Computational Overview of a Pd-Catalyzed Olefin Bis-Alkoxycarbonylation Process

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Supporting Info

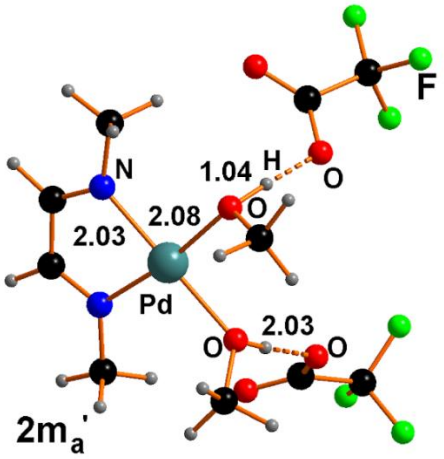


Figure S1. Optimized structure of the compound $[(N\text{-}N)Pd(CH_3OH)_2]^{+2}2[TFA]^-$, **2ma'.**

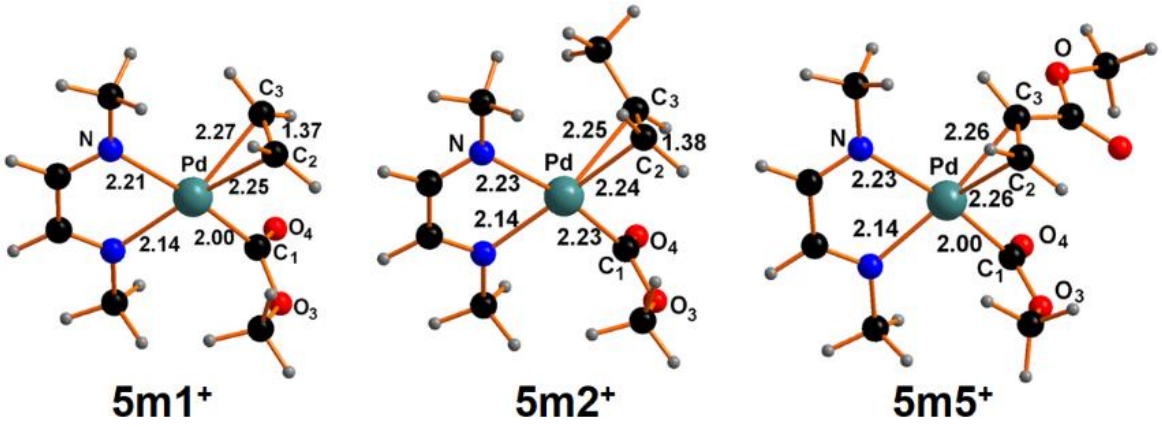
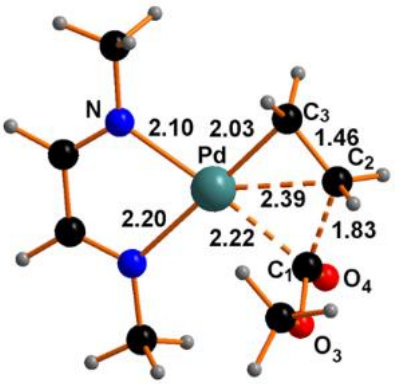
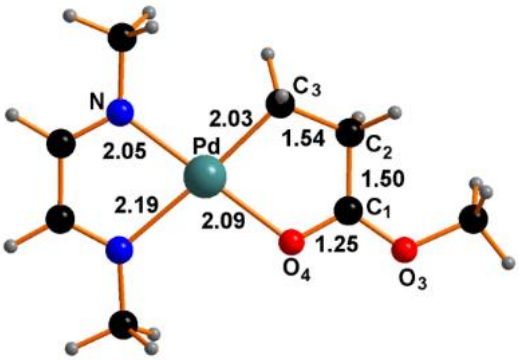


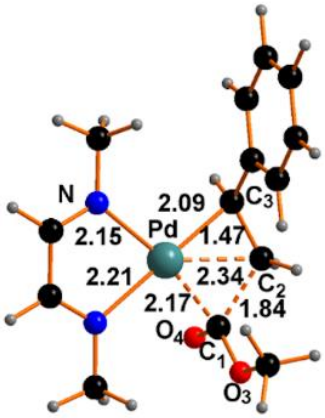
Figure S2. Optimized structures of the three η^2-alkene complexes **5m1**$^+$ (ethylene), **5m2**$^+$ (propene) and **5m5**$^+$ (methylacrylate).



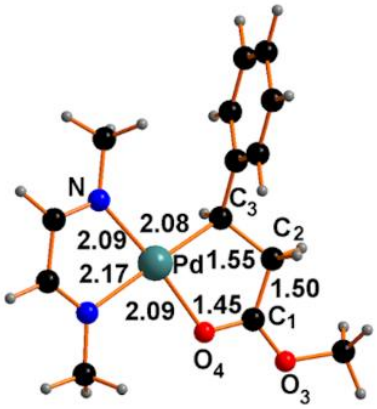
5-6m1$_{TS}^{+}$



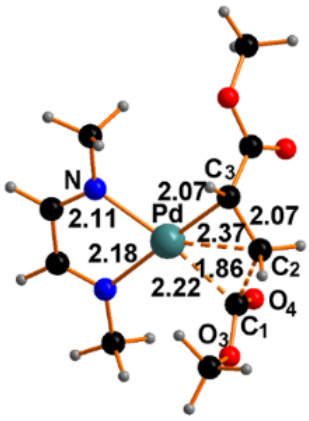
6m1^{+}



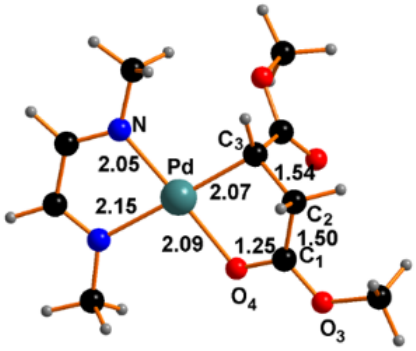
5-6m3$_{TS}^{+}$



6m3^{+}



5-6m5$_{TS}^{+}$



6m5^{+}

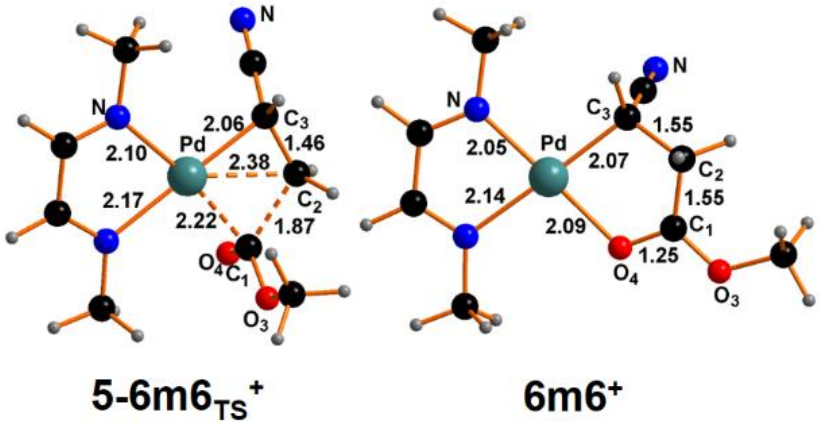


Figure S3. Optimized structures of the pairs of Transition State minimum with general formula **5-6mnTS$^+$/6mn$^+$** with n=1 is related to ethylene, n=3 is related to styrene, n=5 to methylacrylate and n=6 to acrylonitrile.

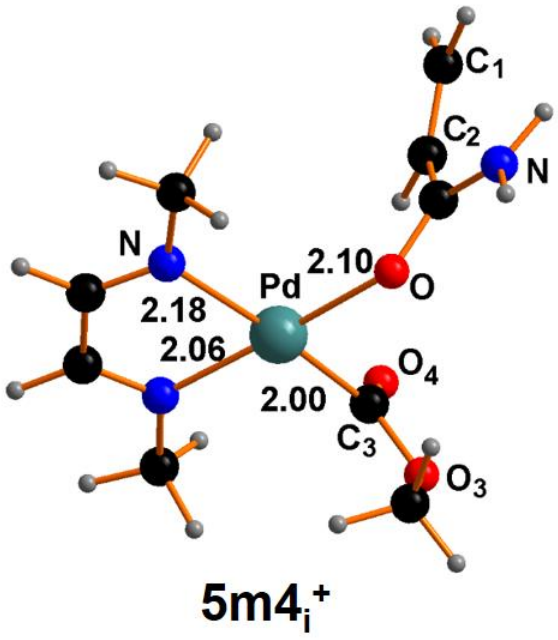


Figure S4. Optimized structure of the isomer **5-6m4$_i$$^+$** where the acrylamide is σ coordinated through O rather than η^2 with the olefin.

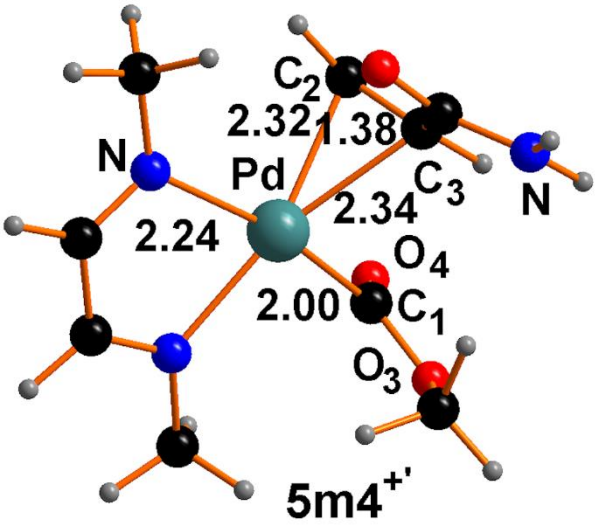


Figure S5. Optimized structure of the **5m4**$^{'+}$.

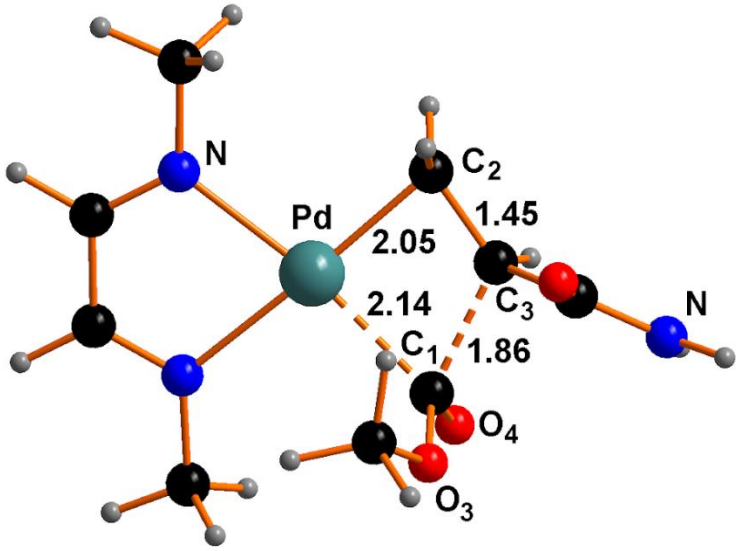


Figure S6. Optimized structure of the Transition State of **5-6m4**$_{TS}^{'+}$ but involving the C_1---C_3 coupling instead of the C_1---C_2 one.

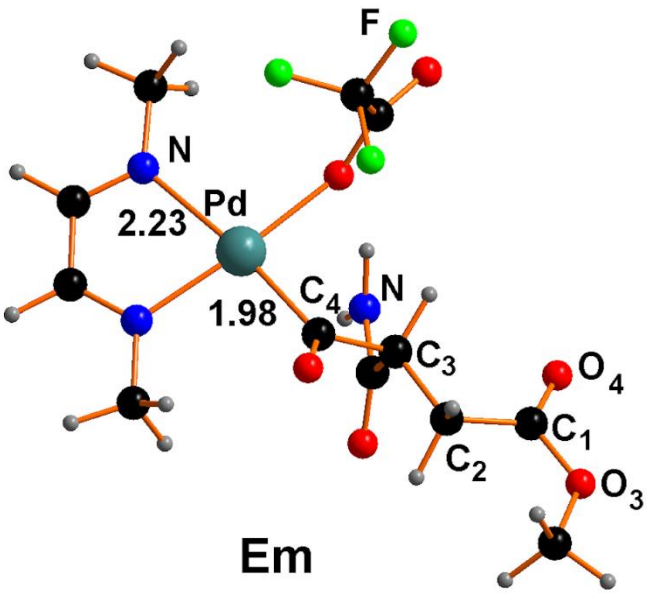


Figure S7. Optimized structure of the former proposed intermediate **Em** in Scheme 2, with a coordinated TFA anion in the palladium coordination sphere

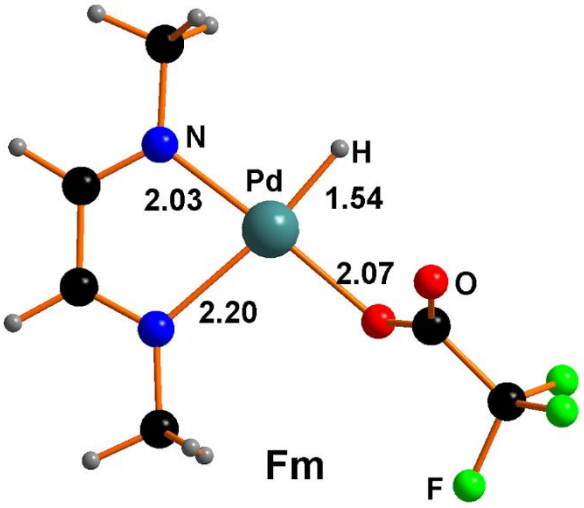


Figure S8. Optimized structure of the compound [(N-N)Pd(TFA)H], **Fm**, proposed as intermediate in Figure 1 and featuring a hydride ligand in the palladium coordination sphere.

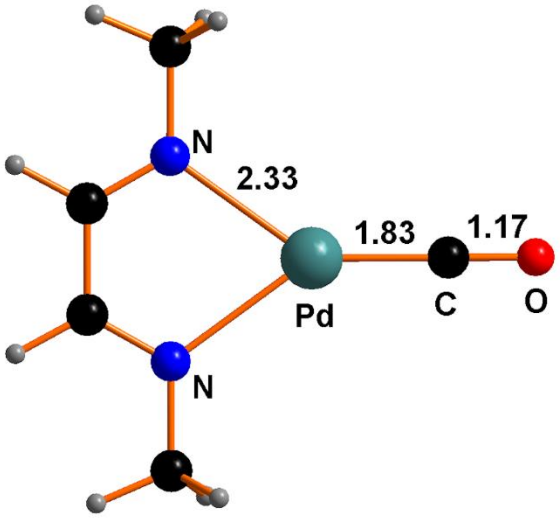


Figure S9. Optimized structure of the compound [(N-N)Pd(CO)].

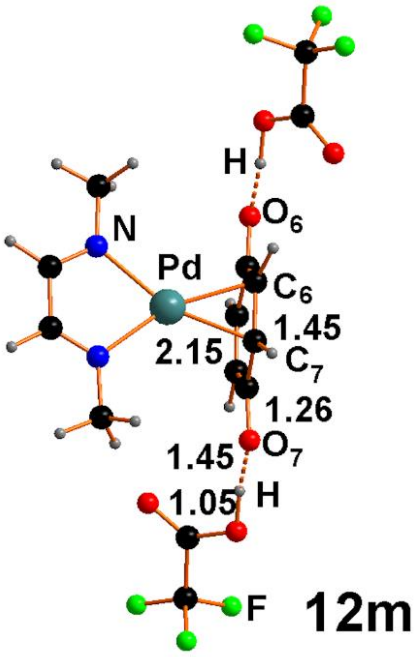


Figure S10. Optimized structure of the compound [(N-N)Pd(η^2-benzoquinone)]*2HTFA, **12m**

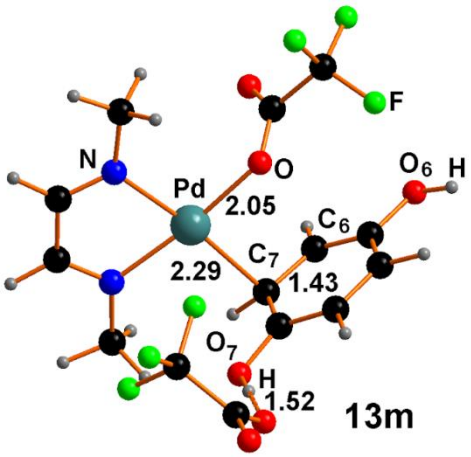


Figure S11. Optimized structure of the compound [(N-N)Pd(TFA)(η^1-H_2BQ)]*HTFA, **13m**

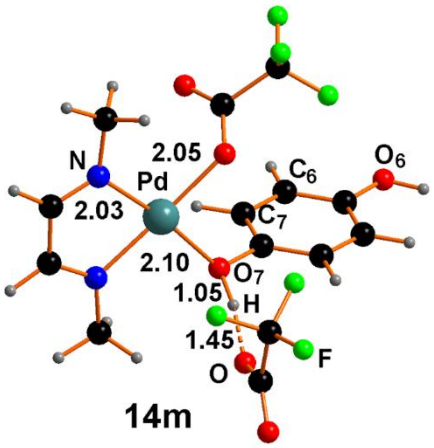


Figure S12. Optimized structure of the compound [(N-N)Pd(TFA)(coordO-H_2BQ)]*TFA^-, **14m**

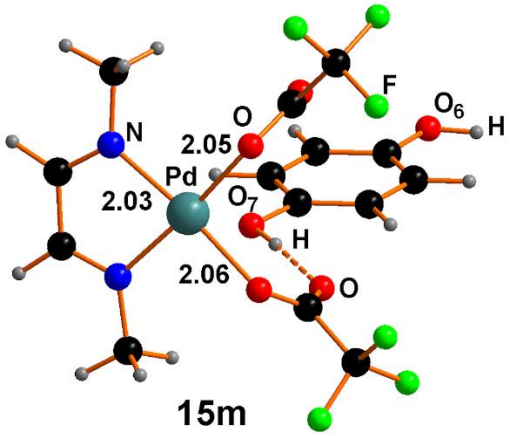


Figure S13. Optimized structure of the compound [(N-N)Pd($TFA)_2$]*H_2BQ, **15m**

Cartesian coordinates, Energies and Thermal Parameters of all the structures optimized in the computational analysis (B3LYP level of theory).

Compound $(NN)Pd(TFA)_2$, **Am**

Cartesian Coordinates

N -5.460660 0.475287 14.065600
Pd -4.676328 -1.209671 13.239059
C -6.695280 0.677178 13.757536
N -6.561335 -1.293734 12.503615
C -7.310466 -0.311630 12.872478
O -2.863731 -1.022557 14.196521
O -4.012172 -2.886196 12.252596
C -1.653711 -0.818022 13.829762
C -3.951680 -4.024328 12.846999
O -4.269886 -4.340518 13.987950
O -0.659782 -0.896064 14.550345
C -1.366960 -0.440149 12.338452
C -3.400676 -5.123177 11.882795
F -3.220672 -6.301559 12.509094
F -4.263495 -5.338489 10.857159
F -2.212082 -4.767793 11.340605
F -0.872332 -1.514514 11.674129
F -2.447735 -0.007042 11.652536
F -0.437859 0.539103 12.265067
C -7.055926 -2.343704 11.621211
H -6.392635 -2.414693 10.756357
H -7.022025 -3.295914 12.157072
H -8.078505 -2.131061 11.299855
C -4.730093 1.378498 14.945624
H -4.328747 0.800796 15.781424
H -3.888319 1.802043 14.391789
H -5.380746 2.176591 15.311499
H -8.344458 -0.219177 12.545969
H -7.254604 1.532096 14.132702

Energy and Thermal parameters

HF=-1447.184317
Zero-point vibrational energy 466750.7 (Joules/Mol)
Zero-point correction= 0.177776 (Hartree/Particle)
Thermal correction to Energy= 0.200704
Thermal correction to Enthalpy= 0.201648
Thermal correction to Gibbs Free Energy= 0.120190
Sum of electronic and zero-point Energies= -1447.006541
Sum of electronic and thermal Energies= -1446.983613
Sum of electronic and thermal Enthalpies= -1446.982669
Sum of electronic and thermal Free Energies= -1447.064127

Compound $[(NN)Pd(TFA)(CH_3OH)]^+[TFA]^-$, **$2m_a$**

Cartesian Coordinates

N 2.926925 -0.254923 0.000063
Pd 0.907196 -0.297885 -0.220631
C 3.415544 0.933658 0.087486
N 1.216894 1.708766 -0.132197
C 2.455266 2.035159 0.009532
O 0.841035 -2.367736 -0.311477
O -1.113814 -0.235518 -0.575667
C -1.960104 0.058009 0.345254
O -1.774526 0.373985 1.515869
C -3.421735 -0.026184 -0.197976
F -4.326491 0.359791 0.721359
F -3.591317 0.760670 -1.287747
F -3.730858 -1.294766 -0.563385
C 0.169742 2.718413 -0.235476
H -0.374812 2.562142 -1.169929
H -0.525270 2.582988 0.596879
H 0.596151 3.724242 -0.212130
C 3.772848 -1.439968 0.055590
H 3.471717 -2.044279 0.915146
H 3.603932 -2.031501 -0.846971
H 4.826360 -1.161945 0.138702
H 2.776213 3.073715 0.063650
H 4.481668 1.116108 0.208192
H 0.461442 -2.705617 -1.219187
C 0.213916 -3.095804 0.765257
H 0.732499 -2.846826 1.692192
H -0.846189 -2.840178 0.850811
H 0.320747 -4.165186 0.562656
O -0.137017 -3.306759 -2.429217
C 0.565482 -3.402781 -3.481561

C -0.185693 -4.163874 -4.625134
O 1.711662 -3.001510 -3.716192
F -0.479645 -5.438729 -4.253278
F 0.526684 -4.243760 -5.769644
F -1.363954 -3.561614 -4.934738

Energy and Thermal parameters

HF=-1562.9340655
Zero-point vibrational energy 605997.5 (Joules/Mol)
Zero-point correction= 0.230812 (Hartree/Particle)
Thermal correction to Energy= 0.257713
Thermal correction to Enthalpy= 0.258657
Thermal correction to Gibbs Free Energy= 0.167171
Sum of electronic and zero-point Energies= -1562.703253
Sum of electronic and thermal Energies= -1562.676353
Sum of electronic and thermal Enthalpies= -1562.675409
Sum of electronic and thermal Free Energies= -1562.766895

Compound $[(NN)Pd(CH_3OH)2]^{+2}2[TFA]^-$, **$2m_a$'**

Cartesian Coordinates

N 0.859464 -2.885948 0.037583
Pd 0.936228 -0.864735 0.154028
C 1.517058 -3.377570 -0.954798
N 2.108235 -1.174865 -1.481704
C 2.213015 -2.417051 -1.808819
O -0.317523 -0.833861 1.805890
O 0.992009 1.209047 0.217147
C 2.769027 -0.130958 -2.255717
H 2.022211 0.605604 -2.570883
H 3.503888 0.362818 -1.613964
H 3.274235 -0.560081 -3.125204
C 0.116658 -3.728574 0.966385
H 0.491082 -3.547321 1.976744
H -0.937976 -3.434636 0.932603
H 0.233726 -4.782606 0.701392
H 2.792994 -2.738270 -2.671926
H 1.558557 -4.447897 -1.147201
H -1.303763 -0.699921 1.504704
C -0.020857 0.036024 2.916333
H 0.964900 -0.231145 3.299864
H -0.033119 1.084218 2.608620
H -0.771914 -0.135856 3.692688
O -2.710376 -0.449299 1.113247
C -3.387082 -1.432406 0.683568
C -4.836832 -1.020648 0.261038
O -3.071720 -2.622735 0.557607
F -5.530834 -0.511081 1.313282
F -5.560629 -2.052054 -0.224913
F -4.818026 -0.062354 -0.701935
C 2.143823 1.971255 0.615762
H 2.895386 2.006133 -0.178344
H 1.819581 2.988149 0.854844
H 2.570473 1.509139 1.506935
H 0.423070 1.713966 -0.488850
O -0.492386 2.523003 -1.322531
C -0.351703 2.587655 -2.580773
O 0.488852 2.057864 -3.319120
C -1.423616 3.507953 -3.255112
F -2.684998 3.163387 -2.891560
F -1.246160 4.806178 -2.887382
F -1.379256 3.471779 -4.604328

Energy and Thermal parameters

HF=-1678.6762889
Zero-point vibrational energy 743837.4 (Joules/Mol)
Zero-point correction= 0.283313 (Hartree/Particle)
Thermal correction to Energy= 0.313439
Thermal correction to Enthalpy= 0.314383
Thermal correction to Gibbs Free Energy= 0.214393
Sum of electronic and zero-point Energies= -1678.392976
Sum of electronic and thermal Energies= -1678.362850
Sum of electronic and thermal Enthalpies= -1678.361906
Sum of electronic and thermal Free Energies= -1678.461895

Compound [(NN)Pd(CO)(CH_3OH)]*[TFA]$^+$, **3m**$^+$

Cartesian Coordinates

N 0.472717 1.860034 0.074702	C -0.917147 -1.851351 -0.658294
Pd -0.294546 -0.027278 -0.286282	O -1.291299 -2.896701 -0.885059
C 1.737626 1.857797 0.299043	O -2.176778 0.736518 -0.610944
N 1.679191 -0.480084 0.032406	H -2.504453 0.579279 -1.611946
C 2.406645 0.552641 0.277623	C -3.252092 0.469778 0.321040
C 2.257162 -1.822346 -0.004648	H -4.097026 1.100475 0.034294
H 1.753886 -2.442519 0.741573	H -3.546316 -0.583103 0.294300
H 2.089299 -2.251167 -0.995852	H -2.914283 0.739763 1.321698
H 3.328308 -1.784708 0.205025	C -3.363807 1.029070 -3.814963
C -0.314162 3.085857 0.070131	O -2.917820 0.252647 -2.908373
H -0.830950 3.165899 -0.888533	O -3.738739 0.741387 -4.952980
H -1.068940 3.018458 0.857882	C -3.418117 2.539304 -3.401976
H 0.327459 3.954386 0.235748	F -4.134043 2.716510 -2.259979
H 3.475452 0.465850 0.464158	F -2.167147 3.020026 -3.160850
H 2.294652 2.772042 0.496617	F -3.970732 3.327136 -4.342960

Energy and Thermal parameters

HF=-1149.8459494
Zero-point vibrational energy 553534.1 (Joules/Mol)
Zero-point correction= 0.210830 (Hartree/Particle)
Thermal correction to Energy= 0.232833
Thermal correction to Enthalpy= 0.233777
Thermal correction to Gibbs Free Energy= 0.154749
Sum of electronic and zero-point Energies= -1149.635119
Sum of electronic and thermal Energies= -1149.613116
Sum of electronic and thermal Enthalpies= -1149.612172
Sum of electronic and thermal Free Energies= -1149.691200

Compound [(NN)Pd(CO)(CH_3OH)]*$[TFA]_{TS}^+$, **3-4m$_{TS}^+$**

Cartesian Coordinates

N 1.639363 1.821450 0.511660	C 0.760981 -2.091883 0.027733
Pd 1.275995 -0.258024 0.142820	O 0.716554 -3.240562 -0.156622
C 2.733295 2.225329 -0.021692	O -0.502548 -1.282038 0.879036
N 3.043588 0.028599 -0.828369	H -1.878428 -1.285812 0.036212
C 3.510969 1.224929 -0.768917	C -0.643010 -1.672190 2.270559
C 3.742190 -1.031908 -1.549941	H -1.082354 -2.673069 2.312057
H 3.974314 -1.837463 -0.848765	H 0.324631 -1.666007 2.775617
H 3.076249 -1.426372 -2.321436	H -1.306909 -0.946546 2.744912
H 4.661097 -0.653308 -2.004134	C -3.505626 -0.489280 -0.802502
C 0.782713 2.714477 1.275239	O -2.708335 -1.493131 -0.499845
H -0.206874 2.725080 0.810160	O -4.533706 -0.607811 -1.428988
H 0.673705 2.309593 2.285778	C -3.045267 0.915878 -0.310403
H 1.189181 3.728802 1.318668	F -2.843384 0.917358 1.027395
H 4.448358 1.493715 -1.253617	F -1.877798 1.265103 -0.900650
H 3.088867 3.252284 0.059632	F -3.954211 1.853508 -0.597099

Energy and Thermal parameters

HF=-1149.8201386

****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 553240.9 (Joules/Mol)
Zero-point correction= 0.210718 (Hartree/Particle)
Thermal correction to Energy= 0.232308
Thermal correction to Enthalpy= 0.233252
Thermal correction to Gibbs Free Energy= 0.155865
Sum of electronic and zero-point Energies= -1149.609420
Sum of electronic and thermal Energies= -1149.587831
Sum of electronic and thermal Enthalpies= -1149.586887
Sum of electronic and thermal Free Energies= -1149.664274

Compound [(NN)Pd($COOCH_3$)(TFA)], **4m**

Cartesian Coordinates

Pd 0.772244 0.200496 0.277752
N 0.637509 2.330835 -0.190928
N 2.604537 0.556995 -0.604017
C 1.704628 2.748094 -0.767495
C 2.785905 1.776524 -0.977690
C 1.140228 -1.725844 0.661566
O 1.954264 -2.066421 1.503611
O 0.477350 -2.704745 -0.002989
C -0.439744 -2.370878 -1.071073
H 0.061633 -1.772510 -1.835897
H -0.745036 -3.328587 -1.492526
H -1.304852 -1.835495 -0.677807
C -0.483023 3.227709 0.042442
H -1.371989 2.805966 -0.435842
H -0.676905 3.271924 1.118098
H -0.292986 4.234337 -0.343222
C 3.667509 -0.426653 -0.802178
H 3.900040 -0.889213 0.159406
H 3.299674 -1.208672 -1.472316
H 4.561951 0.036448 -1.227273
H 1.832471 3.778318 -1.102974
H 3.718279 2.093724 -1.443871
O -1.179436 -0.015738 0.994962
C -1.796844 0.107598 2.106692
O -3.011117 0.002254 2.283846
C -0.921273 0.417405 3.367815
F -1.669941 0.602882 4.473132
F -0.177378 1.542386 3.202511
F -0.062196 -0.597042 3.633665

Energy and Thermal parameters

HF=-1149.4264205
Zero-point vibrational energy 528870.4 (Joules/Mol)
Zero-point correction= 0.201436 (Hartree/Particle)
Thermal correction to Energy= 0.222425
Thermal correction to Enthalpy= 0.223369
Thermal correction to Gibbs Free Energy= 0.149240
Sum of electronic and zero-point Energies= -1149.224984
Sum of electronic and thermal Energies= -1149.203996
Sum of electronic and thermal Enthalpies= -1149.203052
Sum of electronic and thermal Free Energies= -1149.277180

Compound [(NN)Pd($COOCH_3$)(propene)], **5m1**$^+$

Cartesian Coordinates

Pd 0.119828 -0.280065 -0.025236
N 2.295085 -0.009512 0.412974
N 0.389054 1.832171 -0.236745
C 2.617327 1.230095 0.352610
C 1.600535 2.214145 -0.053731
C -1.846260 -0.148008 -0.375271
O -2.294847 -0.177855 -1.504883
O -2.704354 0.035562 0.652327
C -2.240843 0.151396 2.018254
C -0.025335 -2.425160 -0.944789
C -0.006656 -2.471428 0.434721
H -3.146731 0.257684 2.613675
H -1.698466 -0.743633 2.326861
H -1.612946 1.036765 2.139370
H -0.992322 -2.392293 -1.440795
H -0.932336 -2.589674 0.989900

C 3.287853 -0.976011 0.867645
H 4.240905 -0.498524 1.114445
H 2.898010 -1.489609 1.751547
H 3.448905 -1.724176 0.087285
C -0.621098 2.801507 -0.656569
H -1.058326 2.464623 -1.599886
H -1.417054 2.833259 0.092395
H -0.191959 3.799691 -0.779160
H 0.908315 -2.703906 0.972629
H 3.618608 1.586158 0.600348
H 1.896666 3.255369 -0.187022
C 1.142383 -2.676551 -1.849441
H 0.996939 -3.657802 -2.321262
H 1.188527 -1.941545 -2.658855
H 2.094592 -2.694573 -1.317539

Energy and Thermal parameters

HF=-740.954695
Zero-point vibrational energy 672861.4 (Joules/Mol)
Zero-point correction= 0.256279 (Hartree/Particle)
Thermal correction to Energy= 0.274917
Thermal correction to Enthalpy= 0.275861
Thermal correction to Gibbs Free Energy= 0.208757
Sum of electronic and zero-point Energies= -740.698416
Sum of electronic and thermal Energies= -740.679778
Sum of electronic and thermal Enthalpies= -740.678834
Sum of electronic and thermal Free Energies= -740.745938

Compound [(NN)Pd($COOCH_3$)(styrene)], **5m2**$^+$

Cartesian Coordinates

Pd -0.002198 -0.098452 -0.237335
N 2.151082 -0.188640 0.301054
N 0.518964 1.967608 -0.047405
C 2.633159 0.988739 0.459775
C 1.757381 2.151230 0.238631
C -1.879143 0.311158 -0.795965
O -2.185608 0.301499 -1.973566
O -2.811260 0.691846 0.104781
C -2.557147 0.670579 1.529354
C -0.202324 -2.135522 -1.121936
C -0.453277 -2.421588 0.207901
H -3.337796 1.291960 1.966958
H -2.633452 -0.350111 1.905617
H -1.575946 1.085793 1.766252
H 0.806696 -2.220949 -1.514065
H -0.995044 -2.123059 -1.862046
C 3.008371 -1.348082 0.515776
H 4.039646 -1.059226 0.739531
H 2.609360 -1.934655 1.348909
H 2.991692 -1.976358 -0.379302
C -0.336246 3.121268 -0.322025
H -0.732791 3.026289 -1.336435
H -1.179419 3.119028 0.372646
H 0.216441 4.059931 -0.227134
H 0.402754 -2.584654 0.858509
H 3.672472 1.161906 0.742976
H 2.181411 3.153541 0.310847
C -1.741654 -2.767420 0.828033
C -1.760487 -3.040975 2.209968
C -2.938856 -2.894682 0.095748
C -2.943519 -3.417766 2.847386
H -0.841077 -2.955587 2.782867
C -4.119461 -3.269220 0.733786
H -2.950701 -2.708693 -0.973333
C -4.126996 -3.529286 2.110994
H -2.941178 -3.624345 3.913240
H -5.034665 -3.365126 0.157604
H -5.049284 -3.823178 2.603104

Energy and Thermal parameters

HF=-932.7016768
RMSD=4.599e-09
Zero-point vibrational energy 814262.7 (Joules/Mol)
Zero-point correction= 0.310136 (Hartree/Particle)
Thermal correction to Energy= 0.331458
Thermal correction to Enthalpy= 0.332402
Thermal correction to Gibbs Free Energy= 0.258970
Sum of electronic and zero-point Energies= -932.391540
Sum of electronic and thermal Energies= -932.370219
Sum of electronic and thermal Enthalpies= -932.369275
Sum of electronic and thermal Free Energies= -932.442707

Compound [(NN)Pd($COOCH_3$)(ethylene)], **5m3**$^+$

Cartesian Coordinates

Pd 0.018744 0.209332 -0.500873	H -2.193581 0.153661 -2.056723
N -1.151358 -1.503591 0.268210	H -1.018844 1.394182 -2.752191
N 1.546692 -1.132879 0.184202	H -1.192314 2.738326 -0.663750
C -0.384524 -2.411629 0.748326	C -2.597430 -1.667098 0.344389
C 1.075046 -2.225096 0.665715	H -2.878977 -2.599939 0.841731
C 1.320635 1.579760 -1.154293	H -3.020641 -0.819301 0.891062
O 1.684488 1.580436 -2.313790	H -3.010582 -1.655954 -0.668528
O 1.848091 2.489386 -0.306879	C 2.992166 -0.955436 0.062839
C 1.465606 2.533621 1.088224	H 3.233863 -0.770839 -0.987291
C -1.557297 1.017069 -1.888335	H 3.295292 -0.077268 0.638833
C -1.636936 1.750041 -0.726613	H 3.535397 -1.834216 0.420729
H 1.988615 3.397682 1.495725	H -2.330700 1.484488 0.065600
H 0.388060 2.668322 1.195702	H -0.771865 -3.320367 1.211448
H 1.786597 1.628506 1.607845	H 1.730457 -3.025899 1.010385

Energy and Thermal parameters

HF=-701.6342055
Zero-point vibrational energy 600063.8 (Joules/Mol)
Zero-point correction= 0.228552 (Hartree/Particle)
Thermal correction to Energy= 0.245539
Thermal correction to Enthalpy= 0.246484
Thermal correction to Gibbs Free Energy= 0.183679
Sum of electronic and zero-point Energies= -701.405653
Sum of electronic and thermal Energies= -701.388666
Sum of electronic and thermal Enthalpies= -701.387722
Sum of electronic and thermal Free Energies= -701.450527

Compound [(NN)Pd($COOCH_3$)(acrylamide)], **5m4**$^+$

Cartesian Coordinates

Pd 0.474906 0.151732 0.437072	C -0.650352 3.301677 0.214484
N 0.395687 2.322195 -0.054045	H -1.597659 2.938154 -0.194186
N 2.344375 0.476441 -0.556200	H -0.765429 3.407010 1.297746
C 1.450445 2.684938 -0.685332	H -0.417459 4.278036 -0.220541
C 2.509383 1.691747 -0.934925	C 3.406342 -0.502935 -0.780523
C 0.954897 -1.743911 0.868766	H 3.703129 -0.924067 0.183435
O 1.548644 -1.931624 1.911302	H 3.017467 -1.314057 -1.401395
O 0.751272 -2.772162 0.029740	H 4.271414 -0.047301 -1.269681
C 0.089015 -2.627388 -1.248128	H 1.597507 3.706538 -1.038752
C -1.378961 0.169092 1.741764	H 3.424350 2.010404 -1.435813
C -1.743112 -0.285583 0.493791	C -1.300375 -0.782704 2.913804
H 0.114155 -1.594081 -1.597535	O -1.569951 -1.981137 2.795900
H 0.632067 -3.269134 -1.941989	N -0.953545 -0.208671 4.086457
H -0.941860 -2.973141 -1.152866	H -0.896795 -0.780393 4.918445
H -1.429461 1.228118 1.978451	H -0.721686 0.771016 4.164861
H -1.929118 -1.344282 0.350230	H -2.087492 0.389670 -0.282337

Energy and Thermal parameters

HF=-870.3520232
Zero-point vibrational energy 670137.9 (Joules/Mol)

Zero-point correction= 0.255242 (Hartree/Particle)
Thermal correction to Energy= 0.275588
Thermal correction to Enthalpy= 0.276532
Thermal correction to Gibbs Free Energy= 0.204621
Sum of electronic and zero-point Energies= -870.096781
Sum of electronic and thermal Energies= -870.076436
Sum of electronic and thermal Enthalpies= -870.075492
Sum of electronic and thermal Free Energies= -870.147402

Compound [(NN)Pd($COOCH_3$)(methylacrylate)], **5m5**$^+$

Cartesian Coordinates

Pd 0.702040 0.018153 0.379768	C -2.311751 0.868607 0.172061
N 1.308558 2.120467 -0.068622	O -2.317082 2.087863 0.158365
N 2.527079 -0.237836 -0.717060	C -3.921643 0.781797 -1.570239
C 2.378587 2.141478 -0.774021	H -4.433193 -0.009571 -2.114467
C 3.051469 0.871849 -1.091992	H -4.636569 1.408456 -1.033890
C 0.544841 -1.949992 0.718342	H -3.322079 1.393482 -2.247049
O 0.913701 -2.390679 1.787055	C 0.669661 3.382876 0.285363
O 0.105518 -2.791420 -0.233276	H -0.385966 3.333056 0.011563
C -0.416997 -2.310119 -1.497724	H 0.728811 3.508625 1.371681
C -0.675225 0.570680 2.061808	H 1.154394 4.233745 -0.202775
C -1.498029 0.022060 1.103936	C 3.232137 -1.493301 -0.975524
H 0.304991 -1.665042 -2.001424	H 3.443334 -1.977005 -0.017944
H -0.584706 -3.209286 -2.088652	H 2.590377 -2.158287 -1.557717
H -1.358779 -1.781450 -1.345227	H 4.166234 -1.320251 -1.516218
H -0.590446 1.647640 2.159798	H 2.823620 3.071458 -1.130815
H -0.297104 -0.037937 2.876698	H 4.000957 0.897860 -1.628217
H -1.800095 -1.017984 1.164725	O -3.059444 0.098607 -0.627009

Energy and Thermal parameters

HF=-929.517578
Zero-point vibrational energy 714026.7 (Joules/Mol)
Zero-point correction= 0.271958 (Hartree/Particle)
Thermal correction to Energy= 0.293120
Thermal correction to Enthalpy= 0.294065
Thermal correction to Gibbs Free Energy= 0.221384
Sum of electronic and zero-point Energies= -929.245620
Sum of electronic and thermal Energies= -929.224458
Sum of electronic and thermal Enthalpies= -929.223513
Sum of electronic and thermal Free Energies= -929.296194

Compound [(NN)Pd($COOCH_3$)(acrylonitrile)], **5m6**$^+$

Cartesian Coordinates

Pd	0.0310	0.1970	-0.5770	H	0.9270	3.4300	1.1400
N	-1.1410	-1.5830	0.0830	H	1.0490	1.6650	1.4240
N	1.5420	-1.0810	0.2450	H	-2.5030	0.4180	-1.4930
C	-0.3760	-2.4470	0.6400	H	-0.8570	2.9080	-0.6640
C	1.0720	-2.1880	0.6950	C	-2.5750	-1.8420	0.0150
C	1.4030	1.5400	-1.1670	H	-2.8410	-2.7870	0.4980
O	1.7630	1.4950	-2.3240	H	-3.1120	-1.0230	0.5020
O	1.9850	2.3990	-0.3180	H	-2.8790	-1.8760	-1.0360
C	1.5700	2.5520	1.0620	C	2.9860	-0.8500	0.2630
C	-1.7340	1.1770	-1.5970	H	3.3240	-0.6750	-0.7620
C	-1.3940	1.9780	-0.5200	H	3.2020	0.0440	0.8520
H	2.4840	2.7100	1.6330	H	3.5200	-1.7050	0.6870

H -1.8740 1.8250 0.4400
H -0.7580 -3.3750 1.0660
H 1.7280 -2.9520 1.1150
C -1.4400 1.5250 -2.9600
N -1.2620 1.7860 -4.0790

Energy and Thermal parameters

HF=-793.8678138
Zero-point vibrational energy 597901.1 (Joules/Mol)
Zero-point correction= 0.227729 (Hartree/Particle)
Thermal correction to Energy= 0.246241
Thermal correction to Enthalpy= 0.247185
Thermal correction to Gibbs Free Energy= 0.180651
Sum of electronic and zero-point Energies= -793.640085
Sum of electronic and thermal Energies= -793.621573
Sum of electronic and thermal Enthalpies= -793.620629
Sum of electronic and thermal Free Energies= -793.687163

Compound TFA^-

Cartesian Coordinates

O -1.122727 0.002239 -1.096139
C -2.327827 -0.094926 -0.771896
O -3.365788 -0.111445 -1.467204
C -2.544325 -0.200935 0.783828
F -3.833302 -0.393186 1.155193
F -1.832526 -1.229050 1.325376
F -2.127404 0.933204 1.418741

Energy and Thermal parameters

HF=-526.3844232
Zero-point vibrational energy 66658.0 (Joules/Mol)
Zero-point correction= 0.025389 (Hartree/Particle)
Thermal correction to Energy= 0.031464
Thermal correction to Enthalpy= 0.032408
Thermal correction to Gibbs Free Energy= -0.006206
Sum of electronic and zero-point Energies= -526.359035
Sum of electronic and thermal Energies= -526.352959
Sum of electronic and thermal Enthalpies= -526.352015
Sum of electronic and thermal Free Energies= -526.390629

Compound CO

Cartesian Coordinates

C 0.000000 0.000000 -0.003624
O 0.000000 0.000000 1.133624

Energy and Thermal parameters

HF=-113.3160159
Zero-point vibrational energy 13143.8 (Joules/Mol)
Zero-point correction= 0.005006 (Hartree/Particle)
Thermal correction to Energy= 0.007367
Thermal correction to Enthalpy= 0.008311
Thermal correction to Gibbs Free Energy= -0.014131
Sum of electronic and zero-point Energies= -113.311010
Sum of electronic and thermal Energies= -113.308649
Sum of electronic and thermal Enthalpies= -113.307705
Sum of electronic and thermal Free Energies= -113.330147

Compound propene

Cartesian Coordinates

C -0.449357 0.242203 -0.159798
H -0.257703 -0.682369 -0.713729
H 0.115237 0.204641 0.780559
H -1.511570 0.265949 0.115177
C -0.075059 1.456085 -0.962990
C 0.430790 1.438079 -2.202097
H 0.611317 0.503448 -2.730270
H 0.680478 2.355550 -2.728422
H -0.237433 2.419314 -0.476930

Energy and Thermal parameters

HF=-117.9217143
Zero-point vibrational energy 208433.6 (Joules/Mol)
Zero-point correction= 0.079388 (Hartree/Particle)
Thermal correction to Energy= 0.083487
Thermal correction to Enthalpy= 0.084431
Thermal correction to Gibbs Free Energy= 0.054363
Sum of electronic and zero-point Energies= -117.842326
Sum of electronic and thermal Energies= -117.838227
Sum of electronic and thermal Enthalpies= -117.837283
Sum of electronic and thermal Free Energies= -117.867351

Compound styrene

Cartesian Coordinates

C 0.409881 -1.168190 1.832860
C 1.054513 -1.484817 0.697925
H -0.546441 -1.623966 2.070018
H 0.799872 -0.457533 2.556410
H 0.587928 -2.208428 0.029822
C 2.351200 -0.964074 0.224739
C 2.859364 -1.426600 -1.004181
C 3.113282 -0.020928 0.944085
C 4.082649 -0.967394 -1.500783
H 2.286964 -2.154246 -1.574429
C 4.333932 0.438299 0.450029
H 2.752091 0.357486 1.895517
C 4.825934 -0.032034 -0.775263
H 4.452637 -1.340160 -2.451780
H 4.904784 1.165298 1.021021
H 5.777011 0.327887 -1.156890

Energy and Thermal parameters

HF=-309.6711585
Zero-point vibrational energy 349975.3 (Joules/Mol)
Zero-point correction= 0.133299 (Hartree/Particle)
Thermal correction to Energy= 0.140038
Thermal correction to Enthalpy= 0.140982
Thermal correction to Gibbs Free Energy= 0.102136
Sum of electronic and zero-point Energies= -309.537860
Sum of electronic and thermal Energies= -309.531121
Sum of electronic and thermal Enthalpies= -309.530177
Sum of electronic and thermal Free Energies= -309.569022

Compound ethylene

Cartesian Coordinates

C 0.940130 -1.771747 -1.537814
C 0.679664 -2.180960 -0.293096
H 1.958652 -1.675532 -1.906424
H 0.144571 -1.518059 -2.234340
H -0.338971 -2.277698 0.075110

H 1.475256 -2.434204 0.403565

Energy and Thermal parameters

HF=-78.599236
Zero-point vibrational energy 133633.3 (Joules/Mol)
Zero-point correction= 0.050898 (Hartree/Particle)
Thermal correction to Energy= 0.053944
Thermal correction to Enthalpy= 0.054888
Thermal correction to Gibbs Free Energy= 0.028707
Sum of electronic and zero-point Energies= -78.548338
Sum of electronic and thermal Energies= -78.545292
Sum of electronic and thermal Enthalpies= -78.544348
Sum of electronic and thermal Free Energies= -78.570529

Compound acrylamide

Cartesian Coordinates

C 2.211212 -0.664914 0.361976
C 1.631323 0.381211 -0.238537
H 1.658395 -1.388376 0.955425
H 3.283660 -0.819837 0.291846
H 2.228110 1.104591 -0.787623
C 0.181882 0.736915 -0.182730
O -0.180700 1.902918 -0.407960
N -0.703759 -0.241238 0.130948
H -0.439762 -1.212843 0.189620
H -1.688061 -0.014927 0.160036

Energy and Thermal parameters

HF=-247.3244599
Zero-point vibrational energy 207346.0 (Joules/Mol)
Zero-point correction= 0.078974 (Hartree/Particle)
Thermal correction to Energy= 0.084570
Thermal correction to Enthalpy= 0.085515
Thermal correction to Gibbs Free Energy= 0.050409
Sum of electronic and zero-point Energies= -247.245486
Sum of electronic and thermal Energies= -247.239889
Sum of electronic and thermal Enthalpies= -247.238945
Sum of electronic and thermal Free Energies= -247.274051

Compound methyl acrylate

Cartesian Coordinates

C -1.057342 0.208955 2.069051
C -1.692513 -0.544052 1.163655
H -1.228954 1.280054 2.126971
H -0.353712 -0.228785 2.769669
H -1.531141 -1.615392 1.093841
C -2.656107 0.046146 0.201747
O -2.963788 1.227863 0.130445
C -4.124596 -0.460452 -1.598057
H -4.414283 -1.359249 -2.140183
H -4.991735 -0.009383 -1.110741
H -3.663196 0.263527 -2.273259
O -3.168533 -0.900833 -0.609040

Energy and Thermal parameters

HF=-306.4926796
Zero-point vibrational energy 249623.9 (Joules/Mol)
Zero-point correction= 0.095077 (Hartree/Particle)
Thermal correction to Energy= 0.101728
Thermal correction to Enthalpy= 0.102673
Thermal correction to Gibbs Free Energy= 0.064658
Sum of electronic and zero-point Energies= -306.397603
Sum of electronic and thermal Energies= -306.390951
Sum of electronic and thermal Enthalpies= -306.390007
Sum of electronic and thermal Free Energies= -306.428021

Compound acrylonitrile

Cartesian Coordinates

C -2.572018 0.603711 0.000000
H -1.924404 -0.267122 0.000000
H -3.643728 0.436043 0.000000
C -2.084677 1.853488 0.000000
H -2.737498 2.722191 0.000000
C -0.680095 2.131755 0.000000
N 0.456620 2.387333 0.000000

Energy and Thermal parameters

HF=-170.8485971
Zero-point vibrational energy 133239.5 (Joules/Mol)
Zero-point correction= 0.050748 (Hartree/Particle)
Thermal correction to Energy= 0.054895
Thermal correction to Enthalpy= 0.055839
Thermal correction to Gibbs Free Energy= 0.024863
Sum of electronic and zero-point Energies= -170.797849
Sum of electronic and thermal Energies= -170.793702
Sum of electronic and thermal Enthalpies= -170.792758
Sum of electronic and thermal Free Energies= -170.823734

Compound [(NN)Pd($COOCH_3$)(η^1-acrylonitrile)], **5m6$_i$**$^+$

Cartesian Coordinates

Pd 0.355384 -0.081632 0.091460
N 2.213522 -1.212733 0.249101
N 1.729204 1.237276 -0.739267
C 3.205916 -0.549986 -0.220023
C 2.934231 0.786321 -0.770236
C -1.233096 1.090956 -0.268817
O -1.688007 1.165701 -1.395627
O -1.827746 1.805067 0.711540
C -1.322920 1.776483 2.066972
H -1.899953 2.532259 2.598870
H -1.489676 0.796499 2.517482
H -0.261697 2.031322 2.094218
C 2.402020 -2.542740 0.807523
H 3.447285 -2.863272 0.762488
H 2.058593 -2.537139 1.846349
H 1.772582 -3.245869 0.253911
C 1.434516 2.558884 -1.291182
H 0.662650 2.454178 -2.057079
H 1.038029 3.192747 -0.493409
H 2.329466 3.017982 -1.718938

H 4.225446 -0.937651 -0.226829
H 3.748312 1.372152 -1.196142
N -0.901682 -1.447908 0.914350
C -1.591951 -2.272602 1.346583
C -2.470947 -3.257308 1.883620
H -3.474208 -2.912575 2.117478
C -2.080506 -4.526175 2.083327
H -1.077788 -4.866355 1.846909
H -2.777381 -5.249184 2.492970

Energy and Thermal parameters

HF=-793.8887834
Zero-point vibrational energy 596535.7 (Joules/Mol)
Zero-point correction= 0.227208 (Hartree/Particle)
Thermal correction to Energy= 0.246102
Thermal correction to Enthalpy= 0.247046
Thermal correction to Gibbs Free Energy= 0.178209
Sum of electronic and zero-point Energies= -793.661575
Sum of electronic and thermal Energies= -793.642681
Sum of electronic and thermal Enthalpies= -793.641737
Sum of electronic and thermal Free Energies= -793.710574

Transition State [(NN)Pd($COOCH_3$)(acrylamide)], **5-6m4**$_{TS}^{+}$

Cartesian Coordinates

Pd -0.497076 0.156795 0.041098
N 0.145893 2.141822 0.386736
N -2.273755 1.317767 -0.453599
C -0.758759 3.023709 0.155475
C -2.072963 2.577824 -0.327516
C -1.474691 -1.794542 -0.371439
O -1.639926 -1.908357 -1.568737
O -2.454805 -2.131699 0.478352
C -2.339136 -2.011488 1.917028
C 0.219757 -2.093784 0.276293
C 1.156146 -0.995027 0.496749
H -3.346741 -1.803422 2.274726
H -1.988538 -2.961897 2.326043
H -1.675559 -1.192086 2.196765
H 0.479286 -2.712461 -0.579462
H -0.041425 -2.645678 1.174402
H 1.427518 -0.787379 1.531372
C 2.250762 -0.831712 -0.524937
O 2.110897 -1.206330 -1.696660
N 3.384998 -0.236340 -0.081291
C 1.453212 2.556034 0.884889
H 1.613878 2.101652 1.866794
H 2.225515 2.185178 0.206896
H 1.522021 3.644367 0.968266
C -3.559892 0.830415 -0.937573
H -3.389129 0.220039 -1.828362
H -3.999468 0.184521 -0.172628
H -4.243933 1.651823 -1.170424
H -0.574331 4.086795 0.311030
H -2.837646 3.318994 -0.562420
H 3.550500 -0.046280 0.896346
H 4.163791 -0.138954 -0.719013

Energy and Thermal parameters

HF=-870.3256253
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 672650.1 (Joules/Mol)
Zero-point correction= 0.256199 (Hartree/Particle)
Thermal correction to Energy= 0.274954
Thermal correction to Enthalpy= 0.275898
Thermal correction to Gibbs Free Energy= 0.209524
Sum of electronic and zero-point Energies= -870.069426
Sum of electronic and thermal Energies= -870.050671
Sum of electronic and thermal Enthalpies= -870.049727
Sum of electronic and thermal Free Energies= -870.116101

Transition State [(NN)Pd($COOCH_3$)(acrylamide)] of type **5-6m4$_{TS}^{+}$** but involving the C_1---C_3 coupling instead of C_1---C_2 one.

Cartesian Coordinates

Pd	0.5116	0.2288	0.2081
N	2.3207	1.2905	-0.0992
N	1.9823	-1.3832	0.0297
C	3.3467	0.5327	-0.2401
C	3.1679	-0.9253	-0.1399
C	-1.1841	-1.0610	0.4008
O	-1.2565	-1.7325	1.4131
O	-1.5741	-1.5976	-0.7728
C	-1.1948	-1.0620	-2.0691
C	-0.7945	1.7853	0.4831
C	-1.7098	0.6937	0.7475
H	-1.2178	0.0274	-2.0752
H	-0.2043	-1.4364	-2.3318
H	-1.9390	-1.4511	-2.7628
H	-0.9391	2.3565	-0.4313
H	-0.4282	2.3461	1.3406
H	-1.8585	0.5069	1.8069
C	-3.0249	0.7327	-0.0590
O	-3.0820	1.2242	-1.1840
N	-4.0879	0.2379	0.6050
C	2.4580	2.7403	-0.1958
H	1.8116	3.1007	-1.0006
H	2.1165	3.1901	0.7403
H	3.4934	3.0337	-0.3915
C	1.7675	-2.8199	0.1562
H	1.2515	-3.0139	1.1004
H	1.1110	-3.1521	-0.6534
H	2.7077	-3.3780	0.1208
H	4.3408	0.9403	-0.4261
H	4.0414	-1.5751	-0.2069
H	-4.0206	-0.1537	1.5333
H	-4.9983	0.2674	0.1653

Energy and Thermal parameters

HF=-870.315019
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 672650.1 (Joules/Mol)
Zero-point correction= 0.254299 (Hartree/Particle)
Thermal correction to Energy= 0.273954
Thermal correction to Enthalpy= 0.274898
Thermal correction to Gibbs Free Energy= 0.206524
Sum of electronic and zero-point Energies= -870.039426
Sum of electronic and thermal Energies= -870.060671
Sum of electronic and thermal Enthalpies= -870.029727
Sum of electronic and thermal Free Energies= -870.107001

Compound [(NN)Pd(chelate-$COOCH_3$acrylamide)], **6m4^{+}**

Cartesian Coordinates

Pd	-0.797367	0.265760	-0.088338
N	-2.004793	-1.333850	-0.547541
N	-2.724653	0.992185	0.521598
C	-3.252569	-1.146870	-0.281737
C	-3.655035	0.134901	0.307781
C	1.450282	1.971268	-0.228824
O	0.326313	1.976719	0.324156
O	2.225426	3.001454	0.020007
C	3.537312	3.123983	-0.595701
C	1.801427	0.858567	-1.171798
C	1.056347	-0.415180	-0.732712
H	3.902054	4.098669	-0.278474
H	4.195605	2.336541	-0.225682
H	3.450936	3.090755	-1.682660
H	2.881666	0.706149	-1.248572
H	1.448933	1.173540	-2.162660
H	0.945980	-1.113213	-1.564041
C	1.742099	-1.032492	0.455757
O	2.309134	-0.330930	1.312061
N	1.697826	-2.388300	0.569057
C	-1.578601	-2.603737	-1.129158
H	-1.058881	-2.409125	-2.070299
H	-0.883686	-3.087626	-0.438671
H	-2.431678	-3.263412	-1.308447
C	-3.015172	2.294242	1.099995
H	-2.439474	2.400962	2.024314
H	-2.672978	3.067939	0.406243
H	-4.082033	2.422691	1.306837

H -3.997955 -1.913959 -0.487233
H -4.702685 0.325111 0.542964
H 1.450265 -2.974914 -0.213475
H 2.202757 -2.821128 1.330851

Energy and Thermal parameters

HF=-870.3815717
Zero-point vibrational energy 679602.0 (Joules/Mol)
Zero-point correction= 0.258847 (Hartree/Particle)
Thermal correction to Energy= 0.277465
Thermal correction to Enthalpy= 0.278409
Thermal correction to Gibbs Free Energy= 0.211839
Sum of electronic and zero-point Energies= -870.122725
Sum of electronic and thermal Energies= -870.104106
Sum of electronic and thermal Enthalpies= -870.103162
Sum of electronic and thermal Free Energies= -870.169733

Compound [(NN)Pd(CO)($COOCH_3$acrylamide)], **7m4**$^+$

Cartesian Coordinates

Pd 0.968410 -0.113769 -0.263951
N 0.862970 0.718427 1.754716
N 3.018052 -0.265965 0.438283
C 2.001049 0.681241 2.348964
C 3.175879 0.167030 1.632973
C -1.819009 -1.888340 0.546749
O -0.923792 -1.730411 1.361547
O -2.810250 -2.741924 0.867213
C -3.908829 -3.025834 -0.029559
C -1.834172 -1.229590 -0.819194
C -1.043380 0.074298 -0.941114
H -4.485433 -3.803892 0.469046
H -4.533181 -2.140144 -0.168631
H -3.546492 -3.397705 -0.990368
H -2.864493 -1.037758 -1.132335
H -1.436506 -1.971629 -1.523472
H -0.962535 0.312372 -2.005262
C -1.747708 1.246119 -0.293491
O -2.737001 1.094271 0.436530
N -1.255811 2.476049 -0.588880
C -0.286949 1.219842 2.501573
H -0.659665 2.121703 2.011282
H -1.073200 0.464588 2.476664
H -0.014728 1.451048 3.535056
C 4.153201 -0.796917 -0.308768
H 3.930734 -1.826782 -0.602740
H 4.285880 -0.204233 -1.218497
H 5.072384 -0.773035 0.283284
H 2.118802 1.016072 3.379869
H 4.145828 0.159407 2.131911
C 1.286582 -0.781371 -2.009182
O 1.519653 -1.180744 -3.052069
H -0.457138 2.602604 -1.193573
H -1.726654 3.297271 -0.235173

Energy and Thermal parameters

HF=-983.7030387
Zero-point vibrational energy 699166.7 (Joules/Mol)
Zero-point correction= 0.266299 (Hartree/Particle)
Thermal correction to Energy= 0.288025
Thermal correction to Enthalpy= 0.288969
Thermal correction to Gibbs Free Energy= 0.213532
Sum of electronic and zero-point Energies= -983.436740
Sum of electronic and thermal Energies= -983.415014
Sum of electronic and thermal Enthalpies= -983.414069
Sum of electronic and thermal Free Energies= -983.489506

Transition State [(NN)Pd(CO)($COOCH_3$acrylamide)], **7-8m4**$_{TS}^+$

Cartesian Coordinates

Pd 0.828710 -0.337778 -0.183181
N 1.493805 0.056824 1.888586
N 2.867797 -0.884814 -0.227472
C 2.734311 -0.222193 2.047599
C 3.488374 -0.720713 0.883878
C -2.269888 -1.430809 0.320277

O -1.182773 -1.653874 0.834325	C 0.686340 0.509150 3.010519
O -3.324890 -2.119391 0.771374	H 0.176689 1.434801 2.730246
C -4.654583 -1.945218 0.223255	H -0.087891 -0.241324 3.198453
C -2.469489 -0.463535 -0.833422	H 1.285768 0.661608 3.913404
C -1.332833 0.523859 -1.053442	C 3.565160 -1.392226 -1.404185
H -5.263873 -2.694130 0.726425	H 3.061145 -2.300601 -1.745454
H -5.035874 -0.947532 0.450923	H 3.496043 -0.647503 -2.201806
H -4.661217 -2.128362 -0.852893	H 4.615289 -1.607943 -1.186687
H -3.392099 0.104202 -0.678597	H 3.244243 -0.115590 3.006327
H -2.624676 -1.059866 -1.740890	H 4.549360 -0.950167 0.986913
H -1.448804 1.014301 -2.020495	C 0.132641 -0.461153 -1.888039
C -1.269749 1.612985 0.013294	O 0.051524 -0.791418 -3.003232
O -1.900960 1.509089 1.071767	H -0.030401 2.806633 -1.159284
N -0.556363 2.721774 -0.301883	H -0.492933 3.470415 0.373997

Energy and Thermal parameters

HF=-983.6768558
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 696117.5 (Joules/Mol)
Zero-point correction= 0.265137 (Hartree/Particle)
Thermal correction to Energy= 0.286389
Thermal correction to Enthalpy= 0.287333
Thermal correction to Gibbs Free Energy= 0.213944
Sum of electronic and zero-point Energies= -983.411719
Sum of electronic and thermal Energies= -983.390467
Sum of electronic and thermal Enthalpies= -983.389523
Sum of electronic and thermal Free Energies= -983.462911

Compound [(NN)Pd(chelate-COCOOCH$_3$acrylamide)], **8m4**$^+$

Cartesian Coordinates

Pd 0.981957 -0.293790 -0.256945	C -2.039372 1.090881 0.592234
N 2.537643 -1.466243 0.803927	O -2.397880 0.254635 1.426628
N 2.608565 1.016986 -0.254674	N -1.837365 2.391908 0.886840
C 3.629933 -0.804730 0.895054	C 2.429667 -2.811028 1.343897
C 3.660295 0.550730 0.322325	H 1.614752 -2.829375 2.073922
C -1.665593 -1.811028 -0.370630	H 2.156079 -3.491917 0.532063
O -0.471123 -1.792237 -0.032118	H 3.360098 -3.145967 1.813672
O -2.318763 -2.917573 -0.071592	C 2.638307 2.363811 -0.817838
C -3.718320 -3.113789 -0.409919	H 2.303393 2.317668 -1.855195
C -2.332662 -0.708501 -1.153622	H 1.928423 2.988865 -0.268550
C -1.785579 0.697414 -0.874627	H 3.640509 2.795924 -0.755210
H -3.933531 -4.133599 -0.097670	H 4.526642 -1.200415 1.375475
H -4.341847 -2.413315 0.148235	H 4.573755 1.140754 0.395942
H -3.871204 -3.012447 -1.485187	C -0.283860 0.841252 -1.256643
H -3.405539 -0.706830 -0.962847	O 0.035870 1.579910 -2.163554
H -2.201035 -0.951110 -2.216493	H -1.999467 2.716494 1.830826
H -2.321165 1.396288 -1.525679	H -1.601685 3.077177 0.183251

Energy and Thermal parameters

HF=-983.7182096
Zero-point vibrational energy 704457.4 (Joules/Mol)
Zero-point correction= 0.268314 (Hartree/Particle)
Thermal correction to Energy= 0.289080

Thermal correction to Enthalpy= 0.290024
Thermal correction to Gibbs Free Energy= 0.218009
Sum of electronic and zero-point Energies= -983.449896
Sum of electronic and thermal Energies= -983.429129
Sum of electronic and thermal Enthalpies= -983.428185
Sum of electronic and thermal Free Energies= -983.501201

Compound [(NN)Pd(chelate-$COCOOCH_3$acrylamide)(TFA)], **Em**

Cartesian Coordinates

Pd -1.190374 0.439513 0.362199
N -3.388552 0.540664 0.028609
N -1.837443 -1.433066 1.023836
C -3.955532 -0.552172 0.382293
C -3.107703 -1.620218 0.931982
C 4.241198 0.844433 -0.794712
O 3.983167 1.628712 -1.692696
O 5.538508 0.557462 -0.560923
C 5.941965 -0.356612 0.483582
C 3.193657 0.189425 0.082987
C 1.767385 0.523046 -0.358659
H 7.030839 -0.348310 0.462671
H 5.591392 -0.015608 1.460248
H 5.579225 -1.366361 0.277792
H 3.343759 0.520461 1.115630
H 3.340060 -0.894413 0.081338
H 1.658174 1.603828 -0.490470
C 1.421599 -0.156616 -1.698036
O 1.918355 -1.246292 -2.006619
N 0.561644 0.514656 -2.490930
C -4.169799 1.630819 -0.532553
H -4.044183 2.513339 0.101515
H -3.767714 1.875714 -1.520298
H -5.232785 1.380995 -0.614652
C -0.996664 -2.497320 1.566004
H -0.310230 -2.834061 0.783772
H -0.396588 -2.089020 2.381121
H -1.599829 -3.338444 1.918221
H -5.030116 -0.720756 0.288926
H -3.566335 -2.556417 1.250449
H 0.091978 1.352883 -2.162037
H 0.239183 0.073395 -3.341705
C 0.735542 0.143389 0.742049
O 1.106879 -0.267688 1.822048
O -0.737110 2.303242 -0.534154
C -0.737086 3.534318 -0.179745
C -0.931871 3.809685 1.349236
O -0.592653 4.509416 -0.914397
F 0.004771 3.170004 2.093222
F -0.844543 5.120797 1.643615
F -2.148066 3.385476 1.781038

Energy and Thermal parameters

HF=-1510.1159638
Zero-point vibrational energy 774001.9 (Joules/Mol)
Zero-point correction= 0.294802 (Hartree/Particle)
Thermal correction to Energy= 0.323454
Thermal correction to Enthalpy= 0.324398
Thermal correction to Gibbs Free Energy= 0.231668
Sum of electronic and zero-point Energies= -1509.821162
Sum of electronic and thermal Energies= -1509.792510
Sum of electronic and thermal Enthalpies= -1509.791566
Sum of electronic and thermal Free Energies= -1509.880296

Compound [(NN)PdH(TFA)], **Fm**

Cartesian Coordinates

N -2.791602 -0.861323 0.399490
Pd -0.778416 -0.661615 0.198321
C -3.287416 -1.951929 -0.078149
N -1.129786 -2.622190 -0.743908
C -2.377873 -2.919595 -0.705622
O 1.253718 -0.514672 -0.146626
C 2.125230 -0.473194 0.787410
O 1.994848 -0.519712 2.009399
C 3.565447 -0.337485 0.196552
F 4.517874 -0.343558 1.150856
F 3.851684 -1.350937 -0.659588
F 3.702695 0.821854 -0.497466
C -0.167829 -3.529321 -1.346902
H 0.351633 -3.001934 -2.152892
H 0.581009 -3.794644 -0.594181
H -0.639487 -4.436590 -1.738745

C -3.667155 0.123712 1.031912
H -3.327837 0.283516 2.058328
H -3.570638 1.070819 0.495133
H -4.709995 -0.206337 1.027558
H -2.778897 -3.849013 -1.113718
H -4.354906 -2.162456 -0.022757
H -0.748499 0.708404 0.898997

Energy and Thermal parameters

HF=-921.5401164
Zero-point vibrational energy 413004.0 (Joules/Mol)
Zero-point correction= 0.157305 (Hartree/Particle)
Thermal correction to Energy= 0.173390
Thermal correction to Enthalpy= 0.174334
Thermal correction to Gibbs Free Energy= 0.110008
Sum of electronic and zero-point Energies= -921.382811
Sum of electronic and thermal Energies= -921.366726
Sum of electronic and thermal Enthalpies= -921.365782
Sum of electronic and thermal Free Energies= -921.430108

Compound [(NN)Pd(OCH_3)(COCOOCH_3acrylamide)], **9m4**

Cartesian Coordinates

Pd -1.093412 -0.151928 0.134039
N -3.281589 0.090423 -0.297549
N -1.471010 1.852229 0.668870
C -3.683277 1.265855 0.019310
C -2.686856 2.236199 0.491822
C 2.931313 1.261943 -1.007498
O 1.867526 1.567986 -1.521026
O 3.974834 2.102097 -1.176638
C 5.275900 1.828341 -0.609975
C 3.153079 0.004426 -0.194441
C 1.904961 -0.876490 -0.091681
H 5.894530 2.677797 -0.896351
H 5.223120 1.764106 0.479158
H 5.697881 0.910726 -1.026472
H 3.496785 0.280614 0.807446
H 3.970043 -0.571096 -0.641876
H 1.502886 -1.079218 -1.085649
C 2.259629 -2.228403 0.575609
O 3.385207 -2.442255 1.052993
N 1.250989 -3.114454 0.595503
C -4.242160 -0.912241 -0.730694
H -3.978630 -1.244683 -1.738850
H -4.163127 -1.780369 -0.069669
H -5.270245 -0.533943 -0.724763
C -0.481530 2.823959 1.125030
H 0.003261 2.433449 2.021838
H 0.286865 2.922903 0.352619
H -0.938705 3.797004 1.327350
H -4.730731 1.569259 -0.041043
H -2.995150 3.263587 0.688087
H 0.326822 -2.860502 0.170391
H 1.413575 -4.013551 1.029262
C 0.793631 -0.188975 0.758408
O 1.109373 0.303766 1.829927
O -0.961279 -2.094848 -0.517921
C -1.007919 -2.264259 -1.918360
H -0.095563 -1.902450 -2.424482
H -1.108799 -3.336485 -2.150234
H -1.861928 -1.746618 -2.381592

Energy and Thermal parameters

HF=-1099.002462
Zero-point vibrational energy 809209.5 (Joules/Mol)
Zero-point correction= 0.308212 (Hartree/Particle)
Thermal correction to Energy= 0.332564
Thermal correction to Enthalpy= 0.333509
Thermal correction to Gibbs Free Energy= 0.252898
Sum of electronic and zero-point Energies= -1098.694250
Sum of electronic and thermal Energies= -1098.669898
Sum of electronic and thermal Enthalpies= -1098.668953
Sum of electronic and thermal Free Energies= -1098.749564

Compound TS **9-10m4**$_{TS}$

Cartesian Coordinates

Pd	1.3950	-0.1470	-0.2370
N	3.6300	-0.6320	0.0380
N	2.3560	1.7400	-0.2410
C	4.3260	0.4430	0.0710
C	3.6370	1.7290	-0.1190
C	-3.5967	1.2330	-0.6963
O	-3.9368	0.0659	-0.7710
O	-4.3495	2.1483	-1.3519
C	-4.0442	3.5596	-1.3129
C	-2.4184	1.7303	0.1126
C	-1.4360	0.6410	0.6000
H	-4.8592	4.0414	-1.8518
H	-4.0159	3.9288	-0.2858
H	-3.0985	3.7673	-1.8192
H	-2.8166	2.2549	0.9890
H	-1.8571	2.4635	-0.4703
H	-0.6952	1.2012	1.1855
C	-2.0997	-0.2435	1.6763
O	-2.5501	0.3188	2.6901
H	-1.8823	-1.9701	0.6061
H	-2.6125	-2.1284	2.2122
N	-2.1430	-1.5739	1.5099
C	4.2770	-1.9190	0.2320
H	3.8130	-2.4180	1.0890
H	4.0890	-2.5430	-0.6470
H	5.3570	-1.8320	0.3980
C	1.6700	3.0120	-0.4410
H	1.0770	2.9510	-1.3580
H	0.9790	3.1750	0.3920
H	2.3680	3.8530	-0.5060
H	5.4070	0.4460	0.2320
H	4.2250	2.6480	-0.1510
C	-0.5730	0.0760	-0.5680
O	-0.9370	0.2960	-1.7330
O	-0.1690	-1.6050	-0.2610
C	-0.3150	-2.4780	-1.3760
H	-0.5150	-1.9040	-2.2880
H	0.5980	-3.0680	-1.5140
H	-1.1600	-3.1520	-1.1860

Energy and Thermal parameters

HF=-1098.99130
Zero-point vibrational energy 809209.5 (Joules/Mol)
Zero-point correction= 0.308212 (Hartree/Particle)
Thermal correction to Energy= 0.332564
Thermal correction to Enthalpy= 0.333509
Thermal correction to Gibbs Free Energy= 0.252898
Sum of electronic and zero-point Energies= -1098.694250
Sum of electronic and thermal Energies= -1098.649898
Sum of electronic and thermal Enthalpies= -1098.628953
Sum of electronic and thermal Free Energies= -1098.739675

Compound [(NN)Pd], **10m**

Cartesian Coordinates

Pd	-0.775955	0.320812	-0.083472
N	-2.074908	-1.257094	-0.798328
N	-2.668835	0.928993	0.775051
C	-3.265297	-1.123289	-0.247801
C	-3.624569	0.142490	0.321200
C	-1.647414	-2.607525	-1.157411
H	-1.403117	-2.649268	-2.224693
H	-0.729557	-2.842524	-0.605789
H	-2.399566	-3.375316	-0.926538
C	-3.036227	2.297668	1.131532
H	-2.769625	2.494773	2.175870
H	-2.452774	2.989414	0.512608
H	-4.104120	2.511940	0.982500
H	-3.969284	-1.957796	-0.213714
H	-4.673552	0.443821	0.365985

Energy and Thermal parameters

HF=-394.6462373
Zero-point vibrational energy 310585.4 (Joules/Mol)
Zero-point correction= 0.118296 (Hartree/Particle)
Thermal correction to Energy= 0.127267

Thermal correction to Enthalpy= 0.128211
Thermal correction to Gibbs Free Energy= 0.083268
Sum of electronic and zero-point Energies= -394.527942
Sum of electronic and thermal Energies= -394.518970
Sum of electronic and thermal Enthalpies= -394.518026
Sum of electronic and thermal Free Energies= -394.562970

Compound di-ester, **Pm**

Cartesian Coordinates

C -2.091267 -0.373434 -0.526951
O -1.510030 -0.340570 -1.597494
O -3.436282 -0.472803 -0.537221
C -4.205232 -0.537996 0.685499
C -1.388266 -0.324785 0.817029
C 0.126746 -0.132730 0.694799
H -5.239878 -0.649535 0.364343
H -3.912612 -1.402341 1.285809
H -4.098371 0.383063 1.263192
H -1.584333 -1.261340 1.345742
H -1.812904 0.480304 1.422052
H 0.539526 -0.167835 1.713999
C 0.776127 -1.352712 -0.011908
O 0.244835 -2.461479 0.108139
N 1.930481 -1.171519 -0.681224
C 0.457982 1.273130 0.192028
O -0.372178 2.135895 -0.019801
O 1.782454 1.486448 0.088370
C 2.202748 2.813143 -0.320852
H 1.797016 3.046117 -1.306793
H 1.862172 3.549666 0.408741
H 3.289963 2.771299 -0.349417
H 2.391522 -0.273360 -0.713087
H 2.387382 -1.981526 -1.077096

Energy and Thermal parameters

HF=-704.3209784
Zero-point vibrational energy 495390.6 (Joules/Mol)
Zero-point correction= 0.188684 (Hartree/Particle)
Thermal correction to Energy= 0.203000
Thermal correction to Enthalpy= 0.203944
Thermal correction to Gibbs Free Energy= 0.146530
Sum of electronic and zero-point Energies= -704.132294
Sum of electronic and thermal Energies= -704.117978
Sum of electronic and thermal Enthalpies= -704.117034
Sum of electronic and thermal Free Energies= -704.174449

Compound [(NN)Pd(CO)]

Cartesian Coordinates

Pd -0.006602 -1.236119 -0.127009
N -1.365763 0.654739 0.026064
N 1.363371 0.653577 -0.082246
C -0.738186 1.767279 0.058358
C 0.741308 1.766635 -0.000082
C -2.819364 0.649695 0.083326
H -3.204147 0.147957 -0.810257
H -3.134580 0.056874 0.947900
H -3.246183 1.658059 0.152446
C 2.816935 0.647222 -0.139727
H 3.198779 0.054062 0.697329
H 3.129660 0.145174 -1.060837
H 3.248815 1.655186 -0.104462
H -1.251093 2.731258 0.128143
H 1.258950 2.730165 0.029402
C -0.010485 -3.064102 -0.223459
O -0.012715 -4.231860 -0.284989

Energy and Thermal parameters

HF=-508.045452
Zero-point vibrational energy 334937.0 (Joules/Mol)
Zero-point correction= 0.127571 (Hartree/Particle)

Thermal correction to Energy= 0.139228
Thermal correction to Enthalpy= 0.140172
Thermal correction to Gibbs Free Energy= 0.088205
Sum of electronic and zero-point Energies= -507.917881
Sum of electronic and thermal Energies= -507.906224
Sum of electronic and thermal Enthalpies= -507.905280
Sum of electronic and thermal Free Energies= -507.957247

Compound benzoquinone, BQ

Cartesian Coordinates

C 0.672397 1.271833 0.000183
C -0.672394 1.271835 0.000154
C -1.438633 0.000012 0.000237
C -0.672395 -1.271814 0.000118
H -1.254332 -2.188598 0.000064
C 0.672393 -1.271816 0.000136
H 1.254328 -2.188601 0.000119
C 1.438634 0.000009 0.000137
H -1.254322 2.188624 0.000108
H 1.254327 2.188622 0.000191
O -2.670381 0.000011 -0.000042
O 2.670382 0.000005 0.000244

Energy and Thermal parameters

HF=-381.4795518
Zero-point vibrational energy 222961.1 (Joules/Mol)
Zero-point correction= 0.084921 (Hartree/Particle)
Thermal correction to Energy= 0.091186
Thermal correction to Enthalpy= 0.092130
Thermal correction to Gibbs Free Energy= 0.054339
Sum of electronic and zero-point Energies= -381.394630
Sum of electronic and thermal Energies= -381.388366
Sum of electronic and thermal Enthalpies= -381.387422
Sum of electronic and thermal Free Energies= -381.425213

Compound dihydroquinone, H_2BQ

Cartesian Coordinates

C 0.692120 -1.316508 0.080065
C -0.692067 -1.315567 -0.093576
C -1.390273 -0.104942 -0.175173
C -0.694377 1.103391 -0.081654
C 0.694550 1.102479 0.092866
C 1.390543 -0.106796 0.173943
H 1.237194 -2.253240 0.143854
H -1.237216 -2.251577 -0.166546
H -1.226399 2.049171 -0.143659
H 1.226568 2.047593 0.164617
O -2.755903 -0.168380 -0.347031
O 2.755451 -0.172355 0.345202
H 3.128311 0.718802 0.397107
H -3.128203 0.723530 -0.389216

Energy and Thermal parameters

HF=-382.7210562
Zero-point vibrational energy 284057.0 (Joules/Mol)
Zero-point correction= 0.108192 (Hartree/Particle)
Thermal correction to Energy= 0.115035
Thermal correction to Enthalpy= 0.115980
Thermal correction to Gibbs Free Energy= 0.077579
Sum of electronic and zero-point Energies= -382.612865
Sum of electronic and thermal Energies= -382.606021
Sum of electronic and thermal Enthalpies= -382.605077
Sum of electronic and thermal Free Energies= -382.643477

Compound [(NN)Pd(η^2-BQ)], **11m**

Cartesian Coordinates

Pd -0.080941 0.120962 -0.325521	C -2.640554 1.338947 0.311646
C 2.695773 -0.614674 0.320489	H 0.573572 2.970199 1.499755
C 2.614429 0.821985 0.629723	H 2.298689 3.271705 1.123086
C -1.982865 0.876191 -0.912436	C -2.478950 -1.518168 -0.302070
C -1.903917 -0.526997 -1.214092	C -3.025674 -1.017448 0.990848
C 1.671801 -2.624828 -0.420497	H -1.762323 -0.859836 -2.239783
H 2.657384 -3.069618 -0.242160	H -1.901525 1.613088 -1.708211
H 0.919810 -3.137198 0.187382	O -2.542310 -2.733451 -0.566199
H 1.390230 -2.756917 -1.469592	O -2.840156 2.541305 0.566753
C 1.363193 2.836119 0.754151	N 1.638025 -1.204324 -0.105270
H 1.046350 3.355808 -0.155262	N 1.489841 1.416691 0.458433
H -3.394513 -1.772533 1.680468	H 3.642965 -1.139793 0.459771
C -3.100172 0.297158 1.273201	H 3.502421 1.342532 0.994189
H -3.532383 0.659098 2.202697	

Energy and Thermal parameters

HF=-776.2111948
Zero-point vibrational energy 543113.7 (Joules/Mol)
Zero-point correction= 0.206861 (Hartree/Particle)
Thermal correction to Energy= 0.222827
Thermal correction to Enthalpy= 0.223772
Thermal correction to Gibbs Free Energy= 0.162142
Sum of electronic and zero-point Energies= -776.004334
Sum of electronic and thermal Energies= -775.988367
Sum of electronic and thermal Enthalpies= -775.987423
Sum of electronic and thermal Free Energies= -776.049053

Compound [(NN)Pd(η^2-BQ)]*2HTFA, **12m**

Cartesian Coordinates

Pd 0.290532 -0.933091 -0.055851	C 1.228184 1.618585 0.660019
C -0.551977 -3.662162 0.528504	H -0.116420 0.546653 -2.352101
C 0.730396 -3.510799 1.233311	H 2.103577 0.848289 -1.171114
H -1.085742 -4.612837 0.572284	O -2.413371 1.213299 -1.311091
H 1.141343 -4.349935 1.796905	O 2.299356 1.858490 1.287691
C 1.172291 0.955593 -0.623998	H -3.725750 1.601264 -0.806261
C -0.084443 0.787654 -1.293823	O -4.713837 1.896931 -0.608629
C -2.268080 -2.729637 -0.834423	C -5.184557 1.410991 0.508030
H -2.758766 -3.699136 -0.697772	O -4.624136 0.700958 1.320911
H -2.922108 -1.927663 -0.479975	C -6.657492 1.862124 0.723346
H -2.079462 -2.556285 -1.898292	O 4.506238 1.775968 -1.458306
C 2.591077 -2.155979 1.842386	C 5.116232 1.438964 -0.461150
H 3.348307 -1.890323 1.098906	O 4.672576 1.300987 0.757774
H 2.479973 -1.303777 2.519382	H 3.649270 1.524344 0.866161
H 2.914953 -3.038121 2.404856	C 6.633388 1.102547 -0.531752
C -1.308907 1.281919 -0.701522	N 1.324587 -2.375090 1.159625
C -1.228053 1.903129 0.640023	N -1.003160 -2.649583 -0.118952
H -2.154260 2.247947 1.088544	F -6.757528 3.210722 0.732606
C -0.045590 2.063045 1.268990	F -7.143621 1.404790 1.888422
H 0.023232 2.542299 2.241023	F -7.453096 1.399256 -0.268447

F 6.869729 -0.163136 -0.116369
F 7.103749 1.219360 -1.783875
F 7.350064 1.933348 0.259905

Energy and Thermal parameters

HF=-1829.8969177
Zero-point vibrational energy 744266.6 (Joules/Mol)
Zero-point correction= 0.283476 (Hartree/Particle)
Thermal correction to Energy= 0.315465
Thermal correction to Enthalpy= 0.316409
Thermal correction to Gibbs Free Energy= 0.207850
Sum of electronic and zero-point Energies= -1829.613441
Sum of electronic and thermal Energies= -1829.581453
Sum of electronic and thermal Enthalpies= -1829.580508
Sum of electronic and thermal Free Energies= -1829.689067

Transition State ([(NN)Pd(η^2-BQ)]*2HTFA)$_{TS}$, **12-13m$_{TS}$**

Cartesian Coordinates

Pd -1.203800 1.260400 0.162400
C -1.961900 3.218700 -1.783500
C -0.995900 3.874800 -0.909100
C -0.202200 0.876700 2.132400
C -1.279000 0.120000 2.687200
C -3.200100 1.262600 -2.343800
H -3.571000 1.884300 -3.163400
H -2.712500 0.370800 -2.742000
H -4.036300 0.949100 -1.712500
C 0.481300 3.833200 0.947700
H 0.037900 3.982500 1.936200
H 1.348500 3.177200 1.042800
H 0.782300 4.801300 0.540000
C -1.257100 -1.268200 2.664600
C -0.050200 -1.913600 2.235100
H -0.026900 -2.999800 2.264700
C 1.041800 -1.218800 1.756500
H 1.941500 -1.736400 1.441300
C 1.006200 0.198600 1.720200
H -2.152900 0.638600 3.068800
H -0.088500 1.904600 2.455200
O -2.347900 -1.996400 2.919000
O 2.047600 0.932400 1.384000
O -3.467400 -1.834800 0.881500
C -2.797200 -1.572000 -0.164300
O -1.891800 -0.741500 -0.372000
C -3.188200 -2.491300 -1.361100
N -0.503100 3.196500 0.070900
N -2.245200 1.993000 -1.522300
H -0.699800 4.906800 -1.089000
H -2.410700 3.757000 -2.617400
F -4.510800 -2.399900 -1.621900
F -2.916600 -3.780000 -1.058500
F -2.524600 -2.185600 -2.489500
H -2.986500 -1.862200 1.904900
H 2.863400 0.379300 1.031000
O 4.029900 -0.391800 0.600800
C 4.578000 -0.092200 -0.505600
C 5.789400 -1.025400 -0.839000
O 4.294200 0.792400 -1.320900
F 6.723300 -1.002800 0.147500
F 6.419300 -0.686600 -1.984100
F 5.389200 -2.318100 -0.975000

Energy and Thermal parameters

HF=-1829.8663872
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 742276.3 (Joules/Mol)
Zero-point correction= 0.282718 (Hartree/Particle)
Thermal correction to Energy= 0.311644
Thermal correction to Enthalpy= 0.312588
Thermal correction to Gibbs Free Energy= 0.217635
Sum of electronic and zero-point Energies= -1829.583669
Sum of electronic and thermal Energies= -1829.554743
Sum of electronic and thermal Enthalpies= -1829.553799
Sum of electronic and thermal Free Energies= -1829.648752

Compound([(NN)Pd(η^1-HBQ)(TFA)]*HTFA), **13m**

Cartesian Coordinates

Pd 1.236689 0.008804 0.068547	O 2.192566 -2.922369 -1.009718
C 3.094870 2.122496 -0.355953	O -1.366824 1.438549 1.284917
C 3.873318 1.036949 0.237833	C -1.519171 0.952786 0.169287
C 0.822619 -2.129894 0.765937	O -0.689315 0.308028 -0.570434
C -0.474556 -2.088737 1.367715	C -2.893262 1.141578 -0.550598
C 0.972265 2.933472 -1.099489	N 3.253316 -0.053591 0.533039
H 1.548869 3.813082 -1.398173	N 1.836708 1.915607 -0.516468
H 0.461160 2.506708 -1.965520	H 4.939233 1.157973 0.422889
H 0.218927 3.216461 -0.359667	H 3.571912 3.058625 -0.642994
C 3.994550 -1.155974 1.143260	F -3.848055 1.564558 0.299226
H 3.593915 -1.340195 2.144289	F -3.338239 0.001237 -1.124883
H 3.855675 -2.051289 0.533826	F -2.784843 2.071962 -1.534096
H 5.057160 -0.913017 1.219242	H -3.517759 -2.611198 0.617771
C -1.590626 -2.423994 0.633026	H 2.209599 -3.173569 -2.001573
C -1.440253 -2.850741 -0.711860	O 2.269835 -3.652549 -3.450793
H -2.324927 -3.112121 -1.287536	C 2.602531 -3.040282 -4.509355
C -0.197306 -2.959795 -1.305195	C 3.010387 -1.543485 -4.278465
H -0.101441 -3.326876 -2.321114	O 2.650683 -3.458828 -5.672515
C 0.969218 -2.663726 -0.558104	F 2.015227 -0.847674 -3.664888
H -0.573061 -1.782463 2.403493	F 3.304606 -0.884598 -5.418471
H 1.672132 -2.204671 1.434946	F 4.105248 -1.452077 -3.474498
O -2.820182 -2.335664 1.229217	

Energy and Thermal parameters

HF=-1829.895124
Zero-point vibrational energy 753916.4 (Joules/Mol)
Zero-point correction= 0.287152 (Hartree/Particle)
Thermal correction to Energy= 0.318354
Thermal correction to Enthalpy= 0.319298
Thermal correction to Gibbs Free Energy= 0.218316
Sum of electronic and zero-point Energies= -1829.607972
Sum of electronic and thermal Energies= -1829.576770
Sum of electronic and thermal Enthalpies= -1829.575826
Sum of electronic and thermal Free Energies= -1829.676808

Transition State ([(NN)Pd(TFA)(η^1-H_2BQ)]*TFA)$_{TS}$, **13-14m$_{TS}$**

Cartesian Coordinates

Pd -1.203800 1.260400 0.162400	H 0.037900 3.982500 1.936200
C -1.961900 3.218700 -1.783500	H 1.348500 3.177200 1.042800
C -0.995900 3.874800 -0.909100	H 0.782300 4.801300 0.540000
C -0.202200 0.876700 2.132400	C -1.257100 -1.268200 2.664600
C -1.279000 0.120000 2.687200	C -0.050200 -1.913600 2.235100
C -3.200100 1.262600 -2.343800	H -0.026900 -2.999800 2.264700
H -3.571000 1.884300 -3.163400	C 1.041800 -1.218800 1.756500
H -2.712500 0.370800 -2.742000	H 1.941500 -1.736400 1.441300
H -4.036300 0.949100 -1.712500	C 1.006200 0.198600 1.720200
C 0.481300 3.833200 0.947700	H -2.152900 0.638600 3.068800

H -0.088500 1.904600 2.455200
O -2.347900 -1.996400 2.919000
O 2.047600 0.932400 1.384000
O -3.467400 -1.834800 0.881500
C -2.797200 -1.572000 -0.164300
O -1.891800 -0.741500 -0.372000
C -3.188200 -2.491300 -1.361100
N -0.503100 3.196500 0.070900
N -2.245200 1.993000 -1.522300
H -0.699800 4.906800 -1.089000
H -2.410700 3.757000 -2.617400
F -4.510800 -2.399900 -1.621900
F -2.916600 -3.780000 -1.058500
F -2.524600 -2.185600 -2.489500
H -2.986500 -1.862200 1.904900
H 2.863400 0.379300 1.031000
O 4.029900 -0.391800 0.600800
C 4.578000 -0.092200 -0.505600
C 5.789400 -1.025400 -0.839000
O 4.294200 0.792400 -1.320900
F 6.723300 -1.002800 0.147500
F 6.419300 -0.686600 -1.984100
F 5.389200 -2.318100 -0.975000

Energy and Thermal parameters

HF=-1829.8722577
****** 1 imaginary frequency (negative Sign) ******
Zero-point vibrational energy 752429.7 (Joules/Mol)
Zero-point correction= 0.286585 (Hartree/Particle)
Thermal correction to Energy= 0.316199
Thermal correction to Enthalpy= 0.317143
Thermal correction to Gibbs Free Energy= 0.221205
Sum of electronic and zero-point Energies= -1829.585672
Sum of electronic and thermal Energies= -1829.556059
Sum of electronic and thermal Enthalpies= -1829.555115
Sum of electronic and thermal Free Energies= -1829.651052

Compound([(NN)Pd(TFA)(coordO-H_2BQ)]*TFA, **14m**

Cartesian Coordinates

Pd -0.760266 1.025121 -0.661435
C -2.764589 2.966830 -0.971513
C -3.031660 1.981178 -2.017983
C 2.300324 -0.418439 -1.960233
C 3.654927 -0.744728 -1.927699
C -1.369452 3.659801 0.852901
H -2.083655 4.483914 0.923480
H -1.345485 3.100423 1.791197
H -0.366714 4.045128 0.653043
C -2.374135 -0.065821 -3.083148
H -1.462225 -0.090860 -3.685575
H -2.476696 -1.032743 -2.583557
H -3.240762 0.130228 -3.719289
C 4.099432 -1.810127 -1.133884
C 3.183919 -2.541690 -0.369375
H 3.523002 -3.368459 0.249114
C 1.827888 -2.203253 -0.388410
H 1.120571 -2.761475 0.214962
C 1.390402 -1.147633 -1.190367
H 4.372285 -0.183483 -2.517908
H 1.945754 0.400742 -2.577740
O 5.443185 -2.087517 -1.147105
O 0.042399 -0.816455 -1.264274
O 1.895231 2.800049 -0.050706
C 1.613417 1.958340 0.795360
O 0.619341 1.146586 0.855433
C 2.540776 1.792299 2.041253
N -2.230996 0.973260 -2.070437
N -1.737556 2.747764 -0.224392
H -3.859195 2.101447 -2.714500
H -3.399729 3.840067 -0.836619
F 3.618221 2.597181 1.979478
F 2.991390 0.520751 2.159417
F 1.875808 2.092950 3.184769
H 5.638272 -2.833240 -0.561994
H -0.594113 -1.610633 -1.029356
O -1.535746 -2.719618 -0.992447
C -2.328950 -3.174384 -0.110741
C -2.332546 -2.389911 1.245535
O -3.114941 -4.123183 -0.197692
F -1.092891 -1.976142 1.609906
F -2.822823 -3.116715 2.271288
F -3.107016 -1.274350 1.141745

Energy and Thermal parameters

HF=-1829.909385
Zero-point vibrational energy 752408.0 (Joules/Mol)
Zero-point correction= 0.286577 (Hartree/Particle)
Thermal correction to Energy= 0.317777
Thermal correction to Enthalpy= 0.318721
Thermal correction to Gibbs Free Energy= 0.217241
Sum of electronic and zero-point Energies= -1829.622808
Sum of electronic and thermal Energies= -1829.591608
Sum of electronic and thermal Enthalpies= -1829.590664
Sum of electronic and thermal Free Energies= -1829.692144

Compound([(NN)Pd(TFA)$_2$]*H_2BQ, **15m**

Cartesian Coordinates

Pd	1.5984	-0.2047	0.9887
C	1.6112	0.3165	3.7497
C	1.3992	-1.1262	3.6358
C	-4.3509	0.1333	1.6551
C	-5.6149	0.5811	1.2690
C	1.9397	2.4082	2.6200
H	2.0018	2.8088	3.6347
H	2.8615	2.6192	2.0728
H	1.1074	2.8706	2.0832
C	1.1431	-3.0263	2.1937
H	0.2141	-3.1555	1.6322
H	1.9687	-3.3944	1.5801
H	1.0923	-3.5815	3.1334
C	-5.9450	0.6697	-0.0881
C	-5.0016	0.3074	-1.0535
H	-5.2469	0.3732	-2.1107
C	-3.7329	-0.1407	-0.6668
H	-3.0052	-0.4192	-1.4228
C	-3.4002	-0.2311	0.6911
H	-6.3502	0.8640	2.0163
H	-4.0920	0.0644	2.7075
F	-0.2608	-3.1734	-3.0979
F	1.4844	-3.9098	-2.0237
O	-7.2088	1.1209	-0.4091
O	-2.1749	-0.6580	1.1307
O	-0.0391	2.2170	-0.4970
C	1.1403	2.0892	-0.8068
O	2.0291	1.2718	-0.3698
C	1.7483	3.0312	-1.8946
N	1.3450	-1.6035	2.4402
N	1.7305	0.9657	2.6432
H	1.2949	-1.7569	4.5166
H	1.6640	0.8083	4.7191
F	0.8564	3.9375	-2.3369
F	2.1711	2.3214	-2.9700
F	2.8168	3.7156	-1.4177
H	-7.3214	1.1389	-1.3696
H	-1.5964	-0.9111	0.3785
O	-0.6665	-1.5730	-1.0141
C	0.5136	-1.8611	-1.2229
C	0.8440	-2.7881	-2.4344
O	1.5725	-1.5294	-0.5936
F	1.6530	-2.1606	-3.3201

Energy and Thermal parameters

HF=-1829.918607
Zero-point vibrational energy 752408.0 (Joules/Mol)
Zero-point correction= 0.286377 (Hartree/Particle)
Thermal correction to Energy= 0.315277
Thermal correction to Enthalpy= 0.32321
Thermal correction to Gibbs Free Energy= 0.215241
Sum of electronic and zero-point Energies= -1829.622808
Sum of electronic and thermal Energies= -1829.593608
Sum of electronic and thermal Enthalpies= -1829.5790664
Sum of electronic and thermal Free Energies= -1829.7028298