Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting information

Mechanochemical and solvent effects on ligand lability in group 4 Cp_2MXY (X,Y = Cl, OtBu) systems

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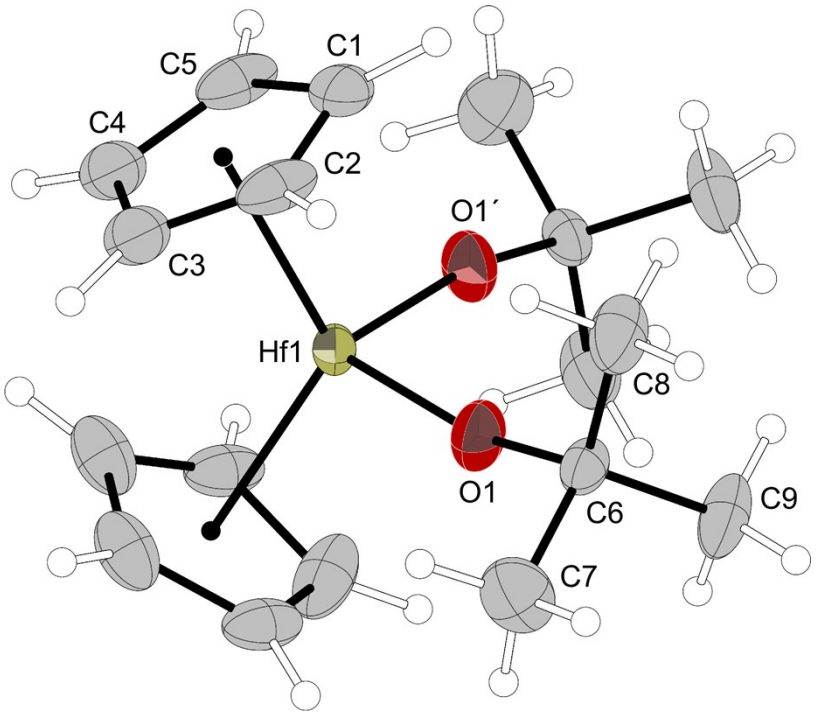
1. Figure S1. Diagram of $Cp_2Hf(OtBu)_2$ (4)



Thermal ellipsoid plot of $Cp_2Hf(OtBu)_2$, illustrating the numbering scheme used in the text. Thermal ellipsoids are shown at the 40% level; hydrogens are drawn with arbitrary radii. Selected bond distances (Å) and angles (deg): Hf–O, 1.915(7); O1–C6, 1.441(13); Hf–Cp´(ring centroid), 2.252; O1–Hf–O1´, 100.1(1); Hf–O1–C6, 166.6(4); Cp–Hf–Cp´, 123.5.

2. Coordinates of Optimized Structures

```
10
[C5H5]-; M06/def2SVPD; ΔG° = -193.18339 au
C     -1.195214    0.123217    0.000003
H     -2.284971    0.235688    0.000006
C     -0.486563   -1.098632    0.000007
H     -0.930220   -2.100335    0.000036
C      0.894539   -0.802234    0.000027
H      1.710134   -1.533678    0.000069
C     -0.252155    1.174779   -0.000013
H     -0.482121    2.245914   -0.000049
C      1.039410    0.602851   -0.000025
H      1.987076    1.152522   -0.000061

10
[C5H5]- (w/PCM,THF); M06/def2SVPD; ΔG° = -193.262988 au
C      1.192246    0.154476   -0.000024
H      2.278017    0.295717   -0.000043
C      0.221516    1.181514    0.000105
H      0.423029    2.257696    0.000190
C     -1.055409    0.575851   -0.000086
H     -2.016657    1.100114   -0.000140
C      0.515525   -1.086048   -0.000067
H      0.985090   -2.075216   -0.000123
C     -0.873885   -0.825835    0.000071
H     -1.669437   -1.578063    0.000118

1
[Cl]-; M06/def2TZVPD; ΔG° = -460.275479 au
Cl     0.000000    0.000000    0.000000

1
[Cl]- (w/PCM,THF); M06/def2TZVPD; ΔG° = -460.372818 au
Cl     0.000000    0.000000    0.000000

14
[OtBu]-; M06/def2SVPD; ΔG° = -232.654056 au
C     -0.000012    0.000044    0.145274
C     -1.339933   -0.534617   -0.431557
H     -2.162126    0.096349   -0.052650
H     -1.382592   -0.550416   -1.540425
H     -1.500729   -1.559139   -0.054476
C      0.207043    1.427598   -0.431756
H     -0.599392    2.079418   -0.054283
H      1.164921    1.823794   -0.053376
H      0.214089    1.472301   -1.540628
C      1.132939   -0.893182   -0.431443
H      2.100579   -0.520813   -0.053674
H      0.996937   -1.920837   -0.053146
H      1.168533   -0.921644   -1.540310
O     -0.000055    0.000241    1.479984

14
[OtBu]- (w/PCM,THF); M06/def2SVPD; ΔG° = -229.741039 au
C     -0.000008   -0.000125    0.133251
C      1.242111   -0.722574   -0.428476
H      1.262495   -1.761949   -0.059843
H      1.271814   -0.746407   -1.534190
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H      2.155805  -0.219136   -0.069573
C     -1.246132  -0.713650   -0.430897
H     -1.271898  -1.754207   -0.065988
H     -2.156927  -0.206523   -0.069726
H     -1.276665  -0.733723   -1.536628
C      0.005662   1.435469   -0.430786
H     -0.884516   1.976324   -0.068539
H      0.898176   1.971248   -0.065943
H      0.007415   1.471980   -1.536541
O     -0.001937   0.000959    1.493553

23
[Cp2TiCl2]; M06/def2TZVPD(Ti,Cl);def2SVP(C,H); ΔG° = -2156.375752 au
C     -1.519159   1.479284   -0.945706
H     -1.206648   2.099228   -1.784252
C     -2.157176   0.223039   -1.039089
C     -1.404520   1.805226    0.434167
H     -2.368253  -0.314315   -1.959010
C     -2.371321  -0.258234    0.263706
H     -0.981876   2.721345    0.841231
C     -1.915898   0.727980    1.177700
H     -2.765228  -1.237074    0.527924
H     -1.919859   0.639429    2.262085
C      2.372327  -0.259799   -0.251073
C      1.921487   0.716145   -1.177970
H      1.931015   0.615825   -2.261244
C      1.404669   1.800707   -0.449051
H      0.982809   2.711576   -0.868494
C      2.151668   0.235917    1.045485
H      2.359028  -0.290927    1.972333
C      1.514106   1.490721    0.935161
H      1.197274   2.119775    1.765154
Ti    -0.000053  -0.046451   -0.000293
Cl     0.0429800 -1.606823   -1.730051
Cl    -0.041320  -1.603021    1.733183
H      2.767582  -1.241488   -0.502540

23
[Cp2TiCl2]; (w/PCM,THF);M06/def2TZVPD(Ti,Cl);def2SVP(C,H); ΔG° = -2156.385781 au
C      1.509054  -1.491381   -0.944677
H      1.197811  -2.114399   -1.781333
C      2.147116  -0.234740   -1.040285
C      1.395690  -1.815628    0.435714
H      2.367805   0.295745   -1.962035
C      2.362134   0.249069    0.262327
H      0.974990  -2.731553    0.844441
C      1.905887  -0.736359    1.177890
H      2.770433   1.222783    0.524067
H      1.915447  -0.652803    2.262760
C     -2.362720   0.248496   -0.258308
C     -1.907398  -0.733359   -1.178047
H     -1.918870  -0.646031   -2.262586
C     -1.394770  -1.814699   -0.440570
H     -0.974286  -2.728982   -0.853177
C     -2.145217  -0.239782    1.042316
H     -2.365045   0.287138    1.966313
C     -1.506494  -1.495549    0.941243
H     -1.193261  -2.121319    1.775062
Ti     0.000075   0.034162   -0.000224
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Cl    -0.044005   1.636038   -1.730308
Cl     0.042564   1.634461    1.731589
H     -2.771878   1.222950   -0.515974

36
[Cp2Ti(OtBu)Cl]; M06/def2TZVPD(Ti,Cl);def2SVP(C,O,H); ΔG° = -1928.803642
au
C     -1.352748  -1.472720   -1.657044
H     -1.349411  -1.151514   -2.697511
C     -0.318107  -2.181833   -1.006508
C     -2.428932  -1.332232   -0.734151
H      0.652842  -2.416282   -1.435211
C     -0.700012  -2.386810    0.325629
H     -3.384820  -0.853689   -0.935693
C     -2.017050  -1.867703    0.491611
H     -0.085125  -2.815671    1.114448
H     -2.580627  -1.858181    1.421913
C     -0.181337   2.388794   -0.073102
C     -0.458584   1.931853   -1.382979
H      0.244824   1.898181   -2.213417
C     -1.792180   1.471527   -1.407410
H     -2.310795   1.067655   -2.274388
C     -1.338903   2.207768    0.706211
H     -1.430805   2.423276    1.766786
C     -2.334309   1.624316   -0.106964
H     -3.337252   1.347468    0.212917
Ti    -0.564332   0.003654    0.018124
Cl    -0.429865  -0.069554    2.384467
H      0.777789   2.751654    0.290451
O      1.214050  -0.058236   -0.231832
C      2.612229  -0.037286   -0.179185
C      3.135993  -1.422616   -0.537840
H      2.859130  -1.688824   -1.569621
H      4.233146  -1.457609   -0.461552
H      2.718874  -2.175073    0.148616
C      3.022828   0.327047    1.240665
H      4.119609   0.342127    1.333920
H      2.633683   1.318170    1.514992
H      2.613594  -0.402144    1.954433
C      3.127068   0.994870   -1.173775
H      2.765546   2.000979   -0.915411
H      4.227300   1.018803   -1.175269
H      2.787362   0.748736   -2.191371

36
[Cp2Ti(OtBu)Cl];(w/PCM,THF);M06/def2TZVPD(Ti,Cl);def2SVP(C,O,H); ΔG° = -1928.812852 au
C     -1.311752  -1.464232   -1.678013
H     -1.254386  -1.151319   -2.719397
C     -0.323987  -2.192435   -0.976184
C     -2.425515  -1.291415   -0.806699
H      0.657637  -2.457229   -1.360580
C     -0.769385  -2.375345    0.339520
H     -3.360039  -0.794416   -1.056841
C     -2.080862  -1.822362    0.441839
H     -0.201026  -2.820958    1.153768
H     -2.691357  -1.796193    1.341973
C     -0.142194   2.375278   -0.033458
C     -0.345574   1.927709   -1.360272
H      0.404819   1.890207   -2.148141
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C     -1.681759    1.485428   -1.468886
H     -2.151732    1.092628   -2.367935
C     -1.350804    2.210756    0.671235
H     -1.508766    2.434711    1.722379
C     -2.302454    1.645098   -0.203937
H     -3.328017    1.384286    0.050674
Ti    -0.566721    0.004812    0.019131
Cl    -0.514813   -0.057834    2.430466
H      0.796695    2.727642    0.389234
O      1.216180   -0.103950   -0.143521
C      2.617213   -0.062572   -0.157949
C      3.140594   -1.446276   -0.521820
H      2.832636   -1.724253   -1.541376
H      4.239850   -1.469047   -0.481497
H      2.752904   -2.196810    0.184113
C      3.082111    0.324140    1.239123
H      4.181143    0.362161    1.282806
H      2.687073    1.311360    1.519021
H      2.724573   -0.410425    1.975111
C      3.078733    0.963213   -1.183961
H      2.726554    1.971306   -0.921035
H      4.177627    0.989256   -1.232630
H      2.697840    0.704104   -2.183519

49
[Cp2Ti(OtBu)2]; M06/def2TZVPD(Ti);def2SVP(C,O,H); ΔG° = -1701.227549 au
Ti    -0.021069   -0.662061    0.007849
C      1.170985   -1.967815   -1.651645
H      2.178628   -2.312071   -1.421494
C     -0.038949   -2.658742   -1.374933
C      0.831538   -0.768438   -2.313758
H     -0.123342   -3.633070   -0.898892
C     -1.109656   -1.858734   -1.808118
H      1.526994    0.004246   -2.631000
C     -0.566300   -0.683737   -2.388988
H     -2.169016   -2.074508   -1.677208
H     -1.133278    0.160889   -2.774954
C      0.917558   -2.420288    1.394111
H      1.512422   -3.201629    0.925506
C      1.408284   -1.213895    1.913937
C     -0.494554   -2.432602    1.576408
H      2.446595   -0.889362    1.897056
C      0.310884   -0.478054    2.432344
H     -1.178223   -3.224223    1.274298
C     -0.849263   -1.249280    2.253338
H      0.353608    0.528438    2.845883
H     -1.863007   -0.937017    2.490639
O      1.077247    0.794556   -0.068322
O     -1.636779    0.193198    0.093947
C      2.206234    1.615932   -0.055097
C     -2.477871    1.304867    0.045113
C      1.989533    2.745206   -1.058407
H      2.877399    3.392859   -1.118628
H      1.790903    2.337305   -2.060658
H      1.130114    3.362788   -0.762572
C      3.444044    0.812114   -0.444985
H      4.344865    1.441939   -0.393433
H      3.586616   -0.042252    0.232121
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H     3.360115   0.427807  -1.471515
C     2.385560   2.201790   1.343060
H     2.590660   1.413203   2.081376
H     3.224952   2.913342   1.364816
H     1.473679   2.736563   1.647970
C    -1.669293   2.538740  -0.330723
H    -2.309675   3.433656  -0.361992
H    -0.868305   2.700841   0.405659
H    -1.201128   2.408029  -1.317802
C    -3.567368   1.043284  -0.989304
H    -3.131829   0.922299  -1.991975
H    -4.113851   0.122585  -0.735412
H    -4.287402   1.875186  -1.027774
C    -3.105787   1.496828   1.422057
H    -3.689658   0.607356   1.703646
H    -2.322615   1.658101   2.178634
H    -3.779912   2.366965   1.433564

49
[Cp2Ti(OtBu)2];(w/PCM,THF);M06/def2TZVPD(Ti);def2SVP(C,O,H);ΔG° = -1701.231317
au
Ti   -0.016279  -0.662260   0.008803
C     1.188767  -1.938475  -1.662363
H     2.207867  -2.251628  -1.437657
C     0.003044  -2.664652  -1.372310
C     0.807018  -0.749062  -2.322297
H    -0.047487  -3.639321  -0.892196
C    -1.096188  -1.895972  -1.792620
H     1.476162   0.044441  -2.645695
C    -0.593966  -0.706415  -2.383185
H    -2.147044  -2.146420  -1.652174
H    -1.190555   0.119554  -2.765451
C     0.957292  -2.405711   1.388209
H     1.568470  -3.170685   0.913459
C     1.423057  -1.192045   1.915488
C    -0.454961  -2.449010   1.571202
H     2.454486  -0.846050   1.898305
C     0.310417  -0.480971   2.436592
H    -1.121642  -3.252720   1.262511
C    -0.834569  -1.275541   2.252358
H     0.331452   0.524137   2.855800
H    -1.854618  -0.985316   2.491645
O     1.067288   0.801379  -0.072821
O    -1.640855   0.181097   0.104433
C     2.192115   1.633052  -0.059545
C    -2.485941   1.291805   0.050116
C     1.968392   2.758295  -1.065460
H     2.848645   3.416984  -1.114971
H     1.788001   2.348844  -2.070514
H     1.098068   3.364497  -0.777716
C     3.434020   0.836349  -0.448347
H     4.328846   1.475154  -0.404204
H     3.586942  -0.012436   0.233347
H     3.347817   0.445880  -1.472482
C     2.363235   2.223436   1.337121
H     2.576096   1.439599   2.078028
H     3.196121   2.942573   1.355949
H     1.445864   2.750911   1.639347
C    -1.696800   2.517384  -0.389471
H    -2.342718   3.408571  -0.413601
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H     -0.865883    2.700620    0.307476
H     -1.271986    2.367464   -1.393415
C     -3.608343    0.998200   -0.939321
H     -3.203743    0.837536   -1.949449
H     -4.153361    0.091786   -0.635240
H     -4.324013    1.833525   -0.985658
C     -3.067225    1.524876    1.441200
H     -3.634249    0.641835    1.773136
H     -2.259885    1.716696    2.164793
H     -3.747148    2.390612    1.445856

53
[CpTi(OtBu)3]; M06/def2TZVPD(Ti);def2SVPD(C,O,H); ΔG° = -1740.763928 au
Ti     0.057616   -0.134380    0.564218
O      1.391651   -0.800769   -0.450300
O      0.226503    1.661884    0.383246
O     -1.408819   -0.501799   -0.407879
C     -0.388854    2.746333   -0.276499
6     -0.343934    2.502567   -1.779522
H     -0.873387    1.572521   -2.031290
H     -0.814066    3.333114   -2.328346
H      0.699020    2.413603   -2.118722
C      0.393736    3.999941    0.083794
H      0.375633    4.161257    1.171838
H      1.442452    3.896885   -0.232095
H     -0.033445    4.887722   -0.407615
C     -1.828967    2.857280    0.209681
H     -2.385362    1.937632   -0.027215
H     -1.848232    3.007263    1.300305
H     -2.340159    3.709119   -0.264632
C      2.681430   -0.730957   -1.000117
C      3.241204    0.669110   -0.790093
H      2.584834    1.416437   -1.258328
H      3.308529    0.903433    0.283099
H      4.246575    0.756942   -1.229615
C      3.557533   -1.767146   -0.310284
H      3.123320   -2.771137   -0.428462
H      4.571511   -1.775121   -0.738313
H      3.641238   -1.546206    0.764643
C      2.559829   -1.036000   -2.486769
H      1.883405   -0.311114   -2.964641
H      3.540143   -0.982084   -2.984392
H      2.148877   -2.045227   -2.635944
C     -2.327543   -1.315128   -1.089572
C     -3.536842   -1.543507   -0.193971
H     -3.248370   -2.075542    0.724181
H     -3.985236   -0.578833    0.088842
H     -4.301526   -2.143227   -0.710405
C     -2.739565   -0.583284   -2.359566
H     -1.859533   -0.402704   -2.995446
H     -3.467758   -1.174804   -2.934493
H     -3.197621    0.386534   -2.113001
C     -1.642830   -2.629531   -1.437672
H     -0.745695   -2.434679   -2.043441
H     -1.330240   -3.156579   -0.523651
H     -2.317747   -3.288512   -2.004570
C      1.136542   -0.354451    2.674736
H      2.153284    0.024958    2.771426
C     -0.051024    0.380459    2.906594
C      0.768168   -1.663322    2.274455
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H     -0.103808    1.435049    3.170684
C     -1.146678   -0.453789    2.610986
H      1.451688   -2.459496    1.984614
C     -0.637778   -1.723264    2.223642
H     -2.197195   -0.164203    2.628998
H     -1.229935   -2.583048    1.913718

53
[CpTi(OtBu)3];(w/PCM,THF);M06/def2TZVPD(Ti);def2SVP(C,O,H);ΔG° = -1740.766372 au
Ti     0.003330   -0.051586    0.660908
O      1.250568   -0.395636   -0.585091
O     -0.189181    1.770908    0.646094
O     -1.498583   -0.630870   -0.151675
C     -0.702131    2.730904   -0.259212
C     -0.307796    2.382790   -1.688794
H     -0.733299    1.414352   -1.987878
H     -0.674978    3.151403   -2.386110
H      0.786629    2.327599   -1.782851
C     -0.109347    4.077677    0.128170
H     -0.368235    4.324945    1.168171
H      0.987631    4.050469    0.040298
H     -0.489614    4.878261   -0.524997
C     -2.218552    2.753738   -0.118913
H     -2.637083    1.762605   -0.349783
H     -2.500331    3.020062    0.910943
H     -2.664534    3.492807   -0.802507
C      2.525280   -0.489013   -1.171063
C      3.347256    0.718624   -0.740143
H      2.853958    1.649251   -1.058188
H      3.457488    0.742384    0.354196
H      4.351684    0.688510   -1.188140
C      3.185493   -1.785092   -0.722028
H      2.556382   -2.646133   -0.994003
H      4.166010   -1.907837   -1.205695
H      3.339641   -1.794777    0.366319
C      2.337375   -0.491938   -2.682306
H      1.827274    0.427083   -3.006094
H      3.308591   -0.551167   -3.196156
H      1.730373   -1.356827   -2.989051
C     -2.139332   -1.565216   -0.990822
C     -3.535599   -1.811712   -0.439686
H     -3.481089   -2.221076    0.579893
H     -4.101861   -0.868950   -0.405565
H     -4.087120   -2.525807   -1.069954
C     -2.216396   -0.967665   -2.388805
H     -1.205271   -0.780064   -2.780873
H     -2.733302   -1.652787   -3.077664
H     -2.768813   -0.016120   -2.368396
C     -1.331877   -2.856385   -1.014993
H     -0.307060   -2.657713   -1.364184
H     -1.282123   -3.303186   -0.010850
H     -1.795201   -3.590268   -1.691590
C      1.555047   -0.712499    2.376872
H      2.624396   -0.648219    2.182311
C      0.751740    0.308041    2.921309
C      0.720470   -1.825761    2.091180
H      1.082319    1.311135    3.183772
C     -0.584485   -0.160185    2.962469
H      1.036394   -2.758833    1.624947
C     -0.597065   -1.487263    2.468882
H     -1.453850    0.413585    3.281595
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H    -1.481181  -2.109276    2.340797

57
[Ti(OtBu)4]; M06/def2TZVP(Ti);def2SVP(C,O,H); ΔG° = -1780.275483 au
Ti   -0.069741  -0.015819  -0.223398
O    -1.432051  -0.275311  -1.381809
O    -0.617561  -0.367809   1.453569
O     0.474165   1.700293  -0.301915
O     1.281807  -1.126634  -0.620041
C    -2.816098  -0.007240  -1.490481
C     2.428810  -1.394181  -1.396187
C     0.949470   2.762718   0.502790
C    -0.533453  -1.358411   2.463324
C     0.880656  -1.356040   3.025650
H     1.610161  -1.556055   2.225225
H     1.112631  -0.381359   3.480123
H     0.993452  -2.130054   3.799892
C    -1.543484  -0.994259   3.538807
H    -1.325149   0.006292   3.940740
H    -2.561323  -0.985745   3.122008
H    -1.513439  -1.717476   4.367806
C    -0.859972  -2.711642   1.846068
H    -0.840627  -3.504003   2.609558
H    -1.861600  -2.693576   1.391561
H    -0.124679  -2.965504   1.066927
C    -3.570513  -1.031802  -0.655648
H    -3.339004  -2.049331  -1.004312
H    -3.278588  -0.948646   0.402586
H    -4.657777  -0.875869  -0.729741
C    -3.192069  -0.124928  -2.958444
H    -4.267222   0.060819  -3.104963
H    -2.627044   0.605214  -3.555810
H    -2.957352  -1.132355  -3.331432
C    -3.086763   1.400858  -0.977692
H    -2.819007   1.479112   0.088292
H    -2.490775   2.132240  -1.543558
H    -4.151490   1.660935  -1.081545
C     2.789236  -2.855991  -1.185136
H     2.984850  -3.048337  -0.119336
H     1.959505  -3.501807  -1.507562
H     3.687570  -3.128543  -1.759253
C     2.088799  -1.119406  -2.853700
H     1.240938  -1.744703  -3.169854
H     1.806975  -0.062583  -2.985917
H     2.947343  -1.333622  -3.508247
C     3.553100  -0.485400  -0.923116
H     4.479367  -0.679599  -1.484855
H     3.274741   0.569962  -1.067317
H     3.752285  -0.652904   0.146637
C     1.565614   3.797103  -0.424829
H     1.943284   4.660285   0.144596
H     2.403371   3.356520  -0.985322
H     0.817080   4.155016  -1.146279
C     1.992138   2.221944   1.471747
H     2.394930   3.027527   2.104656
H     1.544524   1.460555   2.128144
H     2.827349   1.765050   0.921200
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C    -0.228960   3.350501   1.264918
H     0.095950   4.187262   1.902116
H    -0.989932   3.723573   0.564001
H    -0.686935   2.582470   1.907134

57
[Ti(OtBu)4];(w/PCM,THF);M06/def2TZVPD(Ti);def2SVP(C,O,H);ΔG° = -1780.283087au
Ti   -0.032362  -0.035892   0.420563
O    -0.123335  -1.656958  -0.356220
O     1.437427   0.102584   1.465166
O    -1.483761   0.259090   1.467223
O     0.034261   1.149746  -0.919152
C    -0.180225  -2.301438  -1.618340
C     0.277016   2.439189  -1.441437
C    -2.893555   0.128393   1.411740
C     2.808558  -0.253311   1.495669
C     3.458428   0.156325   0.181322
H     2.997559  -0.377976  -0.664129
H     3.343178   1.238690   0.019768
H     4.533480  -0.078699   0.187443
C     3.447485   0.492687   2.655816
H     3.345929   1.579061   2.513029
H     2.959283   0.219467   3.602518
H     4.518389   0.250731   2.733959
C     2.912576  -1.757867   1.696828
H     3.966061  -2.075225   1.731342
H     2.430689  -2.050226   2.641334
H     2.413639  -2.291045   0.872963
C     1.139381  -2.069181  -2.339183
H     1.302834  -0.992011  -2.496714
H     1.975165  -2.473448  -1.748272
H     1.139993  -2.566766  -3.320801
C    -1.334412  -1.713625  -2.418423
H    -1.417039  -2.206208  -3.398944
H    -2.285066  -1.857111  -1.882452
H    -1.178153  -0.636022  -2.581612
C    -0.400401  -3.783142  -1.362320
H     0.423521  -4.192792  -0.759214
H    -1.342896  -3.942864  -0.818100
H    -0.447884  -4.340886  -2.310123
C     0.664373   3.355760  -0.290392
H    -0.142246   3.381403   0.459400
H     1.581372   2.991706   0.197704
H     0.841313   4.381660  -0.646064
C     1.404611   2.331510  -2.456214
H     2.317414   1.947948  -1.977905
H     1.119710   1.648307  -3.270764
H     1.629174   3.315731  -2.893892
C    -0.999093   2.921543  -2.113179
H    -0.847917   3.910104  -2.571867
H    -1.303168   2.215780  -2.900881
H    -1.815852   2.999256  -1.381322
C    -3.244641  -1.351774   1.378806
H    -4.335687  -1.493995   1.343977
H    -2.800991  -1.832079   0.493397
H    -2.856313  -1.856225   2.275938
C    -3.404563   0.827396   0.160265
H    -4.502573   0.776104   0.104110
H    -3.105920   1.886483   0.170077
H    -2.991680   0.355674  -0.745490
C    -3.463764   0.786888   2.657564
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H     -4.561632    0.709439    2.672873
H     -3.068392    0.301768    3.561923
H     -3.190711    1.852075    2.687138

45
[Cp3Ti(OtBu)]; M06/def2TZVP(Ti);def2SVP(C,O,H); ΔG° = -1661.699330 au
C      1.246624  -1.053689   -1.082825
C      2.664079  -0.772711   -1.302889
C      3.407103  -1.776115   -0.740427
C      2.508169  -2.765369   -0.196764
C      1.222966  -2.352119   -0.423497
C     -0.751951   1.703662   -1.826847
C     -0.941356   2.516690   -0.683500
C      0.334586   2.939040   -0.241122
C      1.307131   2.330580   -1.054931
C      0.628336   1.577727   -2.046946
C      0.517741  -0.753372    2.105877
C     -0.389094   0.261426    2.453262
C      0.258061   1.504218    2.280904
C      1.592307   1.248052    1.865018
C      1.744147  -0.144641    1.735693
C     -2.633134  -1.009398   -0.180211
C     -2.716015  -1.682561   -1.545121
C     -2.746713  -2.055760    0.922544
C     -3.725249   0.042046   -0.030561
H      0.542134  -0.933786   -1.916105
H      3.066070   0.097446   -1.823560
H      4.496846  -1.824320   -0.707533
H      2.809501  -3.686700    0.304677
H      0.311374  -2.893202   -0.165559
H     -1.533227   1.193938   -2.386248
H     -1.896483   2.782390   -0.231342
H      0.533267   3.596986    0.601314
H      2.386819   2.420635   -0.947407
H      1.099764   1.000761   -2.838779
H      0.310224  -1.819904    2.074439
H     -1.433005   0.126377    2.729835
H     -0.186587   2.478180    2.476182
H      2.352468   1.996074    1.647566
H      2.634290  -0.668572    1.392842
H     -1.906145  -2.418579   -1.655158
H     -3.677703  -2.202950   -1.668443
H     -2.621454  -0.939630   -2.350541
H     -2.699076  -1.588201    1.916689
H     -3.700527  -2.599207    0.848128
H     -1.928084  -2.785471    0.838743
H     -3.653199   0.792708   -0.831397
H     -4.723189  -0.418566   -0.079736
H     -3.628605   0.555644    0.938517
O     -1.393103  -0.373416   -0.085607
Ti     0.137406   0.553593    0.112354

45
[Cp3Ti(OtBu)];(w/PCM,THF);M06/def2TZVP(Ti);def2SVP(C,O,H); ΔG° = -1661.707109 au
C      1.257031  -1.068088   -1.090854
C      2.667032  -0.770495   -1.312126
C      3.423718  -1.757466   -0.730786
C      2.535763  -2.748969   -0.175462
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C	1.243638	-2.353563	-0.414111
C	-0.776382	1.691816	-1.824821
C	-0.957379	2.507202	-0.680995
C	0.321898	2.936257	-0.252052
C	1.289096	2.327556	-1.072334
C	0.602652	1.569178	-2.056574
C	0.516049	-0.735413	2.111564
C	-0.394061	0.279557	2.451509
C	0.250165	1.523328	2.271366
C	1.585922	1.269324	1.858109
C	1.741003	-0.124213	1.737052
C	-2.625207	-1.025902	-0.176397
C	-2.703004	-1.703248	-1.538919
C	-2.738401	-2.067013	0.930556
C	-3.716914	0.025950	-0.032558
H	0.532837	-0.933049	-1.903742
H	3.056543	0.101389	-1.839857
H	4.514320	-1.786145	-0.685067
H	2.846243	-3.653711	0.351395
H	0.336361	-2.895310	-0.141822
H	-1.560862	1.179372	-2.377304
H	-1.908620	2.771387	-0.219636
H	0.525978	3.598111	0.585881
H	2.369309	2.424197	-0.974596
H	1.067023	0.993062	-2.853462
H	0.307365	-1.802176	2.086144
H	-1.437993	0.143581	2.727768
H	-0.198227	2.497419	2.456530
H	2.341992	2.019534	1.633595
H	2.633217	-0.646896	1.397258
H	-1.895257	-2.443011	-1.641817
H	-3.665690	-2.221597	-1.661788
H	-2.604518	-0.963810	-2.347004
H	-2.692651	-1.594714	1.922519
H	-3.692724	-2.609315	0.855865
H	-1.920448	-2.798199	0.850748
H	-3.647140	0.772821	-0.836917
H	-4.712874	-0.438811	-0.080304
H	-3.622591	0.543416	0.934532
O	-1.382030	-0.388788	-0.081001
Ti	0.134042	0.554453	0.108913