Supplementary Information

Computational Study of Multiple Pathways and Ion-Pairing in Oxidative Addition of Iodomethane to a Binuclear Organoplatinum(II) Complex containing Imine and Phosphine Bridging Ligands

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Energy parameters and coordinates for calculated species

All calculations related to thermodynamic effects are obtained using M06/BS1; single-point data, listed immediately after BS1 data, are calculated using BS2 and M06L-D3, and are followed by Cartesian coordinates.

1A
E(RM06) = -2463.77005035
Zero-point correction= 0.666275 (Hartree/Particle)
Thermal correction to Energy= 0.710994
Thermal correction to Enthalpy= 0.711938
Thermal correction to Gibbs Free Energy= 0.585485
Sum of electronic and zero-point Energies= -2463.103776
Sum of electronic and thermal Energies= -2463.059056
Sum of electronic and thermal Enthalpies= -2463.058112
Sum of electronic and thermal Free Energies= -2463.184565
E(RM06L) = -2465.58612179

Pt 1.82543 1.05789 -1.62712
C 1.19324 1.69242 -3.50821
H 1.01499 0.82319 -4.16291
H 0.25463 2.26666 -3.44128
H 1.94807 2.32801 -3.99909
Pt -1.10398 -0.7594 -1.5016
C -1.2896 -2.63183 -2.35478
H -0.64114 -2.70275 -3.24419
H -1.02299 -3.4623 -1.68241
H -2.32435 -2.80028 -2.69399
C -2.29241 -0.11013 -3.0964
H -1.91782 -0.48978 -4.06093
H -3.32714 -0.47506 -2.98118
H -2.32947 0.98989 -3.15771
C -2.20082 5.73217 1.33041
C -1.04296 5.19698 0.812
C -1.06932 3.88908 0.29209
C -2.2693 3.14251 0.30919
C -3.44391 3.70698 0.8415
C -3.4006 4.98816 1.34373
H 1.02312 3.76536 -0.31898
H -2.19693 6.74197 1.73563
H -0.11154 5.7612 0.79729
C 0.06384 3.24836 -0.26214
C -2.20613 1.83409 -0.22539
H -4.3642 3.12517 0.84803

H -4.30036 5.43823 1.75819
H -3.09228 1.19831 -0.25306
N -1.10777 1.29866 -0.70829
N 0.04651 2.02096 -0.72994
C 3.45626 0.25827 -2.60177
H 4.40337 0.60231 -2.15344
H 3.47832 0.53513 -3.66734
H 3.44238 -0.84362 -2.55101
C 0.89851 -0.33052 1.45999
H 0.14499 0.45345 1.621
H 1.15868 -0.75581 2.44004
P 2.36183 0.46548 0.64465
P 0.09454 -1.59808 0.36845
C 2.58139 2.02653 1.59072
C 3.59762 2.88357 1.14576
C 1.77198 2.43023 2.65457
C 3.79049 4.12279 1.74482
H 4.23616 2.57844 0.31328
C 1.95997 3.67834 3.24807
H 0.98612 1.77782 3.03436
C 2.96318 4.52712 2.79233
H 4.58252 4.77934 1.38774
H 1.31747 3.98381 4.07275
H 3.10584 5.50236 3.25518
C 3.77562 -0.53434 1.26088
C 3.99974 -0.66513 2.63777
C 4.64541 -1.15935 0.36598
C 5.0675 -1.41976 3.10753
H 3.33528 -0.17188 3.34927
C 5.71927 -1.91252 0.83879
H 4.47885 -1.06973 -0.70545
C 5.92999 -2.04511 2.20682
H 5.23151 -1.51804 4.17968
H 6.38772 -2.40096 0.13086
H 6.76796 -2.63474 2.57581
C 1.42667 -2.83085 0.13495
C 2.00972 -3.4931 1.22311
C 1.91198 -3.0718 -1.15274
C 3.05749 -4.38402 1.0218
H 1.64354 -3.31116 2.23484
C 2.96367 -3.9642 -1.35379
H 1.46609 -2.54781 -1.9993
C 3.53469 -4.62041 -0.26762
H 3.50914 -4.89109 1.87341
H 3.33554 -4.14356 -2.36167
H 4.35706 -5.31748 -0.42282
C -1.08342 -2.40622 1.52047
C -1.27972 -3.79108 1.51476
C -1.91529 -1.6073 2.31608
C -2.27504 -4.36567 2.30165
H -0.64744 -4.43082 0.89884
C -2.90414 -2.1844 3.10601
H -1.79661 -0.52248 2.32081
C -3.08643 -3.5657 3.10078
H -2.41294 -5.44589 2.29042
H -3.53641 -1.55134 3.72702
H -3.86159 -4.01699 3.71805

1B
E(RM06) = -2463.75203911

Zero-point correction= 0.667639 (Hartree/Particle)
Thermal correction to Energy= 0.712091
Thermal correction to Enthalpy= 0.713035
Thermal correction to Gibbs Free Energy= 0.588177
Sum of electronic and zero-point Energies= -2463.084400
Sum of electronic and thermal Energies= -2463.039948
Sum of electronic and thermal Enthalpies= -2463.039004
Sum of electronic and thermal Free Energies= -2463.163862
E(RM06) = -2464.43586437

Pt 1.83257 1.03035 -1.57197
C 1.20772 1.66023 -3.44966
H 0.99956 0.78066 -4.07877
H 0.2822 2.25498 -3.38245
H 1.97687 2.26923 -3.94974
Pt -1.15598 -0.74139 -1.44917
C -1.41146 -2.61759 -2.2692
H -0.80675 -2.70244 -3.18663
H -1.13124 -3.44746 -1.60193
H -2.46495 -2.76305 -2.55272
C -2.34655 -0.10086 -3.03964
H -1.99899 -0.53396 -3.98977
H -3.39258 -0.41731 -2.89132
H -2.32921 0.99618 -3.14576
C -2.16742 5.86666 1.14192
C -1.00399 5.27778 0.70321
C -1.04524 3.95687 0.21634
C -2.2688 3.25021 0.1874
C -3.44986 3.87139 0.63893
C -3.39121 5.16347 1.10774
H 1.07233 3.74416 -0.28862
H -2.15026 6.88724 1.51896
H -0.05438 5.8107 0.72532
C 0.09225 3.2653 -0.26245
C -2.2195 1.92356 -0.30294
H -4.39002 3.32252 0.60954
H -4.297 5.65487 1.45731
H -3.11918 1.30926 -0.36316
N -1.11515 1.33841 -0.70935
N 0.05908 2.02581 -0.69558
C 3.44864 0.22073 -2.5557
H 4.39727 0.60012 -2.13996
H 3.44128 0.46176 -3.6288
H 3.44693 -0.87826 -2.46634
C 0.8973 -0.37659 1.50252
H 0.14864 0.40808 1.68172
H 1.15663 -0.82352 2.47351
P 2.36012 0.43176 0.69058
P 0.07357 -1.613 0.37806
C 2.55938 1.99259 1.64939
C 3.56362 2.86327 1.20365
C 1.7442 2.39326 2.70973
C 3.73898 4.1067 1.79777
H 4.20001 2.5646 0.36786
C 1.91211 3.64653 3.29803
H 0.96787 1.73086 3.09289
C 2.90479 4.50594 2.84133
H 4.52299 4.77168 1.43863
H 1.26535 3.94598 4.12174
H 3.03523 5.48441 3.30113

C 3.7751 -0.55711 1.3233
C 3.98668 -0.70628 2.69945
C 4.66121 -1.15765 0.42859
C 5.05476 -1.45865 3.16969
H 3.31456 -0.22304 3.41089
C 5.73644 -1.9073 0.90198
H 4.50194 -1.05078 -0.64235
C 5.93257 -2.06093 2.26905
H 5.20979 -1.57021 4.24197
H 6.41738 -2.37711 0.19356
H 6.7725 -2.64785 2.63811
C 1.42026 -2.81542 0.0735
C 2.04308 -3.51171 1.11682
C 1.87253 -2.9954 -1.23574
C 3.09658 -4.37754 0.85192
H 1.70196 -3.37785 2.14478
C 2.93017 -3.86319 -1.49995
H 1.39606 -2.43899 -2.04421
C 3.54 -4.55401 -0.45811
H 3.58152 -4.90799 1.67031
H 3.27597 -3.9952 -2.52423
H 4.36719 -5.23208 -0.6645
C -1.04532 -2.47432 1.55435
C -1.19812 -3.86372 1.55082
C -1.8761 -1.70907 2.38218
C -2.14474 -4.47279 2.37027
H -0.56963 -4.47944 0.9078
C -2.81543 -2.31832 3.20552
H -1.79745 -0.62022 2.37968
C -2.95142 -3.70427 3.20234
H -2.24918 -5.55669 2.35657
H -3.44778 -1.70801 3.84901
H -3.689 -4.18282 3.84461

2A
E(RM06) = -2515.05357238
Zero-point correction= 0.705891 (Hartree/Particle)
Thermal correction to Energy= 0.754614
Thermal correction to Enthalpy= 0.755559
Thermal correction to Gibbs Free Energy= 0.620303
Sum of electronic and zero-point Energies= -2514.347681
Sum of electronic and thermal Energies= -2514.298958
Sum of electronic and thermal Enthalpies= -2514.298014
Sum of electronic and thermal Free Energies= -2514.433270
E(RM06L) = -2803.40199190

Pt 0.20211 2.13095 -0.98769
C -1.02797 2.94014 -2.48408
H -0.51165 3.01004 -3.45476
H -1.92687 2.31375 -2.62856
H -1.36755 3.95618 -2.21617
Pt -1.40315 -1.81119 -0.93941
C -0.8627 -3.78305 -1.22675
H -0.17547 -3.84946 -2.07861
H -0.37475 -4.17818 -0.32622
H -1.75825 -4.38224 -1.43706
C -2.6756 -2.09999 -2.56376
H -2.18052 -2.72777 -3.31469
H -3.61863 -2.5787 -2.26842
H -2.88092 -1.11462 -3.00571

C -2.86205 -2.63714 0.2921
H -3.20493 -1.87407 1.00182
H -3.70694 -2.98914 -0.31148
H -2.44619 -3.48428 0.8497
C -5.88027 3.35932 1.27147
C -4.50388 3.40256 1.26387
C -3.79462 2.36194 0.63526
C -4.4905 1.29468 0.02841
C -5.89744 1.26697 0.04367
C -6.57648 2.29373 0.66104
H -1.78518 3.16337 0.89005
H -6.4443 4.15678 1.75085
H -3.9584 4.22452 1.72462
C -2.38593 2.33315 0.51579
C -3.69537 0.26882 -0.53419
H -6.42459 0.43837 -0.42642
H -7.66434 2.28811 0.68234
H -4.17763 -0.61105 -0.9592
N -2.38138 0.28171 -0.55931
N -1.71584 1.37261 -0.08431
C 1.73483 3.13603 -1.93668
H 2.66205 3.19467 -1.34619
H 1.42345 4.16666 -2.17144
H 1.97037 2.63888 -2.89203
I 0.46514 -0.91203 -3.01704
C 0.67253 0.06587 1.82249
H -0.2459 0.58886 2.12009
H 1.24985 -0.13672 2.73758
P 1.55702 1.27034 0.73044
P 0.13459 -1.56863 1.1141
C 2.01372 2.58204 1.93548
C 3.20251 3.30057 1.76015
C 1.12768 2.97982 2.94374
C 3.50252 4.38376 2.58084
H 3.90747 3.0089 0.98111
C 1.43318 4.05979 3.76753
H 0.18964 2.44599 3.09944
C 2.62021 4.7652 3.58802
H 4.43374 4.92882 2.43326
H 0.73876 4.34903 4.55516
H 2.85727 5.61005 4.23265
C 3.17182 0.49232 0.35571
C 4.0196 0.04606 1.37718
C 3.57452 0.35582 -0.97436
C 5.24335 -0.5358 1.06795
H 3.72355 0.15651 2.42182
C 4.80217 -0.22623 -1.28419
H 2.9142 0.69667 -1.77112
C 5.63518 -0.67357 -0.26398
H 5.89361 -0.88719 1.86823
H 5.10432 -0.32889 -2.32551
H 6.5943 -1.13104 -0.50304
C 1.69687 -2.53242 1.13663
C 2.34059 -2.82344 2.34736
C 2.28249 -2.94732 -0.06129
C 3.53631 -3.53119 2.35652
H 1.90511 -2.49928 3.293
C 3.48826 -3.64616 -0.051
H 1.80346 -2.70708 -1.01117
C 4.1112 -3.94567 1.15609

H 4.02422 -3.75566 3.30389
H 3.93904 -3.95511 -0.99305
H 5.05012 -4.49741 1.16346
C -0.78761 -2.23131 2.5604
C -0.69211 -3.58071 2.91851
C -1.73241 -1.42868 3.21025
C -1.50721 -4.10823 3.91618
H 0.02325 -4.23246 2.41734
C -2.54339 -1.9559 4.21044
H -1.86509 -0.38362 2.92462
C -2.43289 -3.29738 4.56663
H -1.41619 -5.15979 4.18402
H -3.26881 -1.31471 4.70892
H -3.06936 -3.71032 5.34755

2B
E(RM06) = -2515.03209637
Zero-point correction= 0.707177 (Hartree/Particle)
Thermal correction to Energy= 0.755581
Thermal correction to Enthalpy= 0.756525
Thermal correction to Gibbs Free Energy= 0.622702
Sum of electronic and zero-point Energies= -2514.324919
Sum of electronic and thermal Energies= -2514.276516
Sum of electronic and thermal Enthalpies= -2514.275572
Sum of electronic and thermal Free Energies= -2514.409395
E(RM06L) = -2803.38594037

Pt 0.18079 2.14605 -0.94208
C -1.04417 2.95697 -2.43396
H -0.52024 3.00345 -3.40001
H -1.94151 2.32868 -2.57948
H -1.37271 3.97927 -2.1779
Pt -1.42867 -1.83008 -0.86961
C -0.89001 -3.80183 -1.15521
H -0.23242 -3.87131 -2.02926
H -0.36919 -4.18868 -0.26958
H -1.79063 -4.40517 -1.32789
C -2.69835 -2.136 -2.49098
H -2.19773 -2.76668 -3.23445
H -3.63939 -2.61881 -2.19193
H -2.89706 -1.15742 -2.9491
C -2.88751 -2.63657 0.3886
H -3.23002 -1.87151 1.09886
H -3.74007 -2.99531 -0.20259
H -2.48391 -3.48253 0.95829
C -5.96305 3.4706 0.97432
C -4.58892 3.49442 1.03959
C -3.85986 2.41479 0.5041
C -4.53806 1.32708 -0.08579
C -5.94481 1.31996 -0.14439
C -6.64138 2.3836 0.38177
H -1.84834 3.19677 0.82991
H -6.5392 4.29993 1.3795
H -4.05784 4.33439 1.48476
C -2.44737 2.35954 0.46803
C -3.72783 0.26708 -0.55702
H -6.46039 0.47734 -0.60275
H -7.72878 2.39226 0.34267
H -4.19264 -0.62936 -0.9669
N -2.41488 0.26622 -0.51608

N -1.75969 1.3656 -0.05441
C 1.68244 3.2013 -1.87593
H 2.60461 3.27878 -1.28002
H 1.33857 4.22308 -2.09614
H 1.92399 2.71248 -2.83289
I 0.3996 -0.91046 -2.88335
C 0.6894 0.05242 1.84555
H -0.2296 0.5737 2.14514
H 1.26874 -0.14716 2.76027
P 1.55683 1.2733 0.74443
P 0.14711 -1.58432 1.14315
C 2.04003 2.54899 1.98142
C 3.24204 3.24884 1.82974
C 1.15853 2.94502 2.99375
C 3.5582 4.30707 2.67551
H 3.94375 2.9611 1.04686
C 1.47891 3.99825 3.844
H 0.20716 2.42836 3.12893
C 2.68017 4.68334 3.68686
H 4.49946 4.83832 2.54246
H 0.78559 4.28447 4.6339
H 2.93029 5.50916 4.35089
C 3.16216 0.49422 0.3342
C 4.04171 0.04394 1.32605
C 3.52369 0.36911 -1.00838
C 5.25859 -0.52722 0.97684
H 3.779 0.14816 2.38023
C 4.74589 -0.20081 -1.35765
H 2.83188 0.70404 -1.78044
C 5.61181 -0.64861 -0.36689
H 5.93398 -0.88224 1.7544
H 5.01478 -0.29481 -2.40861
H 6.56741 -1.09574 -0.63818
C 1.7181 -2.53524 1.13774
C 2.37827 -2.83446 2.33757
C 2.29374 -2.92872 -0.07172
C 3.58038 -3.52971 2.32561
H 1.94622 -2.53139 3.292
C 3.5061 -3.61514 -0.08118
H 1.80554 -2.67659 -1.01408
C 4.14515 -3.92309 1.11392
H 4.08021 -3.76241 3.26488
H 3.94924 -3.90409 -1.0328
H 5.08959 -4.46548 1.10394
C -0.73367 -2.2614 2.612
C -0.62782 -3.61427 2.95374
C -1.6609 -1.47107 3.30001
C -1.41223 -4.15455 3.96798
H 0.076 -4.25724 2.42584
C -2.44175 -2.00983 4.31702
H -1.8019 -0.42256 3.03135
C -2.31927 -3.35406 4.65478
H -1.31223 -5.20913 4.21996
H -3.15302 -1.37562 4.84408
H -2.93174 -3.77718 5.44914

2aA
E(RM06) = -2515.06378006
Zero-point correction= 0.705893 (Hartree/Particle)
Thermal correction to Energy= 0.754541

Thermal correction to Enthalpy= 0.755485
Thermal correction to Gibbs Free Energy= 0.622235
Sum of electronic and zero-point Energies= -2514.357887
Sum of electronic and thermal Energies= -2514.309239
Sum of electronic and thermal Enthalpies= -2514.308295
Sum of electronic and thermal Free Energies= -2514.441545
E(RM06L) = -2803.41086075

Pt -2.13883 0.72377 -1.06176
C -3.50724 -0.04992 -2.44232
H -4.44962 -0.37048 -1.97082
H -3.76216 0.73431 -3.17635
H -3.09655 -0.90464 -3.00354
Pt 1.29594 -2.15739 -0.69791
C 3.1061 -2.17002 -1.69951
H 3.00914 -1.59805 -2.63231
H 3.90089 -1.72471 -1.08595
H 3.39635 -3.19909 -1.94838
C 0.82351 -3.78886 -1.90492
H 0.81364 -3.47027 -2.95606
H 1.55649 -4.59711 -1.78444
H -0.17069 -4.16861 -1.62887
C 2.06073 -3.58936 0.58899
H 2.1408 -3.16358 1.59544
H 1.35967 -4.43405 0.60209
H 3.04486 -3.93167 0.24443
C -5.3634 -2.4136 2.0912
C -4.14357 -2.26803 2.71466
C -2.96957 -2.31608 1.94034
C -3.04993 -2.50247 0.54403
C -4.30388 -2.66542 -0.07574
C -5.44322 -2.61845 0.6968
H -1.52383 -2.06116 3.554
H -6.2799 -2.37697 2.6768
H -4.07074 -2.11839 3.79118
C -1.6621 -2.18277 2.4772
C -1.82516 -2.47422 -0.16947
H -4.35463 -2.81838 -1.15314
H -6.4194 -2.73904 0.23126
H -1.81801 -2.58798 -1.25387
N -0.65907 -2.31994 0.41513
N -0.56513 -2.19147 1.76548
C -3.82449 1.4415 -0.10614
H -3.64267 2.40111 0.39969
H -4.14404 0.70983 0.65642
H -4.65653 1.57507 -0.81279
I 0.02871 -0.35095 -2.62521
C 0.60917 0.83062 1.48605
H 0.00239 0.11428 2.05465
H 1.06852 1.5201 2.21064
P -0.63512 1.77827 0.47276
P 1.95884 -0.18962 0.73956
C -1.51778 2.5891 1.8713
C -1.80409 3.95692 1.86021
C -2.0553 1.79604 2.89281
C -2.59868 4.52185 2.85594
H -1.41176 4.59169 1.06548
C -2.84388 2.36134 3.88887
H -1.87691 0.71868 2.90874
C -3.11816 3.72745 3.87303

H -2.81186 5.58962 2.83241
H -3.25102 1.72993 4.67758
H -3.73951 4.16969 4.65021
C 0.31914 3.15972 -0.26491
C 1.25773 3.89381 0.46968
C 0.06098 3.5203 -1.59083
C 1.9339 4.95723 -0.11774
H 1.45576 3.6466 1.51351
C 0.73936 4.58567 -2.17989
H -0.67849 2.95554 -2.16234
C 1.67881 5.30144 -1.44484
H 2.66442 5.52019 0.4621
H 0.53031 4.85493 -3.21413
H 2.21167 6.13338 -1.90307
C 3.15042 1.06092 0.10784
C 3.90413 1.82621 1.0079
C 3.29841 1.28551 -1.26296
C 4.79018 2.79116 0.54355
H 3.80075 1.66789 2.08189
C 4.1819 2.25813 -1.72706
H 2.71407 0.7029 -1.97407
C 4.93022 3.00905 -0.82592
H 5.37136 3.37753 1.25383
H 4.28578 2.42388 -2.79836
H 5.62419 3.76535 -1.18984
C 2.83479 -0.7872 2.2402
C 4.1277 -1.30361 2.07396
C 2.24251 -0.84842 3.50396
C 4.81012 -1.8656 3.14578
H 4.60751 -1.26811 1.09442
C 2.92833 -1.41443 4.57786
H 1.23951 -0.45811 3.67025
C 4.20958 -1.925 4.40237
H 5.81456 -2.25978 2.99917
H 2.45416 -1.45046 5.55755
H 4.74221 -2.36729 5.2427

2aB
E(RM06) = -2515.05106681
Zero-point correction= 0.707048 (Hartree/Particle)
Thermal correction to Energy= 0.755587
Thermal correction to Enthalpy= 0.756531
Thermal correction to Gibbs Free Energy= 0.623223
Sum of electronic and zero-point Energies= -2514.344018
Sum of electronic and thermal Energies= -2514.295480
Sum of electronic and thermal Enthalpies= -2514.294536
Sum of electronic and thermal Free Energies= -2514.427844
E(RM06L) = -2803.40317258

Pt 0.99485 -1.40879 -1.40708
C 1.93205 0.20346 -2.34423
H 3.02964 0.16063 -2.26562
H 1.67791 0.17488 -3.41707
H 1.58604 1.17277 -1.9509
Pt -1.10074 0.08928 2.19265
C -3.05182 0.74347 2.40606
H -3.26627 1.4718 1.61201
H -3.76725 -0.08499 2.32344
H -3.19346 1.23547 3.37728
C -0.62383 2.11168 2.36112

H -0.85319 2.62074 1.41601
H -1.19736 2.58075 3.17125
H 0.44771 2.21703 2.5835
C -0.85314 0.08124 4.25383
H -0.53125 -0.91875 4.5663
H -0.07018 0.80856 4.5049
H -1.78357 0.35634 4.76535
C 5.97074 -0.94258 1.1461
C 5.09259 -1.62512 1.9577
C 3.74123 -1.23392 1.98897
C 3.30125 -0.15503 1.19402
C 4.21373 0.53781 0.37599
C 5.53154 0.14078 0.35638
H 3.013 -2.71435 3.41788
H 7.01765 -1.2377 1.11035
H 5.42555 -2.45988 2.57345
C 2.74673 -1.8681 2.78007
C 1.92109 0.16212 1.26525
H 3.86226 1.36628 -0.23725
H 6.24553 0.66306 -0.27716
H 1.51119 0.9826 0.67621
N 1.07879 -0.47169 2.05073
N 1.48954 -1.51265 2.81878
C 2.64423 -2.46669 -2.06047
H 2.40974 -3.51953 -2.27347
H 3.4251 -2.43922 -1.2812
H 3.05795 -2.01448 -2.97276
I -1.21835 0.30775 -0.70556
C -0.58937 -3.50742 1.26145
H 0.3534 -3.37974 1.8106
H -0.94216 -4.53387 1.44598
P -0.09798 -3.33904 -0.53461
P -1.76255 -2.33364 2.07857
C 0.93397 -4.86391 -0.62837
C 0.74488 -5.82267 -1.62606
C 2.0287 -4.99792 0.23382
C 1.61911 -6.90022 -1.7472
H -0.08776 -5.72768 -2.32248
C 2.8959 -6.07734 0.11827
H 2.22537 -4.23336 0.98904
C 2.6923 -7.03362 -0.8739
H 1.45809 -7.63739 -2.53248
H 3.74175 -6.16727 0.79869
H 3.37563 -7.87594 -0.9696
C -1.60332 -3.81613 -1.46762
C -2.42657 -4.88151 -1.08681
C -1.90121 -3.11138 -2.63703
C -3.53319 -5.22486 -1.85379
H -2.19939 -5.4599 -0.19028
C -3.00848 -3.45779 -3.40775
H -1.25506 -2.2837 -2.93614
C -3.82602 -4.51161 -3.01504
H -4.17136 -6.0512 -1.54296
H -3.22946 -2.90004 -4.31639
H -4.69392 -4.78238 -3.61486
C -3.40552 -2.83412 1.41696
C -4.00091 -4.02807 1.84452
C -4.06088 -2.05599 0.45925
C -5.22441 -4.43252 1.32489
H -3.50707 -4.64729 2.59414

C -5.28426 -2.46602 -0.06444
H -3.60707 -1.13062 0.10589
C -5.86847 -3.6511 0.36831
H -5.67692 -5.36148 1.66921
H -5.77779 -1.85225 -0.81609
H -6.82766 -3.96793 -0.03879
C -1.84542 -3.01252 3.78344
C -2.89091 -2.56815 4.60416
C -0.8701 -3.84809 4.3305
C -2.9601 -2.95532 5.93573
H -3.65774 -1.9067 4.1968
C -0.93952 -4.23423 5.66773
H -0.0398 -4.20355 3.72223
C -1.9813 -3.78954 6.47232
H -3.77993 -2.60146 6.55879
H -0.17243 -4.88913 6.0784
H -2.03264 -4.09099 7.51725

3A
E(RM06) = -2554.77823149
Zero-point correction= 0.746792 (Hartree/Particle)
Thermal correction to Energy= 0.796641
Thermal correction to Enthalpy= 0.797586
Thermal correction to Gibbs Free Energy= 0.661472
Sum of electronic and zero-point Energies= -2554.031439
Sum of electronic and thermal Energies= -2553.981590
Sum of electronic and thermal Enthalpies= -2553.980646
Sum of electronic and thermal Free Energies= -2554.116760
E(RM06L) = -2843.1790061

Pt 0.30601 2.20052 -1.22552
C -0.91299 2.89903 -2.76884
H -0.42262 2.7377 -3.73824
H -1.84968 2.32039 -2.74674
H -1.14213 3.96776 -2.6593
Pt -1.36544 -1.65412 -0.9396
C -0.70604 -3.54132 -1.45662
H 0.01715 -3.45285 -2.27731
H -0.23182 -4.0327 -0.59747
H -1.5565 -4.14973 -1.79039
C -2.57916 -1.81709 -2.62761
H -2.00563 -2.2601 -3.4521
H -3.46622 -2.43618 -2.43995
H -2.89154 -0.8033 -2.91779
C -2.78119 -2.70562 0.15946
H -3.11473 -2.08538 1.00176
H -3.63597 -2.96585 -0.47663
H -2.33453 -3.62695 0.55083
C -5.81973 3.42677 1.52962
C -4.45855 3.5379 1.34895
C -3.76858 2.47797 0.7332
C -4.4643 1.32621 0.31307
C -5.8548 1.2291 0.50093
C -6.51662 2.27529 1.10517
H -1.81135 3.39885 0.70008
H -6.3708 4.23632 2.00354
H -3.91338 4.42526 1.66634
C -2.38172 2.50507 0.45442
C -3.67658 0.29818 -0.25518
H -6.38286 0.33507 0.17349

H -7.59182 2.2178 1.26131
H -4.1521 -0.63418 -0.55793
N -2.37599 0.37114 -0.42741
N -1.71671 1.52708 -0.1169
C 1.86535 3.00515 -2.31374
H 2.73233 3.17071 -1.6625
H 1.55388 3.96135 -2.75163
H 2.12636 2.30687 -3.11806
I 0.49482 -0.29696 -2.64368
C 0.66066 0.18885 1.72777
H -0.25241 0.76599 1.92574
H 1.17318 0.02915 2.68923
P 1.66583 1.31299 0.65973
P 0.1004 -1.47284 1.116
C 2.12352 2.63145 1.84829
C 3.24689 3.41539 1.55671
C 1.32631 2.96839 2.94633
C 3.56764 4.51127 2.3499
H 3.88154 3.16639 0.70489
C 1.65349 4.06461 3.74196
H 0.44199 2.38205 3.19538
C 2.77074 4.8388 3.44481
H 4.44626 5.10929 2.11337
H 1.02941 4.3112 4.59956
H 3.02284 5.69578 4.06715
C 3.27683 0.49121 0.3852
C 4.00772 0.01481 1.48088
C 3.82225 0.39717 -0.89685
C 5.25429 -0.5681 1.28947
H 3.60236 0.10392 2.48991
C 5.07553 -0.18234 -1.08557
H 3.2661 0.77302 -1.75396
C 5.78868 -0.66849 0.00498
H 5.81233 -0.94498 2.1455
H 5.49316 -0.24978 -2.08882
H 6.76716 -1.12326 -0.14203
C 1.63502 -2.47067 1.19395
C 2.20543 -2.81727 2.42561
C 2.27974 -2.84693 0.01237
C 3.38941 -3.54423 2.47067
H 1.72194 -2.52166 3.35709
C 3.47368 -3.56276 0.06025
H 1.8551 -2.56568 -0.95167
C 4.02393 -3.91917 1.28782
H 3.82136 -3.81406 3.43309
H 3.97269 -3.84178 -0.86663
H 4.95325 -4.48567 1.32419
C -0.8742 -2.03871 2.56374
C -0.92235 -3.40284 2.87561
C -1.72461 -1.16086 3.246
C -1.78676 -3.87439 3.85844
H -0.28265 -4.10907 2.34525
C -2.58819 -1.63531 4.2298
H -1.73462 -0.09472 3.01731
C -2.62201 -2.99206 4.53832
H -1.80734 -4.93791 4.09088
H -3.23745 -0.93757 4.75634
H -3.29888 -3.36161 5.30677
C 0.24048 4.08034 -0.34005
H 0.11562 3.96996 0.74515

H 1.18083 4.61414 -0.52361
H -0.5895 4.66272 -0.75898

4A
E(RM06) = -2148.69993708
Zero-point correction= 0.620115 (Hartree/Particle)
Thermal correction to Energy= 0.664807
Thermal correction to Enthalpy= 0.665751
Thermal correction to Gibbs Free Energy= 0.539963
Sum of electronic and zero-point Energies= -2148.079822
Sum of electronic and thermal Energies= -2148.035130
Sum of electronic and thermal Enthalpies= -2148.034186
Sum of electronic and thermal Free Energies= -2148.159974
E(RM06L) = -2723.16842698

C 3.48766 -0.94994 -0.93871
H 4.00803 -1.08518 0.01835
H 3.41965 -1.90734 -1.47095
H 4.03913 -0.2295 -1.55499
Pt 1.58698 -0.22653 -0.55314
C 2.55031 1.62233 -0.49295
H 1.84222 2.37655 -0.12173
H 3.40359 1.55793 0.19595
H 2.91529 1.92321 -1.48384
Pt -1.05419 0.38979 2.57824
C -3.00098 1.01102 2.91963
H -3.37931 1.48298 2.00385
H -3.62805 0.15251 3.19198
H -3.01469 1.74256 3.73651
C -0.58835 2.38218 2.98717
H -1.22011 3.03203 2.36607
H -0.75481 2.62944 4.04416
H 0.46696 2.55833 2.73495
C -0.91556 0.05872 4.62026
H -0.1282 0.70689 5.02458
H -1.86837 0.28775 5.11548
H -0.6502 -0.99118 4.79581
C 1.39679 0.06921 -2.59376
H 2.27423 -0.31806 -3.12816
H 1.29858 1.14529 -2.78271
H 0.4914 -0.44322 -2.93979
I -1.05675 0.99824 -0.27682
C -0.51174 -3.02038 0.98989
H 0.29666 -3.29382 1.67913
H -1.02778 -3.95944 0.73422
P 0.46614 -2.49219 -0.51179
P -1.66519 -1.97604 2.01398
C 1.6094 -3.93989 -0.491
C 1.34688 -5.11917 -1.19471
C 2.73267 -3.88382 0.34331
C 2.20391 -6.21124 -1.08295
H 0.46753 -5.19473 -1.83331
C 3.58414 -4.9778 0.4583
H 2.93893 -2.97822 0.91525
C 3.3243 -6.14212 -0.26048
H 1.98822 -7.12253 -1.6388
H 4.45466 -4.91813 1.10976
H 3.99304 -6.99723 -0.1755
C -0.5774 -2.81817 -1.97495
C -1.96889 -2.90812 -1.9173

C 0.05781 -2.90776 -3.22273
C -2.71422 -3.08551 -3.08179
H -2.48519 -2.84637 -0.96199
C -0.68622 -3.09444 -4.38151
H 1.14592 -2.84438 -3.28689
C -2.07615 -3.17911 -4.31366
H -3.79917 -3.15701 -3.0175
H -0.1786 -3.1718 -5.34163
H -2.65879 -3.32126 -5.22241
C -3.30157 -2.30975 1.24913
C -3.79138 -3.62237 1.19546
C -4.03501 -1.28679 0.64398
C -4.9811 -3.90377 0.53509
H -3.23568 -4.43442 1.66592
C -5.22826 -1.56982 -0.01789
H -3.66414 -0.26414 0.67001
C -5.70007 -2.87709 -0.07628
H -5.34846 -4.92796 0.4959
H -5.78712 -0.76313 -0.48943
H -6.63072 -3.09895 -0.59633
C -1.7627 -2.95993 3.5632
C -2.9445 -2.88826 4.31362
C -0.65385 -3.60755 4.11705
C -3.01771 -3.46176 5.57828
H -3.82015 -2.38071 3.90728
C -0.73134 -4.18598 5.38201
H 0.293 -3.66151 3.58072
C -1.91066 -4.11393 6.11626
H -3.94601 -3.40019 6.14419
H 0.14015 -4.69271 5.7935
H -1.968 -4.56418 7.10585
I 1.78304 -0.3559 2.37054

4B
E(RM06) = -2148.69341165
Zero-point correction= 0.621217 (Hartree/Particle)
Thermal correction to Energy= 0.665838
Thermal correction to Enthalpy= 0.666782
Thermal correction to Gibbs Free Energy= 0.541318
Sum of electronic and zero-point Energies= -2148.072194
Sum of electronic and thermal Energies= -2148.027574
Sum of electronic and thermal Enthalpies= -2148.026630
Sum of electronic and thermal Free Energies= -2148.152094
E(RM06L) = -2723.16466239

C 3.5018 -0.92937 -0.90244
H 4.02235 -1.04284 0.05741
H 3.45512 -1.89529 -1.42216
H 4.04923 -0.21049 -1.52398
Pt 1.58877 -0.22321 -0.53928
C 2.5378 1.62884 -0.46093
H 1.8062 2.37588 -0.12541
H 3.36119 1.57387 0.26307
H 2.93785 1.92127 -1.44038
Pt -1.05512 0.39398 2.56828
C -2.99708 1.04191 2.89103
H -3.36367 1.52403 1.97563
H -3.64201 0.19451 3.15815
H -3.00997 1.77298 3.7082
C -0.56896 2.37912 2.96873

H -1.16457 3.02876 2.31398
H -0.76761 2.6421 4.01594
H 0.49767 2.52334 2.75048
C -0.92843 0.07276 4.61388
H -0.13978 0.71994 5.01658
H -1.88277 0.30613 5.10413
H -0.66575 -0.97597 4.79931
C 1.41444 0.08241 -2.58074
H 2.2998 -0.29401 -3.11047
H 1.30933 1.15877 -2.76265
H 0.51398 -0.43034 -2.93946
I -1.05173 0.98135 -0.28204
C -0.52926 -3.02649 0.97369
H 0.27481 -3.31331 1.66217
H -1.05145 -3.95949 0.70863
P 0.46132 -2.48878 -0.51993
P -1.67215 -1.97618 2.00876
C 1.59636 -3.94514 -0.49673
C 1.32804 -5.12672 -1.19411
C 2.72167 -3.89037 0.33445
C 2.17923 -6.22196 -1.07782
H 0.4486 -5.19782 -1.83323
C 3.56711 -4.98795 0.45412
H 2.9344 -2.98148 0.8988
C 3.30041 -6.15418 -0.25733
H 1.95932 -7.13471 -1.62958
H 4.43987 -4.9279 1.10229
H 3.96545 -7.0118 -0.16942
C -0.57899 -2.81627 -1.98494
C -1.97062 -2.89691 -1.93254
C 0.05975 -2.91148 -3.22989
C -2.71198 -3.07477 -3.0984
H -2.49147 -2.81855 -0.98085
C -0.68049 -3.09823 -4.39029
H 1.14831 -2.85137 -3.28915
C -2.07031 -3.17683 -4.32675
H -3.79748 -3.13511 -3.03657
H -0.17008 -3.178 -5.34863
H -2.65033 -3.3173 -5.23739
C -3.31347 -2.32228 1.25547
C -3.81139 -3.63244 1.22265
C -4.0427 -1.30536 0.63583
C -5.00365 -3.91769 0.56977
H -3.26256 -4.43798 1.71196
C -5.23913 -1.59198 -0.0179
H -3.66099 -0.2864 0.63982
C -5.71837 -2.89652 -0.05473
H -5.37761 -4.94001 0.54833
H -5.79289 -0.78924 -0.50153
H -6.65225 -3.12083 -0.56791
C -1.75322 -2.96695 3.55588
C -2.92994 -2.90993 4.31473
C -0.63355 -3.59998 4.10415
C -2.98864 -3.48552 5.57835
H -3.81342 -2.41183 3.91391
C -0.69606 -4.18056 5.36798
H 0.31349 -3.63328 3.56647
C -1.87151 -4.12508 6.10836
H -3.91343 -3.4338 6.15077
H 0.18541 -4.67303 5.77512

H -1.9168 -4.5758 7.09826
I 1.76452 -0.38031 2.37651

5A
E(RM06) = -2515.04532789
Zero-point correction= 0.704172 (Hartree/Particle)
Thermal correction to Energy= 0.753491
Thermal correction to Enthalpy= 0.754435
Thermal correction to Gibbs Free Energy= 0.616041
Sum of electronic and zero-point Energies= -2514.341156
Sum of electronic and thermal Energies= -2514.291837
Sum of electronic and thermal Enthalpies= -2514.290892
Sum of electronic and thermal Free Energies= -2514.429287
E(RM06L) = -2803.39584357

Pt 1.81652 1.05041 -1.61561
C 1.16763 1.678 -3.49329
H 0.98609 0.80678 -4.14436
H 0.22804 2.25004 -3.42035
H 1.91738 2.31381 -3.99177
Pt -1.13229 -0.73744 -1.47051
C -1.32759 -2.61231 -2.32059
H -0.6035 -2.72905 -3.14446
H -1.16148 -3.44098 -1.61289
H -2.3321 -2.74353 -2.75383
C -2.34709 -0.09251 -3.04744
H -1.96228 -0.43933 -4.02062
H -3.36858 -0.49651 -2.9366
H -2.42309 1.00669 -3.08594
C -2.15783 5.77706 1.33058
C -1.0032 5.22815 0.81896
C -1.04129 3.91913 0.30268
C -2.24987 3.18709 0.31559
C -3.4211 3.76483 0.84094
C -3.36599 5.04656 1.3407
H 1.05196 3.76784 -0.29978
H -2.14479 6.78797 1.73285
H -0.06631 5.78323 0.80622
C 0.08629 3.26267 -0.24524
C -2.20079 1.8774 -0.21636
H -4.34766 3.19216 0.84335
H -4.26239 5.50781 1.7501
H -3.09685 1.25346 -0.24649
N -1.10735 1.3259 -0.69141
N 0.05587 2.03417 -0.70962
C 3.42821 0.22884 -2.60425
H 4.38312 0.58602 -2.18331
H 3.4285 0.48053 -3.6763
H 3.41856 -0.87148 -2.52686
C 0.8992 -0.32339 1.4765
H 0.14996 0.46376 1.64203
H 1.1601 -0.75215 2.45478
P 2.36377 0.4655 0.65594
P 0.08639 -1.58575 0.38483
C 2.59221 2.02769 1.59803
C 3.60641 2.88291 1.14514
C 1.79142 2.43283 2.66783
C 3.80523 4.12227 1.7421
H 4.23821 2.57635 0.30798
C 1.98544 3.68091 3.25929

H 1.00756 1.78157 3.05366
C 2.98624 4.52821 2.7955
H 4.59531 4.77772 1.37869
H 1.34951 3.98766 4.08857
H 3.13352 5.50358 3.25664
C 3.77714 -0.53602 1.27037
C 3.99507 -0.67981 2.64697
C 4.65665 -1.14418 0.37349
C 5.06536 -1.43228 3.11433
H 3.3241 -0.19808 3.36027
C 5.73285 -1.8956 0.84392
H 4.49628 -1.04205 -0.69777
C 5.93668 -2.0423 2.21154
H 5.2245 -1.54083 4.18623
H 6.40869 -2.37138 0.13441
H 6.77646 -2.63052 2.57865
C 1.42037 -2.81378 0.13467
C 2.0177 -3.47437 1.2163
C 1.89287 -3.05286 -1.15803
C 3.06607 -4.36177 1.0035
H 1.66169 -3.29428 2.23199
C 2.94581 -3.94126 -1.37063
H 1.43682 -2.52986 -1.99958
C 3.53087 -4.5956 -0.29093
H 3.52819 -4.8679 1.85003
H 3.30774 -4.11843 -2.38252
H 4.3542 -5.28947 -0.4551
C -1.07695 -2.40425 1.54522
C -1.25461 -3.79194 1.55227
C -1.91635 -1.61006 2.33755
C -2.23782 -4.3734 2.34937
H -0.61725 -4.42872 0.93865
C -2.89299 -2.19358 3.13836
H -1.81546 -0.52301 2.32939
C -3.05612 -3.57758 3.14674
H -2.36037 -5.45553 2.3487
H -3.53301 -1.56282 3.75423
H -3.82017 -4.03417 3.77397
C -4.39755 -2.32038 -0.26704
H -4.86158 -2.70018 -1.17971
H -3.36466 -1.99945 -0.44382
H -4.47375 -3.03719 0.55363
I -5.50543 -0.54562 0.32181

5B
E(RM06) = -2515.02915161
Zero-point correction= 0.705172 (Hartree/Particle)
Thermal correction to Energy= 0.754563
Thermal correction to Enthalpy= 0.755507
Thermal correction to Gibbs Free Energy= 0.616564
Sum of electronic and zero-point Energies= -2514.323979
Sum of electronic and thermal Energies= -2514.274589
Sum of electronic and thermal Enthalpies= -2514.273645
Sum of electronic and thermal Free Energies= -2514.412588
E(RM06L) = -2803.38503071

Pt 1.83032 1.01526 -1.56212
C 1.17677 1.5948 -3.4461
H 0.98074 0.69855 -4.05545
H 0.24058 2.17282 -3.38273

H 1.92936 2.20806 -3.9659
Pt -1.18067 -0.73487 -1.43549
C -1.43818 -2.61916 -2.24536
H -0.75525 -2.74827 -3.10064
H -1.25093 -3.44284 -1.53725
H -2.46349 -2.73947 -2.62868
C -2.41393 -0.10835 -2.99936
H -2.08455 -0.54228 -3.95585
H -3.45548 -0.43163 -2.82679
H -2.40884 0.98818 -3.10902
C -2.14173 5.89301 1.11338
C -0.97885 5.29033 0.69157
C -1.02909 3.96944 0.20579
C -2.2609 3.27915 0.15952
C -3.4414 3.91334 0.59348
C -3.37352 5.20489 1.06299
H 1.09147 3.7286 -0.27273
H -2.11763 6.91385 1.48946
H -0.02407 5.81328 0.72508
C 0.10535 3.26181 -0.25748
C -2.22388 1.95231 -0.33041
H -4.3867 3.37375 0.54883
H -4.27785 5.70771 1.39981
H -3.13507 1.35481 -0.40147
N -1.12179 1.35027 -0.71724
N 0.06157 2.02197 -0.68875
C 3.45082 0.21369 -2.54545
H 4.395 0.61556 -2.14061
H 3.43319 0.4395 -3.62172
H 3.46953 -0.88365 -2.44074
C 0.89792 -0.37077 1.50846
H 0.14836 0.41336 1.68627
H 1.15146 -0.82124 2.47929
P 2.36517 0.43782 0.70426
P 0.08 -1.60437 0.37742
C 2.56289 1.99685 1.66525
C 3.56844 2.86716 1.22197
C 1.74643 2.39605 2.72512
C 3.74436 4.1093 1.81863
H 4.20561 2.56922 0.38641
C 1.91504 3.64798 3.31586
H 0.96845 1.73398 3.10545
C 2.90933 4.50712 2.86204
H 4.52941 4.77425 1.46178
H 1.26744 3.94667 4.13915
H 3.04018 5.48454 3.32393
C 3.77654 -0.55392 1.34051
C 3.97264 -0.72147 2.71682
C 4.67715 -1.13579 0.44802
C 5.0386 -1.47553 3.18912
H 3.28999 -0.25142 3.42707
C 5.74995 -1.88757 0.9235
H 4.53183 -1.01157 -0.62298
C 5.92974 -2.06103 2.29044
H 5.18133 -1.60177 4.26146
H 6.44231 -2.34304 0.21681
H 6.76764 -2.64984 2.6611
C 1.42967 -2.79902 0.0578
C 2.06013 -3.49843 1.09455
C 1.87383 -2.97333 -1.25486

C 3.11303 -4.36181 0.81967
H 1.72497 -3.36959 2.12508
C 2.93033 -3.83946 -1.52919
H 1.39373 -2.41264 -2.05807
C 3.5478 -4.53327 -0.49394
H 3.60377 -4.89465 1.633
H 3.26978 -3.96707 -2.55613
H 4.37419 -5.20978 -0.7083
C -1.02927 -2.48437 1.54975
C -1.17345 -3.87548 1.53421
C -1.86596 -1.7311 2.38214
C -2.11741 -4.49716 2.34736
H -0.54011 -4.48206 0.88718
C -2.80222 -2.3528 3.2007
H -1.80156 -0.64098 2.38217
C -2.92956 -3.73985 3.18637
H -2.21453 -5.58165 2.32549
H -3.44135 -1.75015 3.84477
H -3.66308 -4.22808 3.8261
C -4.37386 -2.15024 -0.10201
H -4.97734 -2.46447 -0.95613
H -3.38196 -1.80248 -0.41627
H -4.31743 -2.92614 0.66475
I -5.38397 -0.44082 0.79111

6A
E(RM06) = -2515.06554553
Zero-point correction= 0.706456 (Hartree/Particle)
Thermal correction to Energy= 0.755212
Thermal correction to Enthalpy= 0.756156
Thermal correction to Gibbs Free Energy= 0.618952
Sum of electronic and zero-point Energies= -2514.359089
Sum of electronic and thermal Energies= -2514.310334
Sum of electronic and thermal Enthalpies= -2514.309389
Sum of electronic and thermal Free Energies= -2514.446594
E(RM06L) = -2803.41644515

Pt 1.89002 0.47812 -1.65108
C 1.61805 1.13674 -3.6071
H 1.30665 0.3382 -4.29607
H 0.88507 1.95535 -3.66232
H 2.59026 1.52213 -3.95918
Pt -1.0007 -0.3804 -1.50154
C -1.20224 -2.16157 -2.50654
H -0.26772 -2.32328 -3.06636
H -1.36412 -3.00318 -1.81995
H -2.03601 -2.11938 -3.21911
C -1.61088 0.48989 -3.29409
H -0.87839 0.24374 -4.07281
H -2.5959 0.1148 -3.59991
H -1.66417 1.58096 -3.16809
C -0.4114 6.18475 1.45821
C 0.49789 5.40099 0.78181
C 0.0894 4.14215 0.30608
C -1.23263 3.69196 0.53085
C -2.14857 4.50738 1.21964
C -1.73276 5.74012 1.67339
H 1.9826 3.54339 -0.6061
H -0.11102 7.16072 1.8338
H 1.52258 5.73127 0.61535

C 0.9511 3.26163 -0.39216
C -1.55898 2.40571 0.0338
H -3.16554 4.15092 1.38363
H -2.42966 6.3823 2.20789
H -2.56405 1.99645 0.16596
N -0.69402 1.64382 -0.58829
N 0.58206 2.07176 -0.80203
C 3.00759 -1.01065 -2.52405
H 3.92007 -0.56295 -2.95409
H 2.45666 -1.48835 -3.34848
H 3.3177 -1.79238 -1.81656
C 0.83785 -0.38135 1.61031
H 0.33899 0.59367 1.71887
H 1.01204 -0.78087 2.61929
P 2.38323 -0.03393 0.6651
P -0.32865 -1.45273 0.65912
C 3.03601 1.47677 1.48107
C 4.02513 2.20414 0.80641
C 2.55981 1.94882 2.70708
C 4.52084 3.38719 1.34463
H 4.3951 1.85193 -0.15851
C 3.04796 3.14118 3.23703
H 1.8017 1.39494 3.25997
C 4.02508 3.86228 2.5572
H 5.28693 3.94581 0.80908
H 2.66289 3.50441 4.1886
H 4.40271 4.79509 2.97286
C 3.60347 -1.31522 1.13898
C 3.4422 -2.17952 2.22484
C 4.77365 -1.39328 0.37302
C 4.42603 -3.11748 2.52678
H 2.5456 -2.13989 2.8413
C 5.75773 -2.32626 0.68126
H 4.91714 -0.71863 -0.47157
C 5.58128 -3.1959 1.7545
H 4.28323 -3.79241 3.36969
H 6.662 -2.37699 0.07687
H 6.34657 -3.93349 1.99067
C 0.50242 -3.08106 0.64229
C 0.49349 -3.91104 1.76953
C 1.23825 -3.46046 -0.48364
C 1.21253 -5.10116 1.76638
H -0.07274 -3.62482 2.6565
C 1.97231 -4.64421 -0.47816
H 1.24961 -2.8188 -1.36441
C 1.95638 -5.46611 0.64494
H 1.19923 -5.74285 2.64604
H 2.55 -4.9249 -1.35785
H 2.52408 -6.39525 0.64796
C -1.73468 -1.67111 1.80148
C -2.65555 -2.69353 1.53393
C -1.9903 -0.77902 2.84675
C -3.80164 -2.82692 2.30851
H -2.47385 -3.39079 0.71393
C -3.1412 -0.91617 3.61989
H -1.29887 0.03192 3.07194
C -4.04624 -1.93765 3.3539
H -4.50779 -3.62733 2.094
H -3.32985 -0.21516 4.43149
H -4.94715 -2.03904 3.95677

C -3.02282 -0.42557 -1.0665
H -3.49623 0.44733 -1.53161
H -3.12374 -0.37788 0.02462
H -3.47113 -1.34877 -1.45314
I -5.45926 1.75445 1.53849

7A
E(RM06) = -2515.06980847
Zero-point correction= 0.706878 (Hartree/Particle)
Thermal correction to Energy= 0.755233
Thermal correction to Enthalpy= 0.756177
Thermal correction to Gibbs Free Energy= 0.621800
Sum of electronic and zero-point Energies= -2514.362931
Sum of electronic and thermal Energies= -2514.314576
Sum of electronic and thermal Enthalpies= -2514.313631
Sum of electronic and thermal Free Energies= -2514.448008
E(RM06L) = -2803.41739512

Pt -0.7856 -1.38431 -1.82948
C -0.43111 -1.41958 -3.87401
H -1.1233 -0.78199 -4.44231
H 0.60127 -1.12145 -4.11156
H -0.58064 -2.45922 -4.21194
Pt -0.43174 1.5951 -1.8093
C -2.1623 2.43453 -2.53422
H -2.74937 1.6156 -2.98104
H -2.74871 2.92093 -1.74363
H -1.94074 3.1737 -3.31487
C 0.26502 1.82556 -3.76043
H -0.36985 1.23771 -4.43467
H 0.23098 2.87801 -4.06963
H 1.30217 1.46579 -3.82362
C 6.00779 -1.41679 -0.59336
C 4.77194 -1.96924 -0.85099
C 3.66469 -1.11674 -1.01041
C 3.82557 0.28323 -0.89321
C 5.09491 0.82934 -0.63347
C 6.17038 -0.0194 -0.49089
H 2.15699 -2.65363 -1.39884
H 6.87377 -2.06341 -0.46816
H 4.63746 -3.04661 -0.93554
C 2.35654 -1.58697 -1.28359
C 2.65697 1.07005 -1.03738
H 5.20612 1.90845 -0.53976
H 7.15848 0.38793 -0.28754
H 2.70012 2.1568 -0.94713
N 1.47782 0.55522 -1.28027
N 1.32212 -0.79121 -1.41282
C -2.71814 -1.86639 -2.33539
H -2.86194 -2.95124 -2.1887
H -2.94168 -1.64029 -3.38858
H -3.45619 -1.34028 -1.71257
C -0.39403 -0.03151 1.40227
H 0.68569 0.09619 1.23727
H -0.57434 -0.0174 2.48661
P -0.91418 -1.61629 0.603
P -1.23948 1.37498 0.55633
C 0.39478 -2.82084 1.04381
C 0.27318 -4.10297 0.49021
C 1.51534 -2.51299 1.81594

C 1.26311 -5.05623 0.70099
H -0.60086 -4.35223 -0.1171
C 2.51299 -3.46651 2.01472
H 1.6335 -1.52634 2.26565
C 2.3904 -4.73549 1.45747
H 1.15948 -6.04947 0.26671
H 3.38861 -3.20839 2.61009
H 3.17156 -5.47803 1.61265
C -2.31531 -2.20208 1.63377
C -2.17824 -2.27628 3.02614
C -3.50123 -2.63518 1.03835
C -3.22303 -2.75163 3.80851
H -1.24694 -1.96765 3.50398
C -4.54673 -3.1164 1.82563
H -3.61338 -2.59617 -0.04361
C -4.41122 -3.16885 3.20841
H -3.10917 -2.80189 4.89026
H -5.46957 -3.4481 1.352
H -5.22917 -3.54165 3.82306
C -3.00396 1.08169 0.94034
C -3.43058 1.0565 2.27501
C -3.92555 0.83154 -0.078
C -4.75725 0.77772 2.57943
H -2.72059 1.24738 3.08129
C -5.25763 0.56019 0.22873
H -3.60238 0.8392 -1.11685
C -5.67329 0.53435 1.5559
H -5.07881 0.74902 3.61939
H -5.96777 0.36731 -0.57406
H -6.71305 0.31912 1.79755
C -0.80404 2.82823 1.56585
C -1.62243 3.96299 1.51363
C 0.40859 2.88577 2.25745
C -1.23461 5.13369 2.15626
H -2.56808 3.93168 0.96938
C 0.79308 4.06042 2.89951
H 1.06787 2.01735 2.30347
C -0.02612 5.18449 2.84953
H -1.87937 6.0103 2.11688
H 1.73725 4.08991 3.44256
H 0.27507 6.10226 3.352
C 0.31077 3.50094 -1.49638
H 1.1317 3.68359 -2.19932
H 0.67722 3.54348 -0.46282
H -0.48463 4.24064 -1.64754
I 3.7511 0.66597 3.12528

7B
E(RM06) = -2515.04993583
Zero-point correction= 0.708228 (Hartree/Particle)
Thermal correction to Energy= 0.756439
Thermal correction to Enthalpy= 0.757383
Thermal correction to Gibbs Free Energy= 0.623362
Sum of electronic and zero-point Energies= -2514.341708
Sum of electronic and thermal Energies= -2514.293497
Sum of electronic and thermal Enthalpies= -2514.292553
Sum of electronic and thermal Free Energies= -2514.426574
E(RM06L) = -2803.40101538

Pt -0.77337 -1.35563 -1.77216

C -0.41243 -1.37016 -3.81318
H -1.09771 -0.72369 -4.37841
H 0.62256 -1.07849 -4.0461
H -0.5699 -2.4064 -4.15666
Pt -0.37302 1.59838 -1.74784
C -2.07875 2.4678 -2.49804
H -2.66524 1.66402 -2.97062
H -2.67827 2.95336 -1.71709
H -1.83134 3.21395 -3.26392
C 0.35634 1.83648 -3.6867
H -0.28399 1.27367 -4.37622
H 0.35337 2.89288 -3.98417
H 1.38371 1.44966 -3.74778
C 6.06295 -1.52454 -0.86658
C 4.80343 -2.05216 -1.04207
C 3.70423 -1.1792 -1.12562
C 3.89781 0.21544 -1.01075
C 5.19123 0.73626 -0.83454
C 6.25752 -0.13125 -0.77101
H 2.13921 -2.68431 -1.40403
H 6.92235 -2.18774 -0.79336
H 4.64016 -3.12729 -1.10237
C 2.37127 -1.62282 -1.30271
C 2.73398 1.02172 -1.05361
H 5.32674 1.81025 -0.72033
H 7.2626 0.25718 -0.62234
H 2.80049 2.10533 -0.94466
N 1.53144 0.53295 -1.22673
N 1.34541 -0.80902 -1.35975
C -2.70311 -1.81369 -2.30126
H -2.82247 -2.91028 -2.24847
H -2.93689 -1.50458 -3.33003
H -3.44412 -1.35604 -1.63187
C -0.4044 -0.01517 1.46564
H 0.67976 0.12001 1.32451
H -0.59865 0.00112 2.54753
P -0.90875 -1.60292 0.66019
P -1.24757 1.37844 0.594
C 0.39846 -2.80661 1.10734
C 0.28153 -4.08641 0.54691
C 1.50796 -2.50309 1.89605
C 1.26475 -5.0427 0.77012
H -0.58439 -4.33075 -0.0737
C 2.49928 -3.46055 2.10691
H 1.63754 -1.51564 2.34157
C 2.38085 -4.72708 1.54538
H 1.16368 -6.03507 0.33294
H 3.36655 -3.19696 2.71115
H 3.15591 -5.47358 1.71301
C -2.31496 -2.19618 1.67931
C -2.19398 -2.26744 3.07261
C -3.48602 -2.64824 1.07061
C -3.2394 -2.75875 3.84286
H -1.27086 -1.95026 3.56066
C -4.53309 -3.14342 1.84563
H -3.58352 -2.60957 -0.01263
C -4.41291 -3.19471 3.22909
H -3.13619 -2.8097 4.92562
H -5.44504 -3.48935 1.36134
H -5.23136 -3.58187 3.83413

C -3.02225 1.06473 0.92193
C -3.48372 1.02622 2.24425
C -3.92072 0.83565 -0.1211
C -4.81767 0.75055 2.51314
H -2.79467 1.21087 3.06979
C -5.26082 0.56754 0.14986
H -3.57084 0.85728 -1.151
C -5.70865 0.52416 1.46513
H -5.16399 0.71023 3.54459
H -5.95186 0.3908 -0.67304
H -6.75494 0.31066 1.67825
C -0.88744 2.84971 1.60824
C -1.74057 3.95712 1.52468
C 0.30334 2.95143 2.33044
C -1.40459 5.14595 2.16115
H -2.67516 3.88931 0.96517
C 0.63567 4.14523 2.96554
H 0.99751 2.11173 2.40222
C -0.21479 5.24243 2.88097
H -2.07551 6.00127 2.09636
H 1.56883 4.20333 3.52455
H 0.0468 6.17596 3.37664
C 0.38238 3.49125 -1.38886
H 1.18971 3.70064 -2.10049
H 0.76479 3.5028 -0.35956
H -0.4111 4.23974 -1.50033
I 3.59292 0.80334 2.66199

8A
E(RM06) = -2503.48440573
Zero-point correction= 0.707149 (Hartree/Particle)
Thermal correction to Energy= 0.752883
Thermal correction to Enthalpy= 0.753828
Thermal correction to Gibbs Free Energy= 0.627841
Sum of electronic and zero-point Energies= -2502.777257
Sum of electronic and thermal Energies= -2502.731522
Sum of electronic and thermal Enthalpies= -2502.730578
Sum of electronic and thermal Free Energies= -2502.856565
E(RM06L) = -2505.35427038

Pt -0.81261 -1.37411 -1.85417
C -0.51905 -1.4109 -3.90717
H -1.20003 -0.74119 -4.45145
H 0.51799 -1.15353 -4.17056
H -0.72055 -2.44077 -4.2473
Pt -0.42437 1.5971 -1.81223
C -2.13801 2.45618 -2.55186
H -2.73789 1.64015 -2.98648
H -2.71592 2.9638 -1.76857
H -1.90266 3.17936 -3.34319
C 0.29181 1.81196 -3.75768
H -0.35606 1.24527 -4.43744
H 0.29163 2.86606 -4.06312
H 1.31799 1.4208 -3.81409
C 5.96751 -1.51701 -0.5718
C 4.74386 -2.03846 -0.9313
C 3.64266 -1.17198 -1.0516
C 3.79816 0.21195 -0.80217
C 5.05536 0.72668 -0.43843
C 6.12318 -0.13663 -0.3268

H 2.13996 -2.67109 -1.58402
H 6.82848 -2.17494 -0.47453
H 4.61244 -3.10305 -1.11976
C 2.34102 -1.61563 -1.39308
C 2.64086 1.01627 -0.94717
H 5.16608 1.79356 -0.25166
H 7.10188 0.24671 -0.04603
H 2.68619 2.09569 -0.79412
N 1.4707 0.52678 -1.27061
N 1.31135 -0.80875 -1.48385
C -2.76489 -1.82411 -2.31165
H -2.91306 -2.91185 -2.19457
H -3.01776 -1.5635 -3.35005
H -3.47821 -1.31136 -1.65073
C -0.39383 -0.01308 1.39039
H 0.68301 0.12767 1.22498
H -0.57882 -0.00932 2.47343
P -0.89045 -1.60377 0.58642
P -1.24847 1.38846 0.54915
C 0.44854 -2.77766 1.02608
C 0.3389 -4.06801 0.48965
C 1.57058 -2.44879 1.7889
C 1.33851 -5.00901 0.70756
H -0.53544 -4.33411 -0.10969
C 2.57541 -3.39253 1.99971
H 1.67743 -1.45594 2.22575
C 2.46357 -4.66912 1.45813
H 1.24287 -6.00817 0.2855
H 3.44944 -3.12414 2.59158
H 3.25142 -5.40246 1.62216
C -2.26946 -2.21361 1.63279
C -2.11139 -2.29482 3.02254
C -3.46235 -2.64806 1.05272
C -3.14269 -2.77737 3.81813
H -1.17386 -1.98611 3.48779
C -4.49522 -3.13436 1.85343
H -3.59067 -2.60496 -0.02702
C -4.33905 -3.19357 3.2337
H -3.0124 -2.83367 4.89772
H -5.42416 -3.46597 1.39197
H -5.14704 -3.57097 3.85857
C -3.01094 1.0885 0.93527
C -3.43085 1.03395 2.27126
C -3.93876 0.86978 -0.08459
C -4.75695 0.75313 2.5757
H -2.71597 1.20384 3.07808
C -5.27043 0.59638 0.2228
H -3.6212 0.90362 -1.12463
C -5.67878 0.53737 1.55104
H -5.0738 0.70093 3.61617
H -5.98593 0.42772 -0.58059
H -6.71807 0.32005 1.79264
C -0.82253 2.84245 1.56474
C -1.64263 3.97488 1.48659
C 0.37013 2.90766 2.29067
C -1.27809 5.14998 2.13385
H -2.57373 3.93775 0.91831
C 0.73131 4.08753 2.93786
H 1.02656 2.04034 2.36022
C -0.08976 5.20837 2.85982

H -1.92519 6.02345 2.07265
H 1.6577 4.12647 3.50871
H 0.1945 6.12898 3.36676
C 0.34629 3.49273 -1.50531
H 1.2178 3.62746 -2.15659
H 0.64229 3.56481 -0.45114
H -0.41429 4.24814 -1.73681

9A
E(RM06) = -2566.33753940
Zero-point correction= 0.743962 (Hartree/Particle)
Thermal correction to Energy= 0.797136
Thermal correction to Enthalpy= 0.798080
Thermal correction to Gibbs Free Energy= 0.652141
Sum of electronic and zero-point Energies= -2565.593578
Sum of electronic and thermal Energies= -2565.540403
Sum of electronic and thermal Enthalpies= -2565.539459
Sum of electronic and thermal Free Energies= -2565.685399
E(RM06L) = -3141.21923697

Pt -1.45989 -1.13127 -0.70995
C -2.01469 -2.56677 -2.13109
H -2.4983 -3.45363 -1.69179
H -2.73631 -2.11595 -2.83579
H -1.15231 -2.90758 -2.72638
Pt 2.96377 -0.529 -1.06818
C 4.00541 0.83118 -2.22843
H 3.57248 0.84251 -3.23875
H 3.95144 1.84293 -1.80565
H 5.0608 0.53698 -2.3031
C 3.61576 -1.95097 -2.44605
H 2.88577 -2.02812 -3.26328
H 4.59305 -1.67779 -2.86459
H 3.7052 -2.92375 -1.94198
C 4.74468 -0.90071 -0.0812
H 4.48787 -1.30545 0.9066
H 5.34017 -1.62942 -0.64471
H 5.31615 0.02779 0.03063
C -0.80148 -5.86152 2.02774
C -0.00746 -4.89316 2.60187
C 0.6797 -3.99005 1.76971
C 0.54524 -4.07645 0.36757
C -0.2586 -5.08187 -0.20386
C -0.92237 -5.95934 0.6247
H 1.69214 -2.84504 3.32591
H -1.34041 -6.56569 2.65863
H 0.09951 -4.81462 3.68309
C 1.52443 -2.95606 2.25205
C 1.2228 -3.09152 -0.3943
H -0.35048 -5.14672 -1.28732
H -1.55047 -6.73853 0.19743
H 1.14573 -3.08831 -1.48167
N 1.96906 -2.15467 0.1459
N 2.14191 -2.08942 1.49174
C -2.94796 -1.98147 0.4479
H -3.38002 -1.27352 1.17063
H -2.5277 -2.83238 1.01273
H -3.76183 -2.36921 -0.18402
I 0.4821 -0.12902 -2.5776
C 0.73059 0.82374 1.63525

H 0.94859 -0.13254 2.12879
H 0.65758 1.59022 2.42238
P -0.96315 0.58434 0.88893
P 2.2365 1.1944 0.62557
C -1.87917 0.35675 2.47093
C -3.03012 1.08552 2.77953
C -1.49603 -0.68945 3.32004
C -3.77817 0.77954 3.91529
H -3.35954 1.89404 2.12684
C -2.23746 -0.98947 4.45684
H -0.61941 -1.29613 3.08275
C -3.38415 -0.25576 4.75661
H -4.67427 1.35691 4.13977
H -1.92312 -1.80494 5.10704
H -3.96968 -0.49435 5.64312
C -1.46978 2.26084 0.34434
C -1.28953 3.39558 1.1442
C -2.10726 2.39744 -0.89181
C -1.73381 4.63947 0.70994
H -0.81285 3.3085 2.12147
C -2.55707 3.64247 -1.32635
H -2.2497 1.51358 -1.51617
C -2.36797 4.76475 -0.52614
H -1.58646 5.51635 1.33929
H -3.05639 3.73117 -2.29071
H -2.71596 5.74051 -0.86217
C 1.9901 2.94981 0.13295
C 2.06901 3.9639 1.09705
C 1.67994 3.29174 -1.1856
C 1.84414 5.28977 0.74667
H 2.30633 3.71749 2.13252
C 1.44843 4.62104 -1.53443
H 1.60288 2.51457 -1.945
C 1.53202 5.62091 -0.57073
H 1.90885 6.06758 1.50629
H 1.20424 4.87177 -2.56568
H 1.35431 6.65984 -0.84474
C 3.51995 1.36749 1.92895
C 4.69641 2.05374 1.59673
C 3.42231 0.77099 3.18869
C 5.74464 2.14686 2.50438
H 4.79475 2.52619 0.6178
C 4.47524 0.86463 4.09754
H 2.52573 0.22657 3.48122
C 5.6368 1.55018 3.75924
H 6.64908 2.68784 2.23023
H 4.37954 0.40016 5.07788
H 6.45704 1.62242 4.47168
C -4.80815 0.18757 -2.00515
H -3.80319 -0.13809 -1.71247
H -5.41278 -0.64976 -2.36021
H -4.77804 0.99917 -2.73543
I -5.76092 0.96103 -0.21315

9B
E(RM06) = -2566.32395385
Zero-point correction= 0.744187 (Hartree/Particle)
Thermal correction to Energy= 0.797890
Thermal correction to Enthalpy= 0.798835
Thermal correction to Gibbs Free Energy= 0.649300

Sum of electronic and zero-point Energies= -2565.579767
Sum of electronic and thermal Energies= -2565.526063
Sum of electronic and thermal Enthalpies= -2565.525119
Sum of electronic and thermal Free Energies= -2565.674653
E(RM06L) = -3141.21098063

Pt 1.35588 1.21218 -0.37406
C 2.04291 2.66008 -1.71678
H 2.34309 3.5981 -1.22438
H 2.93008 2.26538 -2.2419
H 1.29319 2.89332 -2.48995
Pt -2.89937 0.39055 -1.32787
C -3.72037 -1.01137 -2.60681
H -3.18043 -0.9752 -3.56286
H -3.64267 -2.02575 -2.19376
H -4.77905 -0.78685 -2.79276
C -3.4159 1.77669 -2.79473
H -2.59078 1.87265 -3.51282
H -4.32012 1.46409 -3.33229
H -3.60786 2.74836 -2.31756
C -4.80776 0.70657 -0.58221
H -4.69815 1.10753 0.43405
H -5.34301 1.42462 -1.21559
H -5.36685 -0.23571 -0.5511
C 0.08023 6.02886 2.08187
C -0.74511 5.04139 2.57137
C -1.21635 4.04529 1.69637
C -0.84038 4.06449 0.33715
C -0.00313 5.08626 -0.14916
C 0.44934 6.0527 0.72032
H -2.39833 2.897 3.12696
H 0.45516 6.80254 2.74916
H -1.03732 5.01882 3.62061
C -2.06309 2.97573 2.08967
C -1.3301 3.00697 -0.47073
H 0.28844 5.08668 -1.19841
H 1.1042 6.84302 0.35911
H -1.07658 2.9583 -1.52951
N -2.12394 2.06309 -0.01552
N -2.49852 2.03929 1.28849
C 2.60216 2.15154 0.98361
H 3.01285 1.4546 1.72935
H 2.03176 2.92992 1.5191
H 3.44271 2.6423 0.47078
I -0.24274 0.07934 -2.48639
C -1.02053 -0.83383 1.67046
H -1.3516 0.12316 2.09471
H -1.02805 -1.57483 2.4849
P 0.74784 -0.52162 1.15018
P -2.35221 -1.28669 0.46799
C 1.44151 -0.27321 2.83998
C 2.59311 -0.93697 3.26857
C 0.89435 0.7199 3.6613
C 3.17566 -0.62408 4.4944
H 3.05566 -1.69368 2.63496
C 1.46881 1.02411 4.88905
H 0.02082 1.28612 3.33021
C 2.61383 0.35166 5.3096
H 4.07791 -1.14769 4.80811
H 1.02755 1.79744 5.51661

H 3.07052 0.59515 6.26761
C 1.38652 -2.17763 0.68836
C 1.1341 -3.32324 1.45115
C 2.21109 -2.2794 -0.43445
C 1.69423 -4.54359 1.09438
H 0.50872 -3.26397 2.34288
C 2.77885 -3.50048 -0.78902
H 2.40069 -1.38707 -1.03357
C 2.52029 -4.63285 -0.02509
H 1.48797 -5.42952 1.69373
H 3.42656 -3.56129 -1.66276
H 2.96277 -5.5895 -0.29931
C -1.97515 -3.03779 0.0499
C -2.17965 -4.04745 0.99978
C -1.44561 -3.37812 -1.19698
C -1.86309 -5.36759 0.7057
H -2.59585 -3.80205 1.97735
C -1.12568 -4.70195 -1.4886
H -1.26503 -2.60333 -1.94134
C -1.33464 -5.69695 -0.54049
H -2.02917 -6.14255 1.45275
H -0.70847 -4.95028 -2.46304
H -1.08655 -6.73198 -0.77127
C -3.7975 -1.48678 1.58626
C -4.89122 -2.22667 1.11678
C -3.90226 -0.84814 2.82385
C -6.05436 -2.33045 1.86916
H -4.83104 -2.73197 0.15125
C -5.06956 -0.95214 3.577
H -3.07546 -0.25703 3.21456
C -6.14707 -1.69073 3.10288
H -6.89256 -2.9121 1.48883
H -5.13201 -0.45196 4.54235
H -7.05873 -1.76955 3.69285
C 4.91596 0.18465 -1.02418
H 3.87103 0.43666 -0.80734
H 5.50185 1.08179 -1.23517
H 5.00065 -0.54474 -1.83288
I 5.74277 -0.72513 0.76564

10A
E(RM06) = -2566.34549653
Zero-point correction= 0.744468 (Hartree/Particle)
Thermal correction to Energy= 0.797897
Thermal correction to Enthalpy= 0.798841
Thermal correction to Gibbs Free Energy= 0.650170
Sum of electronic and zero-point Energies= -2565.601028
Sum of electronic and thermal Energies= -2565.547599
Sum of electronic and thermal Enthalpies= -2565.546655
Sum of electronic and thermal Free Energies= -2565.695326
E(RM06L) = -3141.22429454

Pt 1.00236 1.60276 -0.61145
C 0.95094 3.20694 -1.93709
H 1.43794 4.1016 -1.52716
H 1.4567 2.91885 -2.86993
H -0.09844 3.43765 -2.16913
Pt -2.93264 -0.2071 -1.1099
C -3.54204 -1.82731 -2.24142
H -3.03414 -1.78972 -3.21521

H -3.29923 -2.77467 -1.74377
H -4.62613 -1.78706 -2.40851
C -3.91068 0.94638 -2.54409
H -3.18533 1.27385 -3.30126
H -4.70685 0.37343 -3.0359
H -4.3587 1.82464 -2.05888
C -4.77455 -0.31462 -0.17585
H -4.66292 0.14441 0.81534
H -5.52318 0.22961 -0.76358
H -5.08045 -1.36155 -0.07224
C -1.48829 6.233 1.8558
C -1.78296 5.03076 2.46011
C -2.04591 3.90756 1.65471
C -2.0094 4.02236 0.24746
C -1.71955 5.26244 -0.35483
C -1.45883 6.34965 0.44911
H -2.38117 2.455 3.2469
H -1.2772 7.109 2.46586
H -1.81186 4.93331 3.54434
C -2.33 2.61502 2.16751
C -2.24385 2.83606 -0.4888
H -1.69943 5.34208 -1.44099
H -1.22759 7.31325 -0.00021
H -2.23346 2.85493 -1.57915
N -2.47796 1.67251 0.07679
N -2.53448 1.55356 1.42961
C 1.40798 2.89291 0.94567
H 2.30276 2.59442 1.50613
H 0.52417 2.8229 1.59938
H 1.5268 3.91944 0.57814
I -0.38227 0.05293 -2.60363
C -0.4803 -0.92534 1.68599
H -0.91982 -0.02041 2.12699
H -0.25162 -1.62757 2.50291
P 1.10515 -0.34696 0.935
P -1.83841 -1.65469 0.65894
C 2.06839 0.0617 2.44095
C 3.46276 -0.05978 2.40157
C 1.46857 0.62612 3.57232
C 4.24121 0.38096 3.46683
H 3.95379 -0.50387 1.53357
C 2.24993 1.05666 4.64117
H 0.38558 0.73802 3.63426
C 3.63654 0.94099 4.58918
H 5.32471 0.27939 3.41527
H 1.76951 1.48518 5.51943
H 4.24464 1.28327 5.42494
C 1.97583 -1.82428 0.30161
C 2.14154 -2.95086 1.11704
C 2.55599 -1.80631 -0.96831
C 2.86662 -4.04431 0.65905
H 1.71178 -2.97177 2.11974
C 3.2841 -2.90281 -1.42529
H 2.44169 -0.92935 -1.60444
C 3.43824 -4.02112 -0.61319
H 2.98803 -4.91824 1.29755
H 3.73875 -2.87427 -2.4143
H 4.00946 -4.87767 -0.96782
C -1.17812 -3.30784 0.20467
C -1.03556 -4.30031 1.18338

C -0.77939 -3.58279 -1.10598
C -0.51071 -5.54423 0.85349
H -1.33641 -4.10205 2.21252
C -0.24924 -4.82886 -1.43393
H -0.87154 -2.81715 -1.87593
C -0.11827 -5.81094 -0.457
H -0.40515 -6.30739 1.62302
H 0.06112 -5.02921 -2.45834
H 0.2926 -6.78583 -0.71525
C -3.06066 -2.08503 1.96003
C -4.03295 -3.04719 1.65382
C -3.12468 -1.43114 3.19342
C -5.04146 -3.34947 2.56136
H -4.00052 -3.57154 0.69727
C -4.13747 -1.73512 4.1012
H -2.38723 -0.67775 3.46616
C -5.0975 -2.69137 3.7883
H -5.78614 -4.10257 2.30855
H -4.16905 -1.22095 5.06061
H -5.8872 -2.92685 4.49987
C 3.04277 1.74229 -0.89019
H 3.54035 1.21257 -0.07102
H 3.35889 2.79007 -0.91945
H 3.21659 1.25281 -1.85626
I 6.5662 -0.32569 -0.40462

10B
E(RM06) = -2566.31162844
Zero-point correction= 0.748238 (Hartree/Particle)
Thermal correction to Energy= 0.800410
Thermal correction to Enthalpy= 0.801354
Thermal correction to Gibbs Free Energy= 0.658418
Sum of electronic and zero-point Energies= -2565.563390
Sum of electronic and thermal Energies= -2565.511219
Sum of electronic and thermal Enthalpies= -2565.510274
Sum of electronic and thermal Free Energies= -2565.653211
E(RM06L) = -3141.19481989

Pt 1.41117 1.17194 -0.30638
C 1.98126 2.71366 -1.58515
H 2.59424 3.472 -1.08034
H 2.55901 2.28755 -2.41739
H 1.08772 3.19332 -2.00897
Pt -2.65481 0.36569 -1.36017
C -3.49695 -1.04501 -2.61272
H -2.92431 -1.06333 -3.54974
H -3.47397 -2.04399 -2.1595
H -4.53792 -0.7823 -2.83991
C -3.1133 1.71715 -2.88167
H -2.24762 1.82608 -3.54846
H -3.96989 1.36688 -3.47073
H -3.37102 2.69071 -2.44123
C -4.56474 0.76294 -0.66578
H -4.46323 1.18694 0.34203
H -5.06159 1.47898 -1.33073
H -5.15268 -0.16017 -0.62004
C -0.14789 6.40786 1.75857
C -0.78406 5.32953 2.3312
C -1.16924 4.24967 1.51603
C -0.90498 4.28254 0.12932

C -0.26255 5.39818 -0.44192
C 0.11173 6.44308 0.37197
H -2.03797 2.97974 3.06174
H 0.16102 7.24681 2.37876
H -0.98748 5.29717 3.40063
C -1.80173 3.07491 1.99928
C -1.29431 3.14114 -0.61257
H -0.06224 5.41601 -1.51232
H 0.6158 7.308 -0.05395
H -1.12925 3.09961 -1.68965
N -1.87028 2.08927 -0.07348
N -2.13686 2.04983 1.25793
C 1.90753 2.33508 1.32725
H 2.69757 1.87812 1.9366
H 0.98976 2.40728 1.93226
H 2.2231 3.33657 1.00883
I 0.04062 -0.02055 -2.51961
C -0.93005 -0.90583 1.72457
H -1.20409 0.08769 2.10621
H -0.9939 -1.6265 2.55488
P 0.83594 -0.73859 1.19185
P -2.25102 -1.3036 0.49022
C 1.67091 -0.55132 2.81233
C 3.00223 -0.9697 2.9282
C 1.07927 0.13577 3.87817
C 3.72915 -0.69237 4.08087
H 3.49527 -1.50939 2.11665
C 1.80502 0.39663 5.03622
H 0.04466 0.47721 3.81663
C 3.13252 -0.01001 5.13672
H 4.76802 -1.01291 4.13921
H 1.33001 0.92303 5.86305
H 3.70177 0.20491 6.03955
C 1.38291 -2.39231 0.65093
C 1.15061 -3.51229 1.45857
C 2.12445 -2.53437 -0.52206
C 1.63594 -4.75639 1.08136
H 0.59829 -3.41101 2.39404
C 2.62363 -3.78075 -0.89087
H 2.32984 -1.66753 -1.14724
C 2.37526 -4.89044 -0.09327
H 1.44828 -5.6241 1.71203
H 3.22508 -3.8725 -1.79297
H 2.77148 -5.86401 -0.37707
C -1.95567 -3.0726 0.09779
C -2.25811 -4.06375 1.04075
C -1.38319 -3.4446 -1.12109
C -1.99959 -5.40021 0.76387
H -2.70438 -3.7915 1.99755
C -1.11481 -4.78375 -1.39098
H -1.12774 -2.68427 -1.85923
C -1.42781 -5.76178 -0.45359
H -2.24229 -6.162 1.50309
H -0.65683 -5.05844 -2.33961
H -1.22153 -6.80905 -0.66911
C -3.7312 -1.40199 1.57213
C -4.84919 -2.09938 1.09502
C -3.82885 -0.73171 2.79347
C -6.03051 -2.1302 1.82531
H -4.79368 -2.63158 0.14389

C -5.0144 -0.76289 3.52411
H -2.98186 -0.17496 3.19127
C -6.11651 -1.45942 3.04282
H -6.88751 -2.68094 1.44129
H -5.0712 -0.24088 4.47804
H -7.04183 -1.48266 3.6158
C 3.45789 0.75235 -0.29569
H 3.65259 0.10785 0.56413
H 4.04079 1.67629 -0.23314
H 3.62371 0.23844 -1.24945
I 6.29922 -1.26437 0.41711

11A
E(RM06) = -2566.35268892
Zero-point correction= 0.746124 (Hartree/Particle)
Thermal correction to Energy= 0.798618
Thermal correction to Enthalpy= 0.799562
Thermal correction to Gibbs Free Energy= 0.656420
Sum of electronic and zero-point Energies= -2565.606565
Sum of electronic and thermal Energies= -2565.554071
Sum of electronic and thermal Enthalpies= -2565.553127
Sum of electronic and thermal Free Energies= -2565.696269
E(RM06L) = -3141.22900443

Pt 1.44731 1.61434 0.17414
C 1.81185 3.41635 -0.81391
H 2.62685 3.98612 -0.34726
H 2.07147 3.21723 -1.86301
H 0.88935 4.01393 -0.7828
Pt -3.22944 0.18433 -1.29949
C -3.29024 -1.38096 -2.65116
H -2.3362 -1.437 -3.19321
H -3.47563 -2.33311 -2.13743
H -4.09517 -1.21968 -3.37944
C -3.92793 1.30446 -2.90864
H -3.13773 1.35905 -3.66971
H -4.82152 0.84908 -3.3526
H -4.18042 2.31675 -2.5659
C -5.2341 -0.17585 -0.94199
H -5.35787 -0.34758 0.13223
H -5.80107 0.71704 -1.23517
H -5.58704 -1.04222 -1.51519
C -3.9298 6.51362 2.08737
C -4.33935 5.25636 2.47392
C -4.05913 4.15892 1.63897
C -3.37514 4.3567 0.42085
C -2.96942 5.64906 0.03587
C -3.24501 6.71046 0.8682
H -4.90137 2.58523 2.89206
H -4.13341 7.37058 2.7266
H -4.86553 5.09579 3.41388
C -4.38375 2.81433 1.9579
C -3.08847 3.19769 -0.33802
H -2.4344 5.78666 -0.90316
H -2.93223 7.71487 0.58975
H -2.53509 3.27894 -1.27531
N -3.44343 1.98973 0.03439
N -4.10263 1.7842 1.2029
C 2.9334 2.0851 1.54406
H 3.85374 1.53691 1.30577

H 2.58722 1.80866 2.54656
H 3.13025 3.16344 1.51144
I -0.48207 0.96871 -1.95045
C -0.95755 -0.77935 1.74915
H -1.251 0.20804 2.13667
H -0.98211 -1.49788 2.58353
P 0.8313 -0.55821 1.28436
P -2.34063 -1.30584 0.62037
C 1.61791 -0.62937 2.94283
C 2.98436 -0.93404 3.01026
C 0.95352 -0.24635 4.11181
C 3.66601 -0.86865 4.21961
H 3.52452 -1.22313 2.10699
C 1.64005 -0.179 5.32293
H -0.10601 0.0073 4.09404
C 2.99481 -0.48851 5.38035
H 4.72642 -1.11393 4.25501
H 1.10678 0.11563 6.22555
H 3.5286 -0.43486 6.32782
C 1.39431 -2.14108 0.54449
C 1.46771 -3.30483 1.32131
C 1.82298 -2.18391 -0.78471
C 1.97793 -4.47955 0.78129
H 1.13125 -3.292 2.35885
C 2.34379 -3.35916 -1.3222
H 1.74823 -1.294 -1.40702
C 2.42885 -4.50476 -0.53805
H 2.02668 -5.37892 1.39369
H 2.68304 -3.37531 -2.35683
H 2.84016 -5.42295 -0.95502
C -1.89437 -3.04761 0.22691
C -2.09034 -4.07321 1.16111
C -1.32618 -3.36159 -1.0108
C -1.76204 -5.38758 0.847
H -2.50946 -3.84886 2.14158
C -1.00049 -4.67841 -1.32595
H -1.13148 -2.57275 -1.73595
C -1.22758 -5.69432 -0.40227
H -1.92541 -6.17463 1.58167
H -0.56373 -4.90737 -2.29715
H -0.97903 -6.72481 -0.65211
C -3.6782 -1.54348 1.86134
C -4.763 -2.35693 1.50604
C -3.7159 -0.87179 3.08668
C -5.84852 -2.5088 2.36136
H -4.75855 -2.88283 0.54927
C -4.80664 -1.02033 3.9406
H -2.90136 -0.21533 3.39163
C -5.87335 -1.83834 3.58242
H -6.67824 -3.15134 2.07078
H -4.81673 -0.49238 4.89304
H -6.72328 -1.95425 4.25309
C 3.01562 0.91113 -0.99482
H 3.45024 0.01523 -0.53451
H 3.78469 1.69091 -1.06254
H 2.64633 0.67877 -2.00202
I -0.34526 3.01834 2.04566

11B
E(RM06) = -2566.34007860

Zero-point correction= 0.746638 (Hartree/Particle)
Thermal correction to Energy= 0.799253
Thermal correction to Enthalpy= 0.800197
Thermal correction to Gibbs Free Energy= 0.656639
Sum of electronic and zero-point Energies= -2565.593441
Sum of electronic and thermal Energies= -2565.540826
Sum of electronic and thermal Enthalpies= -2565.539881
Sum of electronic and thermal Free Energies= -2565.683440
E(RM06L) = -3141.22056884

Pt 1.40769 1.63502 0.22004
C 1.73943 3.45843 -0.73129
H 2.58805 4.00212 -0.29577
H 1.93474 3.282 -1.798
H 0.82835 4.06317 -0.62455
Pt -3.2096 0.16256 -1.28879
C -3.25292 -1.39875 -2.64592
H -2.30179 -1.43579 -3.19413
H -3.42208 -2.35747 -2.13894
H -4.06295 -1.24647 -3.37026
C -3.90454 1.28183 -2.89871
H -3.11361 1.33904 -3.65798
H -4.79774 0.82868 -3.34537
H -4.15834 2.29311 -2.55314
C -5.21092 -0.22679 -0.92873
H -5.34331 -0.31917 0.15432
H -5.80043 0.62538 -1.29048
H -5.53447 -1.14088 -1.44257
C -3.96385 6.53169 2.00272
C -4.42961 5.28966 2.37097
C -4.11123 4.17361 1.57558
C -3.33066 4.33959 0.41291
C -2.86491 5.61688 0.04758
C -3.18087 6.69596 0.84011
H -5.07596 2.62981 2.77911
H -4.19571 7.40111 2.61502
H -5.02776 5.1556 3.27136
C -4.49063 2.84035 1.88122
C -3.0176 3.16423 -0.30974
H -2.24687 5.72783 -0.84259
H -2.81938 7.6879 0.57666
H -2.38442 3.21168 -1.1982
N -3.44674 1.97286 0.03599
N -4.19039 1.79695 1.15482
C 2.86445 2.13996 1.60906
H 3.83026 1.70641 1.31867
H 2.56151 1.75928 2.59089
H 2.94647 3.23151 1.65914
I -0.48328 0.95957 -1.94068
C -0.94344 -0.80909 1.77388
H -1.22696 0.17873 2.1685
H -0.96567 -1.53469 2.60229
P 0.8387 -0.56829 1.2873
P -2.3322 -1.31439 0.64098
C 1.65217 -0.67847 2.93073
C 3.01288 -1.01034 2.97083
C 1.01912 -0.2889 4.11398
C 3.71732 -0.96911 4.16728
H 3.52907 -1.30261 2.05489
C 1.72798 -0.24708 5.31234

H -0.03001 0.00405 4.11268
C 3.07539 -0.58667 5.34277
H 4.7735 -1.23371 4.18058
H 1.21929 0.05892 6.22509
H 3.62769 -0.55016 6.28036
C 1.39292 -2.13928 0.51186
C 1.46102 -3.32198 1.25924
C 1.82216 -2.15243 -0.81734
C 1.9621 -4.48608 0.69136
H 1.1312 -3.33066 2.2988
C 2.33255 -3.31829 -1.38377
H 1.7543 -1.24565 -1.41555
C 2.40917 -4.4829 -0.62878
H 2.00518 -5.40013 1.28196
H 2.67322 -3.31004 -2.41798
H 2.81365 -5.39359 -1.06852
C -1.90221 -3.06329 0.25866
C -2.12182 -4.08893 1.18676
C -1.31151 -3.37919 -0.96785
C -1.79576 -5.40445 0.87724
H -2.56313 -3.86298 2.15709
C -0.98605 -4.69654 -1.27689
H -1.099 -2.58983 -1.6875
C -1.23874 -5.71216 -0.36082
H -1.98101 -6.19191 1.60632
H -0.52917 -4.9254 -2.23849
H -0.99223 -6.74389 -0.60772
C -3.67713 -1.52002 1.87976
C -4.75392 -2.35647 1.5571
C -3.73289 -0.78548 3.06733
C -5.844 -2.47487 2.41058
H -4.73941 -2.92665 0.62664
C -4.82686 -0.90259 3.92065
H -2.93093 -0.09852 3.3372
C -5.8824 -1.74772 3.59746
H -6.66735 -3.13591 2.14475
H -4.84873 -0.32719 4.84507
H -6.73569 -1.83896 4.26766
C 2.99494 0.98394 -0.96006
H 3.46149 0.09594 -0.5139
H 3.74279 1.78457 -1.02282
H 2.63868 0.75168 -1.97239
I -0.42219 2.9223 2.09417

12A
E(RM06) = -2566.33534981
Zero-point correction= 0.745414 (Hartree/Particle)
Thermal correction to Energy= 0.798453
Thermal correction to Enthalpy= 0.799397
Thermal correction to Gibbs Free Energy= 0.651894
Sum of electronic and zero-point Energies= -2565.589936
Sum of electronic and thermal Energies= -2565.536897
Sum of electronic and thermal Enthalpies= -2565.535952
Sum of electronic and thermal Free Energies= -2565.683456
(RM06L) = -3141.21419719

1 78 0 0.413377 -1.605944 -1.240698
2 6 0 0.627078 -1.402075 -3.287719
3 1 0 -0.403662 -1.367777 -3.681230
4 1 0 1.149679 -0.463337 -3.515637

5 1 0 1.157090 -2.242328 -3.752449
6 78 0 -1.729477 0.889192 -2.123151
7 6 0 -3.499085 0.348617 -3.012064
8 1 0 -3.293510 -0.578262 -3.570866
9 1 0 -4.292271 0.163886 -2.276741
10 1 0 -3.837804 1.118572 -3.716175
11 6 0 -1.201695 1.599482 -3.996443
12 1 0 -1.040227 0.713680 -4.628107
13 1 0 -1.987242 2.219424 -4.444207
14 1 0 -0.270018 2.176827 -3.928292
15 6 0 4.492637 3.762225 0.204438
16 6 0 4.084667 2.445695 0.190466
17 6 0 2.827764 2.133297 -0.356637
18 6 0 1.999665 3.155981 -0.868686
19 6 0 2.434942 4.492268 -0.853823
20 6 0 3.672592 4.782109 -0.322366
21 1 0 2.925903 -0.024530 -0.083690
22 1 0 5.461709 4.023078 0.624498
23 1 0 4.712198 1.648489 0.588080
24 6 0 2.319268 0.814614 -0.429070
25 6 0 0.725553 2.760490 -1.340597
26 1 0 1.786285 5.274095 -1.245603
27 1 0 4.023662 5.811571 -0.298493
28 1 0 0.027539 3.509108 -1.716604
29 7 0 0.309286 1.516741 -1.345935
30 7 0 1.133926 0.523647 -0.912089
31 6 0 -0.156550 -3.541447 -1.610683
32 1 0 0.401074 -4.225147 -0.956198
33 1 0 0.036903 -3.818061 -2.654919
34 1 0 -1.231055 -3.637393 -1.402148
35 6 0 -1.207776 -0.062049 1.447535
36 1 0 -0.604940 0.851129 1.326740
37 1 0 -1.646737 -0.041100 2.455691
38 15 0 -0.096609 -1.524435 1.226492
39 15 0 -2.519426 0.026069 0.144938
40 6 0 1.421708 -1.124122 2.159496
41 6 0 2.377904 -2.144606 2.258570
42 6 0 1.707676 0.138167 2.682140
43 6 0 3.605767 -1.897596 2.860763
44 1 0 2.160495 -3.138078 1.858301
45 6 0 2.942688 0.382766 3.280174
46 1 0 0.981732 0.949671 2.627905
47 6 0 3.893222 -0.629507 3.365273
48 1 0 4.345224 -2.694045 2.927675
49 1 0 3.155318 1.375391 3.676725
50 1 0 4.860680 -0.434124 3.825049
51 6 0 -0.863857 -2.834344 2.249192
52 6 0 -1.120627 -2.582115 3.603340
53 6 0 -1.167159 -4.086703 1.713410
54 6 0 -1.693985 -3.565005 4.399966
55 1 0 -0.867641 -1.614414 4.039608
56 6 0 -1.738359 -5.071973 2.516780
57 1 0 -0.970624 -4.296630 0.664741
58 6 0 -2.005047 -4.811373 3.856349
59 1 0 -1.894064 -3.360649 5.450442
60 1 0 -1.977025 -6.044343 2.088590
61 1 0 -2.452814 -5.581035 4.483043
62 6 0 -3.403839 -1.567338 0.233741
63 6 0 -4.012711 -1.966299 1.431650
64 6 0 -3.483825 -2.395111 -0.887861

65 6 0 -4.679584 -3.182486 1.502701
66 1 0 -3.963715 -1.323445 2.311660
67 6 0 -4.154002 -3.615283 -0.814444
68 1 0 -3.022349 -2.087851 -1.827258
69 6 0 -4.749586 -4.007924 0.379732
70 1 0 -5.146873 -3.489570 2.436987
71 1 0 -4.211600 -4.254242 -1.694256
72 1 0 -5.274759 -4.959914 0.438251
73 6 0 -3.719512 1.214362 0.837529
74 6 0 -5.065058 1.142710 0.456922
75 6 0 -3.287582 2.275347 1.637302
76 6 0 -5.961185 2.121015 0.875161
77 1 0 -5.418535 0.318068 -0.162988
78 6 0 -4.187315 3.252924 2.051789
79 1 0 -2.242326 2.359647 1.937427
80 6 0 -5.523792 3.179014 1.670015
81 1 0 -7.007217 2.054710 0.580281
82 1 0 -3.835372 4.073375 2.676424
83 1 0 -6.227739 3.943775 1.994085
84 6 0 -2.545854 2.743298 -1.759392
85 1 0 -2.264135 3.427374 -2.565970
86 1 0 -2.126824 3.059992 -0.796033
87 1 0 -3.634140 2.638795 -1.699652
88 53 0 0.249993 4.005425 2.479084
89 6 0 2.364786 -2.268920 -1.378459
90 1 0 2.700099 -2.348253 -0.337544
91 1 0 2.928541 -1.516017 -1.938830
92 1 0 2.396506 -3.237126 -1.886358
93 53 0 6.076588 -1.378297 -0.560105

12B
E(RM06) = -2566.29439432
Zero-point correction= 0.747513 (Hartree/Particle)
Thermal correction to Energy= 0.799957
Thermal correction to Enthalpy= 0.800901
Thermal correction to Gibbs Free Energy= 0.656505
Sum of electronic and zero-point Energies= -2565.546881
Sum of electronic and thermal Energies= -2565.494437
Sum of electronic and thermal Enthalpies= -2565.493493
Sum of electronic and thermal Free Energies= -2565.637889
E(RM06L) = -3141.17830583

Pt 1.18437 -1.06158 -1.11928
C 1.3248 -0.89071 -3.18221
H 0.50354 -1.47874 -3.62477
H 1.23445 0.16451 -3.47478
H 2.27137 -1.28806 -3.57023
Pt -1.85712 0.00782 -2.10016
C -3.06445 -1.38566 -3.01615
H -2.41137 -2.0072 -3.6499
H -3.58895 -2.02937 -2.29988
H -3.80684 -0.89967 -3.66102
C -1.70278 0.84867 -3.99139
H -0.98272 0.22874 -4.54597
H -2.65772 0.85048 -4.52975
H -1.31717 1.87479 -3.92642
C 2.17 5.68374 -0.16623
C 2.45474 4.33702 -0.10524
C 1.47839 3.42356 -0.53925
C 0.2346 3.88066 -1.02326

C -0.03541 5.2573 -1.08355
C 0.92987 6.14192 -0.65667
H 2.62264 1.61933 -0.1587
H 2.91088 6.40702 0.16746
H 3.41385 3.96698 0.25712
C 1.67014 2.02214 -0.50956
C -0.70169 2.88389 -1.39088
H -1.00704 5.60249 -1.43295
H 0.73161 7.21123 -0.68499
H -1.6922 3.17011 -1.74562
N -0.44856 1.59717 -1.34816
N 0.76532 1.15859 -0.91062
C 1.69373 -3.03467 -1.38205
H 2.53152 -3.28556 -0.71599
H 2.00427 -3.23201 -2.41634
H 0.83961 -3.6795 -1.13657
C -1.06955 -0.42902 1.48541
H -1.04623 0.66279 1.33587
H -1.48879 -0.61189 2.48556
P 0.65468 -1.09154 1.34149
P -2.1686 -1.08843 0.15843
C 1.7027 0.10059 2.24018
C 3.04716 -0.25763 2.41221
C 1.26369 1.3569 2.66275
C 3.94057 0.63635 2.98794
H 3.40058 -1.23899 2.08523
C 2.16582 2.2504 3.23622
H 0.2261 1.67225 2.54661
C 3.50084 1.89502 3.39442
H 4.98745 0.36018 3.09572
H 1.80877 3.23066 3.55048
H 4.20747 2.60045 3.82791
C 0.65094 -2.55261 2.44443
C 0.27425 -2.3966 3.78442
C 1.03743 -3.81043 1.98211
C 0.26061 -3.49139 4.63804
H 0.00061 -1.41143 4.16595
C 1.03158 -4.9053 2.84343
H 1.33134 -3.94355 0.94361
C 0.6389 -4.74814 4.16716
H -0.0355 -3.3626 5.67769
H 1.33216 -5.88381 2.47225
H 0.63332 -5.60418 4.84007
C -2.07395 -2.91022 0.28347
C -2.4179 -3.54427 1.485
C -1.69268 -3.6844 -0.81324
C -2.3634 -4.92755 1.58597
H -2.73196 -2.95254 2.34581
C -1.64244 -5.07344 -0.71248
H -1.42695 -3.20156 -1.75454
C -1.97514 -5.69302 0.48678
H -2.62132 -5.41117 2.52652
H -1.34386 -5.66732 -1.57491
H -1.93704 -6.77811 0.56666
C -3.86124 -0.74388 0.74836
C -4.92045 -1.54474 0.30058
C -4.13231 0.38537 1.52254
C -6.23063 -1.2102 0.62111
H -4.72247 -2.43771 -0.29341
C -5.44673 0.71847 1.83627

H -3.33034 1.04045 1.86586
C -6.49595 -0.07462 1.38465
H -7.04813 -1.84016 0.27409
H -5.63803 1.60977 2.43221
H -7.52392 0.18849 1.62837
C -3.53601 1.18173 -1.83086
H -3.66872 1.82575 -2.70588
H -3.33597 1.76133 -0.92012
H -4.39955 0.52281 -1.69619
I -2.04529 3.62647 1.86331
C 3.23589 -0.60616 -1.21622
H 3.48044 -0.39444 -0.16964
H 3.32353 0.26463 -1.8693
H 3.79288 -1.46201 -1.60826
I 5.8082 1.50606 -0.51488

13A
E(RM06) = -2566.36418405
Zero-point correction= 0.746773 (Hartree/Particle)
Thermal correction to Energy= 0.798987
Thermal correction to Enthalpy= 0.799931
Thermal correction to Gibbs Free Energy= 0.657192
Sum of electronic and zero-point Energies= -2565.617411
Sum of electronic and thermal Energies= -2565.565197
Sum of electronic and thermal Enthalpies= -2565.564253
Sum of electronic and thermal Free Energies= -2565.706992
E(RM06L) = -3141.24295335

Pt 0.09701 1.80531 -1.69158
C -0.72668 1.91121 -3.60989
H 0.07474 2.0397 -4.35003
H -1.24987 0.96685 -3.81973
H -1.43234 2.74839 -3.70368
Pt 0.29621 -2.37783 -1.01462
C 1.84654 -3.73454 -1.15886
H 2.59884 -3.34188 -1.85442
H 2.30309 -3.90123 -0.17502
H 1.46609 -4.68998 -1.54234
C -0.33603 -3.16659 -2.8428
H 0.53169 -3.38113 -3.4805
H -0.91651 -4.08958 -2.71114
H -0.96113 -2.40936 -3.3383
C -0.64787 -3.94657 -0.02897
H -1.37363 -3.5403 0.68705
H -1.15306 -4.59547 -0.75485
H 0.0947 -4.53679 0.52014
C -6.49653 0.06595 -1.40145
C -5.34861 0.82229 -1.48154
C -4.10554 0.18223 -1.32841
C -4.04244 -1.20601 -1.10819
C -5.22318 -1.96715 -1.03164
C -6.4339 -1.32633 -1.17457
H -2.86878 1.93833 -1.53322
H -7.46842 0.54295 -1.50971
H -5.38508 1.8981 -1.64568
C -2.8681 0.8637 -1.36286
C -2.74701 -1.75273 -0.96903
H -5.16417 -3.04012 -0.85686
H -7.35875 -1.89621 -1.11321
H -2.64126 -2.82647 -0.82597

N -1.63244 -1.05614 -1.01081
N -1.69251 0.29593 -1.20804
C 1.39005 3.26298 -2.37625
H 1.88127 3.77416 -1.53926
H 0.82735 3.99996 -2.96316
H 2.14145 2.78696 -3.01888
I 1.68003 -0.41259 -2.60658
C 0.49234 0.31098 1.60419
H -0.60119 0.35732 1.48297
H 0.71962 0.49443 2.66597
P 1.12294 1.71061 0.57619
P 0.98332 -1.43357 1.21197
C 0.64467 3.15941 1.59146
C 1.37734 4.3464 1.46374
C -0.50933 3.15455 2.37882
C 0.95952 5.50395 2.11173
H 2.28367 4.36942 0.85717
C -0.92515 4.315 3.02656
H -1.10781 2.24957 2.48859
C -0.19439 5.49173 2.89293
H 1.54007 6.41928 2.00684
H -1.82728 4.29185 3.63716
H -0.52095 6.39898 3.39868
C 2.9451 1.73483 0.76759
C 3.49992 1.75232 2.05383
C 3.78898 1.82168 -0.34142
C 4.87647 1.83594 2.22228
H 2.85199 1.70712 2.93052
C 5.16931 1.91119 -0.17067
H 3.36986 1.81602 -1.34575
C 5.71327 1.91422 1.10915
H 5.29887 1.84015 3.22622
H 5.81723 1.98066 -1.04301
H 6.79177 1.98254 1.24394
C 2.7379 -1.53611 1.72952
C 3.08933 -1.48645 3.08473
C 3.74448 -1.64606 0.7665
C 4.42336 -1.56266 3.4671
H 2.31665 -1.39206 3.84819
C 5.08185 -1.70918 1.15145
H 3.48401 -1.67019 -0.29202
C 5.4211 -1.6772 2.50066
H 4.68548 -1.52808 4.52344
H 5.85857 -1.7862 0.39196
H 6.4662 -1.73548 2.80117
C 0.10172 -2.3368 2.54136
C 0.62386 -3.54621 3.01684
C -1.16916 -1.93608 2.96478
C -0.10419 -4.32738 3.90794
H 1.60676 -3.88636 2.68826
C -1.89655 -2.72054 3.85627
H -1.61994 -1.01159 2.60239
C -1.36696 -3.91712 4.32985
H 0.31792 -5.26256 4.27269
H -2.88293 -2.38751 4.17784
H -1.93644 -4.53036 5.02637
C -1.04009 3.42907 -1.07693
H -1.66344 3.11126 -0.22869
H -0.38451 4.24394 -0.74704
H -1.67056 3.78674 -1.90085

I -3.99328 1.05012 2.45855

13B
E(RM06) = -2566.34470775
Zero-point correction= 0.751268 (Hartree/Particle)
Thermal correction to Energy= 0.802160
Thermal correction to Enthalpy= 0.803104
Thermal correction to Gibbs Free Energy= 0.665793
Sum of electronic and zero-point Energies= -2565.593440
Sum of electronic and thermal Energies= -2565.542548
Sum of electronic and thermal Enthalpies= -2565.541604
Sum of electronic and thermal Free Energies= -2565.678915
E(RM06L) = -3141.22634356

Pt 0.28456 2.25465 -1.14736
C -0.82028 3.0636 -2.72561
H -0.2534 2.97313 -3.66151
H -1.75181 2.48871 -2.82917
H -1.05835 4.1235 -2.55835
Pt -1.38816 -1.61926 -0.8284
C -0.74207 -3.4645 -1.49568
H -0.0884 -3.32167 -2.36515
H -0.19219 -3.99173 -0.70559
H -1.60551 -4.07225 -1.7947
C -2.70571 -1.68598 -2.44536
H -2.21667 -2.15001 -3.31139
H -3.61702 -2.25285 -2.21103
H -2.97033 -0.65201 -2.70793
C -2.71378 -2.77313 0.28134
H -3.01785 -2.2229 1.18149
H -3.59243 -3.02707 -0.32498
H -2.22646 -3.70359 0.5938
C -6.09317 3.59269 0.8442
C -4.75554 3.75539 0.56688
C -3.97543 2.61662 0.30111
C -4.55883 1.33725 0.31337
C -5.92761 1.1855 0.59928
C -6.67817 2.30858 0.86304
H -2.09447 3.63554 0.00541
H -6.70959 4.4611 1.06642
H -4.28801 4.73845 0.57808
C -2.58989 2.66744 0.02583
C -3.68574 0.25928 0.04633
H -6.36991 0.19073 0.61901
H -7.73658 2.21025 1.09539
H -4.08012 -0.75622 0.03591
N -2.40343 0.38142 -0.2144
N -1.83542 1.62409 -0.23825
C 1.91059 3.08485 -2.1111
H 2.77367 3.152 -1.4373
H 1.65244 4.0934 -2.45723
H 2.16012 2.46162 -2.97908
I 0.35843 -0.20726 -2.61743
C 0.63578 0.17097 1.80467
H -0.29332 0.73167 2.00122
H 1.14163 0.03563 2.77343
P 1.62916 1.29219 0.7183
P 0.12458 -1.504 1.18726
C 2.16836 2.5842 1.89859
C 3.35995 3.27962 1.6553

C 1.34031 2.99577 2.94514
C 3.71064 4.3669 2.44755
H 4.02379 2.96756 0.84789
C 1.69516 4.08482 3.73551
H 0.39193 2.49617 3.14944
C 2.87774 4.77331 3.48778
H 4.64094 4.89799 2.25137
H 1.0292 4.39081 4.54126
H 3.15301 5.62758 4.1043
C 3.218 0.44421 0.37592
C 3.99137 -0.02844 1.44361
C 3.72184 0.35117 -0.92248
C 5.23535 -0.59912 1.21083
H 3.62451 0.06168 2.46701
C 4.974 -0.21402 -1.15424
H 3.13161 0.71602 -1.76063
C 5.72868 -0.69187 -0.08972
H 5.82388 -0.9716 2.048
H 5.3565 -0.27719 -2.17164
H 6.70744 -1.13448 -0.26913
C 1.67984 -2.47396 1.19471
C 2.2827 -2.8567 2.39987
C 2.28811 -2.82357 -0.01323
C 3.46146 -3.59204 2.39299
H 1.82226 -2.58801 3.35104
C 3.47461 -3.5522 -0.01728
H 1.83867 -2.51321 -0.95693
C 4.05616 -3.94447 1.18355
H 3.91739 -3.89074 3.3357
H 3.94266 -3.8131 -0.96511
H 4.97922 -4.52234 1.17871
C -0.77608 -2.14329 2.64952
C -0.80036 -3.52024 2.90574
C -1.58655 -1.29768 3.41207
C -1.60635 -4.0341 3.91509
H -0.18407 -4.19946 2.31509
C -2.39229 -1.81578 4.42214
H -1.61837 -0.22097 3.23712
C -2.40468 -3.18305 4.67584
H -1.61035 -5.10603 4.10708
H -3.008 -1.133 5.00634
H -3.03522 -3.58759 5.46601
C 0.25266 4.0732 -0.1438
H -0.22452 3.92667 0.83546
H 1.27548 4.43273 0.02086
H -0.29551 4.82132 -0.73075
I -2.51902 2.57915 3.70513

14A
E(RM06) = -2566.35612170
Zero-point correction= 0.748527 (Hartree/Particle)
Thermal correction to Energy= 0.800362
Thermal correction to Enthalpy= 0.801306
Thermal correction to Gibbs Free Energy= 0.658935
Sum of electronic and zero-point Energies= -2565.607595
Sum of electronic and thermal Energies= -2565.555760
Sum of electronic and thermal Enthalpies= -2565.554816
Sum of electronic and thermal Free Energies= -2565.697186
E(RM06L) = -3141.23500462

Pt -0.87086 -1.66589 -0.63278
C -0.42472 -3.20096 -1.9747
H -0.90937 -3.00931 -2.94153
H 0.66652 -3.21298 -2.1234
H -0.75155 -4.18111 -1.60128
Pt 2.56639 0.66834 -1.37789
C 2.90384 2.45348 -2.36124
H 2.1247 2.59484 -3.12103
H 2.88837 3.29273 -1.65427
H 3.88415 2.42127 -2.85393
C 3.41606 -0.20955 -3.06853
H 3.0454 0.29267 -3.97154
H 4.51263 -0.15431 -3.05595
H 3.10018 -1.26261 -3.09439
C 4.46949 1.01169 -0.61727
H 4.57892 0.47637 0.33488
H 5.22823 0.66723 -1.33046
H 4.60877 2.08459 -0.43964
C 4.11428 -5.36954 2.21259
C 2.87735 -4.77516 2.09222
C 2.74025 -3.66271 1.24243
C 3.854 -3.16986 0.53267
C 5.10956 -3.79057 0.66172
C 5.22777 -4.87955 1.49701
H 0.60649 -3.38878 1.47773
H 4.23964 -6.23112 2.86499
H 2.01079 -5.15058 2.63411
C 1.50962 -3.00546 1.00672
C 3.62621 -2.02067 -0.25914
H 5.96313 -3.40207 0.10867
H 6.19118 -5.37193 1.61172
H 4.45836 -1.567 -0.79657
N 2.46173 -1.42371 -0.37984
N 1.36035 -1.96091 0.22439
C -2.7701 -1.72309 -1.443
H -3.49157 -1.28145 -0.74417
H -3.05231 -2.76382 -1.64359
H -2.76259 -1.16062 -2.38449
I 0.03665 0.21342 -2.62157
C 0.30342 0.80089 1.70395
H 0.81587 -0.10686 2.04836
H 0.08865 1.41676 2.591
P -1.28364 0.16943 0.98956
P 1.53426 1.7303 0.67025
C -2.12411 -0.43473 2.50298
C -3.52126 -0.51618 2.49062
C -1.4243 -0.9416 3.6029
C -4.20561 -1.08691 3.558
H -4.08824 -0.12464 1.64374
C -2.11315 -1.50715 4.67369
H -0.33583 -0.90387 3.64093
C -3.5027 -1.58367 4.65334
H -5.29368 -1.13733 3.53077
H -1.55671 -1.88855 5.52861
H -4.03732 -2.02779 5.49142
C -2.29333 1.63159 0.55307
C -2.53495 2.62292 1.51319
C -2.88892 1.73841 -0.70542
C -3.34504 3.70984 1.20864
H -2.09366 2.54235 2.50769

C -3.70231 2.82844 -1.00823
H -2.72289 0.96575 -1.45391
C -3.92954 3.81374 -0.05361
H -3.52164 4.4792 1.95905
H -4.16897 2.89623 -1.98965
H -4.56833 4.66379 -0.28845
C 0.74779 3.37619 0.5083
C 0.56721 4.19838 1.62851
C 0.25698 3.79367 -0.73169
C -0.08093 5.42137 1.50339
H 0.93362 3.88285 2.60585
C -0.40042 5.01573 -0.8529
H 0.37422 3.15493 -1.60679
C -0.56601 5.83103 0.26241
H -0.2142 6.05435 2.37927
H -0.78466 5.32757 -1.82283
H -1.07781 6.78746 0.1667
C 2.86911 1.98061 1.90184
C 3.61069 3.16736 1.90439
C 3.29202 0.91752 2.70848
C 4.73663 3.29533 2.71235
H 3.31311 4.00129 1.26809
C 4.4158 1.04944 3.5188
H 2.76259 -0.03631 2.70063
C 5.14073 2.23825 3.52292
H 5.30035 4.22684 2.70507
H 4.72735 0.21589 4.14631
H 6.02137 2.33927 4.15496
C -1.64476 -3.0628 0.69762
H -1.28758 -2.8373 1.71084
H -2.74019 -3.00897 0.70119
H -1.33491 -4.07331 0.40354
I -6.83613 0.24872 0.1255

14B
E(RM06) = -2566.31898183
Zero-point correction= 0.747949 (Hartree/Particle)
Thermal correction to Energy= 0.799981
Thermal correction to Enthalpy= 0.800925
Thermal correction to Gibbs Free Energy= 0.658509
Sum of electronic and zero-point Energies= -2565.571033
Sum of electronic and thermal Energies= -2565.519001
Sum of electronic and thermal Enthalpies= -2565.518057
Sum of electronic and thermal Free Energies= -2565.660472
E(RM06L) = -3141.20114421

Pt -0.89613 -1.6439 -0.66636
C -0.44557 -3.17182 -2.01084
H -0.94913 -2.99896 -2.97064
H 0.64214 -3.15607 -2.18365
H -0.74191 -4.15884 -1.62917
Pt 2.58927 0.6864 -1.32958
C 2.91537 2.44683 -2.35805
H 2.16211 2.54322 -3.14925
H 2.84597 3.30572 -1.67857
H 3.91364 2.42763 -2.81282
C 3.45197 -0.23111 -2.99307
H 3.10109 0.2575 -3.91037
H 4.54943 -0.18996 -2.96833
H 3.11804 -1.27846 -3.00886

C 4.48854 1.04991 -0.56007
H 4.58497 0.58624 0.43126
H 5.25567 0.65351 -1.23774
H 4.64935 2.12898 -0.45189
C 4.03908 -5.56792 2.03068
C 2.80256 -4.98179 1.8803
C 2.70128 -3.78588 1.14535
C 3.85279 -3.20416 0.57681
C 5.10904 -3.8183 0.7362
C 5.19117 -4.98716 1.45845
H 0.54781 -3.54152 1.26907
H 4.13448 -6.49371 2.59408
H 1.90822 -5.42796 2.31252
C 1.47994 -3.11369 0.90094
C 3.65524 -1.99067 -0.12228
H 5.99302 -3.3632 0.29193
H 6.15444 -5.47481 1.59233
H 4.50882 -1.47982 -0.56705
N 2.49075 -1.40071 -0.27032
N 1.36604 -1.9936 0.22506
C -2.77437 -1.68773 -1.53218
H -3.49886 -1.17671 -0.88719
H -3.08952 -2.72843 -1.67067
H -2.70718 -1.19303 -2.50858
I 0.0835 0.23222 -2.60371
C 0.31979 0.80892 1.68663
H 0.84765 -0.1069 1.98351
H 0.11419 1.38491 2.60242
P -1.28302 0.18334 0.98333
P 1.53633 1.77814 0.68033
C -2.07865 -0.42742 2.51718
C -3.47505 -0.49937 2.54157
C -1.34976 -0.95461 3.58949
C -4.12945 -1.08528 3.61937
H -4.07338 -0.11442 1.71139
C -2.00954 -1.53051 4.67154
H -0.25923 -0.92324 3.59672
C -3.39971 -1.5989 4.68718
H -5.21713 -1.13792 3.60881
H -1.4325 -1.92675 5.50618
H -3.91357 -2.05491 5.53195
C -2.28095 1.64988 0.56303
C -2.47918 2.66206 1.51038
C -2.92715 1.72771 -0.67125
C -3.29552 3.74386 1.2131
H -2.00835 2.59597 2.49236
C -3.7547 2.80862 -0.96217
H -2.80301 0.93434 -1.40527
C -3.93568 3.81615 -0.02391
H -3.44392 4.52894 1.95317
H -4.27904 2.8409 -1.915
H -4.59227 4.6556 -0.24678
C 0.73789 3.41641 0.51015
C 0.62802 4.28227 1.60608
C 0.1694 3.78489 -0.71204
C -0.02469 5.50134 1.47304
H 1.05971 4.00675 2.56867
C -0.49735 5.00006 -0.83737
H 0.22735 3.10996 -1.5659
C -0.58824 5.8609 0.25092

H -0.09986 6.17044 2.32869
H -0.9499 5.26891 -1.79014
H -1.10571 6.81354 0.1494
C 2.85043 2.05926 1.93104
C 3.64117 3.21222 1.85329
C 3.20542 1.06475 2.84856
C 4.7457 3.37226 2.68233
H 3.39089 3.99666 1.13811
C 4.3112 1.22626 3.67836
H 2.62662 0.1439 2.92686
C 5.08409 2.37978 3.59753
H 5.34461 4.2786 2.61108
H 4.56598 0.44562 4.3934
H 5.94821 2.50606 4.24726
C -1.74924 -3.01196 0.64273
H -1.29644 -2.90349 1.63833
H -2.82322 -2.80985 0.7415
H -1.61296 -4.03511 0.26954
I -6.43337 -0.54068 -0.07556

15B
E(RM06) = -2566.31990353
Zero-point correction= 0.745653 (Hartree/Particle)
Thermal correction to Energy= 0.798981
Thermal correction to Enthalpy= 0.799925
Thermal correction to Gibbs Free Energy= 0.650515
Sum of electronic and zero-point Energies= -2565.574251
Sum of electronic and thermal Energies= -2565.520923
Sum of electronic and thermal Enthalpies= -2565.519979
Sum of electronic and thermal Free Energies= -2565.669388
E(RM06L) = -3141.20718752

1 78 0 0.744093 -1.305782 -1.146935
2 6 0 1.422506 -1.290159 -3.113737
3 1 0 0.602134 -1.365836 -3.842571
4 1 0 1.987786 -0.367636 -3.324016
5 1 0 2.087334 -2.153416 -3.273645
6 78 0 -1.591109 0.354063 -2.053719
7 6 0 -2.832849 -0.785574 -3.233812
8 1 0 -2.235214 -1.624402 -3.622151
9 1 0 -3.696980 -1.173006 -2.679022
10 1 0 -3.202705 -0.194690 -4.081605
11 6 0 -0.784993 1.145207 -3.808944
12 1 0 0.301337 0.992580 -3.793323
13 1 0 -1.203810 0.656891 -4.698741
14 1 0 -0.986871 2.224304 -3.868205
15 6 0 3.750133 4.792336 -0.114041
16 6 0 3.681816 3.420208 -0.205498
17 6 0 2.446952 2.819591 -0.509808
18 6 0 1.297776 3.615990 -0.707026
19 6 0 1.386797 5.015706 -0.609706
20 6 0 2.604451 5.588782 -0.319394
21 1 0 3.114399 0.737392 -0.473038
22 1 0 4.696716 5.272799 0.125087
23 1 0 4.557369 2.792999 -0.039825
24 6 0 2.272896 1.418200 -0.618989
25 6 0 0.088076 2.929014 -0.988267
26 1 0 0.491474 5.620936 -0.738725
27 1 0 2.684618 6.670154 -0.232038
28 1 0 -0.836597 3.480427 -1.160301

29 7 0 0.011336 1.624205 -1.081732
30 7 0 1.121921 0.857289 -0.893719
31 6 0 0.423372 -3.298997 -1.541475
32 1 0 1.386033 -3.828446 -1.421604
33 1 0 0.093983 -3.455184 -2.579982
34 1 0 -0.314478 -3.763896 -0.876587
35 6 0 -1.391574 -0.187315 1.447902
36 1 0 -1.117440 0.874366 1.349920
37 1 0 -1.853994 -0.313039 2.436682
38 15 0 0.138745 -1.208002 1.227269
39 15 0 -2.568832 -0.526521 0.068729
40 6 0 1.435473 -0.294606 2.153092
41 6 0 2.657163 -0.953109 2.351654
42 6 0 1.303325 1.031023 2.568792
43 6 0 3.724466 -0.292947 2.948684
44 1 0 2.772925 -1.995418 2.043529
45 6 0 2.379161 1.693788 3.157002
46 1 0 0.372046 1.584889 2.442411
47 6 0 3.590206 1.037416 3.344073
48 1 0 4.665799 -0.818630 3.102355
49 1 0 2.252065 2.731672 3.463982
50 1 0 4.429078 1.555729 3.806069
51 6 0 -0.112152 -2.669307 2.307096
52 6 0 -0.637522 -2.529004 3.597035
53 6 0 0.309725 -3.928512 1.876342
54 6 0 -0.770348 -3.636095 4.424803
55 1 0 -0.929153 -1.545969 3.969490
56 6 0 0.176153 -5.037984 2.708357
57 1 0 0.745650 -4.043365 0.885385
58 6 0 -0.370139 -4.894179 3.977850
59 1 0 -1.180016 -3.515965 5.426439
60 1 0 0.504177 -6.016037 2.360028
61 1 0 -0.475191 -5.761183 4.628190
62 6 0 -3.002544 -2.293322 0.271110
63 6 0 -3.532450 -2.734500 1.491219
64 6 0 -2.824491 -3.209170 -0.765690
65 6 0 -3.861797 -4.071022 1.671298
66 1 0 -3.694439 -2.026016 2.304840
67 6 0 -3.157207 -4.550239 -0.584659
68 1 0 -2.410336 -2.877355 -1.715699
69 6 0 -3.670637 -4.981450 0.632656
70 1 0 -4.264371 -4.404801 2.626205
71 1 0 -3.008055 -5.256329 -1.400108
72 1 0 -3.928296 -6.029811 0.774863
73 6 0 -4.112176 0.318563 0.552268
74 6 0 -5.340396 -0.166243 0.084982
75 6 0 -4.072692 1.525027 1.254046
76 6 0 -6.508709 0.549110 0.322886
77 1 0 -5.387638 -1.111450 -0.457953
78 6 0 -5.244525 2.237785 1.488608
79 1 0 -3.129480 1.938659 1.615580
80 6 0 -6.462351 1.752892 1.023170
81 1 0 -7.460436 0.162715 -0.038793
82 1 0 -5.190261 3.177584 2.036605
83 1 0 -7.378855 2.311718 1.205912
84 6 0 -3.067427 1.795712 -2.200192
85 1 0 -3.054867 2.258204 -3.192827
86 1 0 -2.855687 2.539767 -1.418867
87 1 0 -4.044253 1.334710 -2.014632
88 53 0 -1.267760 4.113739 2.122538

89 6 0 4.275947 -1.827027 -1.080255
90 1 0 3.437590 -1.630359 -0.403686
91 1 0 4.114601 -1.367062 -2.056556
92 1 0 4.459491 -2.899339 -1.174414
93 53 0 6.057422 -0.921888 -0.226427

Iodide in acetone
E(RM06) = -11.5715594473
Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.016848
Sum of electronic and zero-point Energies= -11.571559
Sum of electronic and thermal Energies= -11.570143
Sum of electronic and thermal Enthalpies= -11.569199
Sum of electronic and thermal Free Energies= -11.588408
E(RM06L) = -298.049042033

Iodomethane in acetone
E(RM06) = -51.2636159544
Zero-point correction= 0.036524 (Hartree/Particle)
Thermal correction to Energy= 0.039695
Thermal correction to Enthalpy= 0.040639
Thermal correction to Gibbs Free Energy= 0.010755
Sum of electronic and zero-point Energies= -51.227092
Sum of electronic and thermal Energies= -51.223921
Sum of electronic and thermal Enthalpies= -51.222977
Sum of electronic and thermal Free Energies= -51.252861
E(RM06L)

C 0.17524 1.69306 0.
H 0.50005 0.65188 0.
H 0.50028 2.21375 0.90169
H 0.50028 2.21375 -0.90169
I -1.99804 1.69304 0.

Iodomethane in benzene
E(RM06) = -51.2620102164
Zero-point correction= 0.036677 (Hartree/Particle)
Thermal correction to Energy= 0.039838
Thermal correction to Enthalpy= 0.040782
Thermal correction to Gibbs Free Energy= 0.010916
Sum of electronic and zero-point Energies= -51.225333
Sum of electronic and thermal Energies= -51.222172
Sum of electronic and thermal Enthalpies= -51.221228
Sum of electronic and thermal Free Energies= -51.251094
E(RM06L) = -337.796281817

C 0.1708 1.69312 -0.00005
H 0.50157 0.65337 0.00009
H 0.50188 2.21293 0.90045
H 0.50183 2.21304 -0.90048
I -1.99827 1.69301 -0.00001

Phthalazine in acetone
E(RM06) = -417.630061881
Zero-point correction= 0.123324 (Hartree/Particle)
Thermal correction to Energy= 0.130000

Thermal correction to Enthalpy= 0.130944
Thermal correction to Gibbs Free Energy= 0.092090
Sum of electronic and zero-point Energies= -417.506738
Sum of electronic and thermal Energies= -417.500062
Sum of electronic and thermal Enthalpies= -417.499118
Sum of electronic and thermal Free Energies= -417.537972
E(RM06L) = -418.039317873

1 6 0 -2.191631 -1.084943 0.001464
2 6 0 -1.403857 0.096003 0.001517
3 6 0 -2.116949 1.313671 0.001798
4 6 0 -3.532307 1.204652 0.001988
5 1 0 0.547296 -0.840387 0.001098
6 1 0 -1.697163 -2.059301 0.001251
7 6 0 0.005268 0.104663 0.001311
8 6 0 -1.419854 2.538444 0.001873
9 1 0 -4.139625 2.113057 0.002200
10 6 0 -0.043467 2.528588 0.001668
11 6 0 0.670187 1.309827 0.001388
12 1 0 -1.979063 3.473415 0.002086
13 1 0 0.507264 3.467441 0.001721
14 1 0 1.758536 1.330185 0.001232
15 7 0 -4.191424 0.073401 0.001919
16 7 0 -3.500744 -1.106042 0.001651

Phthalazine in benzene
E(RM06) = -417.624418502
Zero-point correction= 0.123338 (Hartree/Particle)
Thermal correction to Energy= 0.130013
Thermal correction to Enthalpy= 0.130957
Thermal correction to Gibbs Free Energy= 0.092108
Sum of electronic and zero-point Energies= -417.501080
Sum of electronic and thermal Energies= -417.494405
Sum of electronic and thermal Enthalpies= -417.493461
Sum of electronic and thermal Free Energies= -417.532311
E(RM06L) = -418.034220794

C -2.19387 -1.08361 0.00147
C -1.40356 0.09604 0.00152
C -2.11659 1.3136 0.0018
C -3.53202 1.20206 0.00199
H 0.54926 -0.83726 0.00109
H -1.70373 -2.06053 0.00125
C 0.00572 0.1071 0.00131
C -1.41766 2.53743 0.00187
H -4.14306 2.10843 0.0022
C -0.04222 2.52906 0.00167
C 0.67124 1.31085 0.00139
H -1.97583 3.47323 0.00208
H 0.50802 3.46825 0.00173
H 1.75965 1.33079 0.00123
N -4.19102 0.07206 0.00192
N -3.50188 -1.10485 0.00165

TS-2A/2aA
E(RM06) = -2515.04390375
Zero-point correction= 0.705244 (Hartree/Particle)
Thermal correction to Energy= 0.753497
Thermal correction to Enthalpy= 0.754441

Thermal correction to Gibbs Free Energy= 0.620599
Sum of electronic and zero-point Energies= -2514.338660
Sum of electronic and thermal Energies= -2514.290406
Sum of electronic and thermal Enthalpies= -2514.289462
Sum of electronic and thermal Free Energies= -2514.423305
E(RM06L) = -2803.39164759

Pt 0.44933 2.22105 -1.18484
C -0.65144 3.15782 -2.68924
H -0.10637 3.14697 -3.64817
H -1.60339 2.61901 -2.84221
H -0.88908 4.20986 -2.45805
Pt -1.52427 -1.96744 -0.83341
C -0.79999 -3.85721 -1.26191
H -0.13809 -3.80996 -2.13626
H -0.24455 -4.26419 -0.40656
H -1.63917 -4.52941 -1.48713
C -2.82929 -2.31712 -2.42021
H -2.28524 -2.8007 -3.24141
H -3.67238 -2.9571 -2.12818
H -3.2079 -1.34644 -2.76997
C -2.82829 -2.98648 0.42238
H -3.17077 -2.30277 1.21034
H -3.68926 -3.35685 -0.14739
H -2.31443 -3.83802 0.8837
C -5.98417 3.42435 0.89523
C -4.61098 3.45015 0.79608
C -3.93367 2.28378 0.39376
C -4.65998 1.10956 0.10108
C -6.06426 1.10027 0.20667
C -6.71053 2.25009 0.60039
H -1.90452 3.08048 0.41928
H -6.52245 4.31867 1.20294
H -4.04259 4.35222 1.01793
C -2.52744 2.20176 0.23824
C -3.89851 -0.01975 -0.2803
H -6.61486 0.18914 -0.02263
H -7.79516 2.26002 0.68702
H -4.39967 -0.96226 -0.50209
N -2.58776 -0.01163 -0.37964
N -1.88134 1.12452 -0.13924
C 1.6957 3.85213 -1.26278
H 2.74151 3.5544 -1.09077
H 1.40976 4.57414 -0.48049
H 1.63327 4.35824 -2.23675
I 0.1484 -0.63939 -2.78759
C 0.68776 0.07227 1.68674
H -0.21651 0.64028 1.93981
H 1.24542 -0.09925 2.62055
P 1.63881 1.24154 0.59785
P 0.0967 -1.59513 1.10617
C 2.08656 2.52082 1.84559
C 3.38206 3.03861 1.93727
C 1.07292 3.10509 2.61691
C 3.66065 4.10423 2.79107
H 4.18639 2.61114 1.33872
C 1.35402 4.16218 3.47547
H 0.04715 2.7406 2.54636
C 2.65039 4.66592 3.5646
H 4.67605 4.49366 2.85005

H 0.55524 4.59783 4.07413
H 2.86977 5.49678 4.23332
C 3.242 0.43408 0.24745
C 4.02825 -0.13714 1.25518
C 3.71799 0.44812 -1.06655
C 5.26591 -0.69069 0.94826
H 3.67751 -0.13839 2.28842
C 4.95914 -0.10643 -1.37368
H 3.10701 0.89899 -1.85088
C 5.73179 -0.67612 -0.36673
H 5.87108 -1.13572 1.73725
H 5.3212 -0.0893 -2.40048
H 6.70253 -1.10953 -0.60343
C 1.6461 -2.57838 1.09663
C 2.30831 -2.90367 2.28743
C 2.20821 -2.96839 -0.12232
C 3.49401 -3.629 2.25822
H 1.89479 -2.5928 3.24716
C 3.40344 -3.68349 -0.15058
H 1.71423 -2.70175 -1.05715
C 4.04111 -4.02353 1.03862
H 3.99537 -3.88249 3.19117
H 3.83353 -3.97627 -1.10722
H 4.97043 -4.59093 1.01658
C -0.77248 -2.14758 2.6287
C -0.72423 -3.48713 3.03148
C -1.64808 -1.27852 3.29097
C -1.51266 -3.93999 4.08533
H -0.06926 -4.19046 2.51677
C -2.4345 -1.73253 4.34595
H -1.74327 -0.23693 2.98168
C -2.36827 -3.06392 4.74719
H -1.45728 -4.9847 4.38748
H -3.10425 -1.04 4.8536
H -2.98436 -3.41832 5.572

TS-2B/2aB
E(RM06) = -2515.02665340
Zero-point correction= 0.705866 (Hartree/Particle)
Thermal correction to Energy= 0.754065
Thermal correction to Enthalpy= 0.755009
Thermal correction to Gibbs Free Energy= 0.621020
Sum of electronic and zero-point Energies= -2514.320788
Sum of electronic and thermal Energies= -2514.272589
Sum of electronic and thermal Enthalpies= -2514.271644
Sum of electronic and thermal Free Energies= -2514.405634
E(RM06L) = -2803.37966475

Pt 0.2632 2.21708 -0.97517
C -0.97477 3.0793 -2.40683
H -0.46519 3.1206 -3.38226
H -1.87655 2.45252 -2.535
H -1.29362 4.10257 -2.14633
Pt -1.52984 -1.97379 -0.72991
C -0.82464 -3.88316 -1.08938
H -0.18975 -3.87609 -1.98405
H -0.24499 -4.25658 -0.23479
H -1.67282 -4.56013 -1.25865
C -2.79838 -2.36858 -2.33323
H -2.25071 -2.93706 -3.09424

H -3.68335 -2.94443 -2.02814
H -3.10113 -1.41072 -2.77721
C -2.87958 -2.91078 0.54931
H -3.2352 -2.18297 1.29235
H -3.73351 -3.30175 -0.01913
H -2.40086 -3.74581 1.0751
C -5.97819 3.5979 0.40761
C -4.61977 3.52569 0.61494
C -3.9384 2.33737 0.28906
C -4.64832 1.23899 -0.24216
C -6.03899 1.32968 -0.4452
C -6.68818 2.49888 -0.12168
H -1.91849 2.97649 0.8158
H -6.51617 4.51226 0.64983
H -4.06238 4.37136 1.01522
C -2.54108 2.16171 0.4407
C -3.88726 0.08093 -0.53094
H -6.57928 0.47862 -0.85735
H -7.7619 2.58334 -0.27684
H -4.37525 -0.81613 -0.91309
N -2.58793 0.00593 -0.35855
N -1.89001 1.06918 0.11282
C 1.48951 3.84541 -1.22788
H 2.54131 3.52725 -1.29655
H 1.38145 4.51542 -0.36053
H 1.23446 4.40482 -2.13821
I 0.13183 -0.68236 -2.6619
C 0.73373 0.04623 1.80994
H -0.16214 0.59574 2.12515
H 1.33654 -0.15078 2.7101
P 1.60765 1.25677 0.69256
P 0.12614 -1.60448 1.19144
C 2.1406 2.49905 1.94587
C 3.4232 3.05461 1.91732
C 1.20508 3.02436 2.84572
C 3.76581 4.09404 2.7781
H 4.16554 2.67442 1.2159
C 1.55053 4.05404 3.71292
H 0.18668 2.63346 2.86863
C 2.83435 4.59284 3.68165
H 4.77006 4.51365 2.73981
H 0.81168 4.44196 4.413
H 3.10439 5.4034 4.35662
C 3.18879 0.46043 0.22942
C 4.0516 -0.10785 1.17344
C 3.56137 0.47613 -1.11677
C 5.2629 -0.65811 0.77406
H 3.7824 -0.10935 2.23099
C 4.77727 -0.07455 -1.51623
H 2.88351 0.91501 -1.85057
C 5.62587 -0.64198 -0.57235
H 5.92649 -1.10339 1.51442
H 5.05763 -0.0579 -2.56816
H 6.57687 -1.07275 -0.88313
C 1.68662 -2.57281 1.12976
C 2.36987 -2.92335 2.30157
C 2.23679 -2.92013 -0.10669
C 3.56318 -3.63245 2.23681
H 1.96249 -2.65036 3.27557
C 3.43948 -3.61875 -0.16938

H 1.73171 -2.62593 -1.02727
C 4.09717 -3.98545 0.99953
H 4.0789 -3.90819 3.15565
H 3.8612 -3.8728 -1.14046
H 5.03288 -4.54057 0.94845
C -0.69657 -2.21415 2.72089
C -0.62668 -3.5645 3.08237
C -1.56183 -1.37734 3.43452
C -1.38099 -4.05685 4.14252
H 0.02312 -4.244 2.53086
C -2.31443 -1.86955 4.49599
H -1.67328 -0.32849 3.1567
C -2.22508 -3.21078 4.85464
H -1.30852 -5.10996 4.40972
H -2.97633 -1.19977 5.04301
H -2.8146 -3.59619 5.68478

TS-5A/6A
E(RM06) = -2515.02825307
Zero-point correction= 0.704212 (Hartree/Particle)
Thermal correction to Energy= 0.752638
Thermal correction to Enthalpy= 0.753582
Thermal correction to Gibbs Free Energy= 0.619223
Sum of electronic and zero-point Energies= -2514.324041
Sum of electronic and thermal Energies= -2514.275615
Sum of electronic and thermal Enthalpies= -2514.274671
Sum of electronic and thermal Free Energies= -2514.409030
E(RM06L) = -2803.37871375

Pt 2.03301 0.34737 -1.6285
C 1.79184 0.7351 -3.66594
H 1.20338 -0.06689 -4.1419
H 1.26491 1.68933 -3.83346
H 2.76241 0.78373 -4.18588
Pt -1.14686 -0.369 -1.32233
C -1.69264 -2.10357 -2.29539
H -0.89008 -2.37307 -3.00295
H -1.84643 -2.95646 -1.61699
H -2.61469 -1.96234 -2.87951
C -1.80983 0.59144 -3.06097
H -1.23928 0.23056 -3.93153
H -2.87492 0.39438 -3.25823
H -1.67054 1.68302 -2.98759
C 0.06717 6.37395 0.87727
C 0.81857 5.52049 0.09966
C 0.35782 4.20818 -0.11257
C -0.85844 3.77998 0.46611
C -1.61514 4.66675 1.25389
C -1.14856 5.94766 1.4526
H 2.03648 3.49048 -1.31267
H 0.41075 7.39129 1.0529
H 1.75984 5.83787 -0.34714
C 1.07767 3.24207 -0.85645
C -1.25663 2.44854 0.18809
H -2.55379 4.33037 1.69147
H -1.72231 6.64439 2.06025
H -2.20792 2.06801 0.56431
N -0.53605 1.61371 -0.52086
N 0.67381 2.00393 -1.01507
C 3.30881 -1.14891 -2.24344

H 4.28333 -0.7126 -2.52339
H 2.91526 -1.66498 -3.13433
H 3.4931 -1.90572 -1.46561
C 0.8457 -0.53506 1.6407
H 0.33558 0.411 1.87374
H 1.07412 -1.03242 2.59463
P 2.36978 -0.02403 0.71564
P -0.38113 -1.50907 0.6521
C 2.83303 1.53305 1.58423
C 3.61686 2.46464 0.89221
C 2.42223 1.8312 2.888
C 3.97205 3.67284 1.48426
H 3.93641 2.24482 -0.12831
C 2.76801 3.04559 3.47515
H 1.82958 1.11718 3.45974
C 3.53908 3.96922 2.7742
H 4.57789 4.38917 0.93081
H 2.43541 3.26778 4.48802
H 3.80416 4.91958 3.23498
C 3.69619 -1.17743 1.24221
C 3.46306 -2.36726 1.93358
C 5.00804 -0.85753 0.86641
C 4.52031 -3.21815 2.25089
H 2.45301 -2.65273 2.22341
C 6.06234 -1.70205 1.19216
H 5.20903 0.05944 0.30966
C 5.8203 -2.88723 1.88519
H 4.31883 -4.14441 2.78786
H 7.07677 -1.43666 0.8984
H 6.64566 -3.55179 2.13559
C 0.40014 -3.15279 0.47171
C 0.41729 -4.08439 1.51632
C 1.07034 -3.4453 -0.71925
C 1.10405 -5.28536 1.37127
H -0.1 -3.86685 2.4517
C 1.76541 -4.64401 -0.85951
H 1.05794 -2.7205 -1.53487
C 1.78164 -5.56434 0.18493
H 1.11316 -6.00543 2.1882
H 2.29079 -4.85758 -1.78969
H 2.32101 -6.50389 0.07485
C -1.73552 -1.7905 1.85315
C -2.69658 -2.76641 1.55025
C -1.93558 -0.96842 2.96632
C -3.82123 -2.92323 2.35131
H -2.56324 -3.40982 0.67884
C -3.06714 -1.12585 3.76587
H -1.21151 -0.19845 3.22945
C -4.00958 -2.10196 3.46235
H -4.55617 -3.68824 2.10556
H -3.20531 -0.48217 4.63326
H -4.89305 -2.22298 4.08708
C -3.59898 -0.05586 -0.49693
H -3.60706 0.88015 -1.04148
H -3.14947 -0.11323 0.48594
H -3.87557 -0.96981 -1.00909
I -5.93424 0.32513 0.51241

TS-5B/7B
E(RM06) = -2515.00733673

Zero-point correction= 0.705809 (Hartree/Particle)
Thermal correction to Energy= 0.754088
Thermal correction to Enthalpy= 0.755032
Thermal correction to Gibbs Free Energy= 0.620679
Sum of electronic and zero-point Energies= -2514.301528
Sum of electronic and thermal Energies= -2514.253249
Sum of electronic and thermal Enthalpies= -2514.252305
Sum of electronic and thermal Free Energies= -2514.386658
E(RM06L) = -2803.36239438

Pt 0.93543 -0.39767 0.11348
C 1.6425 1.55875 0.23667
H 0.82704 2.24931 0.49881
H 2.42878 1.65232 1.00347
H 2.06082 1.87948 -0.72997
Pt -0.60168 -0.0926 2.94832
C -2.30019 1.06289 2.8192
H -2.20178 1.69699 1.92265
H -3.22581 0.47711 2.72219
H -2.40017 1.7267 3.68997
C 0.30389 1.68997 3.55785
H 0.25413 2.42345 2.74025
H -0.19541 2.12845 4.43473
H 1.36604 1.53055 3.80916
C 6.17995 -2.20344 4.14622
C 5.55297 -1.79451 2.99059
C 4.16799 -1.54543 3.0149
C 3.44003 -1.7212 4.21372
C 4.09817 -2.13611 5.38695
C 5.45372 -2.37184 5.34431
H 3.90061 -1.0125 0.90627
H 7.25036 -2.39885 4.14129
H 6.10653 -1.66228 2.06226
C 3.42282 -1.14692 1.87792
C 2.05229 -1.44365 4.1557
H 3.52913 -2.26 6.30752
H 5.97628 -2.69138 6.24352
H 1.43903 -1.52675 5.05474
N 1.43176 -1.06489 3.06342
N 2.12671 -0.94293 1.8969
C -0.14823 0.35924 -1.46753
H 0.52015 0.56705 -2.31947
H -0.60946 1.31518 -1.17312
H -0.94629 -0.31006 -1.81803
C -0.60959 -3.34349 1.42167
H 0.19577 -3.54297 2.14199
H -1.11873 -4.30089 1.23974
P 0.23907 -2.69302 -0.0975
P -1.7228 -2.10787 2.2384
C 1.65496 -3.87902 -0.22302
C 1.98783 -4.50468 -1.42818
C 2.48468 -4.09413 0.88533
C 3.11309 -5.31917 -1.5204
H 1.36011 -4.36644 -2.30728
C 3.60819 -4.90776 0.7944
H 2.25898 -3.62429 1.84313
C 3.92805 -5.52295 -0.41257
H 3.34838 -5.80104 -2.46815
H 4.23344 -5.06116 1.67359
H 4.8063 -6.16196 -0.48666

C -0.81463 -3.18581 -1.51191
C -1.89289 -4.06893 -1.42325
C -0.48846 -2.64211 -2.76147
C -2.63988 -4.38679 -2.55354
H -2.17946 -4.50813 -0.46956
C -1.22579 -2.97236 -3.8929
H 0.35499 -1.95534 -2.84468
C -2.30988 -3.83907 -3.78846
H -3.48816 -5.06383 -2.46254
H -0.95777 -2.5419 -4.85634
H -2.89738 -4.08766 -4.67089
C -3.11915 -1.98879 1.06198
C -4.13958 -2.9451 1.0293
C -3.11287 -0.95824 0.11784
C -5.13458 -2.87351 0.06089
H -4.15773 -3.74999 1.76534
C -4.10025 -0.89916 -0.86172
H -2.31969 -0.2095 0.14338
C -5.11212 -1.85388 -0.8884
H -5.92965 -3.61767 0.04532
H -4.07806 -0.09817 -1.59937
H -5.88941 -1.80196 -1.64934
C -2.40607 -3.05049 3.65151
C -3.49044 -2.49519 4.34585
C -1.80035 -4.20342 4.15855
C -3.9584 -3.08396 5.51282
H -3.96672 -1.58763 3.97068
C -2.26949 -4.78958 5.33302
H -0.95907 -4.66365 3.64178
C -3.34596 -4.23221 6.01128
H -4.79567 -2.6364 6.04532
H -1.78658 -5.68674 5.71689
H -3.70327 -4.68284 6.93522
C -0.93389 -0.50482 5.44709
H -0.0516 0.09754 5.61338
H -0.86876 -1.55034 5.17774
H -1.90498 -0.02407 5.46681
I -0.98211 -1.20203 7.96246

TS-7A/12A
E(RM06) = -2566.31668498
Zero-point correction= 0.743455 (Hartree/Particle)
Thermal correction to Energy= 0.796397
Thermal correction to Enthalpy= 0.797341
Thermal correction to Gibbs Free Energy= 0.649119
Sum of electronic and zero-point Energies= -2565.573230
Sum of electronic and thermal Energies= -2565.520288
Sum of electronic and thermal Enthalpies= -2565.519344
Sum of electronic and thermal Free Energies= -2565.667566
E(RM06L) = -3141.19688609

1 78 0 1.103371 -1.012555 -1.154183
2 6 0 1.472729 -0.827346 -3.195157
3 1 0 0.646392 -1.251731 -3.784033
4 1 0 1.594199 0.233141 -3.466769
5 1 0 2.390373 -1.372003 -3.464818
6 78 0 -1.805348 -0.034037 -2.086289
7 6 0 -2.927949 -1.456414 -3.056226
8 1 0 -2.211829 -2.163091 -3.505871
9 1 0 -3.598249 -1.996916 -2.376000

10 1 0 -3.525162 -1.001074 -3.856277
11 6 0 -1.524162 0.776121 -3.980283
12 1 0 -0.916717 0.062609 -4.554963
13 1 0 -2.476224 0.931500 -4.502326
14 1 0 -0.989531 1.733207 -3.907343
15 6 0 2.099256 5.751570 -0.153161
16 6 0 2.424634 4.413037 -0.128405
17 6 0 1.465485 3.474383 -0.548850
18 6 0 0.190253 3.902797 -0.976278
19 6 0 -0.121726 5.273564 -1.005104
20 6 0 0.830619 6.181396 -0.597083
21 1 0 2.678879 1.690312 -0.269802
22 1 0 2.827689 6.491827 0.171067
23 1 0 3.401824 4.068996 0.208528
24 6 0 1.703886 2.079294 -0.568022
25 6 0 -0.731491 2.886490 -1.326688
26 1 0 -1.110009 5.593602 -1.331622
27 1 0 0.603753 7.245331 -0.607655
28 1 0 -1.742467 3.148389 -1.641759
29 7 0 -0.443027 1.608142 -1.297960
30 7 0 0.806155 1.197569 -0.937544
31 6 0 1.272384 -3.029164 -1.543471
32 1 0 2.330214 -3.336218 -1.548510
33 1 0 0.858096 -3.258479 -2.537261
34 1 0 0.737088 -3.636830 -0.803932
35 6 0 -1.148854 -0.458348 1.485322
36 1 0 -1.144610 0.634713 1.363696
37 1 0 -1.543593 -0.678547 2.486939
38 15 0 0.588783 -1.050941 1.261255
39 15 0 -2.263818 -1.092592 0.158851
40 6 0 1.595437 0.162385 2.205427
41 6 0 2.925033 -0.182372 2.488615
42 6 0 1.141791 1.438651 2.548237
43 6 0 3.782121 0.736783 3.084630
44 1 0 3.300589 -1.178306 2.241258
45 6 0 2.000746 2.355050 3.151347
46 1 0 0.115439 1.748941 2.351835
47 6 0 3.323019 2.011173 3.413110
48 1 0 4.812605 0.453487 3.294256
49 1 0 1.624457 3.344662 3.410889
50 1 0 3.994535 2.730496 3.878812
51 6 0 0.751034 -2.553791 2.292157
52 6 0 0.140780 -2.651795 3.547917
53 6 0 1.578811 -3.588880 1.849490
54 6 0 0.326229 -3.786407 4.328628
55 1 0 -0.476734 -1.837024 3.927941
56 6 0 1.764723 -4.724824 2.634898
57 1 0 2.090962 -3.501834 0.891238
58 6 0 1.130860 -4.828188 3.868503
59 1 0 -0.155805 -3.856755 5.302437
60 1 0 2.409880 -5.527029 2.280428
61 1 0 1.272169 -5.717309 4.480923
62 6 0 -2.201181 -2.908906 0.360363
63 6 0 -2.493782 -3.471330 1.610375
64 6 0 -1.841685 -3.743105 -0.698396
65 6 0 -2.405197 -4.844790 1.797883
66 1 0 -2.789175 -2.831209 2.442964
67 6 0 -1.755538 -5.121419 -0.509940
68 1 0 -1.613192 -3.316258 -1.673623
69 6 0 -2.029710 -5.670707 0.738013

70 1 0 -2.624219 -5.272682 2.775050
71 1 0 -1.467719 -5.762406 -1.342010
72 1 0 -1.957971 -6.746969 0.887024
73 6 0 -3.937913 -0.671524 0.755642
74 6 0 -5.031772 -1.422829 0.307363
75 6 0 -4.160930 0.461813 1.541527
76 6 0 -6.326443 -1.042173 0.644000
77 1 0 -4.874290 -2.312179 -0.304689
78 6 0 -5.458627 0.840446 1.874678
79 1 0 -3.325689 1.068027 1.894195
80 6 0 -6.542395 0.091221 1.425894
81 1 0 -7.170478 -1.635211 0.295240
82 1 0 -5.616599 1.725863 2.489618
83 1 0 -7.557021 0.387992 1.686549
84 6 0 -3.507612 1.116771 -1.941172
85 1 0 -3.555695 1.811072 -2.786487
86 1 0 -3.417308 1.655931 -0.988524
87 1 0 -4.384520 0.460196 -1.931487
88 53 0 -2.114161 3.921844 2.176239
89 6 0 3.529609 -0.721533 -0.952318
90 1 0 3.355509 -0.432083 0.076737
91 1 0 3.548371 0.019854 -1.742273
92 1 0 3.779556 -1.750713 -1.184064
93 53 0 6.102751 -0.152082 -0.44534

TS-9A/10A
E(RM06) = -2566.31940841
Zero-point correction= 0.743218 (Hartree/Particle)
Thermal correction to Energy= 0.796101
Thermal correction to Enthalpy= 0.797045
Thermal correction to Gibbs Free Energy= 0.651874
Sum of electronic and zero-point Energies= -2565.576190
Sum of electronic and thermal Energies= -2565.523308
Sum of electronic and thermal Enthalpies= -2565.522364
Sum of electronic and thermal Free Energies= -2565.667535
E(RM06L) = -3141.19955163

1 78 0 1.468791 1.145636 -0.332936
2 6 0 2.117472 2.603960 -1.681439
3 1 0 2.782938 3.358168 -1.234699
4 1 0 2.663793 2.112946 -2.503600
5 1 0 1.258187 3.127067 -2.129545
6 78 0 -2.728605 0.439449 -1.413204
7 6 0 -3.568561 -0.987864 -2.652838
8 1 0 -2.953404 -1.080822 -3.558940
9 1 0 -3.624683 -1.964976 -2.155817
10 1 0 -4.582402 -0.685945 -2.947510
11 6 0 -3.127679 1.782000 -2.955809
12 1 0 -2.247073 1.858350 -3.607721
13 1 0 -3.987762 1.454668 -3.553660
14 1 0 -3.351396 2.767236 -2.522862
15 6 0 -4.653860 0.854613 -0.780473
16 1 0 -4.571228 1.392880 0.173065
17 1 0 -5.166989 1.477451 -1.522927
18 1 0 -5.211600 -0.077913 -0.638733
19 6 0 0.219193 6.092993 1.988486
20 6 0 -0.588465 5.089751 2.476810
21 6 0 -1.070878 4.108110 1.591254
22 6 0 -0.728316 4.159460 0.222474
23 6 0 0.085760 5.201126 -0.262986

24 6 0 0.553381 6.150619 0.618268
25 1 0 -2.212013 2.929123 3.028162
26 1 0 0.603746 6.856204 2.662164
27 1 0 -0.858218 5.041144 3.530832
28 6 0 -1.896962 3.023988 1.986477
29 6 0 -1.216258 3.106818 -0.591448
30 1 0 0.339087 5.237242 -1.321759
31 1 0 1.187848 6.958214 0.258556
32 1 0 -0.983261 3.078972 -1.655837
33 7 0 -1.968497 2.133656 -0.130034
34 7 0 -2.330762 2.091287 1.178226
35 6 0 2.297375 2.260369 1.197737
36 1 0 2.942214 1.647221 1.844428
37 1 0 1.472087 2.657085 1.813618
38 1 0 2.884899 3.107774 0.818279
39 53 0 -0.020587 -0.039916 -2.495687
40 6 0 -0.975854 -0.775885 1.703626
41 1 0 -1.236003 0.222191 2.080068
42 1 0 -1.052190 -1.483946 2.543326
43 15 0 0.801107 -0.632739 1.190206
44 15 0 -2.316282 -1.181379 0.490554
45 6 0 1.593082 -0.439924 2.839005
46 6 0 2.881011 -0.950452 3.044107
47 6 0 1.011119 0.343247 3.841135
48 6 0 3.568350 -0.685123 4.224505
49 1 0 3.357157 -1.563505 2.276626
50 6 0 1.698182 0.602678 5.024364
51 1 0 0.014469 0.766327 3.707584
52 6 0 2.978634 0.092557 5.217915
53 1 0 4.568637 -1.091160 4.367439
54 1 0 1.227645 1.207773 5.797989
55 1 0 3.515720 0.299044 6.142248
56 6 0 1.312603 -2.340248 0.746324
57 6 0 1.047571 -3.412084 1.607793
58 6 0 2.045594 -2.573424 -0.419638
59 6 0 1.502301 -4.689492 1.301871
60 1 0 0.493119 -3.249592 2.533254
61 6 0 2.507506 -3.852691 -0.723590
62 1 0 2.251656 -1.748602 -1.100150
63 6 0 2.236337 -4.911178 0.136805
64 1 0 1.286514 -5.515923 1.977877
65 1 0 3.080990 -4.016956 -1.634708
66 1 0 2.596616 -5.911805 -0.097359
67 6 0 -2.047752 -2.966045 0.137933
68 6 0 -2.317036 -3.925655 1.122851
69 6 0 -1.544276 -3.383882 -1.096649
70 6 0 -2.091400 -5.274273 0.873753
71 1 0 -2.706089 -3.619371 2.094340
72 6 0 -1.313415 -4.735720 -1.342972
73 1 0 -1.318096 -2.649378 -1.869191
74 6 0 -1.589366 -5.681804 -0.360899
75 1 0 -2.304667 -6.009686 1.648093
76 1 0 -0.916708 -5.046692 -2.308343
77 1 0 -1.411788 -6.738478 -0.555594
78 6 0 -3.782683 -1.250041 1.595628
79 6 0 -4.918807 -1.926586 1.130005
80 6 0 -3.848230 -0.593207 2.827156
81 6 0 -6.088796 -1.948842 1.880080
82 1 0 -4.888235 -2.448198 0.171653
83 6 0 -5.022925 -0.615424 3.577137

84 1 0 -2.986011 -0.056989 3.220981
85 6 0 -6.144174 -1.290303 3.106890
86 1 0 -6.960268 -2.482646 1.504186
87 1 0 -5.055067 -0.103536 4.537779
88 1 0 -7.060058 -1.306189 3.695429
89 6 0 3.885238 0.332526 -0.578143
90 1 0 3.704103 -0.242261 0.319079
91 1 0 4.298779 1.330661 -0.497633
92 1 0 3.573694 -0.037213 -1.547350
93 53 0 6.220570 -0.815244 -0.817028

TS-9B/10B
E(RM06) = -2566.30176782
Zero-point correction= 0.744602 (Hartree/Particle)
Thermal correction to Energy= 0.797457
Thermal correction to Enthalpy= 0.798401
Thermal correction to Gibbs Free Energy= 0.653102
Sum of electronic and zero-point Energies= -2565.557165
Sum of electronic and thermal Energies= -2565.504311
Sum of electronic and thermal Enthalpies= -2565.503367
Sum of electronic and thermal Free Energies= -2565.648666
E(RM06L) = -3141.16950337

Pt 1.43251 1.22304 -0.27093
C 1.97985 2.82299 -1.49401
H 1.90602 3.7837 -0.96408
H 3.02367 2.71042 -1.8253
H 1.35233 2.86239 -2.39693
Pt -2.70156 0.36148 -1.39102
C -3.49179 -1.07203 -2.65352
H -2.90009 -1.08954 -3.57891
H -3.46534 -2.06895 -2.19502
H -4.53189 -0.82799 -2.90602
C -3.15714 1.69929 -2.92264
H -2.29326 1.79372 -3.59381
H -4.0206 1.35276 -3.50406
H -3.40008 2.67896 -2.48713
C -4.63186 0.71858 -0.72857
H -4.55699 1.15303 0.27729
H -5.1358 1.41856 -1.40583
H -5.20017 -0.21731 -0.6862
C -0.13067 6.27544 1.88267
C -0.83008 5.2133 2.40977
C -1.22731 4.16446 1.55995
C -0.90844 4.20983 0.18573
C -0.20714 5.31236 -0.33983
C 0.17726 6.32727 0.50672
H -2.22318 2.91284 3.04335
H 0.18825 7.08967 2.53032
H -1.07626 5.17042 3.46992
C -1.93867 3.01585 1.99319
C -1.30875 3.09631 -0.59306
H 0.02947 5.3414 -1.40253
H 0.727 7.18063 0.11521
H -1.0808 3.05598 -1.65844
N -1.97795 2.07772 -0.10132
N -2.30526 2.03122 1.21435
C 2.24344 2.32944 1.27708
H 2.82542 1.70418 1.96888
H 1.41191 2.78934 1.83838

H 2.88952 3.1339 0.89965
I 0.00512 0.01348 -2.46572
C -0.92722 -0.85242 1.69839
H -1.21651 0.13689 2.07737
H -0.98544 -1.56883 2.53262
P 0.84672 -0.65736 1.1792
P -2.25448 -1.27662 0.47679
C 1.63947 -0.49106 2.83028
C 2.93883 -0.97729 3.01853
C 1.04682 0.25784 3.85173
C 3.62536 -0.72075 4.20068
H 3.42554 -1.56505 2.23832
C 1.7315 0.50532 5.03753
H 0.0421 0.66515 3.72738
C 3.02338 0.01992 5.21344
H 4.63644 -1.10395 4.32675
H 1.25269 1.08344 5.82665
H 3.5611 0.21925 6.13881
C 1.38882 -2.34099 0.68903
C 1.14735 -3.43856 1.52439
C 2.1263 -2.52998 -0.48139
C 1.62344 -4.69798 1.18514
H 0.59367 -3.30908 2.45548
C 2.61791 -3.78996 -0.81371
H 2.31809 -1.68845 -1.14463
C 2.3632 -4.87432 0.01658
H 1.42363 -5.54537 1.83956
H 3.20837 -3.91303 -1.71988
H 2.7475 -5.86031 -0.24009
C -1.94399 -3.04862 0.10164
C -2.24113 -4.03544 1.05065
C -1.37138 -3.4273 -1.11536
C -1.97751 -5.37286 0.78285
H -2.68867 -3.75886 2.00566
C -1.09834 -4.76746 -1.3768
H -1.12086 -2.67115 -1.8594
C -1.40561 -5.74076 -0.43266
H -2.2173 -6.13045 1.52748
H -0.64206 -5.04637 -2.32512
H -1.19661 -6.78885 -0.64197
C -3.72419 -1.3852 1.57392
C -4.84223 -2.08627 1.1022
C -3.8182 -0.71932 2.79794
C -6.01939 -2.12438 1.83877
H -4.78985 -2.61442 0.14854
C -4.99948 -0.75737 3.53514
H -2.97156 -0.15881 3.19146
C -6.10163 -1.45698 3.05838
H -6.87649 -2.67685 1.45727
H -5.0534 -0.23714 4.4903
H -7.02411 -1.48441 3.63587
C 3.75741 0.46869 -0.53777
H 3.61571 -0.25355 0.25266
H 4.23304 1.41315 -0.30507
H 3.54605 0.21879 -1.5708
I 6.16518 -0.71183 -0.83997

TS-15B/12B
E(RM06) = -2566.29122924
Zero-point correction= 0.746137 (Hartree/Particle)

Thermal correction to Energy= 0.798355
Thermal correction to Enthalpy= 0.799300
Thermal correction to Gibbs Free Energy= 0.654623
Sum of electronic and zero-point Energies= -2565.545092
Sum of electronic and thermal Energies= -2565.492874
Sum of electronic and thermal Enthalpies= -2565.491930
Sum of electronic and thermal Free Energies= -2565.636606
E(RM06L) = -3141.17586694

Pt -0.87813 -1.3898 -1.6695
C -0.83242 -1.12177 -3.73596
H -1.28269 -0.16037 -4.0243
H 0.20705 -1.15022 -4.09663
H -1.40139 -1.92039 -4.23334
Pt -0.17178 1.6871 -1.67707
C -1.71555 2.86036 -2.36501
H -2.30204 2.23788 -3.05973
H -2.36375 3.22362 -1.55779
H -1.33057 3.728 -2.91517
C 0.75334 1.98826 -3.51511
H 0.69607 1.0399 -4.06697
H 0.26465 2.77972 -4.0965
H 1.8107 2.25045 -3.37258
C 6.00836 -2.0225 -1.27053
C 4.70738 -2.45838 -1.38871
C 3.66999 -1.50939 -1.35865
C 3.96157 -0.13861 -1.1978
C 5.29527 0.28841 -1.07896
C 6.3011 -0.65102 -1.1199
H 2.01624 -2.9043 -1.58436
H 6.82405 -2.74232 -1.28872
H 4.46645 -3.51535 -1.4994
C 2.302 -1.85742 -1.4688
C 2.85116 0.7425 -1.15251
H 5.51134 1.34476 -0.93058
H 7.33753 -0.33575 -1.02072
H 3.00365 1.81452 -1.02847
N 1.60842 0.34331 -1.28139
N 1.32804 -0.981 -1.44463
C -2.89477 -1.6369 -2.00053
H -3.0978 -2.65529 -2.36658
H -3.2393 -0.93818 -2.77732
H -3.48385 -1.46413 -1.09302
C -0.45415 0.04909 1.53329
H 0.62516 0.24467 1.43593
H -0.69243 0.10337 2.60448
P -0.80184 -1.61769 0.80687
P -1.28217 1.38637 0.56814
C 0.60183 -2.66095 1.35869
C 0.472 -4.04825 1.19929
C 1.8186 -2.13913 1.80385
C 1.54739 -4.89094 1.45662
H -0.47599 -4.48121 0.87068
C 2.89125 -2.98772 2.06782
H 1.96921 -1.06934 1.95507
C 2.76246 -4.3604 1.88534
H 1.43328 -5.96404 1.3134
H 3.83039 -2.55476 2.41166
H 3.60495 -5.021 2.08335
C -2.19799 -2.30748 1.76605

C -2.28151 -2.142 3.15298
C -3.1466 -3.0972 1.11264
C -3.32141 -2.72465 3.86561
H -1.52184 -1.57048 3.68789
C -4.18632 -3.68414 1.82974
H -3.06806 -3.26223 0.03829
C -4.27981 -3.48939 3.20262
H -3.37894 -2.59077 4.94456
H -4.92052 -4.29808 1.31113
H -5.09328 -3.94661 3.76348
C -3.06944 1.025 0.71493
C -3.61981 0.79754 1.98321
C -3.90057 0.9918 -0.4044
C -4.97188 0.51431 2.12057
H -2.98726 0.84532 2.87057
C -5.25953 0.71868 -0.2652
H -3.48318 1.16292 -1.39507
C -5.79271 0.47173 0.99435
H -5.3862 0.32311 3.10903
H -5.89651 0.68961 -1.14782
H -6.85304 0.24982 1.10303
C -1.10061 2.87855 1.604
C -2.06119 3.89507 1.52538
C 0.05301 3.08038 2.36439
C -1.86188 5.09519 2.1987
H -2.97408 3.74616 0.94702
C 0.24804 4.28361 3.03499
H 0.82842 2.31527 2.42977
C -0.7058 5.2925 2.95132
H -2.61555 5.87876 2.13774
H 1.15742 4.42209 3.6182
H -0.55171 6.23487 3.47445
C 0.70075 3.46172 -1.07547
H 1.19188 3.94108 -1.92854
H 1.42274 3.18708 -0.29425
H -0.0758 4.11445 -0.66283
I 3.59289 1.45441 2.25323
C -0.35759 -3.60502 -2.20184
H 0.07223 -3.77582 -1.22067
H 0.28228 -3.38802 -3.05005
H -1.35226 -3.99066 -2.40475
I 0.62038 -6.18809 -2.51661