DFT studies of two-electron oxidation, photochemistry, and radical transfer between metal centres in the formation of platinum(IV) and palladium(IV) selenolates from diphenyldiselenide and metal(II) reactants

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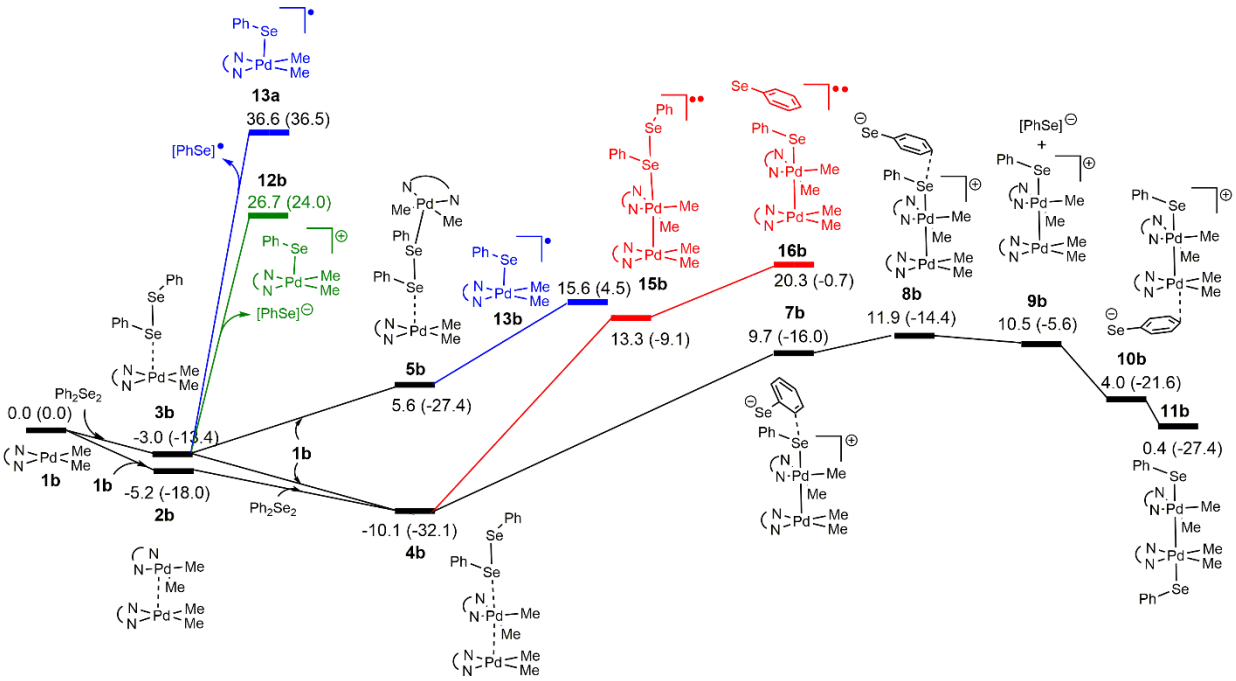
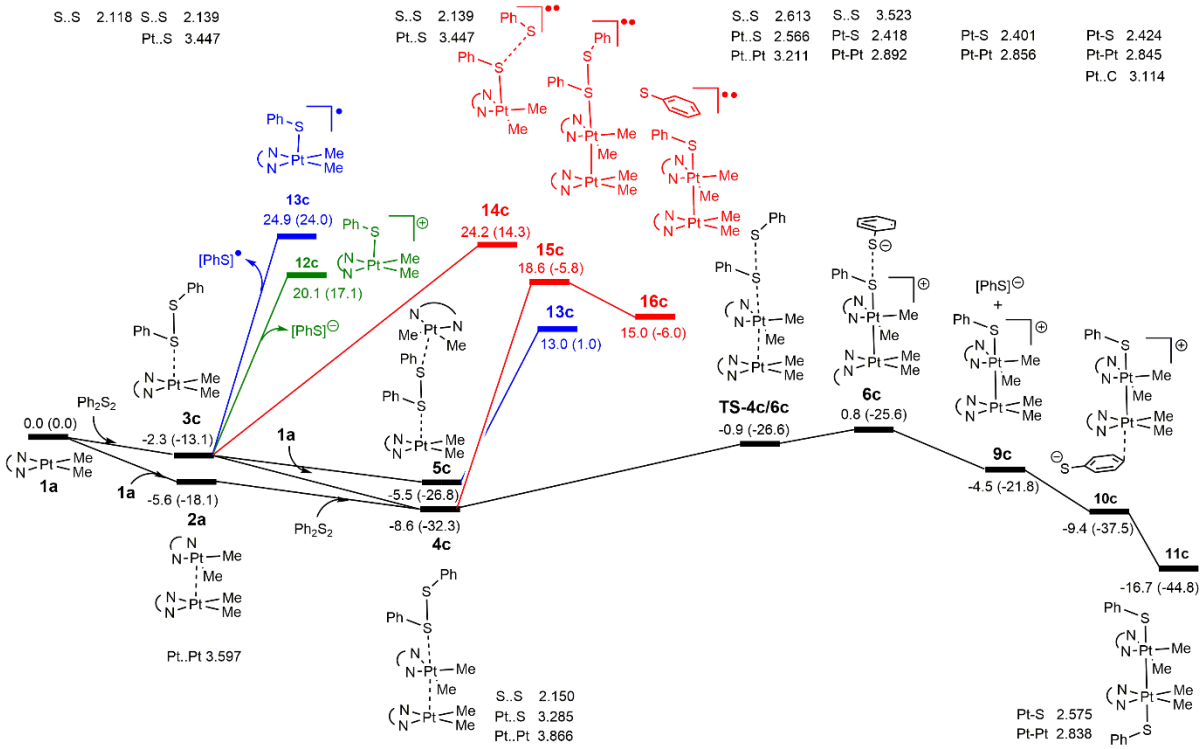
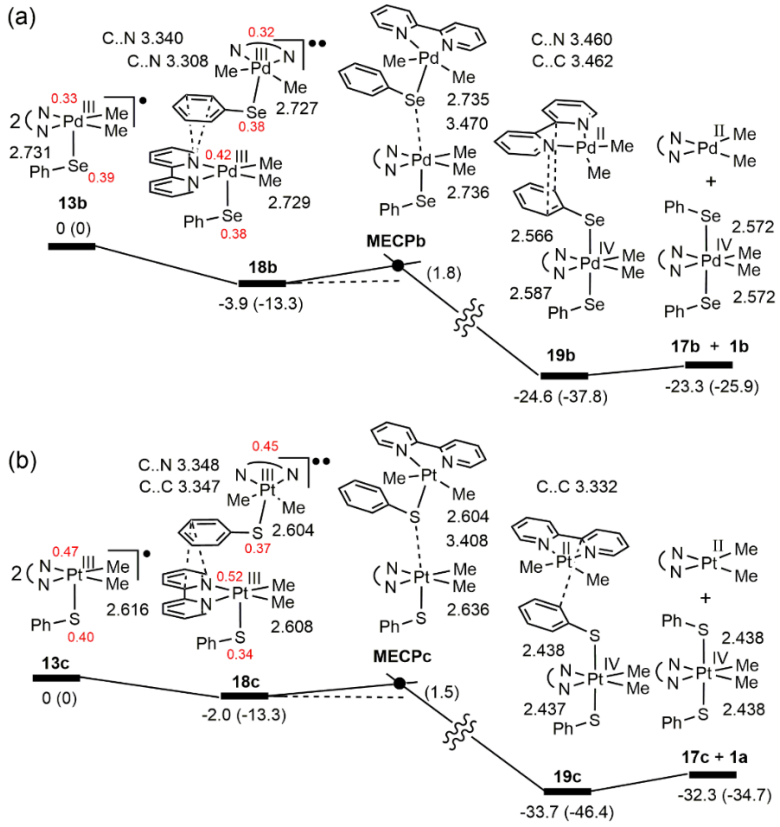
I. **Fig. ESI-1.** Energy profile for the reaction of $Me_2Pd(bipy)$ with Ph_2Se_2 showing high energy species (blue, red, green) omitted from Fig. 1b.
The activation barrier for fragmentation of **5b** to give **13b** is estimated as ΔG 31.9 kcal mol^{-1} using the protocol developed by Hartwig and Hall (J. F. Hartwig, K. S. Cook, M. Hapke, C. D. Incarvito, Y. Fan, C. E. Webster and M. B. Hall, *J. Am. Chem. Soc.*, 2005, **127**, 2538; C. S. Wei, C. A. Jiménez-Hoyos, M. F. Videa, J. F. Hartwig and M. B. Hall, *J. Am. Chem. Soc.*, 2010, **132**, 3078).



II **Fig. ESI-2.** Energy profile for the reaction of $PtMe_2(bipy)$ with Ph_2S_2.

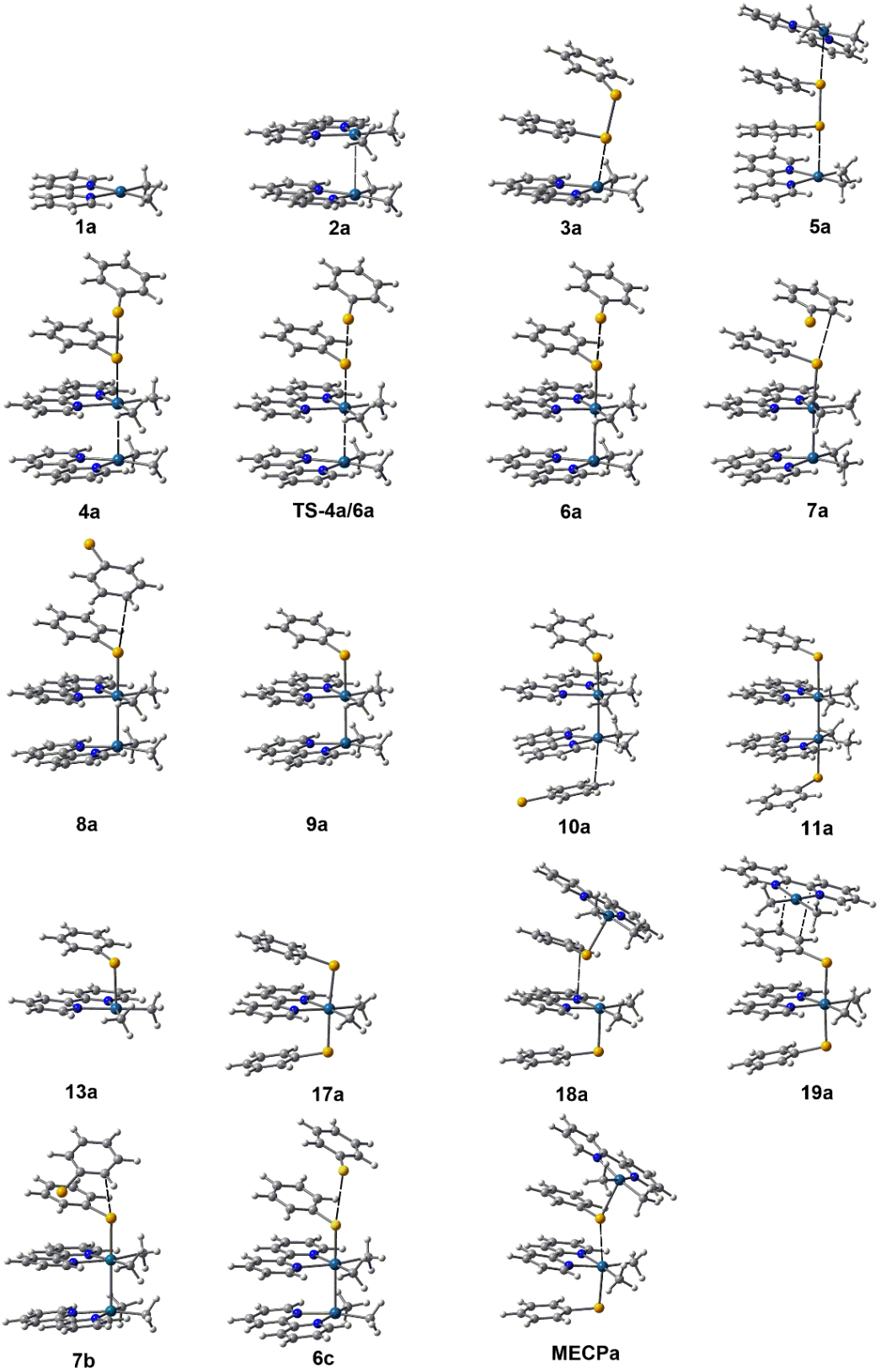


III. **Fig. ESI-3.** Energy profiles for the transformation of doublets $[M^{III}Me_2(bipy)]^{\bullet}$ to $M^{IV}Me_2(bipy)(EPh)_2$ and $M^{II}Me_2(bipy)$ for the (a) Pd/Se system, and (b) the Pt/S system.

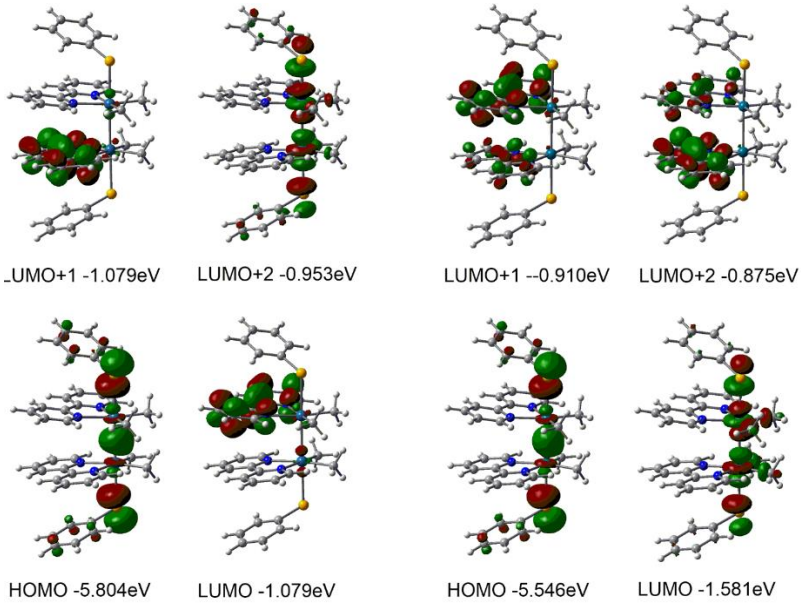


IV. Fig. ESI-4. Gaussview diagrams for structures

Structures are provided for the Pt/Se system (Fig. 1a and Scheme 3), one structure that differs slightly in appearance from these for the Pd/Se system (**7b**, orientation of $PhSe^-$), and structure **6c** for the Pt/S system as this does not have analogues in the Pt/Se and Pd/Se systems.



V. Fig. ESI-5. HOMO and LUMO's for $[PtMe_2(bipy)(SePh)]_2$ (**11a**) and $[PdMe_2(bipy)(SePh)]_2$ (**11b**)



$[PtM4e_2(bipy)(SePh)]_2$ (**11a**) $[PdMe_2(bipy)(SePh)]_2$ (**11b**)

VI. TD-DFT description of the excitation of $[MMe_2(bipy)(SePh)]_2$ (**11a-c**)

$[PtMe_2(bipy)(SePh)]_2$ (**11a**)

Excitation 1: Energy: 445 nm Oscillator Strength: 0.13
HOMO – LUMO Coeff: 0.7

Excitation 2: Energy: 444 nm Oscillator Strength: 0.06
HOMO – LUMO+1 Coeff: 0.7

Excitation 3: Energy: 418 nm Oscillator Strength: 1.75
HOMO – LUMO+2 Coeff: 0.7

Excitation 4: Energy: 402 nm Oscillator Strength: 0.01
HOMO-9 – LUMO+2 Coeff: 0.11
HOMO-8 – LUMO+2 Coeff: 0.13
HOMO-4 – LUMO Coeff: 0.11
HOMO-4 – LUMO+1 Coeff: 0.17
HOMO-4 – LUMO+2 Coeff: 0.27
HOMO-3 – LUMO Coeff: 0.13
HOMO-3 – LUMO+2 Coeff: 0.56

Excitation 5: Energy: 399 nm Oscillator Strength: 0.00
HOMO-6 – LUMO+2 Coeff: 0.11
HOMO-4 – LUMO+1 Coeff: 0.12
HOMO-4 – LUMO+2 Coeff: 0.56
HOMO-3 – LUMO Coeff: 0.18
HOMO-3 – LUMO+1 Coeff: 0.14
HOMO-3 – LUMO+2 Coeff: 0.26

Excitation 6: Energy: 352 nm Oscillator Strength: 0.00
HOMO-6 – LUMO+2 Coeff: 0.13
HOMO-4 – HOMO-1 Coeff: 0.61
HOMO-3 – HOMO-1 Coeff: 0.24

[$PdMe_2(bipy)(SePh)]_2$ (**11b**)

Excitation 1: Energy: 547 nm Oscillator Strength: 1.52
HOMO – LUMO Coeff: 0.7

Excitation 2: Energy: 482 nm Oscillator Strength: 0.00
HOMO-4 – HOMO-1 Coeff: 0.47
HOMO-3 – HOMO-1 Coeff: 0.49

Excitation 3: Energy: 479 nm Oscillator Strength: 0.00
HOMO-4 – HOMO-1 Coeff: 0.49
HOMO-3 – HOMO-1 Coeff: 0.47

Excitation 4: Energy: 460 nm Oscillator Strength: 0.02
HOMO-2 – LUMO+1 Coeff: 0.65
HOMO-2 – LUMO+2 Coeff: 0.24

Excitation 5: Energy: 451 nm Oscillator Strength: 0.04
HOMO-2 – LUMO+1 Coeff: 0.24
HOMO-2 – LUMO+2 Coeff: 0.65

Excitation 6: Energy: 370 nm Oscillator Strength: 0.00
HOMO-16 – LUMO Coeff: 0.12
HOMO-14 – LUMO Coeff: 0.11
HOMO-13 – LUMO Coeff: 0.25
HOMO-11 – LUMO Coeff: 0.13
HOMO-10 – LUMO Coeff: 0.56

[$PtMe_2(bipy)(SPh)]_2$ (**11c**)

Excitation 1: Energy: 458 nm Oscillator Strength: 0.03
HOMO – LUMO Coeff: 0.58
HOMO – LUMO+1 Coeff: 0.38

Excitation 2: Energy: 458 nm Oscillator Strength: 0.02
HOMO – LUMO Coeff: 0.38
HOMO – LUMO+1 Coeff: 0.58

Excitation 3: Energy: 393 nm Oscillator Strength: 1.69
HOMO – LUMO+2 Coeff: 0.69

Excitation 4: Energy: 375 nm Oscillator Strength: 0.00
HOMO-4 – LUMO+2 Coeff: 0.23
HOMO-2 – LUMO+1 Coeff: 0.26
HOMO-1 – LUMO+2 Coeff: 0.576

Excitation 5: Energy: 371 nm Oscillator Strength: 0.01
HOMO-5 – LUMO+2 Coeff: 0.21
HOMO-2 – LUMO+2 Coeff: 0.56
HOMO-1 – LUMO+1 Coeff: 0.31

Excitation 6: Energy: 345 nm Oscillator Strength: 0.00
HOMO-4 – LUMO+2 Coeff: 0.20
HOMO-2 – LUMO+1 Coeff: 0.43
HOMO-1 – LUMO Coeff: 0.47
HOMO-1 – LUMO+2 Coeff: 0.13

VII. Energies of calculated species and Cartesian coordinates

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

1a

E(RM06) = -694.162743930
Zero-point correction= 0.232147 (Hartree/Particle)
Thermal correction to Energy= 0.247050
Thermal correction to Enthalpy= 0.247995
Thermal correction to Gibbs Free Energy= 0.189054
Sum of electronic and zero-point Energies= -693.930597
Sum of electronic and thermal Energies= -693.915694
Sum of electronic and thermal Enthalpies= -693.914749
Sum of electronic and thermal Free Energies= -693.973690
E(RM06) = -694.340714667

N 1.14746300 -1.34124800 -0.32089100
C 0.98003800 -2.64894000 -0.54906700
C 2.00948900 -3.57039500 -0.42974900
C 3.26660600 -3.11085000 -0.05760200
C 3.44606500 -1.75572800 0.18127200
C 2.36715800 -0.88357700 0.04377000
N 1.34842700 1.29758400 0.09452300
C 1.38702600 2.61910800 0.29538700
C 2.53605800 3.29054400 0.68647700
C 3.69763000 2.55385700 0.87779900
C 3.66557000 1.18180700 0.67276600
C 2.47593100 0.57090000 0.27960000
H -0.02397500 -2.95449400 -0.83905600
H 1.82237300 -4.62224300 -0.62664200
H 0.45213600 3.15213100 0.13259100
H 2.51181400 4.36635700 0.83535800
H 4.62149400 3.03848800 1.18405900
H 4.10270900 -3.79809500 0.04630200
C -1.80734600 1.65653500 -0.69897100
H -2.66043100 1.49202500 -0.02071200
H -1.38613100 2.64925200 -0.46608900
H -2.21790200 1.70339400 -1.72072100
H 4.56783800 0.59603600 0.82112800
H 4.42533600 -1.38679900 0.47125100
C -1.92470200 -1.11614200 -1.08412600
H -1.64591600 -1.63734400 -2.01668300
H -2.07143300 -1.88605100 -0.30648700
H -2.89618600 -0.62900600 -1.25486200
Pt -0.42025000 0.15816000 -0.52474400

1b

E(RM06) = -702.683812152
Zero-point correction= 0.231353 (Hartree/Particle)
Thermal correction to Energy= 0.246444
Thermal correction to Enthalpy= 0.247389
Thermal correction to Gibbs Free Energy= 0.188431
Sum of electronic and zero-point Energies= -702.452459
Sum of electronic and thermal Energies= -702.437368
Sum of electronic and thermal Enthalpies= -702.436424
Sum of electronic and thermal Free Energies= -702.495381
E(RM06) = -702.889819315

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C 2.01429300 -3.57189300 -0.43572400
C 3.26772100 -3.10875700 -0.05765500
C 3.44371400 -1.75279900 0.18195200
C 2.36221400 -0.88371400 0.03909500
N 1.35271000 1.30601300 0.08356900
C 1.39768700 2.62513000 0.28395300
C 2.54649400 3.29359100 0.68470300
C 3.70099400 2.54944500 0.88609900
C 3.66335500 1.17718500 0.68022400
C 2.47246200 0.57409600 0.27655300
H -0.01790500 -2.95846300 -0.85296400
H 1.83062700 -4.62425300 -0.63352600
H 0.46697200 3.16475000 0.11393500
H 2.52733400 4.36959500 0.83346400

H 4.62508900 3.02825000 1.20123700
H 4.10518600 -3.79392400 0.05058600
C -1.83272700 1.64086000 -0.70495200
H -2.67839100 1.47102200 -0.02241800
H -1.37970100 2.61619800 -0.46226400
H -2.23290900 1.68898500 -1.72844800
Pd -0.43313700 0.16275900 -0.53132000
H 4.56184500 0.58788700 0.83733800
H 4.42164100 -1.38360800 0.47613700
C -1.94088900 -1.10092900 -1.07628100
H -1.62935300 -1.61733600 -1.99937900
H -2.05379800 -1.85184200 -0.27674900
H -2.91666400 -0.62993900 -1.25274400

2a
E(RM06) = -1388.34635298
Zero-point correction= 0.466082 (Hartree/Particle)
Thermal correction to Energy= 0.497093
Thermal correction to Enthalpy= 0.498037
Thermal correction to Gibbs Free Energy= 0.403019
Sum of electronic and zero-point Energies= -1387.880271
Sum of electronic and thermal Energies= -1387.849260
Sum of electronic and thermal Enthalpies= -1387.848316
Sum of electronic and thermal Free Energies= -1387.943334
E(RM06) = -1388.71233308

N 0.70595800 -1.50394500 -0.37766500
C 0.34892600 -2.76867200 -0.62665300
C 1.23460500 -3.83304400 -0.53414600
C 2.55053200 -3.56797600 -0.17590900
C 2.92637400 -2.25776100 0.08829500
C 1.98129500 -1.23724000 -0.01004500
N 1.28892600 1.06431800 0.10170700
C 1.49570800 2.35000700 0.40439500
C 2.69932800 2.82409200 0.90655700
C 3.73652200 1.91993400 1.09920700
C 3.52783900 0.58273300 0.79186700
C 2.28944600 0.17426000 0.29712000
H -0.69280500 -2.92120100 -0.90834400
H 0.89211700 -4.84326700 -0.74234600
H 0.65334800 3.01879900 0.23640500
H 2.81240200 3.87956900 1.13808600
H 4.69727000 2.24759200 1.48903600
H 3.27971100 -4.37098700 -0.09846000
C -1.68765200 1.94412200 -0.88968200
H -2.45624600 2.03770200 -0.10422700
H -1.05000600 2.84401800 -0.84370100
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H 4.32557000 -0.13684800 0.95349200
H 3.95201700 -2.04024800 0.37302800
C -2.27891200 -0.77327500 -1.25667600
H -2.14258900 -1.14264000 -2.28824600
H -2.45920400 -1.65146900 -0.61047900
H -3.19429000 -0.16131200 -1.24312900
C -0.81186300 -2.77956400 2.59969900
C -3.00476300 -2.23391900 2.07144700
C -3.30814500 -3.54541500 1.73499900
C -2.30642300 -4.50308200 1.83960000
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C 1.80033000 -0.43471400 3.57827100
C 2.92247400 -1.21715700 3.81367900
C 2.80994100 -2.59359100 3.66596500
C 1.58988800 -3.13107200 3.27769400
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H -4.30807900 -3.80131900 1.39581700
H -2.49936800 -5.54182200 1.58247800
H -0.25316800 -4.85338700 2.35062000
H 1.83661000 0.64886200 3.68618100
H 3.85807000 -0.74852000 4.10760700
H 3.66087700 -3.24579300 3.84780200
H 1.48978100 -4.20625500 3.15863400
N -1.79328200 -1.85531300 2.49368600
N 0.62075900 -0.94522800 3.21147100
C -3.08609400 1.04224600 2.69933600

H -3.49348800 0.78777700 1.70542100
H -3.77772100 0.63444500 3.45785800
H -3.10298400 2.13930500 2.78931900
C -0.57424800 2.10691800 3.33598600
H -0.75724300 2.76725900 2.47133300
H -1.10470200 2.54987000 4.19501800
H 0.50711900 2.14413600 3.55571000
Pt -1.22658500 0.20497200 2.92739800
Pt -0.60339800 0.22467600 -0.61475100

2b
E(RM06) = -1405.38961879
Zero-point correction= 0.464592 (Hartree/Particle)
Thermal correction to Energy= 0.495851
Thermal correction to Enthalpy= 0.496796
Thermal correction to Gibbs Free Energy= 0.402204
Sum of electronic and zero-point Energies= -1404.925027
Sum of electronic and thermal Energies= -1404.893767
Sum of electronic and thermal Enthalpies= -1404.892823
Sum of electronic and thermal Free Energies= -1404.987415
E(RM06) = -1405.81030914

N 0.66780700 -1.47476500 -0.34579400
C 0.29520200 -2.73269800 -0.59138400
C 1.16713300 -3.81074200 -0.50482600
C 2.48560700 -3.56094800 -0.14783600
C 2.87931200 -2.25470100 0.11301000
C 1.94642200 -1.22260500 0.01140800
N 1.30973800 1.10057600 0.09237400
C 1.54951400 2.38299800 0.37395700
C 2.76558800 2.83774600 0.86731700
C 3.77790900 1.90975500 1.07415000
C 3.53486100 0.57304400 0.78858000
C 2.28497900 0.18972200 0.30079800
H -0.75102700 -2.87425400 -0.86567700
H 0.81200500 -4.81693100 -0.71210600
H 0.72487700 3.07223000 0.19653300
H 2.90644900 3.89358300 1.08158900
H 4.74726600 2.21815100 1.45882600
H 3.20515700 -4.37279000 -0.06987500
C -1.69292300 2.00176900 -0.90657400
H -2.50185700 2.09563800 -0.16670500
H -1.02288000 2.87232500 -0.80934500
H -2.14422600 2.02231800 -1.90992500
Pd -0.62912800 0.28539300 -0.58070600
H 4.31470100 -0.16281900 0.96367800
H 3.90871900 -2.05182500 0.39486600
C -2.32531300 -0.67534200 -1.19819400
H -2.17542000 -1.04346200 -2.22678300
H -2.47278900 -1.54349700 -0.53300600
H -3.23671800 -0.06216200 -1.17762500
C -0.78965300 -2.81263700 2.60771200
C -2.98964000 -2.31191500 2.08286100
C -3.26850600 -3.62787300 1.73770800
C -2.24710900 -4.56419900 1.84043000
C -0.99599200 -4.15324000 2.28018700
C 0.52360500 -2.29549800 3.05498600
C 1.80782900 -0.43107400 3.53929100
C 2.92418000 -1.20341200 3.83499700
C 2.81069900 -2.58396900 3.73981200
C 1.59783600 -3.13567900 3.34725200
H -3.75302100 -1.53676100 2.01618000
H -4.26209600 -3.90307200 1.39476900
H -2.41781700 -5.60547800 1.57723000
H -0.18544300 -4.87388200 2.34593900
H 1.84477700 0.65666200 3.60716100
H 3.85312000 -0.72532800 4.13501600
H 3.65472900 -3.22985800 3.97049600
H 1.49531100 -4.21515600 3.27977800
N -1.78863100 -1.91094700 2.50747300
N 0.63953800 -0.95275500 3.16056000
Pd -1.23539300 0.18454500 2.86204500
C -3.10859700 0.99373100 2.73770400
H -3.47311900 0.84826000 1.70782600
H -3.76213800 0.43275500 3.42700700

H -3.17645600 2.06256700 2.98219900
C -0.59845400 2.10542300 3.16582400
H -0.98067400 2.77655100 2.38285600
H -0.93368700 2.49399000 4.13992500
H 0.50441000 2.12944100 3.13380700

3a
E(RM06) = -1175.76410207
Zero-point correction= 0.414725 (Hartree/Particle)
Thermal correction to Energy= 0.444722
Thermal correction to Enthalpy= 0.445666
Thermal correction to Gibbs Free Energy= 0.349643
Sum of electronic and zero-point Energies= -1175.349378
Sum of electronic and thermal Energies= -1175.319380
Sum of electronic and thermal Enthalpies= -1175.318436
Sum of electronic and thermal Free Energies= -1175.414459
E(RM06) = -1176.12149807

N -2.18788800 0.96685000 -1.23479300
C -1.94031600 1.78403600 -2.26306300
C -2.23732300 3.13868700 -2.23355600
C -2.81713400 3.66089700 -1.08463800
C -3.07475300 2.81628100 -0.01374100
C -2.74883800 1.46441600 -0.11094400
N -2.73224500 -0.79683400 0.71866700
C -2.90539100 -1.70916600 1.67985300
C -3.34843200 -1.38550900 2.95412200
C -3.61449900 -0.05199800 3.23969700
C -3.43129000 0.90006500 2.24716000
C -2.98692300 0.50324500 0.98663000
H -1.48487900 1.32272500 -3.13824400
H -2.01837500 3.76199800 -3.09597200
H -2.67273800 -2.73772500 1.40859700
H -3.47367600 -2.16499300 3.70031900
H -3.95599500 0.24817100 4.22742800
H -3.07033900 4.71635300 -1.01929600
C -1.72021000 -3.24474400 -1.24121500
H -0.70457900 -3.60439200 -1.46553600
H -2.01247600 -3.65643400 -0.26109700
H -2.39477700 -3.66996600 -2.00218100
H -3.61605000 1.94791100 2.46545400
H -3.53460400 3.21342200 0.88651500
C -0.99217500 -1.30202400 -3.12444600
H -1.74965000 -1.07139500 -3.89310600
H -0.18878700 -0.54940400 -3.19910100
H -0.55546100 -2.28281900 -3.36122300
Se 0.76005800 -1.33106000 0.05117300
Se 3.09836900 -1.59159200 1.18471500
C 3.93745300 -0.10772900 0.25082300
C 4.39269400 -0.26252300 -1.06203100
C 4.04532900 1.13427100 0.88064800
C 4.95343900 0.81848600 -1.73531000
H 4.29718100 -1.22916000 -1.55650700
C 4.61810800 2.21015200 0.20562000
H 3.66281000 1.26256000 1.89341500
C 5.06864400 2.05536800 -1.10193700
H 5.30421300 0.69401600 -2.75870800
H 4.69705800 3.17679100 0.70110700
H 5.50869100 2.89895900 -1.63100200
C 0.59329100 0.52155600 0.64023700
C 0.14725600 0.81744500 1.92951400
C 0.93777200 1.55204400 -0.23455500
C 0.04774000 2.14378700 2.34064100
H -0.11775200 0.00829900 2.61143400
C 0.83003000 2.87814700 0.17883900
H 1.29512500 1.31499500 -1.23780700
C 0.38779400 3.17460100 1.46542100
H -0.30304500 2.37210600 3.34633700
H 1.10049800 3.68058500 -0.50632400
H 0.30752000 4.21116800 1.78855300
Pt -1.84397400 -1.19556000 -1.26328000

3b
E(RM06) = -1184.28500434
Zero-point correction= 0.413431 (Hartree/Particle)

Thermal correction to Energy= 0.443757
Thermal correction to Enthalpy= 0.444701
Thermal correction to Gibbs Free Energy= 0.348128
Sum of electronic and zero-point Energies= -1183.871573
Sum of electronic and thermal Energies= -1183.841247
Sum of electronic and thermal Enthalpies= -1183.840303
Sum of electronic and thermal Free Energies= -1183.936876
E(RM06) = -1184.67081345

N -2.16870800 0.95793900 -1.27238400
C -1.90862900 1.75917600 -2.30747400
C -2.15122300 3.12587300 -2.28353200
C -2.68408700 3.67585600 -1.12515500
C -2.95522400 2.84694000 -0.04508200
C -2.69282600 1.48073500 -0.14475300
N -2.72183400 -0.77166100 0.71829900
C -2.92305000 -1.66457200 1.68969400
C -3.38152000 -1.31850100 2.95361600
C -3.63814400 0.02201400 3.21233000
C -3.42698100 0.95615400 2.20819900
C -2.96157100 0.53402700 0.96264400
H -1.48478300 1.27732700 -3.18836400
H -1.92469000 3.73612700 -3.15342100
H -2.70150600 -2.70140000 1.43820500
H -3.52853200 -2.08447300 3.70991700
H -3.99569600 0.34195500 4.18825200
H -2.88885600 4.74184100 -1.05805000
C -1.69537700 -3.25938500 -1.22408900
H -0.68508300 -3.62552900 -1.45095300
H -1.98424800 -3.61828300 -0.22336300
H -2.39006900 -3.67699700 -1.96853000
Pd -1.81795800 -1.21654900 -1.25741400
H -3.61030200 2.00809500 2.40692700
H -3.37447800 3.27012400 0.86315000
C -0.99203100 -1.36712500 -3.11733200
H -1.77691400 -1.12214200 -3.85136600
H -0.19236500 -0.61118200 -3.17654700
H -0.56815100 -2.34937200 -3.36090300
Se 0.81752000 -1.35865700 0.03039400
Se 3.14832200 -1.59974200 1.12289400
C 3.94941100 -0.08523500 0.20498500
C 4.41163400 -0.21712700 -1.10779700
C 4.01882100 1.15337200 0.84645500
C 4.94242300 0.88512800 -1.77035100
H 4.34508300 -1.18191800 -1.61037900
C 4.56107000 2.25101600 0.18120000
H 3.63115600 1.26180200 1.85962000
C 5.01933200 2.11945000 -1.12616800
H 5.29955500 0.77974100 -2.79361200
H 4.61080000 3.21546800 0.68447600
H 5.43579000 2.97986100 -1.64711200
C 0.59634600 0.46887200 0.67375200
C 0.16119700 0.71165700 1.97767300
C 0.88188400 1.53482300 -0.17984700
C 0.01059000 2.02135000 2.42418400
H -0.05931300 -0.12551200 2.64119400
C 0.71859400 2.84386100 0.26804300
H 1.23253300 1.33792500 -1.19417100
C 0.28377300 3.08741200 1.56806800
H -0.33261900 2.20898900 3.44081600
H 0.93796600 3.67475100 -0.40114600
H 0.15946900 4.11106700 1.91761500

3c
E(RM06) = -1961.93469979
Zero-point correction= 0.416649 (Hartree/Particle)
Thermal correction to Energy= 0.445745
Thermal correction to Enthalpy= 0.446689
Thermal correction to Gibbs Free Energy= 0.353021
Sum of electronic and zero-point Energies= -1952.996879
Sum of electronic and thermal Energies= -1952.967784
Sum of electronic and thermal Enthalpies= -1952.966839
Sum of electronic and thermal Free Energies= -1953.060508
E(RM06) = -1953.79720682

N -2.46125200 1.03073100 -1.22242400
C -2.31106900 1.89567500 -2.22803100
C -2.70741500 3.22378000 -2.14856300
C -3.28749000 3.66524000 -0.96629200
C -3.43890200 2.77283600 0.08586700
C -3.01191000 1.45339000 -0.06577900
N -2.79215600 -0.82010100 0.70542300
C -2.85193300 -1.75883000 1.65269500
C -3.25286600 -1.49746300 2.95578200
C -3.60238300 -0.19392300 3.28475800
C -3.53800500 0.78853700 2.30681000
C -3.12732900 0.44997100 1.01714100
H -1.85345500 1.49682700 -3.13335800
H -2.56564800 3.88754400 -2.99707100
H -2.56059000 -2.76321600 1.34658700
H -3.28337200 -2.29916000 3.68845000
H -3.91720700 0.06045900 4.29418000
H -3.62077400 4.69501900 -0.85996600
C -1.70355400 -3.13830400 -1.38226900
H -0.64678600 -3.38507500 -1.55699000
H -2.01155600 -3.57568300 -0.41792000
H -2.30090100 -3.59975400 -2.18284300
Pd -1.98365500 -1.11365900 -1.32980900
H -3.78754800 1.81535000 2.55910700
H -3.89678000 3.10742300 1.01236000
C -1.22884900 -1.13577500 -3.22754600
H -2.02089800 -0.80706100 -3.92060900
H -0.40677000 -0.40067000 -3.25892000
H -0.84411700 -2.10500500 -3.57108500
C 3.74565600 -0.22487200 0.23731300
C 4.25087900 -0.59498900 -1.01244900
C 3.97029000 1.06276300 0.73015900
C 4.97805700 0.32157400 -1.76255900
H 4.06248300 -1.59873300 -1.39194400
C 4.70827200 1.97336300 -0.02159000
H 3.55371200 1.34822600 1.69602900
C 5.20909200 1.60447500 -1.26664900
H 5.37037700 0.03399800 -2.73641100
H 4.88299500 2.97647900 0.36340300
H 5.78068400 2.31915300 -1.85613100
C 0.51360300 0.50046800 0.57759700
C 0.03422800 0.86294400 1.83884000
C 0.73909500 1.47808100 -0.39342600
C -0.22510100 2.19920300 2.12132200
H -0.13328900 0.09327100 2.59301900
C 0.46884800 2.81379600 -0.10879100
H 1.12926100 1.18543300 -1.36895400
C -0.01436100 3.17411300 1.14613300
H -0.60406600 2.48029500 3.10303900
H 0.64051100 3.57455000 -0.86866600
H -0.22528200 4.21900600 1.36826300
S 0.88446600 -1.20387900 0.19342300
S 2.76738400 -1.36525600 1.19868100

4a

E(RM06) = -1869.95326365
Zero-point correction= 0.649402 (Hartree/Particle)
Thermal correction to Energy= 0.695360
Thermal correction to Enthalpy= 0.696304
Thermal correction to Gibbs Free Energy= 0.565538
Sum of electronic and zero-point Energies= -1869.303861
Sum of electronic and thermal Energies= -1869.257904
Sum of electronic and thermal Enthalpies= -1869.256960
Sum of electronic and thermal Free Energies= -1869.387726
E(RM06) = -1870.49229387

N -3.74862800 1.08515300 -0.23458700
C -3.64497900 2.36741700 -0.59901300
C -3.90436200 3.41963500 0.26812300
C -4.28990600 3.12266800 1.56931400
C -4.39830700 1.79265400 1.95360600
C -4.11877500 0.78451600 1.03185200
N -3.92454900 -1.52294200 0.37122100
C -3.94922000 -2.83496400 0.62654800
C -4.24653200 -3.35507500 1.87829300

C -4.53619900 -2.46920900 2.90870800
C -4.51197700 -1.10582900 2.65049300
C -4.19606300 -0.65228500 1.37004300
H -3.33950200 2.54537900 -1.63005700
H -3.79997600 4.44486900 -0.07707000
H -3.71656200 -3.48792800 -0.21285600
H -4.24959300 -4.43040900 2.03263300
H -4.77649800 -2.83209700 3.90510200
H -4.50438100 3.91546000 2.28185500
C -3.42136600 -2.28540100 -2.77722000
H -2.42927200 -2.41134000 -3.23655700
H -3.65029000 -3.20193000 -2.20699500
H -4.15811900 -2.20808600 -3.59350900
H -4.72608400 -0.40378000 3.45121100
H -4.69745500 1.55022900 2.96934100
C -3.18522700 0.44571400 -3.31585000
H -4.12424300 0.95619800 -3.59314900
H -2.41633600 1.22245700 -3.16140900
H -2.87205400 -0.16849100 -4.17326400
C -0.43116100 2.07819100 0.07746800
C 0.00668900 1.95034400 -2.19841200
C 0.06692200 3.33117600 -2.32266900
C -0.11825600 4.10239500 -1.18204900
C -0.36239400 3.47039000 0.02916100
C -0.72159200 1.33551500 1.32375400
C -1.04576700 -0.73479000 2.31889200
C -1.22046100 -0.16843900 3.57439900
C -1.14381200 1.21410000 3.68791700
C -0.89177900 1.97237400 2.55284700
H 0.15865600 1.29705200 -3.05689100
H 0.26047100 3.78244100 -3.29169300
H -0.07201500 5.18769800 -1.23068600
H -0.51289000 4.06595900 0.92519300
H -1.09160100 -1.81458500 2.17708900
H -1.41403700 -0.80324700 4.43490900
H -1.27411600 1.70126000 4.65131100
H -0.81884300 3.05320900 2.63379700
N -0.23644600 1.34024400 -1.03500000
N -0.81120700 -0.00871500 1.22382100
C 0.19730100 -1.34495000 -2.70824800
H -0.60176900 -1.02547100 -3.39460700
H 1.12888700 -0.81395400 -2.96149400
H 0.36962800 -2.42161600 -2.84637800
C -0.56756300 -2.86907200 -0.47203500
H -1.42457500 -3.23433500 -1.05685800
H 0.32172900 -3.44111500 -0.77540000
H -0.75301200 -3.07120400 0.59542000
Se 2.17802200 -1.31876500 0.04896000
Se 4.77533800 -2.06626600 0.94368000
C 2.58084000 0.53579000 0.50154700
C 2.98058400 1.42467300 -0.49807500
C 2.46037300 0.98407600 1.81855900
C 3.23838200 2.75695400 -0.18506100
H 3.08307300 1.07123700 -1.52493000
C 2.73158900 2.31403000 2.13117400
H 2.15421200 0.28773000 2.60078800
C 3.11485100 3.20332200 1.12888500
H 3.54432000 3.44652600 -0.97107500
H 2.63291000 2.65750500 3.16039700
H 3.32013200 4.24446700 1.37293900
C 5.72326100 -0.65536400 0.00829900
C 5.92615200 -0.72464700 -1.37549400
C 6.19576200 0.46121500 0.70694700
C 6.58999700 0.30094600 -2.04305200
H 5.55472800 -1.58725700 -1.92966100
C 6.86751100 1.48062200 0.03732800
H 6.02585500 0.53307100 1.78151700
C 7.06516500 1.40632500 -1.33936200
H 6.74010000 0.23355600 -3.12008700
H 7.23101100 2.34288500 0.59554900
H 7.58728100 2.20584200 -1.86258000
Pt -0.35803300 -0.84730900 -0.79604700
Pt -3.47642400 -0.61696700 -1.58451400

4b
E(RM06) = -1886.99354342
Zero-point correction= 0.646266 (Hartree/Particle)
Thermal correction to Energy= 0.693196
Thermal correction to Enthalpy= 0.694140
Thermal correction to Gibbs Free Energy= 0.560151
Sum of electronic and zero-point Energies= -1886.347277
Sum of electronic and thermal Energies= -1886.300347
Sum of electronic and thermal Enthalpies= -1886.299403
Sum of electronic and thermal Free Energies= -1886.433393
E(RM06) = -1887.59245179

N -3.80013200 1.14817300 -0.20777500
C -3.70123600 2.43291200 -0.55558300
C -3.96209100 3.47667200 0.32312400
C -4.34790600 3.16177100 1.61952200
C -4.44919000 1.82667800 1.98909500
C -4.16217600 0.83146700 1.05474600
N -3.94895600 -1.47300100 0.37987800
C -3.93577200 -2.78353700 0.63343800
C -4.18888600 -3.31558300 1.89115600
C -4.47474500 -2.43768100 2.92902300
C -4.48552100 -1.07309500 2.67385900
C -4.21044300 -0.61143500 1.38621100
H -3.39626400 2.62516100 -1.58507800
H -3.86007700 4.50662900 -0.00885000
H -3.71057100 -3.43074700 -0.21357600
H -4.16314300 -4.39102700 2.04366400
H -4.68324700 -2.80732000 3.93031100
H -4.56711200 3.94509500 2.34133400
C -3.52389200 -2.18630400 -2.81128400
H -2.52254400 -2.31493100 -3.24744300
H -3.77318800 -3.08494400 -2.22258100
H -4.25026000 -2.09335000 -3.63241200
Pd -3.55356400 -0.54761300 -1.58853700
H -4.69208300 -0.37859600 3.48322500
H -4.74715700 1.57253700 3.00235000
C -3.27810000 0.52099100 -3.31059200
H -4.21478300 1.05585500 -3.54002100
H -2.48753400 1.26502900 -3.11413600
H -2.98938700 -0.07321500 -4.18792500
C -0.44780200 2.04704600 0.05303200
C 0.01365600 1.95407700 -2.21502900
C 0.01154600 3.33761100 -2.33389100
C -0.21431000 4.09255100 -1.18963000
C -0.44002000 3.44213500 0.01567400
C -0.72439500 1.28419600 1.29290600
C -0.99969700 -0.79663600 2.27024800
C -1.20465900 -0.24607200 3.52918000
C -1.17007300 1.13721100 3.65194800
C -0.92822000 1.90944900 2.52365100
H 0.20057100 1.31427800 -3.07778200
H 0.18924000 3.80326800 -3.29936000
H -0.21593700 5.17936700 -1.23113700
H -0.62386500 4.02595500 0.91344900
H -1.01553400 -1.87701500 2.12148300
H -1.39087700 -0.89200800 4.38328100
H -1.32625100 1.61471000 4.61657300
H -0.89136200 2.99172900 2.61186200
N -0.20673600 1.32517100 -1.05890500
N -0.77129000 -0.06019600 1.18237100
Pd -0.26134600 -0.86821000 -0.83065500
C 0.33187300 -1.34710200 -2.72666400
H -0.49196700 -1.05925400 -3.39826200
H 1.22611800 -0.74473800 -2.95179400
H 0.57042700 -2.40760900 -2.87829000
C -0.46343500 -2.89313200 -0.57212000
H -1.28331500 -3.23976400 -1.21851800
H 0.44701800 -3.45375400 -0.82399400
H -0.72065500 -3.08559000 0.48232300
Se 2.38708800 -1.38541100 0.12597400
Se 4.77463100 -2.01943800 1.06351100
C 2.65265800 0.50093200 0.53937200
C 3.01595400 1.38318200 -0.47906700
C 2.48051500 0.97158700 1.84226900

C 3.19347400 2.73528800 -0.19640800
H 3.15694800 1.00914100 -1.49384700
C 2.66890300 2.32219600 2.12287600
H 2.19861700 0.27854900 2.63627200
C 3.02000300 3.20552000 1.10320100
H 3.47268200 3.42215000 -0.99437000
H 2.53085000 2.68671600 3.14014700
H 3.16190600 4.26237300 1.32356600
C 5.75982400 -0.67163100 0.07068300
C 6.01705200 -0.83665500 -1.29378400
C 6.19001700 0.48812000 0.72051400
C 6.69786400 0.15186400 -1.99833000
H 5.67406500 -1.73742200 -1.80299300
C 6.88082800 1.46910000 0.01303100
H 5.96987800 0.62699400 1.77890300
C 7.13227800 1.30500700 -1.34632600
H 6.89299900 0.01919100 -3.06153200
H 7.21324200 2.37053500 0.52597100
H 7.66650500 2.07548600 -1.89972800

4c

E(RM06) = -2647.59894893
Zero-point correction= 0.650635 (Hartree/Particle)
Thermal correction to Energy= 0.695861
Thermal correction to Enthalpy= 0.696805
Thermal correction to Gibbs Free Energy= 0.567833
Sum of electronic and zero-point Energies= -2646.948314
Sum of electronic and thermal Energies= -2646.903088
Sum of electronic and thermal Enthalpies= -2646.902144
Sum of electronic and thermal Free Energies= -2647.031116
E(RM06) = -2648.17073179

N -3.49222000 0.92618900 -1.14606200
C -3.64424500 1.53108000 -2.32933500
C -3.84504100 2.89819000 -2.45590000
C -3.88455100 3.66952200 -1.30117100
C -3.72414500 3.04863100 -0.06995000
C -3.53123400 1.66830000 -0.01472800
N -3.27925200 -0.41580400 1.16282600
C -3.12019400 -1.13583300 2.27800300
C -3.05456000 -0.56606700 3.54162300
C -3.14657200 0.81619100 3.64742100
C -3.30309400 1.57086400 2.49314100
C -3.36957900 0.93114200 1.25593000
H -3.60330500 0.88068500 -3.20215000
H -3.96568600 3.34018800 -3.44120100
H -3.03798200 -2.21255200 2.14079800
H -2.92708000 -1.19827400 4.41623900
H -3.09153100 1.30692800 4.61665000
H -4.04130300 4.74426500 -1.35389800
C -3.17545500 -3.23700900 -0.46570900
H -2.17240000 -3.61676200 -0.72310200
H -3.35100000 -3.45390100 0.60207900
H -3.90660700 -3.82292000 -1.04584300
H -3.36472300 2.65325400 2.56361600
H -3.76123600 3.64066500 0.84024100
C -3.29947700 -1.76081000 -2.85183200
H -4.28650800 -1.55973000 -3.30425900
H -2.55448700 -1.15438200 -3.39872000
H -3.06182100 -2.82013700 -3.03428700
C -0.09689200 1.66442200 -0.62511500
C 0.12261000 0.17746100 -2.39138500
C -0.11226400 1.17121900 -3.33089200
C -0.36009600 2.46161300 -2.87794400
C -0.35084900 2.71008400 -1.51251100
C -0.05324700 1.85072600 0.84001100
C 0.18270400 0.84277200 2.91401700
C 0.12548200 2.06130800 3.57573600
C -0.03730300 3.21596100 2.82006200
C -0.12918700 3.10823400 1.43969100
H 0.31197900 -0.85266400 -2.69098400
H -0.10685500 0.92940100 -4.39044700
H -0.56206000 3.26934500 -3.57814600
H -0.54793200 3.71422800 -1.14650200
H 0.30689000 -0.09055100 3.46190500

H 0.20587900 2.09514800 4.65894100
H -0.08582400 4.19216500 3.29682100
H -0.23376200 4.00448600 0.83397400
N 0.12920200 0.41132400 -1.07542900
N 0.09341600 0.73112500 1.58490200
C 0.67602900 -2.71530400 -0.81733800
H -0.13587200 -2.78077600 -1.56240600
H 1.62451600 -2.55512900 -1.36146900
H 0.74147300 -3.69160200 -0.31249600
C 0.39968000 -2.51930300 1.96044600
H -0.41406200 -3.25502400 1.83813700
H 1.35012000 -3.07735300 1.96472000
H 0.28102300 -2.05230300 2.95433900
C 3.37174600 0.75749600 0.31570300
C 3.42957500 0.65529800 -1.07532600
C 3.26191300 2.01149900 0.92076800
C 3.35998400 1.80343900 -1.85927400
H 3.52888400 -0.32801700 -1.53684000
C 3.20177500 3.15662200 0.13411900
H 3.22855900 2.08290000 2.00834000
C 3.24342700 3.05317000 -1.25604300
H 3.39747300 1.72062100 -2.94450900
H 3.11085500 4.13323200 0.60784200
H 3.18977800 3.95082600 -1.87002800
C 6.36908100 -0.62598900 0.36609300
C 6.57165200 -1.86058700 -0.25766100
C 6.79062800 0.55036300 -0.25888900
C 7.19453800 -1.91429600 -1.49912000
H 6.23152600 -2.77190600 0.23318500
C 7.42192500 0.48963000 -1.49825800
H 6.61025200 1.50994000 0.22542400
C 7.62179700 -0.74022300 -2.11868000
H 7.35143900 -2.87599700 -1.98450000
H 7.75014900 1.40712000 -1.98360200
H 8.11080400 -0.78623300 -3.09015400
Pt 0.34008700 -1.13378000 0.44839100
Pt -3.29254500 -1.22942200 -0.86977500
S 3.48659200 -0.72831800 1.30173800
S 5.53066600 -0.52290100 1.93656800

5a
E(RM06) = -1869.94297252
Zero-point correction= 0.648197 (Hartree/Particle)
Thermal correction to Energy= 0.694810
Thermal correction to Enthalpy= 0.695754
Thermal correction to Gibbs Free Energy= 0.561270
Sum of electronic and zero-point Energies= -1869.294776
Sum of electronic and thermal Energies= -1869.248163
Sum of electronic and thermal Enthalpies= -1869.247218
Sum of electronic and thermal Free Energies= -1869.381703
E(RM06) = -1870.48748698

N -4.89127300 1.11894500 -0.42682000
C -5.12702000 2.10774800 -1.29542500
C -5.39160800 3.41019900 -0.89810400
C -5.40826600 3.69388200 0.46164900
C -5.15592800 2.67285700 1.36681300
C -4.89809300 1.38537100 0.89818700
N -4.43199200 -0.95565500 1.20677500
C -4.13671300 -2.01542900 1.96624000
C -4.01425000 -1.94428400 3.34618300
C -4.20504000 -0.71334400 3.96250800
C -4.50496300 0.39166700 3.17957800
C -4.61001700 0.24820700 1.79631700
H -5.10048700 1.83042900 -2.34832700
H -5.58034800 4.17787100 -1.64339400
H -3.99183400 -2.95520900 1.43610200
H -3.77292500 -2.83669800 3.91685900
H -4.11645600 -0.61080800 5.04141300
H -5.61343300 4.70051400 0.81819000
C -4.22814100 -2.94597400 -1.39628100
H -3.38032800 -3.09876200 -2.08295800
H -4.02273100 -3.52794800 -0.48167600
H -5.11857800 -3.38247400 -1.87843100
H -4.63771500 1.36292800 3.64746800

H -5.16528500 2.88434000 2.43216400
C -4.60129600 -0.69414700 -3.02271600
H -5.56641200 -0.23875900 -3.30571400
H -3.79969600 -0.00015300 -3.33402100
H -4.48477200 -1.61925700 -3.60646900
Se -1.26159300 -1.02352100 -0.59126700
Se 1.27571700 -1.17193000 -0.15490100
C 1.76832500 0.27760500 -1.36315800
C 2.28836400 -0.01069400 -2.62696900
C 1.63369400 1.60514300 -0.95127600
C 2.67709500 1.02607300 -3.47117500
H 2.39894600 -1.04870400 -2.94221200
C 2.01099500 2.63881800 -1.80600900
H 1.23747900 1.83215700 0.03949400
C 2.53731000 2.35154000 -3.06251300
H 3.09115600 0.79743200 -4.45230000
H 1.90264400 3.67293100 -1.47882600
H 2.84175100 3.16045100 -3.72475700
C -1.44603500 0.71388400 0.27566100
C -1.33905400 0.82764800 1.66284500
C -1.65774600 1.85351600 -0.50160800
C -1.42109800 2.08017800 2.26602100
H -1.18354600 -0.06513500 2.27040100
C -1.75058900 3.10372900 0.10655100
H -1.74308800 1.75957200 -1.58513200
C -1.62570200 3.21942800 1.48888600
H -1.33493000 2.16396300 3.34892300
H -1.91600300 3.99022600 -0.50446000
H -1.69265200 4.19766100 1.96239600
C 5.06975300 1.43879600 -0.36873000
C 5.64414300 2.42468600 -1.16979000
C 6.34802900 2.05802500 -2.30809000
C 6.46051200 0.71101200 -2.62804000
C 5.86395700 -0.21721100 -1.78765400
H 5.55240500 3.47512200 -0.90872800
H 6.80232600 2.81968500 -2.93733600
H 6.99921000 0.37760100 -3.51066300
H 5.91930700 -1.28552300 -1.99240900
C 4.28878400 1.74820700 0.84683700
C 3.96674800 3.05292100 1.22053200
C 3.18728800 3.27066400 2.34724000
H 4.30011300 3.89800500 0.62505100
C 3.10948600 0.90801700 2.65828300
C 2.74501300 2.17745500 3.08282200
H 2.92389300 4.28382800 2.64158700
H 2.78450400 0.01933800 3.19707300
H 2.12993400 2.29796400 3.97027900
N 3.86323900 0.69182200 1.57539700
N 5.19066100 0.13062700 -0.68616100
C 3.56086600 -2.52533200 2.17813700
H 4.36474300 -3.13349800 2.62487300
H 3.07908200 -1.95643000 2.99147500
H 2.81212800 -3.22396000 1.77269200
C 4.77855800 -2.99861100 -0.30217600
H 4.35547200 -2.93684800 -1.32068700
H 5.87396800 -3.09574600 -0.39871200
H 4.39973900 -3.92191300 0.16043900
Pt 4.30672900 -1.28680600 0.72153000
Pt -4.51118200 -0.95546900 -0.99006400

5b
E(RM06) = -1886.98580998
Zero-point correction= 0.645657 (Hartree/Particle)
Thermal correction to Energy= 0.693009
Thermal correction to Enthalpy= 0.693953
Thermal correction to Gibbs Free Energy= 0.557408
Sum of electronic and zero-point Energies= -1886.340153
Sum of electronic and thermal Energies= -1886.292801
Sum of electronic and thermal Enthalpies= -1886.291857
Sum of electronic and thermal Free Energies= -1886.428402
E(RM06) = -1887.58474445

N -2.11630800 2.84854700 4.34980400
C -2.29909400 3.96298000 3.63830800
C -2.15297200 5.23473600 4.17567400

C -1.80118900 5.34370500 5.51473500
C -1.60720800 4.18812400 6.25889300
C -1.77139300 2.94361300 5.65086500
N -1.84674100 0.53457000 5.70029600
C -1.65387200 -0.64310700 6.29847100
C -1.18921400 -0.76486900 7.60107000
C -0.91035100 0.39788300 8.30867100
C -1.10268600 1.62541000 7.69133200
C -1.57110800 1.66894300 6.37770600
H -2.57217500 3.82035800 2.59286300
H -2.31425600 6.11174200 3.55482200
H -1.88091900 -1.52474400 5.69974800
H -1.04963100 -1.74843000 8.04106900
H -0.54038600 0.35272400 9.33035100
H -1.67800200 6.31875400 5.98051600
C -2.73471100 -1.11058800 2.96356700
H -2.07965600 -1.39908400 2.12937000
H -2.54922400 -1.79462000 3.80807700
H -3.77878200 -1.22892200 2.63611300
Pd -2.37673600 0.81167200 3.56737600
H -0.86610800 2.53971600 8.22801100
H -1.33706300 4.26497200 7.30819600
C -2.80173900 1.32000400 1.63526800
H -3.73950000 1.89972900 1.62718200
H -1.97933200 1.96829200 1.28856500
H -2.90230100 0.47748600 0.93883300
Se 0.64641500 0.06836400 3.06670500
Se 3.06086000 -0.75490500 2.71323400
C 3.62729600 0.74572000 1.60606200
C 3.68778200 0.60731100 0.21731500
C 4.00018500 1.95166900 2.20336500
C 4.12218400 1.67111300 -0.56849000
H 3.40462300 -0.33960000 -0.24378800
C 4.42698100 3.01577300 1.41160800
H 3.95712800 2.05923500 3.28797800
C 4.49535300 2.87490100 0.02810800
H 4.17749700 1.55694600 -1.65026900
H 4.71691000 3.95441800 1.88326900
H 4.83746200 3.70463300 -0.58843900
C 1.16107000 1.62315700 4.12393600
C 1.61838900 1.46990100 5.43408400
C 1.08267600 2.89652300 3.55782200
C 2.01285000 2.58619200 6.16677700
H 1.66782300 0.47479500 5.87830700
C 1.46323900 4.01257400 4.29991600
H 0.72493400 3.01140400 2.53371000
C 1.93384000 3.85840600 5.60153500
H 2.37176000 2.46196100 7.18787400
H 1.39265300 5.00532300 3.85710900
H 2.23745700 4.73054400 6.17840300
C 7.22175900 0.57143100 1.29418400
C 7.81350100 1.43469800 0.37206100
C 7.92249500 1.04577200 -0.95604700
C 7.43101500 -0.19509400 -1.33982300
C 6.85391000 -1.00032800 -0.36732900
H 8.19779400 2.40252300 0.68113500
H 8.38675900 1.70952000 -1.68180100
H 7.49170300 -0.53977600 -2.36846600
H 6.45245800 -1.98305100 -0.61413700
C 7.06517200 0.91897500 2.72548000
C 7.39227500 2.17935800 3.22724900
C 7.19249000 2.45313600 4.57268500
H 7.78101300 2.95473900 2.57319000
C 6.37157100 0.23077100 4.82465800
C 6.66849000 1.46182100 5.39342300
H 7.43872600 3.43419000 4.97227200
H 5.95482500 -0.57822700 5.42410700
H 6.48996200 1.63187400 6.45162700
Pd 5.94856500 -1.90793700 2.51296700
N 6.56625100 -0.04121400 3.53212500
N 6.75414400 -0.63505900 0.91259000
C 5.36687400 -3.08065500 4.08599400
H 6.01221400 -3.96831500 4.16826300
H 5.44611500 -2.49792300 5.01855300
H 4.32822200 -3.42181300 3.97316800

C 5.43520800 -3.50744300 1.35105900
H 4.77995200 -3.12379300 0.55088100
H 6.35392300 -3.91274000 0.89580100
H 4.91255300 -4.31908500 1.87357000

5c

E(RM06) = -2647.59238345
Zero-point correction= 0.649571 (Hartree/Particle)
Thermal correction to Energy= 0.695542
Thermal correction to Enthalpy= 0.696486
Thermal correction to Gibbs Free Energy= 0.563686
Sum of electronic and zero-point Energies= -2646.942812
Sum of electronic and thermal Energies= -2646.896842
Sum of electronic and thermal Enthalpies= -2646.895898
Sum of electronic and thermal Free Energies= -2647.028698
E(RM06) = -2648.16156797

N -2.06694800 3.09510900 4.71871200
C -2.30303600 4.29492400 4.17726000
C -2.07678700 5.48356200 4.85535400
C -1.58108200 5.41933900 6.15171700
C -1.32301800 4.17725900 6.71372600
C -1.57277300 3.02164300 5.97433700
N -1.66468100 0.63255500 5.69536500
C -1.42383600 -0.61794700 6.10290900
C -0.83330900 -0.91436400 7.32252600
C -0.47599000 0.13860900 8.15562300
C -0.71778700 1.43893400 7.73710900
C -1.31235200 1.66442600 6.49605800
H -2.69276800 4.28724900 3.16012800
H -2.28942200 6.43345300 4.37264900
H -1.71787600 -1.40730200 5.41323800
H -0.65999400 -1.94915800 7.60448600
H -0.00929400 -0.04730900 9.12001800
H -1.39377900 6.32594000 6.72223500
C -2.89354900 -0.65341600 2.94351700
H -2.34350600 -0.80814300 2.00118600
H -2.61445900 -1.47248700 3.62831600
H -3.96631800 -0.76107500 2.71364700
H -0.42914800 2.27124000 8.37261600
H -0.93241500 4.11535200 7.72543000
C -3.17434700 1.95627100 1.96694700
H -4.02840000 2.63098600 2.15314800
H -2.37778700 2.55445100 1.48851800
H -3.50225500 1.19938000 1.23884200
C 3.29680700 0.36052500 1.34893300
C 3.41061100 -0.12206800 0.04324100
C 3.73158800 1.65364100 1.65576500
C 3.96758700 0.68096200 -0.94751900
H 3.07012900 -1.13130400 -0.18721100
C 4.27102700 2.45796400 0.65671300
H 3.65476300 2.02310200 2.67933000
C 4.39481000 1.97190900 -0.64297100
H 4.06504300 0.29842000 -1.96239700
H 4.61356700 3.46355800 0.90002200
H 4.83177400 2.59827700 -1.41913600
C 1.13111500 1.61790400 3.82265000
C 1.69386600 1.56422400 5.10025900
C 0.92382100 2.85146500 3.20289600
C 2.05948100 2.74093500 5.74536500
H 1.85153100 0.59747300 5.58074800
C 1.28288000 4.02728000 3.85648300
H 0.48723000 2.88240900 2.20443700
C 1.85494400 3.97333400 5.12490800
H 2.49476700 2.69658200 6.74323600
H 1.12175100 4.98769500 3.36911500
H 2.13847300 4.89297500 5.63439600
C 7.09505700 0.78948700 1.63786900
C 7.78122700 1.72206600 0.86115600
C 8.17563700 1.38351600 -0.42518600
C 7.86772500 0.12002900 -0.91440900
C 7.19309000 -0.76210300 -0.08336700
H 8.01500500 2.70681800 1.25590300
H 8.71446300 2.10224200 -1.03804300
H 8.14782500 -0.18623400 -1.91851700

H 6.93534000 -1.76770000 -0.41332800
C 6.60923600 1.08515900 3.00109400
C 6.65281900 2.36566900 3.55238700
C 6.13292800 2.58414600 4.82022200
H 7.06797900 3.19683300 2.98916700
C 5.57434200 0.26751600 4.90778300
C 5.58351900 1.51397600 5.51596600
H 6.15290000 3.58072600 5.25512200
H 5.14585200 -0.59952700 5.40806000
H 5.16344100 1.63511300 6.51075500
N 6.07181800 0.05003700 3.68594400
N 6.82499700 -0.44674900 1.16317800
C 5.13132500 -3.06667700 4.01761200
H 5.76998200 -3.95050100 4.17886400
H 5.02484700 -2.55178700 4.98814100
H 4.13449600 -3.43594800 3.72679600
C 5.78001600 -3.45106600 1.32124100
H 5.16717100 -3.18553100 0.44117500
H 6.78366700 -3.72829100 0.95374900
H 5.33483900 -4.34812000 1.77697400
S 2.65397600 -0.69784000 2.63854900
S 0.70116200 0.12027800 2.94332800
Pt -2.48074800 1.19039300 3.73815300
Pt 5.90448300 -1.83348200 2.57531200

6a
E(RM06) = -1869.95293093
Zero-point correction= 0.648921 (Hartree/Particle)
Thermal correction to Energy= 0.695171
Thermal correction to Enthalpy= 0.696116
Thermal correction to Gibbs Free Energy= 0.564653
Sum of electronic and zero-point Energies= -1869.304010
Sum of electronic and thermal Energies= -1869.257760
Sum of electronic and thermal Enthalpies= -1869.256815
Sum of electronic and thermal Free Energies= -1869.388278
E(RM06) = -1870.49058197

N -3.05573600 0.86372200 -0.52896800
C -2.96635600 1.55099700 -1.67214000
C -3.21560700 2.91409100 -1.75258300
C -3.57529000 3.58774500 -0.59225400
C -3.67351000 2.87794100 0.59736100
C -3.40950000 1.50877100 0.60619700
N -3.24887900 -0.63648000 1.69084100
C -3.29049300 -1.42477000 2.76941900
C -3.57257300 -0.94911300 4.04221500
C -3.82734200 0.40778700 4.19729800
C -3.78914400 1.23151200 3.08100100
C -3.49245700 0.68643400 1.83206500
H -2.68147300 0.97563300 -2.55315300
H -3.12390400 3.42707600 -2.70624100
H -3.08476000 -2.47966500 2.59761000
H -3.58984600 -1.63313400 4.88598900
H -4.05248600 0.82450100 5.17597400
H -3.77920700 4.65562400 -0.60820700
C -2.85930500 -3.34684600 -0.10723700
H -1.89902300 -3.80761700 -0.37931700
H -3.08284700 -3.61580000 0.93895100
H -3.63854400 -3.80069500 -0.74134600
H -3.97739800 2.29546300 3.19206600
H -3.95534500 3.39614700 1.50939600
C -2.60259800 -1.73371200 -2.36129500
H -3.57527900 -1.59396800 -2.86479800
H -1.88207600 -1.04024100 -2.82588000
H -2.26335900 -2.75955900 -2.56772700
C 0.23140700 1.67649800 -1.17456400
C 0.56811200 -0.00560300 -2.73836200
C 0.68124400 0.90505000 -3.77902100
C 0.57344300 2.25795600 -3.48240800
C 0.35377100 2.64740900 -2.16863800
C -0.02778300 2.01279900 0.24292700
C -0.35548000 1.22048900 2.39792600
C -0.44653700 2.50403200 2.91882800
C -0.32899100 3.57725200 2.04432200
C -0.11579600 3.32943500 0.69534300

H 0.65763400 -1.07736400 -2.91178600
H 0.85499300 0.55481400 -4.79252100
H 0.66182000 3.00773500 -4.26499300
H 0.26619300 3.70343800 -1.92942000
H -0.43611000 0.34503700 3.04267100
H -0.60744100 2.64831500 3.98378500
H -0.39512000 4.60020200 2.40709400
H -0.00540100 4.16256400 0.00722000
N 0.34655600 0.36679000 -1.47481300
N -0.16613000 0.97814300 1.09925200
C 0.63076900 -2.75663600 -0.84053200
H -0.17151800 -2.94535800 -1.56805500
H 1.58032400 -2.59154700 -1.37250100
H 0.74587600 -3.64078700 -0.19849400
C -0.04809800 -2.28472500 1.84737300
H -0.89079000 -2.96951700 1.68351200
H 0.85268700 -2.88808000 2.03193000
H -0.24652900 -1.68073800 2.74713800
C 3.19058200 0.69940000 0.08545800
C 3.59631300 0.62024000 -1.24804300
C 3.15567000 1.94197600 0.72289800
C 3.94421600 1.77567100 -1.94294400
H 3.63729300 -0.35120900 -1.74227800
C 3.51415600 3.09526400 0.02904000
H 2.84819900 2.00396200 1.76794300
C 3.90200900 3.01430800 -1.30722000
H 4.25531600 1.70524900 -2.98479700
H 3.48099500 4.06064100 0.53310900
H 4.17664600 3.91680200 -1.85118000
C 6.29969600 -0.65397000 0.43365800
C 6.39461300 -1.67437700 -0.52215800
C 6.80000300 0.61351200 0.11130200
C 6.97886700 -1.43290000 -1.76277800
H 6.00189800 -2.66455600 -0.28793300
C 7.38682800 0.85107800 -1.12864300
H 6.71645200 1.42282200 0.83721700
C 7.48011000 -0.16964200 -2.07174200
H 7.04515900 -2.23992000 -2.49215400
H 7.76805000 1.84546500 -1.36062300
H 7.93905000 0.01738800 -3.04140100
Pt 0.15411300 -1.05617600 0.20752900
Pt -2.82649500 -1.31361500 -0.36603900
Se 5.46247200 -0.98105000 2.15291500
Se 2.67703100 -0.91751800 1.04636200

6c

E(RM06) = -2647.59448716
Zero-point correction= 0.652521 (Hartree/Particle)
Thermal correction to Energy= 0.697170
Thermal correction to Enthalpy= 0.698114
Thermal correction to Gibbs Free Energy= 0.573448
Sum of electronic and zero-point Energies= -2646.941966
Sum of electronic and thermal Energies= -2646.897317
Sum of electronic and thermal Enthalpies= -2646.896373
Sum of electronic and thermal Free Energies= -2647.021039
E(RM06) = -2648.16135764

N -3.10867700 0.89841800 -0.49175600
C -3.05711400 1.57114400 -1.64529800
C -3.34918700 2.92481500 -1.74052400
C -3.71304400 3.60193600 -0.58400100
C -3.77731600 2.90496300 0.61578800
C -3.47405700 1.54442500 0.63866600
N -3.23208200 -0.57934200 1.75743200
C -3.25042400 -1.35346600 2.84652800
C -3.55219200 -0.86914700 4.11159000
C -3.85548600 0.47978500 4.24471500
C -3.84500500 1.28767300 3.11622000
C -3.52484200 0.73562500 1.87655300
H -2.76358900 0.99403300 -2.52221800
H -3.28497600 3.42759900 -2.70171500
H -3.00878400 -2.40338600 2.69153800
H -3.54760200 -1.54040000 4.96553300
H -4.09813900 0.90300800 5.21631100
H -3.94748000 4.66325900 -0.61032200

C -2.87728700 -3.30744300 -0.03621700
H -1.95659500 -3.80691200 -0.36498300
H -3.05036500 -3.56204500 1.02222500
H -3.71335600 -3.72274100 -0.62268100
H -4.07492800 2.34476100 3.21112100
H -4.06532500 3.42721900 1.52337400
C -2.67857400 -1.70822400 -2.30212400
H -3.67843500 -1.55483100 -2.74485900
H -1.97806100 -1.02350100 -2.80495400
H -2.36714500 -2.73914100 -2.52218100
C 0.10043900 1.70290500 -1.23454800
C 0.40893500 0.03807900 -2.82330000
C 0.52625500 0.96109200 -3.85236800
C 0.42469100 2.31038900 -3.53824700
C 0.21431200 2.68520300 -2.21866600
C -0.12626900 2.02732200 0.19210500
C -0.41180700 1.21883200 2.34708100
C -0.47480700 2.49839100 2.88207000
C -0.36936400 3.57784200 2.01384500
C -0.19233800 3.34068000 0.65754400
H 0.48819100 -1.03177600 -3.01273400
H 0.69563300 0.62276200 -4.87051300
H 0.51059800 3.06921600 -4.31225400
H 0.13334800 3.73870700 -1.96707000
H -0.49168100 0.33862500 2.98548700
H -0.60789000 2.63464300 3.95181700
H -0.41745000 4.59804300 2.38683600
H -0.09231300 4.17938900 -0.02507900
N 0.19565400 0.39658000 -1.55474400
N -0.25696900 0.98813300 1.04247500
C 0.47223100 -2.75292200 -0.95160600
H -0.35186000 -2.93762500 -1.65118300
H 1.40489900 -2.57044700 -1.50297800
H 0.61260200 -3.63082400 -0.30836700
C -0.11597600 -2.29886900 1.76511800
H -0.94084600 -3.00509000 1.62242700
H 0.81237800 -2.86411600 1.92090000
H -0.30435600 -1.68531400 2.65849800
C 2.96312500 0.51738300 -0.01681100
C 3.45007200 0.46780200 -1.32871200
C 2.99730600 1.73454400 0.67490900
C 3.93273600 1.61661600 -1.94483800
H 3.44687000 -0.48344300 -1.86119300
C 3.48852400 2.88202600 0.05969500
H 2.63596400 1.77260600 1.70329300
C 3.95041100 2.82673600 -1.25356300
H 4.30725100 1.56408100 -2.96626500
H 3.50611800 3.82320800 0.60818100
H 4.33233200 3.72532700 -1.73588100
C 6.27173100 -0.77576200 0.30409400
C 6.23225000 -1.67115200 -0.78441100
C 6.82358000 0.49600600 0.05303600
C 6.72472300 -1.32148800 -2.03733800
H 5.80529200 -2.66342800 -0.62810900
C 7.31407700 0.84648600 -1.19902300
H 6.85850700 1.21836100 0.87011000
C 7.27427900 -0.05935900 -2.25856700
H 6.68110000 -2.04698300 -2.85088000
H 7.73237600 1.84283300 -1.34982400
H 7.66367300 0.21364900 -3.23859700
Pt 0.02574500 -1.05948400 0.12266900
Pt -2.82641000 -1.27950000 -0.30566500
S 2.35087200 -0.94951500 0.77679200
S 5.67809500 -1.22505800 1.90036500

7a
E(RM06) = -1869.94980509
Zero-point correction= 0.651094 (Hartree/Particle)
Thermal correction to Energy= 0.696511
Thermal correction to Enthalpy= 0.697455
Thermal correction to Gibbs Free Energy= 0.569802
Sum of electronic and zero-point Energies= -1869.298711
Sum of electronic and thermal Energies= -1869.253295
Sum of electronic and thermal Enthalpies= -1869.252350
Sum of electronic and thermal Free Energies= -1869.380003

E(RM06) = -1870.48499486

N -3.32587500 1.25012700 -0.17066300
C -3.31880700 2.41503600 -0.82454800
C -3.57883200 3.63024500 -0.20559100
C -3.85787700 3.62828000 1.15433700
C -3.87382900 2.41945900 1.83847800
C -3.60849700 1.23524400 1.15222700
N -3.39821200 -1.16320600 1.02923200
C -3.42103100 -2.38709800 1.56833600
C -3.64096300 -2.60948000 2.91978900
C -3.85459100 -1.50932100 3.74122400
C -3.85274900 -0.23883700 3.18274400
C -3.62254700 -0.08750900 1.81556800
H -3.08997000 2.36577000 -1.88891300
H -3.55469800 4.54981500 -0.78400800
H -3.25520500 -3.21490200 0.88007200
H -3.64257100 -3.62278400 3.31081900
H -4.02619600 -1.63563900 4.80728900
H -4.06399300 4.55581400 1.68276600
C -3.09195800 -2.68354200 -1.76426100
H -2.30279200 -3.28110600 -1.28420500
H -4.07046600 -3.10489900 -1.47367300
H -2.98879400 -2.78868900 -2.85350100
H -4.02089300 0.62611900 3.81748400
H -4.09642200 2.40926900 2.90134600
C -2.93117500 -0.19522700 -3.07469500
H -3.92852300 -0.33381900 -3.52618700
H -2.65423500 0.86647200 -3.17773700
H -2.21466300 -0.79017700 -3.65627200
C -0.13822300 2.41211700 -0.71806000
C -0.01854900 1.77785300 -2.94792200
C 0.07150800 3.09397800 -3.37754800
C 0.05298400 4.10046500 -2.41888300
C -0.04923700 3.75734500 -1.07871000
C -0.25066300 1.97412900 0.69183200
C -0.43655600 0.18543300 2.16260800
C -0.47559100 1.02438500 3.26835900
C -0.39668500 2.39394600 3.05554700
C -0.28268500 2.87292500 1.75678000
H -0.00412300 0.95207900 -3.65780600
H 0.15575800 3.31631000 -4.43735000
H 0.12253100 5.14586500 -2.70950300
H -0.05521600 4.53794000 -0.32343400
H -0.49380200 -0.89776300 2.27383300
H -0.56808500 0.60366200 4.26586900
H -0.42238400 3.08907900 3.89128600
H -0.22153600 3.94337700 1.58419600
N -0.12897200 1.44605000 -1.65956700
N -0.33057100 0.64450000 0.91361800
C 0.11957700 -1.75819400 -2.60071200
H -0.76770100 -2.37499200 -2.77395200
H 0.26193300 -1.06871300 -3.44506600
H 0.99914400 -2.41307200 -2.53562600
C -0.05590800 -2.45235100 0.12306500
H 0.18937800 -3.29191600 -0.53960500
H 0.71793100 -2.38397700 0.90094900
H -1.03232400 -2.63270200 0.58922600
Se 2.40144500 -0.63253000 -0.89237600
Se 5.37106300 -2.75449700 1.76230000
C 2.81129700 0.92112500 0.19709800
C 3.07068600 2.15171000 -0.41226000
C 2.87304100 0.81307200 1.58974700
C 3.38136400 3.26555300 0.36472700
H 3.02326900 2.23702100 -1.49892100
C 3.17561000 1.92870700 2.36349900
H 2.68125400 -0.15015100 2.06406800
C 3.43069400 3.15592400 1.75216300
H 3.57977500 4.22223400 -0.11688500
H 3.21375600 1.83958200 3.44844600
H 3.66856200 4.02764300 2.35968000
C 5.78374600 -1.33808800 0.48959500
C 5.67964700 -1.55278200 -0.89304300
C 6.19371400 -0.06749300 0.91975000
C 5.98681700 -0.54500900 -1.80632000

H 5.36104500 -2.53032500 -1.25779200
C 6.49541100 0.93981400 0.00847700
H 6.27378400 0.13285200 1.98895000
C 6.39899300 0.70928800 -1.36311200
H 5.90753600 -0.74916000 -2.87475600
H 6.80911200 1.91750300 0.37622600
H 6.64417000 1.49577400 -2.07569400
Pt -0.14947900 -0.65798200 -0.87718000
Pt -3.05401500 -0.74608800 -1.10803700

7b
E(RM06) = -1886.97848568
Zero-point correction= 0.648680 (Hartree/Particle)
Thermal correction to Energy= 0.694582
Thermal correction to Enthalpy= 0.695526
Thermal correction to Gibbs Free Energy= 0.567372
Sum of electronic and zero-point Energies= -1886.329806
Sum of electronic and thermal Energies= -1886.283904
Sum of electronic and thermal Enthalpies= -1886.282959
Sum of electronic and thermal Free Energies= -1886.411113
E(RM06) = -1887.56821957

N -3.31674300 1.14922500 -0.26403000
C -3.20227800 2.45337700 -0.52269500
C -3.59028300 3.43970500 0.37514700
C -4.12493100 3.04236400 1.59318200
C -4.25647200 1.68622300 1.86421700
C -3.84596500 0.75219200 0.91332000
N -3.58148700 -1.51047000 0.11577300
C -3.65896200 -2.83423800 0.26741500
C -4.10584200 -3.44012100 1.43415200
C -4.49295800 -2.62354300 2.48862800
C -4.42271500 -1.24551100 2.33582800
C -3.95972200 -0.70874200 1.13430400
H -2.77459300 2.71441900 -1.49156300
H -3.46912700 4.48863600 0.11811200
H -3.34364300 -3.43454400 -0.58512100
H -4.14391200 -4.52333000 1.50614000
H -4.84602200 -3.05127900 3.42385400
H -4.44130400 3.77761000 2.32922800
C -2.72350000 -2.01192700 -3.02986700
H -1.71816900 -2.15182000 -3.44462900
H -3.03546700 -2.93491000 -2.51599900
H -3.42151000 -1.81408200 -3.85681400
Pd -2.84017900 -0.46599900 -1.70158700
H -4.71574300 -0.60059100 3.15903200
H -4.68062100 1.36954500 2.81253400
C -2.36088800 0.68298100 -3.31539500
H -3.32238700 1.05155400 -3.70900900
H -1.75904600 1.53923000 -2.97801800
H -1.82715500 0.16177000 -4.12040600
C -0.08287300 2.14602100 0.20536800
C 0.58037600 2.11405400 -2.01550000
C 0.71088000 3.49504900 -2.06031700
C 0.42658100 4.21627200 -0.90775300
C 0.02925100 3.53677600 0.23527200
C -0.49985700 1.35830600 1.38875500
C -0.93605600 -0.73943000 2.26811700
C -1.17966400 -0.22532900 3.53530100
C -1.08359600 1.14870000 3.71235800
C -0.73771400 1.94810800 2.63057100
H 0.79416000 1.50323800 -2.89242700
H 1.02785300 3.98370300 -2.97720800
H 0.51338100 5.30011500 -0.89417300
H -0.19772100 4.09566100 1.13849600
H -0.99168500 -1.81282800 2.08328800
H -1.43427700 -0.89289500 4.35407900
H -1.26553500 1.59830400 4.68556400
H -0.64003300 3.02126000 2.76711700
N 0.19202500 1.45780200 -0.92025300
N -0.62308800 0.02572700 1.22249000
Pd -0.02986500 -0.75437500 -0.81406800
C 0.73848000 -1.16875200 -2.66510100
H -0.02458500 -0.78066700 -3.34918600
H 1.68146000 -0.61715300 -2.75590500

H 0.91140200 -2.23729200 -2.82766900
C -0.29065300 -2.78645200 -0.62945000
H -1.03921800 -3.05919500 -1.38011300
H 0.62866700 -3.35984000 -0.79227300
H -0.66498000 -2.95659300 0.38838500
Se 2.23267700 -1.31459700 0.14814300
C 2.79445200 0.45469600 0.69558600
C 3.42256700 1.30993500 -0.21714100
C 2.60072900 0.86651500 2.01694000
C 3.84262100 2.57201700 0.18878000
H 3.57431000 0.98332800 -1.24664400
C 3.02893200 2.12897400 2.41935700
H 2.13622400 0.18721800 2.73546700
C 3.64525000 2.98234800 1.50787100
H 4.32709600 3.23735600 -0.52439400
H 2.88201400 2.44210600 3.45282400
H 3.97708900 3.97002800 1.82410200
C 4.48969400 -2.60639100 2.18053000
C 5.48014200 -2.36495300 1.22776700
C 6.33421700 -1.27245100 1.35718000
C 6.18124600 -0.42492100 2.45421800
C 5.19403100 -0.66721400 3.40519900
C 4.32802000 -1.76426700 3.29183600
H 3.83442500 -3.47103400 2.06879900
H 5.58449100 -3.04454000 0.38114400
H 7.11193200 -1.08682200 0.61780800
H 6.83989800 0.43597800 2.57335900
H 5.08449500 0.01114100 4.25239300
Se 2.93408100 -2.09301900 4.60836500

8a

E(RM06) = -1869.94944717
Zero-point correction= 0.651041 (Hartree/Particle)
Thermal correction to Energy= 0.696375
Thermal correction to Enthalpy= 0.697320
Thermal correction to Gibbs Free Energy= 0.569928
Sum of electronic and zero-point Energies= -1869.298406
Sum of electronic and thermal Energies= -1869.253072
Sum of electronic and thermal Enthalpies= -1869.252128
E(RM06) = -1870.48528800

N -2.99530600 1.05747200 -0.35633500
C -2.78229300 2.31973200 -0.73966600
C -3.32952700 3.40981700 -0.07678700
C -4.13423900 3.17086000 1.02933200
C -4.36847200 1.86006000 1.42462300
C -3.78797500 0.81227400 0.71169100
N -3.38332200 -1.52788500 0.29312100
C -3.52009100 -2.82518400 0.58347400
C -4.25779800 -3.28199200 1.66664400
C -4.88706800 -2.34474500 2.47594300
C -4.75481100 -0.99618600 2.17489000
C -3.99030900 -0.60754400 1.07531600
H -2.14026100 2.45276200 -1.61044100
H -3.11807300 4.41788300 -0.42287200
H -3.01107500 -3.52124200 -0.08097700
H -4.33278000 -4.34777900 1.86238800
H -5.47634500 -2.65641900 3.33477400
H -4.58017200 3.99409200 1.58202300
C -1.96899200 -2.43540800 -2.53454600
H -0.90946800 -2.61554000 -2.75750300
H -2.36714300 -3.31344600 -2.00059100
H -2.50653900 -2.35185700 -3.49332800
H -5.23959100 -0.25685100 2.80551800
H -4.99951500 1.66590700 2.28679400
C -1.50560600 0.24916900 -3.08151300
H -2.35434300 0.67682700 -3.64385300
H -0.85437600 1.07993000 -2.76936500
H -0.93781900 -0.39544000 -3.76677400
C -0.00658000 2.03789000 0.81592700
C 1.08506800 1.87609300 -1.22703500
C 1.26588700 3.24951400 -1.30432800
C 0.78349900 4.03489900 -0.26505400
C 0.14653500 3.42430100 0.80620500
C -0.67306700 1.31824600 1.92409200

C -1.32313000 -0.73017300 2.79686100
C -1.80753700 -0.14770500 3.95990100
C -1.72502300 1.23345700 4.08510100
C -1.14930800 1.97234300 3.06044800
H 1.45256700 1.21354300 -2.00959600
H 1.77640400 3.68372500 -2.15901000
H 0.90388600 5.11530900 -0.28243100
H -0.23289100 4.03286500 1.62183900
H -1.36583700 -1.80956300 2.65135100
H -2.24105600 -0.76872800 4.73901300
H -2.09520700 1.73422600 4.97632300
H -1.06210800 3.05026000 3.15998600
N 0.46092100 1.28778400 -0.20298800
N -0.78802200 -0.02123000 1.80109000
C 1.29087500 -1.43799200 -1.68004600
H 0.73856900 -1.11210800 -2.56912200
H 2.26064500 -0.92393200 -1.62912400
H 1.47137700 -2.51904900 -1.73509800
C -0.07355400 -2.93153500 0.28653400
H -0.66303600 -3.35060300 -0.53602100
H 0.88348500 -3.46859300 0.33600900
H -0.60502900 -3.08310800 1.23748000
Se 2.29205400 -1.28893900 1.36829900
C 2.72373200 0.50512200 1.96710600
C 3.51713700 1.33979900 1.17394100
C 2.28148000 0.95128800 3.21507700
C 3.85828900 2.61114300 1.62509300
H 3.86689900 0.98661200 0.20293700
C 2.62563000 2.22384800 3.66393000
H 1.67276300 0.29489200 3.83863300
C 3.41366800 3.05354500 2.87016500
H 4.47881200 3.25704800 1.00552800
H 2.27956000 2.56529300 4.63866100
H 3.68753200 4.04628100 3.22343200
C 5.49376000 -0.32755200 4.32888000
C 6.53703200 0.11185800 3.49990100
C 6.87108800 -0.68708400 2.39406000
C 6.19796800 -1.87762800 2.13592400
C 5.16633000 -2.30400100 2.97277700
C 4.81949400 -1.51681300 4.06975500
H 5.20823100 0.27690600 5.19052300
H 7.67869900 -0.37005200 1.73349000
H 6.48706700 -2.48250200 1.27581600
H 4.64626600 -3.24121800 2.77727100
H 4.01155700 -1.83196200 4.73206400
Se 7.49389000 1.76967500 3.87488600
Pt -2.28985300 -0.72202500 -1.46117900
Pt 0.18872100 -0.91022400 -0.02605200

8b

E(RM06) = -1886.97665919
Zero-point correction= 0.649155 (Hartree/Particle)
Thermal correction to Energy= 0.694846
Thermal correction to Enthalpy= 0.695790
Thermal correction to Gibbs Free Energy= 0.568659
Sum of electronic and zero-point Energies= -1886.327504
Sum of electronic and thermal Energies= -1886.281813
Sum of electronic and thermal Enthalpies= -1886.280869
Sum of electronic and thermal Free Energies= -1886.408000
E(RM06) = -1887.56598553

N -3.02555700 1.02839100 -0.28099700
C -2.83984700 2.29805300 -0.64755600
C -3.37507400 3.37291800 0.05089700
C -4.14169400 3.10522100 1.17695100
C -4.34590600 1.78500000 1.55845600
C -3.77676500 0.75651400 0.80775900
N -3.37184100 -1.57642900 0.33720700
C -3.48030400 -2.87623000 0.62035000
C -4.16024700 -3.35678700 1.73165700
C -4.76005600 -2.43558600 2.58049900
C -4.65624400 -1.08214700 2.28956200
C -3.94877100 -0.67327100 1.15873800
H -2.22926800 2.45513900 -1.53770300
H -3.18694400 4.38914800 -0.28518800

H -2.99621400 -3.56079000 -0.07535500
H -4.21399800 -4.42557400 1.91837000
H -5.30440700 -2.76315400 3.46293700
H -4.58025200 3.91355200 1.75715500
C -1.99138900 -2.40173000 -2.54545700
H -0.93395500 -2.56244800 -2.78788500
H -2.37347900 -3.27237400 -1.98913100
H -2.55709100 -2.30575900 -3.48422500
H -5.11678700 -0.35608800 2.95316000
H -4.94734500 1.56980600 2.43667200
C -1.56260500 0.25954500 -3.04141500
H -2.43938500 0.65186000 -3.58235500
H -0.95113600 1.10317600 -2.68882500
H -0.96751000 -0.35405300 -3.72968100
C 0.07386000 2.09877800 0.69778000
C 1.13455400 1.90443300 -1.35394900
C 1.27812800 3.27940400 -1.47861500
C 0.78822600 4.08328800 -0.45750300
C 0.18299200 3.48886200 0.64121000
C -0.55947000 1.39808400 1.83928700
C -1.17857100 -0.62922000 2.77210900
C -1.65306400 -0.02309200 3.92814900
C -1.57602800 1.36089400 4.01872100
C -1.02425800 2.07809300 2.96561900
H 1.50359300 1.23077000 -2.12715500
H 1.76204500 3.70014400 -2.35538200
H 0.87576400 5.16576600 -0.51131200
H -0.20728800 4.11276200 1.44009300
H -1.21867000 -1.71283500 2.65464600
H -2.07268500 -0.62741700 4.72787000
H -1.93560200 1.88155100 4.90303500
H -0.94570700 3.15900600 3.03679100
N 0.54761800 1.32965200 -0.30222100
N -0.65760500 0.05599000 1.75388600
C 1.37220700 -1.42182800 -1.72579900
H 0.72779900 -1.11416000 -2.55716800
H 2.31201400 -0.85726800 -1.71129400
H 1.58183100 -2.49566200 -1.76383900
C 0.03162400 -2.88653600 0.24213300
H -0.59053900 -3.23867000 -0.58640000
H 0.96953400 -3.45247900 0.27158700
H -0.49343500 -2.98326600 1.20148700
Se 2.41048000 -1.30836700 1.28428900
C 2.81969800 0.49081100 1.85926200
C 3.57796800 1.33640000 1.04124500
C 2.37140600 0.94779900 3.10270100
C 3.87999200 2.62643600 1.46355800
H 3.92511300 0.97710300 0.07167600
C 2.67409100 2.24048800 3.52152800
H 1.78199200 0.28705400 3.73959500
C 3.42826700 3.07896300 2.70362200
H 4.46883000 3.28220100 0.82403900
H 2.32105100 2.59203800 4.49003200
H 3.66630900 4.08919900 3.03223400
C 5.18456300 -0.64049800 4.60135900
C 6.19771800 -0.00347100 3.86559000
C 6.56923000 -0.57369700 2.63567800
C 5.96362700 -1.73392600 2.16902500
C 4.96014600 -2.35809300 2.91363700
C 4.57733800 -1.79964200 4.13434400
H 4.87437800 -0.21519700 5.55628300
H 7.35326700 -0.09846200 2.04560300
H 6.27882900 -2.16125700 1.21652500
H 4.50586100 -3.28365300 2.56225600
H 3.79511400 -2.27518100 4.72760600
Se 7.05171500 1.61267200 4.52180000
Pd -2.31681800 -0.72687600 -1.42446600
Pd 0.30786800 -0.87107700 -0.06617600

9a
E(RM06) = -1629.02223547
Zero-point correction= 0.560538 (Hartree/Particle)
Thermal correction to Energy= 0.598292
Thermal correction to Enthalpy= 0.599236
Thermal correction to Gibbs Free Energy= 0.490765

Sum of electronic and zero-point Energies= -1628.461698
Sum of electronic and thermal Energies= -1628.423944
Sum of electronic and thermal Enthalpies= -1628.423000
E(RM06) = -1629.47218793

N 1.24700700 0.57483000 1.02885800
C 0.95983300 1.33135900 2.09211400
C 1.28229900 2.67972300 2.16423200
C 1.93416200 3.25848400 1.08341000
C 2.24420500 2.47326600 -0.01976400
C 1.89290100 1.12434400 -0.02431600
N 1.80562300 -1.06391400 -1.03448800
C 2.03830400 -1.91753400 -2.03593800
C 2.65554700 -1.54056600 -3.22039300
C 3.05538800 -0.21787300 -3.36130200
C 2.82450400 0.67132800 -2.32076200
C 2.19054800 0.22567100 -1.16154300
H 0.44473600 0.82913800 2.91109800
H 1.01938100 3.25433700 3.04819700
H 1.71058800 -2.94351800 -1.87781600
H 2.81617700 -2.27273200 -4.00643600
H 3.54350800 0.12253700 -4.27114200
H 2.20308700 4.31183600 1.09446600
C 0.89141900 -3.64935000 0.79102600
H -0.10218200 -4.09200400 0.93539000
H 1.28386200 -3.98305600 -0.18302100
H 1.55572300 -4.04602100 1.57613400
H 3.12960300 1.70829900 -2.42416000
H 2.75865500 2.91868900 -0.86614300
C 0.26258200 -1.88581800 2.83970700
H 1.13937800 -1.72433200 3.49125200
H -0.50536700 -1.14735200 3.11606100
H -0.13316500 -2.88943900 3.04809400
C -1.99719000 1.53453700 0.90227100
C -2.75070000 0.02374100 2.49673000
C -3.05510900 1.03586000 3.39557800
C -2.81133900 2.34895400 3.01309300
C -2.28321900 2.60101600 1.75461300
C -1.43209300 1.72755200 -0.45205700
C -0.68862400 0.72720600 -2.40860700
C -0.44793800 1.95296000 -3.01376700
C -0.70902300 3.10650300 -2.28513600
C -1.20811900 2.99307200 -0.99454000
H -2.92818600 -1.02222800 2.74362200
H -3.47334100 0.79211100 4.36786100
H -3.03259600 3.17407300 3.68563300
H -2.08823700 3.62510800 1.45006700
H -0.49930000 -0.20585100 -2.93944200
H -0.06217500 1.99149000 -4.02878400
H -0.53442300 4.08880000 -2.71720500
H -1.43334000 3.89054300 -0.42596300
N -2.22938600 0.26380200 1.29045300
N -1.15241100 0.61420100 -1.16252200
C -2.52716200 -2.90955600 0.87874600
H -1.89825100 -3.06888200 1.76233500
H -3.54725900 -2.64012400 1.18492600
H -2.57085900 -3.83162400 0.28586100
C -1.30477700 -2.71378700 -1.65550400
H -0.57317600 -3.43386200 -1.27530600
H -2.20018900 -3.26362300 -1.97529300
H -0.88977100 -2.18703000 -2.52700600
Se -3.95932900 -1.17069500 -1.42392200
C -4.68784700 0.51202200 -0.78441900
C -5.42918100 0.55478800 0.40116500
C -4.49737000 1.68384400 -1.52287300
C -5.96757200 1.75894900 0.84433000
H -5.57909300 -0.35976300 0.97597500
C -5.03816400 2.88728200 -1.07551900
H -3.92365400 1.65182100 -2.44977600
C -5.77015100 2.92647400 0.10839700
H -6.54087900 1.78639000 1.76978400
H -4.88479600 3.79640900 -1.65519500
H -6.19180600 3.86736800 0.45746500
Pt -1.73717600 -1.33371700 -0.18062700
Pt 0.89637400 -1.60717200 0.91754800

9b
E(RM06) = -1646.04759074
Zero-point correction= 0.559484 (Hartree/Particle)
Thermal correction to Energy= 0.597276
Thermal correction to Enthalpy= 0.598220
Thermal correction to Gibbs Free Energy= 0.489658
Sum of electronic and zero-point Energies= -1645.488107
Sum of electronic and thermal Energies= -1645.450315
Sum of electronic and thermal Enthalpies= -1645.449371
Sum of electronic and thermal Free Energies= -1645.557933
E(RM06) = -1646.55086654
N -3.10947200 1.24268600 -0.38182500
C -2.76172100 2.48990200 -0.70482800
C -3.17907500 3.60147800 0.01570700
C -4.00231800 3.39723500 1.11478200
C -4.37618500 2.10179700 1.44956800
C -3.91566200 1.03316000 0.68085500
N -3.78465400 -1.31854100 0.14779300
C -4.05558300 -2.60300000 0.38950700
C -4.81200700 -3.02781300 1.47370900
C -5.31469700 -2.06421600 2.33823500
C -5.04270400 -0.72580800 2.08938800
C -4.26685800 -0.37467500 0.98452800
H -2.11639300 2.59697700 -1.57773900
H -2.86034200 4.59625800 -0.28392000
H -3.64343200 -3.32247400 -0.31721500
H -4.99808400 -4.08689500 1.62747900
H -5.91328400 -2.34751700 3.20057900
H -4.35532300 4.23631400 1.70945300
C -2.52420100 -2.20930100 -2.76879600
H -1.50369500 -2.50085000 -3.04333300
H -3.01301000 -3.04006700 -2.23686300
H -3.08975400 -1.99082100 -3.68656100
Pd -2.61816700 -0.55100300 -1.58123600
H -5.42574300 0.03233200 2.76602200
H -5.02505900 1.93735200 2.30467300
C -1.76111200 0.38922400 -3.17188900
H -2.60090000 0.88306800 -3.68749000
H -1.06304500 1.15460400 -2.80410300
H -1.24234500 -0.26535300 -3.88303500
C 0.08491100 1.83016100 0.61889000
C 1.12407900 1.60394100 -1.44112400
C 1.45151800 2.95178100 -1.49226500
C 1.06722400 3.75896300 -0.42932300
C 0.38097400 3.19378400 0.63669000
C -0.64488000 1.16275100 1.72230700
C -1.51333400 -0.81391400 2.56117800
C -1.92756200 -0.20481600 3.73856900
C -1.69127100 1.15573000 3.88806400
C -1.04354300 1.84579200 2.87201500
H 1.40522000 0.92932400 -2.24952300
H 1.99269400 3.34950100 -2.34592900
H 1.29973800 4.82113200 -0.42520700
H 0.07602000 3.82048500 1.46966500
H -1.68247600 -1.87880500 2.39696000
H -2.42689700 -0.78803000 4.50751500
H -2.00174200 1.67870900 4.78944100
H -0.84197100 2.90643500 2.99000700
N 0.45808500 1.05832300 -0.42115500
N -0.90132200 -0.15329500 1.57794100
Pd -0.06479800 -1.10421500 -0.29668900
C 0.93361600 -1.70198700 -1.98361200
H 0.33723400 -1.27918100 -2.79900000
H 1.93404900 -1.25727800 -1.93733100
H 1.00825800 -2.79069300 -2.06556200
C -0.57326700 -3.08454900 -0.06923900
H -1.22907000 -3.33095700 -0.90908300
H 0.29599500 -3.75101300 -0.06455300
H -1.10401400 -3.15331100 0.88852200
Se 1.96643800 -1.82816300 1.01438600
C 2.58581400 -0.12901300 1.70507100
C 3.45456600 0.66652700 0.94873800
C 2.18598300 0.29582200 2.97648300
C 3.91353400 1.87578600 1.46001000

H 3.76290200 0.33452100 -0.04301400
C 2.64992400 1.50623400 3.48468300
H 1.50701700 -0.32230400 3.56446200
C 3.50946600 2.29749700 2.72649200
H 4.58635400 2.49342900 0.86728300
H 2.33380000 1.83312300 4.47419200
H 3.86883600 3.24506200 3.12379000

9c
E(RM06) = -2017.84724876
Zero-point correction= 0.562136 (Hartree/Particle)
Thermal correction to Energy= 0.599107
Thermal correction to Enthalpy= 0.600051
Thermal correction to Gibbs Free Energy= 0.494024
Sum of electronic and zero-point Energies= -2017.285113
Sum of electronic and thermal Energies= -2017.248142
Sum of electronic and thermal Enthalpies= -2017.247198
Sum of electronic and thermal Free Energies= -2017.353225
E(RM06) = -2018.31028423

N -3.04352800 1.06656600 -0.22496400
C -2.87527500 2.33659200 -0.60496600
C -3.42247900 3.40731100 0.08828100
C -4.18287800 3.13838600 1.21863300
C -4.37075800 1.81895400 1.61015100
C -3.79133800 0.79144400 0.86725900
N -3.35204600 -1.53755800 0.40846800
C -3.44913500 -2.83986400 0.69143000
C -4.13210300 -3.32212400 1.79916300
C -4.74756600 -2.40597200 2.64222300
C -4.65649600 -1.05217300 2.34932500
C -3.94663900 -0.63694600 1.22350200
H -2.27225600 2.49213800 -1.49968100
H -3.24925600 4.42308800 -0.25642000
H -2.95309900 -3.51892400 0.00019200
H -4.17644100 -4.39093400 1.98731200
H -5.29496000 -2.73773800 3.52097200
H -4.63004000 3.94556900 1.79346800
C -2.08020000 -2.38346800 -2.49982000
H -1.03872500 -2.54018800 -2.80664000
H -2.42041400 -3.27479500 -1.94896000
H -2.69268100 -2.29478500 -3.41204800
H -5.13089600 -0.32940100 3.00646200
H -4.96842700 1.60237800 2.49040000
C -1.69176400 0.31281000 -3.03983800
H -2.58597800 0.71519400 -3.54746200
H -1.04895000 1.16082800 -2.76061600
H -1.14670800 -0.31228300 -3.76043800
C 0.04634200 2.08565600 0.62065600
C 1.04240200 1.89751400 -1.46833700
C 1.22122200 3.26947300 -1.57076100
C 0.78457900 4.06840400 -0.52167700
C 0.19615900 3.47212200 0.58496700
C -0.56172300 1.37978900 1.77109000
C -1.14004300 -0.65948400 2.71220600
C -1.58062100 -0.06052700 3.88475800
C -1.51658100 1.32407100 3.97731900
C -1.00173100 2.05068300 2.91202400
H 1.37117800 1.22530000 -2.25994800
H 1.69315700 3.69213800 -2.45295300
H 0.90327500 5.14847400 -0.55897300
H -0.14511100 4.09141400 1.40929100
H -1.17264400 -1.74230900 2.59013400
H -1.96843900 -0.67152800 4.69521600
H -1.85738900 1.83805600 4.87275600
H -0.93390200 3.13216700 2.98358100
N 0.46526000 1.32289300 -0.40969200
N -0.66012300 0.03723600 1.68094200
C 1.21529900 -1.42480800 -1.91018400
H 0.62846600 -1.06512900 -2.76338000
H 2.20424700 -0.94728400 -1.90005500
H 1.34866600 -2.51106000 -1.98464700
C -0.00669200 -2.90045600 0.15979300
H -0.63610900 -3.34067600 -0.62043000
H 0.96230900 -3.41620800 0.16784700

H -0.48166300 -3.03469200 1.14236000
C 2.73729500 0.41240500 1.61151900
C 3.49444900 1.28906700 0.82230900
C 2.37665800 0.80259400 2.90728300
C 3.86739400 2.53449700 1.31422900
H 3.78511100 0.98226000 -0.18297800
C 2.75317100 2.04914300 3.39830100
H 1.79594600 0.11957600 3.52798800
C 3.49397200 2.91867500 2.60183600
H 4.45093600 3.20967500 0.69013500
H 2.46355200 2.34196700 4.40653700
H 3.78668900 3.89440500 2.98560200
S 2.28584800 -1.19461600 1.00221700
Pt 0.22586700 -0.87933300 -0.19128800
Pt -2.36127100 -0.69005500 -1.38686300

10a
E(RM06) = -1869.96235301
Zero-point correction= 0.651214 (Hartree/Particle)
Thermal correction to Energy= 0.696422
Thermal correction to Enthalpy= 0.697366
Thermal correction to Gibbs Free Energy= 0.570942
Sum of electronic and zero-point Energies= -1869.311139
Sum of electronic and thermal Energies= -1869.265931
Sum of electronic and thermal Enthalpies= -1869.264987
Sum of electronic and thermal Free Energies= -1869.391411
E(RM06) = -1870.49895666

N 1.20823400 0.58741200 1.01669100
C 0.93558700 1.33677700 2.08777300
C 1.28863600 2.67604000 2.17636200
C 1.95395500 3.25335100 1.10172300
C 2.25134500 2.47460900 -0.00787400
C 1.87693500 1.13112600 -0.02386800
N 1.75451000 -1.04383500 -1.05445400
C 1.99382700 -1.89611500 -2.05396100
C 2.65151500 -1.52611600 -3.21861600
C 3.08430200 -0.21119500 -3.34039200
C 2.84365500 0.67738700 -2.30290400
C 2.17363900 0.23616500 -1.16159000
H 0.40756600 0.83610000 2.89992400
H 1.03639500 3.24669300 3.06625600
H 1.63763400 -2.91517200 -1.91165100
H 2.81728800 -2.25731600 -4.00486500
H 3.60816800 0.12210400 -4.23321700
H 2.24578600 4.30066200 1.12562900
C 0.91018200 -3.63599400 0.77174300
H -0.07971400 -4.09484700 0.89084100
H 1.33167900 -3.95611200 -0.19519400
H 1.56380900 -4.02760400 1.56830600
H 3.18864300 1.70363500 -2.38159700
H 2.78651400 2.91212100 -0.84494700
C 0.25835600 -1.88032300 2.83311500
H 1.12267300 -1.68361300 3.49090900
H -0.54108700 -1.17386300 3.10317300
H -0.09955800 -2.89883700 3.04027000
C -1.99865400 1.52834600 0.89337600
C -2.74947000 0.02300900 2.49366900
C -3.05133700 1.03767800 3.39035000
C -2.80793900 2.34977700 3.00359300
C -2.28316700 2.59758900 1.74317100
C -1.43621100 1.71749800 -0.46236800
C -0.70392200 0.71119100 -2.41954400
C -0.45513800 1.93498000 -3.02539000
C -0.70494400 3.09072000 -2.29618400
C -1.20306200 2.98131000 -1.00495900
H -2.92729500 -1.02221900 2.74348100
H -3.46714300 0.79680500 4.36446500
H -3.02701000 3.17698500 3.67437100
H -2.08900200 3.62064400 1.43455800
H -0.52244900 -0.22336400 -2.95040400
H -0.07022900 1.97050000 -4.04085100
H -0.52156100 4.07148800 -2.72817700
H -1.41843400 3.88057000 -0.43535400
N -2.22989600 0.25874800 1.28569600

N -1.16602100 0.60200800 -1.17272800
C -2.50760000 -2.91745200 0.89413800
H -1.86861900 -3.08118700 1.76962200
H -3.52440100 -2.64944500 1.21367300
H -2.56038900 -3.83893700 0.30045900
C -1.30766400 -2.72513400 -1.64831000
H -0.57771300 -3.44889700 -1.27159900
H -2.20721000 -3.27064800 -1.96507300
H -0.89253300 -2.20172300 -2.52189800
Se -3.98602300 -1.18076000 -1.40774200
C -4.70642000 0.50941500 -0.77655700
C -5.44392500 0.56376000 0.41109800
C -4.50905200 1.67836600 -1.51801500
C -5.97311000 1.77332300 0.85112600
H -5.59800400 -0.34713300 0.99077900
C -5.03969300 2.88760700 -1.07376000
H -3.93633800 1.63948600 -2.44533800
C -5.76954600 2.93711800 0.11106200
H -6.54361100 1.80783000 1.77823100
H -4.87972000 3.79353000 -1.65689200
H -6.18375300 3.88231400 0.45760500
C 4.39745700 -2.00790300 0.64463300
C 3.85747600 -1.75343300 1.90740500
C 3.99563800 -0.47557000 2.45385500
C 4.64803400 0.52826700 1.74792300
C 5.19525000 0.28715900 0.47575400
C 5.05145800 -1.00383700 -0.06042700
H 4.29581600 -3.00062500 0.20206200
H 3.36873200 -2.54711600 2.47085100
H 3.58255800 -0.25903000 3.44057900
H 4.74175500 1.52245400 2.18665800
H 5.46021700 -1.21740000 -1.04903000
Se 6.11877800 1.68766700 -0.50140800
Pt -1.73819500 -1.34020500 -0.17806700
Pt 0.88539700 -1.58943500 0.90290600

10b
E(RM06) = -1886.98761494
Zero-point correction= 0.649194 (Hartree/Particle)
Thermal correction to Energy= 0.694912
Thermal correction to Enthalpy= 0.695856
Thermal correction to Gibbs Free Energy= 0.567533
Sum of electronic and zero-point Energies= -1886.338421
Sum of electronic and thermal Energies= -1886.292703
Sum of electronic and thermal Enthalpies= -1886.291759
Sum of electronic and thermal Free Energies= -1886.420082
E(RM06) = -1887.57747464

N 1.22792000 0.60491500 0.99601600
C 0.96199500 1.35810100 2.06417400
C 1.33107200 2.69328900 2.15731000
C 2.00917000 3.26095800 1.08571000
C 2.29857800 2.47857800 -0.02356800
C 1.90478100 1.13978700 -0.04105600
N 1.76150800 -1.03089000 -1.08517800
C 1.99698000 -1.87752800 -2.08834100
C 2.66124200 -1.50978800 -3.25086800
C 3.10533400 -0.19808000 -3.36340200
C 2.87031000 0.68621800 -2.32077600
C 2.19293100 0.24389600 -1.18361900
H 0.42374400 0.86603100 2.87589100
H 1.08358600 3.26695300 3.04674600
H 1.63421300 -2.89641100 -1.95414200
H 2.82305300 -2.23830200 -4.04056800
H 3.63466600 0.13637800 -4.25270400
H 2.31609700 4.30406900 1.11115700
C 0.89557200 -3.61239300 0.77757400
H -0.09100900 -4.07304300 0.90466400
H 1.31561000 -3.89762400 -0.19949900
H 1.56412400 -3.97562800 1.57192600
Pd 0.87833500 -1.56949900 0.87604800
H 3.22520400 1.70942100 -2.39440400
H 2.84251000 2.91038300 -0.85811300
C 0.23942000 -1.86324800 2.79447700
H 1.12942700 -1.68540000 3.41907300

H -0.52839300 -1.11546500 3.03736700
H -0.15086300 -2.86702700 3.00499300
C -2.02118300 1.51127800 0.93483400
C -2.79113000 0.00524800 2.51969500
C -3.09011900 1.01498700 3.42363200
C -2.83470300 2.32723000 3.04609000
C -2.30006200 2.57829600 1.79035400
C -1.44773800 1.70838100 -0.41706200
C -0.71858500 0.72177900 -2.38100100
C -0.44763000 1.94971200 -2.97035200
C -0.68369300 3.09806100 -2.22543600
C -1.18992100 2.97704200 -0.93832500
H -2.97757100 -1.03974700 2.76675600
H -3.51183900 0.77087100 4.39446100
H -3.05097000 3.15227800 3.72058400
H -2.09725100 3.60207200 1.48976300
H -0.54482700 -0.20656200 -2.92631500
H -0.05595300 1.99375300 -3.98299200
H -0.48188300 4.08240600 -2.64110300
H -1.39065200 3.87169900 -0.35624900
N -2.26711100 0.24205600 1.31507000
N -1.19212300 0.59971100 -1.14075500
Pd -1.78813500 -1.35060400 -0.16645500
C -2.57055400 -2.92064100 0.89361600
H -1.88422400 -3.04976000 1.73668000
H -3.56749000 -2.60810600 1.22533500
H -2.64362400 -3.83554300 0.29718100
C -1.36341700 -2.73852700 -1.62509700
H -0.60648000 -3.41456500 -1.21866500
H -2.24913000 -3.30871800 -1.92692800
H -0.97533700 -2.17120100 -2.48036300
Se -3.99747300 -1.22314600 -1.41760200
C -4.70162800 0.46950300 -0.79273200
C -5.45434100 0.52699800 0.38602100
C -4.47909500 1.63899300 -1.52782400
C -5.97634000 1.74002000 0.82235700
H -5.62368800 -0.38387200 0.96108600
C -5.00581500 2.85092900 -1.08849700
H -3.88873600 1.59648000 -2.44372500
C -5.75183000 2.90319800 0.08648100
H -6.55890200 1.77891400 1.74156200
H -4.82859400 3.75741300 -1.66558300
H -6.16135100 3.85159000 0.42975300
C 4.37710500 -2.01353100 0.64769400
C 3.84397800 -1.73011800 1.90647300
C 4.01142000 -0.44949000 2.43687400
C 4.68795000 0.52955700 1.71886300
C 5.23057600 0.25858300 0.45106800
C 5.05642600 -1.03459600 -0.06910600
H 4.24949000 -3.00835300 0.21678100
H 3.32936400 -2.50277000 2.47603700
H 3.59938300 -0.21030100 3.41890500
H 4.80247900 1.52794400 2.14320500
H 5.46004200 -1.27041300 -1.05461800
Se 6.18844000 1.62485800 -0.54265300

10c
E(RM06) = -2647.61049599
Zero-point correction= 0.653296 (Hartree/Particle)
Thermal correction to Energy= 0.697460
Thermal correction to Enthalpy= 0.698404
Thermal correction to Gibbs Free Energy= 0.576346
Sum of electronic and zero-point Energies= -2646.957200
Sum of electronic and thermal Energies= -2646.913036
Sum of electronic and thermal Enthalpies= -2646.912092
Sum of electronic and thermal Free Energies= -2647.034150
E(RM06) = -2648.18053396

N 1.22139400 0.59040000 1.01341800
C 0.95175400 1.34200300 2.08366100
C 1.31364700 2.67869600 2.17242800
C 1.98929000 3.25011200 1.10083600
C 2.28649700 2.46864100 -0.00649800
C 1.89903200 1.12854500 -0.02415900
N 1.75011800 -1.04133200 -1.06121800

C 1.97561100 -1.89214600 -2.06526500
C 2.63135200 -1.52450700 -3.23148000
C 3.07969600 -0.21424200 -3.34943800
C 2.85560600 0.67214900 -2.30684700
C 2.18519600 0.23352100 -1.16429900
H 0.41895600 0.84530900 2.89519100
H 1.06156400 3.25191100 3.06076400
H 1.60898600 -2.90776700 -1.92537200
H 2.78412500 -2.25392000 -4.02205400
H 3.60289400 0.11625300 -4.24361700
H 2.28983500 4.29489200 1.12644100
C 0.90354000 -3.63191200 0.76347500
H -0.08719900 -4.08771400 0.88660100
H 1.31909000 -3.95071300 -0.20638300
H 1.56008500 -4.02683200 1.55580500
H 3.21561900 1.69341900 -2.37940600
H 2.83426300 2.89903700 -0.83890100
C 0.26665200 -1.87848700 2.83114200
H 1.13588500 -1.69309400 3.48525400
H -0.52465600 -1.16593900 3.10823200
H -0.09980400 -2.89465600 3.03495300
C -1.97744100 1.53902500 0.91494400
C -2.72212000 0.03112200 2.51549500
C -3.02971000 1.04460900 3.41150100
C -2.79536300 2.35774800 3.02276600
C -2.27063700 2.60753100 1.76273600
C -1.41647200 1.73066600 -0.44152700
C -0.69558700 0.72882000 -2.40483600
C -0.44496300 1.95385700 -3.00767200
C -0.68554300 3.10768300 -2.27241900
C -1.17830700 2.99558300 -0.97933600
H -2.89559700 -1.01487700 2.76527700
H -3.44481300 0.80238700 4.38558300
H -3.02109900 3.18440600 3.69203400
H -2.08418600 3.63156300 1.45271300
H -0.51997900 -0.20466900 -2.93963400
H -0.06504300 1.99172600 -4.02492900
H -0.49877100 4.08932600 -2.70101900
H -1.38487000 3.89364700 -0.40463700
N -2.20316300 0.26892800 1.30796000
N -1.15225400 0.61732800 -1.15670400
C -2.50309700 -2.90902100 0.89995200
H -1.87074400 -3.07111000 1.78032700
H -3.52303700 -2.64156200 1.20880500
H -2.54767400 -3.82934200 0.30405700
C -1.31299800 -2.71084700 -1.64545200
H -0.60414800 -3.45583800 -1.27039000
H -2.22671500 -3.22392500 -1.97384800
H -0.87672000 -2.18599100 -2.50770000
C -4.58736700 0.36798200 -0.77674200
C -5.34928900 0.42077400 0.39874000
C -4.43146800 1.53526600 -1.53522200
C -5.92724500 1.61548800 0.81180200
H -5.47994800 -0.48802700 0.98734000
C -5.01401200 2.72983700 -1.12167800
H -3.84583400 1.49836000 -2.45446100
C -5.75881300 2.77409100 0.05410900
H -6.51216700 1.64369300 1.73016800
H -4.88214400 3.63005500 -1.72056300
H -6.21283500 3.70883700 0.37858400
C 4.37510700 -2.02036300 0.63334900
C 3.83159000 -1.77297000 1.89788900
C 3.97847500 -0.49568200 2.44797800
C 4.62445800 0.50983000 1.74331000
C 5.16635500 0.28941300 0.45654600
C 5.02300300 -1.01416800 -0.06971500
H 4.27610100 -3.01224400 0.18736900
H 3.35012100 -2.57015800 2.46239500
H 3.57144500 -0.28194600 3.43826400
H 4.72004100 1.50359200 2.18366100
H 5.42943800 -1.22241900 -1.06088300
S -3.86303700 -1.16144600 -1.31987500
S 5.96928000 1.56713600 -0.43760400
Pt -1.73540000 -1.32917900 -0.16976200
Pt 0.88846200 -1.58538800 0.89912900

11a
E(RM06) = -1869.97416938
Zero-point correction= 0.651667 (Hartree/Particle)
Thermal correction to Energy= 0.696705
Thermal correction to Enthalpy= 0.697649
Thermal correction to Gibbs Free Energy= 0.572742
Sum of electronic and zero-point Energies= -1869.322503
Sum of electronic and thermal Energies= -1869.277465
Sum of electronic and thermal Enthalpies= -1869.276521
Sum of electronic and thermal Free Energies= -1869.401428
E(RM06) = -1870.50963026

N -3.38290600 0.91004900 -0.00425800
C -3.36602200 2.20002800 -0.35436000
C -3.68565800 3.22103400 0.52831700
C -4.03716200 2.87976300 1.83013300
C -4.06936400 1.54135100 2.19201900
C -3.74695000 0.56386800 1.24818700
N -3.45166600 -1.72257700 0.54537700
C -3.47042600 -3.04016900 0.76215100
C -3.79312400 -3.59794700 1.99093500
C -4.12509300 -2.74321400 3.03544200
C -4.12637800 -1.37504700 2.81045700
C -3.78072800 -0.88251600 1.55101700
H -3.07723000 2.41154700 -1.38460800
H -3.64991100 4.25588400 0.19838700
H -3.20819900 -3.66903600 -0.08731600
H -3.78383900 -4.67703000 2.11677200
H -4.38692900 -3.13604400 4.01508000
H -4.28825500 3.64781300 2.55783400
C -2.91705000 -2.40518000 -2.65857000
H -1.90367300 -2.56394800 -3.04229200
H -3.23721600 -3.29849000 -2.09861200
H -3.60425700 -2.28028100 -3.50771400
H -4.39144800 -0.69788900 3.61734000
H -4.35474900 1.26447400 3.20305500
C -2.77345200 0.33722100 -3.14337800
H -3.74501900 0.75091500 -3.45305400
H -2.08479000 1.17189100 -2.95138600
H -2.37159900 -0.25733300 -3.97461200
C -0.19260400 2.14777800 0.04008500
C 0.17411900 2.02485700 -2.24833100
C 0.29786800 3.40167800 -2.36105000
C 0.16520500 4.17070700 -1.21075400
C -0.07283000 3.53789300 -0.00018200
C -0.44107400 1.40614200 1.29425400
C -0.74245900 -0.66101100 2.30026600
C -0.82715300 -0.09916600 3.56590100
C -0.72744400 1.28297300 3.67960500
C -0.52941500 2.04040500 2.53500200
H 0.27646000 1.37542900 -3.11694800
H 0.49504200 3.85243800 -3.32966900
H 0.25214300 5.25384200 -1.25230400
H -0.17377000 4.13026600 0.90473000
H -0.81778200 -1.73931500 2.15844200
H -0.97634100 -0.73562300 4.43412500
H -0.79532600 1.76810300 4.65046300
H -0.43080300 3.11920400 2.61526300
N -0.08013100 1.41318900 -1.08721100
N -0.57038700 0.06571100 1.19293000
C 0.26966600 -1.27770300 -2.78940700
H -0.49150900 -0.93204700 -3.49902400
H 1.22752300 -0.78262200 -3.00990300
H 0.40954600 -2.36067400 -2.91431700
C -0.34771600 -2.80117400 -0.49572100
H -1.06372300 -3.30793000 -1.15297700
H 0.64114600 -3.25950700 -0.64742000
H -0.64699000 -2.97265000 0.55042500
Se 2.36319300 -0.98322500 -0.15402900
Se -5.71938700 -0.74833300 -1.93488300
C 2.83479700 0.83306500 0.33972000
C 3.22879900 1.75863700 -0.63594400
C 2.76532100 1.25244000 1.67402300
C 3.53513900 3.06979400 -0.28572300

H 3.28522300 1.44433800 -1.67911300
C 3.07952800 2.56427400 2.02345500
H 2.45852200 0.54297500 2.44395200
C 3.46104700 3.47889100 1.04535000
H 3.83128400 3.77838700 -1.05886600
H 3.01791500 2.87212600 3.06711200
H 3.70286600 4.50497400 1.31767800
C -6.56304100 -0.81565700 -0.18904600
C -6.87120500 -2.04531900 0.40878500
C -6.86908500 0.36219500 0.50421800
C -7.46116300 -2.09358000 1.66797400
H -6.63616800 -2.96999500 -0.11942900
C -7.46134500 0.31159000 1.76431500
H -6.63709300 1.32726500 0.05128900
C -7.75645200 -0.91549000 2.35276500
H -7.68750200 -3.05906400 2.11977500
H -7.68774600 1.23946600 2.28932200
H -8.21784300 -0.95501800 3.33818200
Pt -0.25031200 -0.77535600 -0.86335700
Pt -3.03647200 -0.76294200 -1.42113000

11b
E(RM06) = -1886.99770037
Zero-point correction= 0.650174 (Hartree/Particle)
Thermal correction to Energy= 0.695438
Thermal correction to Enthalpy= 0.696383
Thermal correction to Gibbs Free Energy= 0.571506
Sum of electronic and zero-point Energies= -1886.347526
Sum of electronic and thermal Energies= -1886.302262
Sum of electronic and thermal Enthalpies= -1886.301318
Sum of electronic and thermal Free Energies= -1886.426194
E(RM06) = -1887.58717290

N -3.38259400 0.91527000 0.00544300
C -3.36315900 2.20530200 -0.33742300
C -3.67965100 3.22645200 0.54761500
C -4.03125500 2.88075200 1.84782100
C -4.06572900 1.54071700 2.20456500
C -3.74517500 0.56678900 1.25570600
N -3.45628400 -1.72170700 0.55231700
C -3.47731200 -3.03744300 0.77070000
C -3.80011100 -3.59736300 1.99938500
C -4.12996300 -2.74114200 3.04315200
C -4.12863000 -1.37275900 2.81753700
C -3.78182300 -0.88219900 1.55699000
H -3.07484400 2.42330700 -1.36708800
H -3.64166400 4.26248200 0.22130400
H -3.21672000 -3.66945300 -0.07816000
H -3.79241500 -4.67649300 2.12577700
H -4.39224400 -3.13283500 4.02327100
H -4.28058600 3.64640400 2.57886900
C -2.93362000 -2.37047000 -2.69289900
H -1.91650300 -2.50806800 -3.07178400
H -3.24912200 -3.24353800 -2.10272600
H -3.63173700 -2.23223500 -3.52749300
Pd -3.04758800 -0.75998100 -1.42453100
H -4.39208100 -0.69569000 3.62511500
H -4.35114100 1.26172300 3.21506600
C -2.75854600 0.33030800 -3.14094900
H -3.74202200 0.69829500 -3.46169900
H -2.11025800 1.17622800 -2.87817700
H -2.30156500 -0.24584700 -3.95346800
C -0.17575100 2.16084500 0.04169600
C 0.18694700 2.04261900 -2.24371100
C 0.30610600 3.42057000 -2.35833700
C 0.17474900 4.18703700 -1.20646500
C -0.05917100 3.55182600 0.00413900
C -0.42750900 1.41882900 1.29769200
C -0.74423000 -0.64074000 2.30470900
C -0.82967000 -0.07869400 3.57107900
C -0.72016100 1.30259000 3.68264800
C -0.51419900 2.05700000 2.53710300
H 0.28811300 1.39623300 -3.11570400
H 0.49794200 3.87323700 -3.32723500
H 0.25825000 5.27062200 -1.24659800

H -0.16087500 4.14381800 0.90927500
H -0.82715200 -1.71965700 2.16661800
H -0.98654200 -0.71294600 4.43970100
H -0.78704400 1.78996500 4.65260500
H -0.40853600 3.13522000 2.61710300
N -0.06003200 1.42833200 -1.08435100
N -0.56301200 0.08088600 1.19729200
Pd -0.22667000 -0.76944500 -0.86125100
C 0.30154800 -1.27915500 -2.77605200
H -0.47777700 -0.91552900 -3.45360700
H 1.25181600 -0.76131900 -2.96096400
H 0.44417400 -2.35895600 -2.90172300
C -0.34772300 -2.79407000 -0.52927400
H -1.07579800 -3.26750300 -1.19519200
H 0.63837400 -3.25122300 -0.68206500
H -0.65415400 -2.92344500 0.51880300
Se 2.35631200 -1.01163000 -0.12720400
Se -5.72057700 -0.74813500 -1.92436700
C 2.83908400 0.79873300 0.36517000
C 3.23775900 1.72158100 -0.61170900
C 2.77317500 1.21892400 1.69965300
C 3.55324200 3.03039700 -0.26240900
H 3.28900600 1.40650400 -1.65482900
C 3.09707400 2.52830200 2.04806500
H 2.46114900 0.51201800 2.46961700
C 3.48381900 3.43988400 1.06899700
H 3.85303900 3.73700200 -1.03588300
H 3.03872900 2.83730700 3.09152800
H 3.73275800 4.46440300 1.34078100
C -6.56580000 -0.79911500 -0.18238700
C -6.87854500 -2.02403700 0.42377800
C -6.86921400 0.38468100 0.50268000
C -7.47229500 -2.06189400 1.68116200
H -6.64331000 -2.95291600 -0.09676000
C -7.46485000 0.34432100 1.76112100
H -6.63160000 1.34573200 0.04444100
C -7.76589600 -0.87801600 2.35686200
H -7.70272500 -3.02344000 2.13920100
H -7.68932700 1.27626700 2.27966500
H -8.22989100 -0.90926800 3.34136200

11c
E(RM06) = -2647.62293952
Zero-point correction= 0.651377 (Hartree/Particle)
Thermal correction to Energy= 0.696063
Thermal correction to Enthalpy= 0.697007
Thermal correction to Gibbs Free Energy= 0.573246
Sum of electronic and zero-point Energies= -2663.993806
Sum of electronic and thermal Energies= -2663.949120
Sum of electronic and thermal Enthalpies= -2663.948176
Sum of electronic and thermal Free Energies= -2664.071937
E(RM06) = -2665.26757338

N 1.19740100 0.91364200 1.04619400
C 0.82790900 1.41186300 2.22935400
C 0.90682900 2.76206800 2.53688300
C 1.39517500 3.62944400 1.56597700
C 1.79871200 3.11414000 0.34356200
C 1.70292300 1.74103900 0.10781700
N 2.01975600 -0.22244100 -1.25399800
C 2.40992700 -0.83568800 -2.37423100
C 2.91423500 -0.15404800 -3.47226500
C 3.03386600 1.22774100 -3.39054900
C 2.64981100 1.86800500 -2.22208200
C 2.13912800 1.11969400 -1.16043600
H 0.45016600 0.69192400 2.95577300
H 0.58494100 3.11739600 3.51222000
H 2.30488600 -1.91895700 -2.38858800
H 3.20749900 -0.70153200 -4.36370000
H 3.42585000 1.80368800 -4.22552900
H 1.46859300 4.69706600 1.75913500
C 1.64504900 -3.22507900 0.03167200
H 0.74444700 -3.73361800 -0.32735000
H 2.40783900 -3.22710700 -0.76351700
H 2.05509900 -3.77955700 0.88762800

H 2.74257600 2.94754600 -2.14580600
H 2.19839700 3.78134600 -0.41469300
C 0.64845100 -2.07490000 2.35134600
H 1.51818900 -2.39442700 2.94431800
H 0.09870500 -1.31410100 2.92627300
H -0.00920200 -2.94238600 2.21540400
C -2.15497600 1.07695300 1.25517000
C -2.47176000 -0.92416900 2.38615400
C -2.95163300 -0.27645000 3.51502300
C -3.02426100 1.11145100 3.49706800
C -2.62700300 1.79306400 2.35632300
C -1.71052200 1.73603600 0.00888900
C -0.81516400 1.47177000 -2.11286900
C -0.89153300 2.83094600 -2.37958100
C -1.39349000 3.66766700 -1.38900800
C -1.81039000 3.11483100 -0.18727900
H -2.39257400 -2.00962700 2.34865300
H -3.25684600 -0.85280300 4.38392500
H -3.38795900 1.66096700 4.36209300
H -2.67702500 2.87803300 2.33327600
H -0.43109700 0.77432600 -2.85766100
H -0.55873600 3.21626800 -3.33974600
H -1.46847400 4.74028100 -1.55148000
H -2.22489900 3.75635100 0.58515800
N -2.07297400 -0.27005400 1.29159100
N -1.19564900 0.93753000 -0.94974600
C -1.75395900 -3.20342700 -0.00918800
H -1.05979600 -3.58302900 0.74830300
H -2.77799400 -3.20750300 0.39376100
H -1.73102200 -3.87374300 -0.88007000
C -0.63507000 -2.05611100 -2.30817000
H 0.15103100 -2.80384800 -2.14736000
H -1.46520400 -2.53737900 -2.84604600
H -0.23350000 -1.25270600 -2.94513800
C -4.59409700 -0.05490100 -0.72882400
C -5.27258800 -0.51212700 0.41293900
C -4.72305500 1.29923700 -1.07339200
C -6.04516800 0.35191700 1.18002400
H -5.18306100 -1.56282700 0.69282700
C -5.49741500 2.16419400 -0.30472000
H -4.20811400 1.67008500 -1.96087000
C -6.16069200 1.69644100 0.82675900
H -6.55991300 -0.02599800 2.06321100
H -5.58001700 3.21203200 -0.59326600
H -6.76686600 2.37216000 1.42810300
C 4.58338600 -0.03311100 0.70452400
C 5.21206100 -0.37924200 -0.50326100
C 4.71092900 1.28942200 1.15667600
C 5.92490500 0.56293000 -1.23479100
H 5.12405500 -1.40400000 -0.86768200
C 5.43221900 2.23091500 0.42737300
H 4.23267100 1.57548500 2.09472000
C 6.03828500 1.87493200 -0.77483700
H 6.39416200 0.27198600 -2.17455200
H 5.51377000 3.25196900 0.79996800
H 6.59889800 2.61154100 -1.34826300
S 3.64932800 -1.22752100 1.62322200
S -3.60579000 -1.15577200 -1.70658100
Pt 1.29232400 -1.27027400 0.56659300
Pt -1.32361700 -1.26081300 -0.53487500

12a
E(RM06) = -934.805487329
Zero-point correction= 0.325678 (Hartree/Particle)
Thermal correction to Energy= 0.347494
Thermal correction to Enthalpy= 0.348438
Thermal correction to Gibbs Free Energy= 0.274070
Sum of electronic and zero-point Energies= -934.479809
Sum of electronic and thermal Energies= -934.457994
Sum of electronic and thermal Enthalpies= -934.457050
Sum of electronic and thermal Free Energies= -934.531418
E(RM06) = -935.070158997

N 1.14428900 -1.48316900 -0.31211200
C 0.93539200 -2.79094900 -0.48518200

C 1.94511200 -3.73358000 -0.35637500
C 3.22221400 -3.28737400 -0.04364200
C 3.44208100 -1.92831800 0.13655100
C 2.38088200 -1.03618300 -0.00181800
N 1.46194200 1.19532100 -0.08441000
C 1.54369900 2.52157100 0.05194500
C 2.71437900 3.16271700 0.42933500
C 3.83814400 2.38590600 0.67446600
C 3.75285000 1.00609100 0.54239900
C 2.54539500 0.42585700 0.16067700
H -0.07993600 -3.08860100 -0.74081500
H 1.72817500 -4.78699000 -0.50611200
H 0.63606500 3.08528200 -0.15626600
H 2.73508800 4.24413300 0.52568100
H 4.77768800 2.84591400 0.97030700
H 4.04653800 -3.98895400 0.05674700
C -1.55488000 1.75675000 -1.03559400
H -1.83729800 2.08054600 -0.02091100
H -0.97500300 2.54467100 -1.53411300
H -2.45585300 1.55358600 -1.62452400
Pt -0.37078100 0.11102400 -0.73826600
H 4.62673500 0.39373700 0.74240700
H 4.44136700 -1.57301600 0.36826500
C -2.03289800 -1.03253200 -1.13205200
H -2.66574300 -0.64078200 -1.93676200
H -1.73977300 -2.06059500 -1.37870200
H -2.59877100 -1.01987000 -0.18810900
C 1.85974500 0.39352300 -3.22225400
C 2.79196900 -0.64875600 -3.22927300
C 4.15273800 -0.35679400 -3.25011400
C 4.58069100 0.96894300 -3.25464100
C 3.65119200 2.00895100 -3.24833400
C 2.29036500 1.72470900 -3.23713900
H 2.45036500 -1.68389700 -3.21194900
H 4.87952200 -1.16718600 -3.25517400
H 5.64529700 1.19473200 -3.26362800
H 3.98846200 3.04387400 -3.25253200
H 1.55667000 2.53091900 -3.22727700
Se -0.03289800 -0.01028000 -3.19827000

12b
E(RM06) = -943.320441127
Zero-point correction= 0.325070 (Hartree/Particle)
Thermal correction to Energy= 0.346966
Thermal correction to Enthalpy= 0.347910
Thermal correction to Gibbs Free Energy= 0.273790
Sum of electronic and zero-point Energies= -942.995371
Sum of electronic and thermal Energies= -942.973475
Sum of electronic and thermal Enthalpies= -942.972531
Sum of electronic and thermal Free Energies= -943.046651
E(RM06) = -943.610853938

N 1.17181100 -1.47290900 -0.34249500
C 0.97629200 -2.77946000 -0.53168500
C 1.98557400 -3.72116100 -0.38851800
C 3.25177800 -3.27263400 -0.03781500
C 3.45999200 -1.91433100 0.16065900
C 2.39801500 -1.02537000 0.00171500
N 1.47943100 1.20833800 -0.08193200
C 1.56399700 2.53211900 0.06692200
C 2.72683700 3.17108500 0.47296800
C 3.84417100 2.39053500 0.73450500
C 3.75859500 1.01226500 0.58862600
C 2.55662000 0.43718900 0.17964400
H -0.03047300 -3.08319500 -0.81467200
H 1.77673700 -4.77394600 -0.55407900
H 0.66264800 3.10255600 -0.15285900
H 2.74654700 4.25177800 0.57846700
H 4.77849600 2.84617900 1.05304200
H 4.07636400 -3.97155600 0.07868800
C -1.50591900 1.76108200 -1.08624400
H -1.74742200 2.01049100 -0.04178900
H -0.90052700 2.54028400 -1.56203200
H -2.40907900 1.57189200 -1.67174100
Pd -0.32931800 0.12255900 -0.79392200

H 4.62800700 0.39758100 0.80069100
H 4.45123200 -1.55814100 0.42348700
C -1.99361600 -1.01248400 -1.15730900
H -2.66261200 -0.62916400 -1.93279500
H -1.67754800 -2.03293900 -1.39525000
H -2.46789600 -0.95293800 -0.16700400
C 1.77643100 0.37808100 -3.25542000
C 2.70247000 -0.67123600 -3.25007300
C 4.06478700 -0.38889800 -3.24457200
C 4.50228300 0.93408500 -3.23001000
C 3.58032000 1.98107500 -3.23400300
C 2.21819800 1.70674400 -3.25337600
H 2.35321700 -1.70379000 -3.24258500
H 4.78594900 -1.20429200 -3.24093800
H 5.56850100 1.15190700 -3.21505900
H 3.92530400 3.01335600 -3.22285800
H 1.49082700 2.51847800 -3.25152700
Se -0.11580200 -0.01028500 -3.25442000

12c
E(RM06) = -1323.62909968
Zero-point correction= 0.326952 (Hartree/Particle)
Thermal correction to Energy= 0.348298
Thermal correction to Enthalpy= 0.349242
Thermal correction to Gibbs Free Energy= 0.276443
Sum of electronic and zero-point Energies= -1323.302147
Sum of electronic and thermal Energies= -1323.280801
Sum of electronic and thermal Enthalpies= -1323.279857
Sum of electronic and thermal Free Energies= -1323.352656
E(RM06) = -1323.90481793

N -1.20013300 0.55574800 -1.05813400
C -1.13050000 0.99101500 -2.31932800
C -1.37661400 2.31039500 -2.66924500
C -1.70745200 3.20554300 -1.66134500
C -1.77010900 2.75752700 -0.34850100
C -1.50540600 1.41974400 -0.06503400
N -1.18911300 -0.41525400 1.47084600
C -1.21815600 -0.96740800 2.68611500
C -1.60226800 -0.26384700 3.81856100
C -1.97787200 1.06442100 3.66844400
C -1.94794300 1.64094300 2.40556500
C -1.54548700 0.87714700 1.31177000
H -0.87317300 0.24825200 -3.07261500
H -1.30890500 2.61893400 -3.70817600
H -0.92706600 -2.01433800 2.74910000
H -1.61153600 -0.75477300 4.78712100
H -2.29748700 1.65119200 4.52597000
H -1.91179200 4.24867100 -1.88934700
C -0.35997800 -3.41050700 0.30684900
H 0.73638000 -3.45507900 0.22930800
H -0.66691700 -3.48070800 1.35746600
H -0.80115100 -4.24486500 -0.24949200
H -2.25496100 2.67481500 2.28069300
H -2.01543200 3.45590800 0.44548000
C -0.63108300 -2.38286400 -2.31016400
H -1.33613400 -1.90997400 -3.00539100
H 0.40433400 -2.14429800 -2.59975900
H -0.78458200 -3.46665900 -2.32978400
S -3.03926400 -2.39761100 -0.43356900
C -3.98777400 -0.90503700 -0.48762100
C -4.25495400 -0.28107700 -1.71468800
C -4.48311500 -0.34716900 0.69843300
C -4.98053400 0.90177100 -1.74871100
H -3.87475600 -0.72540400 -2.63432100
C -5.22487400 0.82805700 0.65666800
H -4.27589300 -0.83866600 1.64902000
C -5.46390600 1.45711000 -0.56332200
H -5.17531700 1.39163200 -2.70090600
H -5.60812900 1.25935000 1.57958000
H -6.03382100 2.38380600 -0.59278900
Pt -0.86348600 -1.56385100 -0.44377400

13a
E(UM06) = -934.956022415
Zero-point correction= 0.323789 (Hartree/Particle)
Thermal correction to Energy= 0.346048
Thermal correction to Enthalpy= 0.346992
Thermal correction to Gibbs Free Energy= 0.270470
Sum of electronic and zero-point Energies= -934.632233
Sum of electronic and thermal Energies= -934.609974
Sum of electronic and thermal Enthalpies= -934.609030
Sum of electronic and thermal Free Energies= -934.685553
E(UM06) = -935.218623831

N 1.09617300 -1.45799200 -0.32305500
C 0.89483700 -2.76912100 -0.48638200
C 1.91511100 -3.70385000 -0.39890300
C 3.20218100 -3.24998800 -0.13458700
C 3.41805300 -1.88995000 0.02722500
C 2.34428400 -1.00467800 -0.07609200
N 1.39511400 1.20847600 -0.12294800
C 1.47203900 2.53734200 -0.00682200
C 2.65313800 3.19707500 0.29950000
C 3.80113900 2.43772400 0.48513400
C 3.72602700 1.05751900 0.36326000
C 2.50381700 0.45851000 0.06090400
H -0.12927800 -3.07250000 -0.69810500
H 1.69932800 -4.75936400 -0.53796800
H 0.54454200 3.08488300 -0.16817800
H 2.66434300 4.27978500 0.38709900
H 4.74991500 2.91246400 0.72368900
H 4.03364700 -3.94678400 -0.06070700
C -1.70567000 1.72335900 -0.83197200
H -1.97878700 2.09369400 0.17008700
H -1.18277800 2.52748100 -1.37362600
H -2.62975200 1.49177000 -1.37904300
H 4.61855900 0.45645600 0.50967500
H 4.42320900 -1.52342000 0.21382600
C -2.13059900 -1.02775500 -0.94916200
H -2.60910700 -0.79179500 -1.91065500
H -1.87859100 -2.09998100 -0.94941900
H -2.86739400 -0.84608000 -0.15127600
C 2.00911300 0.36823900 -3.28921700
C 2.93460400 -0.68262500 -3.25380300
C 4.30092100 -0.42004200 -3.18281900
C 4.76198800 0.89326800 -3.13642400
C 3.84736100 1.94560300 -3.16681400
C 2.48289700 1.68700200 -3.24447600
H 2.57820400 -1.71341200 -3.27403200
H 5.00704800 -1.24954000 -3.15384500
H 5.82966200 1.09762600 -3.07560500
H 4.19908600 2.97601600 -3.12501800
H 1.76928300 2.51190400 -3.25846400
Se 0.10572900 0.01088400 -3.34929900
Pt -0.44817700 0.11273400 -0.63924700

13b
E(UM06) = -943.476430547
Zero-point correction= 0.322741 (Hartree/Particle)
Thermal correction to Energy= 0.345261
Thermal correction to Enthalpy= 0.346206
Thermal correction to Gibbs Free Energy= 0.268981
Sum of electronic and zero-point Energies= -943.153690
Sum of electronic and thermal Energies= -943.131169
Sum of electronic and thermal Enthalpies= -943.130225
Sum of electronic and thermal Free Energies= -943.207450
E(UM06) = -943.766173789

N 1.11036100 -1.45774400 -0.33799600
C 0.92085500 -2.76809000 -0.50724700
C 1.94523100 -3.69945500 -0.41633800
C 3.22646300 -3.23744700 -0.14024900
C 3.43159000 -1.87634500 0.03021800
C 2.35138500 -0.99852500 -0.07743600
N 1.39520000 1.21524300 -0.10624500
C 1.47109400 2.54107400 0.02274500
C 2.64988600 3.20342600 0.33694200

C 3.79804600 2.44404800 0.51842500
C 3.72519100 1.06448300 0.38417800
C 2.50347900 0.46720000 0.07355600
H -0.09960600 -3.07964900 -0.72872700
H 1.73746800 -4.75594400 -0.56092600
H 0.54345900 3.09081600 -0.13513700
H 2.65919900 4.28549000 0.43379200
H 4.74596600 2.91789000 0.76278900
H 4.06238000 -3.92867100 -0.06228700
C -1.71844300 1.70523900 -0.83452200
H -1.97277900 2.00272800 0.19467900
H -1.16401500 2.51255900 -1.33449700
H -2.63634800 1.49770900 -1.39620600
Pd -0.44373200 0.11457000 -0.68627200
H 4.61937900 0.46490800 0.52682900
H 4.43298200 -1.50591100 0.22905100
C -2.13345600 -1.00059200 -1.00107500
H -2.60974200 -0.76114900 -1.95979200
H -1.83808800 -2.06024500 -0.99824700
H -2.84710400 -0.81316100 -0.18627000
C 1.98310100 0.37658300 -3.29535900
C 2.89293800 -0.68870400 -3.27502500
C 4.26250600 -0.44751200 -3.19776300
C 4.74275900 0.85810600 -3.13008200
C 3.84409400 1.92453600 -3.14507900
C 2.47639600 1.68745500 -3.22882600
H 2.52110600 -1.71346900 -3.31138600
H 4.95637300 -1.28760500 -3.18041700
H 5.81327700 1.04541300 -3.06415900
H 4.21133400 2.94865900 -3.08636500
H 1.77492700 2.52267700 -3.23010800
Se 0.07610800 0.05033900 -3.36673300

13c
E(UM06) = -1323.77929574
Zero-point correction= 0.324440 (Hartree/Particle)
Thermal correction to Energy= 0.346378
Thermal correction to Enthalpy= 0.347322
Thermal correction to Gibbs Free Energy= 0.271977
Sum of electronic and zero-point Energies= -1323.454856
Sum of electronic and thermal Energies= -1323.432918
Sum of electronic and thermal Enthalpies= -1323.431973
Sum of electronic and thermal Free Energies= -1323.507319
E(UM06) = -1324.05771439

N -1.20474800 0.47954800 -1.06257400
C -1.16272200 0.90050000 -2.32986500
C -1.43526500 2.21045200 -2.69495700
C -1.76411400 3.11676100 -1.69526600
C -1.81208100 2.68279900 -0.37803100
C -1.53096000 1.34968600 -0.08190800
N -1.18746800 -0.47096800 1.45860700
C -1.21568000 -1.01473200 2.67879300
C -1.60834900 -0.31071700 3.80711900
C -1.99640800 1.01508900 3.65288800
C -1.97597000 1.58186000 2.38742500
C -1.56547200 0.81511600 1.29625600
H -0.89867300 0.14946300 -3.07312700
H -1.38561100 2.50540600 -3.73929300
H -0.91121800 -2.05831400 2.74403600
H -1.61157900 -0.79694500 4.77850800
H -2.31802800 1.60365700 4.50874500
H -1.98044100 4.15514900 -1.93483700
C -0.22691200 -3.43178300 0.29938200
H 0.82796300 -3.64198200 0.06523000
H -0.35341900 -3.46897100 1.39295900
H -0.83898600 -4.23207200 -0.14087500
H -2.29716100 2.61067200 2.25322800
H -2.06387800 3.38572400 0.41044400
C -0.35617800 -2.36310800 -2.28073100
H -1.14874700 -2.05906100 -2.98264900
H 0.60468200 -1.95367300 -2.63391100
H -0.29181800 -3.45958300 -2.29454900
S -3.27086900 -2.36610900 -0.43415100
C -4.14597200 -0.83347000 -0.46781300

C -4.40444000 -0.17943800 -1.68515700
C -4.58530300 -0.22238200 0.71824600
C -5.07739800 1.03566700 -1.71388800
H -4.05943600 -0.63987800 -2.61202100
C -5.26144800 0.99332100 0.68706700
H -4.38703200 -0.71383300 1.67178100
C -5.51016600 1.62895700 -0.52749900
H -5.26342200 1.52653900 -2.66877100
H -5.59071500 1.44942900 1.62047300
H -6.03717100 2.58139100 -0.55114200
Pt -0.77374700 -1.58757300 -0.42719900

14a
E(UM06) = -1175.73088285
Zero-point correction= 0.414309 (Hartree/Particle)
Thermal correction to Energy= 0.444605
Thermal correction to Enthalpy= 0.445549
Thermal correction to Gibbs Free Energy= 0.347364
Sum of electronic and zero-point Energies= -1175.316574
Sum of electronic and thermal Energies= -1175.286278
Sum of electronic and thermal Enthalpies= -1175.285334
Sum of electronic and thermal Free Energies= -1175.383519
E(UM06) = -1176.07760048

N -2.70854800 0.83194900 -1.33585600
C -2.98996100 1.52796700 -2.44057700
C -3.37795500 2.85959500 -2.41033200
C -3.46367400 3.49097200 -1.17632000
C -3.16458800 2.77341200 -0.02699200
C -2.79290700 1.43324300 -0.12940600
N -2.06100900 -0.66236700 0.81267200
C -1.70815100 -1.44304400 1.83800400
C -1.74335400 -1.01424200 3.15665800
C -2.17294400 0.28153600 3.41531600
C -2.53732300 1.09694600 2.35387600
C -2.46112200 0.60617300 1.05065600
H -2.89842000 0.98862400 -3.38222000
H -3.60125900 3.38214500 -3.33609500
H -1.38292700 -2.45030000 1.58423700
H -1.44386800 -1.68725500 3.95502000
H -2.22349400 0.65794300 4.43416400
H -3.75592200 4.53589200 -1.10512800
C -1.38029200 -3.22495900 -1.16544100
H -0.40692000 -3.39047200 -1.64938500
H -1.28973000 -3.51599700 -0.10742600
H -2.11706600 -3.88715400 -1.64498300
H -2.86836800 2.11313800 2.54599800
H -3.21631100 3.26380100 0.94043800
C -2.07128300 -1.67252200 -3.33837300
H -3.08062300 -2.04328600 -3.57807800
H -1.88232500 -0.75672100 -3.91894700
H -1.34118400 -2.42987600 -3.65495000
Se 0.59333700 -0.34178500 -1.60762400
Se 2.00345000 -2.03875800 0.65721600
C 3.42724800 -0.73505400 0.73927400
C 4.33126400 -0.60344900 -0.32432700
C 3.55431500 0.11482200 1.84670100
C 5.33633500 0.35757700 -0.27970800
H 4.23897000 -1.25898000 -1.19028700
C 4.56731700 1.06772100 1.89142500
H 2.85062600 0.02799400 2.67473700
C 5.45861800 1.19511800 0.82804600
H 6.03080900 0.45075800 -1.11351300
H 4.65671200 1.71910200 2.75975700
H 6.24683600 1.94523900 0.86200700
C 0.50392800 1.37801300 -0.71808200
C 0.58167600 1.47823700 0.67438800
C 0.33503100 2.53768700 -1.48506300
C 0.49715200 2.72413900 1.29024700
H 0.71076000 0.57491000 1.27257100
C 0.24208900 3.77821300 -0.86167100
H 0.26440900 2.46356900 -2.57068100
C 0.32395300 3.87584000 0.52680000
H 0.55861700 2.78957100 2.37639300
H 0.10207800 4.67390400 -1.46541700

H 0.25248700 4.84821100 1.01102800
Pt -1.96998800 -1.26237100 -1.32743900

14b
E(UM06) = -1184.25110629
Zero-point correction= 0.413385 (Hartree/Particle)
Thermal correction to Energy= 0.443829
Thermal correction to Enthalpy= 0.444774
Thermal correction to Gibbs Free Energy= 0.346750
Sum of electronic and zero-point Energies= -1183.837721
Sum of electronic and thermal Energies= -1183.807277
Sum of electronic and thermal Enthalpies= -1183.806333
Sum of electronic and thermal Free Energies= -1183.904357
E(UM06) = -1184.62476459

N -2.75061700 0.83432400 -1.33720400
C -3.04577700 1.53203400 -2.43557900
C -3.44224700 2.86205200 -2.40217200
C -3.52034500 3.49014500 -1.16635000
C -3.20895100 2.77102100 -0.02091200
C -2.83149200 1.43246200 -0.13068900
N -2.07297800 -0.65559900 0.81150600
C -1.72354100 -1.43291800 1.83854900
C -1.77547800 -1.01047900 3.15967300
C -2.22121900 0.27985600 3.41668200
C -2.58672800 1.09295000 2.35346100
C -2.49241400 0.60460100 1.04983500
H -2.95935200 0.99713300 -3.38099900
H -3.67639800 3.38520900 -3.32505400
H -1.38425900 -2.43717900 1.58798700
H -1.47689300 -1.68243600 3.95939500
H -2.28524500 0.65377000 4.43585200
H -3.81625000 4.53384900 -1.09022500
C -1.27046900 -3.17209200 -1.21971700
H -0.32383200 -3.32276800 -1.75288400
H -1.12764500 -3.40351400 -0.15421900
H -2.03942500 -3.83169500 -1.64514100
Pd -1.91020000 -1.22889800 -1.34350200
H -2.93456700 2.10347200 2.54617600
H -3.25393400 3.26044500 0.94743700
C -1.99687100 -1.63849400 -3.34827300
H -3.01687700 -1.99958500 -3.54745600
H -1.81531900 -0.69616800 -3.88335700
H -1.26825600 -2.38687200 -3.67950100
Se 0.60893900 -0.30352100 -1.61004300
Se 1.99365600 -2.03882500 0.63111100
C 3.44718700 -0.76842200 0.71465600
C 4.36009600 -0.66263700 -0.34419700
C 3.59031100 0.07957300 1.82145800
C 5.39119400 0.27013800 -0.29455300
H 4.25424700 -1.31616000 -1.21012000
C 4.62879500 1.00431800 1.87101100
H 2.88035400 0.01216900 2.64589300
C 5.53003400 1.10515400 0.81311700
H 6.09282400 0.34300400 -1.12438700
H 4.73122300 1.65401600 2.73912700
H 6.33892300 1.83272100 0.85120300
C 0.48593600 1.40200300 -0.70086200
C 0.56756200 1.48890600 0.69250900
C 0.29295000 2.56634400 -1.45533700
C 0.46421400 2.72668500 1.32109500
H 0.71243300 0.58122300 1.28043000
C 0.18399100 3.79878400 -0.81933700
H 0.21733600 2.50147900 -2.54119700
C 0.27063800 3.88333100 0.56973600
H 0.52780700 2.78262100 2.40755900
H 0.02721100 4.69833800 -1.41313000
H 0.18622000 4.84949700 1.06424400

14c
E(UM06) = -1953.37460806
Zero-point correction= 0.416162 (Hartree/Particle)
Thermal correction to Energy= 0.445502
Thermal correction to Enthalpy= 0.446446
Thermal correction to Gibbs Free Energy= 0.351503

Sum of electronic and zero-point Energies= -1952.958446
Sum of electronic and thermal Energies= -1952.929106
Sum of electronic and thermal Enthalpies= -1952.928162
Sum of electronic and thermal Free Energies= -1953.023105
E(UM06) = -1953.75338987

N -1.83106800 0.76106800 -1.17566000
C -1.31612900 1.48707700 -2.17218300
C -1.54977900 2.84739400 -2.30862800
C -2.35756200 3.47310800 -1.36822100
C -2.89254700 2.72332900 -0.33011300
C -2.60987700 1.36053500 -0.24867200
N -2.85892600 -0.81650800 0.75484700
C -3.28045600 -1.63745300 1.72035500
C -4.00873000 -1.19752900 2.81562200
C -4.29967300 0.15815800 2.90973100
C -3.85511800 1.01575500 1.91442300
C -3.13025100 0.50314700 0.83830900
H -0.69145600 0.94838600 -2.88361400
H -1.10848000 3.39437300 -3.13689400
H -3.01655200 -2.68764200 1.60389200
H -4.33268200 -1.90472200 3.57381600
H -4.86275000 0.54860700 3.75400300
H -2.57286800 4.53655800 -1.43905300
C -1.42692600 -3.45531900 -0.70633700
H -0.38881300 -3.80680900 -0.61641900
H -1.97319500 -3.76127300 0.19967400
H -1.88291000 -3.95360100 -1.57490800
H -4.06012200 2.07952800 1.99042200
H -3.52927900 3.20375100 0.40657000
C -0.36957200 -1.71625700 -2.60780700
H -1.02933100 -1.67153700 -3.48990600
H 0.37933100 -0.91196600 -2.68469600
H 0.16115300 -2.67755200 -2.61457000
C 3.51332100 -0.18074500 -0.98852600
C 3.15799300 0.14956800 -2.31227800
C 4.10993100 0.81421100 -0.18832700
C 3.37269200 1.42910800 -2.80578800
H 2.70705800 -0.61809700 -2.94073900
C 4.33339100 2.08878400 -0.68999200
H 4.37977000 0.56898200 0.83824100
C 3.95910200 2.40433900 -1.99657000
H 3.08704800 1.66943800 -3.82881400
H 4.79252700 2.84641200 -0.05683000
H 4.12706300 3.40699700 -2.38572100
C 0.32492600 0.42812900 1.33416000
C -0.27554300 0.80202700 2.54668500
C 0.84448300 1.43161600 0.50106100
C -0.35161600 2.14154600 2.91411300
H -0.69058500 0.03004400 3.19583400
C 0.77286400 2.76742600 0.87696000
H 1.30411300 1.15118800 -0.44720500
C 0.17191200 3.12962900 2.08244000
H -0.82702700 2.41435000 3.85561600
H 1.18589700 3.53210200 0.21920700
H 0.11271100 4.17742500 2.37209800
S 0.38231400 -1.27217700 0.86640300
S 3.17907500 -1.76028500 -0.33781800
Pt -1.50622600 -1.41205900 -0.92885300

15a
E(UM06) = -1869.92448059
Zero-point correction= 0.647502 (Hartree/Particle)
Thermal correction to Energy= 0.694390
Thermal correction to Enthalpy= 0.695334
Thermal correction to Gibbs Free Energy= 0.560077
Sum of electronic and zero-point Energies= -1869.276979
Sum of electronic and thermal Energies= -1869.230091
Sum of electronic and thermal Enthalpies= -1869.229146
Sum of electronic and thermal Free Energies= -1869.364404
E(UM06) = -1870.45947544

N -3.52525900 0.96566000 0.25951600
C -3.59295600 2.27425800 -0.00721000
C -3.63879500 3.24345500 0.98533600

C -3.61737400 2.83025900 2.31161800
C -3.54532100 1.47270400 2.59420800
C -3.49635900 0.55277900 1.54757500
N -3.39727100 -1.68429000 0.66323300
C -3.26606700 -3.00793700 0.79850900
C -3.13350600 -3.63099300 2.03118200
C -3.14214700 -2.84058700 3.17408400
C -3.27448000 -1.46564000 3.04041500
C -3.39482700 -0.90514600 1.76864100
H -3.61122400 2.54475200 -1.06324200
H -3.68789000 4.29494800 0.71502400
H -3.26643600 -3.58334100 -0.12538700
H -3.02660800 -4.71074500 2.08518700
H -3.04255400 -3.28619700 4.16083200
H -3.65529200 3.55465100 3.12166400
C -3.91186900 -2.20183100 -2.53108000
H -3.11804100 -2.24879700 -3.29071100
H -3.92215500 -3.16244500 -1.98869300
H -4.87513000 -2.10653300 -3.05822200
H -3.26641300 -0.83627700 3.92592600
H -3.52919600 1.13940900 3.62783500
C -3.96517300 0.56285000 -2.89401600
H -4.97954100 0.99334000 -2.82566800
H -3.24662800 1.39968000 -2.91725400
H -3.89086100 0.03068500 -3.85401500
C -0.37760400 2.26706900 -0.52895000
C -0.66633200 2.23306000 -2.83247200
C -0.66004400 3.61823200 -2.91180000
C -0.49721100 4.34289100 -1.73699500
C -0.34841000 3.66253900 -0.53733600
C -0.24736300 1.47157700 0.71129800
C -0.17412300 -0.64124300 1.66518100
C 0.02845100 -0.12303700 2.93755800
C 0.08226600 1.25701900 3.08438800
C -0.05854800 2.06101200 1.96130000
H -0.78371700 1.61404400 -3.72154400
H -0.77765500 4.10911400 -3.87379400
H -0.48189400 5.43016000 -1.75202000
H -0.21691000 4.22261500 0.38416200
H -0.22066400 -1.71696900 1.49817700
H 0.13588400 -0.79464700 3.78563200
H 0.23465100 1.70794500 4.06222800
H -0.00560300 3.14115500 2.06347200
N -0.53626100 1.57598700 -1.67672700
N -0.31672400 0.12757000 0.58335100
C -0.59965400 -1.06106700 -3.52947000
H -1.57869600 -0.72921700 -3.90552900
H 0.19775200 -0.51241500 -4.05560700
H -0.48501800 -2.13155700 -3.75097000
C -0.40743200 -2.67242200 -1.24407600
H -1.29886700 -3.15566900 -1.66961400
H 0.48379500 -3.10021500 -1.72821600
H -0.35928200 -2.90709800 -0.16760100
Se 2.31444400 -0.58156500 -1.71558400
Se 3.02037000 -2.43834100 0.77818100
C 2.74006700 1.21609900 -1.13145000
C 2.83613900 2.24415900 -2.07862700
C 2.93226200 1.51369900 0.22147000
C 3.11482700 3.54574200 -1.67332400
H 2.67858800 2.02145400 -3.13498300
C 3.22739700 2.81556400 0.61848500
H 2.86041900 0.72114400 0.96599400
C 3.31470300 3.83674400 -0.32410900
H 3.17595300 4.33855200 -2.41814800
H 3.38134800 3.02853800 1.67664300
H 3.53915400 4.85515300 -0.01146200
C 4.52959700 -1.35429900 1.30799500
C 5.64005200 -1.21405700 0.46442200
C 4.50449300 -0.64512000 2.51735400
C 6.68839200 -0.36855700 0.81416000
H 5.66988700 -1.76160400 -0.47760100
C 5.56241200 0.18683600 2.87086100
H 3.63841700 -0.73610200 3.17394900
C 6.65358800 0.33510300 2.01702200
H 7.54055900 -0.26155700 0.14425100

H 5.52925100 0.73081700 3.81401000
H 7.47565900 0.99509400 2.28851700
Pt -0.48202000 -0.63064900 -1.51775500
Pt -3.62156400 -0.62291200 -1.25362800

15b
E(UM06) = -1886.96606250
Zero-point correction= 0.646657 (Hartree/Particle)
Thermal correction to Energy= 0.693343
Thermal correction to Enthalpy= 0.694287
Thermal correction to Gibbs Free Energy= 0.561018
Sum of electronic and zero-point Energies= -1886.319406
Sum of electronic and thermal Energies= -1886.272719
Sum of electronic and thermal Enthalpies= -1886.271775
Sum of electronic and thermal Free Energies= -1886.405044
E(UM06) = -1887.55604799

N -3.10254000 1.24430300 -0.49026800
C -2.76402700 2.48549500 -0.84490900
C -3.08320100 3.60302400 -0.08403600
C -3.78724100 3.41223300 1.09751700
C -4.14217100 2.12253500 1.47236600
C -3.78651200 1.04752800 0.65780300
N -3.78084000 -1.29655900 0.09182300
C -4.03917300 -2.57864400 0.35881400
C -4.65337600 -3.00088300 1.53063500
C -5.01698700 -2.03820800 2.46374400
C -4.75110100 -0.70294000 2.19329700
C -4.12452700 -0.35461700 0.99618000
H -2.20848600 2.58031000 -1.77908200
H -2.77972900 4.59264700 -0.41564600
H -3.73531900 -3.29572100 -0.40295500
H -4.83868100 -4.05810800 1.69899900
H -5.50071600 -2.32026100 3.39597700
H -4.06095600 4.25676700 1.72559500
C -2.78357500 -2.21892200 -2.91555800
H -1.75748200 -2.51511600 -3.17125300
H -3.26870200 -3.04155500 -2.36497200
H -3.34127600 -2.04262200 -3.84744800
Pd -2.78990300 -0.54442000 -1.74178100
H -5.01815100 0.05528500 2.92395400
H -4.69610400 1.96620700 2.39350600
C -2.00833800 0.37944000 -3.38979500
H -2.81469800 0.97191600 -3.85285000
H -1.21495000 1.06417800 -3.04797200
H -1.58934000 -0.29710000 -4.14635700
C 0.16330800 1.83613700 0.38656200
C 1.11663700 1.52243600 -1.70189300
C 1.40786700 2.87332800 -1.83737300
C 1.03650100 3.73089300 -0.80854200
C 0.40977600 3.20835100 0.31321600
C -0.46724800 1.20625800 1.56964300
C -1.27544600 -0.73566900 2.53462800
C -1.59873000 -0.08569100 3.71941300
C -1.33562400 1.27464700 3.81161700
C -0.75774200 1.92544400 2.72986100
H 1.38897400 0.80927900 -2.48140200
H 1.91632800 3.23118600 -2.72892000
H 1.23522600 4.79817500 -0.87466200
H 0.11493000 3.87182000 1.12146600
H -1.45695600 -1.80522800 2.41639800
H -2.04577000 -0.63957600 4.54087300
H -1.56696600 1.82643700 4.71990100
H -0.52564200 2.98416200 2.80296500
N 0.50580900 1.01751900 -0.62730400
N -0.73814600 -0.11274600 1.48625200
Pd -0.00338300 -1.13349600 -0.38673200
C 0.79493100 -1.82052400 -2.14595200
H 0.20617900 -1.34891600 -2.94492000
H 1.83634000 -1.47062200 -2.15768500
H 0.76965500 -2.91139600 -2.25410900
C -0.58636000 -3.08394400 -0.11403500
H -1.26689100 -3.37790700 -0.92293000
H 0.27819000 -3.75981800 -0.09187500
H -1.10998300 -3.12436200 0.85387200

Se 2.26334700 -1.74257300 1.04864900
Se 4.76537000 -1.60021000 -0.91186700
C 2.58209500 -0.11418400 2.04284600
C 3.09192100 1.02472300 1.41089700
C 2.26875800 -0.05984700 3.40626400
C 3.29245800 2.19680900 2.13373000
H 3.32213800 0.99482800 0.34541800
C 2.46316300 1.11821200 4.12173600
H 1.85955400 -0.94056800 3.90234400
C 2.97528600 2.25032100 3.48956000
H 3.68881000 3.07636000 1.62543300
H 2.20993300 1.15155300 5.18081400
H 3.12815000 3.16934300 4.05284000
C 4.61170400 -0.00538600 -1.99166100
C 4.01564900 -0.05119500 -3.26197900
C 5.11392500 1.22109800 -1.52742700
C 3.93334500 1.09538300 -4.04674600
H 3.62436900 -0.99691100 -3.63719000
C 5.02442000 2.36584500 -2.31211900
H 5.58319000 1.26955200 -0.54435400
C 4.43641200 2.30734400 -3.57520300
H 3.47704100 1.04074700 -5.03432800
H 5.42320500 3.30819300 -1.93881100
H 4.37432000 3.20259000 -4.19215000

15c
E(UM06) = -2647.54894091
Zero-point correction= 0.646945 (Hartree/Particle)
Thermal correction to Energy= 0.692315
Thermal correction to Enthalpy= 0.693259
Thermal correction to Gibbs Free Energy= 0.565483
Sum of electronic and zero-point Energies= -2646.901996
Sum of electronic and thermal Energies= -2646.856626
Sum of electronic and thermal Enthalpies= -2646.855682
Sum of electronic and thermal Free Energies= -2646.983458
E(UM06) = -2648.12496296

N -3.14116100 0.59952500 -1.02704000
C -2.91134600 1.60746000 -1.88003400
C -3.33146400 2.90511100 -1.66524500
C -4.06881000 3.17672400 -0.49619700
C -4.30943800 2.15622400 0.39570800
C -3.82600200 0.85490200 0.14438600
N -3.41650800 -1.44560500 0.69677400
C -3.48480900 -2.48135700 1.54784300
C -4.10266300 -2.42539300 2.77995500
C -4.71113300 -1.21023300 3.15685800
C -4.64789900 -0.13587400 2.30323600
C -3.97500500 -0.24203300 1.06367400
H -2.35005800 1.34496900 -2.77915500
H -3.10249000 3.67988500 -2.39288400
H -3.00923300 -3.40066200 1.20638900
H -4.12170300 -3.30021600 3.42414400
H -5.22319700 -1.11985800 4.11289500
H -4.43515200 4.18067600 -0.29092200
C -2.18548500 -3.49555200 -1.52041400
H -1.14441300 -3.71820900 -1.78783000
H -2.42645300 -4.03848200 -0.59221900
H -2.83477100 -3.88951700 -2.32099300
H -5.10384000 0.80871400 2.59136700
H -4.85947900 2.36249900 1.31125500
C -1.93730400 -1.33561400 -3.27607800
H -2.85018800 -1.23829200 -3.89042700
H -1.31884900 -0.44029000 -3.44624000
H -1.37743400 -2.21048900 -3.63753800
C 0.11962300 2.01044700 -1.02978400
C 0.97061700 0.74624100 -2.78905700
C 1.19785300 1.86850900 -3.56530400
C 0.87279600 3.11712300 -3.03142700
C 0.33697100 3.18568700 -1.75828300
C -0.46832100 1.99916500 0.31572400
C -1.19354700 0.71277200 2.11179300
C -1.62598800 1.82857200 2.80949100
C -1.45755400 3.08239500 2.22548700
C -0.87262900 3.16197300 0.97000200

H 1.21119000 -0.25226100 -3.15304200
H 1.62123600 1.76642800 -4.56077400
H 1.03841300 4.02660700 -3.60444000
H 0.08008200 4.15237600 -1.33352100
H -1.30258700 -0.28699700 2.53290600
H -2.09173900 1.70941600 3.78467800
H -1.78079700 3.98570900 2.73763300
H -0.74545200 4.13233700 0.49730900
N 0.44393500 0.80608200 -1.55777300
N -0.62180800 0.78117300 0.90369300
C 1.08404200 -2.31844600 -1.45419600
H 0.62442400 -2.33774000 -2.45358500
H 2.13601100 -1.99411600 -1.55370500
H 1.08015900 -3.34096600 -1.04987000
C -0.05200700 -2.47371300 1.10237300
H -0.57704800 -3.34172000 0.68153400
H 0.95446900 -2.79549400 1.41739200
H -0.60131500 -2.13364100 1.99558400
C 2.83547200 1.43095800 1.23446400
C 3.39842100 1.39070700 -0.04591900
C 2.56073800 2.65637300 1.84395200
C 3.71023100 2.57857800 -0.69781900
H 3.58256400 0.42836500 -0.52624600
C 2.85378100 3.84160300 1.17502400
H 2.11268200 2.67468300 2.83734300
C 3.43490700 3.80253200 -0.08997500
H 4.15156900 2.54918000 -1.69280200
H 2.63277600 4.79771900 1.64659300
H 3.66881600 4.73045000 -0.60924200
C 5.02632400 -1.38125100 1.28474300
C 4.47696600 -2.48062800 0.61931900
C 6.15225800 -0.73842600 0.76877400
C 5.04581100 -2.92031300 -0.56994500
H 3.59492900 -2.97515900 1.02751200
C 6.73036100 -1.19783600 -0.41250100
H 6.56259100 0.12748600 1.28675800
C 6.17387500 -2.28118700 -1.08556400
H 4.61061300 -3.77037900 -1.09336000
H 7.60839200 -0.69600600 -0.81497600
H 6.61849100 -2.63130700 -2.01529700
S 2.41252300 -0.09129400 2.06790300
S 4.28873300 -0.75232300 2.78664500
Pt -2.51362400 -1.47533300 -1.30709200
Pt 0.12567100 -0.94808000 -0.26125900

16a
E(UM06) = -1869.91415588
Zero-point correction= 0.647360 (Hartree/Particle)
Thermal correction to Energy= 0.694016
Thermal correction to Enthalpy= 0.694960
Thermal correction to Gibbs Free Energy= 0.560655
Sum of electronic and zero-point Energies= -1869.266796
Sum of electronic and thermal Energies= -1869.220140
Sum of electronic and thermal Enthalpies= -1869.219195
Sum of electronic and thermal Free Energies= -1869.353501
E(UM06) = -1870.44688347

N -3.11796300 1.22435800 -0.49668200
C -2.83028300 2.46026600 -0.91812900
C -3.16518600 3.59783500 -0.19715800
C -3.83285800 3.44063300 1.01094900
C -4.13078900 2.15924700 1.45533300
C -3.75685600 1.05895200 0.68490400
N -3.61572300 -1.30398200 0.24481200
C -3.76473100 -2.58601900 0.59460700
C -4.31677000 -2.97795900 1.80589100
C -4.73769800 -1.99130300 2.68932400
C -4.57806500 -0.65894400 2.33575700
C -4.00313100 -0.33594900 1.10679200
H -2.30903000 2.52770800 -1.87318100
H -2.90227300 4.57996100 -0.58119400
H -3.42407100 -3.32053400 -0.13333500
H -4.41339100 -4.03392400 2.04229500
H -5.18058100 -2.25278200 3.64733200
H -4.11873900 4.30455100 1.60610400

C -2.69224900 -2.35785700 -2.71698300
H -1.65362900 -2.60522700 -2.98585000
H -3.10273800 -3.20061700 -2.13483300
H -3.27072200 -2.28506800 -3.65219800
H -4.88701700 0.12080300 3.02618900
H -4.64954800 2.02601800 2.40027100
C -2.10215600 0.29529700 -3.38286900
H -2.90959700 0.90808300 -3.82056200
H -1.25875400 0.96869100 -3.15007500
H -1.76165900 -0.41160900 -4.15410700
C 0.15995700 1.97123300 0.35973200
C 1.04224400 1.69816900 -1.77034700
C 1.24809600 3.06087000 -1.92244500
C 0.88541600 3.90266500 -0.87551700
C 0.33967700 3.35368800 0.27421500
C -0.40873400 1.31068600 1.55390300
C -1.02927900 -0.68558000 2.55646700
C -1.44129000 -0.04232100 3.71611800
C -1.32689700 1.34026500 3.77717700
C -0.80090300 2.02154700 2.68805200
H 1.30887700 0.99233900 -2.55637200
H 1.68278100 3.44688400 -2.84019700
H 1.02893200 4.97787000 -0.95169100
H 0.05903800 4.00291800 1.09895600
H -1.09551300 -1.76941100 2.46145100
H -1.84624600 -0.62024400 4.54274900
H -1.63792300 1.88698100 4.66439700
H -0.69959900 3.10234000 2.72887000
N 0.50757100 1.16698700 -0.66538000
N -0.53535200 -0.03451000 1.50182000
C 0.99919500 -1.66078200 -2.14747200
H 0.34722200 -1.31067600 -2.96283600
H 2.00686100 -1.23814900 -2.28403300
H 1.07385100 -2.75564000 -2.21146500
C -0.11364600 -2.99184400 0.04640200
H -0.83158300 -3.41026900 -0.67557700
H 0.81783600 -3.57346900 -0.01217100
H -0.52660400 -3.11413600 1.06165200
Se 2.77930000 -1.16409200 0.79826000
C 2.74707500 0.30698000 2.05547400
C 3.10230000 1.60220600 1.65488100
C 2.34464300 0.10146600 3.38494000
C 3.05264400 2.66182700 2.55608200
H 3.41564500 1.77854200 0.62461500
C 2.29248400 1.16049100 4.28253400
H 2.06616000 -0.90231300 3.70832900
C 2.64555600 2.44734800 3.87408600
H 3.32713400 3.66369900 2.22587100
H 1.97496200 0.98257000 5.30996100
H 2.59947600 3.27890000 4.57590000
Pt -2.77373200 -0.59973700 -1.66203900
Pt 0.22966200 -1.00145600 -0.35312000
C 5.47726100 -0.63517000 4.92260000
C 5.87153100 0.38901300 4.03988600
C 6.26954400 0.05254300 2.73171900
C 6.28801100 -1.27413500 2.32670700
C 5.90483200 -2.28185900 3.21394900
C 5.49715800 -1.95947300 4.51004500
H 5.15818100 -0.37532100 5.93108600
H 6.56398700 0.84389900 2.04359300
H 6.60081800 -1.52864600 1.31542900
H 5.92313600 -3.32214300 2.89348000
H 5.19741400 -2.74745100 5.19867000
Se 5.87250200 2.19994000 4.60905100

16b

E(RM06) = -1886.97665919
Zero-point correction= 0.649155 (Hartree/Particle)
Thermal correction to Energy= 0.694846
Thermal correction to Enthalpy= 0.695790
Thermal correction to Gibbs Free Energy= 0.568659
Sum of electronic and zero-point Energies= -1886.327504
Sum of electronic and thermal Energies= -1886.281813
Sum of electronic and thermal Enthalpies= -1886.280869
Sum of electronic and thermal Free Energies= -1886.408000

E(RM06) = -1887.56598553

N -3.02555700 1.02839100 -0.28099700
C -2.83984700 2.29805300 -0.64755600
C -3.37507400 3.37291800 0.05089700
C -4.14169400 3.10522100 1.17695100
C -4.34590600 1.78500000 1.55845600
C -3.77676500 0.75651400 0.80775900
N -3.37184100 -1.57642900 0.33720700
C -3.48030400 -2.87623000 0.62035000
C -4.16024700 -3.35678700 1.73165700
C -4.76005600 -2.43558600 2.58049900
C -4.65624400 -1.08214700 2.28956200
C -3.94877100 -0.67327100 1.15873800
H -2.22926800 2.45513900 -1.53770300
H -3.18694400 4.38914800 -0.28518800
H -2.99621400 -3.56079000 -0.07535500
H -4.21399800 -4.42557400 1.91837000
H -5.30440700 -2.76315400 3.46293700
H -4.58025200 3.91355200 1.75715500
C -1.99138900 -2.40173000 -2.54545700
H -0.93395500 -2.56244800 -2.78788500
H -2.37347900 -3.27237400 -1.98913100
H -2.55709100 -2.30575900 -3.48422500
H -5.11678700 -0.35608800 2.95316000
H -4.94734500 1.56980600 2.43667200
C -1.56260500 0.25954500 -3.04141500
H -2.43938500 0.65186000 -3.58235500
H -0.95113600 1.10317600 -2.68882500
H -0.96751000 -0.35405300 -3.72968100
C 0.07386000 2.09877800 0.69778000
C 1.13455400 1.90443300 -1.35394900
C 1.27812800 3.27940400 -1.47861500
C 0.78822600 4.08328800 -0.45750300
C 0.18299200 3.48886200 0.64121000
C -0.55947000 1.39808400 1.83928700
C -1.17857100 -0.62922000 2.77210900
C -1.65306400 -0.02309200 3.92814900
C -1.57602800 1.36089400 4.01872100
C -1.02425800 2.07809300 2.96561900
H 1.50359300 1.23077000 -2.12715500
H 1.76204500 3.70014400 -2.35538200
H 0.87576400 5.16576600 -0.51131200
H -0.20728800 4.11276200 1.44009300
H -1.21867000 -1.71283500 2.65464600
H -2.07268500 -0.62741700 4.72787000
H -1.93560200 1.88155100 4.90303500
H -0.94570700 3.15900600 3.03679100
N 0.54761800 1.32965200 -0.30222100
N -0.65760500 0.05599000 1.75388600
C 1.37220700 -1.42182800 -1.72579900
H 0.72779900 -1.11416000 -2.55716800
H 2.31201400 -0.85726800 -1.71129400
H 1.58183100 -2.49566200 -1.76383900
C 0.03162400 -2.88653600 0.24213300
H -0.59053900 -3.23867000 -0.58640000
H 0.96953400 -3.45247900 0.27158700
H -0.49343500 -2.98326600 1.20148700
Se 2.41048000 -1.30836700 1.28428900
C 2.81969800 0.49081100 1.85926200
C 3.57796800 1.33640000 1.04124500
C 2.37140600 0.94779900 3.10270100
C 3.87999200 2.62643600 1.46355800
H 3.92511300 0.97710300 0.07167600
C 2.67409100 2.24048800 3.52152800
H 1.78199200 0.28705400 3.73959500
C 3.42826700 3.07896300 2.70362200
H 4.46883000 3.28220100 0.82403900
H 2.32105100 2.59203800 4.49003200
H 3.66630900 4.08919900 3.03223400
C 5.18456300 -0.64049800 4.60135900
C 6.19771800 -0.00347100 3.86559000
C 6.56923000 -0.57369700 2.63567800
C 5.96362700 -1.73392600 2.16902500
C 4.96014600 -2.35809300 2.91363700

C 4.57733800 -1.79964200 4.13434400
H 4.87437800 -0.21519700 5.55628300
H 7.35326700 -0.09846200 2.04560300
H 6.27882900 -2.16125700 1.21652500
H 4.50586100 -3.28365300 2.56225600
H 3.79511400 -2.27518100 4.72760600
Se 7.05171500 1.61267200 4.52180000
Pd -2.31681800 -0.72687600 -1.42446600
Pd 0.30786800 -0.87107700 -0.06617600

16c
E(UM06) = -2647.56269944
Zero-point correction= 0.648611 (Hartree/Particle)
Thermal correction to Energy= 0.694798
Thermal correction to Enthalpy= 0.695742
Thermal correction to Gibbs Free Energy= 0.562450
Sum of electronic and zero-point Energies= -2646.914088
Sum of electronic and thermal Energies= -2646.867901
Sum of electronic and thermal Enthalpies= -2646.866957
Sum of electronic and thermal Free Energies= -2647.000250
E(UM06) = -2648.12778461

N -3.05954500 1.12760400 -0.46854200
C -2.79398600 2.37281400 -0.87701600
C -3.15142900 3.49720000 -0.14591400
C -3.81482200 3.31561700 1.06105700
C -4.09090000 2.02456000 1.49139000
C -3.69993700 0.93884000 0.70862300
N -3.53277900 -1.41718200 0.23916900
C -3.68979200 -2.70461900 0.56456200
C -4.26319300 -3.11682000 1.75886600
C -4.69861200 -2.14509900 2.65174300
C -4.53615000 -0.80728100 2.32151700
C -3.94097600 -0.46367000 1.10764600
H -2.27324200 2.45951300 -1.83088900
H -2.90790500 4.48781600 -0.52082700
H -3.33754400 -3.42721400 -0.16938000
H -4.36453800 -4.17660500 1.97529300
H -5.15727800 -2.42228100 3.59781800
H -4.11518700 4.16794400 1.66577200
C -2.51660200 -2.42914400 -2.70591300
H -1.46711500 -2.65274700 -2.95100700
H -2.92300700 -3.28413000 -2.13910500
H -3.07402400 -2.36309600 -3.65438900
H -4.86034400 -0.03908000 3.01782700
H -4.60778300 1.87288000 2.43458500
C -1.97845700 0.23464000 -3.34910400
H -2.80069400 0.80536300 -3.81518900
H -1.17527400 0.94905000 -3.09783600
H -1.58301300 -0.46087200 -4.10425200
C 0.19955700 2.06126700 0.39762600
C 1.08993100 1.73115700 -1.72084100
C 1.31082500 3.08789000 -1.90248800
C 0.94762200 3.95706700 -0.87827100
C 0.38969200 3.44006200 0.28014300
C -0.38343400 1.43531600 1.60370900
C -1.06736000 -0.52412400 2.63583400
C -1.45927200 0.14928900 3.78545900
C -1.29498900 1.52731400 3.82785300
C -0.74790300 2.17488200 2.72860600
H 1.35350100 1.00479400 -2.48908400
H 1.75527400 3.44881800 -2.82576100
H 1.09956300 5.02908900 -0.97923800
H 0.10488400 4.11111500 1.08562000
H -1.16710700 -1.60711100 2.55830700
H -1.88273200 -0.40299400 4.62035500
H -1.58387200 2.09653400 4.70837500
H -0.60372000 3.25118300 2.75664700
N 0.54279100 1.23103000 -0.60779000
N -0.55327300 0.09446200 1.57168200
C 1.05939500 -1.63802300 -2.00092700
H 0.43786100 -1.28910600 -2.83951000
H 2.07925100 -1.23812300 -2.11164200
H 1.11167700 -2.73524100 -2.04212200
C -0.09002800 -2.90907500 0.20959100

H -0.75405100 -3.36878300 -0.53726900
H 0.85566800 -3.47002600 0.23135800
H -0.56331700 -2.99816300 1.20177300
C 2.69960000 0.27813900 2.04642800
C 3.11534800 1.56339000 1.65675200
C 2.31025800 0.09206500 3.38690200
C 3.12950600 2.61785600 2.56256300
H 3.42556500 1.72589700 0.62312900
C 2.32123300 1.14601500 4.28992800
H 1.99430400 -0.90157600 3.70746100
C 2.72970900 2.41766800 3.88499800
H 3.45225200 3.60589300 2.23413400
H 2.01101900 0.97592300 5.32104100
H 2.73791800 3.24501100 4.59303200
C 5.47505100 -0.67564400 4.79975600
C 5.84669200 0.37391000 3.92459600
C 6.17187700 0.05115800 2.58499100
C 6.14701900 -1.26303200 2.15111400
C 5.79255300 -2.28575600 3.03553800
C 5.45309900 -1.98730500 4.35825400
H 5.21017000 -0.42843800 5.82688900
H 6.44440200 0.85751400 1.90557800
H 6.40045400 -1.50014800 1.11954200
H 5.77498100 -3.31808200 2.69070100
H 5.17213900 -2.78675800 5.04132700
S 2.65666000 -1.05739300 0.89572000
S 5.91225000 1.99969900 4.47998700
Pt -2.65907300 -0.68066500 -1.64215700
Pt 0.25367400 -0.93059400 -0.24133200

17a
E(RM06) = -1175.79938528
Zero-point correction= 0.416723 (Hartree/Particle)
Thermal correction to Energy= 0.445879
Thermal correction to Enthalpy= 0.446823
Thermal correction to Gibbs Free Energy= 0.355547
Sum of electronic and zero-point Energies= -1175.382663
Sum of electronic and thermal Energies= -1175.353506
Sum of electronic and thermal Enthalpies= -1175.352562
Sum of electronic and thermal Free Energies= -1175.443839
E(RM06) = -1176.15005533

N 1.07059600 -1.41286700 -0.32244200
C 0.89572800 -2.72110900 -0.52467700
C 1.91694500 -3.64509300 -0.36398800
C 3.16994600 -3.17980800 0.02110400
C 3.35382800 -1.82163200 0.22610500
C 2.27981200 -0.94874000 0.04588300
N 1.28545200 1.24371300 0.02642200
C 1.32221900 2.56603600 0.19684800
C 2.47146700 3.23991100 0.58586100
C 3.62445100 2.49841500 0.80805900
C 3.58650700 1.12195900 0.63781000
C 2.39685500 0.51126100 0.24382500
H -0.10315700 -3.03216500 -0.82790800
H 1.72870700 -4.70057200 -0.53833000
H 0.39108500 3.10124700 0.01462100
H 2.45290900 4.31885100 0.71043700
H 4.54767600 2.98447700 1.11447000
H 3.99938600 -3.86930100 0.15898600
C -1.88833000 1.65515700 -0.83725200
H -2.56636000 1.71820200 0.02299500
H -1.33055500 2.59731400 -0.93227400
H -2.47581000 1.51069200 -1.75309900
H 4.48154200 0.53308500 0.81543800
H 4.32962500 -1.44828600 0.52267500
C -2.15613200 -1.06018400 -1.09612600
H -2.39195200 -0.96248200 -2.16362200
H -1.91434500 -2.10919600 -0.87557500
H -3.04011800 -0.77704600 -0.50929000
C 2.87162400 -0.19853900 4.14851100
C 2.17526600 0.99548100 3.96953100
C 0.94742500 0.99887800 3.31381300
C 0.40464600 -0.19401600 2.82468000
C 1.10012200 -1.39098300 3.02023100

C 2.32823500 -1.39132400 3.67850000
H 3.83355600 -0.19910800 4.65833900
H 2.59273500 1.93233000 4.33674000
H 0.40851900 1.93502600 3.16652600
H 0.68320600 -2.32518000 2.64238100
H 2.86460100 -2.32955300 3.81626900
C 1.97147200 0.45783800 -3.06852900
C 2.75699200 -0.69619100 -3.14197800
C 4.14665700 -0.60516600 -3.09399100
C 4.76357600 0.63710400 -2.97158200
C 3.98531500 1.79193400 -2.91034700
C 2.59716200 1.70448800 -2.96195700
H 2.27618100 -1.67167700 -3.22332000
H 4.74739900 -1.51267900 -3.14379100
H 5.84917000 0.70670800 -2.92844300
H 4.46079300 2.76755700 -2.81622900
H 1.98927500 2.60783700 -2.90612400
Se -1.29519100 -0.18166400 1.87416900
Se 0.02839800 0.33360500 -3.10288400
Pt -0.53579200 0.11687800 -0.58537000

17b
E(RM06) = -1184.30900385
Zero-point correction= 0.416078 (Hartree/Particle)
Thermal correction to Energy= 0.445367
Thermal correction to Enthalpy= 0.446311
Thermal correction to Gibbs Free Energy= 0.354855
Sum of electronic and zero-point Energies= -1183.892925
Sum of electronic and thermal Energies= -1183.863637
Sum of electronic and thermal Enthalpies= -1183.862693
Sum of electronic and thermal Free Energies= -1183.954148
E(RM06) = -1184.68504054

N 1.13545800 -1.25644800 -0.20726100
C 1.00090300 -2.58005500 -0.29361200
C 2.03959500 -3.46240100 -0.03100400
C 3.26735800 -2.93324600 0.34791700
C 3.40872600 -1.55726400 0.44657200
C 2.32213600 -0.73252300 0.15220400
N 1.27926100 1.42653400 -0.05569700
C 1.28952300 2.75872600 -0.00475400
C 2.42257000 3.49202100 0.31879600
C 3.59569500 2.79802500 0.58982500
C 3.59092700 1.41257200 0.52936800
C 2.40804600 0.74360400 0.21074900
H 0.01750700 -2.94771700 -0.58646000
H 1.88177400 -4.53353200 -0.12053900
H 0.34829000 3.25842200 -0.23377900
H 2.37926400 4.57701100 0.35260000
H 4.50978600 3.32983300 0.84356600
H 4.10939500 -3.58526900 0.56838200
C -1.96773300 1.64386100 -0.87772600
H -1.52602500 2.57927400 -0.51314600
H -2.20895500 1.72304700 -1.94238200
H -2.86613700 1.40574100 -0.29771800
Pd -0.52073500 0.20356200 -0.59457800
H 4.50470800 0.86302400 0.73608300
H 4.36415300 -1.13554000 0.74422100
C -2.08424700 -1.03289100 -1.11770500
H -2.53727400 -0.70353600 -2.05920100
H -1.64047700 -2.02770400 -1.24619000
H -2.83019800 -1.04576400 -0.31698000
C 2.75129300 -0.85904900 4.12689700
C 2.40809900 0.46654200 3.87316700
C 1.21886500 0.76888200 3.21386200
C 0.36012700 -0.25509700 2.80114200
C 0.70415900 -1.58444600 3.07118400
C 1.89370600 -1.88324200 3.72847900
H 3.68333900 -1.09442000 4.63797000
H 3.07191300 1.27307900 4.18266800
H 0.95820900 1.80729300 3.00666200
H 0.03901300 -2.38666300 2.75126400
H 2.15504200 -2.92246000 3.92470500
C 1.98514900 0.40790600 -3.07839000
C 2.77599700 -0.74515000 -3.04585100

C 4.16473000 -0.64467600 -3.00817600
C 4.77690800 0.60628200 -3.00379700
C 3.99418300 1.75882500 -3.04916300
C 2.60651500 1.66180700 -3.08779800
H 2.29923400 -1.72587600 -3.03757800
H 4.76924700 -1.55042200 -2.97453600
H 5.86230800 0.68382400 -2.96944100
H 4.46622500 2.74065500 -3.04748500
H 1.99495100 2.56386900 -3.11270900
Se -1.28943700 0.15695500 1.85953700
Se 0.04624500 0.27564100 -3.10206400

17c
E(RM06) = -1953.45068206
Zero-point correction= 0.418869 (Hartree/Particle)
Thermal correction to Energy= 0.447042
Thermal correction to Enthalpy= 0.447986
Thermal correction to Gibbs Free Energy= 0.360113
Sum of electronic and zero-point Energies= -1953.031814
Sum of electronic and thermal Energies= -1953.003640
Sum of electronic and thermal Enthalpies= -1953.002696
Sum of electronic and thermal Free Energies= -1953.090570
E(RM06) = -1953.83140467

N 1.17337600 -1.25428600 -0.12119100
C 1.03076800 -2.57817500 -0.19970800
C 2.07752400 -3.45770000 0.03425600
C 3.32062100 -2.92700600 0.35667000
C 3.47338700 -1.54996300 0.42410100
C 2.37663100 -0.72539700 0.17438800
N 1.34940800 1.43209200 -0.11819500
C 1.35233000 2.76552700 -0.08704600
C 2.47826800 3.50264100 0.24873400
C 3.64105600 2.81366200 0.57186600
C 3.63507800 1.42668100 0.55346300
C 2.46576900 0.75082300 0.20453700
H 0.03727600 -2.93998600 -0.46219000
H 1.91567100 -4.52932600 -0.03859600
H 0.41246600 3.25443100 -0.34143300
H 2.43635200 4.58800500 0.25817400
H 4.54664900 3.35063700 0.84397600
H 4.16997700 -3.57880100 0.54706700
C -1.82619700 1.66738500 -1.05305800
H -2.46462800 1.91279200 -0.19438800
H -1.26673300 2.56090500 -1.36485700
H -2.45138300 1.33985200 -1.89282500
H 4.53433100 0.88097900 0.82371000
H 4.44666300 -1.12708500 0.65476200
C -2.05947100 -1.08034500 -0.81366500
H -2.21549200 -1.30507200 -1.87681100
H -1.83931700 -2.00853500 -0.26726100
H -2.97235200 -0.64085000 -0.39332300
C 2.39548500 -1.19884200 4.15902500
C 2.30797000 0.16703000 3.90415300
C 1.23298500 0.67753800 3.18082600
C 0.22849900 -0.17171000 2.70132500
C 0.31906100 -1.54279300 2.97661600
C 1.39509400 -2.05217800 3.69463600
H 3.23797400 -1.59835100 4.72116500
H 3.08347900 0.84203100 4.26469400
H 1.17006800 1.74650900 2.97343100
H -0.46242200 -2.20923900 2.60909300
H 1.45433100 -3.12189300 3.89226000
C 1.75560400 0.33254900 -3.07254400
C 2.71507500 -0.68654400 -3.04880700
C 4.07156400 -0.38629000 -3.14171900
C 4.48982900 0.93637700 -3.26014600
C 3.54173100 1.95822100 -3.29901000
C 2.18680800 1.65881800 -3.21142000
H 2.38887400 -1.72217200 -2.94692600
H 4.80450000 -1.19193900 -3.11500300
H 5.55070800 1.17152200 -3.32809400
H 3.86000500 2.99561500 -3.39595500
H 1.44374500 2.45701000 -3.23746400
S 0.02071600 -0.05249600 -2.93657800

S -1.14118300 0.47896900 1.76493500
Pt -0.46253400 0.20011300 -0.56019600

18a
E(UM06) = -1869.92810792
Zero-point correction= 0.648414 (Hartree/Particle)
Thermal correction to Energy= 0.694815
Thermal correction to Enthalpy= 0.695759
Thermal correction to Gibbs Free Energy= 0.561810
Sum of electronic and zero-point Energies= -1869.279694
Sum of electronic and thermal Energies= -1869.233293
Sum of electronic and thermal Enthalpies= -1869.232349
Sum of electronic and thermal Free Energies= -1869.366298
E(UM06) = -1870.46058569

N -1.89215800 2.92452200 4.47665900
C -2.16949100 4.09875200 3.90261300
C -1.88056700 5.31412200 4.50505500
C -1.27532500 5.30103100 5.75541800
C -0.97706500 4.08350600 6.35013600
C -1.29462400 2.89807400 5.68803900
N -1.30709100 0.49747800 5.48071200
C -0.98199800 -0.73044300 5.89650900
C -0.33926900 -0.97136800 7.10173500
C -0.02810200 0.11644500 7.91011100
C -0.35113400 1.39337400 7.47667100
C -0.98081300 1.56412000 6.24295100
H -2.64187300 4.05013400 2.92230700
H -2.12731100 6.24380000 4.00010700
H -1.24955300 -1.54793000 5.22865500
H -0.09628200 -1.98897100 7.39467000
H 0.46786800 -0.02571600 8.86726000
H -1.03108700 6.23012100 6.26490900
C -2.64195000 -0.91652300 2.80738500
H -2.24729600 -1.04526000 1.78882200
H -2.17257300 -1.67914900 3.44900000
H -3.72591000 -1.10841600 2.77636800
H -0.09632100 2.25045500 8.09305700
H -0.49348700 4.06526600 7.32231900
C -3.23330800 1.64577900 1.85115500
H -4.20623600 2.06912300 2.15227500
H -2.63718300 2.44160700 1.37792500
H -3.41510500 0.86499900 1.10002200
C 1.19090600 2.16735600 3.47507400
C 1.75757900 1.72198100 4.67717100
C 1.32698300 3.51849600 3.12623900
C 2.43769500 2.60773300 5.50933600
H 1.67206400 0.66978400 4.95882800
C 2.02201900 4.39755800 3.95154900
H 0.88167900 3.87792700 2.19741300
C 2.57736300 3.94580000 5.14860600
H 2.86679800 2.24432600 6.44379300
H 2.12192500 5.44346600 3.66306800
H 3.11726000 4.63427900 5.79716400
C 4.37558700 1.62125300 2.03873800
C 4.41876000 2.79942800 1.29388700
C 3.88445300 2.81825400 0.01328200
C 3.31518200 1.65885400 -0.49944400
C 3.29322300 0.52715800 0.30364600
H 4.84761100 3.70522600 1.71306200
H 3.91080800 3.73209000 -0.57573600
H 2.88532900 1.62652300 -1.49677900
H 2.84248800 -0.40221200 -0.04311400
C 4.93550600 1.52196700 3.40236300
C 5.71125400 2.53413400 3.96835900
C 6.21842200 2.37169800 5.24847200
H 5.94010500 3.43553200 3.40667200
C 5.17073600 0.23099600 5.31320700
C 5.94288400 1.19770200 5.94076400
H 6.82832600 3.15207300 5.69757800
H 4.93866300 -0.71262100 5.80583100
H 6.32287000 1.02438000 6.94376800
N 4.67604500 0.38641900 4.08220200
N 3.80862900 0.50493100 1.53492300
C 3.19064400 -2.54131400 4.44427900

H 3.71097300 -3.49721000 4.28488900
H 3.50031400 -2.13608500 5.42147500
H 2.10840200 -2.74477900 4.48531900
C 2.58185200 -2.50509000 1.73919200
H 1.50524300 -2.26837500 1.74801900
H 2.95805800 -2.41210000 0.70721400
H 2.71520100 -3.54992600 2.05341500
Pt -2.26073200 0.96993900 3.52920900
Pt 3.58889800 -1.18450300 2.94971500
C 6.84056600 -0.84344900 1.52886300
C 7.64777800 0.04548200 2.24932300
C 8.19034200 1.16985300 1.63052300
C 7.93006900 1.42702400 0.28689600
C 7.12713000 0.54685500 -0.43843300
C 6.58834900 -0.57908200 0.17555500
H 7.84487600 -0.14247700 3.30557900
H 8.81372300 1.85250900 2.20771100
H 8.35096900 2.30817200 -0.19471500
H 6.91579500 0.74058700 -1.48973300
H 5.95000400 -1.25832200 -0.39144400
Se 6.01924100 -2.36935600 2.39931300
Se 0.21335400 0.95545200 2.32237300

18b
E(UM06) = -1886.97030721
Zero-point correction= 0.646256 (Hartree/Particle)
Thermal correction to Energy= 0.693469
Thermal correction to Enthalpy= 0.694414
Thermal correction to Gibbs Free Energy= 0.558058
Sum of electronic and zero-point Energies= -1886.324052
Sum of electronic and thermal Energies= -1886.276838
Sum of electronic and thermal Enthalpies= -1886.275894
Sum of electronic and thermal Free Energies= -1886.412249
E(UM06) = -1887.55559762

N -1.87929500 3.02279700 4.35232600
C -1.86980700 4.24927600 3.82779300
C -1.33272900 5.34848900 4.48407500
C -0.77751500 5.15236400 5.74156800
C -0.77800900 3.87715500 6.28947300
C -1.34093900 2.82092200 5.57252800
N -1.88701800 0.49038500 5.28126700
C -1.88201200 -0.78441200 5.67574400
C -1.37750000 -1.19607500 6.90153800
C -0.86282800 -0.22785500 7.75525200
C -0.85685400 1.09805100 7.34724100
C -1.36488700 1.43382300 6.09134800
H -2.31428000 4.34992700 2.83788900
H -1.35310100 6.32814400 4.01477300
H -2.29980100 -1.50513600 4.97342900
H -1.39566100 -2.24743600 7.17467400
H -0.46436100 -0.50027400 8.72978400
H -0.34226600 5.98223100 6.29347900
C -3.41839900 -0.49776500 2.49425200
H -2.96583100 -0.74576400 1.52634900
H -3.22653500 -1.31734200 3.20236700
H -4.50229100 -0.36806500 2.36547300
H -0.44637400 1.85918500 8.00427800
H -0.33608300 3.71441900 7.26805000
C -3.38240300 2.07463000 1.60505600
H -4.39539000 2.42347100 1.85767300
H -2.74140600 2.93134500 1.35355000
H -3.43205000 1.40014300 0.74243900
C 0.96678400 1.47714600 3.44979000
C 1.38890500 0.70428600 4.54025700
C 1.40168500 2.80554600 3.35543800
C 2.21384100 1.25363700 5.51935200
H 1.05972000 -0.33258000 4.62632400
C 2.23197400 3.34900300 4.33250800
H 1.08243900 3.41476800 2.50871100
C 2.63582200 2.57754100 5.42149300
H 2.53433000 0.63595400 6.35966400
H 2.56315400 4.38404400 4.24377600
H 3.28805900 3.00289400 6.18368900
C 4.52891200 1.82297900 2.09332100

C 4.43325100 2.89388800 1.20447100
C 3.70366100 2.74623800 0.03257000
C 3.08121700 1.53260500 -0.22794000
C 3.21523100 0.51442300 0.70749700
H 4.91251100 3.84418300 1.42223400
H 3.62183600 3.57498300 -0.66711700
H 2.49683900 1.37069900 -1.12985800
H 2.74078400 -0.45482200 0.55175700
C 5.28762400 1.91225100 3.36182300
C 6.04760700 3.03360400 3.70068600
C 6.73113700 3.05584700 4.90722100
H 6.12360800 3.88032200 3.02452900
C 5.87997400 0.87502200 5.34379300
C 6.64804200 1.95583400 5.75329200
H 7.32777600 3.92335800 5.18002900
H 5.79187500 -0.01670700 5.96488100
H 7.16957900 1.92745200 6.70604800
N 5.21546200 0.85181300 4.18794700
N 3.91831800 0.64965800 1.83205000
C 3.99780300 -2.12759200 5.06382400
H 4.47152600 -3.09644800 4.86154600
H 4.53822600 -1.61879400 5.87654400
H 2.95215700 -2.28952400 5.36410900
C 2.87228000 -2.34266300 2.58822600
H 1.82255200 -2.07871700 2.79070200
H 3.06516400 -2.32059900 1.50532700
H 3.08335100 -3.34948100 2.96784100
C 6.96873200 -0.61747800 1.44854200
C 7.83598900 0.36646200 1.94092500
C 8.24177600 1.42290300 1.12889000
C 7.78377800 1.51697200 -0.18317500
C 6.91742200 0.54383300 -0.68097400
C 6.51277800 -0.51360200 0.12686400
H 8.18865200 0.30521200 2.97136800
H 8.91556900 2.18036000 1.52875000
H 8.09986300 2.34441700 -0.81637500
H 6.55135500 0.61078800 -1.70510900
H 5.82561300 -1.26662400 -0.26132200
Se 6.35900900 -2.06324900 2.58406900
Se -0.20612000 0.72723800 2.10382700
Pd -2.61318800 1.20887000 3.29115700
Pd 4.04434100 -0.88956000 3.42784600

18c
E(UM06) = -2647.57483412
Zero-point correction= 0.649952 (Hartree/Particle)
Thermal correction to Energy= 0.695556
Thermal correction to Enthalpy= 0.696500
Thermal correction to Gibbs Free Energy= 0.566847
Sum of electronic and zero-point Energies= -2646.924882
Sum of electronic and thermal Energies= -2646.879278
Sum of electronic and thermal Enthalpies= -2646.878334
Sum of electronic and thermal Free Energies= -2647.007987
E(UM06) = -2648.13854081

N -1.85911000 2.92770300 4.56325700
C -2.12003000 4.13865700 4.06179300
C -1.84428400 5.31097600 4.74961000
C -1.26737600 5.21406200 6.00977000
C -0.99033400 3.95871700 6.53202200
C -1.29719700 2.82056700 5.78713700
N -1.46476700 0.43528600 5.49891100
C -1.21062300 -0.82495600 5.86306600
C -0.52995300 -1.14856100 7.02744400
C -0.09088200 -0.11133900 7.84296700
C -0.34095000 1.19870100 7.46248000
C -1.02919500 1.45105200 6.27494800
H -2.56939200 4.15727900 3.06988400
H -2.07856300 6.27248700 4.30169800
H -1.56645400 -1.59955300 5.18543400
H -0.34995200 -2.18946600 7.28114900
H 0.44928400 -0.31857100 8.76363100
H -1.03512500 6.10671400 6.58560400
C -2.89564900 -0.78773400 2.76385400
H -2.38177600 -1.00269800 1.81600300

H -2.66053200 -1.59729900 3.47268300
H -3.97971400 -0.80035300 2.57363800
H 0.02013900 2.01653700 8.07928500
H -0.54442100 3.87342500 7.51859000
C -3.08935800 1.82231300 1.80274900
H -4.09777700 2.22320800 1.99722100
H -2.43981000 2.64765200 1.46897700
H -3.15790100 1.09232400 0.98471500
C 1.00774600 1.86084300 3.32748900
C 1.62101900 1.59601600 4.56423800
C 1.16838300 3.14090700 2.76959900
C 2.36197400 2.57490900 5.21866000
H 1.51712000 0.60243400 5.00537600
C 1.91923400 4.11431200 3.41993700
H 0.69466100 3.36035200 1.81153200
C 2.51758000 3.83774500 4.64997100
H 2.82573100 2.34555700 6.17907900
H 2.03655000 5.09766100 2.96523800
H 3.10514300 4.60023400 5.15957800
C 4.47447400 1.73009600 2.11376700
C 4.54537800 2.88760400 1.33989300
C 3.95988100 2.90624500 0.08209300
C 3.30850400 1.76896200 -0.37774800
C 3.27528400 0.65281100 0.44568900
H 5.03491200 3.77997100 1.71953200
H 4.00634900 3.80543400 -0.52788900
H 2.82905400 1.74035900 -1.35223400
H 2.77426400 -0.26350400 0.13551600
C 5.05842000 1.64260000 3.46831400
C 5.85042400 2.65564200 4.01094200
C 6.35827000 2.51366000 5.29292300
H 6.08594900 3.54461100 3.43258100
C 5.28901100 0.38629100 5.40310300
C 6.07136400 1.35724600 6.01026900
H 6.97783700 3.29619500 5.72469100
H 5.04996600 -0.54578200 5.91391000
H 6.45087200 1.20094100 7.01619800
N 4.79137100 0.52366300 4.17123900
N 3.84651300 0.62820200 1.65212000
C 3.36833900 -2.44089100 4.56034400
H 3.87763600 -3.39522600 4.36178400
H 3.72687800 -2.05177900 5.52703000
H 2.28823700 -2.64000600 4.64925000
C 2.68738200 -2.39548600 1.86996600
H 1.61055700 -2.16396200 1.89857800
H 3.04758800 -2.29636500 0.83315000
H 2.83467400 -3.43901500 2.18152000
S 0.04441400 0.63294000 2.50490800
Pt -2.31969600 1.03111400 3.53213200
Pt 3.70337200 -1.06709000 3.06279100
C 6.77816000 -0.82306500 1.60208400
C 7.64389600 0.07667700 2.24419300
C 8.21889900 1.13600300 1.54820800
C 7.93721100 1.32625500 0.19733100
C 7.07849600 0.44023400 -0.45427900
C 6.51128500 -0.62317100 0.23668000
H 7.85790600 -0.06041900 3.30507600
H 8.88566400 1.82255100 2.06976400
H 8.38292200 2.15822500 -0.34559100
H 6.84953000 0.58005400 -1.51053300
H 5.83436200 -1.31055000 -0.27308800
S 6.00570900 -2.14114500 2.49188100

19a
E(RM06) = -1869.97694143
Zero-point correction= 0.649573 (Hartree/Particle)
Thermal correction to Energy= 0.695687
Thermal correction to Enthalpy= 0.696631
Thermal correction to Gibbs Free Energy= 0.564957
Sum of electronic and zero-point Energies= -1869.327368
Sum of electronic and thermal Energies= -1869.281255
Sum of electronic and thermal Enthalpies= -1869.280310
Sum of electronic and thermal Free Energies= -1869.411985
E(RM06) = -1870.51174441

N -1.78951900 3.43618600 4.80579500
C -1.84966500 4.70347700 4.38206000
C -1.55401300 5.78441000 5.19892300
C -1.18211700 5.53479800 6.51465300
C -1.10720000 4.22184700 6.95605300
C -1.40844000 3.18160900 6.07703400
N -1.67838900 0.85616400 5.51631600
C -1.58222400 -0.44791200 5.79454100
C -1.14094300 -0.92871900 7.01966000
C -0.77736700 -0.01054200 7.99663400
C -0.86507000 1.34492500 7.71120900
C -1.31804600 1.75767600 6.45916000
H -2.15191000 4.84206700 3.34491500
H -1.62089900 6.79576300 4.80760600
H -1.87140700 -1.12852500 4.99540100
H -1.08391200 -1.99993700 7.19283200
H -0.42450300 -0.34236100 8.97024600
H -0.94968100 6.35257800 7.19266200
C -2.67214600 -0.00920200 2.51879600
H -1.94746900 -0.14474800 1.69756100
H -2.63101100 -0.91456500 3.14839200
H -3.67333500 0.03046700 2.05947600
H -0.57004000 2.07233800 8.46202400
H -0.81394000 4.01551800 7.98138100
C -2.68915000 2.71320700 1.84763800
H -3.53005700 3.40881600 2.01713800
H -1.81497100 3.31833600 1.54595100
H -2.95743800 2.07159500 0.99489600
C 1.56816900 1.02857100 3.96928100
C 1.83761100 1.49412300 5.25984200
C 1.36731900 1.95165900 2.93833300
C 1.90126500 2.86192500 5.51517300
H 1.99713400 0.77790600 6.06748600
C 1.44330400 3.31955700 3.19414700
H 1.14310700 1.59655900 1.93112700
C 1.70888600 3.77816500 4.48195800
H 2.10460300 3.21330400 6.52722700
H 1.28665400 4.02855500 2.38082700
H 1.75771500 4.84747500 4.68381000
C 4.29223600 1.36874800 1.78835700
C 4.30299900 2.45092500 0.90819800
C 3.78365700 2.29749500 -0.36847500
C 3.26657700 1.06416500 -0.74691900
C 3.30179100 0.02765000 0.17432300
H 4.70248700 3.41297500 1.21526400
H 3.78119600 3.13652900 -1.06018200
H 2.84312400 0.90097300 -1.73379400
H 2.91018400 -0.95858300 -0.07147200
C 4.79318500 1.46344900 3.17594700
C 5.31973900 2.64154700 3.70580100
C 5.78915700 2.65259100 5.01041900
H 5.37214100 3.54557900 3.10616000
C 5.18431600 0.35350100 5.17546300
C 5.72711300 1.48612900 5.76379500
H 6.20420600 3.56474600 5.43255700
H 5.11234600 -0.58635900 5.72148400
H 6.08955500 1.44740300 6.78706900
N 4.72481900 0.34337300 3.92255500
N 3.80580800 0.17298500 1.40138100
C 3.92672700 -2.83098000 4.45803100
H 4.79242000 -3.49866600 4.35622800
H 3.99726100 -2.28687400 5.41054900
H 3.00859500 -3.43203100 4.47378900
C 3.12231000 -3.04302100 1.83430000
H 2.06654100 -3.22553200 2.07443500
H 3.21657300 -2.80776100 0.76489600
H 3.69945900 -3.95419300 2.03773400
Pt -2.24966700 1.69706700 3.57430200
Pt 3.86898600 -1.45350800 2.92104200
C 6.97620800 -0.57767600 1.45442400
C 7.67300300 0.33289600 2.25426800
C 8.17334900 1.51230500 1.70583000
C 7.98168600 1.79336600 0.35573300
C 7.29539300 0.88461300 -0.44832900
C 6.79814900 -0.29614800 0.09559700

H 7.81239300 0.12163200 3.31514400
H 8.70849700 2.21677600 2.34168600
H 8.36851800 2.71717700 -0.07111800
H 7.14144900 1.09782400 -1.50550800
H 6.25497600 -1.00265800 -0.53263900
Se 6.24872300 -2.21158200 2.22409400
Se 1.44542000 -0.88357700 3.62500800

19b
E(RM06) = -1887.00695345
Zero-point correction= 0.648250 (Hartree/Particle)
Thermal correction to Energy= 0.694489
Thermal correction to Enthalpy= 0.695433
Thermal correction to Gibbs Free Energy= 0.565039
Sum of electronic and zero-point Energies= -1886.358703
Sum of electronic and thermal Energies= -1886.312465
Sum of electronic and thermal Enthalpies= -1886.311521
Sum of electronic and thermal Free Energies= -1886.441915
E(RM06) = -1887.59564533

N -1.74096200 3.03374500 4.29388600
C -1.84942000 4.06294000 3.45067400
C -1.65251800 5.38144800 3.83843300
C -1.33324800 5.63421900 5.16652500
C -1.20759100 4.56739700 6.04552600
C -1.40854100 3.26766600 5.58022100
N -1.63191600 0.89281700 5.92027600
C -1.48968900 -0.21644700 6.64992100
C -0.98442100 -0.21367500 7.94327600
C -0.60707500 1.00314300 8.49759500
C -0.74661100 2.15931000 7.74311000
C -1.26286100 2.07848300 6.44956800
H -2.11121600 3.80969900 2.42333300
H -1.75629700 6.18467500 3.11397700
H -1.79530900 -1.14572500 6.16994400
H -0.88864500 -1.14576700 8.49340700
H -0.20088300 1.05412900 9.50516200
H -1.18264900 6.65205300 5.51899400
C -2.77241400 -0.99219700 3.46674000
H -2.06691100 -1.48079100 2.77846400
H -2.76913200 -1.54135100 4.42320400
H -3.77975600 -1.05903600 3.02953400
H -0.43054900 3.11326000 8.15611100
H -0.96388600 4.75408400 7.08768500
C -2.63493500 1.22689700 1.81187200
H -3.51832800 1.88080200 1.72296900
H -1.76607200 1.74737400 1.37310200
H -2.81969200 0.30907400 1.23800600
C 1.58308000 1.25949100 4.00914700
C 1.93852500 1.33828700 5.35970400
C 1.50450700 2.43389500 3.25434400
C 2.21718000 2.57132600 5.94282600
H 2.00360700 0.42464000 5.95284600
C 1.78351500 3.66654500 3.83949200
H 1.21816900 2.37890700 2.20278800
C 2.14170900 3.73863900 5.18410200
H 2.49491900 2.61900300 6.99571100
H 1.71786700 4.57508200 3.24110300
H 2.35738200 4.70335300 5.64140600
C 4.40705900 1.68097100 1.96140100
C 4.60467000 2.91994900 1.34939500
C 4.10656700 3.13722200 0.07352500
C 3.42267000 2.11325200 -0.57099000
C 3.27359800 0.90577800 0.09667600
H 5.13303800 3.71754300 1.86351400
H 4.24997000 4.10026600 -0.41098000
H 3.01032500 2.24037900 -1.56802800
H 2.74217400 0.07338200 -0.36457500
C 4.88760500 1.38414700 3.32952100
C 5.59484500 2.31450800 4.09305500
C 6.03718700 1.96184900 5.35910200
H 5.81184000 3.30515200 3.70386800
C 5.05463800 -0.18232600 5.02636700
C 5.76805400 0.68592200 5.84030200
H 6.59220600 2.67713400 5.96168000

H 4.82115600 -1.19456900 5.35668200
H 6.10143100 0.36359200 6.82283800
N 4.61990200 0.15651800 3.81218000
N 3.75570900 0.69240600 1.32106400
C 3.27779800 -2.88239400 3.64624000
H 4.04990800 -3.62230900 3.40747000
H 3.39321200 -2.51465100 4.67382000
H 2.27951200 -3.31440600 3.52230700
C 2.57125200 -2.43015700 1.06716300
H 1.50613700 -2.52925900 1.30516100
H 2.70591400 -1.92771100 0.10094600
H 3.04836200 -3.41559900 1.04074100
C 6.76629000 -0.56723300 1.21342400
C 7.58425300 0.01448200 2.18726900
C 8.28490200 1.18651700 1.91056100
C 8.17324300 1.79159000 0.66142900
C 7.36525600 1.21252800 -0.31621700
C 6.66888400 0.03896000 -0.04458000
H 7.66061500 -0.44767800 3.17209500
H 8.91403600 1.63191400 2.68060100
H 8.71670100 2.71047800 0.44780600
H 7.27307600 1.67959000 -1.29616700
H 6.03134500 -0.40865100 -0.80751700
Se 5.76277400 -2.18454500 1.60521700
Se 1.18130700 -0.45807200 3.19531300
Pd 3.51327300 -1.22497300 2.44782800
Pd -2.21712600 0.94944600 3.79310700

19c
E(RM06) = -2647.62783863
Zero-point correction= 0.651921 (Hartree/Particle)
Thermal correction to Energy= 0.696881
Thermal correction to Enthalpy= 0.697825
Thermal correction to Gibbs Free Energy= 0.570526
Sum of electronic and zero-point Energies= -2646.975917
Sum of electronic and thermal Energies= -2646.930958
Sum of electronic and thermal Enthalpies= -2646.930014
Sum of electronic and thermal Free Energies= -2647.057312
E(RM06) = -2648.19262790

N -1.78317700 3.32410800 4.96682100
C -1.89322100 4.61501600 4.63417200
C -1.59845100 5.64621600 5.51341300
C -1.17511600 5.31902100 6.79606400
C -1.04986300 3.98186000 7.14334500
C -1.35102100 2.99551000 6.20420100
N -1.60371600 0.70614100 5.50562800
C -1.46797800 -0.61053500 5.69219400
C -0.93713900 -1.15906500 6.85113200
C -0.52846200 -0.29794400 7.86146600
C -0.66553000 1.07067000 7.67488500
C -1.20665000 1.55253800 6.48413400
H -2.23556600 4.81495500 3.61975400
H -1.70626200 6.67939500 5.19500600
H -1.79784000 -1.24348300 4.87032400
H -0.84693800 -2.23739600 6.94882700
H -0.10311300 -0.68378000 8.78488900
H -0.94291500 6.09543100 7.52112800
C -2.69374600 0.01333200 2.49841000
H -1.97528300 -0.08225500 1.66652700
H -2.65355900 -0.92367700 3.07984500
H -3.69747300 0.08202600 2.04883200
H -0.33705500 1.75537600 8.45157200
H -0.71932700 3.71454900 8.14299000
C -2.75336000 2.76986900 1.98981200
H -3.61827500 3.41952300 2.21261100
H -1.90720000 3.42727400 1.71967900
H -3.00802300 2.17539800 1.09948400
C 1.54654500 1.11872700 3.71435700
C 1.79216800 1.52665200 5.03205200
C 1.35085200 2.09881900 2.73337800
C 1.86072000 2.87808000 5.35533800
H 1.93534000 0.76822600 5.80421800
C 1.42118500 3.45223400 3.05729700
H 1.14603000 1.78970400 1.70699900

C 1.67883900 3.84678900 4.36781500
H 2.05673000 3.17657900 6.38590300
H 1.27302200 4.20043200 2.27856700
H 1.73381600 4.90456500 4.62181800
C 4.33333000 1.51133900 1.71169200
C 4.31158800 2.57792200 0.81244800
C 3.84940600 2.37086000 -0.47881600
C 3.40844300 1.10545100 -0.84784400
C 3.44961100 0.09448600 0.10096500
H 4.63452100 3.56896500 1.11780300
H 3.82571600 3.19525500 -1.18749600
H 3.03158400 0.90100100 -1.84584700
H 3.10143700 -0.91152300 -0.13035400
C 4.79962100 1.65653400 3.10799600
C 5.36940400 2.83454300 3.59077900
C 5.80149600 2.89257600 4.90779100
H 5.49353800 3.69781700 2.94346200
C 5.08739600 0.63497600 5.17117500
C 5.66406000 1.77186600 5.71794800
H 6.25017000 3.80480500 5.29384000
H 4.96186300 -0.27363400 5.75922300
H 5.99784900 1.77030000 6.75164300
N 4.65863300 0.58283600 3.90916000
N 3.90580200 0.28918200 1.33966100
C 3.62882900 -2.48959300 4.60079200
H 4.49428700 -3.16112200 4.67399000
H 3.57287800 -1.85824500 5.49925300
H 2.70846600 -3.08291200 4.53687600
C 3.11599800 -2.88379600 1.90595400
H 2.02441200 -2.97257600 1.98263100
H 3.40369000 -2.75078600 0.85317300
H 3.58593400 -3.80205900 2.27910600
S 1.46748700 -0.61018600 3.29417500
Pt -2.25331000 1.65804300 3.63988300
Pt 3.79755900 -1.24841700 2.96267000
C 6.88781300 -0.82812100 1.72049600
C 7.63185400 0.17493300 2.35302900
C 8.27900300 1.15605300 1.60612600
C 8.19626100 1.14732000 0.21619400
C 7.46417500 0.14806200 -0.42431200
C 6.81560700 -0.83063800 0.32106600
H 7.69693600 0.18342300 3.44164400
H 8.84957200 1.93190000 2.11548600
H 8.70278000 1.91395100 -0.36776400
H 7.39664800 0.13211800 -1.51141400
H 6.23713700 -1.60981300 -0.17709900
S 6.06649000 -2.08875600 2.67524000

MECPa
E(RM06) = -1869.9258189300
N -1.7956418 2.8702387 4.5783597
C -2.0323430 4.0631855 4.0236054
C -1.8384023 5.2577169 4.7008462
C -1.3760715 5.2051062 6.0102451
C -1.1164196 3.9695290 6.5853469
C -1.3298955 2.8068837 5.8454088
N -1.4064723 0.4131053 5.6015600
C -1.1328836 -0.8305610 6.0076657
C -0.5178733 -1.1084107 7.2189406
C -0.1686457 -0.0412556 8.0394953
C -0.4364558 1.2520947 7.6160135
C -1.0558563 1.4580528 6.3824150
H -2.3952738 4.0473640 2.9968848
H -2.0487783 6.2026270 4.2079163
H -1.4171451 -1.6296964 5.3244975
H -0.3187568 -2.1376124 7.5039437
H 0.3165384 -0.2126926 8.9975518
H -1.2159978 6.1161202 6.5814705
C -2.6705488 -0.9138273 2.8490220
H -2.1137332 -1.1460395 1.9290648
H -2.4500800 -1.6995504 3.5889982
H -3.7449930 -0.9577124 2.6120862
H -0.1425903 2.0936707 8.2364438
H -0.7569342 3.9171970 7.6090100
C -2.8849311 1.6622075 1.8020028

H -3.9043335 2.0571092 1.9457793
H -2.2364533 2.4846292 1.4581911
H -2.9179933 0.9030225 1.0082318
C 1.2678859 2.0364298 3.5850219
C 1.7852236 1.8385148 4.8721251
C 1.3902669 3.3011034 2.9942728
C 2.4140063 2.8793967 5.5496411
H 1.7049876 0.8535220 5.3366699
C 2.0318697 4.3367186 3.6686709
H 0.9824849 3.4675229 1.9956583
C 2.5456264 4.1301056 4.9486632
H 2.8075394 2.7092818 6.5520654
H 2.1270232 5.3125857 3.1931717
H 3.0445403 4.9416210 5.4763119
C 4.4176465 1.6703159 1.9584540
C 4.5393492 2.8299368 1.1928664
C 4.0360608 2.8511707 -0.0996810
C 3.4198327 1.7122217 -0.6050656
C 3.3307966 0.5958399 0.2135569
H 5.0044797 3.7206928 1.6054190
H 4.1194533 3.7524383 -0.7027485
H 3.0080662 1.6844631 -1.6100134
H 2.8487829 -0.3192399 -0.1290764
C 4.9163126 1.5779214 3.3463289
C 5.6942401 2.5769562 3.9329508
C 6.1359876 2.4219941 5.2379712
H 5.9759532 3.4615871 3.3690296
C 5.0188925 0.3170631 5.2885856
C 5.7917961 1.2695914 5.9356617
H 6.7471640 3.1919860 5.7028938
H 4.7317067 -0.6081054 5.7870163
H 6.1166930 1.1034232 6.9591452
N 4.5877338 0.4648409 4.0332574
N 3.8161430 0.5710589 1.4574362
C 3.0722307 -2.4465467 4.3604339
H 3.5831468 -3.4094282 4.2152960
H 3.3660567 -2.0402861 5.3422079
H 1.9862927 -2.6316199 4.3798340
C 2.5690069 -2.4361610 1.6331721
H 1.4881279 -2.2244433 1.6082187
H 2.9745866 -2.3418204 0.6126260
H 2.7158635 -3.4764066 1.9573860
Pt -2.1748258 0.9418190 3.5882986
Pt 3.5170758 -1.0960450 2.8719168
C 6.8146495 -0.8283892 1.5251752
C 7.6206620 0.0856185 2.2153661
C 8.2024963 1.1610442 1.5473259
C 7.9813161 1.3451359 0.1849928
C 7.1713844 0.4458595 -0.5080771
C 6.5936026 -0.6318305 0.1546821
H 7.7866688 -0.0452978 3.2856555
H 8.8279219 1.8625339 2.0988444
H 8.4357062 2.1860818 -0.3364010
H 6.9899234 0.5861509 -1.5732638
H 5.9504903 -1.3276694 -0.3862059
Se 5.9662700 -2.3030739 2.4515199
Se 0.3928897 0.5906101 2.6442111

MECPb
E(RM06) = -1886.9674788400
N -1.7500320 2.8652623 4.5820441
C -1.9872916 4.0577082 4.0325136
C -1.8253365 5.2518421 4.7207875
C -1.3986147 5.1933785 6.0412787
C -1.1413211 3.9559673 6.6152365
C -1.3187177 2.7974981 5.8586168
N -1.3839428 0.4008165 5.6142314
C -1.1157318 -0.8394177 6.0273254
C -0.5153625 -1.1179000 7.2473055
C -0.1691857 -0.0484907 8.0655733
C -0.4286805 1.2445704 7.6338185
C -1.0418946 1.4455716 6.3959060
H -2.3241377 4.0464455 2.9960165
H -2.0338717 6.1973203 4.2283679
H -1.3905293 -1.6425308 5.3435101

H -0.3250674 -2.1467243 7.5404744
H 0.3062439 -0.2176398 9.0291302
H -1.2680284 6.1018800 6.6240473
C -2.6274204 -0.8945288 2.8009494
H -2.0648744 -1.1383590 1.8904208
H -2.4169265 -1.6508114 3.5722315
H -3.7020964 -0.8967657 2.5694592
H -0.1322862 2.0875295 8.2520081
H -0.8127259 3.9007452 7.6491605
C -2.7712840 1.6552425 1.7762447
H -3.7903095 2.0373138 1.9446680
H -2.1014790 2.4828178 1.4979412
H -2.7843936 0.9165548 0.9663279
C 1.2869645 2.0153220 3.5726745
C 1.7815219 1.8324727 4.8708377
C 1.4083080 3.2754836 2.9719379
C 2.3904056 2.8834068 5.5498482
H 1.6978724 0.8506886 5.3416912
C 2.0253926 4.3232642 3.6506342
H 1.0207368 3.4289699 1.9630915
C 2.5199247 4.1306970 4.9403978
H 2.7732855 2.7230583 6.5582838
H 2.1226439 5.2956899 3.1685416
H 3.0050046 4.9505458 5.4683830
C 4.4054216 1.6921087 1.9437516
C 4.5280654 2.8577604 1.1858945
C 4.0243283 2.8879276 -0.1064342
C 3.4099402 1.7517881 -0.6197148
C 3.3281306 0.6291125 0.1927202
H 4.9921025 3.7471333 1.6039662
H 4.1049625 3.7936310 -0.7031422
H 2.9954569 1.7302768 -1.6238213
H 2.8503761 -0.2854935 -0.1598144
C 4.9024872 1.5969286 3.3343764
C 5.6854036 2.5947490 3.9188816
C 6.1239755 2.4409101 5.2260172
H 5.9747545 3.4770712 3.3540710
C 5.0002126 0.3413535 5.2744556
C 5.7772170 1.2902783 5.9242505
H 6.7357404 3.2106250 5.6913188
H 4.7132553 -0.5840718 5.7745806
H 6.1020450 1.1229260 6.9475941
N 4.5662371 0.4889718 4.0219067
N 3.8108686 0.5951507 1.4353217
C 3.0139160 -2.4345544 4.3363508
H 3.5505393 -3.3855040 4.2245499
H 3.2851015 -1.9661524 5.2951924
H 1.9302544 -2.6205895 4.3146956
C 2.5665658 -2.4508849 1.6390708
H 1.4857126 -2.2524948 1.6667720
H 2.9604246 -2.2819677 0.6252424
H 2.7663536 -3.4883131 1.9326386
C 6.7783107 -0.8666836 1.5454698
C 7.5912885 0.0426173 2.2341249
C 8.1750327 1.1171126 1.5666991
C 7.9471062 1.3070179 0.2055849
C 7.1333879 0.4104784 -0.4868980
C 6.5578241 -0.6688774 0.1746587
H 7.7597442 -0.0902288 3.3037969
H 8.8038539 1.8154524 2.1186826
H 8.3997044 2.1500506 -0.3139134
H 6.9424943 0.5552757 -1.5500744
H 5.9130748 -1.3624256 -0.3676458
Se 5.9116096 -2.3280931 2.4740624
Se 0.4521945 0.5485110 2.6334354
Pd -2.0916497 0.9314226 3.5623735
Pd 3.5005357 -1.0939051 2.8575072

MECPc
E(RM06) = -2647.5723841600
N -1.7110041 2.8607915 4.5862054
C -1.9359161 4.0548550 4.0292680
C -1.7825345 5.2464617 4.7216777
C -1.3769248 5.1882251 6.0492524
C -1.1322189 3.9512902 6.6283608

C -1.2993998 2.7925392 5.8713152
N -1.3465755 0.3996884 5.6075235
C -1.0812340 -0.8450854 6.0137305
C -0.5094983 -1.1278390 7.2452527
C -0.1878413 -0.0639899 8.0809496
C -0.4449456 1.2311338 7.6558571
C -1.0301631 1.4414070 6.4066822
H -2.2532906 4.0415790 2.9873669
H -1.9814496 6.1925100 4.2266043
H -1.3342104 -1.6403161 5.3137521
H -0.3210904 -2.1581410 7.5336635
H 0.2682898 -0.2391213 9.0523303
H -1.2503230 6.0973536 6.6325746
C -2.5058134 -0.9104824 2.7901668
H -1.8878191 -1.1464965 1.9111234
H -2.3464461 -1.6966981 3.5451884
H -3.5615660 -0.9410353 2.4807246
H -0.1664957 2.0711212 8.2861369
H -0.8178196 3.8952856 7.6666285
C -2.7047679 1.6784820 1.7721094
H -3.7134905 2.1018516 1.9137283
H -2.0327868 2.4835621 1.4333216
H -2.7576601 0.9236094 0.9758563
C 1.2533647 1.9073477 3.6080362
C 1.7462636 1.8009890 4.9201789
C 1.3958556 3.1367541 2.9429208
C 2.3565563 2.8843657 5.5423036
H 1.6517583 0.8475512 5.4449451
C 2.0123212 4.2173136 3.5644292
H 1.0143936 3.2301507 1.9245415
C 2.4961632 4.0965654 4.8673722
H 2.7321106 2.7803548 6.5607121
H 2.1167651 5.1599904 3.0276972
H 2.9803283 4.9422127 5.3538561
C 4.3910528 1.7492958 1.9588571
C 4.5473075 2.9005162 1.1869641
C 4.0446945 2.9311520 -0.1051299
C 3.3915683 1.8103589 -0.6032618
C 3.2766759 0.6983663 0.2177825
H 5.0402322 3.7785240 1.5942269
H 4.1564169 3.8261037 -0.7123151
H 2.9735138 1.7919654 -1.6059601
H 2.7726199 -0.2055752 -0.1219851
C 4.8894820 1.6508827 3.3462330
C 5.6644643 2.6499741 3.9360110
C 6.1208796 2.4854981 5.2346824
H 5.9330312 3.5434069 3.3797019
C 5.0188317 0.3725971 5.2748925
C 5.7956578 1.3219925 5.9225444
H 6.7308347 3.2563138 5.7004669
H 4.7455375 -0.5611068 5.7658801
H 6.1392253 1.1449679 6.9377769
N 4.5689385 0.5321658 4.0277461
N 3.7658273 0.6631951 1.4593607
C 3.0732652 -2.3971788 4.3392404
H 3.6184089 -3.3396341 4.1834892
H 3.3550556 -1.9910456 5.3246250
H 1.9945895 -2.6197906 4.3574187
C 2.5314584 -2.3522166 1.6190329
H 1.4478356 -2.1553881 1.6186916
H 2.9207237 -2.2296651 0.5952307
H 2.7026538 -3.3949625 1.9216201
S 0.4647732 0.5443380 2.8162550
Pt -2.0313835 0.9371229 3.5633626
Pt 3.4900504 -1.0245460 2.8610744
C 6.6496827 -0.8774895 1.5600294
C 7.4926424 0.0067017 2.2522154
C 8.1276223 1.0540723 1.5915069
C 7.9304317 1.2477065 0.2260335
C 7.1010838 0.3730900 -0.4767812
C 6.4745128 -0.6789436 0.1791794
H 7.6394612 -0.1332659 3.3238610
H 8.7742536 1.7292404 2.1524244
H 8.4183416 2.0740130 -0.2883620
H 6.9414527 0.5137409 -1.5455629

H 5.8211797 -1.3586899 -0.3706961
S 5.7891864 -2.1687102 2.4045994

Ph2S2
E(RM06) = -1259.23428032
Zero-point correction= 0.183382 (Hartree/Particle)
Thermal correction to Energy= 0.195795
Thermal correction to Enthalpy= 0.196739
Thermal correction to Gibbs Free Energy= 0.141837
Sum of electronic and zero-point Energies= -1259.050898
Sum of electronic and thermal Energies= -1259.038486
Sum of electronic and thermal Enthalpies= -1259.037542
Sum of electronic and thermal Free Energies= -1259.092444
E(RM06) = -1259.43372469

C 2.89436100 2.40649400 0.40791500
C 3.17324600 1.22910300 1.10201700
C 2.51442400 0.05180500 0.76922800
C 1.56832600 0.05513200 -0.25940000
C 1.28287600 1.23524800 -0.94975400
C 1.95344500 2.40939400 -0.61732000
H 3.41361600 3.32631200 0.67100900
H 3.90981000 1.22941300 1.90342000
H 2.72086300 -0.87260300 1.30724900
H 0.52794600 1.22962800 -1.73569100
H 1.73200300 3.32964400 -1.15467800
C -1.70879200 0.04535800 0.42202700
C -1.42833900 1.22785000 1.11039300
C -2.10628700 2.39780700 0.77820800
C -3.04976000 2.38839400 -0.24465200
C -3.32366600 1.20868500 -0.93676900
C -2.65727700 0.03553600 -0.60435300
H -0.67161600 1.22739500 1.89463000
H -1.88877200 3.31991100 1.31398800
H -3.57495200 3.30492900 -0.50741900
H -4.06221100 1.20389900 -1.73633100
H -2.85975800 -0.89063100 -1.14084200
S 0.67070700 -1.42813900 -0.67955300
S -0.80230000 -1.43256300 0.84195600

PhS$^-$
E(RM06) = -629.739746933
Zero-point correction= 0.089883 (Hartree/Particle)
Thermal correction to Energy= 0.095440
Thermal correction to Enthalpy= 0.096384
Thermal correction to Gibbs Free Energy= 0.060101
Sum of electronic and zero-point Energies= -629.649864
Sum of electronic and thermal Energies= -629.644307
Sum of electronic and thermal Enthalpies= -629.643363
Sum of electronic and thermal Free Energies= -629.679645
E(RM06) = -629.843279412

C -1.00342600 -0.65340500 0.00005400
C 0.38715600 -0.65339900 0.00055100
C 1.13117300 0.54468600 -0.00001500
C 0.38726200 1.74285100 -0.00100700
C -1.00330500 1.74299100 -0.00148100
C -1.71649000 0.54481800 -0.00098800
H -1.53784100 -1.60435800 0.00046500
H 0.92784900 -1.60098000 0.00134300
H 0.92807100 2.69036700 -0.00143100
H -1.53766200 2.69397400 -0.00224600
H -2.80554800 0.54488500 -0.00137600
S 2.89446200 0.54463100 0.00061300

PhS doublet
E(UM06) = -629.583475578
Zero-point correction= 0.090332 (Hartree/Particle)
Thermal correction to Energy= 0.095927
Thermal correction to Enthalpy= 0.096871
Thermal correction to Gibbs Free Energy= 0.059846
Sum of electronic and zero-point Energies= -629.493144
Sum of electronic and thermal Energies= -629.487549
Sum of electronic and thermal Enthalpies= -629.486604
Sum of electronic and thermal Free Energies= -629.523630

E(UM06) = -629.677943730

C -0.99532500 -0.66936400 0.00006500
C 0.38709100 -0.67488600 0.00056400
C 1.11264800 0.54469000 -0.00002200
C 0.38720000 1.76434100 -0.00101600
C -0.99520600 1.75894900 -0.00148600
C -1.68987000 0.54481700 -0.00098400
H -1.54364900 -1.60889900 0.00047100
H 0.94182800 -1.61116800 0.00134600
H 0.94204900 2.70055700 -0.00141500
H -1.54347200 2.69851500 -0.00227700
H -2.77803900 0.54488400 -0.00134900
S 2.82644500 0.54462400 0.00058400

Ph2Se2
E(RM06) = -481.578042131
Zero-point correction= 0.181329 (Hartree/Particle)
Thermal correction to Energy= 0.194572
Thermal correction to Enthalpy= 0.195517
Thermal correction to Gibbs Free Energy= 0.138311
Sum of electronic and zero-point Energies= -481.396713
Sum of electronic and thermal Energies= -481.383470
Sum of electronic and thermal Enthalpies= -481.382526
Sum of electronic and thermal Free Energies= -481.439732
E(RM06) = -481.757838080

C 2.73175600 2.53400800 0.36046400
C 3.12078300 1.37902600 1.03868200
C 2.59659100 0.14456500 0.67128200
C 1.67672700 0.07062900 -0.37732900
C 1.27873200 1.22578600 -1.05197700
C 1.81611000 2.45749800 -0.68426000
H 3.14438100 3.49826300 0.65167700
H 3.83658100 1.44082100 1.85645500
H 2.89138300 -0.76077400 1.20057000
H 0.53981300 1.16291300 -1.85044900
H 1.50476500 3.35987000 -1.20763300
C -1.67668700 0.07071900 0.37729800
C -1.27856400 1.22585500 1.05187400
C -1.81595100 2.45758500 0.68421000
C -2.73164400 2.53413300 -0.36046200
C -3.12076500 1.37914300 -1.03863000
C -2.59662900 0.14467500 -0.67122400
H -0.53952200 1.16300200 1.85022400
H -1.50449800 3.35992300 1.20757300
H -3.14428000 3.49839800 -0.65162400
H -3.83660200 1.44094400 -1.85636400
H -2.89148300 -0.76065800 -1.20049200
Se 0.88447700 -1.63452300 -0.87516100
Se -0.88457500 -1.63443100 0.87517600

PhSe$^-$
E(RM06) = -240.916994286
Zero-point correction= 0.089409 (Hartree/Particle)
Thermal correction to Energy= 0.095241
Thermal correction to Enthalpy= 0.096185
Thermal correction to Gibbs Free Energy= 0.058343
Sum of electronic and zero-point Energies= -240.827585
Sum of electronic and thermal Energies= -240.821753
Sum of electronic and thermal Enthalpies= -240.820809
Sum of electronic and thermal Free Energies= -240.858651
E(RM06) = -240.999680963

C 1.60232900 -2.81417700 3.70741300
C 1.98202600 -1.47324200 3.69138800
C 1.15146200 -0.50929400 3.12773200
C -0.08566700 -0.85596100 2.56322500
C -0.45345000 -2.20916000 2.58501200
C 0.37777300 -3.17361100 3.14874400
H 2.25208300 -3.56812600 4.14948400
H 2.93671900 -1.17243100 4.12368100
H 1.46331200 0.53554500 3.12300100
H -1.40873500 -2.50733900 2.15212200
H 0.06285000 -4.21746300 3.15062300

Se -1.25513600 0.49824700 1.78035400

PhSe doublet
E(UM06) = -240.742293610
Zero-point correction= 0.089584 (Hartree/Particle)
Thermal correction to Energy= 0.095497
Thermal correction to Enthalpy= 0.096442
Thermal correction to Gibbs Free Energy= 0.057752
Sum of electronic and zero-point Energies= -240.652710
Sum of electronic and thermal Energies= -240.646796
Sum of electronic and thermal Enthalpies= -240.645852
Sum of electronic and thermal Free Energies= -240.684542
E(UM06) = -240.823083870

C 1.59484400 -2.80463400 3.70106400
C 1.98103300 -1.46714800 3.69038400
C 1.15462500 -0.49720500 3.12969100
C -0.06923400 -0.87562100 2.57598200
C -0.46508300 -2.21373700 2.58193100
C 0.37221600 -3.17242800 3.14616900
H 2.24509800 -3.55832800 4.14068100
H 2.93536800 -1.16975300 4.12209800
H 1.46512700 0.54708500 3.12537800
H -1.42022900 -2.51048400 2.14990800
H 0.06134900 -4.21593900 3.14933500
Se -1.22954700 0.47118300 1.79015800

TS-4a/6a
E(RM06) = -1869.95293531
Zero-point correction= 0.648937 (Hartree/Particle)
Thermal correction to Energy= 0.694285
Thermal correction to Enthalpy= 0.695229
Thermal correction to Gibbs Free Energy= 0.567042
Sum of electronic and zero-point Energies= -1869.303998
Sum of electronic and thermal Energies= -1869.258651
Sum of electronic and thermal Enthalpies= -1869.257706
Sum of electronic and thermal Free Energies= -1869.385893
E(RM06) = -1870.49154216

N -3.11330400 0.83926300 -0.56021800
C -3.02673200 1.51654800 -1.70964300
C -3.24246700 2.88499200 -1.79495100
C -3.56256000 3.57589000 -0.63307700
C -3.65496000 2.87722500 0.56348300
C -3.42445400 1.50201900 0.57755500
N -3.27968700 -0.63721000 1.67469300
C -3.30929400 -1.41647100 2.76040600
C -3.55746100 -0.92670700 4.03489000
C -3.78934000 0.43501700 4.18451000
C -3.76075100 1.24968100 3.06135800
C -3.49788100 0.69078300 1.81100200
H -2.77432800 0.92756100 -2.59139500
H -3.15563500 3.38895000 -2.75390000
H -3.12207900 -2.47548400 2.59201800
H -3.56715200 -1.60382900 4.88435300
H -3.98859100 0.86234600 5.16423300
H -3.73985100 4.64845100 -0.65329400
C -2.90538300 -3.36541000 -0.10000000
H -1.93267400 -3.80542600 -0.36490800
H -3.12446400 -3.63113100 0.94820300
H -3.67073700 -3.84551100 -0.73159400
H -3.92923500 2.31748300 3.16764500
H -3.90434000 3.40895200 1.47722900
C -2.67846300 -1.76979800 -2.37261300
H -3.64528100 -1.62884300 -2.88696100
H -1.94992000 -1.08374300 -2.83729700
H -2.34173900 -2.79854500 -2.56953400
C 0.20793100 1.69740700 -1.15595000
C 0.50602100 0.03371100 -2.74720700
C 0.59394900 0.95671400 -3.77950500
C 0.49788800 2.30624000 -3.46394600
C 0.30963500 2.68008900 -2.14071400
C -0.02558000 2.01568100 0.27000800
C -0.32659400 1.19431700 2.41839200
C -0.42561000 2.47076400 2.95510500

C -0.32227800 3.55552500 2.09306600
C -0.11923300 3.32588500 0.73927900
H 0.59084000 -1.03601500 -2.93514500
H 0.74126500 0.61838700 -4.80122700
H 0.57024900 3.06535300 -4.23917500
H 0.23070400 3.73337700 -1.88664000
H -0.39695600 0.31035200 3.05254700
H -0.58203100 2.60086700 4.02258300
H -0.39359400 4.57340400 2.46890400
H -0.02437400 4.16818700 0.06004800
N 0.31782200 0.39111800 -1.47379200
N -0.14267400 0.96919800 1.11582800
C 0.64512000 -2.73382100 -0.87592700
H -0.18209700 -2.92895900 -1.57470800
H 1.57121500 -2.55614200 -1.44524300
H 0.79519000 -3.62263200 -0.24730500
C 0.01503500 -2.28828300 1.83051800
H -0.87266600 -2.92376900 1.70241400
H 0.88975400 -2.94312700 1.95632400
H -0.09987000 -1.69396700 2.75116800
C 3.20978900 0.73074300 0.07068200
C 3.57188700 0.65969000 -1.27587900
C 3.17880700 1.97041800 0.71336700
C 3.88342500 1.82138100 -1.97807800
H 3.60452700 -0.30968400 -1.77507300
C 3.50530600 3.12921100 0.01290800
H 2.90016100 2.02582900 1.76686200
C 3.85230500 3.05666300 -1.33505200
H 4.15876700 1.75861500 -3.03031400
H 3.47851200 4.09258700 0.52101400
H 4.10108100 3.96379200 -1.88359100
C 6.32538000 -0.66147500 0.45982900
C 6.44846500 -1.70513800 -0.46630200
C 6.84955100 0.59483600 0.13418400
C 7.08449900 -1.49541600 -1.68695000
H 6.03644300 -2.68583500 -0.22615600
C 7.49282700 0.79875600 -1.08390300
H 6.74179100 1.41998000 0.83866400
C 7.61085200 -0.24339600 -2.00032700
H 7.17179500 -2.31756900 -2.39663900
H 7.89667100 1.78271900 -1.32086200
H 8.11090200 -0.08190300 -2.95399000
Pt 0.18818900 -1.04496300 0.19814400
Pt -2.90272400 -1.33383800 -0.37974200
Se 5.41390200 -0.93806700 2.15011800
Se 2.74459900 -0.89655800 1.04114000

TS-4c/6c
E(RM06) = -2647.59208875
Zero-point correction= 0.650411 (Hartree/Particle)
Thermal correction to Energy= 0.695040
Thermal correction to Enthalpy= 0.695984
Thermal correction to Gibbs Free Energy= 0.570242
Sum of electronic and zero-point Energies= -2646.941678
Sum of electronic and thermal Energies= -2646.897049
Sum of electronic and thermal Enthalpies= -2646.896105
E(RM06) = -2648.16082860

N -3.19646300 0.89295900 -0.48243800
C -3.17356000 1.60440700 -1.61424000
C -3.43529000 2.96703900 -1.65211900
C -3.73555700 3.61428300 -0.46030400
C -3.75777500 2.88071500 0.71880000
C -3.48238200 1.51446500 0.68518400
N -3.24582400 -0.65036500 1.71276800
C -3.20538500 -1.45955900 2.77594800
C -3.39239400 -1.00943000 4.07515300
C -3.63716500 0.34335000 4.27546500
C -3.68204500 1.18899800 3.17584000
C -3.47793800 0.66921100 1.89779400
H -2.93145000 1.04874500 -2.52041600
H -3.39936200 3.49986300 -2.59868000
H -3.01172900 -2.51017000 2.56769400
H -3.34566100 -1.70977900 4.90432500
H -3.78974200 0.74032100 5.27611100

H -3.95001400 4.68009800 -0.44346000
C -2.92568500 -3.31959600 -0.15755400
H -1.96662700 -3.73925700 -0.49604500
H -3.07480600 -3.61913800 0.89383100
H -3.72386600 -3.79083700 -0.75421800
H -3.86106100 2.25044200 3.32141200
H -3.99188700 3.37810600 1.65560400
C -2.82375600 -1.64668000 -2.39073500
H -3.79837100 -1.43683600 -2.86532700
H -2.07730000 -0.97721700 -2.85176600
H -2.54479300 -2.68089900 -2.64176800
C 0.06541100 1.74124900 -1.26223700
C 0.39808400 0.07923200 -2.84747900
C 0.38259000 0.99226000 -3.89204500
C 0.20339400 2.33607400 -3.58778100
C 0.04547700 2.71437900 -2.26180600
C -0.11211300 2.06417300 0.17077700
C -0.29536700 1.25180900 2.33523300
C -0.40340600 2.52979200 2.86748300
C -0.36291000 3.61016300 1.99511500
C -0.21545100 3.37522600 0.63482000
H 0.53900800 -0.98593100 -3.02795900
H 0.50925000 0.65083400 -4.91550800
H 0.18452200 3.08672900 -4.37428600
H -0.10588400 3.76175800 -2.01611500
H -0.31566900 0.37073000 2.97716200
H -0.51652600 2.66417100 3.93991200
H -0.44037700 4.62892600 2.36737100
H -0.16637900 4.21427700 -0.05330300
N 0.24379800 0.44072900 -1.57086700
N -0.16116300 1.02186500 1.02777500
C 0.64975900 -2.68294200 -0.96071900
H -0.18969700 -2.89876800 -1.63911400
H 1.56039300 -2.49853300 -1.55191600
H 0.82597800 -3.56224500 -0.32549500
C 0.03787000 -2.24007500 1.74054700
H -0.78935400 -2.94521700 1.57730700
H 0.95824400 -2.81726500 1.90956400
H -0.17113900 -1.65141600 2.64872900
C 3.08962300 0.63077800 -0.03444100
C 3.48383600 0.54219700 -1.37348400
C 3.06731700 1.88391600 0.58759400
C 3.82535500 1.68871300 -2.08486800
H 3.51789800 -0.43579200 -1.85425800
C 3.42052400 3.02784900 -0.12079400
H 2.77503400 1.95226700 1.63629700
C 3.79559400 2.93346200 -1.46051100
H 4.12677100 1.60670300 -3.12858900
H 3.39638400 3.99813700 0.37419400
H 4.06873500 3.82979500 -2.01527200
C 6.00005900 -0.74843900 0.41338600
C 6.11131000 -1.79200300 -0.52029100
C 6.64956700 0.46345400 0.12983600
C 6.84256000 -1.62768100 -1.69148200
H 5.60870100 -2.73771300 -0.31521900
C 7.39005000 0.62243100 -1.03660000
H 6.56013800 1.28723500 0.83838100
C 7.48838400 -0.42033700 -1.95563800
H 6.91362400 -2.45072100 -2.40216100
H 7.88747300 1.57187400 -1.23341700
H 8.06445400 -0.29425500 -2.87107100
Pt 0.19978600 -0.99080300 0.11206900
Pt -2.96013600 -1.28104000 -0.37622700
S 2.64772000 -0.84037500 0.86819700
S 5.05085600 -0.93745600 1.88892000