.232122 -2.277091 -1.287268
C -4.932646 -2.953925 -1.680326
P -2.262010 0.670184 1.301838
C -3.900143 1.547661 1.255765
C -2.168137 -0.263268 2.919372
C -1.727091 0.608004 4.096454
C -3.419086 -1.076160 3.242234
C -4.000142 2.610704 2.351621
C -4.163016 2.158387 -0.123220
Ti 0.120682 1.490800 0.500837
C -0.718785 3.318708 -0.192528
C 0.022783 4.634673 -0.501085
C 1.095455 4.904461 0.562864
C -0.971799 5.808464 -0.508024
C 0.689055 4.552908 -1.877438
C 1.011961 1.686808 2.108032
H 0.153500 -3.082770 1.015645
H 2.253080 -4.296850 1.441108
H 4.518501 -0.967387 -0.059527
H 4.648602 0.905105 -1.103941
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H 5.157608 3.282473 -1.463416
H 3.478336 3.747447 -1.130666
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 H 0.273499 3.593894 -1.221338
 F 5.770773 -2.484946 2.057148
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 F -5.448827 -3.122503 -1.137646

MODIFICATIONS ON THE AROMATIC RINGS

(Substituent on the phenyl rings in *para* position to nitrogen atom of the PNP ligand)

H

1

E: -2915.26052784 H: -2914.374697 G: -2914.498622
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 P -2.523757 -0.208857 -0.100464
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 C -3.179361 0.230973 -2.783869
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 C 1.267761 -2.025528 0.516559
 C 3.669810 -2.947037 1.692896
 C 2.450951 -3.557338 1.992247
 C 1.267520 -3.106194 1.417625

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C -0.369328 2.423219 -1.156493
C -0.370843 3.896750 -0.687003
C 1.021688 4.310148 -0.192001
C -0.755193 4.814148 -1.862434
C -1.386395 4.117688 0.443815
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1-2-TS

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5-6-TS

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C 0.178805 3.336672 -2.364570
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H 2.527654 -1.954274 2.401121
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H 4.787819 -0.565632 -1.665997

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 H 0.015289 4.220753 -3.005339
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6

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 C -1.775939 -3.501973 2.403377
 C -3.067317 -3.333932 1.900312
 C -3.318675 -2.258538 1.052585
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C -4.209139 0.561334 -2.625741
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C 2.229446 -0.043052 3.765934
C 1.073997 -0.282254 3.028686
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C 3.909172 -0.044850 -1.533283
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C 0.068251 4.743564 -0.039012
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 C -2.928720 -3.945874 -0.972356
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 C -4.014441 0.579485 -1.084582
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 C -3.024578 0.094377 1.705294
 C -4.399240 -0.525056 1.944698
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 C 1.806336 -2.658751 3.292896
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C 0.266001 3.751140 0.621938
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C 1.113545 4.344090 -0.517366
C 0.845575 4.194204 1.974764
C -0.283121 1.289862 -2.530847
H 0.283058 -3.875331 0.171116
H -1.409729 -5.451556 -0.680264
H -4.222191 -2.234986 -1.143155
H -4.820497 -0.112911 -0.788423
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H -2.259807 -0.581568 2.124031
H -4.562632 -0.673374 3.024154
H -4.502137 -1.507272 1.459364
H -5.209645 0.127157 1.581634
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P -2.453284 -0.008603 -0.052710
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C -4.360072 1.961609 -0.628311
C -3.675945 0.448711 -2.519663
C -2.938088 -0.060318 1.752752
C -4.325288 -0.648848 1.997649
C -2.729264 1.268520 2.476998
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C 2.913959 -1.205971 -1.875516
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C -0.041495 3.892054 0.589030
C -1.411848 4.429239 0.150396
C 1.059819 4.640993 -0.185649
C 0.143294 4.138013 2.093746
C -0.074151 1.414069 -2.244608
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H -4.263245 -2.252056 -1.094949

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H -5.122439 0.030101 1.655002
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H -1.721557 1.663873 2.290539
H -2.852620 1.126291 3.562611
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H -0.036639 2.083004 -3.110260
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C -3.355638 -3.771311 -0.990616
C -3.493732 -2.399402 -0.797610
N -0.090177 -1.390864 0.246405
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C -3.627542 0.537327 -2.578391
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C -4.492705 -0.329752 1.919994
C -2.880134 1.540698 2.442862
C 3.266104 -1.844296 1.732381
C 2.233894 -1.399702 0.902495
C 0.910946 -1.883859 1.068202
C 3.023982 -2.762523 2.750842
C 1.722030 -3.237041 2.930823
C 0.684801 -2.810798 2.111627
P 2.417201 -0.237578 -0.489350
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C 2.806552 -1.397824 -1.905383
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C 0.435851 3.841653 0.649374
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C 1.517070 4.467277 -0.243834
C 0.806793 4.038095 2.127129
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H -4.463621 -1.929058 -0.980858
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H -3.539894 -0.540050 -2.777987
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H -4.635544 -1.311583 1.445823
H -5.241838 0.366671 1.509930

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H -1.860363 1.931972 2.326359
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H 4.281926 -1.469730 1.579859
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H 3.145972 -0.768785 -3.947989
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H 2.047104 0.439714 -3.235002
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H 4.794233 -2.041303 -2.394663
H 4.644919 -1.888676 -0.632188

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C 0.673176 -1.651176 1.173117
C 2.558916 -2.571766 3.059069
C 1.210959 -2.907519 3.186002
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C 2.512067 -1.099535 -3.188389

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C 0.562994 5.169968 0.540996
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H 3.291077 -2.925638 3.787449
H -4.307257 -4.080409 -1.514002

MODIFICATIONS ON THE AROMATIC RINGS

(Substituent on the phenyl rings in *para* position to nitrogen atom of the PNP ligand)

Me

1

E: -3144.06477668 H: -3143.108389 G: -3143.244317
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C 2.338107 3.895265 -0.934407
C 3.593029 3.331444 -0.688776
C 3.651967 2.010485 -0.238298
N 0.076742 1.049684 -0.048071
P 2.493260 -0.488917 0.503113
C 3.964984 -1.172343 -0.417365
C 4.273511 -2.622638 -0.048823
C 3.776444 -1.013466 -1.928336
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C 4.348052 0.035707 2.629431
C 2.601888 -1.770425 3.004862
C -3.564385 1.771060 -0.086275
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C -3.672777 2.836883 0.814646
C -2.513358 3.327834 1.422405
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C 0.796047 -5.277522 -1.754126
C 0.854523 -4.645302 0.653682
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6'

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7'

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Modifications on the phenyl rings in meta position to nitrogen atom of the PNP ligand. (CF₃)

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H 1.015814 -1.662481 4.797724
H -0.366509 -1.495288 3.690336
H 2.934595 0.255339 4.667868
H 1.675324 1.496505 4.808210
H 2.768345 1.508790 3.410354

H 3.150416 -2.018778 4.504303
H 4.545090 -2.891560 3.848028
H 2.904377 -3.365515 3.362298
H 5.357643 -2.553400 1.551285
H 4.500491 -1.512987 0.390450
H 3.789718 -3.063050 0.862662
H 2.366325 -3.724860 -4.045646
H 0.820401 -4.157534 -3.273082
H 2.352161 -4.504291 -2.439760
H 3.810409 -2.588415 -1.601261
H 3.731463 -1.757655 -3.174599
H 3.221334 -0.908094 -1.690940
H 1.547655 -1.286473 -4.282511
H 0.979630 -0.408692 -2.837835
H 0.010989 -1.743887 -3.509912
H -4.906105 2.323668 0.510148
H 4.435759 2.551786 -0.719574
C 2.390957 3.409489 -2.344522
C -2.844111 4.058239 1.000570
F 1.537406 4.414409 -2.104191
F 2.044938 2.890690 -3.530703
F 3.604248 3.950491 -2.490150
F -2.649463 4.816104 -0.086916
F -1.920597 4.427023 1.897077
F -4.037408 4.397030 1.501539

5-6-TS

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C 1.160853 1.077658 0.092978
C 0.764512 2.428677 -0.109345
C 3.429394 1.885085 0.493267
C 3.033023 3.212535 0.298921
C 1.699128 3.462123 0.001622
N 0.217611 0.079273 0.051562
P -1.004068 2.682792 -0.507214
C -1.410861 4.304477 0.308325
C -2.787444 4.831634 -0.099559
C -1.302067 4.135599 1.826157
C -1.021140 2.913200 -2.354742
C -0.237133 4.120779 -2.859241
C -2.442149 2.859337 -2.919040
C 0.302054 -3.597701 0.415083
C 0.000806 -2.255165 0.632294
C 0.593355 -1.244956 -0.167883
C 1.195687 -3.975545 -0.585719
C 1.782288 -2.985860 -1.372649
C 1.485423 -1.638884 -1.175439

P -1.134219 -1.593262 1.904463
C -2.075065 -3.029794 2.599489
C 0.087845 -1.029307 3.203861
C -0.486930 0.075101 4.091532
C 0.731677 -2.165436 3.993465
C -2.854387 -2.610678 3.848984
C -3.022445 -3.590127 1.539510
Ti -1.906569 0.343177 0.333068
C -2.785073 -0.454981 -0.929313
C -3.491750 -1.102627 -2.093620
C -4.853104 -0.430440 -2.339849
C -3.714457 -2.601097 -1.829836
C -2.606128 -0.954938 -3.344196
H 2.866045 -0.180372 0.571966
H 1.381869 4.496865 -0.147618
H -0.656296 5.039603 -0.016733
H -2.816411 5.140412 -1.153260
H -3.042390 5.715385 0.506330
H -3.581448 4.083868 0.054583
H -2.064014 3.435299 2.205564
H -1.464460 5.101965 2.329152
H -0.312662 3.764510 2.133365
H -0.503644 1.991501 -2.674047
H -0.234160 4.132755 -3.960935
H 0.811651 4.101688 -2.529657
H -0.689127 5.068626 -2.524770
H -2.982182 3.806040 -2.771718
H -3.021852 2.052898 -2.447113
H -2.409521 2.669115 -4.003303
H -0.157192 -4.372230 1.033365
H 1.937010 -0.879617 -1.816967
H -1.343724 -3.804581 2.886116
H 0.868771 -0.566004 2.579133
H 0.293105 0.464937 4.764593
H -1.319422 -0.275614 4.720157
H -0.852973 0.923212 3.491245
H 0.017946 -2.656636 4.672892
H 1.555990 -1.776290 4.612017
H 1.155021 -2.932219 3.326583
H -2.199562 -2.313253 4.679842
H -3.469033 -3.453102 4.203157
H -3.537681 -1.773185 3.633674
H -3.555378 -4.469238 1.935077
H -2.499071 -3.894156 0.623028
H -3.768714 -2.833910 1.253134
H -5.373240 -0.885712 -3.199993
H -4.737321 0.644733 -2.547683
H -5.509727 -0.534331 -1.460853
H -4.372197 -2.759291 -0.962031
H -4.183308 -3.089595 -2.701418
H -2.757372 -3.106918 -1.630416
H -3.071972 -1.436198 -4.221606

H -1.622579 -1.421721 -3.179279
H -2.436152 0.104178 -3.587867
C -3.879849 1.080990 1.292584
H -3.656339 0.327993 0.193653
H -3.751317 2.171759 1.214547
H -3.559343 0.755514 2.299176
H -4.959669 0.877733 1.228215
H 3.750655 4.030159 0.378811
H 1.431416 -5.027117 -0.749379
C 2.771810 -3.343402 -2.450366
C 4.866893 1.610772 0.853565
F 4.009574 -2.936896 -2.132939
F 2.466595 -2.762285 -3.617836
F 2.837039 -4.660294 -2.669947
F 5.709436 2.152100 -0.036074
F 5.180904 2.138195 2.046623
F 5.145329 0.306108 0.917990

6

E: -3431.56186199 H: -3430.777911 G: -3430.910501
C 2.423682 0.844136 0.581565
C 1.094349 1.093508 0.181648
C 0.741081 2.433281 -0.128250
C 3.351147 1.876055 0.664961
C 2.999837 3.192206 0.364603
C 1.689204 3.452051 -0.025895
N 0.124035 0.107189 0.142994
P -1.005898 2.688191 -0.615151
C -1.427662 4.342370 0.120764
C -2.810920 4.823800 -0.319575
C -1.318621 4.276665 1.645575
C -0.929475 2.878865 -2.467300
C -0.152883 4.097237 -2.957697
C -2.315651 2.776663 -3.106514
C 0.123583 -3.570728 0.564421
C -0.165385 -2.220842 0.744780
C 0.494730 -1.232397 -0.026200
C 1.064109 -3.977750 -0.381047
C 1.713834 -3.008655 -1.142715
C 1.437770 -1.653258 -0.973028
P -1.382023 -1.503303 1.900723
C -2.456617 -2.877751 2.516426
C -0.258681 -0.970859 3.297772
C -0.844712 0.181268 4.113596
C 0.244128 -2.127797 4.156888
C -3.340769 -2.379942 3.663291
C -3.306089 -3.434638 1.374519
Ti -1.962184 0.408165 0.268878
C -2.724930 -0.434665 -1.156697

C -2.747381 -1.224681 -2.449557
C -3.974772 -0.851193 -3.297166
C -2.797789 -2.731409 -2.142156
C -1.470120 -0.933652 -3.252219
C -3.474969 1.279017 1.523353
H 2.725172 -0.169298 0.849795
H 1.402942 4.482842 -0.247253
H -0.678497 5.059206 -0.255256
H -2.847939 5.056894 -1.392440
H -3.074498 5.744630 0.224060
H -3.590145 4.076161 -0.104945
H -2.079473 3.602774 2.065576
H -1.481954 5.276939 2.076669
H -0.329972 3.928849 1.980401
H -0.369114 1.968201 -2.741286
H -0.092866 4.083312 -4.057645
H 0.877684 4.116088 -2.575202
H -0.648019 5.038995 -2.671568
H -2.887963 3.710012 -3.001216
H -2.899680 1.961086 -2.655791
H -2.218573 2.574485 -4.184828
H -0.388182 -4.326351 1.164952
H 1.943880 -0.911212 -1.593847
H -1.794497 -3.673061 2.899178
H 0.600765 -0.564747 2.739355
H -0.112388 0.519545 4.863738
H -1.762940 -0.101583 4.649852
H -1.084132 1.041701 3.471144
H -0.556640 -2.567137 4.771698
H 1.026416 -1.772356 4.846173
H 0.686090 -2.928358 3.543748
H -2.759353 -2.092907 4.550671
H -4.035088 -3.177538 3.970273
H -3.944362 -1.510777 3.356588
H -3.945537 -4.250630 1.746651
H -2.695308 -3.831734 0.552993
H -3.956849 -2.653028 0.953313
H -3.987697 -1.414655 -4.245376
H -3.978618 0.221474 -3.545179
H -4.910518 -1.076553 -2.760279
H -3.703540 -2.990536 -1.572636
H -2.804803 -3.322039 -3.074153
H -1.920600 -3.037349 -1.551528
H -1.431739 -1.542565 -4.170934
H -0.571861 -1.162462 -2.660144
H -1.423699 0.124808 -3.548624
H -3.737567 -0.172440 -0.739490
H -4.225678 0.497947 1.753245
H -3.111314 1.666083 2.492100
H -4.024538 2.096415 1.020050
H 3.729632 3.998027 0.442395
H 1.286420 -5.035406 -0.521821

C 2.721058 -3.394343 -2.194561
C 4.766055 1.538450 1.061559
F 4.806747 0.603074 2.018707
F 5.431304 2.603503 1.521012
F 5.466447 1.058920 0.024810
F 3.918734 -2.844875 -1.953560
F 2.344794 -2.974940 -3.410714
F 2.901188 -4.715804 -2.271800

6'

E: -3431.55897454 H: -3430.775715 G: -3430.909386
C -2.484128 0.862068 -0.781156
C -1.175364 1.086260 -0.318227
C -0.728369 2.430324 -0.215566
C -3.303573 1.931421 -1.137329
C -2.856771 3.247790 -1.047949
C -1.563469 3.482347 -0.579450
N -0.286912 0.068678 -0.003029
P 0.961325 2.556593 0.475365
C 1.542533 4.271905 0.076446
C 2.850996 4.583883 0.805971
C 1.695797 4.462283 -1.434178
C 0.559183 2.515095 2.305010
C -0.160664 3.767422 2.799074
C 1.750664 2.145281 3.185576
C -0.634752 -3.591069 0.388646
C -0.200869 -2.347308 -0.069346
C -0.771294 -1.157418 0.444759
C -1.636395 -3.691597 1.351708
C -2.202788 -2.521072 1.855957
C -1.779546 -1.270059 1.415998
P 1.031862 -2.051932 -1.390342
C 2.052763 -3.596421 -1.482428
C -0.072092 -2.008836 -2.900164
C 0.569242 -1.260513 -4.069280
C -0.623836 -3.372521 -3.305678
C 3.048823 -3.501834 -2.640349
C 2.772717 -3.845275 -0.157429
Ti 1.792656 0.267633 -0.499225
C 3.077386 -0.271965 0.693358
C 4.533798 -0.361615 1.109965
C 5.029464 1.031381 1.544448
C 5.385586 -0.816827 -0.087826
C 4.721686 -1.343522 2.277153
C 2.746019 1.110298 -2.179962
H -2.856969 -0.159507 -0.875679
H -1.212877 4.513759 -0.495443
H 0.766780 4.964584 0.444451

H 2.724106 4.617369 1.897062
H 3.229732 5.568374 0.489355
H 3.627485 3.836653 0.578410
H 2.522401 3.854546 -1.828334
H 1.920790 5.517835 -1.654520
H 0.786358 4.192318 -1.990715
H -0.147436 1.668489 2.340612
H -0.527233 3.608486 3.825586
H -1.031468 4.020943 2.176040
H 0.511265 4.639867 2.826797
H 2.515727 2.935632 3.207635
H 2.228938 1.220712 2.836304
H 1.411121 1.986351 4.221419
H -0.196263 -4.507499 -0.012989
H -2.228845 -0.364064 1.828327
H 1.362350 -4.433475 -1.680649
H -0.909746 -1.389601 -2.535638
H -0.159661 -1.151173 -4.887835
H 1.444048 -1.789906 -4.476151
H 0.895254 -0.253291 -3.774090
H 0.163429 -4.025940 -3.714078
H -1.387671 -3.253331 -4.090406
H -1.100919 -3.893156 -2.461242
H 2.550692 -3.430702 -3.617729
H 3.686445 -4.399494 -2.662307
H 3.707880 -2.626203 -2.527112
H 3.375000 -4.765034 -0.224053
H 2.079455 -3.957651 0.688301
H 3.443453 -3.007937 0.077768
H 6.094675 1.000538 1.831312
H 4.459573 1.409940 2.405553
H 4.918940 1.754970 0.722000
H 5.244544 -0.141261 -0.945646
H 6.458468 -0.825563 0.168338
H 5.111159 -1.831667 -0.413570
H 5.782432 -1.419155 2.569583
H 4.374032 -2.353934 2.011120
H 4.152299 -1.017020 3.162462
H 3.546371 1.803604 -1.862162
H 3.230600 0.291700 -2.746477
H 2.073898 1.652619 -2.869567
H 2.330156 -0.653851 1.438208
H -1.973129 -4.667017 1.702372
H -3.503339 4.076985 -1.334206
C -3.285315 -2.573637 2.903619
C -4.700431 1.622797 -1.611250
F -2.911158 -1.951124 4.030107
F -3.614854 -3.824763 3.236178
F -4.403785 -1.966948 2.485867
F -5.466639 1.159317 -0.614382
F -4.702994 0.680720 -2.564636
F -5.318810 2.694816 -2.115391

6'-7'-TS

E: -3431.51053839 H: -3430.730339 G: -3430.862072
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C -0.737777 2.411112 -0.190090
C -3.329869 2.048485 -1.124198
C -2.836593 3.347453 -0.969647
C -1.538029 3.511497 -0.499602
N -0.383681 0.025153 -0.091808
P 0.965305 2.459691 0.469664
C 1.607907 4.149812 0.052432
C 2.935985 4.428079 0.756954
C 1.756154 4.304984 -1.462470
C 0.634496 2.405500 2.308587
C -0.047929 3.661149 2.845346
C 1.858283 2.005431 3.131487
C -0.784213 -3.614918 0.421497
C -0.310598 -2.390266 -0.052673
C -0.908458 -1.174631 0.362078
C -1.848552 -3.676786 1.314305
C -2.440865 -2.480474 1.730651
C -1.986276 -1.252048 1.270406
P 1.050368 -2.141418 -1.243999
C 2.119578 -3.653579 -1.130826
C 0.131205 -2.205475 -2.871878
C 0.937253 -1.685427 -4.062335
C -0.501696 -3.564551 -3.161182
C 3.252332 -3.567536 -2.157249
C 2.677640 -3.825220 0.283391
Ti 1.800293 0.223171 -0.527259
C 3.346919 -0.054944 0.479621
C 4.767758 -0.106923 1.000135
C 5.328355 1.322250 1.050669
C 5.648304 -0.958145 0.065563
C 4.790672 -0.715162 2.410074
C 2.753024 0.726602 -2.063259
H -2.960841 -0.060826 -0.971208
H -1.145989 4.523480 -0.372946
H 0.861608 4.876480 0.415707
H 2.833736 4.460644 1.850567
H 3.331575 5.404278 0.435046
H 3.685188 3.662310 0.505757
H 2.539545 3.633718 -1.846708
H 2.047233 5.338918 -1.706376
H 0.824475 4.085306 -2.005028
H -0.083175 1.568553 2.360146
H -0.364726 3.500118 3.888007

H -0.946101 3.925470 2.267239
 H 0.632768 4.527265 2.842983
 H 2.612058 2.805951 3.173010
 H 2.339499 1.111636 2.711429
 H 1.556018 1.785117 4.167684
 H -0.316012 -4.545065 0.090061
 H -2.456448 -0.334371 1.625598
 H 1.486304 -4.525181 -1.368754
 H -0.675446 -1.477825 -2.674394
 H 0.261800 -1.506172 -4.913845
 H 1.693908 -2.411229 -4.395651
 H 1.454793 -0.745576 -3.823280
 H 0.262509 -4.327190 -3.381327
 H -1.153581 -3.494303 -4.046305
 H -1.120482 -3.924735 -2.326060
 H 2.887757 -3.663371 -3.189226
 H 3.977918 -4.378747 -1.988701
 H 3.787478 -2.607820 -2.074754
 H 3.239300 -4.770257 0.351252
 H 1.892495 -3.845553 1.052902
 H 3.371199 -3.008768 0.531573
 H 6.379192 1.324427 1.383905
 H 4.745175 1.944175 1.746267
 H 5.286970 1.795860 0.056717
 H 5.648407 -0.549794 -0.957863
 H 6.693124 -0.984689 0.417686
 H 5.284868 -1.995840 0.010139
 H 5.818223 -0.747746 2.807245
 H 4.401142 -1.746110 2.406412
 H 4.177734 -0.125819 3.109054
 H 3.445497 0.393723 -0.874147
 H 3.549686 0.904784 -2.792471
 H 1.873855 1.406550 -2.229837
 H 2.695953 -0.914363 0.825885
 H -3.454320 4.212769 -1.214334
 H -2.209034 -4.637008 1.685729
 C -3.609855 -2.543009 2.679639
 C -4.741024 1.871003 -1.622137
 F -3.387078 -3.401687 3.683601
 F -4.723345 -2.959831 2.060254
 F -3.889344 -1.357475 3.229558
 F -5.042874 0.594113 -1.874339
 F -5.636126 2.317604 -0.729752
 F -4.954726 2.557846 -2.753227

6'-7"-TS

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 C -1.289399 1.055014 -0.333502

C -0.852748 2.389316 -0.141743
C -3.445814 1.944039 -1.039868
C -3.013257 3.258441 -0.831594
C -1.714673 3.462283 -0.382679
N -0.403435 0.016165 -0.119775
P 0.855726 2.524570 0.483544
C 1.481343 4.184586 -0.068523
C 2.941674 4.354118 0.357132
C 1.342818 4.362758 -1.581676
C 0.559552 2.605447 2.332823
C -0.280740 3.795822 2.788323
C 1.829902 2.468513 3.173709
C -0.605998 -3.643735 0.349493
C -0.189958 -2.388024 -0.099609
C -0.867956 -1.213790 0.309122
C -1.683331 -3.777793 1.216492
C -2.352217 -2.620932 1.631659
C -1.958019 -1.364471 1.196564
P 1.178558 -2.075250 -1.264757
C 2.326615 -3.524658 -1.113878
C 0.302576 -2.199183 -2.913606
C 1.162786 -1.758664 -4.100751
C -0.359035 -3.550517 -3.171977
C 3.501057 -3.355982 -2.082045
C 2.816717 -3.662086 0.328063
Ti 1.784035 0.318299 -0.472486
C 3.323882 -0.020684 0.529093
C 4.737605 -0.097973 1.066430
C 5.306565 1.324951 1.226682
C 5.622526 -0.877211 0.082487
C 4.743558 -0.797635 2.434058
C 2.745854 1.116041 -1.871400
H -2.973476 -0.147625 -0.989000
H -1.366928 4.484591 -0.215317
H 0.868543 4.949096 0.438823
H 3.071757 4.335946 1.447766
H 3.329488 5.319772 -0.003650
H 3.564273 3.555277 -0.074814
H 1.900858 3.578834 -2.115557
H 1.753502 5.341579 -1.876188
H 0.299039 4.322369 -1.922151
H -0.034255 1.684854 2.475776
H -0.513869 3.701221 3.860946
H -1.236958 3.861962 2.250133
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Modifications on the phenyl rings in meta position to nitrogen atom of the PNP ligand. (OMe)

1

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H 4.407316 -0.595547 2.202985
H 0.953975 1.271830 2.527239
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5-6-TS

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6

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C 3.722091 1.936105 -1.258435
C 2.573151 2.337716 -1.952029
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6'

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C 1.019908 -2.831842 2.884334
C -2.245242 2.919256 0.933403
C -1.520541 1.911781 0.302236
C -0.236881 1.562926 0.794782
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C -0.460920 3.269361 2.514064
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H 1.073394 -4.921921 -0.095920
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C 3.812006 3.839079 3.775838
H 4.635702 3.593510 4.458633
H 4.150942 4.635741 3.090613
H 2.962283 4.216801 4.371120
C 6.260647 -1.813075 -1.894717
H 5.948704 -2.371502 -2.794684
H 7.144022 -1.211422 -2.144978
H 6.538599 -2.533636 -1.105665

6'-7"-TS

E: -2986.91589154 H: -2986.081956 G: -2986.206157
C 3.191106 0.146255 -0.653121
C 1.964246 -0.445573 -0.302664
C 1.893847 -1.868177 -0.302307
C 4.307831 -0.625532 -0.980625
C 4.233002 -2.026093 -0.975425
C 3.019046 -2.619388 -0.632229
N 0.819589 0.277433 -0.016402
P 0.291237 -2.533275 0.235855
C 0.149244 -4.221779 -0.527646
C -1.175197 -4.869663 -0.119652
C 0.277991 -4.163090 -2.050215
C 0.588609 -2.786018 2.072040
C 1.623057 -3.862220 2.391868
C -0.683402 -2.972003 2.899413
C -0.009523 3.775310 0.814801
C -0.059596 2.515153 0.224927
C 0.909499 1.531292 0.568959
C 0.956537 4.110374 1.762612
C 1.903527 3.139024 2.118513
C 1.875894 1.872399 1.529979
P -1.240727 1.971491 -1.042618
C -2.762707 3.016363 -0.850234
C -0.384287 2.495240 -2.622933
C -1.033339 1.954192 -3.898694
C -0.122717 3.995923 -2.723196
C -3.808679 2.584910 -1.882951
C -3.314377 2.901729 0.571143
Ti -1.195667 -0.553499 -0.492143
C -2.755867 -0.713347 0.528354
C -4.131245 -1.068302 1.055561
C -4.284110 -2.601255 1.105926
C -5.207215 -0.496174 0.120704
C -4.317991 -0.498838 2.470013
C -1.964384 -1.425805 -1.968458
H 3.297198 1.231048 -0.683403
H 2.960967 -3.711290 -0.625234
H 0.979967 -4.827682 -0.127589
H -1.233717 -5.066599 0.960148
H -1.299943 -5.835248 -0.635065
H -2.023957 -4.224601 -0.396756
H -0.527619 -3.552269 -2.483726
H 0.204900 -5.180306 -2.467559
H 1.235824 -3.733399 -2.375865
H 1.015967 -1.803596 2.339024
H 1.878193 -3.834431 3.463465
H 2.557226 -3.720883 1.829122

H 1.237154 -4.871862 2.177087
H -1.159907 -3.947134 2.719235
H -1.428932 -2.191900 2.695290
H -0.439926 -2.923621 3.972716
H -0.743144 4.535013 0.531742
H 2.630250 1.148755 1.841282
H -2.480208 4.065669 -1.042023
H 0.584656 1.980662 -2.496149
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H -1.907215 2.552082 -4.197585
H -1.364389 0.910915 -3.795123
H -1.060218 4.562684 -2.844788
H 0.503827 4.212667 -3.603435
H 0.404287 4.383702 -1.839471
H -3.513717 2.840885 -2.909602
H -4.769508 3.085557 -1.683689
H -3.975507 1.496682 -1.841540
H -4.267904 3.448029 0.650744
H -2.626620 3.310414 1.324203
H -3.492868 1.847265 0.824972
H -5.270200 -2.892682 1.505792
H -3.510336 -3.054949 1.743884
H -4.185623 -3.037378 0.099063
H -5.064360 -0.851932 -0.912442
H -6.213537 -0.806390 0.446550
H -5.180285 0.603125 0.103477
H -5.319152 -0.741231 2.862624
H -4.205020 0.595772 2.480738
H -3.575091 -0.918600 3.167639
H -2.721167 -1.212364 -0.791900
H -2.621611 -2.023296 -2.607640
H -1.283081 -0.760316 -2.560102
H -1.938972 -0.847910 1.299091
H 5.088578 -2.649582 -1.230715
H 0.959161 5.105262 2.205868
O 5.421853 0.064553 -1.304246
O 2.876897 3.339518 3.031498
C 2.988089 4.592672 3.648078
H 3.841419 4.531641 4.335792
H 3.181674 5.397435 2.917288
H 2.086188 4.848936 4.231323
C 6.589126 -0.637197 -1.633074
H 6.452897 -1.271832 -2.526247
H 7.357800 0.114770 -1.853443
H 6.942777 -1.266336 -0.797385

7'

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C -2.142157 2.013221 -0.986563
C -0.923703 1.590820 -0.442085
C 0.161691 2.505410 -0.404033
C -2.293758 3.306965 -1.494573
C -1.218714 4.205667 -1.469091
C -0.006464 3.786904 -0.920146
N -0.704315 0.290425 0.013499
P 1.653476 1.852748 0.423953
C 3.023444 3.009533 -0.062605
C 4.298299 2.758900 0.745294
C 3.305729 2.927972 -1.563551
C 1.210503 2.216427 2.208785
C 1.266491 3.697494 2.572313
C 1.939086 1.333754 3.220076
C -2.800389 -2.522715 1.136567
C -1.830873 -1.797388 0.450713
C -1.715209 -0.401705 0.677513
C -3.671472 -1.915241 2.042670
C -3.565978 -0.534121 2.254072
C -2.594336 0.211033 1.577148
P -0.671153 -2.420343 -0.811684
C -0.575646 -4.251878 -0.499170
C -1.660210 -2.180675 -2.382187
C -0.827609 -2.316325 -3.657267
C -2.942442 -3.006432 -2.437662
C 0.196994 -4.973191 -1.605571
C 0.030179 -4.551598 0.874815
Ti 1.147955 -0.518744 -0.510130
C 2.498467 -1.960396 0.309428
C 4.017931 -1.797695 0.515934
C 4.657369 -1.134800 -0.711943
C 4.669224 -3.175400 0.729095
C 4.291510 -0.933753 1.750520
C 1.586601 -0.085464 -2.254830
H -2.994342 1.333904 -1.036101
H 0.821762 4.499404 -0.895389
H 2.663107 4.024548 0.176704
H 4.134705 2.826500 1.830494
H 5.058543 3.510577 0.480039
H 4.724187 1.768485 0.525792
H 3.678720 1.931431 -1.842741
H 4.071123 3.671555 -1.838385
H 2.410520 3.119291 -2.171638
H 0.153084 1.902484 2.214771
H 0.820039 3.859442 3.566580
H 0.705279 4.316927 1.856036
H 2.301835 4.071083 2.615795
H 3.014221 1.560857 3.283651

H 1.833259 0.267416 2.972624
H 1.511266 1.487673 4.223839
H -2.898626 -3.598042 0.967078
H -2.536099 1.283065 1.771198
H -1.615450 -4.620818 -0.511072
H -1.929716 -1.114752 -2.280280
H -1.391894 -1.912014 -4.512862
H -0.590821 -3.364945 -3.890764
H 0.116067 -1.757023 -3.575552
H -2.728570 -4.081136 -2.556313
H -3.551635 -2.700936 -3.303458
H -3.560446 -2.874247 -1.537027
H -0.332143 -4.948555 -2.567887
H 0.335539 -6.032151 -1.335522
H 1.196764 -4.534944 -1.755551
H -0.092195 -5.621010 1.109961
H -0.443730 -3.974925 1.682714
H 1.106498 -4.328675 0.887899
H 5.750385 -1.038081 -0.596529
H 4.240620 -0.129172 -0.879685
H 4.468009 -1.723607 -1.624441
H 4.517468 -3.823928 -0.149292
H 5.756554 -3.093800 0.901913
H 4.228723 -3.688371 1.599854
H 5.373053 -0.791610 1.915220
H 3.872042 -1.391913 2.661254
H 3.834446 0.058366 1.638389
H 2.335538 -2.752587 -0.453247
H 2.474812 -0.470104 -2.785667
H 0.984740 0.599923 -2.877543
H 2.037479 -2.352150 1.238659
H -1.310849 5.217855 -1.860671
H -4.416444 -2.517605 2.561172
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O -4.350945 0.160750 3.101407
C -3.720564 4.856969 -2.585656
H -3.040790 5.038890 -3.436450
H -4.754005 4.861941 -2.955170
H -3.606022 5.675390 -1.853400
C -5.343153 -0.515308 3.825106
H -4.915721 -1.281758 4.494966
H -5.854556 0.238211 4.437619
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7"

E: -2986.95374850 H: -2986.116227 G: -2986.241653
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C -2.561772 0.773503 -0.343611

C -3.855616 -1.538607 -1.244516
C -4.551446 -0.322159 -1.214584
C -3.888068 0.818693 -0.760047
N -0.505834 -0.459215 -0.007390
P -1.565271 2.138371 0.325112
C -2.392038 3.717343 -0.181832
C -1.726890 4.914055 0.503090
C -2.379411 3.882252 -1.701711
C -1.841896 1.918879 2.163443
C -3.227898 2.349374 2.636087
C -0.712574 2.498296 3.015740
C 1.848327 -3.063025 1.119622
C 1.322480 -1.985794 0.411201
C 0.003058 -1.549216 0.697737
C 1.121107 -3.723902 2.111210
C -0.180407 -3.290684 2.392495
C -0.728670 -2.213610 1.688696
P 2.129782 -1.060341 -0.944572
C 3.905435 -1.636279 -0.872657
C 1.390934 -1.913303 -2.445452
C 1.679567 -1.200021 -3.767437
C 1.691002 -3.407811 -2.523543
C 4.705598 -1.220038 -2.109175
C 4.622241 -1.200398 0.407690
Ti 0.619417 1.208457 -0.616637
C 1.796660 2.817387 0.182580
C 3.250409 2.783931 0.674058
C 3.696738 4.172511 1.162893
C 4.167025 2.355560 -0.477660
C 3.353005 1.798829 1.846704
C 0.186209 1.630627 -2.362161
H -2.008086 -2.562080 -0.878692
H -4.436522 1.764157 -0.732071
H -3.438820 3.653422 0.161823
H -1.837896 4.888813 1.596567
H -2.185660 5.850800 0.149020
H -0.651038 4.960338 0.270513
H -1.350836 3.991770 -2.074700
H -2.948744 4.782934 -1.982588
H -2.823257 3.021662 -2.222381
H -1.777112 0.821055 2.248741
H -3.393255 2.023312 3.675527
H -4.024983 1.903287 2.021407
H -3.348712 3.444072 2.615271
H -0.636940 3.593326 2.933736
H 0.260705 2.072835 2.731034
H -0.883034 2.258233 4.077522
H 2.855667 -3.424204 0.900368
H -1.746341 -1.903704 1.931004
H 3.843168 -2.737601 -0.871862
H 0.316457 -1.782533 -2.231791
H 0.976870 -1.555219 -4.538165

H 2.694954 -1.402590 -4.137878
H 1.551958 -0.111789 -3.672859
H 2.748776 -3.600558 -2.765962
H 1.088373 -3.869976 -3.321996
H 1.451364 -3.929720 -1.584917
H 4.366232 -1.734117 -3.017795
H 5.766802 -1.478853 -1.965890
H 4.653094 -0.135561 -2.292721
H 5.572958 -1.749824 0.500366
H 4.036462 -1.393968 1.317270
H 4.862142 -0.129742 0.384777
H 4.740631 4.163811 1.522320
H 3.060254 4.522538 1.992105
H 3.627351 4.917326 0.353405
H 4.126945 3.089438 -1.299119
H 5.219823 2.267366 -0.159273
H 3.846556 1.388689 -0.891480
H 4.389010 1.691012 2.210551
H 2.987614 0.800036 1.561326
H 2.739074 2.142595 2.695618
H 1.704200 3.523768 -0.671522
H 0.603596 2.478914 -2.930918
H -0.582534 1.077068 -2.929960
H 1.163665 3.253369 0.979667
H -5.590990 -0.250536 -1.532453
H 1.573164 -4.561768 2.640564
O -4.390403 -2.702582 -1.665602
O -0.975354 -3.844791 3.329846
C -5.721609 -2.726254 -2.103827
H -5.877988 -2.077985 -2.983727
H -5.940814 -3.763101 -2.389228
H -6.424158 -2.425695 -1.307115
C -0.496432 -4.927865 4.080193
H 0.399199 -4.660635 4.667882
H -1.298725 -5.208849 4.774370
H -0.261491 -5.798649 3.443563

Modifications on the phosphine substituents of the PNP ligand

Me

1

E: -2679.61575459 H: -2678.911891 G: -2679.024412
C 3.009675 1.591770 -1.135313
C 2.221734 0.692288 -0.388858
C 2.893985 -0.359808 0.274119
C 4.388092 1.441655 -1.209300

C 5.059287 0.396116 -0.558061
C 4.281037 -0.496388 0.181594
N 0.830802 0.763123 -0.313790
P 1.785930 -1.455217 1.219758
C 2.585834 -3.099357 1.221379
C 1.965278 -0.888853 2.951340
C 6.553838 0.245487 -0.670788
C -1.819887 3.303821 -0.817870
C -1.094920 2.111762 -0.898370
C 0.187968 2.003479 -0.312797
C -1.303670 4.434800 -0.183267
C -0.023325 4.326880 0.379815
C 0.706034 3.147683 0.324722
C -2.087050 5.717269 -0.082925
P -1.696037 0.572965 -1.669908
C -3.499573 0.758323 -1.868678
C -1.070343 0.667167 -3.391915
Ti -0.422213 -0.882899 0.003145
C -1.580327 -0.687140 1.398618
C -2.271741 -0.018515 2.559595
C -2.071249 -0.858165 3.833392
C -3.777537 0.117403 2.276515
C -1.671541 1.379190 2.768797
C -0.420140 -2.756543 -1.058091
C -1.619428 -3.707839 -1.235862
C -2.881134 -2.920101 -1.617332
C -1.329381 -4.731674 -2.347668
C -1.874610 -4.471823 0.070440
H 2.526312 2.411749 -1.670453
H 4.964697 2.155971 -1.804965
H 4.775600 -1.322296 0.702799
H 3.554330 -3.094411 1.743990
H 1.565257 0.132196 3.027367
H 7.075553 1.169335 -0.374933
H 6.858718 0.018990 -1.705444
H 6.926269 -0.567526 -0.030785
H -2.818683 3.359060 -1.260610
H 0.407863 5.190554 0.894954
H 1.686167 3.095857 0.802865
H -3.038471 5.652545 -0.630297
H -1.521863 6.568772 -0.493676
H -2.322780 5.961046 0.965662
H -3.765683 1.642619 -2.467266
H 0.029289 0.669358 -3.363909
H -2.556841 -0.386514 4.704814
H -0.999694 -0.970236 4.060142
H -2.497336 -1.867841 3.715192
H -4.237061 -0.864491 2.078423
H -4.306351 0.572949 3.131148
H -3.950294 0.756337 1.396689
H -2.152664 1.899673 3.614013
H -1.796368 1.999532 1.868130

H -0.592207 1.315213 2.977312
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H -3.743798 -3.589094 -1.776107
H -2.721076 -2.358862 -2.553805
H -3.152340 -2.195649 -0.832371
H -2.166462 -5.438272 -2.484531
H -0.427287 -5.321103 -2.115928
H -1.156031 -4.227888 -3.312791
H -2.108204 -3.787320 0.900900
H -0.986913 -5.056201 0.364194
H -2.717850 -5.175243 -0.031556
H 3.017574 -0.891942 3.273875
H 1.375671 -1.543263 3.610529
H 2.737417 -3.436605 0.186058
H 1.918888 -3.816479 1.723136
H -3.890583 -0.135276 -2.376448
H -3.973478 0.824552 -0.879821
H -1.420017 1.576444 -3.903798
H -1.399801 -0.218578 -3.956585

1-2-TS

E: -2679.56561262 H: -2678.863841 G: -2678.974737
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C 1.742016 -2.364272 0.230483
C 4.308331 -2.256306 -0.811476
C 3.836707 -3.486173 -0.328479
C 2.540185 -3.509800 0.189849
N 1.370870 -0.025524 -0.258908
P 0.055338 -2.272189 0.919965
C -0.588739 -3.984511 0.917898
C 0.336597 -1.929836 2.696428
C 4.698647 -4.721153 -0.374928
C 1.610126 3.665968 -0.393339
C 1.204145 2.354145 -0.651437
C 1.868788 1.254747 -0.053314
C 2.690318 3.950891 0.443421
C 3.355324 2.860037 1.022955
C 2.962455 1.550034 0.788135
C 3.118209 5.365513 0.735263
P -0.181452 1.905352 -1.750056
C -1.189770 3.412733 -1.964990
C 0.631270 1.721893 -3.389670
Ti -0.783832 -0.159864 -0.350802
C -1.661301 0.668103 0.897984
C -2.338513 1.419681 2.013106
C -3.314436 0.511276 2.779957

C -3.100369 2.636928 1.461316
C -1.249009 1.914675 2.981957
C -2.620761 -1.029384 -1.306806
C -4.089972 -1.441741 -1.093455
C -4.960709 -0.196562 -0.889515
C -4.595603 -2.213343 -2.319680
C -4.170522 -2.344154 0.144754
H 3.931750 -0.173929 -1.187629
H 5.316667 -2.200414 -1.233419
H 2.146245 -4.454117 0.578455
H 0.050133 -4.672320 1.492791
H 0.821716 -0.946909 2.777833
H 5.643051 -4.575145 0.173560
H 4.964767 -4.990170 -1.410082
H 4.186283 -5.586283 0.070826
H 1.071899 4.497408 -0.858185
H 4.200140 3.045531 1.693547
H 3.492132 0.732186 1.280974
H 2.949899 5.626541 1.793056
H 2.559449 6.089339 0.124101
H 4.190600 5.514710 0.532476
H -0.618183 4.242712 -2.407407
H 1.356633 0.896877 -3.329128
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H -2.800525 -0.388683 3.152714
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H -2.401852 3.351231 0.999249
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H -0.512432 2.539386 2.453492
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H -2.507183 -0.235151 -0.176322
H -2.521545 -0.425687 -2.232306
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H -2.035295 3.177695 -2.628922
H -1.597690 3.719212 -0.992488
H -0.117269 1.471610 -4.157634
H 1.160977 2.640125 -3.685954

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E: -2481.98219539 H: -2481.445163 G: -2481.540759
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C 1.795128 -0.872187 0.040024
C 2.817685 0.111719 -0.000438
C 3.549068 -2.558789 -0.167820
C 4.560576 -1.588239 -0.211623
C 4.161005 -0.253762 -0.120575
N 0.476703 -0.479193 0.203276
P 2.224797 1.836890 0.078835
C 3.642186 2.828009 0.681996
C 2.082596 2.320545 -1.681080
C 6.008333 -1.974209 -0.368978
C -2.902420 -1.948725 -0.131957
C -1.787486 -1.301160 0.405641
C -0.568871 -1.244247 -0.311362
C -2.854772 -2.582441 -1.375758
C -1.637177 -2.546200 -2.069846
C -0.521708 -1.896183 -1.558294
C -4.062408 -3.262823 -1.965908
P -1.777441 -0.442873 2.021019
C -3.526985 -0.195376 2.485294
C -1.253391 -1.774335 3.181854
Ti -0.116860 1.313173 1.156585
C -1.278160 2.081871 0.149357
C -2.248647 2.495028 -0.928784
C -2.224493 4.024776 -1.092171
C -3.672172 2.052009 -0.551078
C -1.868674 1.832108 -2.264634
H 1.457399 -3.012133 0.002078
H 3.822087 -3.617357 -0.222508
H 4.929432 0.524956 -0.152107
H 4.521235 2.745118 0.025048
H 1.344114 1.653458 -2.146843
H 6.292123 -2.777501 0.328842
H 6.674778 -1.119335 -0.182613
H 6.220037 -2.341199 -1.386958
H -3.842642 -1.961790 0.427356
H -1.567411 -3.025445 -3.051091
H 0.399396 -1.859383 -2.143627
H -4.900379 -3.284930 -1.254193
H -3.840221 -4.302438 -2.253922
H -4.411224 -2.742724 -2.872843
H -4.080198 -1.144137 2.557163
H -0.225241 -2.075704 2.931480
H -2.914668 4.360357 -1.886784
H -1.211619 4.371680 -1.352050
H -2.514709 4.522366 -0.152918

H -3.971456 2.476689 0.420801
H -4.408651 2.379365 -1.306002
H -3.725556 0.954000 -0.483073
H -2.589490 2.085464 -3.062638
H -1.841815 0.736325 -2.159178
H -0.871995 2.162425 -2.595998
H 1.710205 3.352996 -1.752025
H 3.045753 2.228223 -2.206177
H 3.339730 3.885440 0.720062
H 3.921554 2.511902 1.697859
H -3.562626 0.302372 3.465961
H -4.009473 0.463543 1.751812
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H -1.908643 -2.656099 3.112220

5-6-TS

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C 1.968804 -0.876646 0.129447
C 2.835583 0.217989 -0.115426
C 3.955884 -2.277189 0.330244
C 4.815592 -1.193461 0.097020
C 4.222241 0.050857 -0.126438
N 0.600553 -0.650345 0.193770
P 1.959651 1.792667 -0.399692
C 3.172012 3.117106 -0.043346
C 1.766821 1.869130 -2.217796
C 6.311343 -1.373266 0.101596
C -2.545309 -2.585419 -0.104644
C -1.584020 -1.683325 0.361456
C -0.300815 -1.615347 -0.236095
C -2.287494 -3.459817 -1.160536
C -1.013995 -3.395196 -1.746021
C -0.047432 -2.504038 -1.304102
C -3.324944 -4.429543 -1.663195
P -1.868770 -0.539786 1.755163
C -3.678075 -0.296170 1.856643
C -1.524452 -1.581646 3.233093
Ti -0.264135 1.216880 0.825704
C -1.474076 1.856691 -0.239569
C -2.542496 2.410571 -1.141926
C -1.922468 3.437912 -2.105306
C -3.642175 3.095924 -0.312595
C -3.151922 1.258178 -1.958517
H 1.945872 -3.001693 0.553054
H 4.384638 -3.266690 0.517445
H 4.866818 0.914580 -0.317497
H 4.050438 3.074233 -0.705461

H 1.083131 1.063712 -2.521165
 H 6.629661 -2.139641 -0.622977
 H 6.676466 -1.693904 1.091035
 H 6.830140 -0.437934 -0.154723
 H -3.531103 -2.613808 0.369651
 H -0.777853 -4.055236 -2.586638
 H 0.922234 -2.471067 -1.804887
 H -4.261798 -4.347941 -1.093007
 H -2.976457 -5.472073 -1.584770
 H -3.565705 -4.248878 -2.723318
 H -4.215514 -1.222012 2.112546
 H -0.460349 -1.861215 3.226219
 H -2.688572 3.888478 -2.760182
 H -1.166490 2.960295 -2.747176
 H -1.428139 4.250652 -1.549144
 H -3.236639 3.950448 0.253077
 H -4.454455 3.476282 -0.955882
 H -4.082918 2.395427 0.413686
 H -3.911862 1.626793 -2.669410
 H -3.630042 0.516047 -1.300637
 H -2.371312 0.729317 -2.526886
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 H -1.028436 2.785235 1.038907
 H 0.678039 3.294089 2.218928
 H -0.637765 2.410425 3.069879
 H -0.952746 3.987126 2.324439
 H 1.312443 2.832058 -2.493880
 H 2.731920 1.750111 -2.733581
 H 2.678927 4.090868 -0.184159
 H 3.507440 3.049512 1.002164
 H -1.727019 -1.009068 4.151984
 H -2.131978 -2.499736 3.237799
 H -3.892691 0.456656 2.629783
 H -4.043381 0.084849 0.893433

6

E: -2522.51044135 H: -2521.925685 G: -2522.026876
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 C 1.747178 -1.020044 -0.012995
 C 2.767342 -0.053376 -0.178647
 C 3.485360 -2.727411 -0.064044
 C 4.499744 -1.772640 -0.228133
 C 4.107564 -0.434229 -0.281537
 N 0.427440 -0.597899 0.135934
 P 2.164412 1.665740 -0.240879
 C 3.479709 2.689266 0.507973
 C 2.232154 2.106695 -2.016190
 C 5.945069 -2.184769 -0.327329
 C -2.945291 -2.138822 0.047536

C -1.833421 -1.407114 0.474407
C -0.630212 -1.419359 -0.267957
C -2.909984 -2.919199 -1.108599
C -1.711765 -2.931938 -1.838322
C -0.601571 -2.202076 -1.438680
C -4.102347 -3.717436 -1.565728
P -1.810078 -0.320424 1.938752
C -3.552998 0.024945 2.352167
C -1.242417 -1.404339 3.304821
Ti -0.123101 1.274286 0.873389
C -1.279709 2.235446 -0.164936
C -2.177122 2.472921 -1.353596
C -1.605562 3.614544 -2.213159
C -3.592601 2.854850 -0.888646
C -2.246934 1.190677 -2.196176
C 0.556498 2.288851 2.629464
H 1.395572 -3.149717 0.186696
H 3.753934 -3.786733 -0.006150
H 4.875629 0.335492 -0.408444
H 4.438899 2.596828 -0.023512
H 1.519245 1.472045 -2.561348
H 6.109675 -2.883012 -1.163446
H 6.282587 -2.693899 0.589884
H 6.600783 -1.316254 -0.484897
H -3.870597 -2.101812 0.629790
H -1.654595 -3.519119 -2.759801
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H -4.979937 -3.531655 -0.929887
H -3.895484 -4.799540 -1.540226
H -4.380943 -3.466163 -2.601289
H -4.113430 -0.885689 2.613224
H -0.222898 -1.746802 3.074515
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H -0.597288 3.360871 -2.574866
H -1.529490 4.548806 -1.633352
H -3.578208 3.777012 -0.285438
H -4.264819 3.023910 -1.747201
H -4.030166 2.056813 -0.268824
H -2.867566 1.335257 -3.096535
H -2.673517 0.357238 -1.616599
H -1.240655 0.881184 -2.519970
H -1.206674 3.104797 0.549073
H -0.299209 2.479404 3.306722
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H 1.055301 3.261177 2.464969
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H 3.616828 2.397683 1.559039
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H -1.897629 -2.279016 3.434195

H -1.209353 -0.828273 4.242419

6'

E: -2522.50716271 H: -2521.922422 G: -2522.024011

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C -1.817938 -2.085455 -2.248477
C -6.306895 1.051518 0.159967
C 2.384908 2.914806 -0.170783
C 1.509702 1.916380 0.268324
C 0.250999 1.733642 -0.350525
C 2.053112 3.774879 -1.217610
C 0.800330 3.593755 -1.824024
C -0.077851 2.602035 -1.412258
C 2.993801 4.851838 -1.690616
P 1.865293 0.760353 1.635799
C 3.684013 0.685714 1.770035
C 1.354886 1.676651 3.141076
Ti 0.400099 -1.099313 0.654558
C 1.666030 -1.736909 -0.523238
C 2.649234 -2.814048 -0.915523
C 2.327763 -3.321737 -2.331866
C 2.553839 -3.984273 0.074010
C 4.081491 -2.251137 -0.894647
C 0.034976 -2.306987 2.352454
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H -4.483680 3.050279 0.539976
H -4.742446 -1.152681 -0.285059
H -3.783568 -3.322374 -0.334856
H -1.254020 -1.259213 -2.704643
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H -6.776579 0.079995 -0.051839
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H 3.356565 3.032209 0.318473
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H 4.125930 1.650407 2.062208
H 0.270399 1.854077 3.092145
H 3.026596 -4.117499 -2.642170

H 2.393878 -2.506874 -3.070934
H 1.306070 -3.730657 -2.375513
H 1.542390 -4.420715 0.065576
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H 2.758546 -3.645672 1.102195
H 4.816028 -3.011565 -1.211461
H 4.354685 -1.921059 0.119864
H 4.178448 -1.386409 -1.571089
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H 0.947359 -2.321408 2.981215
H -0.788204 -1.895451 2.968645
H 1.618061 -0.886131 -1.249736
H -2.266920 -4.176217 0.069368
H -3.012674 -3.090089 1.269568
H -1.312875 -3.028140 -2.506722
H -2.843079 -2.093814 -2.648879
H 1.565147 1.066841 4.033165
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6'-7'-TS

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C -2.115422 0.101899 0.101711
C -2.381648 -1.276796 -0.093590
C -4.510191 0.393412 0.483892
C -4.773448 -0.969977 0.281155
C -3.679430 -1.786744 -0.006899
N -0.802208 0.555955 0.054478
P -0.889077 -2.256718 -0.429199
C -1.255807 -3.969402 0.086920
C -0.791037 -2.357399 -2.253732
C -6.174367 -1.514904 0.380690
C 0.908249 3.834347 -0.251476
C 0.578619 2.544258 0.170586
C -0.539913 1.856692 -0.363131
C 0.158080 4.505427 -1.218230
C -0.943105 3.821488 -1.755277
C -1.286910 2.539384 -1.349680
C 0.513518 5.893458 -1.683016
P 1.497949 1.565747 1.394662
C 3.196806 2.233474 1.441182
C 0.788273 2.041673 3.012270
Ti 0.873179 -0.787192 0.661707
C 2.343268 -1.442394 -0.281568
C 3.516955 -2.243136 -0.790505
C 3.357127 -3.701588 -0.338593
C 4.834702 -1.674119 -0.234621
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H -3.846542 -2.857152 -0.164446
H -2.094441 -4.410524 -0.472864
H -0.591560 -1.349496 -2.645340
H -6.609002 -1.336945 1.377638
H -6.198075 -2.599187 0.197898
H -6.845481 -1.039768 -0.352972
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H -2.142990 2.043798 -1.811567
H 0.765781 5.907903 -2.755882
H 1.378863 6.292301 -1.133722
H -0.323943 6.594864 -1.539043
H 3.227766 3.285681 1.762521
H -0.266887 1.732408 3.028818
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H 3.314952 -3.777878 0.759695
H 4.840546 -1.700948 0.866488
H 5.705270 -2.247456 -0.595734
H 4.970921 -0.625330 -0.543770
H 4.383168 -2.774632 -2.731295
H 3.663314 -1.146661 -2.680309
H 2.609331 -2.576324 -2.752752
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H 1.854196 -2.231357 3.033047
H 0.206404 -1.828650 2.328679
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H 3.787497 1.629880 2.146283
H 3.655748 2.143957 0.445896
H 1.317965 1.501726 3.811109
H 0.850572 3.126995 3.183956
H -0.358342 -4.583106 -0.080300
H -1.485753 -3.987154 1.161950
H -1.726495 -2.738311 -2.691033
H 0.045856 -3.011592 -2.539132

6'-7"-TS

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C -2.681206 -0.816739 -0.122398
C -4.414425 1.229083 0.569078
C -4.954094 -0.041518 0.314504
C -4.055926 -1.051988 -0.028707
N -0.763105 0.646532 0.079467
P -1.444914 -2.069940 -0.576959

C -2.101953 -3.688044 -0.049637
C -1.528128 -2.148732 -2.408662
C -6.437121 -0.288232 0.409008
C 1.680315 3.413845 -0.211803
C 1.054413 2.234551 0.199494
C -0.216216 1.860248 -0.305824
C 1.088367 4.278505 -1.133202
C -0.170186 3.909406 -1.632438
C -0.808187 2.741395 -1.240316
C 1.763158 5.546878 -1.586174
P 1.734400 1.066191 1.414989
C 3.543279 1.305740 1.423633
C 1.208128 1.751210 3.034449
Ti 0.589776 -1.045286 0.555672
C 2.081087 -1.739185 -0.322719
C 3.360980 -2.444657 -0.700454
C 3.046913 -3.848449 -1.249151
C 4.247742 -2.570507 0.546540
C 4.100701 -1.631756 -1.774377
C 0.637615 -2.311038 1.939918
H -2.680653 2.484383 0.712767
H -5.085259 2.043731 0.859671
H -4.442407 -2.057036 -0.225912
H -3.044656 -3.953758 -0.552149
H -1.223553 -1.173902 -2.817085
H -6.841653 0.046461 1.377345
H -6.675582 -1.356340 0.299965
H -6.987560 0.255900 -0.376088
H 2.662869 3.670721 0.196435
H -0.661859 4.555210 -2.366747
H -1.777592 2.488572 -1.674043
H 1.141077 6.432311 -1.378135
H 1.957544 5.536878 -2.671028
H 2.727891 5.692332 -1.078501
H 3.833663 2.333356 1.690441
H 0.109102 1.735466 3.079093
H 3.967463 -4.385959 -1.533169
H 2.403769 -3.786981 -2.141864
H 2.516741 -4.453772 -0.496871
H 3.732524 -3.121088 1.349953
H 5.182437 -3.106450 0.314643
H 4.510288 -1.577332 0.941698
H 5.047420 -2.119960 -2.059666
H 4.333750 -0.619091 -1.410849
H 3.489181 -1.526465 -2.685048
H 1.606538 -2.363353 0.881432
H 0.829317 -3.214116 2.527956
H 0.345897 -1.437048 2.586395
H 1.411437 -1.507697 -1.208960
H -1.348493 -4.456555 -0.278873
H -2.249446 -3.670933 1.039249
H -0.828425 -2.914885 -2.777215

H -2.544189 -2.382574 -2.761472
H 3.982729 0.615640 2.158974
H 3.942587 1.055854 0.430907
H 1.557252 2.785736 3.173287
H 1.598894 1.121028 3.848170

7'

E: -2522.49940490 H: -2521.914784 G: -2522.015386
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C 1.337014 -1.449563 0.050816
C 2.494266 -0.660274 -0.145923
C 2.801334 -3.317733 0.594641
C 3.953011 -2.536438 0.415057
C 3.768254 -1.204812 0.043169
N 0.080095 -0.855525 -0.057325
P 2.183480 1.060547 -0.673399
C 3.621495 2.037782 -0.115980
C 2.413559 0.982105 -2.495295
C 5.324774 -3.117306 0.637126
C -3.418212 -2.046148 -0.279931
C -2.273755 -1.362982 0.134358
C -1.023876 -1.605019 -0.476076
C -3.369819 -2.995030 -1.304486
C -2.123533 -3.237067 -1.900530
C -0.974812 -2.561932 -1.505950
C -4.601651 -3.727959 -1.767080
P -2.172696 -0.111785 1.455208
C -3.849191 0.590407 1.630178
C -1.932764 -1.091669 2.981759
Ti -0.060658 1.102316 0.618121
C -1.345974 2.710209 0.030383
C -0.808339 4.018988 -0.583815
C 0.323776 4.582014 0.288100
C -1.929302 5.068179 -0.674775
C -0.277837 3.751657 -1.997771
C 0.816983 1.384128 2.226625
H 0.655895 -3.431965 0.594101
H 2.908016 -4.365159 0.892931
H 4.649614 -0.574129 -0.106954
H 4.571574 1.683208 -0.543663
H 1.592007 0.396530 -2.933520
H 5.489915 -3.359161 1.699809
H 6.114118 -2.415285 0.331912
H 5.465642 -4.049253 0.067502
H -4.376481 -1.839478 0.207017
H -2.053658 -3.970743 -2.709347
H -0.024336 -2.769233 -2.002283
H -4.867703 -3.453178 -2.800804

H -5.468932 -3.501395 -1.130310
H -4.450217 -4.818725 -1.751297
H -4.599327 -0.174914 1.880611
H -0.979855 -1.632942 2.893242
H 0.717760 5.528419 -0.119833
H 1.163246 3.871646 0.368354
H -0.029422 4.781653 1.312996
H -2.331007 5.304681 0.323977
H -1.572951 6.011039 -1.125113
H -2.765702 4.697601 -1.289619
H 0.116166 4.669657 -2.465410
H -1.072128 3.356516 -2.652130
H 0.531379 3.006659 -1.979083
H -1.867096 2.949401 0.982118
H 0.735842 2.360999 2.739915
H 1.449184 0.668728 2.781233
H -2.125797 2.283852 -0.635173
H -3.834195 1.341818 2.433753
H -4.139396 1.093010 0.696350
H -2.750190 -1.809832 3.146930
H -1.854257 -0.406576 3.838974
H 3.663785 1.999634 0.981689
H 3.475138 3.085231 -0.419849
H 3.370776 0.504849 -2.754830
H 2.387726 1.993992 -2.927151

7"

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C -1.968144 0.668561 0.066784
C -2.751969 -0.482027 -0.186387
C -4.036003 1.854493 0.571752
C -4.816397 0.713931 0.327765
C -4.142537 -0.447979 -0.048519
N -0.577661 0.584161 -0.013245
P -1.803938 -1.946373 -0.709003
C -2.778405 -3.408608 -0.220070
C -1.924013 -1.930983 -2.538937
C -6.313723 0.750435 0.485875
C 2.217588 3.012135 -0.150205
C 1.410256 1.940485 0.231786
C 0.164361 1.708937 -0.392528
C 1.820319 3.903725 -1.150888
C 0.577017 3.677819 -1.757516
C -0.235047 2.608589 -1.396965
C 2.687129 5.061912 -1.570610
P 1.790428 0.686850 1.497083
C 3.556910 0.889567 1.924011

C 0.940327 1.309445 2.996545
Ti 0.323650 -1.242124 0.503333
C 1.573830 -2.490350 -0.676499
C 3.109083 -2.554983 -0.639180
C 3.627484 -3.738327 -1.474193
C 3.585936 -2.734244 0.808949
C 3.681257 -1.258680 -1.229197
C -0.204960 -2.025252 2.097374
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H -3.763992 -3.447657 -0.708286
H -1.413788 -1.032418 -2.915762
H -6.603377 0.915840 1.536477
H -6.776051 -0.192343 0.159502
H -6.762229 1.564710 -0.104774
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H 0.239115 4.353680 -2.548975
H -1.190647 2.456818 -1.903816
H 2.163905 6.022912 -1.442785
H 2.971804 4.987734 -2.632459
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H 3.775192 1.915463 2.257706
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H 0.222592 -3.009068 2.370604
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H -1.415440 -2.816242 -2.950715
H -2.970605 -1.920567 -2.879325
H -2.213543 -4.311923 -0.495944
H -2.898354 -3.400565 0.872507
H 1.103314 0.599037 3.820548
H 1.299608 2.309229 3.283900
H 3.798560 0.199038 2.745645
H 4.199845 0.641421 1.068386

Modifications on the phosphine substituents of the PNP ligand

^tBu

1

E: -3150.90025767 H: -3149.837901 G: -3149.975237
C -1.059743 -3.619448 -0.430210
C -1.157721 -2.251708 -0.066453
C -2.463936 -1.752285 0.151385
C -2.165176 -4.451284 -0.451098
C -3.446604 -3.984424 -0.120697
C -3.562019 -2.625787 0.156571
N -0.050469 -1.420583 0.031436
P -2.599064 0.053698 0.332906
C -3.674122 0.559975 -1.151983
C -3.990505 2.057550 -1.047108
C -2.800678 0.278911 -2.387068
C -3.447201 0.386885 1.990561
C -4.963572 0.180041 2.033747
C -3.125467 1.835859 2.380928
C -4.633736 -4.910000 -0.086336
C 3.569562 -2.272976 -0.148815
C 2.360596 -1.597995 -0.364304
C 1.187092 -2.029691 0.297673
C 3.685724 -3.328653 0.754341
C 2.535307 -3.691784 1.468578
C 1.321183 -3.063635 1.245886
C 4.993699 -4.041636 0.975056
P 2.125938 -0.091205 -1.371671
C 3.719406 0.943321 -1.343583
C 1.741506 -0.695937 -3.138767
C 1.037649 0.428044 -3.914319
C 2.982762 -1.164903 -3.903116
C 3.523389 2.109621 -2.325827
C 3.810330 1.498747 0.082801
Ti 0.012793 0.692733 0.124290
C 0.611305 1.071183 1.791666
C 1.137979 1.004060 3.208672
C 0.104728 1.583324 4.192240
C 2.431549 1.826853 3.348287
C 1.430383 -0.456240 3.574190
C -0.268040 2.572787 -0.986450
C -0.153882 4.047964 -0.523265
C 1.260705 4.374565 -0.026806
C -0.466532 4.976769 -1.711192
C -1.146729 4.362064 0.603283
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H -4.742949 2.259746 -0.270030
H -4.404807 2.416085 -2.003880
H -3.099908 2.659043 -0.825152

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H -2.556026 -0.791808 -2.468013
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H -5.262217 -0.838078 1.747510
H -5.500699 0.896808 1.396326
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H -2.041315 2.007709 2.385587
H -3.511678 2.042756 3.392918
H -4.545241 -5.652419 0.723734
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H -5.570684 -4.356588 0.073974
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H 2.593835 -4.487110 2.217605
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H -3.027359 -0.270590 4.015859
H -3.103992 -1.607927 2.841577
C -4.988987 -0.207803 -1.346715
H -5.536068 0.250923 -2.187500
H -4.815560 -1.258930 -1.611908
H -5.650585 -0.171925 -0.472360
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1-2-TS

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C -4.275329 -3.228142 0.272187
C -4.090920 -1.849114 0.277918
N -0.399472 -1.476072 0.297062
P -2.562788 0.558977 0.184264
C -3.461593 1.146861 -1.383210
C -3.531418 2.680736 -1.390427
C -2.577893 0.658219 -2.544759
C -3.313655 1.272614 1.763787
C -4.842050 1.333110 1.817930
C -2.733804 2.683090 1.949923
C -5.645567 -3.852296 0.314985
C 3.006429 -2.950586 0.487154
C 1.937306 -2.148933 0.066265
C 0.690090 -2.233899 0.735993
C 2.917626 -3.800940 1.588428
C 1.703127 -3.821302 2.288149
C 0.620872 -3.061459 1.875020
C 4.079281 -4.655577 2.022975
P 2.018532 -0.861846 -1.234922
C 3.789003 -0.181770 -1.359276
C 1.508546 -1.702339 -2.869597
C 1.013448 -0.616527 -3.838493
C 2.627042 -2.520983 -3.520115
C 3.805747 0.802752 -2.541012
C 4.009215 0.612217 -0.066774
Ti 0.126908 0.564923 0.019787

C 0.844076 1.219680 1.463135
C 1.462179 1.581670 2.796538
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C 1.947612 0.270437 3.442701
C 0.349636 2.568081 -1.091664
C 0.803470 4.039584 -0.975626
C 2.324712 4.108136 -0.801410
C 0.412059 4.794522 -2.254058
C 0.112490 4.695994 0.226392
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H -3.208664 -5.105989 0.156881
H -4.977790 -1.215773 0.314187
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H -2.574430 3.156757 -1.132744
H -1.593295 1.148480 -2.553952
H -3.063564 0.889433 -3.507377
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H -5.307323 0.345737 1.688064
H -5.260092 2.019772 1.067449
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H -6.435793 -3.087046 0.312788
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H 3.945750 -2.918134 -0.061323
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H -0.312857 -3.095772 2.439600
H 4.957873 -4.498801 1.380419
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H 3.920340 -0.026920 0.824491
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H 0.068855 3.193808 3.312189
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H 2.667605 5.150152 -0.695283
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H -0.679522 4.778636 -2.407164
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C -2.794154 0.359451 2.886503
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H -1.709747 0.187744 2.795406
H -2.986389 0.831340 3.864110
C -4.875380 0.594527 -1.605631
H -5.309712 1.081376 -2.495143
H -4.867385 -0.486295 -1.799069
H -5.550524 0.794537 -0.762731
C 4.965006 -1.160791 -1.520715
H 4.793237 -1.955911 -2.254718
H 5.847636 -0.591282 -1.856670
H 5.244743 -1.623182 -0.565554
C 0.329717 -2.643139 -2.582107
H 0.605373 -3.453353 -1.891815
H -0.529033 -2.112290 -2.152134
H 0.004627 -3.104942 -3.528853

A

E: -2953.28479677 H: -2952.390443 G: -2952.512998
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C -2.464088 -1.066342 0.376874
C -2.186634 -3.565748 1.575680
C -3.470732 -3.156850 1.186079
C -3.569480 -1.904700 0.584978
N -0.080149 -0.637879 0.656437
P -2.587364 0.568904 -0.425783
C -3.338121 0.290981 -2.140208
C -3.565064 1.664247 -2.787777
C -2.245532 -0.462397 -2.916458
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C -3.421715 3.114907 0.293607
C -4.671392 -4.041441 1.396126
C 3.553697 -1.082002 1.294231

C 2.351156 -0.818687 0.624332
C 1.122943 -0.883216 1.327190
C 3.599850 -1.370998 2.656595
C 2.382774 -1.377414 3.354655
C 1.178453 -1.141536 2.711018
C 4.899640 -1.657498 3.361413
P 2.243531 -0.297394 -1.130567
C 3.767013 0.739561 -1.583534
C 2.214344 -1.928778 -2.099066
C 2.232226 -1.630630 -3.603726
C 3.350082 -2.889251 -1.728489
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C 4.048552 1.679277 -0.405356
Ti -0.008610 1.003758 -0.632435
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C 0.899970 3.426491 1.279145
C 1.821945 4.505430 0.678728
C 1.634363 2.684570 2.412003
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H -2.052472 -4.554249 2.026330
H -4.556391 -1.565470 0.265798
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H -3.758975 1.537977 -3.865812
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H -1.301491 0.108774 -2.972159
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H -5.361687 0.296916 0.971616
H -5.616040 1.554479 -0.272227
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H -2.349685 3.327336 0.176353
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H 0.246983 -1.144407 3.280627
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H 5.053776 -0.974784 4.211920
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H 1.430894 -0.931693 -3.893069
H 4.341269 -2.512713 -2.008174
H 3.202832 -3.845414 -2.258502
H 3.354219 -3.109477 -0.650703
H 3.024450 1.017782 -3.650907
H 4.160914 2.258740 -3.086273
H 2.484843 2.262825 -2.486761

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C -3.066543 1.420337 2.103423
H -1.968351 1.506680 2.099115
H -3.468063 2.177946 2.795977
H -3.328154 0.427029 2.495780
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H 4.937672 -0.611263 -2.871596
H 5.850493 0.714180 -2.135252
H 5.391920 -0.683864 -1.149541
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H 0.829871 -2.889204 -0.687368
H 0.015751 -1.983769 -1.977040
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5-6-TS

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C 3.569555 -3.254476 -1.410370
C 3.650911 -1.940333 -0.960713
N 0.099929 -0.951192 -0.548493
P 2.612779 0.536422 -0.000278
C 3.608947 0.433251 1.611395
C 3.994018 1.845490 2.070989
C 2.628084 -0.183845 2.623774
C 3.463622 1.574392 -1.326645
C 4.970270 1.356863 -1.486534
C 3.183393 3.050936 -1.006805
C 4.793841 -4.050726 -1.778512
C -3.538001 -1.648365 -0.837803
C -2.314321 -1.227307 -0.300591
C -1.136074 -1.318382 -1.086817

C -3.664751 -2.102085 -2.150158
C -2.507598 -2.114863 -2.940901
C -1.278839 -1.735863 -2.425260
C -4.990960 -2.546197 -2.709108
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6

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6'

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H 0.275318 -1.233681 -2.860176
H 1.090194 -2.588257 -3.669587

7'

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7"

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C 2.883758 -1.244000 -2.217093
C 3.057759 -0.423867 -3.500172
C 4.117770 -2.119697 -1.965054
C 3.622198 2.349404 -1.440416
C 3.717831 1.645522 0.965506
Ti -0.014072 0.852209 -0.670715
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C 0.404538 4.030998 0.807297
C -0.682315 5.113071 0.657973
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C 0.390589 3.521171 2.255134
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Modifications on the phosphine substituents of the PNP ligand

NMe₂

1

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C 1.810058 -3.850130 1.527099
C 0.688046 -3.134136 1.131761
C 4.307628 -4.253016 1.608408
P 2.124786 -0.102621 -1.105035
C 0.604587 -0.526130 -3.313770
C 2.623881 -1.874368 -3.110336
C 4.349783 0.965423 -2.325448
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Ti 0.073691 0.885996 0.142764
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C 1.944403 0.277670 3.537881
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C 1.594713 3.171078 -2.169099
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C 0.436406 4.707166 -0.588956
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1-2-TS

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Modifications on the phosphine substituents of the PNP ligand

Ph

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C 3.091769 3.479291 -2.060705
C 3.307193 2.254698 -1.429615
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C 5.743037 -0.345059 2.540340
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H 6.807232 -0.098838 2.535931
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C 2.354674 -0.069056 1.246665
C 1.060484 -0.241869 1.794546
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6

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H -4.030858 4.857123 2.302982

6'

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C 1.633976 3.927645 1.385260
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H -4.373274 0.868096 5.257902
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C 3.070825 -0.698587 -3.051870
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C 3.629437 -1.440420 -4.090670
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H -7.100545 1.894156 -3.058088
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C -2.942749 1.950656 2.042765
C -2.997590 -0.391272 2.633748
C -3.152203 2.295747 3.374796
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C -3.199828 -0.042914 3.970050
H -2.938269 -1.443654 2.346274
C -3.279343 1.297275 4.342402
H -3.211108 3.348504 3.660191
H -3.295137 -0.827442 4.724101
H -3.437005 1.566865 5.389178

6'-7"-TS

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C -0.973378 -3.664230 -0.172195
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C -2.413312 -1.738712 -0.280853
C -2.048845 -4.466224 -0.530492
C -3.325132 -3.939636 -0.780770
C -3.481245 -2.559113 -0.647769
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C -4.464501 -4.830597 -1.201021
C 3.254012 -1.520990 1.882030
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C 0.934018 -1.772018 1.112794
C 3.063610 -2.410267 2.936074
C 1.784056 -2.977192 3.062983
C 0.751598 -2.671547 2.191795
C 4.163694 -2.748171 3.907382
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C -0.006674 2.347707 -0.265107
C -0.008166 3.853643 -0.175725
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H -2.140361 4.021406 -0.629085
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H 1.468302 4.116009 -1.772512
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H -0.742350 0.071140 -2.690577

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C 4.460444 1.806971 -0.796278
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C 5.224465 2.911172 -0.419456
H 4.573158 1.389886 -1.799882
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H 5.689022 4.321195 1.149055
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H -7.351040 0.813607 -0.665587
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H -2.412595 -1.624625 2.332414
C -3.078584 1.022785 4.368686
H -3.439223 3.046852 3.697900
H -2.683230 -1.068563 4.732780
H -3.200090 1.266599 5.426563

7'

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C -0.865753 -2.046550 -0.040131
C -2.179219 -1.615913 -0.326558
C -1.575884 -4.305542 -0.574220
C -2.877167 -3.878160 -0.881625
C -3.157754 -2.516904 -0.749978
N 0.095629 -1.087905 0.287438
P -2.420939 0.166997 -0.014319
C -3.922618 -4.860188 -1.341290
C 3.312061 -0.919561 2.104025
C 2.334280 -0.763526 1.119823
C 1.053864 -1.341982 1.264909
C 3.065479 -1.665714 3.259039
C 1.797571 -2.252657 3.389815
C 0.808580 -2.097513 2.426494
C 4.112411 -1.837957 4.328507
P 2.520103 0.138402 -0.452080
Ti -0.034357 0.710652 -0.744083
C 0.294694 2.723400 -0.141441
C -0.691935 3.890855 -0.359299
C -1.277246 3.833227 -1.777616
C 0.042674 5.230932 -0.179805
C -1.842106 3.831120 0.653026
C -0.378451 0.460410 -2.549976
H 0.423355 -3.779192 0.035822
H -1.326823 -5.366308 -0.673531
H -4.163042 -2.150002 -0.978640
H -3.624425 -5.350442 -2.281884
H -4.889488 -4.366691 -1.515180
H -4.081675 -5.657265 -0.597678
H 4.289964 -0.448078 1.965679
H 1.571660 -2.837228 4.286789
H -0.175571 -2.547020 2.574552
H 3.774866 -1.425391 5.292873
H 5.049154 -1.329214 4.059344
H 4.345438 -2.901433 4.497050
H -1.928591 4.700664 -1.977553
H -1.879018 2.921936 -1.924170
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H -0.636341 6.090574 -0.315124
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H -2.535460 4.677736 0.517744
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H -2.429247 2.907598 0.539870
H 1.203294 2.916555 -0.754614
H -0.541627 1.182981 -3.366560
H -0.459693 -0.589327 -2.892036

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H 2.878988 2.296489 1.447967
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C 4.491706 -3.071658 -2.136864
H 4.230422 -2.283143 -0.147757
C 4.185734 -2.928175 -3.490740
H 3.122641 -1.766805 -4.970312
H 5.122034 -3.898402 -1.801623
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C -1.946007 0.852894 2.642701
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C -2.144286 0.799018 4.022578
H -1.110341 1.425772 2.234746
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7"

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C 1.837290 4.202395 0.773709
C 3.130968 3.844867 0.362205
C 3.362270 2.501246 0.071476
N 0.049988 0.931559 0.628581
P 2.559724 -0.227771 -0.213010
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C -3.356795 0.778381 2.093801
C -2.294677 0.651782 1.191163
C -0.985188 1.030796 1.557121
C -3.163728 1.239235 3.394348
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C -0.792273 1.486173 2.878060
C -4.304699 1.374682 4.367700
P -2.449991 0.116237 -0.543579
Ti 0.104352 -0.298248 -1.040687
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C -0.160300 -3.393960 -0.468815
C 1.243536 -4.004352 -0.559775
C -1.203844 -4.505008 -0.653114
C -0.339836 -2.769114 0.925554
C 0.451609 0.652897 -2.594421
H -0.182893 3.588566 1.178464
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H 4.386729 5.412328 1.175958
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H -1.662078 1.937667 4.781978
H 0.209155 1.776415 3.201851
H -4.424132 2.417263 4.703184
H -4.140648 0.761682 5.268387
H -5.256536 1.058200 3.917655
H 1.446871 -4.693586 0.276854
H 2.011346 -3.216502 -0.539391
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H -1.108481 -4.970741 -1.647489
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H -2.226100 -4.102398 -0.570215
H -0.252135 -3.520051 1.728925
H -1.329614 -2.298199 1.025214
H 0.423180 -1.998345 1.128312
H -1.325696 -2.331482 -2.003780
H 0.333258 0.064106 -3.525876
H 0.802810 1.679204 -2.790007

H 0.380624 -2.498231 -2.403761
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H 4.494979 -3.889148 2.533935
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C -4.935422 -2.783757 -1.980874
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H -3.599555 -1.774182 1.517469
C -5.284690 -3.532130 -0.855882
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H -5.064250 -3.743636 1.281454
H -5.928441 -4.408410 -0.958568
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C -4.748891 1.645094 -1.214686
C -3.265142 3.564947 -2.591422
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C -5.386495 2.748567 -1.776277
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C -4.644882 3.711667 -2.462579
H -2.681203 4.311750 -3.133968
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Substitution of phosphorus atoms on the PNP ligand

As

1

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C  -2.516105  -1.331032  -0.663073
C  -2.112051  -3.700501  -2.049923
C  -3.408932  -3.170456  -1.999204
C  -3.581459  -1.976600  -1.294846
N  -0.152978  -1.180801  -0.122640
C  -4.151829  1.239956  -0.510939
C  -4.461415  2.556310  0.201057
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C  -3.310119  -0.327670  2.086390
C  -4.665813  -1.019233  2.018307
C  -3.266201  0.773739  3.143334
C  -4.558244  -3.860904  -2.685674
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C  2.235994  -1.504754  0.199588
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C  3.099327  -3.322517  1.578939
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C  0.706146  -3.080225  1.196137
C  4.249140  -4.050654  2.223940
C  4.275337  0.546992  -0.835520
C  2.092159  -0.759413  -2.678836
C  1.737548  0.263679  -3.755947
C  3.220794  -1.699337  -3.087182
C  4.696853  1.472444  -1.975690
C  4.628668  1.145444  0.523423
Ti 0.004996  0.876110  0.220879
C  0.480647  1.234052  1.938451
C  0.903864  0.986791  3.368217
C  0.417696  2.119929  4.286240
C  2.438147  0.903405  3.441848
C  0.321115  -0.351739  3.845468
C  -0.447908  2.608310  -0.989101
C  0.314072  3.942143  -1.125224
C  1.800954  3.697865  -1.402473
C  -0.274981  4.756843  -2.290714
C  0.175469  4.767992  0.160476
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H  -1.936135  -4.631231  -2.597960
H  -4.583654  -1.540316  -1.237918
H  -5.017489  0.566381  -0.398587
H  -4.764484  2.405892  1.246589
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H -0.488790 2.110932 -1.985825
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H 2.347519 4.643251 -1.560027
H 1.935021 3.079483 -2.305404
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H 0.234031 5.728660 -2.412735
H -1.346803 4.957452 -2.128409

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H -0.884161 4.929396 0.418794
H 0.647440 5.758777 0.051310
As -2.630984 0.316150 0.344775
As 2.356311 0.086010 -0.905119

1-2-TS

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H 1.601827 3.852899 2.630686
H -1.172005 2.381442 -2.530932
H 0.471922 1.883491 -3.004606
H -0.881464 0.717034 -3.119625
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As 2.368906 -0.179254 -0.905644

6'-7'-TS

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C -1.951573 -4.180481 -0.892766
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C -4.530672 2.373968 -0.246532
C -3.992538 0.908506 -2.231511
C -2.898826 0.250481 2.087344
C -4.289455 -0.300426 2.381319
C -2.607603 1.562744 2.809310
C -4.394152 -4.554910 -1.453491
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C 2.346702 -1.246880 0.717291
C 1.022754 -1.690869 0.938757
C 3.214916 -2.645852 2.518256
C 1.902120 -3.089434 2.736235
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C 4.355980 -3.142262 3.367382

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C 2.839060 -1.163188 -2.258693
C 2.604884 -0.474959 -3.601091
C 4.201085 -1.842037 -2.169272
C 4.465315 1.936806 -1.531372
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C 0.422079 4.293156 2.152328
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C -4.100593 2.774692 -0.533695
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C -2.750049 1.774328 2.797025
C -4.768312 -4.274356 -1.310714
C 3.274778 -1.897293 1.467432
C 2.239856 -1.370195 0.691751
C 0.897575 -1.766804 0.894641
C 3.037698 -2.834589 2.475103
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C 0.663906 -2.710980 1.921041
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C 4.167517 0.777850 -0.364010
C 2.795572 -1.319751 -2.265425
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Substitution of nitrogen atom with phosphorus atom

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H 1.444903 2.323751 -3.105015
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6

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Substitution of nitrogen atom with phosphorus atom and replacement of ⁱPr groups with ^tBu groups

1

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6

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H 3.191230 -1.603742 2.458479
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H 1.845842 1.684755 -2.275641
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6'

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C 2.364686 -1.642738 -0.170522
C 1.748666 -4.369866 -0.165973
C 3.043748 -3.974430 0.192348
C 3.320477 -2.608484 0.177774
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C -0.154252 4.141825 -0.212534
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 C 4.290185 0.109157 -2.845914
 C 3.634737 2.353874 -1.906293

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C -4.448637 -3.059717 -1.101276
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C -5.823060 -3.673343 -1.067157
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C -3.089401 2.157355 2.092227
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C -0.418215 4.786381 1.121289
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C 0.577823 4.794182 -1.167514
C 0.437961 1.494958 2.101921
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7'

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 C 3.019373 -2.778972 0.268267
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C 1.804236 4.513175 -0.774911
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Modified version of the PNP ligand backbone (B)

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1-2-TS

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H 2.058657 1.652353 -2.892175
H 4.789038 1.373781 -1.742435
H 4.656360 -0.011387 -0.642969
H 3.406480 1.256244 -0.623305
H 1.090802 5.550418 0.638022
H -0.122313 4.395576 1.232075
H -0.136353 4.898376 -0.474680
H 1.720911 4.149906 -2.044398
H 2.879043 4.883822 -0.902981
H 3.091641 3.200885 -1.430840
H 2.970184 4.087596 1.508842
H 3.032271 2.356582 1.077541
H 1.736903 2.952471 2.121103
C 2.507357 -1.677089 0.023761
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H 1.868506 -2.559832 0.175902
C -2.811344 -0.063061 1.398609
H -2.279237 0.566386 2.126457
H -3.854520 -0.142763 1.739468
C -2.143531 -1.418180 1.438939
C 2.531922 -0.868643 1.301868
C -2.511395 3.006404 1.652303
H -2.897139 2.497661 2.547701
H -1.444511 2.759038 1.534396
H -2.589085 4.089821 1.836011
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H -5.935870 -0.761214 -1.434859
H -5.068018 -1.132398 0.061732
C 4.242203 -1.050347 -3.057695
H 3.789744 -1.521201 -3.941796
H 5.134332 -0.502423 -3.404469
H 4.592578 -1.843811 -2.379390
C 2.092448 -3.532189 -2.590068
H 2.974031 -3.326547 -3.208147

H 2.436792 -3.889371 -1.608164
H 1.551507 -4.369131 -3.063021

5-6-TS

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C 2.590650 4.096547 1.347809
C 3.095133 2.796535 1.253756
N 0.038907 0.694289 1.067664
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C 4.302084 -1.328487 -2.380578
C 3.211654 0.887490 -2.124819
C 3.306904 -2.517355 0.664900
C 4.806092 -2.581535 0.971787
C 2.912370 -3.634525 -0.311913
C 3.499396 5.297846 1.354287
C -3.508337 1.061087 2.216653
C -1.144360 0.670226 1.851113
C -3.453323 0.524722 3.502642
C -2.212621 0.059531 3.957384
C -1.089162 0.134455 3.147168
C -4.676818 0.443635 4.377858
P -2.032722 0.695966 -1.423014
C -3.634134 -0.157651 -1.947293
C -1.510827 1.995932 -2.705532
C -0.093270 2.415627 -2.287272
C -1.439187 1.367853 -4.103849
C -3.268869 -1.301468 -2.902740
C -4.230649 -0.751523 -0.662001
Ti 0.012756 -0.742907 -0.442628
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C -1.431548 -3.496960 0.534222
C -0.423134 -4.633697 0.780531
C -2.448212 -4.004798 -0.504211
C -2.158105 -3.190169 1.855813
C 0.391629 -1.739518 -2.581056
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H 0.760800 5.217357 1.591842
H 4.180959 2.655141 1.265977
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H 2.831788 1.671292 -1.452712

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H 2.346205 -0.208709 2.165755
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C 2.528984 -2.726125 1.976613
H 2.931710 -2.115278 2.797618
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H 2.617821 -3.780448 2.284641
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H -5.614619 0.186458 -2.734471
H -4.923271 1.623080 -1.960826
C -2.397671 3.246880 -2.755296
H -3.432975 3.025152 -3.042396
H -2.415923 3.786376 -1.797483
H -1.991714 3.945138 -3.506455
H -0.330762 -2.215931 -3.261668

6

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C 3.028966 3.811903 1.456204
C 3.388079 2.463001 1.424131
N 0.127807 0.747360 0.810326
P 2.604356 -0.976330 -0.238707
C 3.808691 -0.227769 -1.510453
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C 4.698893 -2.897755 0.398750
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C -1.696366 0.312981 4.028666
C -0.695591 0.337462 3.068466
C -4.111166 0.617518 4.722674
P -2.180235 0.720542 -1.375291
C -3.824730 -0.133893 -1.749159
C -1.766351 2.002043 -2.714715
C -0.329886 2.458138 -2.413655
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C -4.353677 -0.639389 -0.398932
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C -0.647446 -4.525067 1.188157
C -2.749484 -3.901534 0.044017
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H 4.900593 -3.903236 0.805134
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H 4.425486 5.260645 0.659697
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H 2.586477 -4.086892 1.830487
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H 5.695386 -0.669149 -0.442506
H 5.812676 0.550647 -1.720602
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C -2.675946 3.238536 -2.718493
H -3.719500 3.003414 -2.959904
H -2.659062 3.778476 -1.760717
H -2.314878 3.942628 -3.486867
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6'

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C -3.282769 -2.867301 0.822280
N -0.096022 -0.927385 0.761398
P -2.618612 0.890296 -0.018799
C -3.771508 0.417341 -1.458071
C -4.007176 1.626600 -2.373503
C -3.043293 -0.660328 -2.278713
C -3.269566 2.445801 0.854989
C -4.790059 2.511742 1.030939
C -2.777183 3.668788 0.069677
C -3.841104 -5.317331 0.513316
C 3.255402 -1.641073 2.283772
C 0.968646 -1.102973 1.690550
C 3.022878 -1.384411 3.634234
C 1.733039 -0.981448 4.005161
C 0.734183 -0.846095 3.051790
C 4.110371 -1.537606 4.665017
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C 3.872725 0.452202 -1.484462
C 1.847907 -1.440375 -2.919087
C 0.407480 -1.945947 -2.741097

C 1.890575 -0.507693 -4.136657
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C 4.360343 0.692701 -0.047123
Ti 0.071672 0.791953 -0.382468
C 0.781789 2.172334 0.621601
C 1.270375 3.589414 0.885112
C 1.103674 4.469158 -0.361878
C 2.757946 3.586792 1.282977
C 0.481555 4.223121 2.046282
C -0.257474 1.752109 -2.281564
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H -4.350997 -2.677074 0.968021
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H -4.518636 1.288187 -3.289981
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H -2.765981 -1.537563 -1.677126
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H 5.914063 0.268993 -2.164003
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C 2.760553 -2.648638 -3.170028
H 3.806254 -2.367389 -3.343940
H 2.733747 -3.377769 -2.347126
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6'-7'-TS

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C -3.128499 -0.643896 -2.246923
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C -2.718857 3.770353 -0.270181
C -4.018953 -5.123803 1.110928
C 3.313933 -1.554708 2.205053

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C 1.940506 -0.664001 3.946635
C 0.877505 -0.598573 3.057847
C 4.347636 -1.220335 4.492115
P 2.060140 -0.694442 -1.402862
C 3.727580 0.112553 -1.793130
C 1.463355 -1.758673 -2.854819
C 0.052541 -2.213336 -2.454393
C 1.361846 -0.907325 -4.125777
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C 4.387514 0.454638 -0.447533
Ti 0.139591 0.792779 -0.425347
C 1.020461 2.261402 0.339215
C 1.593477 3.583798 0.815802
C 0.593972 4.722607 0.578308
C 2.899223 3.936368 0.080694
C 1.881340 3.464742 2.321838
C -0.076276 1.719702 -2.148281
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H -1.282212 -5.324853 1.052227
H -4.437378 -2.424869 1.216842
H -4.737251 2.407650 -1.952908
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H -2.818943 -1.484710 -1.608729
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H 2.349949 -0.622716 -4.516223
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 H 0.527890 2.346875 -2.823059
 H -1.115780 1.692469 -2.514697
 C 2.452105 -1.977854 -0.123104
 H 3.467845 -2.376385 -0.264074
 H 1.760041 -2.807087 -0.326770
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 H -3.967103 -0.184321 1.594990
 C -2.450868 -1.620074 1.066541
 C 2.252166 -1.498256 1.291497
 C -2.299066 2.789943 1.991721
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 H -1.232643 2.560400 1.840295
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 H -5.817456 -0.258057 -1.739246
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 H 4.858911 -1.749752 -2.106371
 C 2.313164 -3.006642 -3.131612
 H 3.309897 -2.770746 -3.522426
 H 2.433943 -3.643428 -2.242972
 H 1.802183 -3.617877 -3.894265
 H 1.666130 1.392491 0.669433

6'-7"-TS

E: -3072.30049249 H: -3071.302330 G: -3071.432004
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 C -1.855955 -4.177328 1.287274
 C -3.216590 -3.848625 1.294022
 C -3.540802 -2.493762 1.210315
 N -0.209287 -0.863165 0.830263

P -2.509756 1.045584 -0.208312
C -3.595174 0.450341 -1.652439
C -3.724416 1.533742 -2.730280
C -2.860292 -0.742775 -2.281197
C -3.101716 2.754280 0.379888
C -4.625008 2.908640 0.464851
C -2.523167 3.824778 -0.556194
C -4.277177 -4.911958 1.413219
C 3.141829 -1.245764 2.465085
C 0.838355 -0.891403 1.781338
C 2.897059 -0.756223 3.748468
C 1.589561 -0.352580 4.046201
C 0.591619 -0.418321 3.083346
C 3.998976 -0.640711 4.768984
P 2.119712 -0.861792 -1.313021
C 3.781207 -0.043320 -1.700382
C 1.691515 -2.144759 -2.648179
C 0.248998 -2.581804 -2.355259
C 1.731963 -1.500515 -4.040004
C 3.541976 1.084104 -2.715712
C 4.249867 0.569686 -0.372815
Ti 0.082661 0.771256 -0.559344
C 0.926660 2.222214 0.299601
C 1.692360 3.477858 0.685251
C 0.739441 4.643093 1.010208
C 2.610895 3.918455 -0.462661
C 2.532658 3.180491 1.939289
C -0.090201 1.715760 -2.204400
H 0.169831 -3.485096 1.171533
H -1.550508 -5.223520 1.385521
H -4.593682 -2.201088 1.283196
H -4.368464 2.367962 -2.419054
H -4.182637 1.089412 -3.629731
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H 4.355151 0.399605 4.852206
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H 2.731139 1.751471 -2.392013
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H 4.630034 -0.193145 0.321083
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H 0.037437 4.378291 1.814732
H 0.149639 4.937315 0.129332
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H 3.119552 4.863100 -0.210297
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H 3.235139 2.352032 1.769458
H 1.887994 2.894438 2.785595
H 0.509371 2.364152 -1.000358
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H 0.254919 0.783892 -2.713726
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H 3.484456 -2.328781 0.116051
H 1.794223 -2.817741 0.005804
C -2.989876 -0.042728 1.202281
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C 2.145738 -1.328735 1.484282
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C 4.874801 -0.982899 -2.215793
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H 5.828762 -0.430956 -2.262002
H 5.032825 -1.847175 -1.552253
C 2.583304 -3.394286 -2.640508
H 3.635338 -3.174432 -2.857160
H 2.536183 -3.936977 -1.685443
H 2.228011 -4.089767 -3.419407
H 0.335212 1.808544 1.161977

7'

E: -3072.33940155 H: -3071.338033 G: -3071.466039
C -0.735728 -3.237104 1.056091
C -1.105335 -1.876270 0.983785
C -1.671180 -4.262856 1.112913
C -3.043110 -3.992159 1.116307
C -3.418179 -2.647203 1.122794
N -0.149734 -0.860473 0.855628
P -2.548618 0.969740 -0.082300
C -3.731805 0.484064 -1.488178
C -3.897797 1.636768 -2.486919
C -3.077955 -0.689928 -2.232451
C -3.045595 2.653993 0.637259
C -4.552305 2.847753 0.840348
C -2.496887 3.757772 -0.278089
C -4.067219 -5.096640 1.117238
C 3.257793 -1.501142 2.306413
C 0.955448 -0.976776 1.740325
C 3.099112 -1.053698 3.617754
C 1.835038 -0.578794 3.988559
C 0.795969 -0.543047 3.068954
C 4.248166 -1.053554 4.591561
P 2.073002 -0.775392 -1.340649
C 3.749912 0.032786 -1.716078
C 1.537157 -1.887903 -2.781508
C 0.104953 -2.321011 -2.436264
C 1.505491 -1.087958 -4.089297
C 3.488261 1.325925 -2.499666
C 4.413266 0.389226 -0.374828
Ti 0.062271 0.789389 -0.502837
C 1.090672 2.228325 0.618469
C 1.549003 3.701508 0.654796
C 0.675130 4.508814 1.623820
C 1.493509 4.373416 -0.723228
C 3.002695 3.758658 1.162122
C -0.232619 1.375964 -2.215714
H 0.324499 -3.494315 1.076173
H -1.323228 -5.299427 1.153881
H -4.481400 -2.397453 1.205461
H -4.508982 2.458336 -2.088034
H -4.410788 1.258291 -3.386744
H -2.925301 2.042034 -2.802712
H -2.159154 -0.364784 -2.736896
H -3.772311 -1.064862 -3.003081
H -2.839657 -1.531640 -1.565901
H -4.722981 3.802853 1.365270
H -4.994993 2.053668 1.460888
H -5.105853 2.898130 -0.107207
H -2.995766 3.781601 -1.254924
H -1.421577 3.627193 -0.457759

H -2.652255 4.741511 0.195537
H -3.710473 -5.978143 1.671023
H -4.299974 -5.429615 0.091571
H -5.013273 -4.771157 1.575506
H 4.230773 -1.898008 1.999007
H 1.665660 -0.227888 5.010711
H -0.185319 -0.164375 3.365395
H 3.926836 -1.368764 5.595912
H 4.682985 -0.045171 4.691585
H 5.053882 -1.728184 4.267208
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H 0.936549 -0.154889 -3.972318
H 1.017729 -1.691418 -4.872732
H 2.513110 -0.839787 -4.452495
H 2.995872 1.143607 -3.464756
H 4.444364 1.838450 -2.699264
H 2.846651 2.012191 -1.932214
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H 4.798708 -0.501528 0.140080
H 3.741508 0.908743 0.322019
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H 0.670261 4.059720 2.630297
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H 0.464425 4.422561 -1.109815
H 1.878355 5.405453 -0.671481
H 2.102673 3.834776 -1.464684
H 3.348682 4.799099 1.284718
H 3.687533 3.262220 0.455957
H 3.101443 3.250378 2.134954
H 1.951062 1.613029 0.246454
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H 0.253591 2.318864 -1.843337
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H 3.466714 -2.419360 -0.128883
H 1.759129 -2.851005 -0.203097
C -2.956647 -0.186201 1.291161
H -2.393565 0.216571 2.145916
H -4.024210 -0.155112 1.553030
C -2.492955 -1.599418 1.081374
C 2.220494 -1.476301 1.365347
C -2.362946 2.767156 2.012554
H -2.871676 2.161384 2.776163
H -1.304980 2.470276 1.979319
H -2.403622 3.814267 2.352771
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H 4.905417 -1.818009 -1.989613
C 2.388859 -3.151415 -2.969249
H 3.416280 -2.937057 -3.285693
H 2.431146 -3.771871 -2.062263
H 1.928710 -3.770974 -3.757123
H 0.956368 1.862267 1.655566

7"

E: -3072.34016654 H: -3071.337727 G: -3071.467524
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C -1.161102 -1.937819 0.768863
C -1.755917 -4.317526 0.694276
C -3.122107 -4.029246 0.776661
C -3.476580 -2.686074 0.912545
N -0.179737 -0.931787 0.714622
P -2.548327 0.985150 -0.072222
C -3.661365 0.527630 -1.547103
C -3.813651 1.721508 -2.499679
C -2.943545 -0.596817 -2.311684
C -3.163594 2.610766 0.714985
C -4.689314 2.743721 0.800805
C -2.589928 3.789699 -0.083089
C -4.162748 -5.116222 0.715569
C 3.094995 -1.687784 2.393678
C 0.853524 -1.093023 1.677099
C 2.829452 -1.335399 3.716334
C 1.546422 -0.857374 4.011663
C 0.590294 -0.738394 3.013184
C 3.877433 -1.458107 4.791208
P 2.205826 -0.678099 -1.283739
C 3.880017 0.186907 -1.444999
C 1.815858 -1.690780 -2.840267
C 0.371269 -2.183093 -2.664087
C 1.872879 -0.789948 -4.079698
C 3.656852 1.514618 -2.180992
C 4.348663 0.482080 -0.010995
Ti 0.124986 0.780183 -0.487123
C 0.963750 2.253040 0.724521
C 1.550212 3.679845 0.736220
C 0.881564 4.485093 1.867465
C 1.318306 4.419862 -0.587797
C 3.058851 3.637690 1.010926
C -0.209502 1.451248 -2.161169
H 0.248193 -3.567686 0.653338
H -1.423927 -5.357666 0.625237
H -4.533198 -2.431464 1.047080
H -4.467963 2.506307 -2.095286
H -4.271190 1.372314 -3.440286

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H -3.584045 -0.935398 -3.143465
H -2.734842 -1.471288 -1.678741
H -4.936649 3.659387 1.363992
H -5.152657 1.900930 1.335740
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H -1.495903 3.739527 -0.143957
H -2.862035 4.738153 0.409629
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H -4.418321 -5.365524 -0.328133
H -5.094480 -4.813250 1.216222
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H -0.407098 -0.362565 3.254446
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H 4.201503 -0.467232 5.148977
H 4.769879 -1.987227 4.427216
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H -0.323182 -1.338498 -2.583292
H 0.236651 -2.818347 -1.776198
H 1.278152 0.124297 -3.933751
H 1.454285 -1.333111 -4.943195
H 2.902202 -0.506303 -4.343318
H 3.304730 1.373885 -3.212078
H 4.603552 2.078835 -2.224936
H 2.916315 2.132870 -1.656999
H 5.175778 1.210425 -0.039069
H 4.726564 -0.420857 0.488316
H 3.549096 0.904691 0.613023
H 1.317837 5.494379 1.957337
H 1.002358 3.977521 2.838249
H -0.198180 4.605419 1.684464
H 0.255192 4.437809 -0.869304
H 1.664072 5.464532 -0.517387
H 1.866622 3.946259 -1.415911
H 3.464412 4.658173 1.110077
H 3.604204 3.146185 0.194483
H 3.283705 3.095155 1.943572
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H -0.648235 1.650272 -3.147109
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C -2.980551 -0.246240 1.229388
H -2.424160 0.097841 2.114152
H -4.050936 -0.218132 1.481409
C -2.537220 -1.649108 0.927895
C 2.142240 -1.576962 1.372343
C -2.621205 2.679510 2.155744

H -3.164067 2.003980 2.832467
H -1.549311 2.447140 2.231668
H -2.759710 3.702383 2.542074
C -5.046316 0.009679 -1.136145
H -5.617447 0.720365 -0.526596
H -5.636248 -0.186883 -2.047167
H -4.978656 -0.940707 -0.589605
C 4.973702 -0.621310 -2.148517
H 4.774257 -0.757616 -3.220366
H 5.931064 -0.080004 -2.063232
H 5.119785 -1.611910 -1.690915
C 2.721080 -2.913738 -3.044851
H 3.770352 -2.650534 -3.223036
H 2.682063 -3.614431 -2.197813
H 2.370235 -3.467509 -3.931798
H 1.328057 1.692772 1.608586

Modified version of the PNP ligand backbone (C)

1

E: -2992.64142314 H: -2991.719511 G: -2991.849857
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C 1.178147 1.856275 -0.475648
C 2.497454 1.379551 -0.493196
C 1.932703 4.156148 -0.329433
C 3.254535 3.709671 -0.373431
C 3.519529 2.322586 -0.453432
N 0.051159 1.069763 -0.491682
P 2.542214 -0.442841 -0.546548
C 3.105771 -0.777340 -2.296402
C 3.378729 -2.253927 -2.584038
C 2.069512 -0.214256 -3.271772
C 3.892998 -1.006295 0.600400
C 5.324779 -0.811499 0.102466
C 3.642446 -2.445279 1.060296
C 4.407598 4.681602 -0.331037
C -3.270621 2.619126 -0.085742
C -2.348464 1.591534 -0.259296
C -0.996622 1.948916 -0.362915
C -2.878865 3.976499 -0.024463
C -1.527254 4.306829 -0.133641
C -0.569288 3.298470 -0.297651
C -3.929702 5.041330 0.168717

P -2.623869 -0.211837 -0.380588
C -4.165434 -0.474489 0.629923
C -3.103707 -0.385860 -2.183764
C -3.043635 -1.827572 -2.690742
C -4.419464 0.296241 -2.551778
C -4.826033 -1.836729 0.426289
C -3.847661 -0.230935 2.104461
Ti 0.011349 -0.938630 0.120333
C 0.213473 -0.872160 1.920454
C 0.506112 -0.218437 3.248884
C 1.715313 -0.893030 3.919614
C -0.709731 -0.343382 4.182776
C 0.814523 1.267648 3.014698
C 0.169803 -2.939282 -0.694353
C -0.433462 -4.240299 -0.121350
C -1.882741 -4.012287 0.324451
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H 4.045436 -0.211511 -2.418745
H 4.134445 -2.687730 -1.914349
H 3.752650 -2.366044 -3.614416
H 2.463243 -2.857735 -2.498053
H 1.102321 -0.732769 -3.167208
H 2.411959 -0.355836 -4.309145
H 1.895281 0.860898 -3.120587
H 3.731363 -0.344747 1.468864
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H 5.539699 0.228098 -0.179306
H 5.548595 -1.449385 -0.765842
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H 5.081639 4.471993 0.514889
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H -1.220408 5.354923 -0.074223
H -4.677278 5.023687 -0.640637
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H -2.281756 0.168964 -2.670062
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H -3.834410 -2.457380 -2.256667
H -2.077937 -2.301525 -2.467902
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H -4.439763 1.348732 -2.234234
H -5.130269 -2.009592 -0.615284
H -5.735756 -1.896888 1.044806

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H 1.526017 -1.963446 4.101663
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H -0.022318 1.766196 2.500343
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H 5.406277 -0.941275 1.910507
H 5.096087 0.005839 3.376082
H 5.000750 0.792863 1.790933
H 4.175552 -3.114274 0.689597
H 4.524283 -3.338870 -1.034885
H 2.834635 -3.288000 -0.469695
H 4.140773 -1.578494 -2.689740
H 3.636438 0.065548 -2.229828
H 2.445935 -1.254254 -2.253419
H 0.730765 -4.149782 -3.887293
H 1.794854 -3.484626 -2.623911
H 1.009004 -2.394417 -3.792076
H -1.525105 -2.032866 -3.698618
H -1.742537 -3.797344 -3.818711
H -2.504912 -2.892779 -2.489229
H -0.615042 -5.341243 -2.102383
H -1.345979 -4.427532 -0.759740
H 0.413851 -4.642959 -0.823901
H -0.064982 -1.013403 -1.836949
H -0.333455 -2.220971 2.899807
H -1.239933 -3.163439 1.680847
H 0.526252 -3.312785 1.771060

6'-7'-TS

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C -2.473663 0.317460 -1.618582
C -1.723469 2.201703 -3.613103
C -3.067053 2.037065 -3.267246
C -3.423944 1.099757 -2.269602
N -0.065406 -0.126532 -1.401786
P -2.629350 -0.924046 -0.285399
C -3.175087 0.117717 1.164562
C -3.525225 -0.721977 2.393105
C -2.081494 1.140582 1.481885
C -4.018956 -2.083278 -0.710505
C -5.416703 -1.471304 -0.774055
C -3.988393 -3.314705 0.200414

C -4.149995 2.828227 -3.958681
C 3.352177 0.485067 -2.620437
C 2.352001 -0.074728 -1.831206
C 1.035123 0.352443 -2.058398
C 3.065602 1.456088 -3.608859
C 1.746385 1.875118 -3.805050
C 0.711074 1.328424 -3.036148
C 4.190840 2.009860 -4.448157
P 2.410373 -1.306763 -0.485795
C 3.675227 -2.583849 -0.955265
C 3.083971 -0.316418 0.951501
C 3.141498 -1.105667 2.260029
C 4.407418 0.391664 0.669903
C 3.626579 -3.752342 0.033704
C 3.424320 -3.069731 -2.383927
Ti -0.153103 -1.920556 -0.209269
C -0.381906 -3.613821 -0.966168
C -0.638340 -5.072114 -1.291453
C 0.598519 -5.703299 -1.953817
C -1.824524 -5.169803 -2.267159
C -0.962349 -5.849037 -0.007195
C -0.044794 -2.602291 1.543526
H -1.451296 2.922606 -4.389612
H -4.482493 1.005428 -2.014254
H -4.074526 0.665153 0.834242
H -4.451485 -1.296456 2.253975
H -3.676736 -0.066452 3.265526
H -2.720408 -1.432364 2.642762
H -1.157838 0.649152 1.829219
H -2.417947 1.815006 2.285202
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H -5.498844 -0.689662 -1.540450
H -5.717198 -1.038778 0.193463
H -4.447321 -3.111231 1.178541
H -2.958819 -3.655689 0.375146
H -4.555662 -4.139945 -0.258504
H -4.793543 2.178308 -4.574357
H -3.726044 3.595549 -4.622311
H -4.804485 3.339308 -3.234777
H 4.391569 0.167336 -2.489103
H 1.528834 2.622405 -4.573746
H 4.968253 2.481402 -3.825647
H 3.828627 2.768043 -5.157259
H 4.683658 1.217048 -5.034139
H 4.670138 -2.109290 -0.910203
H 2.295999 0.451345 1.054755
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H 4.019775 -1.768734 2.292363
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H 4.341889 1.070478 -0.191432
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H 4.138908 -3.868098 -2.639825
H 3.531854 -2.266354 -3.125613
H 2.411155 -3.487893 -2.483484
H 0.423107 -6.767909 -2.181057
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H 0.842490 -5.197973 -2.902105
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H -2.009410 -6.216193 -2.563478
H -2.743737 -4.777395 -1.809299
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H -1.833208 -5.424579 0.513989
H -0.111936 -5.832384 0.693501
H 0.200070 -3.078379 -1.775444
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H 0.055280 -3.250905 2.419246
H -0.191458 -3.491281 0.417900

6'-7"-TS

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C -2.425891 0.597025 -1.679856
C -1.567925 2.851474 -3.179915
C -2.916615 2.698985 -2.848755
C -3.325827 1.575551 -2.093629
N -0.050054 -0.043813 -1.633785
P -2.696045 -0.929834 -0.714984
C -3.786577 -0.421329 0.701638
C -4.084826 -1.621254 1.600455
C -3.138091 0.718367 1.487355
C -3.749518 -1.973177 -1.867376
C -5.180324 -1.468377 -2.047700
C -3.737135 -3.465207 -1.533482
C -3.945747 3.713152 -3.283332
C 3.427334 0.808881 -2.498742
C 2.393076 0.084500 -1.912189
C 1.084336 0.555922 -2.109693
C 3.189298 1.989419 -3.240524
C 1.881207 2.453410 -3.397418
C 0.812006 1.746444 -2.834554
C 4.355593 2.724424 -3.854098
P 2.405685 -1.456010 -0.928115
C 3.010088 -2.719945 -2.154224

C 3.716846 -1.262233 0.383698
C 3.481074 -2.226613 1.550332
C 5.162554 -1.322960 -0.108845
C 3.237188 -4.084075 -1.509854
C 2.007867 -2.814741 -3.305834
Ti -0.147513 -1.635177 -0.176298
C -0.236847 -3.500662 0.007252
C -0.301973 -4.919892 0.530836
C -0.229354 -5.920205 -0.633149
C -1.622729 -5.134354 1.295908
C 0.868635 -5.160146 1.496024
C -0.182573 -1.354524 1.680250
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H -4.382088 1.497000 -1.819154
H -4.729009 -0.053260 0.262321
H -4.661071 -2.401722 1.082385
H -4.674377 -1.304514 2.475406
H -3.148660 -2.072882 1.966029
H -2.163762 0.403386 1.892970
H -3.787035 1.008459 2.329245
H -2.976287 1.609110 0.862678
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H -5.683192 -2.045706 -2.840002
H -5.217576 -0.411182 -2.343169
H -5.773904 -1.593998 -1.128360
H -4.246876 -3.681726 -0.582750
H -2.718350 -3.868172 -1.466576
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H -4.502578 4.119036 -2.423528
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H 4.026944 3.633960 -4.377275
H 4.888506 2.096022 -4.586098
H 3.965964 -2.334650 -2.548814
H 3.517421 -0.239245 0.748258
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H 3.680600 -3.271001 1.266837
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H 0.699281 -5.798630 -1.210808

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H 0.852731 -4.435739 2.325940
H 1.837141 -5.057903 0.984985
H -0.884454 -3.329272 -0.903408
H 0.518427 -0.506534 1.453999
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H -0.196962 -2.659878 1.170634

7'

E: -2835.52573772 H: -2834.722518 G: -2834.841768
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C 1.458446 3.917894 0.015019
C 2.811528 3.608034 -0.139378
C 3.207553 2.265074 -0.348346
N -0.102769 0.668249 -0.233227
P 2.425044 -0.580699 -0.656157
C 2.616189 -0.702408 -2.509574
C 2.954705 -2.118933 -2.972762
C 1.343248 -0.194816 -3.191486
C 3.994353 -1.196036 0.125463
C 5.293947 -0.701118 -0.509155
C 3.988058 -2.726166 0.247648
C 3.866949 4.684804 -0.083874
C -3.577836 1.817033 0.144018
C -2.538171 0.916204 -0.057531
C -1.233534 1.427912 -0.069201
C -3.334401 3.200798 0.321299
C -2.024866 3.687172 0.274496
C -0.951898 2.807516 0.074515
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C -3.982516 -1.623506 0.400882
C -2.831100 -0.868851 -2.271339
C -2.422090 -2.165944 -2.969842
C -4.248899 -0.438395 -2.640668
C -4.105944 -3.103725 0.034403
C -3.914441 -1.426788 1.916408
Ti 0.035506 -1.401821 0.141688
C -0.228342 -1.569141 2.235495
C 0.784017 -1.211805 3.337540
C 1.911179 -2.250004 3.363544
C 0.084647 -1.204718 4.707696

C 1.377632 0.179406 3.082822
C 0.167838 -3.044041 -0.670486
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H 4.272890 2.063287 -0.481336
H 3.447288 -0.025174 -2.771326
H 3.959211 -2.434670 -2.658878
H 2.928910 -2.164367 -4.073179
H 2.227081 -2.847915 -2.584736
H 0.485652 -0.846260 -2.957623
H 1.479083 -0.201860 -4.284565
H 1.086154 0.831418 -2.892378
H 3.917957 -0.774502 1.143189
H 6.155281 -1.099742 0.050438
H 5.381092 0.393014 -0.504927
H 5.394603 -1.045998 -1.549711
H 4.290452 -3.205897 -0.694222
H 2.996514 -3.122987 0.508221
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H 3.419430 5.680346 0.047820
H 4.468100 4.710349 -1.007030
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H -4.866093 -1.084220 0.019160
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H -4.327612 -0.296662 -3.730294
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H -3.782423 -0.370784 2.194955
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H 2.456964 -2.262531 2.409258
H 1.514487 -3.265112 3.528915
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H -0.726353 -0.459035 4.732124
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H 0.589441 0.946709 3.018948
H 1.939154 0.212910 2.136731
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H 0.163392 -3.475780 0.368527

H -1.053666 -0.823742 2.263268

7"

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C 2.950494 3.529487 0.560845
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C 1.991057 0.472393 -3.100506
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C 5.441350 -0.755204 -0.213274
C 4.012295 -2.753468 0.374190
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C -1.141127 1.475107 0.060199
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C -1.862566 3.745396 0.530618
C -0.824519 2.822622 0.364977
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C -3.010989 -0.749072 -2.333800
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C -4.152218 0.192091 -2.710690
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Ti 0.070537 -1.390573 -0.313145
C 0.202024 -2.661919 1.377628
C 0.287257 -2.083123 2.802955
C 1.558343 -1.239546 2.964628
C 0.319009 -3.223657 3.833949
C -0.933687 -1.198638 3.083475
C 0.069074 -2.422497 -1.830644
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H 4.401390 1.992540 0.146256
H 3.999157 0.323622 -2.345446
H 4.256771 -2.139861 -2.595024
H 3.598097 -1.472312 -4.098926
H 2.518921 -2.308680 -2.951572
H 1.045855 -0.092828 -3.103830
H 2.294193 0.628816 -4.148083
H 1.800870 1.461028 -2.657859

H 3.954970 -0.836132 1.332163
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H 3.062363 -3.099112 0.803440
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H 1.037653 -3.367907 1.202803
H 0.020450 -2.609549 -2.911804
H 0.176825 -3.374463 -1.251795
H -0.713213 -3.283231 1.277476

Modified version of the PNP ligand backbone (D)

1

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C -0.553571 -3.289092 0.321654
C 1.842297 -4.563600 -0.477153
C 0.663489 -5.295168 -0.451587
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C 5.081873 -1.313479 0.343925
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C 2.123686 2.002124 -2.970962
C 4.083753 2.614462 -1.488800
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Ti -0.543989 0.520322 0.141507
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C -1.401163 1.119069 3.247953
C -2.847538 1.542274 3.555462
C -0.455854 2.106921 3.953720
C -1.145806 -0.286121 3.812907
C -1.703927 1.432049 -1.492951
C -2.076177 2.884339 -1.879591
C -0.993749 3.490193 -2.772695
C -3.397100 2.884377 -2.670842
C -2.266637 3.760977 -0.635864
H 2.787169 -5.046323 -0.742864
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H -4.169616 -1.814561 -3.457422
H -3.640018 -0.262483 -2.782308
H -1.214255 -1.213274 -2.900548
H -1.901788 -2.712814 -3.556219
H -0.836302 -2.777580 -2.140133
H -3.639491 -0.844939 1.850534
H -5.888873 -1.793566 1.455873
H -4.650926 -3.002755 1.087801
H -5.493329 -2.159614 -0.230788
H -5.010323 0.494324 -0.550828
H -3.891792 1.256701 0.604484
H -5.471970 0.657964 1.154045
H 1.627766 -7.154525 -1.001389
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C -3.512398 0.783284 3.083018
C -1.374188 1.974474 2.565098
C -4.328390 0.186870 -0.113149
C -5.419051 1.231808 0.129736
C -4.723723 -1.192533 0.409023
C -0.245090 6.561286 -0.302022
C 4.297809 0.226606 -0.999238
C 2.948746 -0.108311 -0.920763
C 2.008520 0.936653 -0.719614
C 4.789838 1.544296 -0.899650
C 3.869226 2.566014 -0.724189
C 2.503975 2.264100 -0.647916
C 6.270563 1.807620 -0.992881
P 1.652033 -2.030108 0.560540
C 1.905198 -3.870463 0.640253
C 2.705437 -1.307961 1.921052
C 1.936783 -1.135702 3.232222
C 4.051300 -2.004633 2.111370
C 1.382550 -4.486912 1.937906
C 1.306228 -4.551734 -0.587240
Ti -0.618823 -0.845021 0.054751
C -1.263764 -1.733055 -1.404121
C -1.961221 -2.704731 -2.330280
C -0.966921 -3.210615 -3.391763
C -3.123672 -1.996262 -3.050297
C -2.520335 -3.900499 -1.548132
C -1.383996 -1.947447 1.731490
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H -2.151617 4.662077 -0.577583
H -3.328139 2.535134 1.836347
H -4.546025 0.550237 2.795491
H -3.557570 1.350067 4.026569
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H -0.766989 1.068913 2.729560
H -1.471800 2.484623 3.536767
H -0.819040 2.641679 1.894348

H -4.188911 0.091725 -1.203466
H -6.350064 0.917046 -0.367922
H -5.157306 2.222103 -0.270792
H -5.648074 1.351904 1.198936
H -4.902047 -1.194156 1.494439
H -3.942847 -1.932957 0.192860
H -5.654649 -1.524675 -0.077965
H 0.714891 7.096843 -0.274136
H -0.796881 6.821143 0.616099
H -0.825284 6.959505 -1.150022
H 5.018477 -0.583950 -1.149659
H 4.202300 3.605671 -0.657345
H 6.823692 1.294629 -0.189296
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H 6.685035 1.449736 -1.949090
H 2.999799 -4.006066 0.607897
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H 1.610433 -2.092620 3.666513
H 1.043659 -0.509895 3.091471
H 3.941927 -3.004854 2.559221
H 4.687888 -1.411292 2.786790
H 4.597827 -2.112246 1.161976
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H 0.301530 -4.326000 2.060443
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H 0.222985 -4.377871 -0.643614
H -1.451956 -3.920375 -4.083026
H -0.114548 -3.724259 -2.923966
H -0.570052 -2.375969 -3.992066
H -2.775139 -1.094123 -3.578218
H -3.590957 -2.662413 -3.795158
H -3.904010 -1.695278 -2.336050
H -3.043396 -4.600592 -2.220381
H -3.235110 -3.575901 -0.778197
H -1.721146 -4.459250 -1.040121
H -0.742392 -0.915308 -1.983423
H -0.855075 -1.801074 2.690153
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C 2.558029 -1.555591 -0.978967
H 1.861109 -1.752785 -1.810003
H 3.445276 -2.190049 -1.127027
C -2.313901 2.036938 -0.852613
H -3.177707 2.714693 -0.915370
H -2.257919 1.491039 -1.810635
H -1.232152 -3.001674 1.430848

6'-7'-TS

E: -2914.03004367 H: -2913.171054 G: -2913.290850
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C 0.796616 2.093394 -0.600379
C -0.322607 2.960709 -0.703696
C 2.267413 4.084210 -0.502626
C 1.166300 4.926716 -0.520776
C -0.107782 4.334399 -0.642756
N 0.866146 0.701526 -0.596832
P -2.292510 1.341550 0.428634
C -2.175113 2.308521 2.023413
C -3.076107 1.711177 3.108504
C -0.728908 2.361354 2.527261
C -4.101197 1.208370 -0.002815
C -4.893366 2.506206 0.166863
C -4.812146 0.015247 0.633120
C 1.300430 6.425419 -0.438681
C 4.319002 -0.768617 -0.945326
C 2.928451 -0.795741 -0.884242
C 2.233130 0.430720 -0.693543
C 5.091133 0.407471 -0.853981
C 4.415940 1.608320 -0.704088
C 3.017100 1.615178 -0.638967
C 6.594115 0.336133 -0.936854
P 1.134328 -2.337394 0.490707
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C 1.442954 -1.598211 3.207690
C 3.382040 -2.877034 2.162862
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C 0.134532 -4.663172 -0.676960
Ti -0.836053 -0.770125 0.156717
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C -2.740781 -2.195643 -2.245221
C -1.939061 -2.938795 -3.327149
C -3.639559 -1.154476 -2.936703
C -3.629335 -3.196414 -1.491574
C -1.780375 -1.800312 1.421643
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H -0.980589 4.992123 -0.713568
H -2.512018 3.336509 1.803793
H -4.144929 1.788910 2.870995
H -2.914144 2.244390 4.058614
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H -0.338873 1.348763 2.725246
H -0.686545 2.917683 3.477228
H -0.047062 2.852425 1.822853
H -4.022991 1.001821 -1.082876
H -5.895951 2.388857 -0.274585
H -4.418569 3.363081 -0.333004

H -5.035510 2.770779 1.225376
H -5.012775 0.173069 1.702945
H -4.213642 -0.900362 0.540356
H -5.783113 -0.150827 0.139254
H 0.836596 6.822206 0.479479
H 0.808716 6.924475 -1.289264
H 2.355774 6.734541 -0.436102
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H 4.968121 2.551207 -0.650364
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H 7.048914 1.332277 -0.835098
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H 1.926895 -4.593722 0.502188
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H 0.724322 -0.780310 3.051574
H 3.033670 -3.849086 2.545140
H 4.081015 -2.464316 2.907655
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H 0.622871 -4.371371 -1.618561
H -0.884744 -4.250719 -0.680106
H -2.612785 -3.439808 -4.041233
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H -1.306787 -2.240438 -3.898987
H -3.037427 -0.366405 -3.415438
H -4.261667 -1.626604 -3.715511
H -4.316767 -0.678059 -2.213129
H -4.339956 -3.683099 -2.178527
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H -3.030152 -3.986477 -1.013010
H -0.807947 -1.227315 -1.760883
H -1.644231 -0.901096 2.078087
H -2.065615 -1.910468 -0.011893
C 2.238956 -2.125964 -0.966583
H 1.583652 -2.184209 -1.851768
H 2.976370 -2.939477 -1.048333
C -1.720734 2.463628 -0.904871
H -2.409140 3.312197 -1.028593
H -1.783536 1.846914 -1.818255
H -2.399127 -2.560746 1.907584

6'-7"-TS

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C -0.242788 3.026586 -0.640762
C 2.398495 4.035096 -0.459727
C 1.334122 4.922434 -0.432085
C 0.034215 4.387289 -0.545716
N 0.856614 0.716179 -0.600380
P -2.268585 1.381291 0.378322
C -2.151524 2.227313 2.041130
C -3.046032 1.549854 3.082446
C -0.704265 2.252279 2.543460
C -4.076982 1.342235 -0.076842
C -4.825407 2.645286 0.214381
C -4.835972 0.125373 0.445250
C 1.532143 6.411597 -0.314534
C 4.238413 -0.889684 -1.026118
C 2.849572 -0.861263 -0.932079
C 2.209045 0.390981 -0.720612
C 5.058947 0.253278 -0.939207
C 4.437098 1.478238 -0.754457
C 3.041281 1.541749 -0.661757
C 6.555554 0.121599 -1.057085
P 1.102347 -2.354067 0.545657
C 0.784954 -4.184708 0.634754
C 2.295890 -1.967060 1.923039
C 1.579051 -1.584555 3.219541
C 3.376869 -3.023231 2.138156
C 0.026317 -4.581385 1.900896
C 0.060008 -4.676320 -0.616279
Ti -0.879159 -0.695116 0.146172
C -1.818097 -1.447757 -1.283920
C -2.769807 -2.145068 -2.238969
C -1.966287 -2.891192 -3.319382
C -3.661307 -1.100635 -2.934078
C -3.658508 -3.147402 -1.489414
C -2.005831 -1.550626 1.400791
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H -0.809702 5.084274 -0.583722
H -2.492083 3.267161 1.894344
H -4.115910 1.642985 2.853060
H -2.882951 2.012614 4.068956
H -2.809918 0.477228 3.168119
H -0.305940 1.230080 2.655812
H -0.663917 2.725903 3.537394
H -0.029014 2.808470 1.882014
H -4.004994 1.234282 -1.172351
H -5.823647 2.609372 -0.250239
H -4.313509 3.531979 -0.186779

H -4.976373 2.803199 1.292794
H -4.977939 0.157514 1.535034
H -4.300752 -0.800785 0.208117
H -5.834946 0.080922 -0.018315
H 2.599388 6.676891 -0.322074
H 1.099807 6.803749 0.620825
H 1.047967 6.951799 -1.144069
H 4.720033 -1.860759 -1.182581
H 5.029194 2.396296 -0.696129
H 6.848602 -0.306625 -2.029508
H 6.966898 -0.539912 -0.277181
H 7.052934 1.097726 -0.960869
H 1.784361 -4.651884 0.658808
H 2.787377 -1.054310 1.549178
H 2.315311 -1.269163 3.975729
H 0.999848 -2.415285 3.649926
H 0.892861 -0.738230 3.064267
H 2.968651 -3.951551 2.568105
H 4.137527 -2.645001 2.839419
H 3.896529 -3.277246 1.201557
H 0.591588 -4.354864 2.816254
H -0.167452 -5.665855 1.897079
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H 0.622561 -4.467665 -1.538087
H -0.929358 -4.206027 -0.705697
H -2.638665 -3.400993 -4.028794
H -1.305267 -3.649923 -2.876232
H -1.338919 -2.193008 -3.896683
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H -4.287189 -1.571981 -3.710230
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C 2.106746 -2.164485 -0.984550
H 1.389004 -2.190881 -1.820949
H 2.805228 -3.004752 -1.119330
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H -2.316223 3.490853 -0.892279
H -1.766275 2.076890 -1.815616
H -2.899531 -2.055239 1.782806

7'

E: -2914.07331609 H: -2913.210794 G: -2913.333239
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C 0.958209 1.947392 -0.546532
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C 2.656358 3.757559 -0.602064
C 1.666449 4.725619 -0.570748
C 0.328992 4.283560 -0.541819
N 0.884950 0.551244 -0.504992
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C -2.160620 1.181651 3.527547
C 0.035047 2.009760 2.604047
C -3.880866 1.634532 0.682911
C -4.350396 2.959547 1.290436
C -4.712842 0.463631 1.202621
C 1.980488 6.199066 -0.582783
C 4.173442 -1.285440 -0.755737
C 2.786335 -1.169867 -0.709284
C 2.215621 0.130014 -0.602971
C 5.060391 -0.190657 -0.738316
C 4.507403 1.078229 -0.686127
C 3.116571 1.226842 -0.626259
C 6.548548 -0.419230 -0.795831
P 0.692711 -2.487312 0.519350
C 0.212801 -4.284076 0.488181
C 1.622399 -2.163955 2.092490
C 0.689963 -1.859138 3.266869
C 2.668633 -3.224275 2.428278
C -0.623421 -4.725864 1.686329
C -0.506940 -4.596210 -0.825060
Ti -0.979870 -0.725026 -0.155169
C -1.443822 -0.892605 -2.193697
C -2.715619 -1.219008 -2.991510
C -2.444765 -1.036836 -4.495532
C -3.842230 -0.264529 -2.573911
C -3.166651 -2.665215 -2.755668
C -2.157699 -1.669047 0.891047
H 3.711478 4.044500 -0.633536
H -0.462736 5.039845 -0.526227
H -1.839659 3.059109 2.516072
H -3.249933 1.319757 3.554010
H -1.770931 1.479647 4.513503
H -1.963316 0.106321 3.397354
H 0.473712 1.030882 2.358190
H 0.284480 2.235535 3.653032
H 0.529642 2.758870 1.974238
H -4.045031 1.689411 -0.406909
H -5.406078 3.134436 1.029471
H -3.778980 3.826328 0.927399

H -4.286717 2.949666 2.389355
H -4.622578 0.337642 2.291257
H -4.418819 -0.485592 0.738783
H -5.776406 0.642664 0.977423
H 3.065308 6.378045 -0.562536
H 1.540976 6.714208 0.286625
H 1.579685 6.689769 -1.484758
H 4.598123 -2.292211 -0.828415
H 5.149847 1.963565 -0.694997
H 6.903134 -0.997639 0.072914
H 7.100239 0.531950 -0.808679
H 6.836107 -0.983182 -1.697969
H 1.168911 -4.835864 0.506433
H 2.154459 -1.230030 1.843537
H 1.270826 -1.458532 4.112635
H 0.158862 -2.753837 3.622791
H -0.071170 -1.112824 2.998808
H 2.207737 -4.188490 2.693935
H 3.269696 -2.898977 3.292270
H 3.365350 -3.393121 1.593409
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H 0.102027 -4.358929 -1.710289
H -1.446549 -4.028573 -0.893221
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7"

E: -2914.07331630 H: -2913.210797 G: -2913.333270
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C 0.957505 1.947807 -0.546387
C -0.057174 2.945156 -0.534960
C 2.655127 3.758474 -0.601739
C 1.664937 4.726234 -0.570126
C 0.327603 4.283781 -0.541273
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C 6.548436 -0.417256 -0.797377
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C 0.692094 -1.858261 3.267348
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Ti -0.979666 -0.725348 -0.155235
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C -2.715135 -1.220170 -2.991625
C -2.444297 -1.037946 -4.495645
C -3.842354 -0.266327 -2.574231
C -3.165222 -2.666657 -2.755659
C -2.157446 -1.669728 0.890695
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H -1.841272 3.057987 2.516229
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H 5.149168 1.965134 -0.695264
H 6.836394 -0.974590 -1.703521
H 6.902667 -1.002052 0.067193
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H 1.170714 -4.835196 0.507600
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H 0.161297 -2.753009 3.623593
H -0.069253 -1.112044 2.999647
H 2.209973 -4.187307 2.694124
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MODIFICATIONS OF CH^tBu LIGAND (OMe)

1

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6

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H -0.129192 3.724417 -2.142580
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H -4.715074 4.232052 -0.276400
H -3.794695 4.485295 -1.779281
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6'

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C -4.089221 -1.245849 -0.305288
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C -3.701595 3.481287 -0.481421
C -3.835284 1.656574 -2.217271

C -2.672593 1.304101 1.973561
C -4.128257 1.200833 2.420714
C -1.977057 2.549917 2.518289
C -5.660831 -3.204299 -0.674660
C 2.837903 -2.372523 1.309497
C 1.830516 -1.706349 0.605091
C 0.510074 -1.676601 1.102503
C 2.579618 -3.029526 2.513799
C 1.263499 -2.999004 2.998225
C 0.250520 -2.338264 2.316891
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6'-7'-TS

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C -3.861610 2.959310 -0.351574
C -3.828826 1.242113 -2.190057
C -2.519321 0.785992 1.953027
C -3.923556 0.490270 2.475330
C -1.957151 2.091984 2.515966
C -5.349745 -3.805931 -0.832943
C 3.111427 -2.250773 1.312737
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Ti 0.069579 0.714410 -0.754895
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C 0.869713 3.820441 0.225713
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C 2.052214 4.318168 -0.622262
C -0.029921 1.363722 -2.519165
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H -2.964234 1.741355 -2.654610
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7'

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7"

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MODIFICATIONS OF CH^tBu LIGAND (H)

1

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6

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C -3.602216 1.872273 -0.103409
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7'

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7"

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C 1.469070 3.888005 0.350943
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H -0.940718 0.588049 -2.734964
H 0.772122 2.397396 1.781502
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MODIFICATIONS OF CH^tBu LIGAND (CF₃)

1

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H -0.187641 -2.070519 4.011786
H 1.032324 -1.384701 2.913001
H -1.771930 -4.066200 2.963194
H -0.321343 -4.873018 2.339275
H -1.609934 -4.391515 1.217693
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H -0.614381 3.103363 -2.464092
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H 0.830909 2.329085 2.796872
H -0.253861 0.978796 3.272959

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F -4.240517 3.446738 -1.177196
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6

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C 3.014191 -2.949927 -2.055438
C 4.202643 -2.291000 -1.709863
C 4.079956 -1.104766 -0.985910
N 0.419726 -0.711938 -0.587596
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C 4.122490 2.237888 2.341983
C 3.954846 -0.281325 2.451621
C 2.892148 2.323195 -0.879762
C 4.298736 2.376517 -1.468897
C 2.438571 3.680383 -0.339823
C 5.545167 -2.846437 -2.106500
C -3.092441 -1.759380 -1.165006
C -1.894180 -1.439840 -0.528089
C -0.753267 -1.078497 -1.276022
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C -2.071051 -1.370113 -3.294005
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C -4.519188 -2.018391 -3.237458
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C 0.172010 -3.052054 2.749809
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C -3.991966 -0.143694 1.855321
Ti 0.091159 0.558495 1.028340
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C -1.522453 2.939182 -0.505741
C -1.385957 4.424450 -0.127664
C -3.020738 2.622781 -0.579780
C -0.923742 2.689066 -1.898177
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H -4.183721 0.010843 0.785982
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H 0.130463 2.996750 -1.896372
H -0.897942 2.425427 1.567053
H -0.472081 0.865619 3.624066
H 0.951549 -0.193590 3.592794
H 1.136473 1.571931 3.390622
F -3.669418 3.433869 -1.439064
F -3.265759 1.374562 -0.994964
F -3.633805 2.773616 0.604357

6'

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N -0.703907 -1.084355 0.364425
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C -3.507457 2.346279 -0.807998
C -3.134061 3.821882 -0.657713
C -3.663734 1.964926 -2.281338
C -2.343882 1.626828 1.864362
C -3.767981 1.795121 2.388718
C -1.425018 2.762622 2.310058
C -6.258416 -2.399918 -0.349012
C 2.329114 -2.950656 1.393535
C 1.440228 -2.178552 0.638600
C 0.149662 -1.886037 1.129560
C 1.980713 -3.453952 2.647596
C 0.695385 -3.159470 3.127579
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C 2.947046 -4.265719 3.469665
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C 3.591764 -1.412347 -1.220778
C 1.157316 -2.937871 -2.108520
C 0.758436 -2.482246 -3.512539
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Ti 0.103692 0.475157 -0.789780
C 1.237404 1.693988 0.015954
C 1.926166 3.027738 -0.214332
C 0.884132 4.143098 -0.428232
C 2.842255 2.972855 -1.450873
C 2.775677 3.401144 1.000810
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H -5.070471 0.062547 -0.347886
H -4.470650 2.179875 -0.296451
H -3.169788 4.157998 0.387920
H -3.839439 4.447408 -1.227378
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H -2.751901 2.197679 -2.849637
H -4.492299 2.536510 -2.728972
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 H -1.771983 3.745483 1.956911
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 H 3.642108 2.229293 -1.333399
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 H -1.042485 0.496832 -3.300441
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6'-7'-TS

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C -6.672850 -0.629342 -0.846892
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C 0.620969 -2.977303 -2.222433
C 0.713874 -2.444302 -3.652186
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C 3.889590 -1.488319 0.261011
Ti 0.248516 0.450978 -0.766186
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C 2.691562 2.703111 -0.309267
C 2.048053 4.037019 -0.715069
C 3.817734 2.348517 -1.300118
C 3.314038 2.871602 1.079516
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H -5.206158 -2.898016 -0.407884
H -4.841155 1.374759 -0.533576
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H -0.865871 4.385297 -0.540912
H -1.743025 2.998547 -2.595387
H -3.310061 3.846237 -2.580389
H -3.257395 2.073979 -2.451725
H -1.808372 0.791217 2.287512
H -3.278766 2.298710 3.598725
H -4.100663 1.787913 2.110264
H -3.405449 3.426957 2.237818
H -0.748349 3.678156 2.302045
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H 2.341031 -4.015171 1.025048

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 C -5.113597 1.405526 0.138126
 C -4.440923 0.184208 0.159242
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 C -2.311461 -4.014893 1.044787
 C -3.331048 -2.155439 2.393315
 C -2.258974 -1.950078 -1.828379
 C -3.693908 -2.196780 -2.287627

C -1.337727 -3.095691 -2.249800
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C 1.124071 2.451973 -0.542145
C -0.161614 2.079292 -0.996258
C 1.445976 3.956492 -2.437666
C 0.177679 3.568397 -2.896778
C -0.607699 2.658291 -2.204612
C 2.280214 4.947428 -3.206429
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C 3.888250 0.945890 2.402689
C 4.032657 0.980805 -0.112495
Ti 0.171772 -0.499817 0.751236
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C 2.410061 -2.920083 0.136088
C 1.649731 -4.237637 0.389553
C 3.512819 -2.751578 1.191472
C 3.063751 -3.010785 -1.246463
C 0.085592 -1.245449 2.471534
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H -5.023040 -0.732226 0.296857
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H -2.386497 -1.977059 2.928485
H -3.912585 -2.901003 2.959004
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H -1.889561 -1.029909 -2.315451
H -3.717434 -2.344967 -3.379247
H -4.357569 -1.351772 -2.055585
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H 2.500316 4.585399 -4.223673
H 3.241436 5.136985 -2.707024
H 3.776431 2.708924 1.158019
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H 0.335805 2.961875 4.365573

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H 1.332761 4.685939 1.108642
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H 1.218171 -4.211126 1.400448
H 3.050547 -2.641738 2.183615
H 4.178139 -3.627056 1.218105
H 4.118315 -1.855366 1.001684
H 0.976761 -1.778995 1.509584
H 0.168593 -1.919939 3.329066
H -0.159901 -0.195481 2.778687
H 0.805803 -1.660182 -0.734529
F 2.155671 -3.164432 -2.224297
F 3.898313 -4.058925 -1.334769
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7'

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C -0.093726 4.716497 -0.963345
C 1.302749 4.762860 -1.081875
C 2.016066 3.609479 -0.749248
N -0.645619 1.203453 0.151234
P 2.196487 0.897419 0.229990
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C 4.882873 0.001182 0.160185
C 3.933948 0.975673 -1.958723
C 2.261180 1.210371 2.075996
C 3.256723 2.292606 2.486021
C 2.396048 -0.061363 2.911949
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C -2.808461 0.286913 0.706041
C -1.789273 1.229975 0.952329
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C -2.787838 -0.163753 -3.528037
C -4.703708 0.507864 -2.007825
C -3.566543 -3.116876 -1.806737
C -3.193838 -3.046955 0.685327
Ti 0.188042 -0.499319 -0.685687
C 0.258108 -2.611571 -0.261508
C 1.433715 -3.598917 -0.376138
C 2.260224 -3.333590 -1.641554
C 0.922251 -5.051369 -0.387912
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H 5.907058 0.206169 -0.189817
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H 1.631662 -0.805372 2.646102
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