

Electronic Supporting Information

DFT characterisation of a Pd^{II}→I^{III} adduct, and a Pd^{II} complex formed after oxidative alkenylation of Pd^{II} by [Ph(alkenyl)I^{III}]⁺, in Pd-mediated synthesis of benzofurans involving Pd^{IV}, annulation and chain-walking

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Table ESI-1. Second-generation energy decomposition analysis (EDA) based on absolutely localised orbitals (ALMO-EDA2) for interaction between the iodonium and palladium fragments in adducts **5** and **4**. The energies are given in kcal mol⁻¹.

adduct	5	4
ΔE_{int}	-17.2	-13.1
$\Delta E(\text{PAULI})$	29.3	22.5
$\Delta E(\text{ELEC})$	-24.0	-21.9
$\Delta E(\text{SOL})$	8.1	8.6
$\Delta E(\text{DISP})$	-17.2	-11.3
$\Delta E(\text{POL})$	-3.4	-2.3
$\Delta E(\text{CT})$	-10.0	-8.7

The following formula expresses the interaction energy (ΔE_{int}) between the iodonium and palladium fragments. Here, $\Delta E(\text{PAULI})$ is the Pauli repulsion, $\Delta E(\text{ELEC})$ is the electrostatic interactions, $\Delta E(\text{SOL})$ is the solvation energy, ΔE_{disp} is the dispersion interaction, $\Delta E(\text{POL})$ is polarization energy and $\Delta E(\text{CT})$ is charge transfer energy.

$$\Delta E_{\text{int}} = \Delta E(\text{PAULI}) + \Delta E(\text{ELEC}) + \Delta E(\text{SOL}) + \Delta E(\text{DISP}) + \Delta E(\text{POL}) + \Delta E(\text{CT})$$

The EDA calculations indicate that orbital, dispersive, and electrostatic interactions all contribute to the stability of these adducts (Table ESI-1). The calculations indicate that the primary contribution of orbital interactions to the stability of these adducts comes from charge transfer from the Pd d_{z^2} orbital to the LUMO of the iodonium reagent. This claim is supported by the contour plots of natural orbitals for chemical bonds (NOCV) for this specific interaction in structures **5** and **4** (Figure ESI-1).

Figure ESI-1 Contour plots of NOCV for charge transfer from the Pd d_{z^2} orbital to the LUMO of the iodonium reagent in adducts **5** (left) and **4** (right).

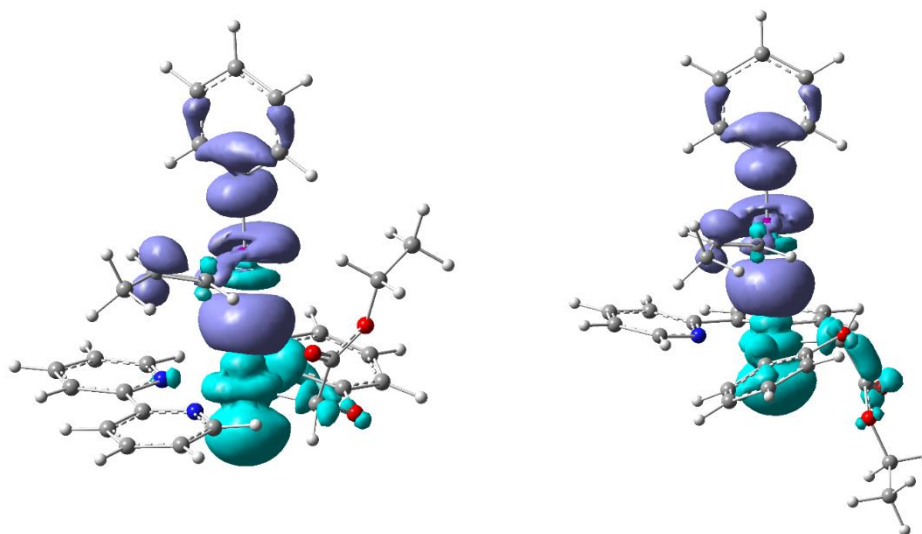


Figure ESI-2. Potential energy scans for those steps in the sequence **18** → **22** for which transition states could not be identified, illustrating inflection points (**18** → **19**, **20** → **21**) and a “barrierless” process for **19** → **20**.

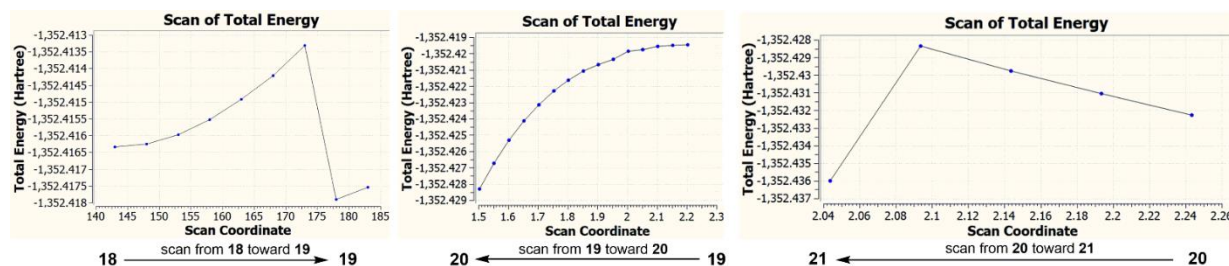
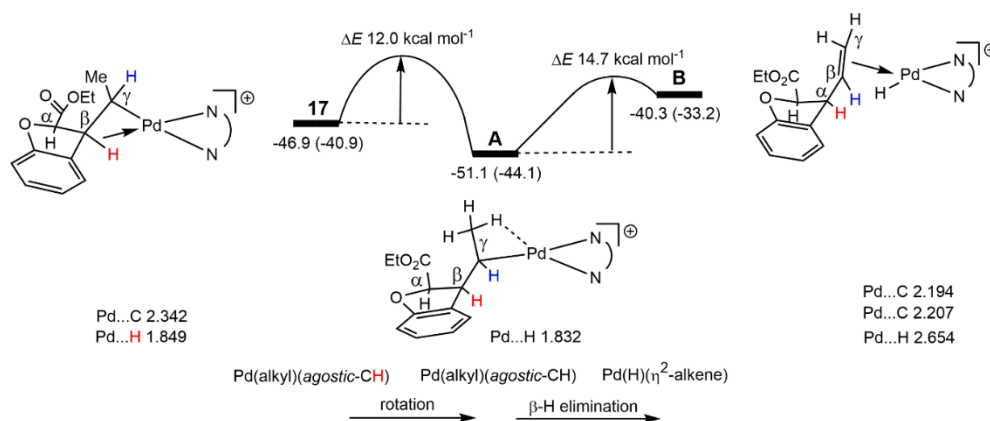


Figure ESI-3. Chain-walking from **17** (Fig. 3a) to **B** containing the benzofuran skeleton in the isomeric form corresponding to the high energy isomer **26** (Scheme 2). Selected interatomic distances (Å) are shown; energies ΔG (ΔH) are in kcal mol⁻¹.



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 M06-D3, and are followed by Cartesian coordinates.

1

E(RM06) = -1235.34617903
Zero-point correction= 0.342643 (Hartree/Particle)
Thermal correction to Energy= 0.365411
Thermal correction to Enthalpy= 0.366355
Thermal correction to Gibbs Free Energy= 0.289432
Sum of electronic and zero-point Energies= -1235.003536
Sum of electronic and thermal Energies= -1234.980768
Sum of electronic and thermal Enthalpies= -1234.979824
Sum of electronic and thermal Free Energies= -1235.056747
E(RM06L) = -1236.48566061

C -3.42168 -3.14911 0.04711
C -2.09052 -1.35771 0.6627
C -3.2198 -0.59223 0.94864
C -4.48202 -1.13881 0.76295
C -4.58904 -2.44676 0.31198
H -3.45775 -4.18144 -0.29327
H -3.12123 0.41874 1.33334
H -5.36976 -0.55071 0.98534
H -5.55378 -2.92636 0.16994
C -0.72049 -0.86111 0.90801
C -0.45814 0.46122 1.2616
C 1.52718 -1.39195 1.08891
C 0.84514 0.84732 1.5428
H -1.26096 1.1911 1.31318
C 1.8584 -0.09807 1.46823
H 2.29345 -2.15573 0.9858
H 1.06147 1.87708 1.81889
H 2.89336 0.15304 1.68648
Pd -0.3087 -3.69268 -0.07519
N 0.27578 -1.76887 0.80541
N -2.20307 -2.62167 0.19684
C -0.82972 -5.43368 -0.94701
C -1.95421 -5.74224 -1.71307
C 0.13298 -6.44997 -0.79059
C -2.16353 -7.03071 -2.21947
H -2.69431 -4.97075 -1.93416
C -0.05378 -7.73877 -1.27984
C -1.2209 -8.0273 -1.9857
H -3.06232 -7.24895 -2.79573
H 0.7199 -8.49099 -1.12934
H -1.37843 -9.0329 -2.3747
C 1.47489 -4.72723 -0.10859
H 2.02471 -4.48515 0.81068
O 1.27478 -6.13587 -0.13516
C 2.2275 -4.29329 -1.31957
O 2.30244 -4.89428 -2.37128

O 2.82388 -3.10084 -1.11232
C 3.49464 -2.51601 -2.23595
H 4.34474 -3.15323 -2.51579
H 2.8058 -2.48779 -3.09062
C 3.93608 -1.13703 -1.82521
H 4.48457 -0.65666 -2.64446
H 3.07143 -0.50781 -1.57616
H 4.59677 -1.1802 -0.94911

2

E(RM06) = -784.313728431
Zero-point correction= 0.175520 (Hartree/Particle)
Thermal correction to Energy= 0.192448
Thermal correction to Enthalpy= 0.193392
Thermal correction to Gibbs Free Energy= 0.127382
Sum of electronic and zero-point Energies= -784.138208
Sum of electronic and thermal Energies= -784.121281
Sum of electronic and thermal Enthalpies= -784.120337
Sum of electronic and thermal Free Energies= -784.186346
E(RM06L) = -1071.44761232

C 0.33179 -3.9629 3.17576
C 1.64403 -4.03349 2.96775
H -0.19494 -3.20023 3.747
H 2.05916 -4.84487 2.36606
C 2.59862 -3.0382 3.52436
H 3.35123 -3.53999 4.14734
H 3.14267 -2.54138 2.70947
H 2.09195 -2.27492 4.12559
C -1.38369 -6.4498 4.11499
C -0.33737 -6.68095 4.99199
C -0.6246 -7.37417 6.16624
C -1.92004 -7.81589 6.42098
C -2.94157 -7.56824 5.50864
C -2.68564 -6.87175 4.32828
H 0.6722 -6.33219 4.78196
H 0.17515 -7.57057 6.87792
H -2.13478 -8.359 7.33941
H -3.95381 -7.91396 5.70991
H -3.47324 -6.67301 3.6039
I -0.96851 -5.37383 2.28869
F -3.50142 -5.6695 -0.06321
F -4.68451 -7.62007 0.09434
F -4.64025 -6.16095 1.85387
F -2.76538 -7.34082 1.30258

3

E(RM06) = -1235.34609123
Zero-point correction= 0.342072 (Hartree/Particle)
Thermal correction to Energy= 0.365107
Thermal correction to Enthalpy= 0.366051
Thermal correction to Gibbs Free Energy= 0.287458
Sum of electronic and zero-point Energies= -1235.004019
Sum of electronic and thermal Energies= -1234.980984
Sum of electronic and thermal Enthalpies= -1234.980040
Sum of electronic and thermal Free Energies= -1235.058634

E(RM06L) = -1236.48567819

C -3.39445 -3.34621 -0.19973
C -2.61627 -1.283 0.50853
C -3.91979 -0.79108 0.56421
C -4.97946 -1.61734 0.21731
C -4.71636 -2.92597 -0.16193
H -3.14319 -4.36716 -0.4776
H -4.11643 0.22604 0.89073
H -5.99984 -1.24271 0.25931
H -5.51276 -3.61792 -0.42217
C -1.4492 -0.48004 0.93064
C -1.55319 0.86448 1.28188
C 0.82273 -0.4612 1.39812
C -0.42399 1.54758 1.71224
H -2.50489 1.38371 1.21926
C 0.78711 0.87406 1.77737
H 1.75636 -1.01981 1.38587
H -0.49488 2.59702 1.99009
H 1.69774 1.36716 2.10712
Pd -0.26476 -3.16883 0.2053
N -0.26285 -1.12557 0.98599
N -2.36591 -2.54874 0.10386
C -0.24293 -5.01455 -0.59906
C -1.12012 -5.58772 -1.52053
C 0.87113 -5.78623 -0.21619
C -0.95333 -6.90283 -1.97099
H -1.95549 -5.00607 -1.91522
C 1.05693 -7.0965 -0.64585
C 0.12439 -7.65717 -1.51778
H -1.66587 -7.33063 -2.67581
H 1.93465 -7.65292 -0.31839
H 0.25927 -8.68237 -1.86151
C 1.66492 -3.78763 0.59347
H 1.92036 -3.43107 1.60009
O 1.78933 -5.2074 0.59126
C 2.55601 -3.1256 -0.39686
O 2.94485 -1.97267 -0.29096
O 2.87239 -3.90648 -1.43703
C 3.6721 -3.30244 -2.46381
H 3.13031 -2.43982 -2.87502
H 4.60358 -2.92807 -2.01879
C 3.92985 -4.35418 -3.50819
H 4.53489 -3.93547 -4.32154
H 4.47159 -5.2069 -3.0802
H 2.98801 -4.72301 -3.93347

4

E(RM06) = -1595.19530082

Zero-point correction= 0.503373 (Hartree/Particle)

Thermal correction to Energy= 0.539016

Thermal correction to Enthalpy= 0.539960

Thermal correction to Gibbs Free Energy= 0.429621

Sum of electronic and zero-point Energies= -1594.691928

Sum of electronic and thermal Energies= -1594.656285

Sum of electronic and thermal Enthalpies= -1594.655341

Sum of electronic and thermal Free Energies= -1594.765680
E(RM06L) = -1883.20521223

C -3.49146 -2.81 0.34918
C -2.26792 -0.84559 0.4712
C -3.39826 -0.14712 0.89332
C -4.60524 -0.81792 1.03484
C -4.65522 -2.17887 0.7661
H -3.48239 -3.87811 0.13921
H -3.33984 0.91169 1.12823
H -5.49228 -0.28131 1.36424
H -5.57293 -2.75041 0.87602
C -0.93905 -0.20558 0.36549
C -0.75815 1.17159 0.47946
C 1.3463 -0.51992 0.10435
C 0.52515 1.6983 0.41462
H -1.60811 1.83629 0.60604
C 1.59966 0.83971 0.22913
H 2.14849 -1.22847 -0.09519
H 0.67851 2.77165 0.5026
H 2.6203 1.20783 0.16822
Pd -0.39646 -3.13133 -0.20739
N 0.11266 -1.03296 0.17236
N -2.33094 -2.16645 0.18694
C -0.86296 -5.03659 -0.66414
C -2.04489 -5.54694 -1.19872
C 0.19026 -5.94429 -0.45223
C -2.20787 -6.91987 -1.42363
H -2.86361 -4.87408 -1.46055
C 0.05034 -7.31263 -0.65594
C -1.16795 -7.79764 -1.13302
H -3.14733 -7.29657 -1.82685
H 0.89388 -7.9774 -0.47251
H -1.29046 -8.86685 -1.3023
C 1.45745 -4.03906 -0.27342
H 2.07698 -3.59732 0.51868
O 1.37464 -5.43968 -0.02613
C 2.05894 -3.70212 -1.59466
O 2.59478 -2.63055 -1.82903
O 1.92761 -4.66987 -2.50515
C 2.41418 -4.37577 -3.82511
H 1.89012 -3.48852 -4.20481
C -0.75984 -5.35326 2.72659
C -2.00564 -5.75461 2.94764
H 0.07624 -5.93097 2.33681
H -2.75524 -5.05484 3.3249
C -2.43416 -7.15575 2.68195
H -2.73708 -7.64839 3.61602
H -3.30977 -7.16002 2.01915
H -1.63428 -7.74235 2.21441
H 3.48309 -4.13234 -3.7644
C -0.05052 -3.51757 5.222
C -1.20288 -3.35813 5.98139
C -1.09906 -3.50187 7.36308
C 0.1309 -3.79253 7.94745
C 1.26968 -3.94283 7.16102

C 1.18963 -3.8057 5.77675
H -2.15931 -3.12552 5.5167
H -1.9868 -3.38291 7.98146
H 0.20284 -3.9019 9.02782
H 2.22945 -4.1698 7.6214
H 2.07322 -3.92319 5.15235
I -0.19592 -3.31974 3.07829
C 2.15782 -5.5895 -4.67556
H 2.50815 -5.41068 -5.69926
H 2.68662 -6.46519 -4.27908
H 1.08594 -5.82138 -4.71342

5

E(RM06) = -1595.19986166
Zero-point correction= 0.503588 (Hartree/Particle)
Thermal correction to Energy= 0.538784
Thermal correction to Enthalpy= 0.539728
Thermal correction to Gibbs Free Energy= 0.433208
Sum of electronic and zero-point Energies= -1594.696274
Sum of electronic and thermal Energies= -1594.661078
Sum of electronic and thermal Enthalpies= -1594.660134
Sum of electronic and thermal Free Energies= -1594.766654
E(RM06L) = -1883.21063062

C -2.53598 2.31692 -2.10345
C -1.07223 3.10321 -0.49191
C -0.85589 4.26481 -1.23246
C -1.51016 4.43924 -2.44397
C -2.38035 3.45289 -2.88566
H -3.21941 1.52809 -2.40648
H -0.18445 5.03826 -0.87092
H -1.34672 5.34282 -3.02705
H -2.93334 3.55048 -3.81597
C -0.43236 2.8786 0.8217
C 0.36162 3.84404 1.43961
C -0.07676 1.41415 2.58283
C 0.94769 3.56569 2.66688
H 0.52377 4.81258 0.9757
C 0.73321 2.32444 3.24863
H -0.25161 0.41995 2.98741
H 1.56688 4.31348 3.15746
H 1.17692 2.05598 4.20364
Pd -2.01891 0.33693 0.34285
N -0.65288 1.68075 1.40523
N -1.88863 2.12616 -0.94994
C -3.35762 -0.91765 -0.52409
C -3.80905 -0.98977 -1.84355
C -3.86877 -1.88092 0.36822
C -4.78057 -1.91463 -2.24194
H -3.3998 -0.32259 -2.60413
C -4.83486 -2.81151 -0.00237
C -5.30024 -2.81358 -1.31518
H -5.1272 -1.92703 -3.27472
H -5.19634 -3.53207 0.73032
H -6.05797 -3.53585 -1.6164
C -2.17937 -1.16287 1.74842

H -2.18004 -0.6644 2.72663
O -3.38974 -1.8928 1.63368
C -0.96322 -2.01291 1.62477
O 0.13753 -1.68373 2.04364
O -1.18054 -3.16054 0.97434
C -0.0357 -3.99572 0.74852
H 0.75412 -3.39517 0.27204
C 1.24967 -0.05392 -0.72256
C 1.83046 1.02813 -1.2281
H 1.34919 -0.48474 0.27503
H 1.60649 1.34485 -2.25065
C 2.79181 1.85603 -0.44908
H 3.777 1.85586 -0.93491
H 2.44966 2.90054 -0.42104
H 2.90628 1.49192 0.57897
H 0.35115 -4.34033 1.71671
C 1.38978 -2.04399 -3.18906
C 1.66529 -1.43028 -4.40415
C 2.64829 -1.99572 -5.2139
C 3.32368 -3.14078 -4.80056
C 3.02592 -3.73442 -3.57679
C 2.04486 -3.18802 -2.75271
H 1.13099 -0.53592 -4.71946
H 2.88289 -1.53475 -6.17157
H 4.08927 -3.57629 -5.43973
H 3.55591 -4.62964 -3.25707
H 1.80397 -3.64692 -1.79447
I -0.1219 -1.18014 -1.91875
C -0.4791 -5.13695 -0.12521
H 0.36499 -5.80834 -0.3253
H -1.27216 -5.71834 0.36073
H -0.8648 -4.7695 -1.08619

6

E(RM06) = -1595.19735445
Zero-point correction= 0.503553 (Hartree/Particle)
Thermal correction to Energy= 0.538669
Thermal correction to Enthalpy= 0.539613
Thermal correction to Gibbs Free Energy= 0.433679
Sum of electronic and zero-point Energies= -1594.693801
Sum of electronic and thermal Energies= -1594.658685
Sum of electronic and thermal Enthalpies= -1594.657741
Sum of electronic and thermal Free Energies= -1594.763675
E(RM06L) = -1883.20626186

C 3.21833 1.88618 -1.49332
C 3.6788 -0.35259 -1.12132
C 4.65175 -0.33761 -2.11999
C 4.89697 0.83614 -2.81921
C 4.17575 1.97619 -2.49416
H 2.64213 2.75922 -1.19502
H 5.23399 -1.22745 -2.34177
H 5.65692 0.85915 -3.59728
H 4.34784 2.92475 -2.99572
C 3.4137 -1.54936 -0.29607
C 3.97389 -2.79261 -0.58488

C 2.36708 -2.41838 1.5797
C 3.7111 -3.87088 0.24864
H 4.60373 -2.92866 -1.45938
C 2.90072 -3.68114 1.35951
H 1.71099 -2.23026 2.42547
H 4.1398 -4.8466 0.0305
H 2.67395 -4.49164 2.0475
Pd 1.55172 0.55193 0.8405
N 2.60172 -1.37825 0.77148
N 2.95403 0.75244 -0.83601
C 0.52673 2.27802 0.80993
C 0.25238 3.11505 -0.27407
C -0.06821 2.60576 2.0439
C -0.52234 4.27346 -0.1252
H 0.63984 2.86983 -1.26657
C -0.84325 3.74785 2.2144
C -1.05687 4.58831 1.12065
H -0.70055 4.92439 -0.98071
H -1.2869 3.96016 3.1864
H -1.65831 5.48791 1.24614
C 0.45951 0.45381 2.59987
H 1.10907 -0.02721 3.34391
O 0.13215 1.75597 3.07754
C -0.79593 -0.32654 2.40993
O -1.92339 0.12575 2.38706
O -0.53606 -1.63973 2.23618
C -1.66358 -2.49668 2.00018
H -2.32736 -2.46468 2.87476
C -0.71011 -0.67591 -1.17978
C -0.18833 -0.99658 -2.35908
H -0.50204 -1.1397 -0.21433
H -0.46605 -0.44184 -3.25778
C 0.78787 -2.11063 -2.51078
H 0.40458 -2.85606 -3.22081
H 1.73396 -1.73293 -2.92515
H 0.99465 -2.60954 -1.55469
H -2.23074 -2.11495 1.1378
C -3.82361 -0.41559 -1.08504
C -4.25253 -0.89426 -2.31556
C -5.33904 -1.76536 -2.32809
C -5.96162 -2.12752 -1.13567
C -5.50496 -1.63031 0.08166
C -4.41749 -0.75908 0.12185
H -3.7576 -0.60178 -3.2401
H -5.69916 -2.15751 -3.27724
H -6.81195 -2.80649 -1.1564
H -5.99185 -1.91949 1.0111
H -4.03197 -0.3779 1.06718
I -2.13626 0.90842 -1.01801
C -1.12774 -3.87794 1.74074
H -1.9559 -4.57699 1.57378
H -0.48756 -3.88848 0.8476
H -0.53955 -4.24055 2.59371

7

E(RM06) = -1595.16273430

Zero-point correction= 0.501387 (Hartree/Particle)
Thermal correction to Energy= 0.536715
Thermal correction to Enthalpy= 0.537659
Thermal correction to Gibbs Free Energy= 0.428754
Sum of electronic and zero-point Energies= -1594.661347
Sum of electronic and thermal Energies= -1594.626019
Sum of electronic and thermal Enthalpies= -1594.625075
Sum of electronic and thermal Free Energies= -1594.733981
E(RM06L) = -1883.21888192

C -1.81729 2.59515 2.46728
C -0.40971 3.32338 0.77754
C -0.1088 4.47432 1.50301
C -0.69755 4.67744 2.74342
C -1.57412 3.72252 3.23811
H -2.46801 1.80755 2.83553
H 0.59091 5.20701 1.11281
H -0.46455 5.57137 3.31742
H -2.05669 3.83263 4.20528
C 0.19106 3.05011 -0.54485
C 0.99228 3.97837 -1.20673
C 0.39525 1.56477 -2.31481
C 1.5043 3.66851 -2.4601
H 1.20685 4.94577 -0.76233
C 1.19609 2.44255 -3.03267
H 0.12098 0.59884 -2.73086
H 2.1283 4.38774 -2.98587
H 1.56188 2.16039 -4.01639
Pd -1.32007 0.46803 0.1147
N -0.08845 1.85351 -1.10303
N -1.25998 2.39474 1.26994
C -2.474 -0.86092 1.11593
C -3.39805 -0.60341 2.12333
C -2.35044 -2.17596 0.64121
C -4.14021 -1.65025 2.67295
H -3.57023 0.40688 2.48871
C -3.07741 -3.22882 1.17925
C -3.9664 -2.95472 2.2134
H -4.85488 -1.44122 3.46699
H -2.95914 -4.23157 0.77289
H -4.54569 -3.76598 2.65055
C -1.30923 -1.20387 -1.10968
H -0.34137 -1.23757 -1.62466
O -1.48503 -2.38038 -0.39025
C -2.42002 -0.86931 -2.07418
O -2.35435 0.09604 -2.81266
O -3.43992 -1.70832 -2.00936
C -4.57754 -1.41699 -2.8536
H -4.91938 -0.39815 -2.63208
C 0.17079 -0.42538 1.16804
C 0.83428 0.20274 2.12745
H 0.35413 -1.44809 0.83011
H 0.57003 1.21056 2.45015
C 2.00689 -0.42905 2.81461
H 2.91268 0.17367 2.65688
H 1.83226 -0.47514 3.89839

H 2.19873 -1.44529 2.44789
H -4.24865 -1.44653 -3.89978
C 3.82167 -1.72439 0.0666
C 4.90494 -1.67656 0.9371
C 5.16507 -2.78113 1.74589
C 4.35209 -3.90956 1.68077
C 3.27497 -3.94055 0.79922
C 3.00131 -2.84477 -0.01784
H 5.53459 -0.79039 0.99348
H 6.0102 -2.75302 2.43184
H 4.56039 -4.76846 2.31611
H 2.63946 -4.8227 0.73943
H 2.16111 -2.87227 -0.71019
I 3.37638 -0.01728 -1.14454
C -5.62549 -2.45059 -2.5514
H -6.51456 -2.26734 -3.16617
H -5.25739 -3.45999 -2.77181
H -5.92205 -2.41075 -1.4957

8

E(RM06) = -1352.35472709
Zero-point correction= 0.413005 (Hartree/Particle)
Thermal correction to Energy= 0.440657
Thermal correction to Enthalpy= 0.441601
Thermal correction to Gibbs Free Energy= 0.353815
Sum of electronic and zero-point Energies= -1351.941722
Sum of electronic and thermal Energies= -1351.914070
Sum of electronic and thermal Enthalpies= -1351.913126
Sum of electronic and thermal Free Energies= -1352.000912
E(RM06L) = -1353.63364523

C -1.7697 -2.37673 -1.24067
C -2.80953 -0.30787 -1.07967
C -3.89798 -0.77765 -1.81178
C -3.89775 -2.08873 -2.26955
C -2.82481 -2.91445 -1.96377
H -0.91566 -2.98957 -0.95845
H -4.753 -0.1381 -2.0118
H -4.74249 -2.46491 -2.84217
H -2.79707 -3.95556 -2.27295
C -2.78862 1.03393 -0.45693
C -3.79679 1.97333 -0.65705
C -1.72925 2.44274 1.05596
C -3.75468 3.17526 0.03764
H -4.6121 1.77548 -1.34635
C -2.7135 3.41196 0.92431
H -0.8867 2.59214 1.72773
H -4.5369 3.91635 -0.11031
H -2.65142 4.33073 1.50073
Pd -0.06223 -0.11204 0.23598
N -1.75923 1.29204 0.37889
N -1.74555 -1.10461 -0.83531
C 1.55763 -1.28174 -0.02947
C 1.71365 -2.31159 -0.95177
C 2.66029 -0.90014 0.7493
C 2.93622 -2.97922 -1.0454

H 0.8992 -2.60127 -1.61351
C 3.88105 -1.55598 0.66996
C 4.00418 -2.6114 -0.22825
H 3.05017 -3.79161 -1.76099
H 4.71585 -1.22263 1.28365
H 4.95326 -3.13861 -0.30643
C 1.45752 0.97609 1.13021
H 1.03666 1.53018 1.97695
O 2.48598 0.15769 1.58807
C 1.83612 1.91497 0.01075
O 1.04861 2.72465 -0.44145
O 3.07838 1.74723 -0.41368
C 3.5011 2.57552 -1.52089
H 2.80802 2.41588 -2.35657
C -0.2633 -1.01999 2.03125
C -1.45031 -1.46934 2.41065
H 0.6593 -1.0557 2.61327
H -2.32131 -1.3982 1.75604
C -1.6669 -2.09403 3.75536
H -2.42914 -1.53849 4.31815
H -2.0334 -3.12359 3.6442
H -0.74467 -2.11639 4.34785
H 3.42809 3.62638 -1.21421
C 4.90847 2.17336 -1.86048
H 5.27098 2.77171 -2.70463
H 5.58062 2.33692 -1.00936
H 4.95554 1.11414 -2.14292

9

E(RM06) = -1352.35090350
Zero-point correction= 0.413400 (Hartree/Particle)
Thermal correction to Energy= 0.440854
Thermal correction to Enthalpy= 0.441799
Thermal correction to Gibbs Free Energy= 0.354723
Sum of electronic and zero-point Energies= -1351.937504
Sum of electronic and thermal Energies= -1351.910049
Sum of electronic and thermal Enthalpies= -1351.909105
Sum of electronic and thermal Free Energies= -1351.996180
E(RM06L) = -1353.63155759

C -3.10814 3.01659 -1.38495
C -1.52233 3.69449 0.17008
C -1.61502 5.00851 -0.28354
C -2.48073 5.31305 -1.3255
C -3.2496 4.30256 -1.88543
H -3.69935 2.19375 -1.78168
H -1.03092 5.79879 0.17927
H -2.55947 6.33634 -1.68542
H -3.95239 4.49681 -2.69081
C -0.65338 3.30621 1.30054
C 0.24319 4.19011 1.89484
C -0.01166 1.61951 2.76684
C 1.01793 3.76018 2.96429
H 0.35002 5.20523 1.52481
C 0.89099 2.45299 3.41232
H -0.11468 0.57388 3.05388

H 1.7208 4.44369 3.43513
H 1.48278 2.0719 4.23993
Pd -2.06692 0.71941 0.53939
N -0.77023 2.03654 1.74701
N -2.25931 2.71429 -0.39827
C -3.24369 -0.50997 -0.55228
C -3.61471 -0.41305 -1.88686
C -3.74576 -1.56894 0.21395
C -4.54977 -1.30519 -2.41871
H -3.19152 0.3548 -2.5348
C -4.67187 -2.46713 -0.29985
C -5.07837 -2.31849 -1.62315
H -4.85814 -1.20556 -3.45792
H -5.04241 -3.27662 0.32667
H -5.80088 -3.01724 -2.04136
C -2.11096 -0.99973 1.71858
H -2.13147 -0.56216 2.72639
O -3.31212 -1.68466 1.49563
C -0.88894 -1.84578 1.5533
O 0.16511 -1.5759 2.10053
O -1.06777 -2.85762 0.71795
C 0.10108 -3.64304 0.39693
H 0.86185 -2.96977 -0.02188
C -0.4367 0.15242 -0.50961
C -0.28412 0.37258 -1.80322
H 0.30683 -0.24491 0.18716
H -1.09221 0.78173 -2.41233
C 1.00756 0.07187 -2.50157
H 0.84326 -0.65921 -3.30467
H 1.41543 0.97951 -2.96618
H 1.75762 -0.33369 -1.81175
H 0.50006 -4.07213 1.32442
C -0.32709 -4.69671 -0.58482
H 0.53418 -5.31561 -0.86276
H -1.09413 -5.34979 -0.15109
H -0.73293 -4.24069 -1.49651

10

E(RM06) = -1595.20928587
Zero-point correction= 0.504440 (Hartree/Particle)
Thermal correction to Energy= 0.539533
Thermal correction to Enthalpy= 0.540477
Thermal correction to Gibbs Free Energy= 0.434402
Sum of electronic and zero-point Energies= -1594.704846
Sum of electronic and thermal Energies= -1594.669753
Sum of electronic and thermal Enthalpies= -1594.668809
Sum of electronic and thermal Free Energies= -1594.774884
E(RM06L) = -1883.21819556

C -2.97151 2.94471 -1.34256
C -1.34999 3.50395 0.2226
C -1.40262 4.83771 -0.17508
C -2.26758 5.21495 -1.19363
C -3.07654 4.25538 -1.78528
H -3.59466 2.16063 -1.76672
H -0.78777 5.58708 0.3141

H -2.31568 6.25462 -1.50907
H -3.78191 4.50662 -2.57235
C -0.49779 3.04524 1.33994
C 0.42393 3.87801 1.97087
C 0.04689 1.30332 2.77681
C 1.16431 3.391 3.04
H 0.57631 4.89865 1.63222
C 0.97112 2.08206 3.4585
H -0.11398 0.26345 3.05333
H 1.88753 4.03333 3.53728
H 1.52684 1.65801 4.2906
Pd -1.95349 0.52172 0.43057
N -0.66874 1.76836 1.74702
N -2.12301 2.5732 -0.37959
C -3.13609 -0.61636 -0.7484
C -3.52315 -0.40314 -2.06393
C -3.64797 -1.72471 -0.0613
C -4.48071 -1.23346 -2.65374
H -3.09179 0.40489 -2.65553
C -4.59388 -2.5645 -0.63478
C -5.01389 -2.30235 -1.93655
H -4.8017 -1.04266 -3.67648
H -4.97221 -3.41516 -0.07083
H -5.75531 -2.95165 -2.39923
C -2.00538 -1.28832 1.47124
H -2.00755 -0.94572 2.51533
O -3.2184 -1.93472 1.20964
C -0.83741 -2.17918 1.17196
O -0.8586 -3.12386 0.41757
O 0.24396 -1.75826 1.8393
C 1.49598 -2.40863 1.53252
H 1.43738 -3.45373 1.86159
C -0.29585 0.05374 -0.62076
C -0.13778 0.26644 -1.91474
H 0.468 -0.26134 0.09415
H -0.96395 0.59637 -2.5469
C 1.19146 0.07488 -2.58057
H 1.10986 -0.66758 -3.38781
H 1.53105 1.01632 -3.03346
H 1.95736 -0.26802 -1.87296
H 1.63144 -2.3988 0.44171
C 0.72991 -3.38138 -3.40023
C 1.48423 -3.24337 -4.56112
C 2.87378 -3.30501 -4.47129
C 3.49158 -3.5061 -3.23998
C 2.71851 -3.65198 -2.09113
C 1.32743 -3.58759 -2.161
H 1.00018 -3.08145 -5.5227
H 3.4727 -3.19478 -5.3741
H 4.57732 -3.55312 -3.17687
H 3.19761 -3.81708 -1.12613
H 0.71979 -3.68629 -1.26062
I -1.39749 -3.19655 -3.50051
C 2.57938 -1.63996 2.23604
H 3.54962 -2.11898 2.05849
H 2.63551 -0.60851 1.86204
H 2.40466 -1.61072 3.31912

11

E(RM06) = -1352.35047437
Zero-point correction= 0.413136 (Hartree/Particle)
Thermal correction to Energy= 0.440609
Thermal correction to Enthalpy= 0.441554
Thermal correction to Gibbs Free Energy= 0.354336
Sum of electronic and zero-point Energies= -1351.937338
Sum of electronic and thermal Energies= -1351.909865
Sum of electronic and thermal Enthalpies= -1351.908921
Sum of electronic and thermal Free Energies= -1351.996139
E(RM06L) = -1353.63083995

C -2.96186 2.94827 -1.35873
C -1.38075 3.53344 0.23864
C -1.47153 4.8717 -0.13682
C -2.33474 5.23747 -1.16116
C -3.10064 4.26178 -1.78335
H -3.55005 2.14999 -1.80678
H -0.88811 5.63251 0.37318
H -2.41341 6.28045 -1.45931
H -3.79942 4.50331 -2.57931
C -0.5143 3.07885 1.34668
C 0.40784 3.91654 1.97006
C 0.08704 1.3247 2.74621
C 1.17911 3.42513 3.01513
H 0.53829 4.94315 1.64059
C 1.01765 2.10616 3.41588
H -0.05351 0.27809 3.00952
H 1.90401 4.07083 3.50555
H 1.60162 1.67746 4.22592
Pd -1.95102 0.54382 0.44022
N -0.66121 1.79581 1.74262
N -2.11857 2.58947 -0.38633
C -3.11243 -0.61413 -0.74346
C -3.44833 -0.44435 -2.07938
C -3.65566 -1.69555 -0.03872
C -4.39105 -1.28833 -2.67313
H -2.99876 0.34851 -2.67736
C -4.58953 -2.54585 -0.61482
C -4.96062 -2.32514 -1.93874
H -4.67439 -1.13126 -3.71235
H -4.99343 -3.37504 -0.03674
H -5.68895 -2.98573 -2.40593
C -2.02803 -1.25555 1.50055
H -2.01049 -0.90727 2.54228
O -3.2617 -1.86618 1.25117
C -0.89129 -2.18429 1.19491
O -0.94731 -3.12883 0.44363
O 0.20849 -1.79697 1.85324
C 1.43319 -2.50003 1.549
H 1.36975 -3.50669 1.98076
C -0.29404 0.06077 -0.59829
C -0.10404 0.33225 -1.87695
H 0.44311 -0.33028 0.10617
H -0.89889 0.74364 -2.50139

C 1.22053 0.08773 -2.53451
H 1.10642 -0.6179 -3.36827
H 1.62329 1.02141 -2.94942
H 1.95303 -0.32553 -1.82955
H 1.51513 -2.60351 0.45843
C 2.56054 -1.69327 2.13056
H 3.51543 -2.19891 1.94478
H 2.60731 -0.69561 1.67237
H 2.44199 -1.57271 3.21503

12

E(RM06) = -1352.41508230
Zero-point correction= 0.414762 (Hartree/Particle)
Thermal correction to Energy= 0.442218
Thermal correction to Enthalpy= 0.443162
Thermal correction to Gibbs Free Energy= 0.355181
Sum of electronic and zero-point Energies= -1352.000320
Sum of electronic and thermal Energies= -1351.972865
Sum of electronic and thermal Enthalpies= -1351.971921
Sum of electronic and thermal Free Energies= -1352.059901
E(RM06L) = -1353.68016492

C 2.05339 1.27378 -2.0439
C 2.88732 -0.42682 -0.70778
C 4.15483 -0.26975 -1.26248
C 4.35876 0.70176 -2.23337
C 3.29092 1.49138 -2.63386
H 1.18434 1.86234 -2.33
H 4.98113 -0.90339 -0.95377
H 5.34447 0.83191 -2.67435
H 3.40105 2.26032 -3.39347
C 2.58789 -1.44429 0.31581
C 3.57284 -2.24038 0.89221
C 0.94898 -2.51822 1.57568
C 3.22071 -3.19958 1.83175
H 4.61544 -2.10926 0.61887
C 1.88517 -3.34982 2.17288
H -0.11054 -2.61812 1.80084
H 3.98671 -3.82232 2.28778
H 1.55779 -4.09362 2.89377
Pd -0.03078 -0.12407 -0.08966
N 1.2883 -1.58535 0.67649
N 1.85194 0.346 -1.10605
C -1.08829 2.55221 0.53779
C -0.60842 3.49985 -0.36809
C -1.70728 1.39091 -0.01777
C -0.72063 3.31976 -1.74748
H -0.1712 4.42283 0.00904
C -1.77864 1.18899 -1.41283
C -1.2807 2.16441 -2.27869
H -0.36054 4.10186 -2.41396
H -2.33952 0.33143 -1.78143
H -1.36613 2.02959 -3.35478
C -1.70107 -0.58874 0.98614
H -1.3918 -0.7097 2.03381
O -2.47521 0.57446 0.81063

C -2.32059 -1.83476 0.4473
O -2.04532 -2.94025 0.87754
O -3.16631 -1.61538 -0.55681
C -3.76951 -2.78439 -1.15018
H -2.9706 -3.43646 -1.52628
C -1.03581 2.70549 1.98848
C -0.32358 3.62815 2.65259
H -1.62822 1.98963 2.56225
H 0.2939 4.34116 2.09961
C -0.30597 3.75718 4.13257
H 0.71558 3.65575 4.52679
H -0.65604 4.75243 4.44352
H -0.94077 3.0028 4.61385
H -4.31112 -3.33133 -0.36825
C -4.68006 -2.30844 -2.24707
H -5.16628 -3.16734 -2.72449
H -5.46113 -1.64818 -1.85074
H -4.11945 -1.76233 -3.01656

13

E(RM06) = -1352.41770387
Zero-point correction= 0.416081 (Hartree/Particle)
Thermal correction to Energy= 0.443002
Thermal correction to Enthalpy= 0.443947
Thermal correction to Gibbs Free Energy= 0.357404
Sum of electronic and zero-point Energies= -1352.001623
Sum of electronic and thermal Energies= -1351.974702
Sum of electronic and thermal Enthalpies= -1351.973757
Sum of electronic and thermal Free Energies= -1352.060299
E(RM06L) = -1353.68446123

C -1.56148 2.63326 1.10946
C -2.88896 0.77584 0.74865
C -3.80791 1.21861 1.69781
C -3.58098 2.41749 2.35844
C -2.43767 3.14336 2.05657
H -0.65478 3.17867 0.86118
H -4.68521 0.62318 1.93589
H -4.28754 2.77361 3.10461
H -2.2135 4.08738 2.54555
C -3.07859 -0.48383 0.01067
C -4.32813 -1.08858 -0.09686
C -2.12867 -2.14799 -1.29366
C -4.46332 -2.26283 -0.82337
H -5.19772 -0.62912 0.36422
C -3.34204 -2.80422 -1.43366
H -1.23851 -2.5553 -1.76003
H -5.43574 -2.74044 -0.91731
H -3.39223 -3.71751 -2.01982
Pd -0.25933 0.26358 -0.65412
N -1.9876 -1.019 -0.58757
N -1.7713 1.48018 0.46375
C 2.76594 1.01308 -0.84255
C 3.57508 1.97927 -0.24193
C 3.15827 -0.32399 -0.77259
C 4.75359 1.60563 0.39812

H 3.29512 3.03014 -0.31154
C 4.33572 -0.71146 -0.15385
C 5.13682 0.26607 0.43111
H 5.38512 2.36504 0.85514
H 4.59937 -1.76694 -0.11722
H 6.06405 -0.02343 0.92252
C 1.0113 -1.36614 -1.02321
H 0.5372 -1.91581 -1.84189
O 2.35795 -1.25111 -1.38581
C 0.85366 -2.10897 0.28956
O 0.1 -3.04503 0.45353
O 1.65289 -1.6161 1.23374
C 1.60977 -2.26462 2.52222
H 0.60094 -2.14008 2.93699
C 1.54704 1.31012 -1.60524
C 0.65024 2.29471 -1.27432
H 1.49052 0.87892 -2.61039
H 0.82199 2.82376 -0.33289
C -0.31663 2.89265 -2.23928
H -1.28189 3.12908 -1.77616
H 0.09854 3.8399 -2.617
H -0.48611 2.23233 -3.09901
H 1.78639 -3.33804 2.38007
C 2.66268 -1.62213 3.38126
H 2.63359 -2.05451 4.38853
H 3.66483 -1.78688 2.9668
H 2.49593 -0.54074 3.466

14

E(RM06) = -1352.39962092
Zero-point correction= 0.416259 (Hartree/Particle)
Thermal correction to Energy= 0.442734
Thermal correction to Enthalpy= 0.443678
Thermal correction to Gibbs Free Energy= 0.359382
Sum of electronic and zero-point Energies= -1351.983361
Sum of electronic and thermal Energies= -1351.956887
Sum of electronic and thermal Enthalpies= -1351.955943
Sum of electronic and thermal Free Energies= -1352.040239
E(RM06L) = -1353.66530784

C -3.91586 -3.53764 0.0203
C -2.91205 -1.45482 0.16765
C -4.14467 -0.84882 0.39554
C -5.29135 -1.6309 0.42907
C -5.17684 -3.00153 0.24218
H -3.78503 -4.60742 -0.13221
H -4.2042 0.22191 0.57192
H -6.26056 -1.17248 0.61223
H -6.04354 -3.65638 0.27052
C -1.65255 -0.69154 0.15469
C -1.60519 0.67571 -0.10601
C 0.65808 -0.77609 0.34995
C -0.37578 1.32012 -0.12836
H -2.51806 1.22688 -0.31723
C 0.77914 0.58273 0.09854
H 1.54019 -1.39103 0.52264

H -0.32207 2.38651 -0.33545
H 1.76329 1.04257 0.07909
Pd -0.75048 -3.57576 0.3257
N -0.52631 -1.39954 0.39002
N -2.80795 -2.78848 -0.03095
C -0.92439 -5.4042 -0.55909
C -1.8084 -5.3213 -1.64464
C -0.16754 -6.57732 -0.43498
C -1.99773 -6.37865 -2.53138
H -2.36104 -4.40115 -1.82557
C -0.37195 -7.64855 -1.31042
C -1.28947 -7.56118 -2.34427
H -2.69777 -6.26873 -3.35781
H 0.23817 -8.53913 -1.16502
H -1.42948 -8.40513 -3.0174
C 1.44605 -5.69439 1.06679
H 2.1122 -6.12185 1.83246
O 0.81792 -6.80778 0.48352
C 2.33546 -4.9131 0.10565
O 2.98723 -3.95248 0.4595
O 2.29944 -5.39754 -1.12207
C 2.97625 -4.63764 -2.14641
H 2.6385 -3.59442 -2.07732
C 0.42179 -4.84597 1.76058
C 0.58341 -3.54388 2.17965
H -0.3473 -5.44786 2.25411
H 1.49239 -3.01593 1.88867
C -0.24162 -2.94977 3.26994
H 0.32023 -3.03749 4.21341
H -0.4351 -1.88237 3.11367
H -1.19575 -3.47677 3.39624
H 4.0548 -4.66261 -1.94664
C 2.61268 -5.26802 -3.46114
H 3.07804 -4.71336 -4.2843
H 2.95666 -6.3084 -3.50777
H 1.52408 -5.2565 -3.60536

15

E(RM06) = -1352.44549284
Zero-point correction= 0.418261 (Hartree/Particle)
Thermal correction to Energy= 0.444251
Thermal correction to Enthalpy= 0.445195
Thermal correction to Gibbs Free Energy= 0.360267
Sum of electronic and zero-point Energies= -1352.027231
Sum of electronic and thermal Energies= -1352.001242
Sum of electronic and thermal Enthalpies= -1352.000297
Sum of electronic and thermal Free Energies= -1352.085226
E(RM06L) = -1353.70639833

C 2.76313 -1.77073 -1.3361
C 3.31098 0.0645 -0.01616
C 4.64278 -0.33965 0.00998
C 5.03121 -1.49076 -0.66048
C 4.07552 -2.21778 -1.35458
H 1.99053 -2.31746 -1.87123
H 5.38167 0.2473 0.54777

H 6.07127 -1.80768 -0.64413
H 4.32823 -3.11946 -1.90526
C 2.85399 1.30485 0.64553
C 3.69647 2.13294 1.3839
C 1.05648 2.72497 1.02923
C 3.1786 3.28927 1.95406
H 4.74575 1.8877 1.52021
C 1.83633 3.59786 1.77602
H -0.00267 2.91168 0.85443
H 3.82552 3.94441 2.53341
H 1.39631 4.49472 2.20351
Pd 0.43387 0.09613 -0.60725
N 1.55268 1.61435 0.4832
N 2.37847 -0.6687 -0.68093
C -1.6605 -2.13094 0.60514
C -0.68323 -2.80155 1.32322
C -2.79748 -1.66585 1.25472
C -0.87289 -2.99585 2.69523
H 0.21554 -3.17258 0.82859
C -3.01689 -1.84823 2.60857
C -2.02652 -2.52791 3.32285
H -0.11516 -3.51766 3.27683
H -3.91882 -1.47421 3.08839
H -2.16057 -2.68775 4.39151
C -2.94787 -0.7804 -0.81799
H -3.6548 -0.89368 -1.64752
O -3.66531 -1.02482 0.40796
C -2.54799 0.68425 -0.73643
O -1.40879 1.12142 -0.56341
O -3.58543 1.47026 -0.8129
C -3.37711 2.90133 -0.64428
H -2.93848 3.05996 0.34842
C -1.79501 -1.79753 -0.85887
C -0.51239 -1.42617 -1.58166
H -2.20048 -2.68597 -1.38157
H 0.15626 -2.29413 -1.48388
C -0.69872 -1.07296 -3.04112
H 0.26782 -0.91953 -3.54048
H -1.22412 -1.88189 -3.57817
H -1.28971 -0.15598 -3.18374
H -2.6563 3.22968 -1.40241
C -4.71726 3.56036 -0.79386
H -4.60541 4.64365 -0.66941
H -5.14115 3.37065 -1.78702
H -5.42111 3.19762 -0.03554

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E(RM06) = -1352.41675525
Zero-point correction= 0.416449 (Hartree/Particle)
Thermal correction to Energy= 0.442268
Thermal correction to Enthalpy= 0.443212
Thermal correction to Gibbs Free Energy= 0.358057
Sum of electronic and zero-point Energies= -1352.000306
Sum of electronic and thermal Energies= -1351.974488
Sum of electronic and thermal Enthalpies= -1351.973544
Sum of electronic and thermal Free Energies= -1352.058698

E(RM06L) = -1353.69361317

C -2.43298 -1.7291 1.4088
C -3.25236 -1.18645 -0.69435
C -3.98498 -0.13185 -0.15337
C -3.91986 0.12192 1.20927
C -3.12787 -0.69019 2.00913
H -1.80987 -2.39322 2.00546
H -4.62135 0.47774 -0.78845
H -4.49074 0.94138 1.63986
H -3.04853 -0.53536 3.08162
C -3.28865 -1.51241 -2.13457
C -3.79574 -0.62712 -3.08348
C -2.80098 -3.06183 -3.77995
C -3.80115 -0.99631 -4.42233
H -4.16678 0.3509 -2.7903
C -3.29812 -2.23852 -4.78189
H -2.39261 -4.04423 -4.01295
H -4.19043 -0.3134 -5.17424
H -3.28048 -2.57016 -5.81652
Pd -1.62701 -3.70764 -0.83513
N -2.79293 -2.71589 -2.49139
N -2.48468 -1.97294 0.09415
C -0.68374 -5.75805 -1.09931
C -2.00667 -6.13164 -1.39483
C 0.26585 -5.65284 -2.14105
C -2.34633 -6.3777 -2.73178
H -2.72206 -6.31022 -0.59255
C -0.06564 -5.87517 -3.46352
C -1.38813 -6.2501 -3.73454
H -3.35838 -6.68772 -2.98237
H 0.68689 -5.82506 -4.2469
H -1.66697 -6.4668 -4.76491
C 1.49334 -5.842 -0.29444
H 1.65951 -6.93345 -0.27713
O 1.516 -5.43368 -1.67432
C 2.65606 -5.22808 0.44529
O 3.54851 -4.58887 -0.05408
O 2.56963 -5.56069 1.73327
C 3.63015 -5.07566 2.58564
H 4.57947 -5.49788 2.23257
C 0.06205 -5.59692 0.22313
C -0.34856 -4.20449 0.68159
H -0.203 -6.36601 0.95693
H -0.96426 -4.24631 1.59016
C 0.67834 -3.10155 0.70745
H 0.21662 -2.12305 0.88936
H 1.4052 -3.25488 1.52296
H 1.24211 -3.03038 -0.23303
H 3.68714 -3.98396 2.48004
C 3.3041 -5.49606 3.99094
H 4.08812 -5.14679 4.67305
H 2.34878 -5.0669 4.3181
H 3.24111 -6.58814 4.07119

E(RM06) = -1352.42714149
Zero-point correction= 0.416862 (Hartree/Particle)
Thermal correction to Energy= 0.442891
Thermal correction to Enthalpy= 0.443836
Thermal correction to Gibbs Free Energy= 0.359754
Sum of electronic and zero-point Energies= -1352.010280
Sum of electronic and thermal Energies= -1351.984250
Sum of electronic and thermal Enthalpies= -1351.983306
Sum of electronic and thermal Free Energies= -1352.067388
E(RM06L) = -1353.69151890

C -0.45793 -0.80362 0.64428
C -2.74151 -1.25097 0.51981
C -3.02404 -0.0692 1.19926
C -1.98315 0.75711 1.60186
C -0.67502 0.38619 1.32337
H 0.54951 -1.13846 0.4061
H -4.04996 0.20503 1.42649
H -2.19744 1.68076 2.13468
H 0.17049 0.99852 1.62437
C -3.79256 -2.19592 0.08311
C -5.15304 -1.92218 0.19831
C -4.24995 -4.27838 -0.83853
C -6.07408 -2.87401 -0.22148
H -5.50141 -0.97521 0.60066
C -5.62056 -4.07718 -0.74502
H -3.8398 -5.20015 -1.24752
H -7.13956 -2.67126 -0.13909
H -6.30816 -4.84795 -1.0821
Pd -1.20109 -3.45357 -0.70536
N -3.3615 -3.36471 -0.43869
N -1.46023 -1.59768 0.24995
C 0.96515 -5.52872 -2.73178
C 0.71064 -5.24611 -4.06381
C 1.9442 -6.45636 -2.38382
C 1.46234 -5.90596 -5.03871
H -0.06341 -4.532 -4.34485
C 2.70977 -7.11278 -3.33199
C 2.45212 -6.81737 -4.67162
H 1.27307 -5.7074 -6.09171
H 3.46902 -7.83312 -3.03587
H 3.0303 -7.32117 -5.44442
C 0.88932 -6.07381 -0.45478
H 0.10898 -6.84967 -0.40059
O 2.05867 -6.63688 -1.0352
C 1.17801 -5.56405 0.93586
O 2.2705 -5.35618 1.40155
O 0.01776 -5.31788 1.54693
C 0.086 -4.58795 2.79099
H 0.60584 -5.20772 3.53193
C 0.43313 -4.96228 -1.43907
C 0.78842 -3.55196 -1.09811
H -0.73927 -5.05568 -1.5058
H 1.35979 -3.42624 -0.16901
C 1.20069 -2.59706 -2.17658
H 1.25036 -1.57261 -1.7852

H 2.20421 -2.85078 -2.55661
H 0.51358 -2.60292 -3.03237
H 0.6853 -3.68155 2.6231
C -1.32464 -4.26588 3.19571
H -1.32269 -3.69628 4.1326
H -1.81984 -3.66035 2.42307
H -1.91057 -5.18036 3.35009

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E(RM06) = -1352.41633686
Zero-point correction= 0.414569 (Hartree/Particle)
Thermal correction to Energy= 0.441279
Thermal correction to Enthalpy= 0.442224
Thermal correction to Gibbs Free Energy= 0.356069
Sum of electronic and zero-point Energies= -1352.001768
Sum of electronic and thermal Energies= -1351.975057
Sum of electronic and thermal Enthalpies= -1351.974113
Sum of electronic and thermal Free Energies= -1352.060268
E(RM06L) = -1353.68300287

C -1.57939 -1.7369 1.41067
C -3.42575 -1.6116 0.01187
C -4.15433 -0.95635 1.00222
C -3.5564 -0.68806 2.2266
C -2.23955 -1.07235 2.43507
H -0.54595 -2.0539 1.54025
H -5.18165 -0.65003 0.82908
H -4.11709 -0.17614 3.00526
H -1.72508 -0.87065 3.37062
C -3.97629 -1.88031 -1.3333
C -5.25648 -1.48972 -1.71504
C -3.59117 -2.76399 -3.45868
C -5.7003 -1.75159 -3.00427
H -5.91122 -0.97875 -1.01577
C -4.8545 -2.39646 -3.89525
H -2.89227 -3.27381 -4.11507
H -6.70043 -1.4492 -3.30607
H -5.15748 -2.618 -4.91467
Pd -1.31964 -3.14028 -1.45833
N -3.16256 -2.51496 -2.21219
N -2.15297 -2.01211 0.23575
C 1.27374 -5.10647 -2.33552
C 2.04202 -4.44832 -3.29407
C 1.30515 -6.50095 -2.26795
C 2.8231 -5.20536 -4.1619
H 2.01802 -3.36403 -3.38383
C 2.0832 -7.27308 -3.11543
C 2.84536 -6.59977 -4.06637
H 3.4204 -4.70654 -4.92223
H 2.08607 -8.35748 -3.03321
H 3.46469 -7.1745 -4.75281
C -0.24164 -5.95191 -0.72939
H -1.27391 -6.0305 -1.09754
O 0.51441 -7.01893 -1.29196
C -0.22563 -6.04986 0.78284
O 0.6984 -6.46603 1.43568

O -1.35731 -5.54428 1.27171
C -1.44141 -5.41546 2.70844
H -1.22899 -6.3924 3.15905
C 0.42746 -4.65571 -1.22035
C 0.56547 -3.51873 -0.4333
H -0.95527 -3.82733 -2.80288
H 0.22042 -3.61453 0.6009
C 1.53073 -2.40288 -0.69371
H 1.29959 -1.54192 -0.05469
H 2.55738 -2.72701 -0.46019
H 1.51657 -2.05753 -1.73276
H -0.6596 -4.71529 3.03559
C -2.82444 -4.92601 3.03442
H -2.92546 -4.79441 4.11819
H -3.02896 -3.96072 2.55089
H -3.58215 -5.64689 2.7039

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E(RM06) = -1352.41841203
Zero-point correction= 0.413684 (Hartree/Particle)
Thermal correction to Energy= 0.440637
Thermal correction to Enthalpy= 0.441581
Thermal correction to Gibbs Free Energy= 0.351052
Sum of electronic and zero-point Energies= -1352.004728
Sum of electronic and thermal Energies= -1351.977775
Sum of electronic and thermal Enthalpies= -1351.976831
Sum of electronic and thermal Free Energies= -1352.067360
E(RM06L) = -1353.68446413

C -2.30298 -1.43595 1.2487
C -3.66007 -1.02326 -0.58487
C -4.36497 -0.05832 0.13018
C -4.01056 0.21332 1.44481
C -2.96239 -0.48974 2.02042
H -1.47525 -2.00504 1.66594
H -5.18911 0.48053 -0.32763
H -4.55405 0.96633 2.01089
H -2.65251 -0.31649 3.04724
C -3.99446 -1.37664 -1.9792
C -5.00208 -0.73759 -2.69603
C -3.53396 -2.74834 -3.80828
C -5.27171 -1.12759 -4.00059
H -5.57812 0.06386 -2.24319
C -4.52753 -2.15158 -4.56877
H -2.92283 -3.55143 -4.2088
H -6.05852 -0.63206 -4.56449
H -4.703 -2.49057 -5.58587
Pd -1.73839 -3.17211 -1.3792
N -3.27252 -2.37325 -2.54682
N -2.63129 -1.69674 -0.01966
C 0.94471 -5.09189 -1.89597
C 2.03179 -4.43309 -2.46958
C 0.59648 -6.36958 -2.34794
C 2.73838 -5.07218 -3.484
H 2.33274 -3.44283 -2.13695
C 1.28167 -7.01937 -3.35951

C 2.3625 -6.34482 -3.92331
H 3.59503 -4.57726 -3.9366
H 0.98465 -8.01276 -3.68728
H 2.92968 -6.82585 -4.71832
C -0.73421 -6.06469 -0.57641
H -1.81296 -5.96507 -0.42215
O -0.49569 -6.87761 -1.71561
C -0.09956 -6.72946 0.64637
O 0.77123 -7.56145 0.59902
O -0.63646 -6.22828 1.75471
C -0.0858 -6.70673 3.00438
H -0.26135 -7.7881 3.06332
C -0.02235 -4.74202 -0.85068
C -0.09077 -3.64269 -0.00793
H -1.35205 -4.15701 -2.52067
H -0.64185 -3.79929 0.92477
C 0.90159 -2.51721 -0.02938
H 0.56243 -1.68494 0.59848
H 1.87522 -2.85193 0.36158
H 1.06422 -2.1233 -1.04021
H 0.99826 -6.53856 2.99099
C -0.76814 -5.95461 4.11149
H -0.38033 -6.2907 5.08026
H -0.58473 -4.87592 4.02552
H -1.85112 -6.12817 4.09708

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E(RM06) = -1352.41947510
Zero-point correction= 0.414699 (Hartree/Particle)
Thermal correction to Energy= 0.441449
Thermal correction to Enthalpy= 0.442394
Thermal correction to Gibbs Free Energy= 0.355162
Sum of electronic and zero-point Energies= -1352.004776
Sum of electronic and thermal Energies= -1351.978026
Sum of electronic and thermal Enthalpies= -1351.977082
Sum of electronic and thermal Free Energies= -1352.064313
E(RM06L) = -1353.68548899

C -1.41894 -3.8461 -4.67057
C -3.48089 -2.80473 -4.56683
C -3.62007 -2.8998 -5.94941
C -2.61272 -3.49138 -6.70066
C -1.484 -3.96802 -6.05223
H -0.55094 -4.20515 -4.12555
H -4.50833 -2.52252 -6.44722
H -2.71512 -3.57377 -7.78034
H -0.66313 -4.43361 -6.5914
C -4.50835 -2.17266 -3.7155
C -5.64434 -1.55861 -4.23782
C -5.19481 -1.64761 -1.55192
C -6.57122 -0.98343 -3.38025
H -5.80989 -1.52243 -5.31024
C -6.34648 -1.02904 -2.0115
H -4.97324 -1.70429 -0.49036
H -7.45971 -0.50255 -3.78282
H -7.04396 -0.59345 -1.30156

Pd -2.52357 -3.12018 -1.70257
N -4.2965 -2.20452 -2.37961
N -2.38585 -3.29025 -3.93789
C 0.04093 -5.05664 -1.96734
C 1.19461 -4.58917 -2.60196
C -0.44233 -6.33543 -2.2749
C 1.80512 -5.39645 -3.55802
H 1.61416 -3.61473 -2.36284
C 0.13496 -7.14145 -3.24071
C 1.26909 -6.64637 -3.88227
H 2.70753 -5.05033 -4.05728
H -0.27148 -8.12508 -3.46391
H 1.75782 -7.2583 -4.63842
C -1.63144 -5.74033 -0.47521
H -2.69025 -5.54543 -0.27603
O -1.52731 -6.68325 -1.53567
C -0.97208 -6.31855 0.77505
O -0.165 -7.21408 0.7734
O -1.39763 -5.6547 1.84555
C -0.79311 -6.02008 3.10856
H -1.01915 -7.07565 3.30367
C -0.84986 -4.51118 -0.94431
C -0.79947 -3.30598 -0.25814
H -2.96139 -2.88404 -0.23716
H -1.23623 -3.29082 0.74086
C 0.15873 -2.19645 -0.55856
H -0.20626 -1.25319 -0.13672
H 1.13689 -2.40747 -0.0977
H 0.31442 -2.04875 -1.63407
H 0.29516 -5.91786 3.01274
C -1.36327 -5.10915 4.15837
H -0.93086 -5.35526 5.1353
H -1.13221 -4.05956 3.93667
H -2.4523 -5.22041 4.22771

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E(RM06) = -1352.43945318
Zero-point correction= 0.416439 (Hartree/Particle)
Thermal correction to Energy= 0.443052
Thermal correction to Enthalpy= 0.443996
Thermal correction to Gibbs Free Energy= 0.356563
Sum of electronic and zero-point Energies= -1352.023014
Sum of electronic and thermal Energies= -1351.996401
Sum of electronic and thermal Enthalpies= -1351.995457
Sum of electronic and thermal Free Energies= -1352.082890
E(RM06L) = -1353.70377393

C -2.12334 -4.77419 -4.58159
C -3.85104 -3.22507 -4.46952
C -4.27848 -3.58675 -5.74441
C -3.59965 -4.57796 -6.44085
C -2.49673 -5.18153 -5.85445
H -1.25364 -5.20843 -4.08927
H -5.13142 -3.09486 -6.2029
H -3.92851 -4.86615 -7.43676
H -1.92668 -5.95376 -6.36353

C -4.50386 -2.15545 -3.68431
C -5.65104 -1.49087 -4.11227
C -4.43492 -0.86815 -1.75317
C -6.18872 -0.48488 -3.31966
H -6.13244 -1.75127 -5.05054
C -5.57168 -0.16058 -2.11874
H -3.91356 -0.6577 -0.82063
H -7.08504 0.04011 -3.64237
H -5.95827 0.62144 -1.47095
Pd -2.2745 -3.14999 -1.93089
N -3.9169 -1.83801 -2.51218
N -2.78413 -3.83467 -3.90102
C 0.2833 -4.66408 -2.05033
C 1.24197 -3.89538 -2.71794
C 0.16469 -6.02451 -2.36915
C 2.06666 -4.51107 -3.65389
H 1.34502 -2.83116 -2.51765
C 0.97739 -6.65686 -3.2958
C 1.93709 -5.87488 -3.93473
H 2.82325 -3.92448 -4.17095
H 0.85845 -7.71667 -3.50943
H 2.59606 -6.33683 -4.66771
C -1.34956 -5.73323 -0.73922
H -2.44617 -5.77614 -0.72805
O -0.86037 -6.63615 -1.72286
C -0.79933 -6.16991 0.61544
O 0.28941 -6.66611 0.77157
O -1.66265 -5.87678 1.58425
C -1.2122 -6.13258 2.93627
H -1.01254 -7.20687 3.03276
C -0.7971 -4.34754 -1.11614
C -0.83097 -3.25807 -0.10366
H -1.77128 -2.56506 -0.28254
H -1.13036 -3.64554 0.87949
C 0.35658 -2.31831 -0.00135
H 0.21215 -1.61856 0.82957
H 1.27597 -2.88817 0.1856
H 0.49298 -1.7269 -0.9133
H -0.2669 -5.59646 3.0905
C -2.29497 -5.66453 3.86626
H -1.99344 -5.84545 4.90465
H -2.48042 -4.58968 3.74611
H -3.23243 -6.2035 3.68263

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E(RM06) = -1352.44095238
Zero-point correction= 0.417007 (Hartree/Particle)
Thermal correction to Energy= 0.443411
Thermal correction to Enthalpy= 0.444355
Thermal correction to Gibbs Free Energy= 0.359048
Sum of electronic and zero-point Energies= -1352.023945
Sum of electronic and thermal Energies= -1351.997541
Sum of electronic and thermal Enthalpies= -1351.996597
Sum of electronic and thermal Free Energies= -1352.081904
E(RM06L) = -1353.70573089

C 1.8619 3.30408 0.90765
C 3.05277 1.86003 -0.46772
C 4.21215 2.61042 -0.28853
C 4.17122 3.74176 0.51664
C 2.97688 4.10159 1.12624
H 0.90119 3.53743 1.36376
H 5.14573 2.31878 -0.76065
H 5.0712 4.33399 0.66615
H 2.90286 4.97892 1.76284
C 3.00133 0.64237 -1.3057
C 4.08685 0.19842 -2.05688
C 1.71926 -1.14841 -2.05312
C 3.96764 -0.95773 -2.81647
H 5.02203 0.75083 -2.05993
C 2.76413 -1.64925 -2.81573
H 0.75315 -1.64947 -2.02488
H 4.81118 -1.3111 -3.40516
H 2.62541 -2.55833 -3.39435
Pd 0.24945 0.83746 -0.18058
N 1.83114 -0.03736 -1.31872
N 1.89882 2.21518 0.1346
C -2.01146 -0.15101 -1.67029
C -1.90042 -0.79855 -2.90336
C -2.85598 0.95657 -1.55336
C -2.60708 -0.28881 -3.9859
H -1.27142 -1.68141 -3.01309
C -3.56494 1.48698 -2.61735
C -3.4229 0.84101 -3.843
H -2.5303 -0.77396 -4.95682
H -4.21314 2.35071 -2.48947
H -3.96984 1.21713 -4.70564
C -1.99255 0.69457 0.4951
H -1.16835 1.47152 0.818
O -2.9162 1.42462 -0.27511
C -2.63206 0.24411 1.79781
O -3.71507 -0.28412 1.83138
O -1.83468 0.47109 2.83082
C -2.27742 -0.0572 4.10662
H -2.49072 -1.12616 3.97514
C -1.39687 -0.39711 -0.36755
C -1.19078 -1.82097 0.09467
H -2.18567 -2.23294 0.33845
H -0.84548 -2.39996 -0.77534
C -0.23726 -2.04793 1.25782
H -0.19311 -3.11641 1.50222
H 0.78034 -1.71515 1.01047
H -0.54729 -1.51568 2.16706
H -3.21243 0.44797 4.37745
C -1.1771 0.19148 5.09763
H -1.47399 -0.19219 6.08064
H -0.25314 -0.31807 4.79564
H -0.97016 1.26412 5.19658

23

E(RM06) = -1352.42855580

Zero-point correction= 0.414532 (Hartree/Particle)

Thermal correction to Energy= 0.441284
Thermal correction to Enthalpy= 0.442228
Thermal correction to Gibbs Free Energy= 0.356902
Sum of electronic and zero-point Energies= -1352.014024
Sum of electronic and thermal Energies= -1351.987272
Sum of electronic and thermal Enthalpies= -1351.986328
Sum of electronic and thermal Free Energies= -1352.071654
E(RM06L) = -1353.69765244

C 1.91701 3.50559 0.95494
C 2.92587 2.05151 -0.56418
C 4.04603 2.87583 -0.62632
C 4.08964 4.03782 0.1308
C 3.00852 4.35903 0.93884
H 1.04485 3.72072 1.5642
H 4.88419 2.61809 -1.26678
H 4.96281 4.68453 0.08585
H 2.99652 5.25755 1.54924
C 2.81875 0.79505 -1.33116
C 3.8597 0.31673 -2.12385
C 1.51629 -1.03707 -1.88018
C 3.70129 -0.87775 -2.81316
H 4.79419 0.86394 -2.20286
C 2.50713 -1.57258 -2.69085
H 0.5689 -1.55467 -1.75294
H 4.50817 -1.25927 -3.43466
H 2.33673 -2.51394 -3.20596
Pd 0.21844 1.11556 0.14954
N 1.65587 0.11467 -1.21898
N 1.87383 2.37977 0.22373
C -1.91909 -0.33386 -1.54919
C -1.81183 -1.13439 -2.69252
C -2.589 0.89195 -1.63734
C -2.3419 -0.65377 -3.88079
H -1.33992 -2.11527 -2.65082
C -3.11294 1.40034 -2.81435
C -2.97295 0.59911 -3.94132
H -2.27492 -1.25874 -4.78264
H -3.62106 2.36115 -2.84117
H -3.37811 0.94477 -4.8904
C -2.00062 0.67796 0.46876
H -0.48913 2.0576 1.15554
O -2.66879 1.49033 -0.41994
C -2.44355 0.89354 1.87729
O -3.15767 1.80767 2.21518
O -1.977 -0.0577 2.67653
C -2.36875 0.01694 4.06564
H -3.46416 -0.01749 4.11584
C -1.51372 -0.48689 -0.16166
C -1.15411 -1.81462 0.45839
H -2.022 -2.12624 1.05989
H -1.07886 -2.54392 -0.36101
C 0.0993 -1.90322 1.31897
H 0.17366 -2.9093 1.75192
H 1.00935 -1.72605 0.73137
H 0.07689 -1.1836 2.14467
H -2.03977 0.98298 4.46855

C -1.72691 -1.14781 4.76562
H -2.04287 -1.16903 5.81514
H -2.02387 -2.09567 4.29791
H -0.63269 -1.07331 4.73924

24

E(RM06) = -729.018290282
Zero-point correction= 0.244877 (Hartree/Particle)
Thermal correction to Energy= 0.259664
Thermal correction to Enthalpy= 0.260608
Thermal correction to Gibbs Free Energy= 0.202405
Sum of electronic and zero-point Energies= -728.773413
Sum of electronic and thermal Energies= -728.758626
Sum of electronic and thermal Enthalpies= -728.757682
Sum of electronic and thermal Free Energies= -728.815886
E(RM06L) = -729.697012157

C -2.20058 -0.48837 -1.60022
C -1.79749 -1.14132 -2.77281
C -2.78652 0.782 -1.68815
C -2.00109 -0.4958 -3.9818
H -1.33632 -2.12772 -2.73245
C -3.00023 1.44503 -2.88927
C -2.59478 0.77873 -4.03778
H -1.6972 -0.97936 -4.9086
H -3.45909 2.43053 -2.92013
H -2.7395 1.25486 -5.0061
C -2.71193 0.26864 0.42878
O -3.10167 1.24697 -0.45615
C -2.91991 0.50201 1.85594
O -2.56208 -0.28002 2.71697
O -3.53861 1.65892 2.09856
C -3.77322 1.9656 3.48508
H -2.81033 1.97224 4.0124
C -2.16664 -0.81492 -0.20101
C -1.59228 -2.05444 0.39697
H -2.11857 -2.29526 1.32781
H -1.75313 -2.89019 -0.29976
C -0.10006 -1.89735 0.67776
H 0.32236 -2.82482 1.08423
H 0.45249 -1.6446 -0.23776
H 0.07232 -1.09541 1.40782
H -4.38735 1.16795 3.92319
C -4.4586 3.3029 3.53716
H -4.65866 3.57826 4.57951
H -3.83108 4.08342 3.08955
H -5.41413 3.2758 2.99908

25

E(RM06) = -728.995834055
Zero-point correction= 0.243918 (Hartree/Particle)
Thermal correction to Energy= 0.258870
Thermal correction to Enthalpy= 0.259815
Thermal correction to Gibbs Free Energy= 0.200628
Sum of electronic and zero-point Energies= -728.751916
Sum of electronic and thermal Energies= -728.736964

Sum of electronic and thermal Enthalpies= -728.736020
Sum of electronic and thermal Free Energies= -728.795206
E(RM06L) = -729.673253523

C -2.13891 -0.38035 -1.44003
C -1.47036 -0.71521 -2.61298
C -2.98582 0.72905 -1.42103
C -1.66573 0.07391 -3.7458
H -0.80498 -1.57785 -2.64368
C -3.20036 1.52428 -2.53394
C -2.52106 1.17716 -3.70283
H -1.14666 -0.17087 -4.67075
H -3.86901 2.38126 -2.48922
H -2.66236 1.78228 -4.59711
C -3.03629 -0.02319 0.7107
O -3.58251 0.92133 -0.21353
C -2.15961 0.67291 1.74096
O -2.05923 0.28818 2.88465
O -1.48706 1.68905 1.21564
C -0.56666 2.36475 2.0976
H 0.15398 1.62942 2.47808
C -2.19022 -0.98663 -0.11269
C -1.63576 -2.13046 0.30883
H -3.86142 -0.50987 1.24598
H -1.04164 -2.69266 -0.41629
C -1.75367 -2.71418 1.67311
H -1.9931 -3.78525 1.61881
H -0.8035 -2.63521 2.22368
H -2.51773 -2.21366 2.27957
H -1.12977 2.75758 2.95383
C 0.09638 3.45432 1.30245
H 0.80809 3.99614 1.93668
H 0.64431 3.03865 0.44793
H -0.64299 4.17117 0.92485

26

E(RM06) = -728.979613668
Zero-point correction= 0.244140 (Hartree/Particle)
Thermal correction to Energy= 0.258828
Thermal correction to Enthalpy= 0.259772
Thermal correction to Gibbs Free Energy= 0.200963
Sum of electronic and zero-point Energies= -728.735473
Sum of electronic and thermal Energies= -728.720786
Sum of electronic and thermal Enthalpies= -728.719842
Sum of electronic and thermal Free Energies= -728.778651
E(RM06L) = -729.655060555

C -2.18193 -0.40149 -1.41233
C -1.48109 -0.70454 -2.56701
C -3.02109 0.70611 -1.37583
C -1.64317 0.11816 -3.68628
H -0.8159 -1.56804 -2.59729
C -3.20619 1.53362 -2.47046
C -2.49888 1.21735 -3.63323
H -1.09827 -0.10046 -4.60293
H -3.86784 2.39562 -2.41657

H -2.61616 1.85026 -4.51178
C -3.01774 -0.02739 0.75988
O -3.63222 0.8692 -0.16999
C -2.08259 0.71253 1.69728
O -1.90035 0.36365 2.84206
O -1.45742 1.72095 1.09872
C -0.47844 2.41908 1.89569
H 0.27172 1.69316 2.23748
H -3.80289 -0.47591 1.37653
H -0.97821 2.82726 2.78339
C 0.11967 3.49366 1.03171
H 0.87369 4.05085 1.60037
H 0.60484 3.06212 0.14757
H -0.64884 4.20016 0.69497
C -2.25492 -1.10337 -0.07779
H -2.89351 -1.99732 -0.15731
C -0.92086 -1.52099 0.45998
H -0.17429 -0.72771 0.57152
C -0.59951 -2.77956 0.74647
H -1.32007 -3.59089 0.63163
H 0.39139 -3.05037 1.1073

A

E(RM06) = -1352.43273699
Zero-point correction= 0.417245 (Hartree/Particle)
Thermal correction to Energy= 0.443210
Thermal correction to Enthalpy= 0.444154
Thermal correction to Gibbs Free Energy= 0.358433
Sum of electronic and zero-point Energies= -1352.015492
Sum of electronic and thermal Energies= -1351.989527
Sum of electronic and thermal Enthalpies= -1351.988583
Sum of electronic and thermal Free Energies= -1352.074304
E(RM06L) = -1353.69691814

C 0.03123 -1.92951 0.90269
C -2.00575 -0.96339 0.3428
C -1.61795 0.24303 0.9201
C -0.36095 0.34287 1.50371
C 0.48185 -0.76025 1.50025
H 0.65167 -2.82353 0.86831
H -2.28082 1.10362 0.91522
H -0.04628 1.27984 1.95765
H 1.47171 -0.7241 1.94674
C -3.32565 -1.16813 -0.29136
C -4.31506 -0.18883 -0.30547
C -4.72969 -2.63591 -1.43106
C -5.53821 -0.45661 -0.90526
H -4.1406 0.77952 0.15472
C -5.75447 -1.70254 -1.47718
H -4.8579 -3.62783 -1.85885
H -6.31564 0.30393 -0.91861
H -6.69753 -1.9586 -1.95202
Pd -1.95382 -3.74907 -0.72971
N -3.54684 -2.37813 -0.86016
N -1.17629 -2.02849 0.3404
C -1.51577 -4.5452 -3.91025

C -1.04037 -3.24294 -3.84804
C -0.81293 -5.50444 -4.63277
C 0.14 -2.92308 -4.5243
H -1.58367 -2.48107 -3.28539
C 0.36519 -5.21742 -5.30425
C 0.83198 -3.90403 -5.2357
H 0.51901 -1.90308 -4.49973
H 0.89321 -5.98756 -5.86235
H 1.75044 -3.64131 -5.75835
C -2.70518 -6.55495 -4.0572
H -3.41515 -6.45234 -4.89159
O -1.3959 -6.73482 -4.59187
C -3.08622 -7.75458 -3.22505
O -2.31632 -8.56643 -2.77181
O -4.40578 -7.73876 -3.02478
C -4.94361 -8.76869 -2.16521
H -4.24864 -8.92562 -1.33135
C -2.68589 -5.21965 -3.24041
C -2.51179 -5.41757 -1.74671
H -3.63449 -4.69359 -3.41268
H -3.4031 -5.84121 -1.26577
C -1.21976 -5.88835 -1.2056
H -1.30593 -6.66626 -0.4413
H -0.45649 -6.13636 -1.9526
H -0.65329 -5.03438 -0.61247
H -5.87251 -8.33977 -1.77635
C -5.19256 -10.03763 -2.93791
H -5.66396 -10.7832 -2.28586
H -5.86306 -9.85153 -3.78594
H -4.25432 -10.45941 -3.31719

B

E(RM06) = -1352.41155451
Zero-point correction= 0.415447 (Hartree/Particle)
Thermal correction to Energy= 0.441459
Thermal correction to Enthalpy= 0.442403
Thermal correction to Gibbs Free Energy= 0.356521
Sum of electronic and zero-point Energies= -1351.996107
Sum of electronic and thermal Energies= -1351.970096
Sum of electronic and thermal Enthalpies= -1351.969151
Sum of electronic and thermal Free Energies= -1352.055034
E(RM06L) = -1353.67780111

C -0.77558 -0.32839 -0.95777
C -2.68212 -0.85839 0.28091
C -2.82129 0.47353 0.65922
C -1.90311 1.41458 0.21155
C -0.85902 1.01066 -0.6083
H 0.01906 -0.69738 -1.60006
H -3.64465 0.78596 1.29435
H -2.00857 2.45687 0.50364
H -0.11869 1.71329 -0.98016
C -3.61529 -1.91769 0.72399
C -4.63113 -1.68844 1.64855
C -4.22887 -4.15139 0.55451
C -5.46342 -2.73721 2.01986

H -4.7743 -0.70656 2.09045
C -5.2652 -3.99343 1.46442
H -4.02838 -5.12086 0.09744
H -6.25835 -2.56915 2.74285
H -5.89105 -4.84107 1.72943
Pd -1.6525 -3.25829 -1.0944
N -3.42819 -3.14656 0.19265
N -1.66198 -1.23779 -0.52848
C -0.3428 -5.17524 -4.02973
C 0.65338 -4.2132 -4.10709
C -0.02313 -6.51604 -4.23609
C 1.96495 -4.62061 -4.36565
H 0.41727 -3.1563 -3.98301
C 1.26915 -6.9489 -4.48019
C 2.26459 -5.97207 -4.53538
H 2.75631 -3.87733 -4.44202
H 1.4868 -8.00315 -4.63623
H 3.29174 -6.27356 -4.73464
C -2.24542 -6.47849 -4.30527
H -2.46704 -6.33152 -5.37411
O -1.11396 -7.33297 -4.17932
C -3.43924 -7.11 -3.63154
O -3.3984 -8.04101 -2.86513
O -4.53776 -6.43701 -3.98112
C -5.77731 -6.85444 -3.36521
H -5.58084 -7.09323 -2.31245
C -1.81293 -5.10457 -3.70191
C -2.14133 -5.0904 -2.22409
H -2.352 -4.29474 -4.20909
H -3.21723 -5.11399 -2.01845
C -1.27607 -5.41667 -1.20125
H -1.65763 -5.7277 -0.22733
H -0.22179 -5.61543 -1.39674
H -0.34789 -3.15806 -1.91879
H -6.41586 -5.96674 -3.41394
C -6.38015 -8.02005 -4.10455
H -7.35218 -8.27553 -3.66517
H -6.53673 -7.77097 -5.16127
H -5.7342 -8.90373 -4.04324

[BF₄]⁻

E(RM06) = -424.460140778
Zero-point correction= 0.014664 (Hartree/Particle)
Thermal correction to Energy= 0.018973
Thermal correction to Enthalpy= 0.019917
Thermal correction to Gibbs Free Energy= -0.012891
Sum of electronic and zero-point Energies= -424.445477
Sum of electronic and thermal Energies= -424.441168
Sum of electronic and thermal Enthalpies= -424.440223
Sum of electronic and thermal Free Energies= -424.473032
E(RM06L) = -424.730531493

B 0.59816 -0.74896 -0.00001
F 1.06412 -0.09034 1.14135
F 1.06377 -2.06662 0.
F -0.79948 -0.7494 0.00001

F 1.06414 -0.09033 -1.14135

Phi

E(RM06) = -242.847962521
Zero-point correction= 0.089756 (Hartree/Particle)
Thermal correction to Energy= 0.095672
Thermal correction to Enthalpy= 0.096616
Thermal correction to Gibbs Free Energy= 0.057983
Sum of electronic and zero-point Energies= -242.758207
Sum of electronic and thermal Energies= -242.752291
Sum of electronic and thermal Enthalpies= -242.751347
Sum of electronic and thermal Free Energies= -242.789980
E(RM06L) = -529.577016462

C -1.66813 -1.1409 0.00005
C -0.27467 -1.15011 0.00056
C 0.40344 0.06394 0.00003
C -0.27457 1.27807 -0.00099
C -1.66801 1.26898 -0.0015
C -2.36499 0.06406 -0.00098
H -2.20776 -2.08673 0.00047
H 0.27078 -2.09171 0.00136
H 0.271 2.2196 -0.00139
H -2.2076 2.21483 -0.0023
H -3.45359 0.06414 -0.00139
I 2.54581 0.06388 0.00075

[Phi(CH=CHMe)]⁺

E(RM06) = -359.829285893
Zero-point correction= 0.159846 (Hartree/Particle)
Thermal correction to Energy= 0.170626
Thermal correction to Enthalpy= 0.171570
Thermal correction to Gibbs Free Energy= 0.121025
Sum of electronic and zero-point Energies= -359.669440
Sum of electronic and thermal Energies= -359.658660
Sum of electronic and thermal Enthalpies= -359.657716
Sum of electronic and thermal Free Energies= -359.708261
E(RM06L) = -646.699276610

C 0.03658 -3.79584 3.32202
C 1.32351 -3.9525 3.03164
H -0.42628 -3.00935 3.91423
H 1.65267 -4.79179 2.41573
C 2.36524 -3.01079 3.52151
H 3.11223 -3.55246 4.11718
H 2.89875 -2.56535 2.67108
H 1.93883 -2.20747 4.13236
C -1.5221 -6.37092 4.36504
C -0.44059 -7.18033 4.68098
C -0.52259 -7.93865 5.84603
C -1.6618 -7.87708 6.64486
C -2.73002 -7.05699 6.29333
C -2.6709 -6.282 5.13653
H 0.44214 -7.221 4.04563
H 0.31004 -8.58183 6.12385
H -1.71677 -8.47546 7.55204

H -3.61758 -7.0103 6.92121
H -3.49543 -5.63139 4.85503
I -1.39891 -5.18505 2.57881

TS-1/3

E(RM06) = -1235.33406114
Zero-point correction= 0.342118 (Hartree/Particle)
Thermal correction to Energy= 0.364322
Thermal correction to Enthalpy= 0.365266
Thermal correction to Gibbs Free Energy= 0.289319
Sum of electronic and zero-point Energies= -1234.991943
Sum of electronic and thermal Energies= -1234.969739
Sum of electronic and thermal Enthalpies= -1234.968795
Sum of electronic and thermal Free Energies= -1235.044742
E(RM06L) = -1236.47254688

C -3.7154 -3.34768 0.33224
C -2.67202 -1.32548 0.75978
C -3.89195 -0.74418 1.10108
C -5.05153 -1.50493 1.03917
C -4.96491 -2.83556 0.65427
H -3.59728 -4.38911 0.03956
H -3.94071 0.2886 1.43515
H -6.00924 -1.06229 1.30426
H -5.84194 -3.47557 0.6076
C -1.39305 -0.5913 0.86383
C -1.33099 0.78572 1.06964
C 0.91887 -0.73888 0.92659
C -0.09403 1.39824 1.2158
H -2.23833 1.38222 1.10324
C 1.05593 0.62236 1.15737
H 1.79567 -1.38208 0.8646
H -0.03298 2.47253 1.3756
H 2.04503 1.05618 1.27715
Pd -0.55908 -3.35288 0.00218
N -0.26809 -1.33443 0.77438
N -2.59782 -2.61644 0.36594
C -0.75315 -5.15639 -0.87272
C -1.85975 -5.70814 -1.52113
C 0.4294 -5.92159 -0.87466
C -1.81967 -6.98991 -2.08153
H -2.78367 -5.13243 -1.60645
C 0.49487 -7.20019 -1.42203
C -0.6463 -7.73567 -2.01773
H -2.70444 -7.39936 -2.56855
H 1.4329 -7.75389 -1.39263
H -0.60731 -8.73518 -2.45005
C 1.37504 -3.95507 -0.13381
H 1.8907 -3.71196 0.80966
O 1.53495 -5.37706 -0.31325
C 2.12324 -3.27906 -1.27014
O 1.64265 -2.58107 -2.13966
O 3.43346 -3.55404 -1.20376
C 4.25422 -3.02359 -2.25825
H 3.87935 -3.39726 -3.22038
H 4.15743 -1.92958 -2.26645

C 5.66784 -3.46413 -1.9931
H 6.33344 -3.08046 -2.7757
H 6.02222 -3.0867 -1.02566
H 5.74218 -4.55864 -1.98495

TS-4/7

E(RM06) = -1595.16273430
Zero-point correction= 0.501387 (Hartree/Particle)
Thermal correction to Energy= 0.536715
Thermal correction to Enthalpy= 0.537659
Thermal correction to Gibbs Free Energy= 0.428754
Sum of electronic and zero-point Energies= -1594.661347
Sum of electronic and thermal Energies= -1594.626019
Sum of electronic and thermal Enthalpies= -1594.625075
Sum of electronic and thermal Free Energies= -1594.733981
E(RM06L) = -1883.17287993

C -3.58921 -2.97934 0.45826
C -2.3901 -0.99509 0.41994
C -3.56613 -0.26298 0.5857
C -4.78018 -0.9288 0.67593
C -4.79739 -2.31575 0.61297
H -3.55012 -4.06761 0.42454
H -3.54041 0.82008 0.65902
H -5.70198 -0.36592 0.80463
H -5.72256 -2.88072 0.68702
C -1.0625 -0.34675 0.33786
C -0.91416 1.03302 0.2094
C 1.24282 -0.62383 0.35837
C 0.36088 1.58241 0.16893
H -1.78141 1.68217 0.12993
C 1.46275 0.74244 0.25022
H 2.07338 -1.32555 0.38594
H 0.487 2.65822 0.06925
H 2.47859 1.127 0.221
Pd -0.44619 -3.35291 0.19401
N 0.01655 -1.15963 0.40355
N -2.4181 -2.34404 0.35352
C -0.87038 -5.19749 -0.52328
C -2.04302 -5.63075 -1.13
C 0.18175 -6.1131 -0.37343
C -2.18868 -6.97263 -1.50532
H -2.86235 -4.93634 -1.3206
C 0.05639 -7.44631 -0.73854
C -1.14968 -7.87351 -1.29468
H -3.11889 -7.30628 -1.96341
H 0.89811 -8.12588 -0.61216
H -1.26467 -8.91639 -1.58653
C 1.42458 -4.23345 -0.00364
H 2.06298 -3.83966 0.79817
O 1.34348 -5.63861 0.15205
C 1.97169 -3.79988 -1.32703
O 2.43752 -2.69012 -1.5167
O 1.88128 -4.73682 -2.26878
C 2.33382 -4.37356 -3.58588
H 1.76057 -3.50112 -3.92604

C -0.57441 -4.43205 2.26453
C -1.76802 -4.73862 2.74967
H 0.33257 -5.03656 2.22663
H -2.55405 -3.99002 2.86376
C -2.10819 -6.16784 3.04814
H -2.45613 -6.27499 4.08577
H -2.91927 -6.50977 2.3878
H -1.24686 -6.83017 2.89767
H 3.39005 -4.08021 -3.52799
C 0.19557 -3.28221 5.22955
C -0.99325 -3.26417 5.95142
C -1.05262 -3.97836 7.1458
C 0.05665 -4.69081 7.59365
C 1.23551 -4.6949 6.85285
C 1.31547 -3.9877 5.65561
H -1.85684 -2.70488 5.59588
H -1.97352 -3.97443 7.72611
H 0.00212 -5.2472 8.52742
H 2.10203 -5.25288 7.20297
H 2.23216 -3.99024 5.06883
I 0.2746 -2.27239 3.35719
C 2.12354 -5.57125 -4.47046
H 2.44736 -5.34337 -5.49297
H 2.70131 -6.43117 -4.10955
H 1.06379 -5.8549 -4.49856

TS-5/9

E(RM06) = -1595.16723958
Zero-point correction= 0.501886 (Hartree/Particle)
Thermal correction to Energy= 0.536648
Thermal correction to Enthalpy= 0.537592
Thermal correction to Gibbs Free Energy= 0.433061
Sum of electronic and zero-point Energies= -1594.665354
Sum of electronic and thermal Energies= -1594.630592
Sum of electronic and thermal Enthalpies= -1594.629648
Sum of electronic and thermal Free Energies= -1594.734179
E(RM06L) = -1883.17617561

C -3.1678 2.76505 -1.61107
C -1.45711 3.41998 -0.18916
C -1.70148 4.76069 -0.48497
C -2.70899 5.09092 -1.38135
C -3.4605 4.07672 -1.95835
H -3.74526 1.937 -2.02006
H -1.12611 5.54932 -0.00888
H -2.90839 6.13432 -1.61553
H -4.26611 4.28809 -2.65631
C -0.40368 3.00277 0.7643
C 0.54935 3.8936 1.25802
C 0.54813 1.26621 1.98158
C 1.51524 3.43873 2.14524
H 0.55342 4.9337 0.94527
C 1.51727 2.10166 2.51926
H 0.52124 0.20072 2.21327
H 2.26282 4.12669 2.53411
H 2.25637 1.70246 3.20872

Pd -1.80147 0.36312 0.05763
N -0.3871 1.70291 1.13023
N -2.19017 2.43971 -0.76176
C -3.26827 -0.73703 -0.75643
C -3.7657 -0.6714 -2.05513
C -3.82447 -1.67279 0.13054
C -4.82515 -1.49735 -2.45112
H -3.32541 0.0187 -2.7797
C -4.86465 -2.51153 -0.25111
C -5.36738 -2.4084 -1.54842
H -5.2202 -1.42486 -3.46329
H -5.26465 -3.23448 0.45826
H -6.18653 -3.05659 -1.85606
C -2.01215 -1.18493 1.44334
H -1.89485 -0.64456 2.39314
O -3.31711 -1.72266 1.3868
C -0.94197 -2.2113 1.32415
O 0.23707 -1.96692 1.53854
O -1.38726 -3.40531 0.94619
C -0.38878 -4.4234 0.75241
H 0.35602 -4.04713 0.03585
C -0.00238 -0.29657 -1.10421
C 0.32831 0.64415 -1.97807
H 0.57575 -0.85848 -0.36534
H -0.35329 0.94333 -2.77771
C 1.61914 1.39436 -1.82951
H 2.22456 1.29565 -2.74222
H 1.42398 2.46639 -1.68062
H 2.20858 1.0274 -0.98023
H 0.12499 -4.59936 1.70629
C 1.00683 -2.9243 -3.00204
C 1.7348 -2.03644 -3.78839
C 3.03594 -2.377 -4.15038
C 3.58561 -3.58782 -3.73763
C 2.8369 -4.46798 -2.96152
C 1.53656 -4.14091 -2.58336
H 1.2969 -1.09604 -4.11948
H 3.61737 -1.69181 -4.76482
H 4.6018 -3.84926 -4.0267
H 3.26288 -5.4177 -2.6429
H 0.94837 -4.83015 -1.979
I -0.97231 -2.3877 -2.41261
C -1.09342 -5.65262 0.25005
H -0.36674 -6.45653 0.08009
H -1.83181 -6.00778 0.9794
H -1.61474 -5.45039 -0.69531

TS-6/10

E(RM06) = -1595.16574544
Zero-point correction= 0.501766 (Hartree/Particle)
Thermal correction to Energy= 0.536568
Thermal correction to Enthalpy= 0.537512
Thermal correction to Gibbs Free Energy= 0.433238
Sum of electronic and zero-point Energies= -1594.663980
Sum of electronic and thermal Energies= -1594.629177
Sum of electronic and thermal Enthalpies= -1594.628233

Sum of electronic and thermal Free Energies= -1594.732508
E(RM06L) = -1883.17547584

C -3.19446 2.76988 -1.50035
C -1.43985 3.37033 -0.1103
C -1.62898 4.71597 -0.4236
C -2.63287 5.07688 -1.31229
C -3.43705 4.08819 -1.86154
H -3.81106 1.96143 -1.89085
H -1.01439 5.4855 0.0343
H -2.78946 6.12436 -1.5604
H -4.24399 4.32412 -2.54998
C -0.40327 2.92484 0.84816
C 0.58778 3.78547 1.32113
C 0.458 1.18922 2.12472
C 1.53086 3.31424 2.22398
H 0.63837 4.81525 0.97928
C 1.46465 1.99202 2.64203
H 0.37533 0.14055 2.4053
H 2.30976 3.97768 2.59346
H 2.17791 1.57845 3.35062
Pd -1.8624 0.31078 0.12175
N -0.44778 1.63511 1.247
N -2.21841 2.41422 -0.66173
C -3.3244 -0.74412 -0.75606
C -3.79457 -0.62121 -2.06078
C -3.90332 -1.70877 0.08281
C -4.85556 -1.41901 -2.50762
H -3.33476 0.09231 -2.74948
C -4.949 -2.51568 -0.34925
C -5.42626 -2.35592 -1.65005
H -5.2314 -1.30241 -3.52298
H -5.36965 -3.2618 0.32306
H -6.24757 -2.98094 -1.99724
C -2.11004 -1.29276 1.44323
H -2.00141 -0.80058 2.42013
O -3.41792 -1.8124 1.34363
C -1.10195 -2.37807 1.2764
O -1.30891 -3.48153 0.82437
O 0.10893 -1.96019 1.69282
C 1.20402 -2.87998 1.53142
H 1.0122 -3.76869 2.14624
C -0.08842 -0.3251 -1.0597
C 0.27039 0.64987 -1.88688
H 0.50959 -0.91344 -0.35977
H -0.40746 1.01065 -2.66404
C 1.58651 1.34864 -1.72006
H 2.17937 1.27876 -2.64358
H 1.43009 2.41787 -1.51459
H 2.17302 0.92029 -0.89741
H 1.24198 -3.20004 0.47993
C 0.97364 -2.93797 -2.78053
C 1.79356 -2.15796 -3.59045
C 3.12598 -2.53295 -3.74761
C 3.61648 -3.6684 -3.10772
C 2.77854 -4.43883 -2.30593

C 1.44416 -4.07692 -2.13342
H 1.40202 -1.27636 -4.09562
H 3.77974 -1.93416 -4.37944
H 4.6581 -3.95626 -3.2374
H 3.16004 -5.32846 -1.80792
H 0.78343 -4.67202 -1.50442
I -1.04573 -2.34262 -2.47188
C 2.45676 -2.15827 1.94529
H 3.32075 -2.82679 1.85203
H 2.63603 -1.27992 1.30932
H 2.39354 -1.82428 2.98911

TS-8/12

E(RM06) = -1352.35103873
Zero-point correction= 0.412244 (Hartree/Particle)
Thermal correction to Energy= 0.439473
Thermal correction to Enthalpy= 0.440417
Thermal correction to Gibbs Free Energy= 0.352637
Sum of electronic and zero-point Energies= -1351.938795
Sum of electronic and thermal Energies= -1351.911566
Sum of electronic and thermal Enthalpies= -1351.910622
Sum of electronic and thermal Free Energies= -1351.998402
E(RM06L) = -1353.62738987

C 1.3051 -1.84547 2.08088
C 2.78158 -0.38039 1.05593
C 3.8225 -0.83878 1.86037
C 3.57763 -1.83693 2.79381
C 2.29175 -2.34347 2.91946
H 0.28119 -2.20274 2.1579
H 4.81534 -0.40696 1.77864
H 4.38304 -2.19898 3.42879
H 2.0456 -3.10645 3.65271
C 2.95461 0.73816 0.10592
C 4.20667 1.25823 -0.21365
C 1.91594 2.32867 -1.22612
C 4.29405 2.35 -1.06682
H 5.11178 0.81574 0.19238
C 3.12859 2.90603 -1.57486
H 0.97967 2.739 -1.59668
H 5.26655 2.76206 -1.32616
H 3.14716 3.76886 -2.2348
Pd 0.02688 0.00194 -0.1976
N 1.82626 1.26858 -0.41649
N 1.54133 -0.9071 1.15889
C -1.57203 -1.2416 -0.25405
C -1.72137 -2.48583 0.36155
C -2.692 -0.65566 -0.86611
C -2.9695 -3.0955 0.40452
H -0.85608 -3.00669 0.769
C -3.9474 -1.25317 -0.82755
C -4.07665 -2.47652 -0.18465
H -3.07905 -4.06753 0.88172
H -4.7948 -0.75726 -1.29666
H -5.05037 -2.96138 -0.14846
C -1.38376 1.19732 -1.11388

H -0.93401 1.72386 -1.96283
O -2.4999 0.49508 -1.55519
C -1.64924 2.14364 0.03059
O -0.85006 3.00252 0.35137
O -2.80931 1.92264 0.63222
C -3.12901 2.784 1.7486
H -2.36235 2.64652 2.52193
C -0.01134 -1.21776 -1.86048
C 0.87233 -2.20658 -1.92804
H -0.60043 -0.8322 -2.69447
H 1.36584 -2.57324 -1.02435
C 1.23259 -2.87693 -3.21658
H 2.30884 -2.78494 -3.41612
H 1.00607 -3.95121 -3.16655
H 0.68553 -2.44761 -4.06446
H -3.08314 3.82506 1.40589
C -4.50039 2.40058 2.228
H -4.78466 3.03309 3.07727
H -5.24546 2.53581 1.43453
H -4.52574 1.35387 2.5553

TS-8/14

E(RM06) = -1352.33064623
Zero-point correction= 0.413316 (Hartree/Particle)
Thermal correction to Energy= 0.440134
Thermal correction to Enthalpy= 0.441078
Thermal correction to Gibbs Free Energy= 0.355680
Sum of electronic and zero-point Energies= -1351.917330
Sum of electronic and thermal Energies= -1351.890513
Sum of electronic and thermal Enthalpies= -1351.889568
Sum of electronic and thermal Free Energies= -1351.974966
E(RM06L) = -1353.60483575

C -3.78771 -3.32296 -0.24037
C -2.53221 -1.37113 -0.29733
C -3.67595 -0.62167 -0.55943
C -4.90258 -1.2609 -0.67412
C -4.96634 -2.63387 -0.4818
H -3.80016 -4.39455 -0.06251
H -3.61673 0.46061 -0.63544
H -5.80217 -0.6844 -0.87696
H -5.90851 -3.17373 -0.51013
C -1.23475 -0.74124 0.00284
C -0.95937 0.59258 -0.28285
C 0.81995 -0.98754 1.04614
C 0.24731 1.13973 0.13468
H -1.67341 1.19954 -0.83255
C 1.14726 0.3438 0.8287
H 1.51592 -1.65534 1.54775
H 0.47679 2.18099 -0.08021
H 2.09684 0.73269 1.18553
Pd -0.73578 -3.68162 0.32398
N -0.33583 -1.52302 0.64346
N -2.59276 -2.72074 -0.1949
C -1.02572 -5.51849 -0.46897
C -2.06802 -5.89401 -1.31232

C 0.0438 -6.41549 -0.32239
C -2.09188 -7.15728 -1.90616
H -2.8786 -5.2069 -1.5411
C 0.03247 -7.68001 -0.89934
C -1.05217 -8.05459 -1.68257
H -2.9283 -7.43074 -2.54704
H 0.88813 -8.33692 -0.75184
H -1.06942 -9.04126 -2.14176
C 1.26989 -4.6874 0.58285
H 2.03546 -4.5059 1.33952
O 1.14956 -6.048 0.38849
C 1.75512 -3.92094 -0.6567
O 2.26021 -2.82156 -0.58411
O 1.64975 -4.63878 -1.76315
C 2.13135 -4.03464 -2.98468
H 1.58721 -3.09436 -3.1414
C -0.03097 -4.53556 2.10084
C 0.11957 -3.72355 3.14781
H -0.26534 -5.59604 2.2006
H 0.43194 -2.68611 3.02118
C -0.13223 -4.17739 4.54787
H 0.77543 -4.06128 5.15729
H -0.91166 -3.56416 5.02042
H -0.44516 -5.22745 4.58695
H 3.19541 -3.79841 -2.85989
C 1.88595 -5.03 -4.08346
H 2.21703 -4.6156 -5.04285
H 2.4381 -5.95985 -3.90012
H 0.81776 -5.27099 -4.16001

TS-12/13

E(RM06) = -1352.40741872
Zero-point correction= 0.415076 (Hartree/Particle)
Thermal correction to Energy= 0.441501
Thermal correction to Enthalpy= 0.442445
Thermal correction to Gibbs Free Energy= 0.357724
Sum of electronic and zero-point Energies= -1351.992343
Sum of electronic and thermal Energies= -1351.965918
Sum of electronic and thermal Enthalpies= -1351.964974
Sum of electronic and thermal Free Energies= -1352.049695
E(RM06L) = -1353.67514115

C 1.05181 -2.37477 1.49392
C 2.56063 -0.65421 1.10162
C 3.43977 -1.17946 2.04566
C 3.09562 -2.34253 2.72102
C 1.88034 -2.95458 2.44384
H 0.08339 -2.80877 1.2489
H 4.37793 -0.67969 2.26894
H 3.7709 -2.76004 3.46434
H 1.56862 -3.8616 2.95435
C 2.8382 0.58029 0.34705
C 4.10331 1.15853 0.30738
C 2.0112 2.22953 -1.07252
C 4.31316 2.30408 -0.448
H 4.93043 0.7061 0.84704

C 3.25035 2.84841 -1.15271
H 1.15059 2.64303 -1.58758
H 5.30063 2.75795 -0.48866
H 3.364 3.73999 -1.76299
Pd 0.06926 -0.09168 -0.43739
N 1.8016 1.12897 -0.33786
N 1.38322 -1.25953 0.83576
C -1.87859 -1.5668 -0.89856
C -2.12699 -2.68662 -0.07489
C -2.70578 -0.43559 -0.72033
C -3.14835 -2.67333 0.85677
H -1.53466 -3.59012 -0.21953
C -3.76117 -0.43468 0.18694
C -3.97983 -1.55229 0.97645
H -3.32949 -3.55156 1.4733
H -4.37492 0.45904 0.27284
H -4.7985 -1.55573 1.69344
C -1.22813 1.26386 -1.28753
H -0.8424 1.63673 -2.24385
O -2.4874 0.66945 -1.50666
C -1.29177 2.37076 -0.27199
O -0.62798 3.38557 -0.35739
O -2.1427 2.11636 0.71956
C -2.25611 3.12122 1.74688
H -1.27257 3.2491 2.21753
C -0.93839 -1.59955 -2.04224
C 0.14621 -2.39791 -2.15622
H -1.20504 -0.96672 -2.89255
H 0.42663 -3.04953 -1.32402
C 1.00084 -2.4645 -3.36915
H 2.04861 -2.23664 -3.12463
H 0.99815 -3.47842 -3.79512
H 0.66258 -1.76383 -4.14253
H -2.53246 4.07402 1.27795
C -3.29632 2.64339 2.72132
H -3.39254 3.36142 3.54434
H -4.2756 2.54656 2.23613
H -3.01961 1.66921 3.14452

TS-13/15

E(RM06) = -1352.38612493
Zero-point correction= 0.415555 (Hartree/Particle)
Thermal correction to Energy= 0.441483
Thermal correction to Enthalpy= 0.442427
Thermal correction to Gibbs Free Energy= 0.359191
Sum of electronic and zero-point Energies= -1351.970570
Sum of electronic and thermal Energies= -1351.944642
Sum of electronic and thermal Enthalpies= -1351.943698
Sum of electronic and thermal Free Energies= -1352.026934
E(RM06L) = -1353.65034865

C -2.07556 2.65339 0.57909
C -3.31383 0.70485 0.30346
C -4.44128 1.32978 0.83149
C -4.36678 2.65612 1.23285
C -3.16109 3.3328 1.11028

H -1.11111 3.14527 0.47535
H -5.3714 0.78128 0.94787
H -5.24286 3.14996 1.64689
H -3.05031 4.36757 1.42225
C -3.31364 -0.71404 -0.10776
C -4.48442 -1.4614 -0.21398
C -2.04047 -2.54877 -0.72108
C -4.40667 -2.79744 -0.58501
H -5.45359 -1.01023 -0.02186
C -3.1629 -3.35715 -0.83938
H -1.04593 -2.95426 -0.89425
H -5.31335 -3.39185 -0.67356
H -3.05277 -4.39919 -1.12683
Pd -0.48049 0.24762 -0.50561
N -2.10775 -1.2626 -0.36895
N -2.14779 1.37863 0.17521
C 3.05003 0.61118 -0.8426
C 3.88144 1.68252 -0.55641
C 3.54697 -0.68042 -0.76564
C 5.20843 1.4274 -0.19404
H 3.51231 2.70498 -0.63291
C 4.85186 -0.96585 -0.42402
C 5.68482 0.1214 -0.13662
H 5.87215 2.25789 0.03785
H 5.20374 -1.99339 -0.36675
H 6.71925 -0.0641 0.14712
C 1.29499 -1.24188 -0.73359
H 0.64318 -1.82817 -1.38797
O 2.61053 -1.63117 -1.06999
C 1.08914 -1.58559 0.73353
O 0.44325 -2.5403 1.10897
O 1.77533 -0.7702 1.52679
C 1.7949 -1.08461 2.93706
H 0.76986 -1.01385 3.32267
C 1.65714 0.6584 -1.35624
C 0.80079 1.76169 -0.99232
H 1.59257 0.38136 -2.41773
H 1.09466 2.303 -0.08316
C 0.21822 2.60503 -2.09061
H -0.62496 3.21648 -1.74627
H 0.98569 3.29903 -2.4703
H -0.1168 1.98978 -2.93662
H 2.13465 -2.12091 3.0556
C 2.72508 -0.09841 3.58582
H 2.80161 -0.30622 4.65943
H 3.72875 -0.16632 3.14685
H 2.3602 0.92865 3.45876

TS-15/16

E(RM06) = -1352.43225054
Zero-point correction= 0.416768 (Hartree/Particle)
Thermal correction to Energy= 0.442419
Thermal correction to Enthalpy= 0.443363
Thermal correction to Gibbs Free Energy= 0.360089
Sum of electronic and zero-point Energies= -1352.015483
Sum of electronic and thermal Energies= -1351.989831

Sum of electronic and thermal Enthalpies= -1351.988887
Sum of electronic and thermal Free Energies= -1352.072161
E(RM06L) = -1353.69204947

C -3.32426 -2.26623 1.52869
C -2.95382 -1.30755 -0.55655
C -3.83671 -0.27345 -0.25351
C -4.46647 -0.24695 0.98317
C -4.20933 -1.26235 1.89379
H -3.10061 -3.08711 2.20761
H -4.04591 0.50342 -0.98376
H -5.15776 0.55676 1.22594
H -4.68422 -1.28879 2.87069
C -2.27095 -1.40592 -1.86485
C -2.27807 -0.37944 -2.80714
C -0.99365 -2.74199 -3.27207
C -1.62135 -0.56709 -4.01708
H -2.77493 0.56468 -2.60169
C -0.97057 -1.76944 -4.2628
H -0.49237 -3.70246 -3.40104
H -1.61707 0.22693 -4.76073
H -0.44731 -1.954 -5.19717
Pd -1.45428 -3.87571 -0.37388
N -1.62445 -2.56345 -2.10997
N -2.70585 -2.29054 0.34339
C -1.22504 -6.27053 -0.8118
C -2.54844 -6.18632 -1.25505
C -0.20065 -6.55206 -1.72152
C -2.80238 -6.33697 -2.62532
H -3.36609 -6.04841 -0.54814
C -0.4322 -6.71449 -3.07354
C -1.75844 -6.59403 -3.50945
H -3.82328 -6.26801 -2.99477
H 0.38001 -6.93948 -3.76105
H -1.97472 -6.71692 -4.56951
C 0.88486 -6.19189 0.239
H 1.4792 -6.84655 0.88192
O 1.00787 -6.6818 -1.11663
C 1.52225 -4.81158 0.18222
O 1.05761 -3.88673 -0.46458
O 2.6544 -4.75597 0.85348
C 3.36289 -3.4899 0.84023
H 3.5623 -3.22087 -0.20404
C -0.62736 -6.22463 0.58838
C -1.24905 -5.03049 1.29568
H -0.82705 -7.16083 1.1376
H -2.27953 -5.28998 1.58549
C -0.51286 -4.40817 2.45216
H -1.05722 -3.54793 2.86292
H -0.40759 -5.14254 3.26869
H 0.49824 -4.05806 2.20665
H 2.70068 -2.72738 1.27124
C 4.62199 -3.67608 1.63724
H 5.18864 -2.73782 1.65154
H 4.39616 -3.95678 2.67304
H 5.25606 -4.45324 1.19383

TS-16/17

E(RM06) = -1352.41675525
Zero-point correction= 0.416449 (Hartree/Particle)
Thermal correction to Energy= 0.442268
Thermal correction to Enthalpy= 0.443212
Thermal correction to Gibbs Free Energy= 0.358057
Sum of electronic and zero-point Energies= -1352.000306
Sum of electronic and thermal Energies= -1351.974488
Sum of electronic and thermal Enthalpies= -1351.973544
Sum of electronic and thermal Free Energies= -1352.058698
E(RM06L) = -1353.67965284

C -0.96938 -1.09512 0.85873
C -3.05707 -1.02018 -0.17394
C -3.33506 0.18971 0.45753
C -2.39385 0.76132 1.30269
C -1.18668 0.10993 1.50893
H -0.0377 -1.63846 0.99828
H -4.28787 0.68699 0.30178
H -2.60868 1.70583 1.79716
H -0.41973 0.51546 2.1629
C -4.02407 -1.68229 -1.07832
C -5.22029 -1.08792 -1.47394
C -4.51819 -3.5838 -2.3163
C -6.08057 -1.78627 -2.31209
H -5.48417 -0.08648 -1.14674
C -5.73219 -3.06026 -2.73988
H -4.19012 -4.57521 -2.62777
H -7.01677 -1.33162 -2.62808
H -6.37889 -3.63991 -3.39283
Pd -1.66079 -3.50535 -0.9366
N -3.68851 -2.91463 -1.51261
N -1.87199 -1.64606 0.03956
C 0.33511 -5.75159 -2.13477
C -0.48686 -5.50162 -3.22278
C 1.60456 -6.28416 -2.33348
C -0.02772 -5.81109 -4.50535
H -1.48418 -5.07046 -3.07734
C 2.08836 -6.59852 -3.59262
C 1.24589 -6.3526 -4.6787
H -0.66443 -5.63274 -5.36953
H 3.08353 -7.01841 -3.72129
H 1.59324 -6.59394 -5.68195
C 1.38137 -6.26415 -0.10506
H 1.00439 -7.25244 0.19828
O 2.30526 -6.43363 -1.17445
C 2.06455 -5.60816 1.06989
O 3.11699 -5.01847 1.03225
O 1.29773 -5.74353 2.15242
C 1.75303 -5.05673 3.33836
H 2.72967 -5.46703 3.62374
C 0.18218 -5.42625 -0.67264
C 0.23363 -3.93187 -0.37226
H -0.74477 -5.84111 -0.23483
H 0.27411 -3.75221 0.71445

C 1.23375 -3.1076 -1.13567
H 1.15701 -2.04205 -0.88194
H 2.26227 -3.42346 -0.88764
H 1.11502 -3.20983 -2.22251
H 1.89293 -3.99568 3.08996
C 0.71411 -5.25977 4.40477
H 1.02574 -4.7533 5.3259
H -0.25369 -4.84491 4.09582
H 0.58114 -6.32542 4.62748

TS-17/18

E(RM06) = -1352.41404633
Zero-point correction= 0.413367 (Hartree/Particle)
Thermal correction to Energy= 0.439411
Thermal correction to Enthalpy= 0.440355
Thermal correction to Gibbs Free Energy= 0.356841
Sum of electronic and zero-point Energies= -1352.000680
Sum of electronic and thermal Energies= -1351.974636
Sum of electronic and thermal Enthalpies= -1351.973692
Sum of electronic and thermal Free Energies= -1352.057205
E(RM06L) = -1353.67974385

C -1.43966 -1.61531 1.45922
C -3.33253 -1.51168 0.11596
C -4.00976 -0.78719 1.0937
C -3.36334 -0.47607 2.28314
C -2.05166 -0.88883 2.47099
H -0.41225 -1.95903 1.5666
H -5.0384 -0.47369 0.94081
H -3.8849 0.08573 3.05465
H -1.50524 -0.66097 3.38203
C -3.94623 -1.88023 -1.17716
C -5.19236 -1.41144 -1.5828
C -3.71964 -3.07983 -3.16063
C -5.70237 -1.80258 -2.81395
H -5.7629 -0.73623 -0.95178
C -4.95727 -2.65296 -3.6189
H -3.09482 -3.74322 -3.75288
H -6.67476 -1.44002 -3.13918
H -5.31792 -2.98396 -4.58877
Pd -1.33372 -3.27601 -1.21363
N -3.22587 -2.70401 -1.97362
N -2.06064 -1.92643 0.31686
C 1.26351 -5.11548 -2.39374
C 1.83884 -4.41104 -3.44346
C 1.57289 -6.46283 -2.20512
C 2.73283 -5.07591 -4.28189
H 1.58232 -3.36789 -3.62388
C 2.46713 -7.1385 -3.01797
C 3.04662 -6.41822 -4.06186
H 3.18649 -4.54424 -5.11571
H 2.69344 -8.18828 -2.8454
H 3.7485 -6.9207 -4.72521
C -0.09305 -6.11188 -0.74708
H -1.03672 -6.40022 -1.23309
O 0.92208 -7.02711 -1.14786

C -0.26708 -6.13532 0.75474
O 0.57876 -6.45187 1.55317
O -1.482 -5.67543 1.05305
C -1.75434 -5.40791 2.44549
H -1.65112 -6.34319 3.00912
C 0.37908 -4.73693 -1.26176
C 0.58907 -3.63949 -0.39766
H -0.94788 -4.27835 -2.3657
H 0.39801 -3.80996 0.6668
C 1.53048 -2.51576 -0.70212
H 1.31938 -1.65073 -0.06101
H 2.56747 -2.83086 -0.50387
H 1.47555 -2.18419 -1.7444
H -0.99491 -4.70403 2.81544
C -3.14323 -4.83868 2.52398
H -3.38084 -4.5766 3.56181
H -3.22949 -3.93103 1.90954
H -3.88663 -5.56495 2.17323

TS-19/20

E(RM06) = -1352.41313209
Zero-point correction= 0.414365 (Hartree/Particle)
Thermal correction to Energy= 0.440303
Thermal correction to Enthalpy= 0.441248
Thermal correction to Gibbs Free Energy= 0.355792
Sum of electronic and zero-point Energies= -1351.998768
Sum of electronic and thermal Energies= -1351.972829
Sum of electronic and thermal Enthalpies= -1351.971885
Sum of electronic and thermal Free Energies= -1352.057340
E(RM06L) = -1353.67949770

C -1.9477 -0.55285 0.66813
C -3.24602 -0.61303 -1.2445
C -3.56589 0.73413 -1.09302
C -3.0428 1.44682 -0.02274
C -2.21964 0.7919 0.88014
H -1.31352 -1.09744 1.35972
H -4.23343 1.22914 -1.79179
H -3.28774 2.49885 0.10442
H -1.79359 1.30028 1.7407
C -3.80399 -1.42724 -2.34271
C -4.53144 -0.87605 -3.39508
C -4.09974 -3.56149 -3.2266
C -5.05734 -1.70589 -4.37525
H -4.68169 0.19723 -3.46199
C -4.84664 -3.07468 -4.28773
H -3.89729 -4.62334 -3.12368
H -5.62564 -1.28142 -5.19963
H -5.2425 -3.76402 -5.02829
Pd -2.25153 -3.43561 -0.79241
N -3.58729 -2.76089 -2.27917
N -2.43257 -1.24593 -0.36631
C 0.43707 -4.68326 -1.42676
C 1.27341 -3.62135 -1.78408
C 0.3458 -5.80246 -2.26722
C 2.00469 -3.71753 -2.96091

H 1.35711 -2.73684 -1.15562
C 1.0594 -5.91085 -3.44924
C 1.89389 -4.84747 -3.78088
H 2.67321 -2.90869 -3.24786
H 0.96994 -6.79374 -4.07753
H 2.47799 -4.89983 -4.698
C -0.82644 -6.39104 -0.47346
H -1.84961 -6.68375 -0.222
O -0.53896 -6.73273 -1.81983
C 0.14923 -7.14455 0.44127
O 1.13446 -7.72805 0.06461
O -0.25679 -7.03672 1.70069
C 0.59635 -7.63047 2.70632
H 0.61595 -8.71527 2.54298
C -0.52523 -4.9015 -0.34971
C -0.85277 -4.1433 0.77287
H -2.5307 -4.88322 -1.25668
H -1.49713 -4.65321 1.49483
C 0.06739 -3.1102 1.35313
H -0.37853 -2.63304 2.23228
H 0.98999 -3.60666 1.69452
H 0.36531 -2.33015 0.64278
H 1.6147 -7.24726 2.56538
C 0.02678 -7.26072 4.0465
H 0.64591 -7.68877 4.84357
H 0.00665 -6.17083 4.175
H -0.99415 -7.64503 4.16107

TS-22/23

E(RM06) = -1352.42682468
Zero-point correction= 0.413436 (Hartree/Particle)
Thermal correction to Energy= 0.439478
Thermal correction to Enthalpy= 0.440422
Thermal correction to Gibbs Free Energy= 0.356983
Sum of electronic and zero-point Energies= -1352.013389
Sum of electronic and thermal Energies= -1351.987347
Sum of electronic and thermal Enthalpies= -1351.986403
Sum of electronic and thermal Free Energies= -1352.069842
E(RM06L) = -1353.69529527

C 1.79664 3.49719 0.81248
C 2.93436 2.00651 -0.56839
C 4.04793 2.84209 -0.57945
C 4.01769 4.03317 0.13324
C 2.87394 4.36972 0.84374
H 0.87665 3.71675 1.34746
H 4.9371 2.57179 -1.14171
H 4.88363 4.69125 0.12942
H 2.80559 5.29182 1.41406
C 2.88955 0.72141 -1.29592
C 3.96512 0.24516 -2.04169
C 1.64504 -1.16085 -1.82908
C 3.85562 -0.97416 -2.69639
H 4.88653 0.81526 -2.1134
C 2.67499 -1.69557 -2.58992
H 0.70413 -1.69529 -1.71078

H 4.68981 -1.35466 -3.28147
H 2.54511 -2.65589 -3.08124
Pd 0.20097 1.00105 0.01095
N 1.74174 0.01393 -1.20044
N 1.82486 2.346 0.12692
C -1.9491 -0.22632 -1.55405
C -1.8213 -0.983 -2.72258
C -2.6697 0.97069 -1.5983
C -2.38808 -0.49014 -3.89087
H -1.29828 -1.93819 -2.72093
C -3.23438 1.49003 -2.7499
C -3.07681 0.7313 -3.90528
H -2.30185 -1.06308 -4.81198
H -3.78506 2.42747 -2.73918
H -3.51154 1.08769 -4.83711
C -2.02697 0.7509 0.49775
H -0.74672 1.88209 0.90698
O -2.75954 1.53458 -0.35903
C -2.52169 0.86527 1.91098
O -3.38025 1.64593 2.24242
O -1.90897 0.00183 2.70614
C -2.33317 -0.00932 4.09008
H -3.41306 -0.20003 4.11535
C -1.49453 -0.40109 -0.17608
C -1.20584 -1.76748 0.41112
H -2.0965 -2.06594 0.98602
H -1.14918 -2.46915 -0.4338
C 0.03024 -1.94649 1.28354
H 0.0392 -2.9628 1.69892
H 0.95625 -1.81485 0.70951
H 0.04526 -1.24115 2.12138
H -2.1518 0.98624 4.51407
C -1.54656 -1.08417 4.78476
H -1.86289 -1.1528 5.83219
H -1.71432 -2.05999 4.31069
H -0.47173 -0.86495 4.76577