

“Supporting Information for”

The role of hypervalent iodine(III) reagents in promoting alkoxylation of unactivated C(sp³)–H bonds catalyzed by palladium(II) complexes

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Content:

Fig. S1 Comparing the calculated mechanisms of oxidative addition from **18** via two different pathways. (page S2)

Fig S2. Wave function analysis carried out along the IRC of **TS**₁₇₋₁₈ and **TS**₁₈₋₁₉. (page S3)

Fig. S3 Comparing the calculated mechanisms of cyclopalladation via removal of α -, β - and γ -C-H protons by the OAc ligand. (page S4)

Table S1. Total potential (E), enthalpy (H) and Gibbs free energies (G) of all structures optimized at the SMD/M06/BS1 level of theory along with the total potential energies calculated by SMD/M06/BS2//SMD/M06/BS1 and Cartesian coordinates for all of the calculated structures. (page S5)

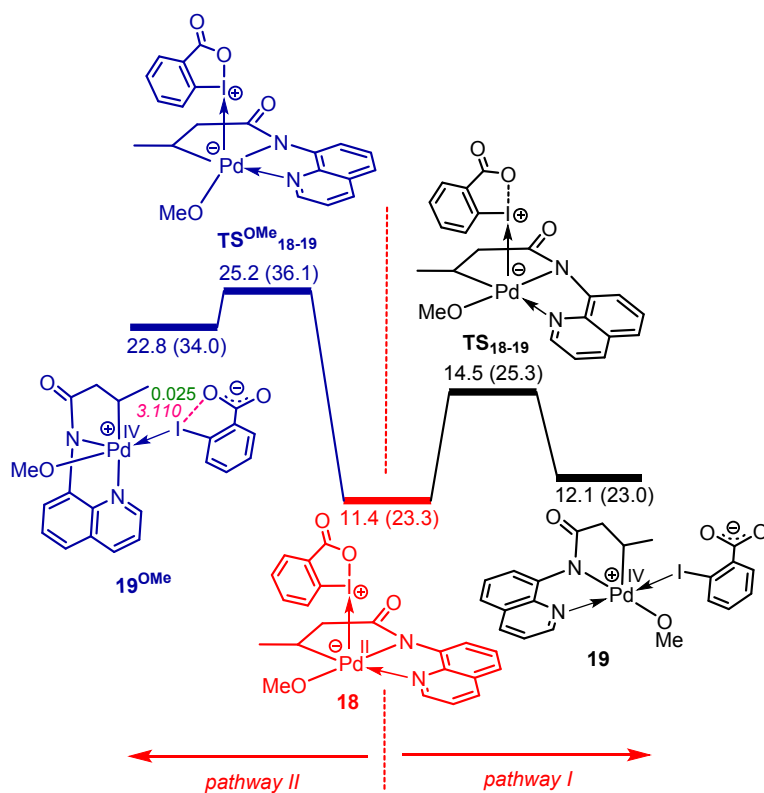
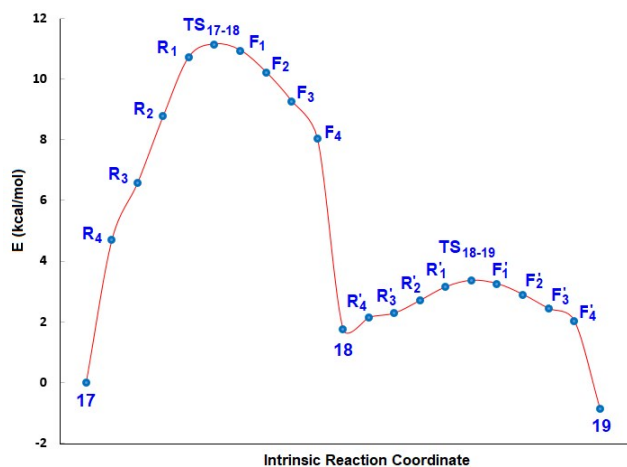
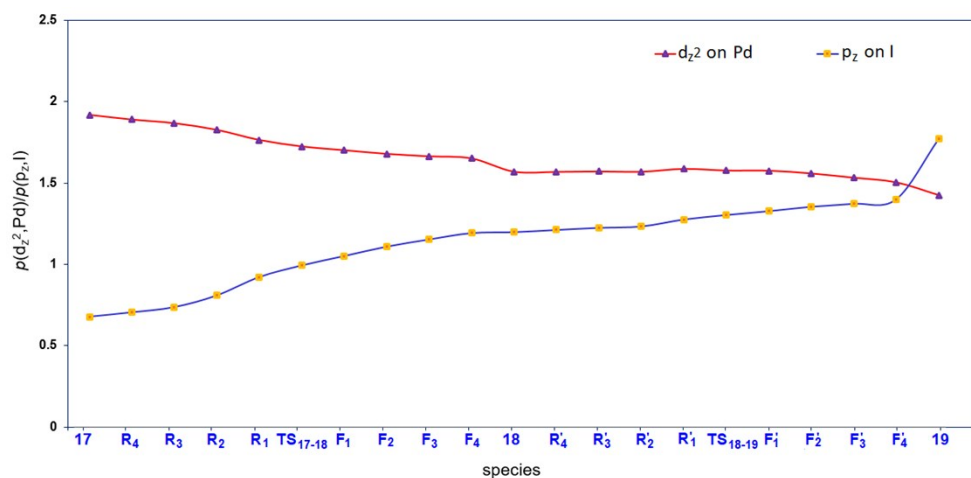


Fig. S1 Comparing the calculated mechanisms of oxidative addition from **18** via pathways I and II. Free energies (potential energies) are given in kcal/mol. The I-O distance (Å) and the WBI value between I and O are annotated in pink and green, respectively. Pathway I involves the migration of the quinoline to the apical position while in pathway II, the isomerization occurs via the movement of the OMe ligand. Although both pathways lead to oxidation of the Pd(II) center, pathway I is computed to be much more favorable than pathway II. This result supports the importance of the isomerization through moving the ligand trans to the strong σ -donor alkyl ligand, as discussed in the oxidative addition section.

(a)



(b)



(c)

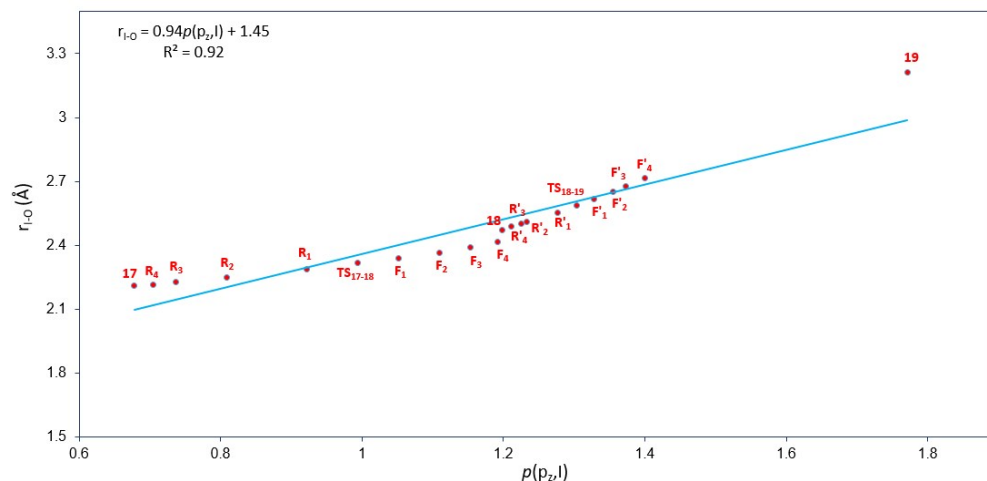


Fig. S2 (a) IRC path for oxidation of Pd(II) to Pd(IV) by BI-OMe (transformation $17 \rightarrow TS_{17-18} \rightarrow 18 \rightarrow TS_{18-19} \rightarrow 19$) calculated at the SDD/MO6/BS1 level of theory. (b) Change in population of the palladium d_z^2 and iodine p_z orbitals upon moving from **17** to **19** obtained by NBO calculations. (d) Correlation between the population of iodine p_z orbital, $p(p_z, I)$, and the I-O^a distance.

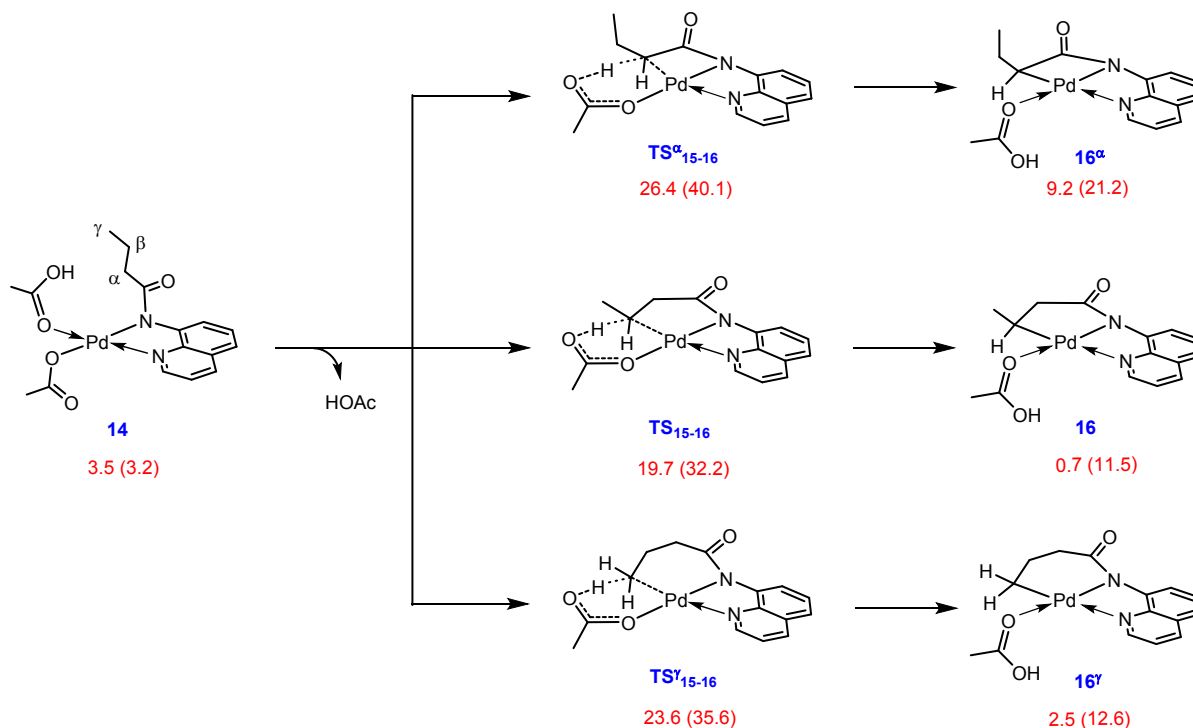


Fig. S3 Comparing the calculated mechanisms of cyclopalladation via removal of α -, β - and γ -C-H protons by the OAc ligand. Free energies (potential energies) are given in kcal/mol. It follows that TS_{15-16} is significantly lower in energy than $\text{TS}^{\alpha}_{15-16}$ and $\text{TS}^{\gamma}_{15-16}$, implying that the C-H activation at the β position is kinetically favoured over other positions. Since TS_{15-16} lies below TS_{17-18} , TS_{18-19} and TS_{21-22} (Figs 3a and 4), the C-H activation in this case is unlikely to be reversible and thus the regioselectivity of the alkoxylation reaction should be controlled by a kinetic preference for deprotonation of the β -C-H bond.

Table S1. Total potential (E), enthalpy (H) and Gibbs free energies (G) of all structures optimized at the SMD/M06/BS1 level of theory along with the total potential energies calculated by SMD/M06/BS2//SMD/M06/BS1 and Cartesian coordinates for all of the calculated structures.

1

E (M06-SMD/BS1) = -688.0848934 au

H (M06-SMD/BS1) = -687.822439 au

G (M06-SMD/BS1) = -687.879235 au

E (M06-SMD/BS2//M06-SMD/BS1) = -688.3457287 au

C	0.10878900	1.51496100	-0.28906900
C	-0.22434700	0.17848100	-0.19636500
C	-1.60661100	-0.17953900	-0.03689900
C	-2.59018800	0.84088200	0.05016300
C	-2.20599500	2.20016900	-0.02329200
C	-0.88295100	2.51490600	-0.19348000
H	1.13442500	1.82780600	-0.44880100
C	-3.93475900	0.43124800	0.20647000
H	-2.97006900	2.97338800	0.04964300
H	-0.57306100	3.55619000	-0.26441200
C	-4.23679700	-0.90487800	0.26198100
C	-3.18421300	-1.83715700	0.15911300
H	-4.71294900	1.19134500	0.27823000
H	-5.26028600	-1.25310900	0.38013900
H	-3.40446400	-2.90582700	0.19652200
N	-1.91996100	-1.49990800	0.01755800
N	0.64616000	-0.91117700	-0.27376800
H	0.14346100	-1.80049100	-0.29910900
C	2.00447200	-1.07760500	-0.18804400
C	2.89417300	0.12123100	-0.02131900
H	2.81654100	0.74169500	-0.92900600
H	2.50720300	0.74270000	0.80218900
C	4.34789100	-0.24274300	0.22957500
H	4.72043300	-0.85272900	-0.60577500
H	4.41616700	-0.87727600	1.12543900
C	5.20745600	0.99698400	0.39779400
H	4.86590900	1.60687400	1.24648100
H	6.25830400	0.73614700	0.57755900
H	5.17073400	1.63157300	-0.49939200
O	2.45284400	-2.22279200	-0.24450200

2 (BI-OMe)

E (M06-SMD/BS1) = -545.7135263 au

H (M06-SMD/BS1) = -545.566294 au

G (M06-SMD/BS1) = -545.617131 au

E (M06-SMD/BS2//M06-SMD/BS1) = -832.3361573 au

C	-2.93306700	0.60943400	0.11731200
C	-1.73941000	-0.11061000	0.06520900
C	-0.56254800	0.59754800	-0.10691500
C	-0.50256400	1.96962600	-0.24512500
C	-1.70894800	2.66807500	-0.18972800
C	-2.91472000	1.99300100	-0.00627000
H	-3.86643700	0.06542700	0.25283400
H	0.44669500	2.47874300	-0.39778500
H	-1.70053400	3.75159700	-0.29393300
H	-3.84692500	2.55281500	0.03515000
I	1.18775700	-0.62872300	-0.15655800
C	-1.70146400	-1.59996200	0.17117900
O	-2.73049200	-2.25551500	0.33617200
O	-0.51921500	-2.11991000	0.06964700
O	2.36312200	1.03535900	-0.32982500
C	2.78933800	1.55094300	0.92062900
H	3.39550400	2.43940400	0.70094200
H	1.94299400	1.85393700	1.55770800
H	3.41054600	0.83260400	1.47695500

3

E (M06-SMD/BS1) = -802.5368415 au

H (M06-SMD/BS1) = -802.239691 au

G (M06-SMD/BS1) = -802.303405 au

E (M06-SMD/BS2//M06-SMD/BS1) = -802.8443413 au

C	-1.63872400	2.26884500	0.03603400
C	-1.10504500	1.09505600	0.51861700
C	-1.78492300	-0.14074100	0.30394600
C	-2.99627800	-0.12244700	-0.44557300
C	-3.51253100	1.10109100	-0.93223000
C	-2.84862100	2.27672000	-0.68716200
H	-1.10697200	3.20111000	0.22201400
C	-3.65127300	-1.35758800	-0.66050000
H	-4.44428400	1.08861600	-1.49760000
H	-3.24427900	3.22128300	-1.05540100
C	-3.11366300	-2.50547900	-0.14119500
C	-1.91624300	-2.40989400	0.60016500
H	-4.57712700	-1.37219200	-1.23575100
H	-3.58823500	-3.47363000	-0.28363600
H	-1.48211700	-3.31518200	1.03056000

N	-1.26706100	-1.28683600	0.82192000
N	0.08430300	1.13692300	1.29008900
C	1.29187400	0.56317700	1.02362000
C	1.45739700	-0.09115700	-0.32605100
H	1.11989800	-1.13326000	-0.22782200
H	0.78911400	0.38278500	-1.05779000
C	2.87191300	-0.08662900	-0.88703600
H	2.79980900	-0.48566400	-1.91787800
C	3.48726000	1.30047200	-0.95454700
H	2.79467600	1.99457600	-1.44955300
H	3.70072700	1.68212500	0.05186600
H	4.42085900	1.30170200	-1.53061700
O	2.19015100	0.61183900	1.86501000
O	3.64683300	-0.99766100	-0.12129500
C	4.89851200	-1.29068200	-0.69175400
H	5.60842200	-0.45239000	-0.60849900
H	5.31334200	-2.14779200	-0.14912300
H	4.80229700	-1.56055100	-1.75799100
H	0.03937400	1.59997600	2.19543500

Pd₃(OAc)₆

E (M06-SMD/BS1) = -1754.105696 au

H (M06-SMD/BS1) = -1753.756817 au

G (M06-SMD/BS1) = -1753.864489 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1754.737721 au

Pd	-1.79376100	0.05833100	-0.00038000
O	-1.93306900	1.20231200	-1.68086200
O	-2.05882800	1.66595200	1.25226600
C	-1.17749700	2.31228700	1.88706000
O	0.07208900	2.27780800	1.67841800
Pd	0.94613200	1.52227700	-0.00058100
C	-1.26857400	2.26109700	-1.88971600
O	-0.24075300	2.63496600	-1.25624700
O	-2.00982800	-1.07482600	1.67950600
O	-2.16675200	-1.52717500	-1.25155100
C	-1.32996900	-2.23455800	-1.88138400
O	-0.08070100	-2.28080400	-1.67342400
Pd	0.84791700	-1.58229500	0.00151400
C	-1.41006400	-2.17055000	1.89461700
O	-0.40580700	-2.60901900	1.26516900
O	1.94875500	-1.19978900	1.67516800

O	2.39957700	-1.11208700	-1.26160400
C	2.59860000	-0.13199100	1.88469000
C	2.58737000	-0.03459900	-1.89519400
O	2.47216200	0.95563100	1.25342200
O	2.00626300	1.07112100	-1.68144200
C	-1.77126700	3.16832100	-2.96880000
H	-2.46582700	3.88838400	-2.51602800
H	-0.94711300	3.72443800	-3.42508700
H	-2.31673400	2.60004400	-3.72824900
C	-1.86505100	-3.13038300	-2.95455600
H	-2.10643100	-4.10127900	-2.50169100
H	-2.77805500	-2.71521200	-3.39099400
H	-1.11075200	-3.29589500	-3.72988500
C	-1.97015800	-3.03994400	2.97673000
H	-1.19300400	-3.67873100	3.40610000
H	-2.43828200	-2.43040200	3.75578500
H	-2.74459800	-3.68172000	2.53609000
C	3.63885300	-0.17638800	2.95997500
H	3.75144100	0.80429700	3.43164200
H	3.39087900	-0.93520800	3.70809400
H	4.59744300	-0.44930000	2.49888400
C	3.61826000	-0.05336900	-2.98027400
H	4.59072000	0.19398700	-2.53410000
H	3.68902700	-1.04659600	-3.43319100
H	3.39165400	0.69942100	-3.74133700
C	-1.65464400	3.23444900	2.96522800
H	-2.57510200	2.85729200	3.42043200
H	-0.88026600	3.37361900	3.72558400
H	-1.86827500	4.21152300	2.51170400

Pd(OAc)₂

E (M06-SMD/BS1) = -584.6589628 au

H (M06-SMD/BS1) = -584.544567 au

G (M06-SMD/BS1) = -584.59454 au

E (M06-SMD/BS2//M06-SMD/BS1) = -584.8738101 au

Pd	0.00003200	0.00004500	-0.01574500
O	-1.76187800	-1.08333600	-0.01316900
C	-2.43934000	-0.00002100	-0.00199700
O	-1.76190300	1.08341200	-0.01314400
O	1.76191200	1.08328100	-0.01359600
C	2.43933000	-0.00013200	-0.00221700

O	1.76174200	-1.08338900	-0.01358200
C	-3.91522900	-0.00003400	0.05424200
H	-4.22654500	-0.00374200	1.10739000
H	-4.31555800	0.90161300	-0.42004900
H	-4.31560600	-0.89852800	-0.42602300
C	3.91518800	-0.00008600	0.05463900
H	4.31572300	-0.90214400	-0.41870200
H	4.31568100	0.89799600	-0.42631200
H	4.22613000	0.00463800	1.10788900

13

E (M06-SMD/BS1) = -1272.796451 au

H (M06-SMD/BS1) = -1272.417225 au

G (M06-SMD/BS1) = -1272.503352 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1273.266857 au

C	2.86726400	-1.07327200	1.63780900
C	1.82154700	-0.46804400	0.98610300
C	1.99305500	0.78683800	0.37041500
C	3.25141200	1.43143600	0.42380600
C	4.31387400	0.79031100	1.10249000
C	4.12368400	-0.43435700	1.69554200
H	2.71896800	-2.04512300	2.10795300
C	3.36893200	2.68921100	-0.21026300
H	5.28124300	1.28854600	1.14436500
H	4.94294900	-0.92405200	2.21669800
C	2.28405000	3.23613300	-0.84923700
C	1.06633600	2.53472000	-0.86172300
H	4.32547400	3.20917500	-0.18312400
H	2.34197600	4.20007900	-1.34673400
H	0.18545400	2.93554800	-1.36113400
N	0.92765200	1.35749200	-0.27582200
N	0.50858200	-1.08171600	0.90218000
H	0.04423700	-1.17053800	1.81728600
C	0.38144500	-2.33426100	0.19260000
C	1.21110800	-2.49284700	-1.04342600
H	2.12354900	-3.04450500	-0.76040100
H	1.54468500	-1.51205000	-1.41068200
C	0.45396300	-3.24816600	-2.12913100
H	0.15945300	-4.23523200	-1.74722400
H	-0.48012100	-2.70704300	-2.35131400
C	1.28970900	-3.39444700	-3.38655400

H	1.56869800	-2.41295100	-3.79544800
H	0.74364500	-3.93816400	-4.16766600
H	2.21909100	-3.94486700	-3.18241000
O	-0.41348800	-3.15062100	0.60241100
Pd	-0.77680000	0.25520600	-0.13174400
O	-1.90028900	1.60206900	-1.16410800
C	-2.50164700	2.46437300	-0.40002500
O	-2.40659200	2.49016600	0.83132700
O	-2.44288800	-0.90362000	0.04783700
C	-2.75347700	-1.23723000	1.26332200
O	-2.13672200	-0.86918300	2.27097200
C	-3.31840500	3.47556700	-1.15835400
H	-2.64395900	4.13792400	-1.71703300
H	-3.92236100	4.07708800	-0.47261000
H	-3.96734600	2.97908600	-1.88893100
C	-3.93042800	-2.16892000	1.35737400
H	-4.33400100	-2.17924300	2.37450300
H	-3.59281300	-3.18341200	1.10386200
H	-4.71433200	-1.89292800	0.64373900

TS₁₃₋₁₄

E (M06-SMD/BS1) = -1272.784221 au
H (M06-SMD/BS1) = -1272.410737 au
G (M06-SMD/BS1) = -1272.49522 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1273.255069 au

C	2.50651100	0.24680700	1.98384200
C	1.49527600	0.28057800	1.05266500
C	1.13974500	1.51292700	0.46101000
C	1.84895300	2.69627800	0.77206900
C	2.89411800	2.62551500	1.72281200
C	3.20271400	1.42772800	2.32115300
H	2.77631100	-0.70251200	2.44557400
C	1.45305500	3.88544100	0.11819600
H	3.43596000	3.53601800	1.97447600
H	3.99928800	1.37706400	3.06055000
C	0.41096700	3.86209300	-0.77574900
C	-0.26844300	2.65443700	-1.01164400
H	1.98289800	4.81183800	0.33662500
H	0.08563900	4.75939800	-1.29476700
H	-1.11971900	2.60372600	-1.68880500
N	0.08363900	1.52819900	-0.41577700

N	0.78266700	-0.88578800	0.62090400
H	0.04891500	-1.54482200	1.41455500
C	1.43384300	-1.79424600	-0.25364800
C	2.73941400	-1.37915000	-0.87193900
H	3.48704000	-1.26192700	-0.07139100
H	2.61461300	-0.36949100	-1.29925800
C	3.24207200	-2.35290300	-1.92327000
H	3.35873800	-3.34826300	-1.47106400
H	2.48403100	-2.46097200	-2.71315900
C	4.55908100	-1.89054400	-2.51997800
H	4.45544200	-0.90639600	-2.99901900
H	4.92456100	-2.59334400	-3.27949400
H	5.33599000	-1.80092100	-1.74718400
O	0.90537000	-2.86997100	-0.48742000
Pd	-0.95164300	-0.21283300	-0.32919100
O	-2.59378200	0.52404000	-1.29158700
C	-3.41743300	1.17452800	-0.52784100
O	-3.26144000	1.34140300	0.68710000
O	-2.02594300	-1.92858800	0.11507300
C	-1.77102800	-2.53987000	1.19651400
O	-0.78442800	-2.28122600	1.95839900
C	-4.59478700	1.75631200	-1.26344600
H	-4.24847900	2.58465600	-1.89597300
H	-5.34267100	2.13478100	-0.56027200
H	-5.04828800	1.00866500	-1.92419000
C	-2.67326100	-3.65967200	1.59634000
H	-2.15389000	-4.60853300	1.40839600
H	-3.60563000	-3.64325700	1.02605900
H	-2.88231400	-3.60508200	2.67022900

14

E (M06-SMD/BS1) = -1272.790432 au

H (M06-SMD/BS1) = -1272.412662 au

G (M06-SMD/BS1) = -1272.496878 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1273.262157 au

C	-2.49010400	1.25001500	-1.51615500
C	-1.43152200	0.91162500	-0.69617800
C	-0.59698500	1.95533400	-0.22447100
C	-0.88569900	3.31448700	-0.48785300
C	-2.00723000	3.62162000	-1.29241700
C	-2.77402800	2.60263700	-1.80324000

H	-3.11490200	0.47106800	-1.94742000
C	-0.01397500	4.28375700	0.05854400
H	-2.23135200	4.66462100	-1.51031900
H	-3.62265400	2.83135300	-2.44531200
C	1.07209300	3.89131500	0.80179400
C	1.32137500	2.52122000	0.98674200
H	-0.21529200	5.33885000	-0.12361900
H	1.75763200	4.61465600	1.23461500
H	2.19173700	2.16849900	1.53731200
N	0.51706200	1.59637100	0.48966800
N	-1.05886500	-0.39070100	-0.29704400
H	-0.26447400	-1.63963900	-1.54606300
C	-1.92406100	-1.27431100	0.30474000
C	-3.39855400	-0.94954000	0.40918200
H	-3.86012000	-1.10776800	-0.57852700
H	-3.53421100	0.11932500	0.63176000
C	-4.12286300	-1.79749500	1.44353100
H	-4.01613100	-2.86061800	1.18682400
H	-3.64234500	-1.66865900	2.42511500
C	-5.59259300	-1.42597400	1.52839600
H	-5.72263000	-0.37202200	1.81336700
H	-6.12030700	-2.03851600	2.27085600
H	-6.09498200	-1.56937600	0.56078900
O	-1.49560600	-2.34263100	0.75550900
Pd	0.89273700	-0.38149300	0.35438000
O	2.79348700	-0.20672900	1.10791500
C	3.70369400	0.07491600	0.22955600
O	3.48871900	0.22079500	-0.98037300
O	1.39759600	-2.38770700	-0.05493900
C	0.97564300	-2.99835700	-1.04921600
O	0.08700500	-2.51061800	-1.87797600
C	5.08074500	0.24906800	0.81327200
H	5.10197200	1.16637400	1.41683300
H	5.83266900	0.32590100	0.02215500
H	5.32649300	-0.58509200	1.48065300
C	1.44400800	-4.36447700	-1.38344900
H	0.62350200	-5.07053800	-1.20153300
H	2.30375000	-4.63716100	-0.76766500
H	1.69908400	-4.42220500	-2.44738800

E (M06-SMD/BS1) = -1043.797608 au
 H (M06-SMD/BS1) = -1043.488065 au
 G (M06-SMD/BS1) = -1043.559153 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -1044.179531 au

C	-3.07704800	1.66597900	0.22314200
C	-1.90648900	0.93814400	0.06276100
C	-2.01879500	-0.47723800	0.00100700
C	-3.26673600	-1.13709400	0.09773700
C	-4.43361100	-0.35733700	0.26106900
C	-4.32191100	1.01017800	0.32031700
H	-3.03403700	2.74669000	0.27499100
C	-3.26982900	-2.54853200	0.02734100
H	-5.39824900	-0.85618000	0.33859100
H	-5.21461000	1.62052500	0.44735200
C	-2.09208000	-3.23735500	-0.12916900
C	-0.88730500	-2.52245300	-0.21711800
H	-4.21981700	-3.07686100	0.10023500
H	-2.06776500	-4.32210100	-0.18534700
H	0.07203600	-3.02117800	-0.34125800
N	-0.86351900	-1.20192100	-0.15383200
N	-0.59389700	1.41886600	-0.04138800
C	-0.24969500	2.73669500	-0.05450800
C	1.22528100	3.04772700	-0.19343300
H	1.42926400	3.91216500	0.45418400
H	1.38073500	3.40319100	-1.22484500
C	2.21260000	1.93966800	0.12272500
H	2.03360500	1.53218700	1.12885900
H	2.16744800	1.13692700	-0.68639400
C	3.66639000	2.37916900	0.02875700
H	3.90039500	2.76494700	-0.97191900
H	4.34477100	1.54547000	0.24706800
H	3.85837000	3.17736800	0.75827600
O	-1.05992900	3.66816700	0.01093800
Pd	0.77184700	-0.03761200	-0.23698800
O	2.04011600	-1.62256100	-0.55304700
C	2.96516200	-1.80407400	0.33718000
O	3.11352200	-1.10275100	1.34494600
C	3.86362800	-2.97694800	0.04735900
H	3.27437400	-3.90269900	0.05690600
H	4.66243000	-3.04947400	0.79145200
H	4.30097600	-2.88144500	-0.95387100

TS₁₅₋₁₆

E (M06-SMD/BS1) = -1043.767238 au

H (M06-SMD/BS1) = -1043.463434 au

G (M06-SMD/BS1) = -1043.531714 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1044.149361 au

C	-3.00387500	1.80766400	0.17628700
C	-1.89143700	0.98615800	0.06675700
C	-2.10885300	-0.42061300	-0.01143600
C	-3.41290900	-0.97063800	0.02858800
C	-4.51904900	-0.09815200	0.14391700
C	-4.30114500	1.25630600	0.21389700
H	-2.87170700	2.88186600	0.23458100
C	-3.53193100	-2.37699000	-0.05296900
H	-5.52400100	-0.51656600	0.17316000
H	-5.14725700	1.93644200	0.30012000
C	-2.40997700	-3.15975500	-0.16659300
C	-1.14819200	-2.54223000	-0.20053400
H	-4.52545700	-2.82360700	-0.02463800
H	-2.47419900	-4.24260800	-0.23137300
H	-0.23432600	-3.12775800	-0.28930900
N	-1.00760500	-1.23044500	-0.12668600
N	-0.55053100	1.37225900	0.01491100
C	-0.06899700	2.62428700	0.23223200
C	1.43898900	2.70302200	0.19093900
C	2.12089100	1.56916100	-0.56203100
H	1.71642600	1.50404200	-1.58548200
O	-0.76061100	3.62192900	0.47199400
Pd	0.74451800	-0.13176000	-0.21048400
O	2.05511300	-1.77394100	-0.29166800
C	3.09578300	-1.55027800	0.39475500
O	3.35482900	-0.40338000	0.88056700
C	4.05509900	-2.66235200	0.65528700
H	5.06185200	-2.35774400	0.34694000
H	4.08946700	-2.85925900	1.73399900
H	3.76172000	-3.57385900	0.12822500
H	2.53094000	0.43054000	0.28506200
C	3.61648500	1.84457800	-0.73191900
H	4.12690800	1.98665400	0.23022500
H	4.12530400	1.03620700	-1.27200800
H	3.73926300	2.76972100	-1.31579600

H	1.78910100	2.72576000	1.23723000
H	1.71518600	3.68055700	-0.23648000

16

E (M06-SMD/BS1) = -1043.800633 au

H (M06-SMD/BS1) = -1043.491717 au

G (M06-SMD/BS1) = -1043.562273 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1044.18242 au

C	-3.22079500	1.40189200	0.17861800
C	-1.98198500	0.78656400	0.05055900
C	-1.95503100	-0.64699600	-0.02312700
C	-3.15662300	-1.39903900	0.04379400
C	-4.39344300	-0.72786900	0.17640600
C	-4.40695500	0.64357500	0.24031600
H	-3.27066400	2.48329000	0.23469700
C	-3.05418900	-2.80800300	-0.02719700
H	-5.31180000	-1.31172900	0.22384600
H	-5.35368400	1.17282000	0.34124500
C	-1.82617400	-3.40572000	-0.15621800
C	-0.68351100	-2.58796900	-0.21811700
H	-3.96573000	-3.40358300	0.02262400
H	-1.71977200	-4.48613600	-0.21235800
H	0.31122900	-3.02409900	-0.32400000
N	-0.74301100	-1.27123800	-0.15610100
N	-0.74005600	1.41885000	0.00315500
C	-0.50693600	2.75412800	0.13740300
C	0.97247500	3.05430500	0.21450100
H	1.16054200	4.07195500	-0.16505300
H	1.21381500	3.08551900	1.29237100
C	1.84656600	2.00501000	-0.46506200
H	1.84160100	2.16558100	-1.55724300
C	3.26295700	1.99156100	0.06064200
H	3.29664100	1.73175800	1.13015900
H	3.90250300	1.28240300	-0.48156300
H	3.72682500	2.98949900	-0.03926100
O	-1.36976300	3.63563000	0.24206300
Pd	0.84154800	0.23337300	-0.30104600
O	2.70525100	-1.44229800	1.53367800
C	3.08751100	-1.61672100	0.28342000
O	2.54139800	-1.04468500	-0.66460900
C	4.23207100	-2.54474000	0.12259400

H	4.01867400	-3.49179600	0.63147200
H	4.43535900	-2.71962700	-0.93606600
H	5.11698100	-2.10717000	0.60186000
H	1.95701400	-0.79614800	1.55574300

17

E (M06-SMD/BS1) = -1360.549985 au
H (M06-SMD/BS1) = -1360.160991 au
G (M06-SMD/BS1) = -1360.250657 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1647.452167 au

C	5.29265000	0.32695600	0.61249300
C	3.94359600	0.22216500	0.29508700
C	3.44997500	-1.06620100	-0.10402800
C	4.32071100	-2.18735900	-0.15255300
C	5.68525500	-2.03073300	0.17992200
C	6.14560800	-0.79197100	0.55130100
H	5.68892700	1.28887200	0.91624600
C	3.77104200	-3.43263900	-0.53582300
H	6.34479200	-2.89652100	0.13498600
H	7.19523300	-0.65704300	0.80958800
C	2.43818500	-3.53108900	-0.84227500
C	1.64623100	-2.37104200	-0.77451400
H	4.42405000	-4.30438500	-0.57791900
H	1.98624700	-4.47558600	-1.13471800
H	0.58162600	-2.41674800	-1.01090400
N	2.12339900	-1.18964400	-0.42845300
N	2.99954900	1.24544000	0.34854700
C	3.23141800	2.53356500	0.72822800
C	1.94938400	3.32579600	0.82881100
H	2.16306800	4.39078900	0.64373100
H	1.64967400	3.26051800	1.89040700
C	0.81470800	2.79548400	-0.04347000
H	0.90559900	3.19510900	-1.06846000
C	-0.54721800	3.11067400	0.53259200
H	-0.68883300	2.63045600	1.51369600
H	-1.36707800	2.78855600	-0.12326400
H	-0.66409300	4.19824800	0.69028900
O	4.33148900	3.01934300	1.02272100
Pd	1.15962300	0.80080700	-0.30328400
C	-6.00513800	0.16022300	0.18855200
C	-4.74262300	-0.38423100	0.42135500

C	-3.66287700	0.15323100	-0.25922600
C	-3.76224900	1.20395700	-1.14903100
C	-5.03562700	1.73248900	-1.36588200
C	-6.14769300	1.21436900	-0.70448100
H	-6.86073800	-0.25441700	0.71906100
H	-2.88906200	1.60755800	-1.65696600
H	-5.15204300	2.56121200	-2.06184300
H	-7.13203400	1.64075000	-0.88633400
I	-1.81778000	-0.80339300	0.24394800
C	-4.52563500	-1.50230000	1.37899400
O	-5.44592400	-2.02542200	1.99730800
O	-3.27908400	-1.87386300	1.50748600
O	-0.82285400	0.45457200	-1.12030200
C	-0.76923600	-0.04014300	-2.45802000
H	-0.34595900	0.76216100	-3.07629600
H	-1.77910000	-0.27953400	-2.82212600
H	-0.13302600	-0.93211900	-2.54387700

7

E (M06-SMD/BS1) = -814.7975368 au

H (M06-SMD/BS1) = -814.558288 au

G (M06-SMD/BS1) = -814.616601 au

E (M06-SMD/BS2//M06-SMD/BS1) = -815.0853943 au

C	-1.46560300	2.37471600	-0.06201600
C	-0.82135600	1.14448600	-0.02562500
C	-1.63567600	-0.03835200	0.01939900
C	-3.05153400	0.06769000	0.03638000
C	-3.66193800	1.34209100	0.00319700
C	-2.87111900	2.46277800	-0.04597000
H	-0.87089200	3.27995000	-0.10017900
C	-3.80199900	-1.13009300	0.08421600
H	-4.74913100	1.40902900	0.01477400
H	-3.32823400	3.45101100	-0.07523800
C	-3.16258500	-2.34237300	0.11254900
C	-1.75638800	-2.36070000	0.09144100
H	-4.89008700	-1.06713300	0.09795100
H	-3.71326900	-3.27889100	0.14974000
H	-1.21508700	-3.30652800	0.11262500
N	-1.02159000	-1.26475600	0.04646300
N	0.55810100	0.94197100	-0.01955400
C	1.52468700	1.90240200	0.06235900

C	2.90398200	1.29842300	0.20488500
H	3.64730600	1.97380800	-0.24726500
H	3.11841600	1.29177100	1.28815100
C	2.98634900	-0.12082400	-0.33664200
H	3.11308200	-0.11154200	-1.43270800
C	4.00814600	-1.00307700	0.33085700
H	3.86113400	-1.03590700	1.42082500
H	3.96974200	-2.03394400	-0.05234100
H	5.03520000	-0.63615100	0.15306300
O	1.32803800	3.12272600	0.07931700
Pd	1.16243800	-0.96175600	-0.10875000

8

E (M06-SMD/BS1) = -1360.558684 au

H (M06-SMD/BS1) = -1360.169958 au

G (M06-SMD/BS1) = -1360.260445 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.42891 au

C	3.75898000	0.16628600	1.99510400
C	2.74913500	0.05052200	1.05412000
C	2.27230300	-1.25517600	0.71462000
C	2.80599500	-2.39439200	1.37178200
C	3.80676000	-2.23166300	2.35591800
C	4.26883400	-0.97278200	2.64805000
H	4.14766100	1.14805400	2.24341800
C	2.31080800	-3.66168300	0.98528900
H	4.20383800	-3.11348900	2.85684600
H	5.04941000	-0.83614500	3.39446200
C	1.36001200	-3.75896500	0.00166500
C	0.89967000	-2.57707800	-0.60878300
H	2.70413200	-4.55108900	1.47712700
H	0.96597000	-4.71995100	-0.31875900
H	0.15939100	-2.61767900	-1.40927000
N	1.33236900	-1.38098400	-0.26699500
N	2.18060500	1.14804400	0.39950500
C	2.03671800	2.42261700	0.88218700
C	1.23334500	3.31079600	-0.03437000
H	1.66616500	4.32278900	-0.02339200
H	0.22079800	3.39569800	0.39141400
C	1.18656600	2.77352800	-1.44158600
H	2.16171700	2.82865500	-1.93982300
C	0.05407200	3.19715600	-2.31430100

H	-0.91783000	3.10448700	-1.81529400
H	0.03494100	2.63578500	-3.25875700
H	0.19697300	4.25955800	-2.57766200
O	2.49048200	2.78775500	1.96215400
Pd	1.06075400	0.71285000	-1.16575500
C	-3.08494400	1.76067700	2.06942800
C	-2.62290300	0.81423700	1.14841800
C	-3.55629000	-0.01217200	0.52097600
C	-4.91617300	0.10689000	0.79271900
C	-5.35737700	1.07625200	1.68873900
C	-4.44088100	1.90383700	2.33024300
H	-2.35456700	2.39294700	2.57400100
H	-5.63188200	-0.55597700	0.30991200
H	-6.42301700	1.17326300	1.88975000
H	-4.78142400	2.65580200	3.03955900
I	-2.96269400	-1.59275600	-0.80066300
C	-1.13605800	0.76457900	0.92176400
O	-0.37997200	0.62730300	1.88269500
O	-0.80251900	0.93885900	-0.31284000
O	2.65014300	0.62251700	-2.34280400
C	3.14499800	-0.65930400	-2.60164500
H	3.65268000	-1.11034700	-1.73081500
H	3.90127300	-0.55390800	-3.39816700
H	2.37458100	-1.35932800	-2.96793900

TS₁

E (M06-SMD/BS1) = -1360.520576 au

H (M06-SMD/BS1) = -1360.134626 au

G (M06-SMD/BS1) = -1360.222711 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.391502 au

C	3.86588600	0.73956700	-1.65876000
C	2.69300300	0.59685000	-0.92710000
C	2.05357100	1.78790400	-0.43714100
C	2.59761400	3.06004700	-0.78341400
C	3.75913000	3.15272600	-1.58030500
C	4.38218000	2.00264200	-1.99449500
H	4.38680400	-0.14839400	-2.00141900
C	1.94484100	4.21307300	-0.28779000
H	4.14728900	4.13750000	-1.83869300
H	5.29208900	2.05306200	-2.59048900
C	0.84269000	4.08377900	0.51456500

C	0.39752000	2.78304100	0.82462200
H	2.34289000	5.19348900	-0.55025700
H	0.32088600	4.94909200	0.91661200
H	-0.46887000	2.64833200	1.47676000
N	0.96573200	1.68530000	0.37299800
N	2.18084500	-0.66436800	-0.60324900
C	2.43797400	-1.79870400	-1.30575600
C	1.98342300	-3.06425300	-0.59278400
H	2.50801000	-3.91557700	-1.06512300
H	0.90388400	-3.21696500	-0.73720900
C	2.36226300	-3.14484200	0.84145800
H	3.42939100	-3.05275700	1.04177300
C	1.57043500	-3.94907000	1.77211400
H	0.49046200	-3.83173900	1.62214700
H	1.85018900	-3.78607900	2.81659300
H	1.82224600	-4.99936700	1.52638500
O	2.95581800	-1.85256100	-2.42161400
Pd	0.95886600	-0.91739300	0.97505200
C	-3.18022300	-1.36015000	-2.48575400
C	-2.74848200	-0.69076300	-1.33464000
C	-3.71748500	-0.14268200	-0.49079000
C	-5.07409100	-0.26784800	-0.77816400
C	-5.47934400	-0.96657700	-1.91137000
C	-4.53014700	-1.51291000	-2.76937000
H	-2.42580600	-1.77030100	-3.15621000
H	-5.81682200	0.18037100	-0.12063700
H	-6.54204600	-1.07185100	-2.12372200
H	-4.84050900	-2.05148200	-3.66288800
I	-3.21417400	1.03402700	1.23131600
C	-1.25922600	-0.62437600	-1.11575000
O	-0.52912200	-0.30760900	-2.05842900
O	-0.88934600	-0.96705100	0.06620100
O	2.54065500	-1.30438600	2.11486100
C	3.74961500	-0.61771100	1.93691100
H	4.30879300	-0.95610300	1.04725000
H	4.37762800	-0.80804400	2.82150500
H	3.59994800	0.47133200	1.85137300

TS₂

E (M06-SMD/BS1) = -1360.522974 au

H (M06-SMD/BS1) = -1360.138011 au

G (M06-SMD/BS1) = -1360.228243 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.395626 au

C	4.33070800	1.29631000	-1.06890500
C	3.30140500	0.78378700	-0.30073500
C	3.62111300	-0.03419200	0.82851600
C	4.99202700	-0.27084400	1.13894800
C	6.01267900	0.29751700	0.34322700
C	5.68072400	1.06686100	-0.74423800
H	4.08253000	1.90184000	-1.93954400
C	5.28075300	-1.08549700	2.25853100
H	7.05306300	0.10753500	0.60662300
H	6.45860100	1.50127200	-1.36996400
C	4.25463200	-1.61682600	2.99427600
C	2.93124000	-1.32952200	2.59879600
H	6.32264000	-1.27770900	2.51588900
H	4.43871000	-2.24721700	3.86126300
H	2.09890200	-1.74721100	3.16947400
N	2.61414100	-0.57560800	1.56731700
N	1.95783700	1.02251200	-0.65591400
C	1.53682200	2.29312700	-0.79398200
C	0.14573200	2.51999900	-1.37169800
H	0.25618900	3.33859200	-2.11746700
H	-0.53231400	2.93596900	-0.61193100
C	-0.48603400	1.48538400	-2.17091400
H	0.16148700	0.84289600	-2.77746100
C	-1.89437100	1.49278800	-2.51016000
H	-2.52310800	2.02400800	-1.78909900
H	-2.26537900	0.48422500	-2.72811800
H	-1.92758500	2.02974200	-3.48058700
O	2.17982300	3.30074500	-0.47180700
Pd	0.79396600	-0.65537400	-0.84651200
C	-2.93984200	2.33213300	1.66458000
C	-2.70345300	1.08165000	1.07935200
C	-3.80860700	0.30954600	0.70420800
C	-5.10486700	0.77512300	0.90624100
C	-5.31313300	2.03310100	1.46454200
C	-4.22811300	2.81493900	1.84577200
H	-2.07990400	2.92837200	1.96713300
H	-5.95723200	0.15775300	0.62877800
H	-6.33087600	2.39317500	1.60562300
H	-4.38377000	3.79665600	2.28896500

I	-3.64200200	-1.67429800	-0.09858000
C	-1.26101400	0.71066500	0.87985100
O	-0.42768300	0.99752800	1.73996800
O	-1.01736300	0.14838800	-0.25774900
O	2.19320800	-1.83005300	-1.63632600
C	1.24500000	-2.80948100	-1.72764800
H	1.45546700	-3.70108800	-1.11395200
H	0.96680700	-3.08340400	-2.75877700
H	0.22127900	-2.44103800	-1.27640700

9a

E (M06-SMD/BS1) = -1044.858926 au

H (M06-SMD/BS1) = -1044.52923 au

G (M06-SMD/BS1) = -1044.601712 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1045.237777 au

C	-1.65432200	2.41914100	-0.57714700
C	-1.00355400	1.24886200	-0.21921100
C	-1.79322400	0.09887600	0.10631800
C	-3.21008600	0.18388600	0.08368800
C	-3.83484500	1.40302500	-0.26204500
C	-3.06092600	2.48890600	-0.58647200
H	-1.07090400	3.29425100	-0.84093400
C	-3.93914100	-0.98517100	0.40478200
H	-4.92268500	1.45614300	-0.27246700
H	-3.53035300	3.43130700	-0.86370100
C	-3.27821400	-2.14345500	0.72401900
C	-1.87048400	-2.13954800	0.71239700
H	-5.02815500	-0.94441100	0.39073100
H	-3.81341400	-3.05541300	0.97614400
H	-1.31113500	-3.04610800	0.94725400
N	-1.16154400	-1.07123500	0.41336800
N	0.38846200	1.11419500	-0.16996500
C	1.32820300	2.10496300	-0.05462300
C	2.73557300	1.56625300	0.02333500
H	3.41557500	2.26631200	-0.48503400
H	3.02770200	1.55491100	1.08516800
C	2.84011100	0.18784200	-0.57795300
H	2.71498600	0.20509300	-1.66763900
C	3.96649900	-0.68466200	-0.13342000
H	4.05166100	-0.73379800	0.95888600
H	3.87516300	-1.70305400	-0.53665900

H	4.91152800	-0.27000600	-0.52508100
O	1.05060900	3.29946100	0.02192300
Pd	1.06463500	-0.73447800	-0.04707700
O	1.54667900	-0.61398200	1.89832800
O	0.83360900	-1.08502700	-2.01591900
C	-0.22439200	-1.93063900	-2.35645900
H	-1.21505000	-1.44512700	-2.27446400
H	-0.09887100	-2.22776800	-3.41247100
H	-0.24935200	-2.86207800	-1.76097300
C	0.76245000	0.13549300	2.77284800
H	0.82538200	1.22549600	2.59138800
H	-0.30513100	-0.15013600	2.75823100
H	1.13235600	-0.03659500	3.79834800

TS₃

E (M06-SMD/BS1) = -1044.824066 au
H (M06-SMD/BS1) = -1044.496194 au
G (M06-SMD/BS1) = -1044.568681 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1045.204914 au

C	-1.51857100	2.21461900	0.16493900
C	-1.05318700	0.98325800	-0.25891600
C	-1.98506700	-0.07651200	-0.48911700
C	-3.37349800	0.18033600	-0.29017100
C	-3.80841400	1.45955800	0.12484500
C	-2.89161100	2.45825800	0.34797700
H	-0.79646200	3.00788700	0.35491100
C	-4.27733300	-0.88432600	-0.51325000
H	-4.87522700	1.63078700	0.26839300
H	-3.21930100	3.44366800	0.67446500
C	-3.79958500	-2.10781200	-0.90274300
C	-2.40662600	-2.25926200	-1.06797200
H	-5.34376900	-0.71076900	-0.36749900
H	-4.46334100	-2.95037000	-1.08243400
H	-2.00704800	-3.22741400	-1.37841200
N	-1.52717800	-1.29861100	-0.87458100
N	0.32538500	0.75575300	-0.41783600
C	1.05210000	1.51887800	-1.26308100
C	2.55342800	1.29363000	-1.27481800
H	3.02623900	2.29131700	-1.34930000
H	2.83057700	0.77041300	-2.20113100
C	3.17372400	0.67853700	-0.09487600

H	2.89992500	1.11087800	0.87394000
C	4.50869200	0.08226900	-0.15348300
H	4.72537800	-0.40333700	-1.10996200
H	4.68825500	-0.60064200	0.68443300
H	5.20947800	0.92776800	-0.01577200
O	0.56654400	2.32683000	-2.06336700
Pd	1.18337000	-0.53692900	0.86664200
O	2.34138300	-1.47141800	-0.49311900
O	0.33133900	0.30765600	2.46357700
C	-0.85435100	-0.32225500	2.83886800
H	-1.70669400	-0.06713700	2.17885700
H	-1.13386500	0.00578500	3.85600400
H	-0.76843200	-1.42638500	2.87083900
C	1.93448500	-1.73975100	-1.79982400
H	1.30836400	-0.94657900	-2.24170000
H	1.34541900	-2.67345800	-1.85118300
H	2.81881300	-1.86474100	-2.45002300

TS₁₇₋₁₈

E (M06-SMD/BS1) = -1360.532226 au

H (M06-SMD/BS1) = -1360.144803 au

G (M06-SMD/BS1) = -1360.232178 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.424154 au

C	4.66813400	0.64764000	1.18624300
C	3.47754900	0.40483300	0.51260700
C	3.30612800	-0.87719300	-0.10527300
C	4.32233700	-1.86463100	-0.00086200
C	5.51670800	-1.57255500	0.69530200
C	5.67265000	-0.33575300	1.26900800
H	4.82077400	1.61173600	1.65678400
C	4.08638400	-3.12046000	-0.60494200
H	6.28986800	-2.33685400	0.76347300
H	6.58906100	-0.09631200	1.80669900
C	2.90585200	-3.35452100	-1.26143200
C	1.95695000	-2.31928400	-1.32773900
H	4.85412900	-3.89090700	-0.53342200
H	2.69060200	-4.31134100	-1.73035600
H	1.01156500	-2.47812700	-1.84534100
N	2.14421900	-1.12960500	-0.78611600
N	2.41387000	1.29571400	0.37797500
C	2.29996400	2.50065400	1.00279200

C	0.95316200	3.13417200	0.74956800
H	1.04502500	4.23099000	0.81383100
H	0.29504600	2.83503300	1.58511600
C	0.33251700	2.70977100	-0.56502500
H	0.93527200	3.07081300	-1.41696100
C	-1.10673400	3.11916600	-0.70978100
H	-1.73944400	2.69767600	0.08500700
H	-1.52948100	2.83583900	-1.68049800
H	-1.17875000	4.21771500	-0.62767500
O	3.14936700	3.03230100	1.72770800
Pd	0.85049200	0.72315300	-0.77029900
C	-5.59917500	-0.54951500	0.39852900
C	-4.25067900	-0.67257000	0.73397700
C	-3.30778900	-0.15209400	-0.14449300
C	-3.64597700	0.48207100	-1.32398700
C	-5.00262200	0.59322000	-1.63267000
C	-5.97540200	0.08200800	-0.77849300
H	-6.33805800	-0.96173600	1.08428300
H	-2.88125300	0.87502400	-1.98636200
H	-5.29171400	1.08961200	-2.55750200
H	-7.02912400	0.17654400	-1.03274700
I	-1.27245700	-0.40988000	0.57125700
C	-3.84606100	-1.35322100	1.99591500
O	-4.67457300	-1.82227100	2.77405000
O	-2.56562100	-1.41526400	2.20806000
O	-0.82798800	0.31271100	-1.89326500
C	-0.81272400	-0.80135500	-2.74199900
H	-1.59737300	-0.66331900	-3.50591100
H	-1.04306200	-1.74638400	-2.21696900
H	0.15134100	-0.92224000	-3.26321700

18

E (M06-SMD/BS1) = -1360.547193 au

H (M06-SMD/BS1) = -1360.159447 au

G (M06-SMD/BS1) = -1360.248961 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.433157 au

C	3.65786800	-1.63387700	1.24921200
C	2.84587200	-0.67281500	0.66330700
C	2.99362300	-0.43279900	-0.74044900
C	3.96719400	-1.13716500	-1.49383400
C	4.78469800	-2.09540300	-0.85211900

C	4.61804400	-2.33183300	0.48990400
H	3.55880700	-1.83879600	2.30918100
C	4.06453600	-0.84582800	-2.87371500
H	5.52825800	-2.63429400	-1.43775700
H	5.23664200	-3.07319100	0.99296600
C	3.23228100	0.08499600	-3.44437700
C	2.28738000	0.73167800	-2.62912000
H	4.80748200	-1.37426500	-3.47078300
H	3.28578500	0.32566600	-4.50293100
H	1.60052100	1.47128000	-3.04342800
N	2.17410200	0.48343800	-1.33840000
N	1.87611300	0.09095000	1.32221100
C	1.66825200	0.14264900	2.67008900
C	0.42438800	0.92291400	3.03484900
H	0.60433000	1.44673700	3.98765900
H	-0.37267400	0.18955900	3.24065800
C	-0.02692200	1.91296700	1.99246100
H	0.67596800	2.76351400	1.89906700
C	-1.45188900	2.35279800	2.08363000
H	-2.14954600	1.50530300	2.05222600
H	-1.72077700	3.07037200	1.29950200
H	-1.59685400	2.85722900	3.05534100
O	2.37872700	-0.38597800	3.52761700
Pd	0.67938800	1.22375900	0.14920100
C	-5.17591100	-0.65349700	-0.90278300
C	-3.91693200	-1.08529100	-0.48285600
C	-2.89017600	-0.14771300	-0.46258900
C	-3.05720300	1.17201300	-0.84490700
C	-4.32833400	1.57002700	-1.26083600
C	-5.38460100	0.66421500	-1.28661100
H	-5.98420400	-1.38306500	-0.92254200
H	-2.22347000	1.87314400	-0.84059700
H	-4.48342200	2.60286400	-1.56878000
H	-6.37200300	0.98581600	-1.61233100
I	-0.98081300	-0.87979500	0.22093600
C	-3.70303700	-2.51748200	-0.09018100
O	-4.64988500	-3.31405700	-0.11018100
O	-2.50390400	-2.82592300	0.24519200
O	-0.28260000	2.47571600	-1.09988100
C	0.45835600	3.65410900	-1.03551800
H	0.18780500	4.28909400	-0.17001000

H	0.30024800	4.24782600	-1.95337600
H	1.55321000	3.46469600	-0.97688400

TS₁₈₋₁₉

E (M06-SMD/BS1) = -1360.544627 au
H (M06-SMD/BS1) = -1360.157707 au
G (M06-SMD/BS1) = -1360.244617 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1647.430003 au

C	-3.68269800	-2.29724900	-0.05417200
C	-2.95512600	-1.12357600	-0.16275600
C	-3.41737700	0.02440600	0.54382100
C	-4.61290300	-0.02290700	1.30353800
C	-5.33710000	-1.23532200	1.37348900
C	-4.86766800	-2.34150700	0.70922400
H	-3.33987800	-3.18977200	-0.56633600
C	-5.00783200	1.15685000	1.97309800
H	-6.24929400	-1.27247000	1.96726400
H	-5.41163300	-3.28265100	0.76839300
C	-4.24005100	2.29221800	1.88279600
C	-3.06424100	2.25513600	1.11484800
H	-5.92444100	1.14657500	2.56224100
H	-4.51760500	3.21082200	2.39294500
H	-2.42333200	3.13277600	1.02834300
N	-2.67378700	1.16947500	0.47295300
N	-1.78958500	-0.94064200	-0.91823200
C	-1.50242000	-1.64374800	-2.04689200
C	-0.27339500	-1.11809400	-2.75142600
H	-0.42281300	-1.22940100	-3.83877900
H	0.59063800	-1.75026300	-2.49659400
C	0.00516700	0.32307700	-2.47224100
H	-0.80743900	0.99878900	-2.78624600
O	-2.14912500	-2.59570900	-2.48849600
Pd	-0.72034100	0.73499800	-0.45332100
C	5.45882100	0.31439700	0.70825600
C	4.25458300	-0.39098400	0.77036700
C	3.09696400	0.29554300	0.41608700
C	3.09212800	1.62874200	0.03884300
C	4.31146400	2.30349000	-0.00628200
C	5.49380300	1.64662200	0.31987000
H	6.36935200	-0.21593900	0.98254700
H	2.15767400	2.14073400	-0.18783600

H	4.32610300	3.35282300	-0.29666600
H	6.44323800	2.17748300	0.28140900
I	1.24855900	-0.81896600	0.46300600
C	4.25561600	-1.82388700	1.24143600
O	5.34237400	-2.37936100	1.47133000
O	3.10962800	-2.36202600	1.38080800
O	0.08323600	2.48444900	0.09610400
C	-0.29819300	3.48266900	-0.80103700
H	0.26936200	3.44763400	-1.75156600
H	-0.11409900	4.47002900	-0.34313400
H	-1.37617500	3.44674200	-1.05942600
C	1.36155700	0.83129200	-2.79033700
H	1.43034400	0.85050500	-3.89426400
H	2.16197600	0.17785000	-2.42389200
H	1.52820600	1.85937100	-2.44916000

19

E (M06-SMD/BS1) = -1360.55137 au

H (M06-SMD/BS1) = -1360.163366 au

G (M06-SMD/BS1) = -1360.251601 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.433692 au

C	-4.25458000	-1.17578700	1.25862600
C	-3.19585300	-0.62299200	0.56810800
C	-3.32439200	0.69864500	0.06658900
C	-4.52448600	1.43022300	0.22435500
C	-5.59156200	0.83070600	0.93477800
C	-5.44550300	-0.43801900	1.44026300
H	-4.17220200	-2.18214700	1.65878500
C	-4.57694500	2.72206800	-0.34541500
H	-6.51372700	1.39288800	1.07329500
H	-6.26279200	-0.89808000	1.99269800
C	-3.48989300	3.22324100	-1.01987700
C	-2.32137100	2.44884500	-1.11308100
H	-5.48889000	3.30909300	-0.24184300
H	-3.50454600	4.21174300	-1.47057500
H	-1.43207900	2.82925600	-1.61208400
N	-2.24955700	1.23751100	-0.59121000
N	-1.98757300	-1.25361000	0.22547800
C	-2.01320100	-2.46452700	-0.40267800
C	-0.82852100	-2.62316300	-1.32682500
H	-1.09878700	-3.31880500	-2.13972600

H	0.03785900	-3.06272400	-0.81262000
C	-0.49248900	-1.31923300	-1.96035300
H	-1.33694700	-0.79683200	-2.42255700
O	-2.90590200	-3.30273900	-0.29929400
Pd	-0.52464000	0.14097100	-0.17820300
C	4.77596000	1.46621800	-0.11517300
C	3.87959800	0.39192800	-0.07223200
C	3.02835400	0.33441500	1.02984000
C	3.05335800	1.27730400	2.05364300
C	3.98242600	2.31136800	1.99627100
C	4.84289600	2.40509300	0.90613900
H	5.43260300	1.54732600	-0.98048600
H	2.34788400	1.21530800	2.88042600
H	4.01850900	3.04723000	2.79765500
H	5.56321100	3.21936600	0.84673000
I	1.47347600	-1.13437100	1.17422600
C	3.89826200	-0.59761000	-1.22930000
O	4.03100800	-0.09845600	-2.37198600
O	3.79322400	-1.81487700	-0.94323200
O	0.65424100	1.74600300	-0.29661700
C	1.15833200	2.12091900	-1.53740300
H	1.99793700	1.48277600	-1.87384500
H	1.54827100	3.15184900	-1.46030500
H	0.39477900	2.12809300	-2.34207200
C	0.80903600	-1.14635300	-2.61509500
H	1.64039700	-1.60208500	-2.06532200
H	1.02745800	-0.10902300	-2.88897300
H	0.70304400	-1.69473000	-3.57378200

20

E (M06-SMD/BS1) = -1360.560484 au

H (M06-SMD/BS1) = -1360.171973 au

G (M06-SMD/BS1) = -1360.25975 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.436952 au

C	-3.28335600	0.86911600	2.17368300
C	-2.51834000	0.36922400	1.14245300
C	-2.83124500	0.75843700	-0.18424600
C	-3.92617300	1.60468000	-0.47092300
C	-4.69430000	2.09456500	0.61240200
C	-4.36663800	1.73490000	1.89687400
H	-3.05600500	0.59178500	3.19950100

C	-4.17788800	1.90105400	-1.82947900
H	-5.53354300	2.75698000	0.40614900
H	-4.95261800	2.11680900	2.73092200
C	-3.37245700	1.37900900	-2.81333300
C	-2.28171000	0.56958800	-2.45307900
H	-5.01696000	2.54804200	-2.08294900
H	-3.54635000	1.59060400	-3.86479500
H	-1.59243800	0.17099100	-3.19544400
N	-2.03804800	0.27801000	-1.18935300
N	-1.48235500	-0.58173200	1.23990800
C	-1.79666000	-1.81241600	1.75400400
C	-1.08237900	-2.91264700	1.01449900
H	-1.65075800	-3.84968500	1.12742700
H	-0.08824600	-3.10151400	1.44872100
C	-0.99530800	-2.57340200	-0.45241300
H	-1.97896900	-2.37301600	-0.89498500
O	-2.61432600	-2.01113900	2.64958600
Pd	-0.29118500	-0.51753700	-0.44401500
C	3.28406700	3.06096800	0.30441300
C	2.51300200	1.90778400	0.48419300
C	3.12314600	0.68627000	0.21334000
C	4.43365000	0.58546600	-0.24048800
C	5.16764300	1.75236400	-0.43501200
C	4.59174600	2.98881600	-0.15931500
H	2.83021100	4.02636200	0.52848400
H	4.88165300	-0.38731700	-0.43521200
H	6.19202500	1.68659300	-0.79687300
H	5.16567900	3.90271400	-0.30192200
I	2.12545700	-1.16577500	0.63730800
C	1.07716700	2.08863000	0.92412400
O	0.87680200	2.60337100	2.03624500
O	0.18742100	1.75524700	0.07829000
O	0.71064600	-0.09157200	-2.15201600
C	0.87742600	-1.03609300	-3.15334900
H	1.54346200	-1.87182600	-2.86595500
H	1.34569800	-0.53631700	-4.02045300
H	-0.07716200	-1.46749700	-3.51777900
C	-0.15395200	-3.48821000	-1.27099400
H	0.87576800	-3.57109900	-0.90120700
H	-0.14934200	-3.24052100	-2.33504000
H	-0.61300200	-4.48913800	-1.17609800

TS₄

E (M06-SMD/BS1) = -1360.515903 au
H (M06-SMD/BS1) = -1360.129131 au
G (M06-SMD/BS1) = -1360.217926 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1647.398345 au

C	-3.98047400	-1.03590900	1.90568900
C	-3.03337000	-0.57797000	1.02086700
C	-3.22304400	0.67827700	0.39598300
C	-4.38003600	1.45178900	0.64100900
C	-5.33364600	0.95509700	1.56264200
C	-5.12815000	-0.25627600	2.17839400
H	-3.84550300	-2.00424300	2.38456000
C	-4.49615700	2.67952700	-0.05019200
H	-6.21950900	1.55154800	1.77603000
H	-5.86225800	-0.63433900	2.88741600
C	-3.51088600	3.07232800	-0.92423800
C	-2.38220800	2.25254100	-1.10657200
H	-5.37357100	3.30291000	0.11888700
H	-3.57779000	4.00790800	-1.47283300
H	-1.57593800	2.53581300	-1.78219300
N	-2.24300600	1.10937900	-0.46021100
N	-1.87970100	-1.28703400	0.59802000
C	-2.11163000	-2.24583200	-0.36351400
C	-0.94454500	-2.53731900	-1.31213100
H	-1.22454300	-3.42695500	-1.91367300
H	-0.03115900	-2.81869700	-0.77651300
C	-0.66813100	-1.52878700	-2.38671400
O	-3.18244800	-2.83160800	-0.51042500
Pd	-0.50969100	-0.02450500	-0.24554500
C	4.72853500	1.97396300	0.08210200
C	4.11681700	0.74162400	0.33920500
C	2.77977900	0.77353600	0.72483500
C	2.06725300	1.95852600	0.87779000
C	2.71276600	3.16858800	0.63720100
C	4.04577700	3.17379300	0.23576000
H	5.76847700	1.96717900	-0.24088600
H	1.01615100	1.93867600	1.16708100
H	2.16710800	4.10239700	0.76238900
H	4.55417400	4.11643300	0.04000700
I	1.67092400	-1.04906700	0.98115100

C	4.93910100	-0.52973500	0.18944700
O	5.83435500	-0.51564500	-0.68472300
O	4.65588300	-1.47279900	0.97155200
O	0.33146400	0.47072100	-2.06767900
C	-1.78137500	-0.97841600	-3.16940600
H	-2.64156700	-0.67648600	-2.56031500
H	-2.11831700	-1.81739000	-3.80719300
H	-1.46803400	-0.16714000	-3.83090100
H	0.27781900	-1.68446600	-2.90600000
C	1.68152500	0.37616700	-2.41321500
H	2.18528600	-0.51142400	-1.98902700
H	2.23906900	1.26694800	-2.07459200
H	1.77443600	0.32425200	-3.51226800

TS₅

E (M06-SMD/BS1) = -1360.523083 au
H (M06-SMD/BS1) = -1360.136401 au
G (M06-SMD/BS1) = -1360.223392 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1647.39785 au

C	-3.75023400	-0.25514200	2.06764100
C	-2.80501700	-0.20599000	1.07182500
C	-2.91693800	0.77922600	0.06126500
C	-3.99596300	1.68976500	0.03947600
C	-4.95008800	1.61795300	1.08376700
C	-4.81987300	0.67066100	2.07050800
H	-3.67662600	-1.01624500	2.84281200
C	-4.03710600	2.61978200	-1.02410100
H	-5.77556400	2.32835400	1.09168400
H	-5.55468700	0.61971500	2.87184800
C	-3.05643300	2.60685500	-1.98672800
C	-2.00517900	1.67714700	-1.89058900
H	-4.85319800	3.34032500	-1.06807400
H	-3.06613600	3.30734800	-2.81744700
H	-1.20136800	1.64829900	-2.62484300
N	-1.93900500	0.80729600	-0.89900400
N	-1.72734800	-1.11403100	0.89624300
C	-2.05739600	-2.26913700	0.22375000
C	-0.94422500	-2.94952100	-0.58236100
H	-1.33926300	-3.94151800	-0.87934200
H	-0.05559500	-3.16764300	0.02584700
C	-0.56687500	-2.35162500	-1.90949000

H	-1.33421400	-1.77472800	-2.42912100
O	-3.18380200	-2.76440300	0.22222800
Pd	-0.28850000	-0.29785000	-0.29562900
C	3.63929100	2.65970400	-0.16576000
C	2.67784700	1.76394100	0.32091200
C	3.12339900	0.48364500	0.64693600
C	4.45030100	0.09099500	0.49745800
C	5.38436500	1.01548000	0.04173500
C	4.97547200	2.30447300	-0.28802200
H	3.30900400	3.65806100	-0.45031800
H	4.75512000	-0.92859100	0.72803600
H	6.42621700	0.71871300	-0.06546800
H	5.69764900	3.03098900	-0.65649100
I	1.78208100	-1.06745900	1.28889200
C	1.24077900	2.25835100	0.40316100
O	0.61590800	2.04951100	1.47327100
O	0.81850300	2.86009100	-0.61429800
O	0.58240300	-0.46979300	-2.16588900
C	0.38788800	-3.11706900	-2.71947000
H	1.31322400	-3.33239700	-2.16722500
H	0.60644000	-2.64519700	-3.67967600
H	-0.08972200	-4.09356800	-2.91299200
C	1.95909700	-0.57916000	-2.37661000
H	2.43968500	-1.35590800	-1.75435100
H	2.45977300	0.37876800	-2.14802000
H	2.16169400	-0.81646800	-3.43417400

TS₆

E (M06-SMD/BS1) = -1360.551752 au

H (M06-SMD/BS1) = -1360.164386 au

G (M06-SMD/BS1) = -1360.251364 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.432426 au

C	-4.00154500	-1.86588700	0.68556200
C	-3.01422000	-0.98598600	0.28527700
C	-3.39221200	0.34155500	-0.05144300
C	-4.74818500	0.74700100	-0.03845800
C	-5.73155200	-0.18733700	0.36223500
C	-5.35243900	-1.45650900	0.72409500
H	-3.73821200	-2.87842400	0.97428900
C	-5.03469600	2.07803100	-0.41625600
H	-6.77481600	0.12337000	0.38893900

H	-6.10334000	-2.17450900	1.04905800
C	-4.01587100	2.92937900	-0.76789000
C	-2.69101400	2.46482200	-0.72820600
H	-6.07072500	2.41499000	-0.41824300
H	-4.20698600	3.95863200	-1.05920600
H	-1.85308300	3.12120800	-0.95674300
N	-2.39904400	1.22137000	-0.39015200
N	-1.64237700	-1.25727500	0.13065100
C	-1.25407500	-2.41953200	-0.44978600
C	0.19085700	-2.39131000	-0.97417800
H	0.27232400	-3.21619300	-1.69590900
H	0.90027400	-2.55583700	-0.15596900
C	0.43842000	-1.12866000	-1.68965900
H	1.17423500	-0.40352800	-1.34765600
O	-1.95565100	-3.41375200	-0.61887600
Pd	-0.53790000	0.48766700	0.15383000
C	4.58505200	0.38202600	-1.37023900
C	3.65813500	-0.26424500	-0.54381600
C	3.15476800	0.46328300	0.53562600
C	3.56122600	1.76494300	0.81384500
C	4.51464900	2.36512000	-0.00389300
C	5.02257800	1.67263600	-1.09914000
H	4.97022100	-0.15890800	-2.23455600
H	3.13011300	2.31240700	1.64980500
H	4.84612600	3.37904000	0.21291700
H	5.75772700	2.14248000	-1.75033200
I	1.56865300	-0.31282600	1.76566600
C	3.28329000	-1.69602800	-0.88776700
O	2.82666100	-1.88515800	-2.05152000
O	3.46260800	-2.56018000	-0.00557700
O	0.30354700	2.30111600	0.11686600
C	0.79729400	2.58491900	-1.15555200
H	1.58253900	1.87643600	-1.48823400
H	1.26101800	3.58752100	-1.14459600
H	0.00955700	2.60479000	-1.93614000
C	-0.20451900	-0.86803500	-2.97131500
H	-0.36586900	0.20117400	-3.15142700
H	-1.11902000	-1.45340700	-3.12596100
H	0.52968800	-1.20012500	-3.73137900

E (M06-SMD/BS1) = -1476.223768 au
 H (M06-SMD/BS1) = -1475.777946 au
 G (M06-SMD/BS1) = -1475.877997 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -1763.157064 au

C	4.27737900	0.27197100	1.79321500
C	3.20748400	0.10913300	0.93626400
C	3.43098800	-0.52261600	-0.31642600
C	4.72482400	-0.93758600	-0.70973900
C	5.79845800	-0.74822200	0.19188900
C	5.56629700	-0.16334800	1.41268900
H	4.12661800	0.73841100	2.76215200
C	4.86046300	-1.51719000	-1.99128300
H	6.79490400	-1.07746900	-0.09866100
H	6.38896100	-0.02408500	2.11177000
C	3.76185600	-1.66454500	-2.80322700
C	2.50266300	-1.25135200	-2.33643900
H	5.84628000	-1.84246500	-2.32203300
H	3.83968100	-2.10506500	-3.79339200
H	1.60288400	-1.38309000	-2.93546600
N	2.35455200	-0.70282100	-1.14449300
N	1.89149600	0.56607700	1.12728200
C	1.67645500	1.86394500	1.49341500
C	0.36781200	2.40175700	0.93575400
H	0.46498900	3.49487700	0.84788800
H	-0.47288800	2.19269200	1.60896300
C	0.13003200	1.85100700	-0.42981600
O	2.45988700	2.56001100	2.13250400
Pd	0.57612700	-0.40625500	-0.11538900
C	-4.75422600	-0.70240900	-0.98987500
C	-3.74419200	-0.27332200	-0.12145300
C	-3.02485900	-1.26041200	0.54815400
C	-3.27565200	-2.61850900	0.37768100
C	-4.30840800	-3.01183900	-0.46775300
C	-5.04822900	-2.05009000	-1.15046900
H	-5.31083900	0.05220600	-1.54418500
H	-2.66741900	-3.36233000	0.88919000
H	-4.52085700	-4.07129200	-0.59942500
H	-5.84957200	-2.35274600	-1.82225500
I	-1.35078700	-0.76465900	1.78853300
C	-3.46221100	1.21171000	-0.01630000
O	-3.40694300	1.82502200	-1.12005000

O	-3.30214500	1.71167600	1.11639300
O	-0.49740000	-1.52506500	-1.38057600
C	-1.07782200	-0.82147100	-2.43527800
H	-1.80358600	-0.05352200	-2.10398100
H	-1.63506200	-1.53491500	-3.06858900
H	-0.33453500	-0.32309100	-3.09057600
H	-0.89483200	1.58111400	-0.70423000
C	-1.73581700	4.11798100	-2.33317100
H	-1.48634500	3.18738000	-2.87435900
H	-0.98770900	4.87705000	-2.59358100
H	-2.71526300	4.46655400	-2.69952500
O	-1.72740900	3.94314500	-0.93521500
H	-2.42453900	3.26509900	-0.76552600
C	1.03571700	2.24035400	-1.52625600
H	0.74537600	3.27418400	-1.79071800
H	0.90924500	1.62716200	-2.42519700
H	2.09006100	2.27720800	-1.22604600

TS₂₁₋₂₂

E (M06-SMD/BS1) = -1476.224708 au

H (M06-SMD/BS1) = -1475.779829 au

G (M06-SMD/BS1) = -1475.875779 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1763.157196 au

C	4.30457100	0.95283300	1.51775800
C	3.24015000	0.46990000	0.78224500
C	3.48499900	-0.55766600	-0.16768100
C	4.79104800	-1.04966300	-0.39993900
C	5.85746900	-0.52549700	0.36764700
C	5.60571800	0.44581600	1.30534100
H	4.14018500	1.72729700	2.26044900
C	4.94513200	-2.04194500	-1.39416900
H	6.86351300	-0.90874000	0.20417500
H	6.42266500	0.84513100	1.90380500
C	3.85185900	-2.49717900	-2.09057800
C	2.58101600	-1.98090500	-1.78681400
H	5.94023700	-2.43649400	-1.59714500
H	3.94286100	-3.25788500	-2.86123100
H	1.68606800	-2.34375300	-2.28960700
N	2.41440800	-1.04931500	-0.86564000
N	1.91108800	0.92665900	0.81030700
C	1.65942300	2.26445500	0.76036800

C	0.31876400	2.57578200	0.11049200
H	0.39472500	3.58547100	-0.32048200
C	0.04247800	1.62486000	-0.99903700
O	2.42895600	3.14982600	1.12466400
Pd	0.62146100	-0.46515700	0.00489900
C	-4.69305300	-1.15247000	-0.94465700
C	-3.71749500	-0.44336100	-0.23510800
C	-3.01372700	-1.14062800	0.74427700
C	-3.24978100	-2.48335200	1.02407200
C	-4.24887200	-3.15229000	0.32398600
C	-4.97103400	-2.48307600	-0.66053500
H	-5.23603400	-0.63299900	-1.73350400
H	-2.65562200	-3.00493500	1.77236300
H	-4.44938900	-4.19943800	0.54326800
H	-5.74655600	-3.00466800	-1.21874600
I	-1.39954700	-0.22760300	1.81875000
C	-3.45678600	1.00027200	-0.61195900
O	-3.27908700	1.20601400	-1.84718200
O	-3.43495000	1.85568200	0.29615600
O	-0.37874100	-2.00517100	-0.78422400
C	-0.98689800	-1.72270300	-2.00694100
H	-1.67626200	-0.85827200	-1.96339900
H	-1.59323300	-2.59647800	-2.30769000
H	-0.26061000	-1.53612100	-2.82421000
H	-0.96163200	1.20580200	-1.09802000
C	-2.19252800	4.53428700	-1.26373900
H	-3.14063700	4.93153900	-1.66168100
H	-1.44314000	5.33365400	-1.31957600
H	-2.35091000	4.28262400	-0.20295200
O	-1.72404300	3.43894500	-2.01509900
H	-2.40400100	2.72091000	-1.97735100
H	-0.49022600	2.58159800	0.85193000
C	0.88482800	1.63962000	-2.20357800
H	0.48101400	2.46705200	-2.81641100
H	0.78851500	0.72711000	-2.80241200
H	1.93803700	1.86543700	-1.99654400

22

E (M06-SMD/BS1) = -1476.287567 au

H (M06-SMD/BS1) = -1475.837983 au

G (M06-SMD/BS1) = -1475.933348 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1763.214848 au

C	4.17404900	0.74701800	1.46234000
C	3.10400200	0.28695500	0.70997400
C	3.35485100	-0.78261200	-0.19740300
C	4.65776500	-1.30212900	-0.39531300
C	5.72367300	-0.78027800	0.37261200
C	5.46726100	0.20913600	1.28896000
H	4.02155500	1.53624500	2.18851000
C	4.81363000	-2.33588800	-1.34599900
H	6.72518800	-1.18487800	0.23379100
H	6.27675500	0.60300000	1.90179200
C	3.72335000	-2.81538500	-2.02887900
C	2.45475300	-2.28122100	-1.74922400
H	5.80805600	-2.74628000	-1.51972400
H	3.81422600	-3.61113800	-2.76350300
H	1.55739800	-2.67108000	-2.22634100
N	2.28625800	-1.30406700	-0.87643700
N	1.78329500	0.77152600	0.70506300
C	1.55617700	2.10063200	0.88075800
C	0.23568300	2.64382300	0.38239800
H	0.08384700	3.60626000	0.88893400
C	0.28068100	2.86320200	-1.13369300
O	2.39158800	2.90261300	1.32697000
Pd	0.50802400	-0.69881600	-0.02448000
C	-4.67683000	-0.57976400	-1.24277400
C	-3.67175200	-0.13321100	-0.38118200
C	-3.18227600	-1.01059200	0.58625200
C	-3.67710200	-2.30322600	0.70770300
C	-4.69971400	-2.72082200	-0.14079900
C	-5.19774200	-1.86108600	-1.11476900
H	-5.04800500	0.09454500	-2.01341700
H	-3.26111200	-2.98468000	1.44722000
H	-5.09507900	-3.73020500	-0.04362800
H	-5.98790500	-2.19255700	-1.78534600
I	-1.51288500	-0.47666500	1.81384900
C	-3.12644100	1.24290200	-0.55134100
O	-2.63800100	1.43764000	-1.76545000
O	-3.12251800	2.08682100	0.32695300
O	-0.47885200	-2.25218000	-0.83005400
C	-1.02927600	-1.88565900	-2.05594700
H	-1.74498600	-1.04422300	-1.98080100

H	-1.58842900	-2.74181600	-2.47638400
H	-0.26569900	-1.59998100	-2.81007400
H	0.29039600	1.87689900	-1.62781400
C	-1.32234100	4.69876700	-1.05933500
H	-2.13253800	5.08189200	-1.68841300
H	-0.49589200	5.42229100	-1.07306500
H	-1.69671000	4.59370900	-0.03146600
O	-0.93613600	3.45491600	-1.61732000
H	-2.14618000	2.31484400	-1.77229400
H	-0.60638600	1.98522600	0.61989200
C	1.48581900	3.65594900	-1.59953600
H	1.37868100	3.90714600	-2.66229300
H	2.40087200	3.06018000	-1.48395300
H	1.62089800	4.58361500	-1.02750200

TS₂₂₋₂₃

E (M06-SMD/BS1) = -1476.278564 au

H (M06-SMD/BS1) = -1475.829362 au

G (M06-SMD/BS1) = -1475.921847 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1763.203942 au

C	4.39793300	0.89066200	1.32871200
C	3.30976300	0.42087300	0.60258900
C	3.45679600	-0.84541000	-0.03108900
C	4.67362800	-1.57234500	0.01618600
C	5.75899600	-1.04033300	0.74624800
C	5.60143100	0.16035500	1.39361600
H	4.32571100	1.83548100	1.85270500
C	4.72747900	-2.81127800	-0.66201700
H	6.69349100	-1.59765600	0.79106700
H	6.42375900	0.57432800	1.97548700
C	3.62380600	-3.28222800	-1.32766800
C	2.44314400	-2.52131100	-1.31212800
H	5.65533700	-3.38224000	-0.64096800
H	3.63698400	-4.23124600	-1.85707600
H	1.52821600	-2.85769900	-1.79744100
N	2.37314000	-1.35880000	-0.69019500
N	2.05584100	1.03495200	0.45206900
C	1.90192100	2.37005800	0.64066900
C	0.51085700	2.93682600	0.45496600
H	0.51511400	3.91425600	0.95393300
C	0.10109300	3.16570200	-0.99344700

O	2.82060700	3.15558200	0.92643600
Pd	0.67300700	-0.23257300	-0.43413600
C	-5.15464600	-0.99411600	-0.52207600
C	-4.11155200	-0.30105300	0.10628900
C	-3.07789400	-1.04615700	0.69026500
C	-3.08953100	-2.43735800	0.63594200
C	-4.12072100	-3.10114200	-0.02198000
C	-5.15626200	-2.37839800	-0.60381000
H	-5.96224900	-0.41539400	-0.96666200
H	-2.28875400	-3.00688600	1.10340900
H	-4.11098900	-4.18859700	-0.06971500
H	-5.96876700	-2.89082100	-1.11454400
I	-1.43982800	-0.19220700	1.76186400
C	-4.23491500	1.18087500	0.06149900
O	-3.08178900	1.82292300	-0.12034100
O	-5.30458300	1.75561400	0.12564800
O	-0.39265500	-1.70374500	-1.28290900
C	-1.33678800	-1.27013500	-2.20161900
H	-2.04735300	-0.52979700	-1.78025300
H	-1.94799900	-2.13187900	-2.53003100
H	-0.88353200	-0.83151500	-3.11276600
O	-0.36809100	1.92594100	-1.53006100
H	-0.25097400	2.31484400	0.94053500
C	-0.98723200	2.07719500	-2.79319600
H	-1.64943500	1.22181400	-2.95292600
H	-0.25128000	2.11629500	-3.61014300
H	-1.59648000	2.99509900	-2.81832100
H	-0.76203800	3.85760100	-0.98266800
C	1.20934700	3.76425300	-1.83730600
H	1.62505700	4.65153700	-1.34256900
H	0.84712300	4.07105100	-2.82587700
H	2.02295700	3.03748000	-1.97995200
H	-3.27204900	2.78247700	-0.15092300

23

E (M06-SMD/BS1) = -1044.945254 au

H (M06-SMD/BS1) = -1044.61157 au

G (M06-SMD/BS1) = -1044.680585 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1045.324937 au

C	2.02621900	2.54274100	-0.52564600
C	1.32436500	1.39558000	-0.18361600

C	2.07268300	0.19755600	-0.01581300
C	3.48405400	0.17437400	-0.12765700
C	4.15832400	1.36881400	-0.46756500
C	3.42886300	2.51488500	-0.66995800
H	1.49311800	3.47368900	-0.67686100
C	4.14075300	-1.05325100	0.11506500
H	5.24290200	1.35699500	-0.56420300
H	3.93748600	3.43875500	-0.94153600
C	3.41535000	-2.16998100	0.44944900
C	2.01566700	-2.08191800	0.51458000
H	5.22688500	-1.09424500	0.03832000
H	3.89631000	-3.12278900	0.65373000
H	1.39365600	-2.94084500	0.76046100
N	1.37817400	-0.94749600	0.27812100
N	-0.05575600	1.26032000	0.01720200
C	-0.84036000	2.30773400	0.36224800
C	-2.28041300	1.97640800	0.69584700
H	-2.79903900	2.93867100	0.77714400
C	-3.04392900	1.09354100	-0.27626700
O	-0.45947300	3.48325100	0.45802600
Pd	-0.62188000	-0.70073300	0.18515200
O	-0.98331800	-2.67400000	0.37487800
C	-0.76667800	-3.37314900	-0.81110900
H	-1.39624100	-3.02027700	-1.65256700
H	-1.00873800	-4.44033200	-0.65921700
H	0.28539500	-3.33317600	-1.15918400
H	-2.70422400	1.26231800	-1.31343900
O	-2.73511300	-0.29160000	0.04635600
H	-2.32384900	1.50987000	1.69357000
C	-4.53236800	1.34956600	-0.16329800
H	-5.11804100	0.79743900	-0.90560800
H	-4.72307900	2.41652300	-0.32804000
H	-4.89102700	1.08646900	0.84201200
C	-3.42795100	-1.23812400	-0.77542000
H	-3.23201200	-1.03593000	-1.83900200
H	-4.50343800	-1.19684600	-0.57488800
H	-3.05072300	-2.22220600	-0.49408200

24

E (M06-SMD/BS1) = -1273.931733 au

H (M06-SMD/BS1) = -1273.529979 au

G (M06-SMD/BS1) = -1273.615439 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1274.407126 au

C	2.38548300	-2.81994000	-0.35694400
C	1.56687100	-1.71877400	-0.16324600
C	2.18437800	-0.48401500	0.17309700
C	3.59168200	-0.35263700	0.24544300
C	4.39185100	-1.49859000	0.03389400
C	3.78682800	-2.69904100	-0.24851600
H	1.94730100	-3.78051700	-0.60308200
C	4.11609400	0.93075900	0.51811000
H	5.47491500	-1.40700600	0.09898500
H	4.39562900	-3.58814600	-0.40502800
C	3.26890400	1.99646000	0.69516400
C	1.88141300	1.78668500	0.63885200
H	5.19649200	1.05901000	0.57617700
H	3.64346500	2.99770000	0.88999400
H	1.18222300	2.60660000	0.78784700
N	1.36355800	0.59208400	0.40440500
N	0.17174400	-1.65851300	-0.27109400
C	-0.53466200	-2.46756300	-1.09655100
C	-1.98735600	-2.08370200	-1.29232300
H	-2.42392400	-2.84342900	-1.95192400
C	-2.84452200	-1.99468700	-0.04358200
O	-0.06897200	-3.44010000	-1.70488000
Pd	-0.59086200	0.06110100	0.47823500
O	-1.31224100	1.81975600	1.20759600
C	-0.93718700	2.13494700	2.51784600
H	-1.30564300	1.39207500	3.24838900
H	-1.36504100	3.11180200	2.79996100
H	0.15837900	2.20734600	2.65315100
H	-2.57263000	-2.79347200	0.66777100
O	-2.58196200	-0.72637500	0.62286000
H	-2.04791800	-1.11945200	-1.82457000
C	-4.31230300	-2.06340200	-0.40648300
H	-4.96855900	-1.93436500	0.46149100
H	-4.53659200	-3.04204800	-0.84793300
H	-4.55278100	-1.28652300	-1.14523100
C	-2.98721800	-0.73596900	1.99773300
H	-2.30467200	-1.36370400	2.58855300
H	-4.01092300	-1.11560600	2.08778400
H	-2.95864000	0.29785200	2.34771600

O	-0.75107800	3.66320700	-0.49518400
C	-0.73358200	3.19262400	-1.72867300
O	-1.00614200	2.03169800	-2.01341800
C	-0.34358400	4.22348700	-2.73874200
H	-1.00335900	5.09571500	-2.65782600
H	-0.39506200	3.81073800	-3.74956000
H	0.67766000	4.56914400	-2.53426400
H	-0.99317500	2.91533200	0.17336700

TS₂₄₋₂₅

E (M06-SMD/BS1) = -1273.931062 au

H (M06-SMD/BS1) = -1273.532867 au

G (M06-SMD/BS1) = -1273.616896 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1274.407334 au

C	-2.24621400	2.94780000	-0.25020300
C	-1.47918700	1.80279000	-0.11060700
C	-2.14829300	0.58558400	0.18304200
C	-3.55887500	0.51518600	0.26776200
C	-4.30710300	1.70475800	0.11405500
C	-3.65056000	2.88664400	-0.12817200
H	-1.76675500	3.89628100	-0.46413300
C	-4.13856800	-0.75401800	0.48880400
H	-5.39247800	1.66038000	0.18889000
H	-4.21936000	3.80811100	-0.24163400
C	-3.33927700	-1.86455200	0.60044300
C	-1.94428100	-1.71661400	0.53392400
H	-5.22290400	-0.83547900	0.55670300
H	-3.75704100	-2.85637200	0.75027000
H	-1.28321400	-2.57685100	0.62106500
N	-1.37425300	-0.53563400	0.35363000
N	-0.08917600	1.67999000	-0.24320500
C	0.64306100	2.47558900	-1.06135800
C	2.06801500	2.02157200	-1.30068500
H	2.52793600	2.76873300	-1.95862900
C	2.94341300	1.87210200	-0.07131800
O	0.21469200	3.49034900	-1.62453000
Pd	0.60206300	-0.08732800	0.43554100
O	1.29177100	-1.89418900	1.13140100
C	0.88297900	-2.26438700	2.42591800
H	1.24689200	-1.54616200	3.17764000
H	1.30014800	-3.25353100	2.67309800

H	-0.21458100	-2.32765600	2.52743700
H	2.73239600	2.67845100	0.65167100
O	2.61874100	0.61485700	0.58956700
H	2.06783500	1.06322900	-1.84687100
C	4.40566500	1.85647100	-0.45990600
H	5.06571500	1.67394100	0.39566200
H	4.68228200	2.82610800	-0.89136400
H	4.58578600	1.07708400	-1.21295400
C	3.02932300	0.59711300	1.96347300
H	2.37354100	1.24572800	2.56168900
H	4.06697900	0.93774400	2.05038700
H	2.96450800	-0.43764800	2.30617300
O	0.59361400	-3.64365500	-0.39413800
C	0.52494900	-3.24161500	-1.63434100
O	0.89724100	-2.13013300	-2.01944800
C	-0.07743800	-4.25019700	-2.56678100
H	0.37131600	-5.23757400	-2.40796800
H	0.04854700	-3.94359000	-3.60904900
H	-1.14997600	-4.34129200	-2.34756100
H	0.94743300	-2.81624300	0.28451200

25

E (M06-SMD/BS1) = -1273.932506 au

H (M06-SMD/BS1) = -1273.530241 au

G (M06-SMD/BS1) = -1273.616406 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1274.409261 au

C	1.86874400	-3.17606000	-0.14311200
C	1.23980800	-1.94695000	-0.04580400
C	2.03878900	-0.80746200	0.22287500
C	3.44650700	-0.89229200	0.32412100
C	4.05475900	-2.16407800	0.21510600
C	3.27010400	-3.27034300	-0.00229600
H	1.28690100	-4.06975100	-0.33784200
C	4.16059000	0.31199600	0.51417600
H	5.13710400	-2.24244600	0.30411100
H	3.73128300	-4.25336900	-0.08132000
C	3.48765900	1.50726100	0.58015300
C	2.08518000	1.51432400	0.49982100
H	5.24654500	0.27602700	0.59389900
H	4.01173000	2.45099900	0.70407500
H	1.51870400	2.44449000	0.54060700

N	1.39215000	0.39626600	0.35034600
N	-0.12626200	-1.66575400	-0.20736700
C	-0.92884100	-2.37281200	-1.04546200
C	-2.27296800	-1.74448800	-1.34479800
H	-2.79394800	-2.42721300	-2.02665900
C	-3.16938400	-1.49780000	-0.14822500
O	-0.60967400	-3.44434900	-1.57094000
Pd	-0.61862900	0.16600900	0.42398600
O	-1.15372400	2.07887900	1.13231600
C	-0.70344000	2.45753800	2.42936500
H	-1.08775900	1.73422600	3.15692800
H	-1.09398700	3.45395400	2.67233800
H	0.39422300	2.47563700	2.49270700
H	-3.11116000	-2.34644200	0.55400000
O	-2.68988900	-0.32244400	0.56857000
H	-2.13082700	-0.79129100	-1.88087700
C	-4.59508100	-1.24720200	-0.58659500
H	-5.24764100	-0.98515600	0.25423100
H	-5.00211500	-2.15112200	-1.05578600
H	-4.62455100	-0.43009900	-1.32024200
C	-3.10713900	-0.31409800	1.94156000
H	-2.53197400	-1.05465800	2.51484100
H	-4.17715000	-0.54104300	2.00825800
H	-2.93423600	0.69274100	2.32856700
O	-0.09276100	3.74124900	-0.49078900
C	0.00809000	3.20131100	-1.64344500
O	-0.60484000	2.17217900	-2.00734400
C	0.98898600	3.84782700	-2.59507000
H	0.97836900	4.93924200	-2.49529600
H	0.78976200	3.56416300	-3.63381800
H	2.00117200	3.50491800	-2.33393700
H	-0.79176400	2.76206600	0.44829400

TS₂₅₋₂₆

E (M06-SMD/BS1) = -1273.92026 au
H (M06-SMD/BS1) = -1273.518798 au
G (M06-SMD/BS1) = -1273.602731 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1274.394729 au

C	-3.08357300	-2.13383700	-0.03778200
C	-2.00623400	-1.26847900	0.03929400
C	-2.26810200	0.12260000	0.07319300

C	-3.58509100	0.63616400	0.07691700
C	-4.66146900	-0.27788800	0.00454300
C	-4.40017100	-1.62568300	-0.05831300
H	-2.91803300	-3.20468200	-0.07762400
C	-3.73581700	2.03936700	0.15748800
H	-5.68101000	0.10421400	-0.00211200
H	-5.22529200	-2.33315700	-0.12204400
C	-2.62864900	2.84840400	0.23324400
C	-1.34678900	2.27227900	0.20726100
H	-4.73916000	2.46388600	0.16231200
H	-2.71729300	3.92906600	0.30361000
H	-0.44002800	2.87882000	0.24450900
N	-1.18315900	0.96187700	0.12389800
N	-0.64294900	-1.59977600	0.10637200
C	-0.19432000	-2.70019600	0.76749700
C	1.28873200	-2.72355600	1.07084600
H	1.49295300	-3.67784800	1.57144300
C	2.21400400	-2.61114800	-0.12325500
O	-0.92247600	-3.62715400	1.13791900
Pd	0.55348500	-0.00077500	-0.14769500
O	1.38570300	1.71266600	-1.71781900
C	0.51294400	1.99714200	-2.79146600
H	0.40864900	1.08236300	-3.38966600
H	0.91589100	2.79015100	-3.43855400
H	-0.48860400	2.30243700	-2.44850500
H	1.83246400	-3.22773700	-0.95402800
O	2.22899300	-1.23128100	-0.59606900
H	1.53568300	-1.92000400	1.78458900
C	3.62735700	-3.00427400	0.24261100
H	4.32387200	-2.85463900	-0.59069900
H	3.65919000	-4.06513200	0.51929600
H	3.97341700	-2.40986000	1.09922500
C	2.54377400	-1.15421100	-1.99496200
H	1.70910700	-1.55598400	-2.58781300
H	3.45580700	-1.72710100	-2.19922700
H	2.70820400	-0.10148000	-2.23212800
O	1.69037000	3.46111300	0.28166600
C	2.09729500	2.65871700	1.16438400
O	2.04968000	1.39396500	1.07344900
C	2.66534300	3.22520700	2.44455500
H	2.90979300	4.28731900	2.33997300

H	3.55663000	2.66626600	2.75242300
H	1.91980200	3.11555900	3.24399600
H	1.43683600	2.48035400	-1.08640200

26

E (M06-SMD/BS1) = -1158.278747 au
H (M06-SMD/BS1) = -1157.933293 au
G (M06-SMD/BS1) = -1158.008275 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1158.702582 au

C	-2.50051800	-2.38732600	-0.66932400
C	-1.62984800	-1.39871000	-0.24124100
C	-2.16791500	-0.11220700	0.02599200
C	-3.55221400	0.15592300	-0.08565200
C	-4.40883700	-0.88174000	-0.51922500
C	-3.87825500	-2.11526800	-0.80834100
H	-2.12453800	-3.37851900	-0.89501500
C	-3.99557600	1.45447200	0.25204200
H	-5.47471700	-0.68214600	-0.61753200
H	-4.53000600	-2.91735900	-1.15093800
C	-3.09632600	2.40190900	0.67604000
C	-1.73302200	2.07320000	0.74298300
H	-5.05736900	1.68649400	0.17572900
H	-3.41117100	3.40448600	0.95219100
H	-0.98843300	2.79835100	1.06537000
N	-1.29263000	0.86812400	0.42064100
N	-0.24883800	-1.50570700	-0.01931000
C	0.35249400	-2.66586900	0.34325100
C	1.78318000	-2.53358700	0.82427500
H	2.12770900	-3.54796700	1.05900900
C	2.77028000	-1.91659200	-0.14662300
O	-0.19614800	-3.77448000	0.33632300
Pd	0.62849800	0.28690100	0.24199200
H	2.57299200	-2.27513400	-1.17099800
O	2.58705400	-0.46965500	-0.16397400
H	1.80887000	-1.95649500	1.76292600
C	4.19166700	-2.22049500	0.27342300
H	4.93152300	-1.72441800	-0.36508400
H	4.37156200	-3.30069000	0.21249100
H	4.35425900	-1.89942400	1.31144600
C	3.08323800	0.11903500	-1.37582200
H	2.41943400	-0.13119900	-2.21508100

H	4.09675000	-0.24349600	-1.58064800
H	3.11547700	1.20002800	-1.22581000
O	0.84301100	2.79899800	-1.45936700
C	1.33195400	3.02739800	-0.34567900
O	1.41969000	2.15747200	0.61071600
C	1.86198200	4.38985200	0.01704700
H	1.90445800	5.03957500	-0.86236500
H	2.85803700	4.30871300	0.46788800
H	1.20195300	4.84616000	0.76701300

TS₂₆₋₂₇

E (M06-SMD/BS1) = -1387.247459 au

H (M06-SMD/BS1) = -1386.834303 au

G (M06-SMD/BS1) = -1386.921115 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1387.765388 au

C	-3.14947000	-2.33195000	0.29395700
C	-2.20659200	-1.31880500	0.20041600
C	-2.68106100	0.01415700	0.14797600
C	-4.06476200	0.31770000	0.14821100
C	-4.99175400	-0.74516200	0.21884700
C	-4.52695200	-2.03570700	0.29903400
H	-2.82865600	-3.36492200	0.36409100
C	-4.43744900	1.67937000	0.10246700
H	-6.05704300	-0.51993100	0.22294000
H	-5.23220600	-2.86214800	0.37122900
C	-3.47224300	2.65444100	0.07394400
C	-2.11818600	2.28230700	0.08684800
H	-5.49585100	1.93763300	0.09925500
H	-3.72645100	3.71052600	0.04661800
H	-1.33223100	3.03168000	0.07755800
N	-1.74405300	1.01359700	0.11518600
N	-0.80837200	-1.46241500	0.21513000
C	-0.21625100	-2.60357100	-0.24333600
C	1.28224400	-2.72764400	-0.10240800
H	1.48909700	-3.80464600	-0.05574200
C	2.05939800	-2.15415700	-1.27798800
O	-0.84081400	-3.53735700	-0.76434800
Pd	0.15490800	0.32291500	0.30328300
H	1.55822700	-2.44137800	-2.22107700
O	2.03815100	-0.72531200	-1.17415500
H	1.64993600	-2.26759300	0.82243500

C	3.49198100	-2.64684400	-1.27054900
H	4.08602400	-2.17796300	-2.06508800
H	3.52908700	-3.73343800	-1.41946700
H	3.96291500	-2.41394600	-0.30375200
C	2.17241300	-0.07542900	-2.42362600
H	1.24020400	-0.14689300	-3.00717900
H	2.99698600	-0.50212500	-3.01360400
H	2.39793700	0.97880400	-2.23052000
O	0.42951800	2.65873200	-1.78199300
C	1.11755900	2.88207000	-0.78724600
O	1.07550300	2.17467800	0.31292400
C	2.12342200	3.99865400	-0.74112400
H	1.98966700	4.67772800	-1.58835400
H	3.13264200	3.56449200	-0.78973800
H	2.05187000	4.55357400	0.20129000
O	3.41078200	1.19112900	1.17904200
C	3.04365000	0.06584000	1.75459500
O	1.87448800	-0.32480800	1.77792600
C	4.15897000	-0.67846000	2.39857200
H	5.05443100	-0.64767200	1.76821500
H	3.86425100	-1.71196000	2.60013300
H	4.40858100	-0.18777600	3.34889400
H	2.59124000	1.65820900	0.84191000

27

E (M06-SMD/BS1) = -1387.254178 au

H (M06-SMD/BS1) = -1386.839304 au

G (M06-SMD/BS1) = -1386.927731 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1387.773875 au

C	2.74251100	2.58252800	0.80753300
C	1.97965000	1.47958500	0.45646900
C	2.67044600	0.32173400	0.02333700
C	4.07561600	0.30665300	-0.15243500
C	4.81166700	1.46399200	0.18530200
C	4.14601000	2.56194000	0.67384200
H	2.25938900	3.47817800	1.18091700
C	4.66019800	-0.88074800	-0.64534400
H	5.89375400	1.45845900	0.06457900
H	4.70511000	3.45152600	0.95957400
C	3.87352400	-1.97142800	-0.92224200
C	2.49304300	-1.90115900	-0.67858100

H	5.73840500	-0.91529000	-0.79782800
H	4.29406800	-2.89676100	-1.30600500
H	1.85082700	-2.76266200	-0.84226000
N	1.92127900	-0.79933400	-0.22008300
N	0.57513600	1.37132300	0.49396900
C	-0.17788900	2.47168800	0.19502700
C	-1.67696700	2.31153600	0.15732900
H	-2.08899500	3.32713400	0.22176200
C	-2.15975700	1.64478700	-1.13363300
O	0.30678600	3.58055600	-0.07060900
Pd	0.03177100	-0.62211100	0.46737200
H	-1.66912800	0.66127400	-1.22568000
C	-4.43611000	2.39922900	-0.94008500
H	-5.44626700	1.97465400	-0.93263500
H	-4.36090000	3.09431000	-1.79047600
H	-4.29486700	2.96695200	-0.00682900
O	-3.54265400	1.31383900	-1.05179500
H	-2.03283900	1.73850400	1.02007000
C	-1.82321500	2.46290500	-2.36604300
H	-2.29916000	2.02724800	-3.25430500
H	-0.73778200	2.46580200	-2.53177400
H	-2.14491600	3.50915300	-2.27105200
O	-0.17444200	-2.68430700	0.50759200
C	-0.74448000	-3.23690100	-0.50306000
O	-1.38854900	-2.60415000	-1.36670100
C	-0.56754500	-4.72241200	-0.61855600
H	0.32189400	-4.91906600	-1.23366100
H	-1.42993400	-5.17407600	-1.11893500
H	-0.40952300	-5.18550800	0.36049700
O	-3.23074600	-1.44502100	0.12683100
C	-2.93120600	-0.76723300	1.19496800
O	-1.78258400	-0.41417800	1.51380200
C	-4.09669600	-0.38511100	2.03175500
H	-4.60042400	0.45797600	1.53705400
H	-3.77288000	-0.07191900	3.02717500
H	-4.81406800	-1.20960200	2.09655300
H	-2.43338900	-1.68651900	-0.43951700

TS₂₇₋₂₈

E (M06-SMD/BS1) = -1387.240301 au

H (M06-SMD/BS1) = -1386.831576 au

G (M06-SMD/BS1) = -1386.920376 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1387.758245 au

C	-2.67638400	-2.42215800	0.78886900
C	-1.91592200	-1.33641200	0.42948800
C	-2.55449700	-0.17046500	-0.04204000
C	-3.95861800	-0.12288200	-0.19963000
C	-4.71527300	-1.25579800	0.18261800
C	-4.08375100	-2.37053400	0.67942400
H	-2.18375200	-3.32895800	1.13767800
C	-4.51412900	1.06639500	-0.72460600
H	-5.79881700	-1.22183800	0.07955400
H	-4.66767200	-3.23898800	0.97731100
C	-3.69609400	2.12065000	-1.05012500
C	-2.31266600	2.01751400	-0.82280200
H	-5.59244200	1.13151200	-0.86483900
H	-4.09466600	3.04411400	-1.46081900
H	-1.63852000	2.84751700	-1.02528600
N	-1.76932800	0.91647600	-0.33405400
N	-0.48024800	-1.34936100	0.41810800
C	0.05440000	-1.99781900	-0.71913700
C	1.54611300	-2.17321200	-0.75530900
H	1.73957900	-3.18098500	-1.14865000
C	2.20844700	-1.10682900	-1.65478600
O	-0.65478400	-2.38473400	-1.63686000
Pd	0.09525800	0.67081400	0.41770400
H	1.65079400	-0.16230300	-1.54262500
C	4.46674200	-1.80015300	-1.26050000
H	5.35987300	-1.43965600	-0.73888800
H	4.74116300	-2.02787300	-2.30188100
H	4.13311900	-2.73005400	-0.77243600
O	3.50185300	-0.77440000	-1.17243900
H	1.97829500	-2.11505600	0.24862700
C	2.19634100	-1.50648200	-3.11582600
H	2.69767800	-0.74600800	-3.72856500
H	1.16022400	-1.60239900	-3.46461000
H	2.68960000	-2.47412100	-3.28015300
O	0.43512400	2.68198400	0.51222400
C	1.39884400	3.11488600	-0.24389700
O	2.07454300	2.40373300	-0.99382800
C	1.62427000	4.59977600	-0.13724900
H	0.72350500	5.13442800	-0.46438500

H	2.47308400	4.90768300	-0.75504800
H	1.80819900	4.88076000	0.90674500
O	1.00872100	-1.52635900	2.41496400
C	1.88683700	-0.59902600	2.33411400
O	1.82995200	0.36741600	1.52361200
C	3.08214200	-0.70677300	3.21700800
H	3.49788500	0.28114100	3.43429900
H	3.84376100	-1.28915300	2.67897700
H	2.83715200	-1.23727600	4.14184500
H	0.22302800	-1.50491400	1.52535500

28

E (M06-SMD/BS1) = -1387.254974 au

H (M06-SMD/BS1) = -1386.840332 au

G (M06-SMD/BS1) = -1386.930035 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1387.771562 au

C	0.04651000	3.24063300	1.34467900
C	-0.36841100	2.01278200	0.89123400
C	-1.53779100	1.89578600	0.11632600
C	-2.29050400	3.05169400	-0.20131700
C	-1.84071100	4.30607200	0.27142600
C	-0.69697500	4.39625100	1.02728100
H	0.95013700	3.31437500	1.94937300
C	-3.45954800	2.87907200	-0.97691900
H	-2.42037200	5.19448000	0.02516700
H	-0.35514000	5.36200500	1.39197400
C	-3.82364000	1.62299700	-1.39340700
C	-3.02419800	0.52271200	-1.04032600
H	-4.05756000	3.75220900	-1.23443100
H	-4.71533400	1.45631000	-1.99108700
H	-3.27505300	-0.48746700	-1.36045200
N	-1.92740800	0.65495400	-0.31398000
N	0.35079000	0.79061200	1.21526200
H	0.30461100	0.58276700	2.22096000
C	1.73489600	0.66390900	0.80481300
C	2.06699500	1.17939800	-0.56196000
H	2.12466400	2.27934500	-0.52465100
H	1.24270400	0.93675100	-1.24933500
C	3.39088800	0.63586500	-1.07130500
H	3.44393300	-0.44649300	-0.85460000
C	3.54037900	0.86151400	-2.56099700

H	2.78446300	0.29011400	-3.11676900
H	4.53036300	0.53726700	-2.90685200
H	3.42115300	1.92688200	-2.80374300
O	2.49988600	0.09873100	1.55182400
Pd	-0.67048300	-0.83185000	0.27325400
O	-1.70664200	-2.27602300	-0.71551300
C	-2.58684200	-2.88967700	0.01685800
O	-2.80227200	-2.63929800	1.20712000
O	0.63456400	-2.23765800	0.96506700
C	1.55057500	-2.57687400	0.10967700
O	1.59380600	-2.17958800	-1.06119600
C	-3.36625900	-3.93684200	-0.73208500
H	-4.02869000	-3.44386100	-1.45599100
H	-3.97156000	-4.53443100	-0.04409700
H	-2.69190500	-4.58910600	-1.29870100
C	2.62655400	-3.46195800	0.67442000
H	3.11031700	-4.03691000	-0.12154400
H	2.23808300	-4.13497300	1.44585300
H	3.38385500	-2.81603400	1.14257600
O	4.41646300	1.30667900	-0.34993800
C	5.56118000	0.51268500	-0.15258300
H	5.33224900	-0.36943100	0.46990200
H	6.30403200	1.12837700	0.36682300
H	5.99854500	0.16507800	-1.10285600

HOAc

E (M06-SMD/BS1) = -228.9646732 au

H (M06-SMD/BS1) = -228.897569 au

G (M06-SMD/BS1) = -228.930026 au

E (M06-SMD/BS2//M06-SMD/BS1) = -229.0665165 au

O	0.76847600	-1.03775700	0.00002200
C	0.08985300	0.11776600	0.00001000
O	0.64331200	1.19948900	0.00000100
C	-1.38381000	-0.10686600	-0.00001000
H	-1.67121300	-0.69052900	0.88301500
H	-1.91115100	0.84997700	0.00013400
H	-1.67107300	-0.69032000	-0.88322100
H	1.72287000	-0.82837900	-0.00010600

MeOH

E (M06-SMD/BS1) = -115.6494595 au

H (M06-SMD/BS1) = -115.593808 au
 G (M06-SMD/BS1) = -115.620851 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -115.7071077 au
 O -0.74575100 0.12375200 -0.00005100
 H -1.13116900 -0.76443900 -0.00017800
 C 0.65877100 -0.01928100 0.00000700
 H 1.09045600 0.98821200 0.00093000
 H 1.02639900 -0.54973100 0.89237600
 H 1.02769400 -0.54837100 -0.89275900

PhICOOH

E (M06-SMD/BS1) = -431.3364793 au
 H (M06-SMD/BS1) = -431.221983 au
 G (M06-SMD/BS1) = -431.267989 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -717.8839585 au
 C 2.65757500 -0.16515700 0.02901900
 C 1.33759400 0.30898000 0.03787600
 C 0.29526000 -0.62847400 0.04153700
 C 0.57234500 -1.99196100 0.03685500
 C 1.89024000 -2.43807900 0.04540100
 C 2.93684100 -1.52317900 0.04142100
 H 3.47243200 0.55518100 0.03060700
 H -0.24280800 -2.71236800 0.02392300
 H 2.09171900 -3.50789100 0.05000200
 H 3.96978100 -1.86464800 0.04567100
 I -1.78409700 -0.11719800 -0.05123700
 C 1.12456600 1.77759200 0.09092200
 O 2.12811000 2.45261200 -0.48150300
 O 0.17563900 2.33444600 0.60538500
 H 1.94949400 3.40641000 -0.36389700

13_H

E (M06-SMD/BS1) = -1233.516136 au
 H (M06-SMD/BS1) = -1233.166631 au
 G (M06-SMD/BS1) = -1233.250029 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -1233.971357 au
 C 2.80357300 -1.50207900 1.30039200
 C 1.79865700 -0.78776500 0.69604200
 C 2.02953000 0.52846700 0.25063700
 C 3.30957900 1.11200200 0.40486000
 C 4.32999500 0.35470900 1.02545500

C	4.07807500	-0.92117200	1.46844200
H	2.61102200	-2.51944700	1.63989200
C	3.48800600	2.43214600	-0.06792600
H	5.31341800	0.80611200	1.14789400
H	4.86337400	-1.49888900	1.95036300
C	2.43683400	3.09908300	-0.64601100
C	1.18977700	2.45955100	-0.75060400
H	4.46372000	2.90465600	0.03685100
H	2.54146500	4.11426300	-1.01830600
H	0.32857000	2.96124400	-1.18968500
N	0.99603900	1.22426800	-0.32110800
N	0.47582600	-1.34423200	0.48311200
H	-0.02753100	-1.57109900	1.35681200
C	0.32441600	-2.44128000	-0.44830300
C	1.26293200	-2.45898000	-1.61517600
H	2.25588000	-2.75072500	-1.23825300
H	1.38025900	-1.43092100	-1.98969800
C	0.80070200	-3.40433600	-2.70540000
H	0.72434600	-4.43308100	-2.33396900
H	-0.18325400	-3.11090100	-3.09282900
O	-0.55966300	-3.24475600	-0.25152500
Pd	-0.76696300	0.21410500	-0.25295200
O	-1.84680100	1.78454700	-0.96410100
C	-2.33369800	2.53865000	-0.02457800
O	-2.17799100	2.33436900	1.18407200
O	-2.50484500	-0.84342800	-0.11661200
C	-2.72723900	-1.40530100	1.03058600
O	-1.98573400	-1.30577200	2.01829600
C	-3.09242300	3.73148600	-0.54025000
H	-2.38248100	4.44454600	-0.98025200
H	-3.63431700	4.22529100	0.27176800
H	-3.79158200	3.43607600	-1.33074800
C	-3.96589000	-2.25666700	1.06509000
H	-4.29132900	-2.42352200	2.09650500
H	-3.72631200	-3.22947900	0.61324000
H	-4.77642800	-1.80849400	0.48063100
H	1.51173400	-3.39546000	-3.53902000

TS_{13-14_H}

E (M06-SMD/BS1) = -1233.503916 au

H (M06-SMD/BS1) = -1233.160993 au

G (M06-SMD/BS1) = -1233.239564 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1233.959952 au

C	2.73440400	-1.04181400	1.49887300
C	1.72043400	-0.52790500	0.72520900
C	1.79416000	0.81452000	0.29191300
C	2.92102000	1.61331300	0.59488800
C	3.95369800	1.05049900	1.38120100
C	3.85078600	-0.24388500	1.83069600
H	2.67633900	-2.07554000	1.83824500
C	2.93370900	2.93787000	0.10065200
H	4.81849600	1.66451800	1.62810200
H	4.64044900	-0.67184900	2.44466000
C	1.87345600	3.40538100	-0.63618700
C	0.77174200	2.56436500	-0.86988700
H	3.79040200	3.57524500	0.31616900
H	1.85584700	4.41803900	-1.02924200
H	-0.10215100	2.90984100	-1.42017100
N	0.73744700	1.32078400	-0.42318700
N	0.58422800	-1.29422100	0.30365900
H	-0.26048200	-1.74277200	1.13513800
C	0.75954000	-2.25219900	-0.72912100
C	2.05130900	-2.24271000	-1.49971800
H	2.87234800	-2.48104900	-0.80749000
H	2.24163200	-1.20848900	-1.82939600
C	2.03862600	-3.20248300	-2.67143900
H	1.88243300	-4.23564500	-2.33818100
H	1.23995800	-2.95482100	-3.38184000
O	-0.14653600	-3.03410800	-0.97030200
Pd	-0.85677900	0.07436600	-0.33616700
O	-2.18720600	1.47394000	-0.99902700
C	-2.65822700	2.24740600	-0.06921500
O	-2.36450200	2.16038800	1.12848100
O	-2.44733800	-1.17561500	0.11792500
C	-2.33284700	-1.96868500	1.10043400
O	-1.24767500	-2.19050800	1.72868700
C	-3.59423700	3.30934900	-0.58107300
H	-3.01990500	4.04692200	-1.15744000
H	-4.09465600	3.81758200	0.24857100
H	-4.34011800	2.87606800	-1.25727300
C	-3.54689100	-2.71380600	1.54637700
H	-3.43319100	-3.76897500	1.26603600

H	-4.45305400	-2.31327500	1.08479300
H	-3.62675000	-2.67081700	2.63832300
H	2.99451600	-3.15982100	-3.20635800

15_H

E (M06-SMD/BS1) = -1004.516779 au
H (M06-SMD/BS1) = -1004.23754 au
G (M06-SMD/BS1) = -1004.307616 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1004.884014 au

C	3.26330000	0.85708800	-0.25297600
C	1.92986100	0.52626600	-0.06019300
C	1.60419700	-0.85400100	0.03663900
C	2.58740100	-1.86671500	-0.06254500
C	3.93354100	-1.48550700	-0.26100900
C	4.24501900	-0.15107000	-0.35087200
H	3.55276600	1.89773900	-0.33099000
C	2.15859100	-3.20921000	0.03993600
H	4.69712600	-2.25761100	-0.34027500
H	5.27917100	0.15336300	-0.50382600
C	0.83008900	-3.49994300	0.23161700
C	-0.09459700	-2.44827300	0.32416000
H	2.89856500	-4.00533400	-0.03576600
H	0.47545600	-4.52357800	0.31393100
H	-1.15584700	-2.63021000	0.48461300
N	0.28609000	-1.18512600	0.22887400
N	0.82945500	1.38738000	0.04984900
C	0.88821500	2.74458800	-0.04231500
C	-0.42588300	3.48396300	0.09456300
H	-0.40892100	4.29330800	-0.64691800
H	-0.40375900	3.97892100	1.07710300
C	-1.70309300	2.68019500	-0.05224700
H	-1.79938100	2.19376000	-1.03499300
H	-1.89286400	1.99626200	0.83163400
O	1.93174500	3.38759600	-0.20022600
Pd	-0.90926000	0.42838800	0.30342300
O	-2.62656400	-0.65411800	0.63007400
C	-3.27585200	-0.96796000	-0.44775700
O	-2.94082500	-0.62480400	-1.58823700
C	-4.47944400	-1.83920300	-0.20899400
H	-4.14057700	-2.86706500	-0.02001100
H	-5.13481300	-1.84326600	-1.08540600

H	-5.03680300	-1.50988600	0.67496700
H	-2.59588000	3.31128300	0.04646800

TS_{15-16_H}

E (M06-SMD/BS1) = -1004.490347 au

H (M06-SMD/BS1) = -1004.216366 au

G (M06-SMD/BS1) = -1004.282263 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1004.858066 au

C	-3.08878300	1.48021600	-0.12175400
C	-1.86950600	0.82413800	-0.03575500
C	-1.88242400	-0.60064400	-0.01054000
C	-3.09293500	-1.33164200	-0.07556800
C	-4.31356000	-0.62428500	-0.16448200
C	-4.29291900	0.74896400	-0.18577100
H	-3.11288300	2.56360300	-0.14206500
C	-3.00719200	-2.74232100	-0.04451700
H	-5.24755000	-1.18208400	-0.21241300
H	-5.22812400	1.30290300	-0.25246800
C	-1.78355900	-3.35826000	0.04528900
C	-0.62410200	-2.56699500	0.10420900
H	-3.92547500	-3.32697700	-0.09230600
H	-1.69025200	-4.44059500	0.07130400
H	0.36522000	-3.01627900	0.17408900
N	-0.67538600	-1.24660700	0.07756000
N	-0.59581700	1.39471500	0.02784700
C	-0.30558600	2.71790900	-0.09739400
C	1.17617300	3.00366900	-0.09795000
C	2.02791100	1.93067300	0.56315000
H	1.81611600	1.83428900	1.63864900
O	-1.14111700	3.61866300	-0.23624100
Pd	0.89751300	0.08358900	0.19763400
O	2.38550400	-1.39129500	0.27709600
C	3.48090500	-1.02031500	-0.24328400
O	3.67820200	0.16849400	-0.63950500
C	4.58749500	-2.01169800	-0.38760700
H	5.44880400	-1.67601800	0.20276500
H	4.90671900	-2.05155100	-1.43566400
H	4.27991500	-3.00664900	-0.05565100
H	2.66240300	0.89888600	-0.17101300
H	1.46996300	3.12232800	-1.15341600
H	1.33273900	3.98650800	0.36979400

H 3.08301400 2.24644000 0.53040300

7_H

E (M06-SMD/BS1) = -775.513721 au

H (M06-SMD/BS1) = -775.303612 au

G (M06-SMD/BS1) = -775.357804 au

E (M06-SMD/BS2//M06-SMD/BS1) = -775.7869354 au

C	-0.94661400	2.44939900	-0.07484300
C	-0.45855600	1.15023500	-0.01928400
C	-1.41178300	0.07889900	0.01361300
C	-2.80422800	0.35305100	0.00116200
C	-3.25436800	1.69170000	-0.04960100
C	-2.33151800	2.70688000	-0.08816000
H	-0.24756900	3.27632300	-0.10541000
C	-3.69202900	-0.74724600	0.03680100
H	-4.32520800	1.89087600	-0.06073400
H	-2.66378500	3.74320500	-0.13123500
C	-3.20151800	-2.02683900	0.08084000
C	-1.80758200	-2.21318800	0.08844500
H	-4.76501600	-0.55590900	0.02785700
H	-3.86009100	-2.89124300	0.10874800
H	-1.38197300	-3.21599700	0.12228500
N	-0.94858500	-1.21111700	0.05599300
N	0.88660700	0.77520800	0.01744700
C	1.96510800	1.61571500	0.08105300
C	3.26464300	0.86177900	0.24259600
H	4.06317700	1.42224500	-0.26637200
H	3.50091600	0.90783000	1.31807300
C	3.15896200	-0.58587300	-0.21179300
H	3.39037500	-0.70015200	-1.28230800
O	1.90698600	2.84877400	0.06405900
Pd	1.23466800	-1.18157500	-0.03775200
H	3.78929400	-1.27062500	0.37414800

17_H

E (M06-SMD/BS1) = -1321.266785 au

H (M06-SMD/BS1) = -1320.907204 au

G (M06-SMD/BS1) = -1320.992877 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1608.1543903 au

C	5.15669400	0.54958500	0.85407900
C	3.84258200	0.39528000	0.43041000

C	3.43279200	-0.90792100	-0.01107700
C	4.34683700	-1.99404100	-0.00353300
C	5.67403900	-1.78792200	0.43619500
C	6.05420900	-0.53620800	0.85302400
H	5.49132400	1.52315700	1.19302500
C	3.87637900	-3.25284900	-0.444440400
H	6.36937200	-2.62642600	0.43539300
H	7.07431300	-0.36401600	1.19403200
C	2.57654400	-3.39701900	-0.85760800
C	1.73541900	-2.27017300	-0.83552400
H	4.56374900	-4.09885900	-0.44696600
H	2.18763700	-4.35299000	-1.19900000
H	0.69432800	-2.34905100	-1.15534700
N	2.14010300	-1.07901600	-0.43596600
N	2.85734100	1.38157900	0.40013300
C	2.99453800	2.67509500	0.81425000
C	1.68456400	3.43199500	0.76895900
H	1.89928100	4.48794300	0.54367000
H	1.30659900	3.41858300	1.80464200
C	0.65556800	2.81131000	-0.16991100
H	0.72167000	3.22779500	-1.18784600
O	4.03740600	3.19008900	1.23604400
Pd	1.10162300	0.84340600	-0.37034400
C	-5.85454400	0.51783900	0.53722800
C	-4.65605500	-0.19415800	0.57565700
C	-3.58187400	0.29490700	-0.14872300
C	-3.62611100	1.44859000	-0.90521200
C	-4.83624700	2.14377900	-0.92817500
C	-5.94070500	1.68314800	-0.21363000
H	-6.70558000	0.14214500	1.10299800
H	-2.75949000	1.80336500	-1.45816300
H	-4.90878300	3.05799100	-1.51442800
H	-6.87462400	2.24044900	-0.24337300
I	-1.83454600	-0.91700900	0.05539500
C	-4.50064300	-1.44499000	1.36647900
O	-5.41893200	-1.92877500	2.01859000
O	-3.30962800	-1.98139600	1.30683600
O	-0.82901600	0.42170800	-1.21676400
C	-0.79802600	0.03119100	-2.58826200
H	-0.37444900	0.87369800	-3.15038600
H	-1.81758400	-0.16771500	-2.95036300

H	-0.17138500	-0.85900800	-2.74723900
H	-0.37661600	2.93215700	0.19108900

TS_{17-18_H}

E (M06-SMD/BS1) = -1321.249538 au

H (M06-SMD/BS1) = -1320.891296 au

G (M06-SMD/BS1) = -1320.974572 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1608.127506 au

C	-4.56963600	1.18699600	-1.02916700
C	-3.42735000	0.70180400	-0.40548100
C	-3.38819600	-0.68993500	-0.06572700
C	-4.48806700	-1.53457700	-0.37070600
C	-5.63098900	-0.99626900	-1.00386500
C	-5.65585300	0.33910500	-1.31991500
H	-4.62111600	2.23654300	-1.29390800
C	-4.38664800	-2.90069500	-0.02252400
H	-6.47006300	-1.65323100	-1.22914400
H	-6.53056100	0.76700600	-1.80767500
C	-3.25220000	-3.37169200	0.58635000
C	-2.20921500	-2.46890300	0.85750000
H	-5.22110300	-3.56429400	-0.24882900
H	-3.14262200	-4.41705200	0.86338400
H	-1.29704800	-2.81459600	1.34234200
N	-2.26831100	-1.18510600	0.55246000
N	-2.28994600	1.43816500	-0.07693500
C	-2.06274300	2.74921600	-0.38384200
C	-0.65419500	3.17588500	-0.03193400
H	-0.65035000	4.25373900	0.19122700
H	-0.05760900	3.05173300	-0.95154300
C	-0.05669700	2.35401300	1.09048000
H	-0.44456600	2.63474400	2.08132500
O	-2.86698500	3.51559200	-0.92416300
Pd	-0.82388500	0.47131600	0.90102800
C	5.66456200	-0.16315100	-0.31174300
C	4.33814400	-0.30268100	-0.72053700
C	3.33725800	-0.04194000	0.20655100
C	3.59272500	0.35720800	1.50410200
C	4.92886200	0.49398600	1.88401700
C	5.95957500	0.23577600	0.98444200
H	6.45105700	-0.37533100	-1.03457000
H	2.78225500	0.54419800	2.20198700

H	5.15632200	0.80644300	2.90176200
H	6.99593500	0.34578400	1.29702000
I	1.35170500	-0.27010800	-0.63077900
C	4.01152200	-0.73175400	-2.10828900
O	4.88511800	-0.97940500	-2.93614500
O	2.74139600	-0.82697000	-2.37532000
O	0.81834000	-0.26025600	1.89690600
C	0.80094400	-1.57170200	2.38459000
H	1.69522700	-1.72461400	3.01309800
H	0.83817100	-2.33137900	1.58291100
H	-0.09197500	-1.77142800	3.00085200
H	1.04041000	2.35966800	1.10906000

18_H

E (M06-SMD/BS1) = -1321.261937 au

H (M06-SMD/BS1) = -1320.903361 au

G (M06-SMD/BS1) = -1320.990104 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1608.13410033 au

C	-3.68710500	-1.86261400	-1.01264700
C	-2.85688900	-0.80626200	-0.66341100
C	-3.11951900	-0.12484000	0.56710900
C	-4.21526700	-0.50284300	1.38327200
C	-5.04541600	-1.57372900	0.98059300
C	-4.77079500	-2.23350600	-0.19188500
H	-3.50328500	-2.40083400	-1.93554800
C	-4.41795700	0.21708800	2.58251400
H	-5.88438700	-1.86043300	1.61305700
H	-5.39832500	-3.06517600	-0.50795100
C	-3.56785400	1.23837100	2.92864800
C	-2.49908300	1.54509000	2.06940800
H	-5.25599500	-0.05571800	3.22350000
H	-3.70089600	1.80541200	3.84622700
H	-1.79291600	2.34104400	2.31014500
N	-2.28699000	0.89404400	0.94108400
N	-1.76604900	-0.33748700	-1.40230700
C	-1.39888900	-0.75263900	-2.65156800
C	-0.05875700	-0.19230500	-3.07773100
H	-0.09787200	0.01326200	-4.15839400
H	0.67490200	-1.00287300	-2.94801500
C	0.36418900	1.03821000	-2.31638900
H	-0.10727900	1.96837000	-2.67377700

O	-2.04868300	-1.51108200	-3.37304900
Pd	-0.63015200	1.06663500	-0.50719200
C	5.33327100	-0.18774700	0.47484500
C	4.04657400	-0.72067900	0.56608000
C	2.98194600	0.10937000	0.23842400
C	3.13449900	1.43065100	-0.14176600
C	4.43335600	1.93435000	-0.22015200
C	5.52838200	1.12827900	0.07818800
H	6.17311800	-0.83269500	0.72888600
H	2.26956200	2.06474700	-0.33068900
H	4.58003400	2.97243100	-0.51386100
H	6.53680800	1.53176200	0.01107400
I	1.03972200	-0.82206500	0.36280900
C	3.83916800	-2.12923700	1.03302700
O	4.80833800	-2.84797800	1.29833700
O	2.61269600	-2.50240100	1.14104100
O	0.31469300	2.58931300	0.41167100
C	-0.30904000	3.75176800	-0.03949700
H	0.01799900	4.05063000	-1.05393500
H	-0.07330800	4.58585700	0.64512900
H	-1.41630700	3.66833300	-0.05775800
H	1.44590400	1.16074300	-2.21394400

TS_{18-19_H}

E (M06-SMD/BS1) = -1321.259296 au
H (M06-SMD/BS1) = -1320.901324 au
G (M06-SMD/BS1) = -1320.98611 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1608.130922 au

C	-3.78078500	-2.28120600	-0.10208000
C	-3.00259500	-1.14131700	-0.19669400
C	-3.50270000	0.06860600	0.36072500
C	-4.78420700	0.11736300	0.96296300
C	-5.55707400	-1.06532500	1.02631600
C	-5.05267800	-2.23213800	0.50686800
H	-3.41022400	-3.21987600	-0.50079500
C	-5.21269200	1.35909900	1.48308500
H	-6.53689600	-1.03113800	1.50033300
H	-5.63697300	-3.14887700	0.56365000
C	-4.39505300	2.46038400	1.40244300
C	-3.13441200	2.32753000	0.79787900
H	-6.19582500	1.42529500	1.94822600

H	-4.69800800	3.42589800	1.79849800
H	-2.45424900	3.17642700	0.72901800
N	-2.71046400	1.18168500	0.29584400
N	-1.74807800	-1.04283200	-0.81357500
C	-1.43100700	-1.73200000	-1.94768700
C	-0.16051900	-1.21695600	-2.58697300
H	-0.26739600	-1.30620800	-3.67956400
H	0.67766700	-1.86585900	-2.29801100
C	0.09399800	0.21280600	-2.23497000
H	-0.59218800	0.93470100	-2.69739400
O	-2.09170600	-2.65096400	-2.43157400
Pd	-0.68569200	0.62508600	-0.30302500
C	5.54419200	0.47722500	0.12497600
C	4.37959100	-0.21703900	0.46021500
C	3.16788600	0.33839200	0.06307300
C	3.07701000	1.53940500	-0.62010300
C	4.25762600	2.20873400	-0.93837200
C	5.48974700	1.67652300	-0.57181300
H	6.49615300	0.04754100	0.43254500
H	2.11041400	1.96495000	-0.87522400
H	4.20225600	3.15477300	-1.47419500
H	6.40887500	2.20231300	-0.82335800
I	1.39416500	-0.78233400	0.56264000
C	4.47349400	-1.49852500	1.24701400
O	5.59189500	-1.94612300	1.54229000
O	3.36025200	-2.03446100	1.56688600
O	0.13277100	2.37372000	0.23801600
C	-0.10551300	3.35399000	-0.72815900
H	0.52681100	3.23492400	-1.62999000
H	0.12266600	4.34396800	-0.29741800
H	-1.15856600	3.38672700	-1.07112800
H	1.13485100	0.54150500	-2.25900300

19_H

E (M06-SMD/BS1) = -1321.263357 au
H (M06-SMD/BS1) = -1320.905492 au
G (M06-SMD/BS1) = -1320.987716 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1608.131926 au

C	-4.11675400	-1.79550600	0.60382100
C	-3.08358900	-0.94895000	0.26270600
C	-3.38291500	0.40447700	-0.03859100

C	-4.71353100	0.88295200	-0.03402900
C	-5.74948000	-0.01444000	0.31889000
C	-5.44573100	-1.31636500	0.63357400
H	-3.90615700	-2.83350900	0.84596800
C	-4.91820500	2.23405700	-0.39275500
H	-6.77596900	0.34783000	0.33912900
H	-6.24099300	-2.00577500	0.91078000
C	-3.84949300	3.03273100	-0.72439000
C	-2.55190300	2.49779100	-0.68323700
H	-5.93314900	2.62970400	-0.40399300
H	-3.98159000	4.07398500	-1.00490500
H	-1.67553100	3.10545600	-0.90191200
N	-2.34087400	1.23530300	-0.35480200
N	-1.72946000	-1.29531500	0.09330000
C	-1.41975200	-2.28519600	-0.81137100
C	-0.13010800	-1.98598200	-1.54350800
H	-0.18676000	-2.43768700	-2.54661000
H	0.73397800	-2.43569200	-1.03524200
C	0.01148500	-0.50637400	-1.69138200
H	-0.72543300	-0.02505700	-2.34255100
O	-2.13227600	-3.25364500	-1.04919300
Pd	-0.53062400	0.37475700	0.15629500
C	4.72230800	0.71395900	-1.16153100
C	3.73122900	-0.11306800	-0.62020000
C	3.16963200	0.29282900	0.58804500
C	3.55824400	1.45101200	1.25547800
C	4.56815000	2.23369100	0.70447100
C	5.14867100	1.86193900	-0.50559400
H	5.15978300	0.43328100	-2.11908900
H	3.07227700	1.74682600	2.18338000
H	4.88928000	3.13712700	1.21977300
H	5.93209000	2.47655200	-0.94583600
I	1.53938800	-0.79765100	1.45157400
C	3.33027300	-1.35795800	-1.39992200
O	3.07233300	-1.17160200	-2.61333600
O	3.30474500	-2.44238000	-0.77255300
O	0.41839600	2.13658600	0.23895300
C	0.98220800	2.56299900	-0.96403300
H	1.84066600	1.94262200	-1.28649300
H	1.36258600	3.58959100	-0.82574200
H	0.25482100	2.59507600	-1.79967400

H 1.02355700 -0.10282900 -1.78908100

21_H

E (M06-SMD/BS1) = -1436.931147 au

H (M06-SMD/BS1) = -1436.514214 au

G (M06-SMD/BS1) = -1436.61058 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1723.850027 au

C	4.30652500	0.30888100	1.76622800
C	3.22681800	0.15192900	0.92282400
C	3.43469200	-0.44589000	-0.34666500
C	4.72396700	-0.84498800	-0.76900600
C	5.80959700	-0.66608600	0.12070000
C	5.59321500	-0.10726800	1.35649500
H	4.16547700	0.75512700	2.74659700
C	4.84121200	-1.39954900	-2.06299100
H	6.80337500	-0.98352200	-0.19121100
H	6.42612400	0.02454700	2.04463500
C	3.72924800	-1.53918700	-2.85843900
C	2.47575400	-1.14314600	-2.36453500
H	5.82259900	-1.71346500	-2.41683300
H	3.79174600	-1.96294700	-3.85687600
H	1.56875400	-1.27488800	-2.95123400
N	2.34476200	-0.61481400	-1.16040300
N	1.90815800	0.58983400	1.14540400
C	1.68963100	1.91312100	1.43222400
C	0.37526600	2.39632800	0.85825900
H	0.46329500	3.47316300	0.65246100
H	-0.44500600	2.26411200	1.57572800
C	0.10843100	1.68378100	-0.42504100
H	0.80921400	1.87689900	-1.24299000
O	2.48243900	2.64128800	2.02045600
Pd	0.58854900	-0.39814700	-0.07835300
C	-4.78630100	-0.38615000	-0.97803700
C	-3.72808500	-0.02464100	-0.13585900
C	-3.07427300	-1.05972600	0.53092200
C	-3.42663200	-2.39721300	0.37183500
C	-4.50037900	-2.71885600	-0.45202000
C	-5.18309000	-1.70855700	-1.12335500
H	-5.29573700	0.40385700	-1.52798800
H	-2.86740200	-3.18120700	0.87890700
H	-4.79098600	-3.76074600	-0.57335000

H	-6.01946900	-1.95392400	-1.77545300
I	-1.37149700	-0.70647400	1.78761600
C	-3.33409600	1.44004500	-0.07449600
O	-3.29585600	2.02235300	-1.19576500
O	-3.07235900	1.94520500	1.03594400
O	-0.49656400	-1.50422700	-1.34427100
C	-1.05670500	-0.81025200	-2.41711300
H	-1.85586700	-0.10777100	-2.11402300
H	-1.51671200	-1.54311000	-3.10298000
H	-0.31212900	-0.23834400	-3.00761800
H	-0.92168900	1.50615200	-0.73610600
C	-1.13188500	3.56161400	-2.84617700
H	-1.06057000	2.48435000	-3.07647800
H	-0.21000200	4.04549200	-3.19114000
H	-1.97325000	3.97573500	-3.42518900
O	-1.26871200	3.80726700	-1.46480700
H	-2.08516500	3.32301400	-1.19026200

TS_{21-22_H}

E (M06-SMD/BS1) = -1436.930447 au

H (M06-SMD/BS1) = -1436.514615 au

G (M06-SMD/BS1) = -1436.60802 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1723.84781 au

C	4.34754400	0.97243900	1.41540500
C	3.26394600	0.49108900	0.70843000
C	3.47751900	-0.54408600	-0.23941800
C	4.77260700	-1.05362900	-0.49287400
C	5.86020600	-0.53322300	0.24746700
C	5.63895100	0.45079500	1.17952400
H	4.20541500	1.75516800	2.15420500
C	4.89457400	-2.05910200	-1.47783600
H	6.85807300	-0.93040700	0.06802600
H	6.47267500	0.84747300	1.75610800
C	3.78149600	-2.50969800	-2.14554800
C	2.52395200	-1.97313100	-1.82504000
H	5.88022000	-2.46850800	-1.69672300
H	3.84679100	-3.28204900	-2.90712200
H	1.61676300	-2.33180800	-2.30747700
N	2.38685500	-1.02628100	-0.91335000
N	1.93896000	0.95361800	0.76377800
C	1.68153400	2.29168000	0.69496800

C	0.33069300	2.57875600	0.06202100
H	0.40757700	3.56243900	-0.42391000
H	-0.46070000	2.64211800	0.82021100
C	0.02753400	1.55602300	-0.96923800
H	0.70751500	1.45687800	-1.81700200
O	2.45631700	3.18201400	1.03392700
Pd	0.62002200	-0.43487000	0.00641400
C	-4.73720000	-0.91985200	-0.94645900
C	-3.71794000	-0.25614700	-0.25372700
C	-3.05219400	-0.97893600	0.73489600
C	-3.35969600	-2.30449400	1.02936200
C	-4.39702500	-2.92610600	0.34170000
C	-5.08858400	-2.22845400	-0.64463600
H	-5.25255800	-0.38208200	-1.74122600
H	-2.79234400	-2.84941100	1.78172300
H	-4.65211400	-3.95860300	0.57322400
H	-5.89588400	-2.71175500	-1.19203100
I	-1.40064700	-0.15169700	1.82378500
C	-3.36282000	1.15396800	-0.68378000
O	-3.23637000	1.30344400	-1.93390600
O	-3.21289500	2.02919600	0.19260800
O	-0.42288200	-1.95189300	-0.77004000
C	-0.97964800	-1.67310700	-2.01902500
H	-1.74526800	-0.87568200	-1.98872200
H	-1.47900100	-2.58509500	-2.39133900
H	-0.22620600	-1.38053400	-2.77888100
H	-0.97508700	1.15731800	-1.09944800
C	-1.63740800	4.33120700	-1.93460300
H	-2.33953600	4.86301400	-2.59667400
H	-0.73820600	4.95114000	-1.83223400
H	-2.11154000	4.22345800	-0.94676600
O	-1.26548900	3.08309100	-2.47899700
H	-2.05165900	2.48677700	-2.38085800

22_H

E (M06-SMD/BS1) = -1437.004094 au

H (M06-SMD/BS1) = -1436.583534 au

G (M06-SMD/BS1) = -1436.675969 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1723.916481 au

C	4.15968200	1.39150900	1.10265800
C	3.13091200	0.69886800	0.48559500

C	3.47028300	-0.48413600	-0.22785500
C	4.81531000	-0.90275000	-0.37758400
C	5.83576800	-0.14887800	0.24566400
C	5.49778100	0.96092800	0.98066300
H	3.93845400	2.28027500	1.68312100
C	5.05626500	-2.07350000	-1.13176200
H	6.87062900	-0.47262600	0.14420200
H	6.27487200	1.53559300	1.48232200
C	4.00661100	-2.77194500	-1.67526500
C	2.69583300	-2.31904800	-1.45057600
H	6.08324700	-2.41211500	-1.26612000
H	4.16321500	-3.67658900	-2.25677000
H	1.83140400	-2.87161800	-1.81525200
N	2.44645700	-1.21993400	-0.76189800
N	1.76589700	1.04069000	0.46709900
C	1.41313300	2.34776000	0.35845100
C	-0.02707700	2.65334000	0.01947300
H	-0.44699800	3.27848900	0.82221800
C	-0.06778500	3.39710900	-1.31094300
O	2.20175700	3.30264800	0.45349300
Pd	0.62670400	-0.64459500	0.01876400
C	-4.49093500	-0.88070500	-1.31409100
C	-3.55900900	-0.30865600	-0.44436400
C	-3.02463600	-1.09587900	0.57616500
C	-3.41002700	-2.42010300	0.74375400
C	-4.36179400	-2.96496900	-0.11488400
C	-4.89897400	-2.19774400	-1.14365500
H	-4.89639200	-0.27556100	-2.12401000
H	-2.96130700	-3.02863000	1.52643400
H	-4.67053100	-4.00013200	0.01843200
H	-5.63295300	-2.62787000	-1.82205600
I	-1.44061800	-0.36805900	1.81859500
C	-3.15831000	1.11223400	-0.64613700
O	-2.63284000	1.32277300	-1.84376100
O	-3.29666900	1.97846800	0.19792700
O	-0.23013500	-2.36616000	-0.56292400
C	-0.80116300	-2.19257700	-1.82201700
H	-1.57023700	-1.39465100	-1.84919000
H	-1.30591200	-3.12780000	-2.12646500
H	-0.05548400	-1.95824600	-2.61027400
H	0.36568900	2.76603500	-2.10073200

C	-1.99660700	4.76410200	-1.03535600
H	-2.96810800	4.94765100	-1.50546300
H	-1.38139600	5.67350900	-1.10696300
H	-2.15635500	4.52033800	0.02432300
O	-1.38528100	3.70304700	-1.74670300
H	-2.29875800	2.26907300	-1.88070600
H	-0.63066900	1.74517200	-0.05899800
H	0.51925800	4.32694300	-1.25498300

1_OMe

E (M06-SMD/BS1) = -763.2571087 au

H (M06-SMD/BS1) = -762.988392 au

G (M06-SMD/BS1) = -763.048036 au

E (M06-SMD/BS2//M06-SMD/BS1) = -763.5502595 au

C	-0.30673300	1.47821200	-0.52285700
C	-0.65443000	0.15420000	-0.35083500
C	-2.01728200	-0.17292700	-0.04448100
C	-2.96775600	0.87053400	0.10983100
C	-2.56760700	2.21856000	-0.04280100
C	-1.26363400	2.50235300	-0.35675000
H	0.70225400	1.75829300	-0.80629900
C	-4.29675900	0.49454700	0.41345200
H	-3.30648800	3.00924200	0.08325300
H	-0.94529000	3.53446500	-0.49294400
C	-4.61548600	-0.83293400	0.53908600
C	-3.59637200	-1.79019900	0.35590600
H	-5.04965400	1.27261600	0.54031600
H	-5.62773600	-1.15607900	0.77072300
H	-3.83239600	-2.85247500	0.44478400
N	-2.34668700	-1.48497800	0.07778400
N	0.19429300	-0.94827100	-0.49126300
H	-0.31609400	-1.83304300	-0.50903300
C	1.54884400	-1.12359000	-0.41485700
C	2.44214500	0.06154200	-0.19528900
H	2.46152800	0.67854400	-1.10658200
H	2.03724800	0.69790400	0.60523500
C	3.85336500	-0.35921000	0.14866200
H	4.29363800	-0.95940000	-0.66685000
H	3.86445400	-0.98912000	1.05680900
O	2.00271600	-2.26385800	-0.51533500
O	4.60590500	0.81373500	0.35590500

C	5.94168000	0.51921400	0.68306000
H	6.46672500	1.46904000	0.83174700
H	6.00869500	-0.07514500	1.61022000
H	6.44107100	-0.04293100	-0.12434700

13_OMe

E (M06-SMD/BS1) = -1347.967023 au

H (M06-SMD/BS1) = -1347.581493 au

G (M06-SMD/BS1) = -1347.671382 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1348.469215 au

C	2.73830400	0.40750100	2.03487900
C	1.62439600	0.49171600	1.23720500
C	1.40252900	1.62875300	0.43627200
C	2.33319400	2.69459300	0.45320600
C	3.47226000	2.58722700	1.28470200
C	3.66801000	1.46840500	2.05772500
H	2.89758200	-0.48083100	2.64560400
C	2.06222500	3.81225200	-0.36873500
H	4.18647800	3.40924800	1.29864600
H	4.54474300	1.39039200	2.69636700
C	0.93008200	3.83085300	-1.14487900
C	0.05276800	2.73353600	-1.10983800
H	2.76074000	4.64798100	-0.37420900
H	0.69310700	4.67440100	-1.78707600
H	-0.85408500	2.71118200	-1.71247500
N	0.28178100	1.67535000	-0.35082500
N	0.64011500	-0.57299000	1.17735800
H	0.12744500	-0.71321200	2.06145400
C	1.05739400	-1.85642200	0.66933100
C	2.01061000	-1.84606200	-0.48173300
H	3.01416000	-2.06712800	-0.08561000
H	2.05640600	-0.85724500	-0.95659300
C	1.58576400	-2.89486700	-1.50850500
H	1.66116300	-3.90592800	-1.07357500
H	0.53648300	-2.72449000	-1.79024900
O	0.57578000	-2.85975800	1.14768400
Pd	-0.92090000	0.05094300	-0.12216500
O	-2.32394400	0.74065400	-1.42148900
C	-3.31298000	1.35757000	-0.84721800
O	-3.41461900	1.53149600	0.37141900
O	-2.08126900	-1.59749800	0.17115900

C	-2.34264500	-1.87315000	1.41219200
O	-1.96693200	-1.19357200	2.37643200
C	-4.34107800	1.87487700	-1.81710900
H	-3.88535200	2.63924500	-2.45974800
H	-5.19117200	2.31106900	-1.28448800
H	-4.68929900	1.06605600	-2.47038600
C	-3.12039500	-3.14518900	1.60655500
H	-3.61285200	-3.14945000	2.58392200
H	-2.41717700	-3.98891600	1.56818000
H	-3.85882200	-3.29008500	0.81092200
O	2.33539500	-2.81092800	-2.69484200
C	3.66044000	-3.27386800	-2.55396200
H	3.68414400	-4.28227700	-2.10871100
H	4.27547400	-2.60155100	-1.93479100
H	4.09844500	-3.31783900	-3.55677200

TS_{13-14_OMe}

E (M06-SMD/BS1) = -1347.954692 au

H (M06-SMD/BS1) = -1347.574858 au

G (M06-SMD/BS1) = -1347.663598 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1348.457651 au

C	-2.09526400	0.75160900	-2.19912500
C	-1.15750200	0.59412400	-1.20606800
C	-0.66332700	1.73318500	-0.53266700
C	-1.15795000	3.02325100	-0.83439000
C	-2.12987500	3.15089000	-1.85453400
C	-2.57611400	2.03821000	-2.52576200
H	-2.47425500	-0.12686000	-2.72050000
C	-0.63409300	4.11123800	-0.09927200
H	-2.50529300	4.14334200	-2.09934400
H	-3.31632800	2.13921300	-3.31671700
C	0.32236900	3.89281600	0.86151600
C	0.78792300	2.58599500	1.08673100
H	-0.99753200	5.11655900	-0.30864500
H	0.74238300	4.70904800	1.44259000
H	1.56729700	2.37764500	1.81802900
N	0.31211400	1.55114600	0.41567900
N	-0.66414000	-0.68529000	-0.78666900
H	0.02652100	-1.41875900	-1.54912800
C	-1.51031100	-1.50924600	-0.00542500
C	-2.75812700	-0.90719800	0.57295600

H	-3.45828100	-0.69726700	-0.24971600
H	-2.52042300	0.06760000	1.02718600
C	-3.39426800	-1.81920700	1.60939100
H	-3.71233300	-2.76813900	1.14409600
H	-2.66456200	-2.06007400	2.39338300
O	-1.19580600	-2.67322500	0.19078000
Pd	1.06621000	-0.32682700	0.32977600
O	2.71431000	0.11230600	1.45013300
C	3.69709800	0.62570700	0.77505100
O	3.67472900	0.83431200	-0.44311700
O	1.89949800	-2.17195200	-0.10420500
C	1.65268500	-2.69364400	-1.23401800
O	0.78831000	-2.25621000	-2.05951200
C	4.88820200	0.98843900	1.62081500
H	4.63437900	1.85627700	2.24411700
H	5.74700300	1.24155200	0.99200900
H	5.14986600	0.16618700	2.29653600
C	2.40336900	-3.92809000	-1.60886500
H	1.76534000	-4.79670000	-1.39758800
H	3.32659900	-4.02162700	-1.03069800
H	2.62090500	-3.92765300	-2.68184900
O	-4.48463000	-1.20569100	2.25990400
C	-5.64003200	-1.11674400	1.45803500
H	-5.53165800	-0.38680300	0.63989000
H	-6.46186300	-0.78903500	2.10421600
H	-5.89922100	-2.09576600	1.02126400

15_OMe

E (M06-SMD/BS1) = -1118.968347 au

H (M06-SMD/BS1) = -1118.652874 au

G (M06-SMD/BS1) = -1118.727167 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1119.381355 au

C	3.03222400	1.94152700	-0.26437400
C	1.94543800	1.10090400	-0.07012200
C	2.20373400	-0.29519300	-0.00233900
C	3.50939300	-0.82601500	-0.13084700
C	4.58673000	0.06681500	-0.32676400
C	4.33477900	1.41514200	-0.38898000
H	2.88016500	3.01176800	-0.32153300
C	3.65748900	-2.22936800	-0.05651300
H	5.59502600	-0.33190200	-0.42545100

H	5.15702200	2.11273300	-0.53982300
C	2.56090600	-3.03402300	0.13347200
C	1.29307200	-2.44457500	0.25529400
H	4.65416600	-2.65847800	-0.15362400
H	2.64883200	-4.11528800	0.19235600
H	0.39327500	-3.03758900	0.40920300
N	1.13522200	-1.13334400	0.19089900
N	0.59293500	1.44910600	0.06673700
C	0.12516900	2.72561300	0.04829800
C	-1.36590400	2.91092700	0.25055900
H	-1.66735200	3.79193200	-0.32961700
H	-1.52582400	3.16187500	1.31041300
C	-2.26108600	1.75656300	-0.12568000
H	-2.11671500	1.42979400	-1.16864000
H	-2.09754300	0.87118600	0.60088200
O	0.83172100	3.73093400	-0.08439100
Pd	-0.60776800	-0.14629100	0.32811700
O	-1.70525700	-1.84624300	0.66590900
C	-2.40171100	-2.24062200	-0.35491300
O	-2.44873300	-1.64378100	-1.43740400
C	-3.15600600	-3.52146500	-0.12148200
H	-2.44219600	-4.34635400	0.00287000
H	-3.81690300	-3.74332400	-0.96469400
H	-3.74300200	-3.45795000	0.80254200
O	-3.58888100	2.09657500	0.10973000
C	-4.49103200	1.10384400	-0.34213200
H	-4.32975600	0.15421100	0.19424200
H	-4.37725900	0.92930100	-1.42319500
H	-5.50168200	1.46683500	-0.13440300

TS_{15-16_OMe}

E (M06-SMD/BS1) = -1118.93653 au

H (M06-SMD/BS1) = -1118.62742 au

G (M06-SMD/BS1) = -1118.695884 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1119.349105 au

C	-2.96634700	2.04752200	-0.19305100
C	-1.95074600	1.10946700	-0.07722400
C	-2.32090100	-0.26528600	-0.00562900
C	-3.67754800	-0.66825500	-0.05216800
C	-4.68125400	0.31974200	-0.17102000
C	-4.31622700	1.64195800	-0.23832300

H	-2.71596300	3.10060500	-0.25029400
C	-3.95164800	-2.05283800	0.02310400
H	-5.72554700	0.01323200	-0.20687600
H	-5.08198500	2.41088100	-0.32978600
C	-2.92382800	-2.95545600	0.13844400
C	-1.60214900	-2.48066300	0.17965100
H	-4.98824200	-2.38685300	-0.01178600
H	-3.10773500	-4.02480100	0.19850600
H	-0.75857600	-3.16337100	0.27049100
N	-1.31774600	-1.19205600	0.11061000
N	-0.57505600	1.34883200	-0.01990900
C	0.01872900	2.56206900	-0.12006700
C	1.53016700	2.50754100	-0.08707700
C	2.08183700	1.28417100	0.61776200
H	1.66732700	1.19949100	1.63198900
O	-0.56612600	3.64340300	-0.26119100
Pd	0.55629400	-0.30270700	0.16914600
O	1.64425500	-2.08878200	0.27086200
C	2.75865500	-1.97409600	-0.32566500
O	3.16572200	-0.86786900	-0.79204100
C	3.62946000	-3.17691500	-0.47605400
H	4.56486400	-3.01093200	0.07233100
H	3.88993500	-3.31020400	-1.53246100
H	3.13823200	-4.07717500	-0.09797000
H	2.30649100	0.07282300	-0.27796000
H	1.87000400	2.55057900	-1.13364700
H	1.89889300	3.42239300	0.40086500
O	3.46937100	1.31452000	0.83037400
C	4.28007400	1.80582100	-0.22354000
H	4.03948600	1.33907100	-1.18839800
H	5.31257400	1.55514200	0.03972200
H	4.19495300	2.89734800	-0.31923300

7_OMe

E (M06-SMD/BS1) = -889.9783836 au
H (M06-SMD/BS1) = -889.732716 au
G (M06-SMD/BS1) = -889.793292 au
E (M06-SMD/BS2//M06-SMD/BS1) = -890.2963307 au

C	1.95750600	2.25209800	0.14518800
C	1.17420400	1.10892000	0.05417700
C	1.84261000	-0.16217900	-0.00942200

C	3.26155000	-0.22267100	0.00971000
C	4.01670000	0.96891900	0.09899200
C	3.36345800	2.17401300	0.16588800
H	1.47192600	3.21991300	0.19783300
C	3.86863400	-1.49802800	-0.06107200
H	5.10411600	0.90643600	0.11519600
H	3.93326400	3.09947000	0.23819100
C	3.09324800	-2.62534300	-0.14441100
C	1.69447900	-2.47830100	-0.15515000
H	4.95666400	-1.56250300	-0.04766300
H	3.53139800	-3.61862900	-0.20086100
H	1.04802700	-3.35375400	-0.21901400
N	1.09041200	-1.30624400	-0.09055600
N	-0.21765000	1.07530400	0.01194100
C	-1.05664400	2.13787900	-0.11464900
C	-2.49366200	1.69914000	-0.31214300
H	-3.18026500	2.45860700	0.09071400
H	-2.66238800	1.66812900	-1.40140500
C	-2.75361100	0.31936100	0.25333300
H	-2.93358800	0.33012000	1.34588200
O	-0.73134200	3.33113300	-0.13045500
Pd	-1.06589200	-0.75021800	0.04214700
O	-3.80936500	-0.29781400	-0.41252300
C	-4.37302000	-1.38575200	0.30229100
H	-4.80110300	-1.04279900	1.25686400
H	-5.16881400	-1.80658500	-0.31930100
H	-3.62459800	-2.16666800	0.50252800

17_OMe

E (M06-SMD/BS1) = -1435.731193 au

H (M06-SMD/BS1) = -1435.335654 au

G (M06-SMD/BS1) = -1435.425373 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1722.663362 au

C	5.22038500	0.42757700	0.80234800
C	3.90512000	0.26653500	0.38567100
C	3.48186900	-1.05100600	-0.00061600
C	4.39052900	-2.14137700	0.05066600
C	5.71896100	-1.92810000	0.48350300
C	6.10963900	-0.66376600	0.84880300
H	5.56266800	1.41261600	1.09831600
C	3.91481700	-3.41390300	-0.34249500

H	6.40728300	-2.77172000	0.51756000
H	7.13082000	-0.48571900	1.18350800
C	2.61642000	-3.56648800	-0.75656100
C	1.78154500	-2.43468800	-0.77716800
H	4.59799200	-4.26272500	-0.31026800
H	2.22420700	-4.53207500	-1.06577600
H	0.74246400	-2.52047200	-1.10268100
N	2.18840400	-1.23227600	-0.41630400
N	2.93436400	1.26350400	0.31733600
C	3.08530200	2.56357700	0.68454600
C	1.77296200	3.31844300	0.64272400
H	1.96216400	4.38852700	0.46492300
H	1.36481400	3.24090300	1.66333300
C	0.79309600	2.72470200	-0.36197700
H	1.04233800	3.04851100	-1.38504400
O	4.13121800	3.10216700	1.07068100
Pd	1.14794800	0.72740600	-0.41861300
C	-5.84063700	0.23560700	0.45519100
C	-4.62371500	-0.44261900	0.52154200
C	-3.55031300	0.07023800	-0.18686000
C	-3.61052100	1.21936300	-0.94985100
C	-4.83864400	1.88095000	-1.00015500
C	-5.94449300	1.39267200	-0.30602100
H	-6.69144200	-0.15918800	1.00811000
H	-2.74014300	1.60143400	-1.47911700
H	-4.92407100	2.79087500	-1.59133500
H	-6.89293200	1.92317600	-0.35848700
I	-1.77605200	-1.09677600	0.04851100
C	-4.44650800	-1.67940000	1.33014200
O	-5.36309200	-2.18170300	1.97087500
O	-3.23940500	-2.18030500	1.30068900
O	-0.79625600	0.24694800	-1.23325300
C	-0.76878600	-0.14673800	-2.60355000
H	-0.37590800	0.70660800	-3.17194600
H	-1.78506700	-0.37683100	-2.95664400
H	-0.11769400	-1.01876600	-2.76638200
O	-0.54648300	3.10468400	-0.18008200
C	-1.11375800	2.79813700	1.07675500
H	-2.20110800	2.89225600	0.97379500
H	-0.78249600	3.49280400	1.86307800
H	-0.86560000	1.76702100	1.38185100

TS_{17-18_0Me}

E (M06-SMD/BS1) = -1435.714267 au

H (M06-SMD/BS1) = -1435.320514 au

G (M06-SMD/BS1) = -1435.410488 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1722.636815 au

C	4.66348700	0.64270400	1.35816200
C	3.50528800	0.39532500	0.63275600
C	3.45650100	-0.79039100	-0.17249600
C	4.56310900	-1.68136600	-0.20046200
C	5.72117400	-1.38840900	0.55448900
C	5.75651700	-0.24440300	1.31149300
H	4.72234600	1.53557300	1.96996000
C	4.45298600	-2.84453400	-0.99602600
H	6.56368200	-2.07809200	0.52041000
H	6.64388900	-0.00475900	1.89579000
C	3.30506700	-3.08432600	-1.70582600
C	2.25990400	-2.14644000	-1.62896500
H	5.29183200	-3.53979300	-1.02919100
H	3.18792700	-3.97149100	-2.32303500
H	1.33770600	-2.30900700	-2.18657100
N	2.32658300	-1.04601700	-0.90299900
N	2.37022600	1.20405700	0.60486100
C	2.11949000	2.24775200	1.43667200
C	0.73564500	2.82178000	1.22225000
H	0.73006600	3.89270700	1.47722100
H	0.05336700	2.32618800	1.93348000
C	0.23944800	2.59981200	-0.18470500
H	0.83662500	3.14094600	-0.94295300
O	2.87351900	2.69769700	2.30789800
Pd	0.86876600	0.69098000	-0.66117300
C	-5.57586300	-0.73528400	0.40139000
C	-4.22672400	-0.90675000	0.71311800
C	-3.28336100	-0.30282500	-0.10883700
C	-3.62130300	0.46197400	-1.20867800
C	-4.97798600	0.62092500	-1.49446700
C	-5.95141800	0.02682000	-0.69597000
H	-6.31637900	-1.21361700	1.04088500
H	-2.85469700	0.91429700	-1.83024500
H	-5.26728700	1.21907100	-2.35698700
H	-7.00545100	0.15876300	-0.93174300

I	-1.24804900	-0.64206000	0.55482600
C	-3.81880500	-1.72344800	1.89120000
O	-4.64786100	-2.27186700	2.61605900
O	-2.53865300	-1.81205300	2.08978100
O	-0.81832700	0.27729500	-1.78006800
C	-0.76422800	-0.75747200	-2.72310900
H	-1.63626400	-0.66525600	-3.39334300
H	-0.81583300	-1.76176600	-2.26561200
H	0.14990100	-0.70941800	-3.33742000
O	-1.09732600	2.89641600	-0.29111100
C	-1.49922100	3.36255500	-1.56952100
H	-0.98272000	4.30239100	-1.81424200
H	-2.57705300	3.54505700	-1.52281300
H	-1.28503100	2.61212400	-2.34372100

19'_OMe

E (M06-SMD/BS1) = -1435.751932 au

H (M06-SMD/BS1) = -1435.35699 au

G (M06-SMD/BS1) = -1435.448883 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1722.665733 au

C	4.23294800	-1.72592800	-0.72848100
C	3.20739700	-0.91680300	-0.27136900
C	3.52807900	0.41995200	0.10111900
C	4.86093000	0.89507400	0.07436600
C	5.88208400	0.02996400	-0.38359400
C	5.55835800	-1.24264100	-0.78398000
H	4.01846000	-2.74168600	-1.04038700
C	5.08891500	2.22366100	0.49909500
H	6.90736100	0.39489400	-0.42101000
H	6.33661800	-1.90893800	-1.15248500
C	4.03808600	3.00784000	0.90792200
C	2.73701300	2.47926900	0.87302100
H	6.10682200	2.61220600	0.49178500
H	4.18586200	4.03247300	1.23838700
H	1.87020400	3.08205400	1.13900800
N	2.50071900	1.23731100	0.49012500
N	1.86093200	-1.26626100	-0.07153300
C	1.52061600	-2.52030600	0.30597700
C	0.16796300	-2.61841700	0.99448300
H	0.20196800	-3.49651800	1.66470000
H	-0.67070400	-2.79313200	0.30621000

C	-0.11729800	-1.48354800	1.87908200
H	0.67824100	-0.98082800	2.44710500
O	2.21683100	-3.53230900	0.19459100
Pd	0.67446300	0.43618000	-0.06846100
C	-4.87165900	0.85680500	0.59534100
C	-3.86894600	0.00581700	0.11188100
C	-3.03014500	0.53375000	-0.87193400
C	-3.18605000	1.82027400	-1.38151000
C	-4.21063800	2.62629400	-0.89518300
C	-5.05055000	2.14288000	0.10269100
H	-5.52456000	0.47075000	1.37646300
H	-2.50563600	2.19890300	-2.14167800
H	-4.34062900	3.63068000	-1.29452200
H	-5.84962600	2.76822300	0.49760200
I	-1.32133200	-0.52805300	-1.62840600
C	-3.81843600	-1.41095300	0.68246400
O	-4.21949500	-1.54002300	1.86307700
O	-3.41335300	-2.32179600	-0.07969400
O	-0.17721600	2.24703900	-0.08942800
C	-0.87061400	2.48935800	1.09230000
H	-1.73724900	1.81244000	1.23450400
H	-1.27569000	3.51759700	1.06907500
H	-0.22938000	2.41748400	1.99571000
O	-1.31992500	-1.20516500	2.14021400
C	-1.65589700	-0.26121100	3.19376600
H	-1.97716500	-0.86306500	4.04726500
H	-2.48717400	0.33391200	2.81326900
H	-0.78166200	0.34898800	3.43875800

22_OMe

E (M06-SMD/BS1) = -1551.470885 au

H (M06-SMD/BS1) = -1551.015221 au

G (M06-SMD/BS1) = -1551.111948 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1838.427742 au

C	4.04386400	-0.02665200	1.78016500
C	2.98074700	-0.21452900	0.91244700
C	3.20242300	-1.02789000	-0.23678000
C	4.47915100	-1.56368800	-0.53247400
C	5.54215900	-1.32643500	0.36956200
C	5.30998700	-0.58611200	1.50223800
H	3.90627900	0.56299400	2.67908300

C	4.61191200	-2.32126900	-1.71811700
H	6.52324800	-1.74748300	0.15448700
H	6.11819600	-0.41433700	2.21157900
C	3.52424900	-2.52854900	-2.53040700
C	2.27918500	-1.99831300	-2.15267500
H	5.58625600	-2.73889400	-1.97049000
H	3.59864000	-3.10767300	-3.44697700
H	1.38074900	-2.18193200	-2.73993500
N	2.13310300	-1.27621200	-1.05649100
N	1.69483000	0.34753900	0.99362000
C	1.55422900	1.63601900	1.40484600
C	0.35155800	2.38958500	0.86828500
H	0.28237100	3.34979300	1.39509800
H	-0.58564500	1.84555200	1.03261200
C	0.50519300	2.63281500	-0.62958100
O	2.38465500	2.24105700	2.09791200
Pd	0.36473100	-0.77677600	-0.11570700
C	-4.78837400	0.06349100	-1.15476100
C	-3.76579500	0.20112000	-0.21258900
C	-3.33014300	-0.93271900	0.47517400
C	-3.89776000	-2.17908100	0.24273000
C	-4.93759200	-2.29162200	-0.67736200
C	-5.38093200	-1.17314700	-1.37586500
H	-5.11779500	0.94191600	-1.70796900
H	-3.52501500	-3.05949700	0.76258100
H	-5.38966900	-3.26566200	-0.85507100
H	-6.18429300	-1.26499700	-2.10393800
I	-1.62832900	-0.85514600	1.77175700
C	-3.14043300	1.53385000	-0.00036200
O	-2.69949400	2.06375000	-1.13526400
O	-3.02157300	2.07214200	1.08336100
O	-0.73349900	-1.94540700	-1.32783000
C	-1.20755000	-1.16952500	-2.38330500
H	-1.83526500	-0.31810200	-2.05261600
H	-1.84095300	-1.79131800	-3.04272700
H	-0.39627700	-0.75197300	-3.01735900
H	0.33181100	1.69627400	-1.19601400
C	-0.47760100	3.81748700	-2.41668200
H	-0.56563600	2.86445600	-2.96304600
H	0.42707200	4.34042700	-2.75057000
H	-1.35344000	4.43932900	-2.62663200

O	-0.45834300	3.59049200	-1.01081600
H	-2.14247000	2.85487300	-0.91610700
O	1.79572000	3.02669100	-1.01074000
C	2.24571300	4.25969200	-0.46131300
H	2.44410400	4.17446600	0.61496000
H	1.52154400	5.06680000	-0.63639600
H	3.17962200	4.50314800	-0.97707600

31

E (M06-SMD/BS1) = -652.4065225 au

H (M06-SMD/BS1) = -652.105395 au

G (M06-SMD/BS1) = -652.164535 au

E (M06-SMD/BS2//M06-SMD/BS1) = -652.6584964 au

C	2.81888900	-1.83750200	-0.38782800
C	3.20255700	-0.38581800	-0.65346400
H	3.42034200	-0.24180200	-1.72340000
C	2.20373000	0.68821600	-0.26775500
C	-0.24922100	1.13484700	0.06616400
C	-0.39882000	2.33253300	-0.87117700
H	0.50590100	2.94999100	-0.83372200
H	-1.24945200	2.96186100	-0.58186200
H	-0.55004000	1.99751100	-1.90596100
C	-0.11291600	1.58794900	1.52260300
H	-0.00360100	0.71681200	2.18395200
H	-1.00172800	2.15026800	1.83653000
H	0.76369600	2.23341900	1.64549100
C	-1.47241400	0.22129400	-0.03196100
C	-2.75808400	0.73656500	0.15166500
H	-2.91039800	1.79669100	0.34554900
C	-3.84217000	-0.12665100	0.08866200
H	-4.85297400	0.25348200	0.22724900
C	-3.62043900	-1.47947300	-0.15331600
H	-4.44214600	-2.18959200	-0.21083700
C	-2.31108400	-1.90255800	-0.32004100
H	-2.08811500	-2.95347500	-0.51076800
N	0.90830700	0.33084000	-0.32971500
O	2.59477000	1.82279600	0.03659000
N	-1.26006900	-1.07782600	-0.26002600
H	4.13073000	-0.13718600	-0.11925100
H	3.63692300	-2.47172300	-0.75856900
C	2.57304500	-2.13756500	1.08239000

H	2.37638800	-3.20517500	1.24457200
H	3.44713500	-1.86275500	1.69006100
H	1.70936200	-1.58092000	1.47480300
H	0.67401200	-0.63764000	-0.53638200
H	1.93971200	-2.12425800	-0.98763300

32 (PIDA)

E (M06-SMD/BS1) = -699.5035232 au

H (M06-SMD/BS1) = -699.293435 au

G (M06-SMD/BS1) = -699.360821 au

E (M06-SMD/BS2//M06-SMD/BS1) = -986.1874142 au

C	0.16764200	-1.51068800	-0.00044200
C	0.79221000	-2.10586000	1.08777800
C	0.94782400	-3.48958700	1.07914200
C	0.47548900	-4.24096000	0.00625800
C	-0.15152600	-3.61879000	-1.07006300
C	-0.30795700	-2.23514000	-1.08550300
H	1.15342300	-1.50802600	1.92239100
H	1.43624800	-3.97867600	1.92001100
H	0.59787500	-5.32263700	0.00896300
H	-0.51787900	-4.20844400	-1.90849600
H	-0.79240200	-1.73612400	-1.92253900
I	-0.06864200	0.60618800	-0.00164800
O	-2.21201000	0.06204700	0.08067000
C	-2.91038100	1.16248100	0.10186700
O	-2.38989400	2.27973800	0.08058900
O	2.13939700	0.54137700	-0.09949700
C	2.58462500	1.76694400	-0.10043900
O	1.83596900	2.74492100	-0.05270900
C	4.07874300	1.87603500	-0.16787800
H	4.44258200	1.39860000	-1.08560300
H	4.38604900	2.92529800	-0.15190000
H	4.52914300	1.34458500	0.67874000
C	-4.39340200	0.94559400	0.15595800
H	-4.65196700	0.39129100	1.06621100
H	-4.92065400	1.90349400	0.14633600
H	-4.71169800	0.33786200	-0.69928300

34

E (M06-SMD/BS1) = -1237.119136 au

H (M06-SMD/BS1) = -1236.700449 au

G (M06-SMD/BS1) = -1236.78654 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1237.580445 au

C	3.33143100	0.26690700	-1.98726600
C	3.26053100	-0.57865800	-0.72266200
H	4.26693400	-0.74594000	-0.31340100
C	2.43239200	-0.08861000	0.43563800
C	0.74119300	1.73722100	1.08792000
C	1.78691800	2.81790900	1.31184300
H	2.71195100	2.36768800	1.69265000
H	1.44244800	3.53811100	2.06372400
H	2.01106700	3.36078700	0.38368200
C	0.31496400	1.10711500	2.41387600
H	-0.32910300	0.23058400	2.26042700
H	-0.25488900	1.85881600	2.97642600
H	1.18136100	0.81137900	3.01102200
C	-0.51261800	2.26338500	0.40850900
C	-0.97561800	3.56385800	0.54735200
H	-0.40971000	4.28656900	1.12957900
C	-2.16962800	3.92878800	-0.06461400
H	-2.54260300	4.94566400	0.03676700
C	-2.87535400	2.99043900	-0.80735300
H	-3.80903900	3.24002500	-1.30385900
C	-2.36401300	1.70813200	-0.91159200
H	-2.86395500	0.92756500	-1.48195100
N	1.29191500	0.72045800	0.10649500
O	2.65262500	-0.42315200	1.57945800
N	-1.21673700	1.36248200	-0.31112100
H	2.85202100	-1.57601100	-0.95291700
H	2.32354300	0.43706200	-2.40062300
C	4.07079500	1.58018800	-1.78762400
H	4.12453900	2.15384900	-2.72136000
H	3.58938200	2.22210500	-1.03437900
H	5.09906100	1.39612700	-1.44648400
H	1.46341600	1.20275900	-0.78293800
H	3.85105000	-0.33021100	-2.74902800
Pd	-0.37045100	-0.49018600	-0.42939400
O	-2.06963400	-1.45579200	-0.99731400
C	-2.98237100	-1.58261200	-0.07998500
O	-2.88493900	-1.15895400	1.07510500
O	0.61114300	-2.27691900	-0.55807200
C	0.67939600	-2.94691700	0.55157100

O	0.11402000	-2.62248700	1.60148800
C	-4.21790400	-2.29460800	-0.56510500
H	-3.95258700	-3.27357100	-0.98195400
H	-4.93515100	-2.42463700	0.25066700
H	-4.68503100	-1.71311900	-1.37028900
C	1.57148100	-4.15703000	0.48340800
H	1.27121200	-4.89818000	1.23112100
H	1.57521500	-4.60702500	-0.51481400
H	2.59808100	-3.83702800	0.71362900

TS₃₄₋₃₅

E (M06-SMD/BS1) = -1237.113665 au

H (M06-SMD/BS1) = -1236.701033 au

G (M06-SMD/BS1) = -1236.78396 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1237.575824 au

C	1.09034900	1.74597600	-2.66317800
C	0.83119000	2.64688900	-1.44819900
H	0.58428900	3.65646700	-1.80805000
C	-0.34943700	2.22188600	-0.60297100
C	-1.22883200	1.20590500	1.45286100
C	-1.91849100	2.48459600	1.91878100
H	-1.15348200	3.18530900	2.27905800
H	-2.58907000	2.26769900	2.76036100
H	-2.49288500	2.97161100	1.12667200
C	-0.68116500	0.50144200	2.70051100
H	-0.12555900	-0.41442100	2.45562700
H	-1.51051000	0.23101300	3.36755700
H	-0.01054200	1.18144100	3.24374600
C	-2.14749500	0.24356800	0.72875900
C	-3.52378700	0.17344800	0.89250000
H	-4.02529900	0.87306600	1.55740800
C	-4.24377400	-0.79068800	0.19702000
H	-5.32356200	-0.85359300	0.31579700
C	-3.57880200	-1.66945200	-0.65175900
H	-4.10989900	-2.43320400	-1.21319300
C	-2.20424300	-1.55981900	-0.77325200
H	-1.61927500	-2.21704700	-1.41420000
N	-0.07516900	1.48736700	0.54973300
O	-1.48888700	2.54002400	-0.94302700
N	-1.52043000	-0.62965100	-0.09233000
H	1.74422400	2.72575300	-0.84443300

H	1.49020900	0.77654200	-2.32443900
C	-0.12475000	1.51039300	-3.54382100
H	0.15775300	0.96876800	-4.45602800
H	-0.89019300	0.91087500	-3.03022100
H	-0.59352800	2.45751100	-3.84693600
H	1.27545300	1.62048500	1.14456400
H	1.88998100	2.21809300	-3.25227100
Pd	0.49077200	-0.38630000	-0.14531800
O	0.87953900	-2.26474400	-0.89520000
C	0.88060000	-3.20749100	-0.00738100
O	0.70439200	-3.02790400	1.20516200
O	2.55531800	-0.12622300	0.08805300
C	3.01965100	0.71997400	0.88863700
O	2.30996200	1.62105500	1.48073800
C	1.09022200	-4.58575100	-0.57609000
H	1.94439200	-4.59468600	-1.26307600
H	1.24774900	-5.31726700	0.22211900
H	0.20249800	-4.87401200	-1.15476000
C	4.47423200	0.73141600	1.19910500
H	4.61407600	0.65002400	2.28367400
H	4.99013600	-0.08791100	0.69325300
H	4.90131100	1.69184600	0.88561100

35

E (M06-SMD/BS1) = -1237.113876 au
H (M06-SMD/BS1) = -1236.698038 au
G (M06-SMD/BS1) = -1236.781972 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1237.576255 au

C	0.96679100	-1.75125000	2.68148500
C	0.73422400	-2.64623400	1.45704300
H	0.48454600	-3.65859500	1.80744300
C	-0.43032300	-2.22302800	0.58612600
C	-1.26759600	-1.17185800	-1.46258900
C	-1.99829400	-2.42235200	-1.94326000
H	-1.25459800	-3.15087800	-2.29308300
H	-2.64593600	-2.17783500	-2.79535500
H	-2.60310900	-2.89011800	-1.16265800
C	-0.68697200	-0.48192500	-2.70404800
H	-0.10459200	0.41505700	-2.45164400
H	-1.49926700	-0.18387500	-3.38047600
H	-0.03152600	-1.18240200	-3.24021400

C	-2.15732900	-0.18063200	-0.74318800
C	-3.53033800	-0.06185700	-0.90668700
H	-4.05542200	-0.74106400	-1.57457600
C	-4.21628000	0.92371000	-0.20666900
H	-5.29337900	1.02448900	-0.32421100
C	-3.52084600	1.77550600	0.64528300
H	-4.02502900	2.55471400	1.21027600
C	-2.15083600	1.61808500	0.76566600
H	-1.54315700	2.25212500	1.40886300
N	-0.13106900	-1.49116700	-0.55346100
O	-1.57484400	-2.55532400	0.90511200
N	-1.50028600	0.66702100	0.08084400
H	1.65937600	-2.71884900	0.87088900
H	1.39052200	-0.78628400	2.35814600
C	-0.27288100	-1.49998100	3.52284600
H	-0.01308000	-0.96515200	4.44577900
H	-1.01164700	-0.88783200	2.98542900
H	-0.76582000	-2.44077500	3.80668300
H	1.37564700	-1.65328000	-1.19864100
H	1.74105300	-2.23376900	3.29575800
Pd	0.50123000	0.35743500	0.13906000
O	0.94146700	2.22746000	0.89415800
C	0.96445700	3.17332200	0.01069100
O	0.78262100	3.00356500	-1.20279800
O	2.57238200	0.05087500	-0.05034000
C	3.06494600	-0.77589500	-0.84411500
O	2.36887600	-1.66638900	-1.48612800
C	1.20827800	4.54423100	0.58398000
H	2.06286000	4.52986500	1.27039800
H	1.38309900	5.27473500	-0.21157200
H	0.32836000	4.85218500	1.16449300
C	4.52563000	-0.80385000	-1.10956000
H	4.70059800	-0.71810000	-2.18864100
H	5.03274700	0.00646300	-0.58129800
H	4.93081600	-1.77124100	-0.78829400

36

E (M06-SMD/BS1) = -1008.110912 au
 H (M06-SMD/BS1) = -1007.763247 au
 G (M06-SMD/BS1) = -1007.837463 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -1008.482903 au

C	0.31830100	-3.00671000	0.18484000
C	-0.99076000	-3.04497400	-0.58810000
H	-1.54106400	-3.95047800	-0.29857600
C	-1.94827600	-1.87678400	-0.43089700
C	-2.21338900	0.56141900	-0.13124300
C	-3.05646500	0.47425600	1.14665300
H	-3.76188700	-0.35995900	1.07584900
H	-3.62644900	1.39926500	1.30479500
H	-2.40584900	0.31446200	2.01892600
C	-3.08655300	0.79004700	-1.36797100
H	-2.46007400	0.90440100	-2.26293100
H	-3.69985200	1.69289900	-1.25629800
H	-3.75722600	-0.06116100	-1.51359600
C	-1.26920500	1.73193600	0.02745100
C	-1.70997200	3.05233000	0.06398700
H	-2.77026700	3.26819600	-0.04572200
C	-0.79804500	4.08031700	0.24399000
H	-1.14039000	5.11259400	0.27042700
C	0.55341500	3.78191900	0.39258900
H	1.29902200	4.55860600	0.53818700
C	0.94278000	2.45797400	0.35575400
H	1.97881700	2.15182600	0.48080100
N	-1.38815100	-0.65805900	-0.29435700
O	-3.17181400	-2.08824300	-0.50097200
N	0.04726100	1.47037000	0.17725000
H	-0.78170300	-3.14047600	-1.66482400
H	1.05383200	-2.22804700	-0.21080300
C	0.16901100	-3.03288400	1.69653800
H	1.13676800	-2.89864400	2.19641300
H	-0.51360200	-2.25601500	2.06774300
H	-0.23719100	-4.00668500	2.00354900
H	0.92019700	-3.87442800	-0.12676800
Pd	0.55439900	-0.46921000	0.06856300
O	2.55352900	-0.19488800	0.54619400
C	3.33456500	-0.03188500	-0.47436100
O	2.95318000	-0.04620500	-1.65249000
C	4.77409000	0.22672600	-0.11852500
H	5.10790700	-0.44533000	0.68011000
H	5.41879600	0.11452300	-0.99557800
H	4.86793700	1.25450700	0.25807000

TS₃₆₋₃₇

E (M06-SMD/BS1) = -1008.084031 au

H (M06-SMD/BS1) = -1007.742553 au

G (M06-SMD/BS1) = -1007.811391 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1008.457194 au

C	1.78133200	-1.89168800	0.15666600
C	0.81635000	-2.87011900	-0.50472500
H	0.99461100	-3.88962200	-0.12698900
C	-0.64906800	-2.54832400	-0.32897900
C	-2.25107400	-0.68077400	-0.06211000
C	-2.82693400	-1.15134200	1.27889200
H	-2.91776200	-2.24287300	1.28578200
H	-3.82042900	-0.71859900	1.45636300
H	-2.16434000	-0.84775200	2.10272800
C	-3.15857600	-1.07818700	-1.22998500
H	-2.75791000	-0.68854500	-2.17583000
H	-4.17514300	-0.68695400	-1.09756700
H	-3.21958900	-2.16838600	-1.29740600
C	-2.14202700	0.83046200	-0.01063400
C	-3.26537100	1.65364500	0.03573100
H	-4.26016500	1.21415400	0.02018800
C	-3.10862200	3.02925000	0.10750800
H	-3.98322600	3.67579400	0.14203300
C	-1.82738000	3.57260400	0.13489200
H	-1.66165800	4.64517600	0.18983600
C	-0.74917700	2.70971900	0.09410500
H	0.27864800	3.06604700	0.11775700
N	-0.89285500	-1.22733400	-0.25775900
O	-1.50795500	-3.44922700	-0.30811600
N	-0.90924400	1.37727600	0.02512200
H	1.00610200	-2.90623100	-1.58928400
H	2.39394100	-0.73716700	-0.42857100
C	1.83773200	-2.00143900	1.67488600
H	2.51563200	-1.24889800	2.10379300
H	0.85234000	-1.86657800	2.14392600
H	2.21144300	-2.99403700	1.97592700
H	2.77832000	-2.19750000	-0.20696500
Pd	0.63678100	0.01630900	-0.02937600
O	2.12550800	1.48939000	0.23037200
C	3.25710600	1.15655600	-0.23049000
O	3.47526100	0.00460000	-0.71443700

C	4.37255000	2.14865700	-0.21751100
H	4.08690400	3.06514400	0.30535200
H	5.25434000	1.70474700	0.25860500
H	4.64715200	2.39006300	-1.25196200

37

E (M06-SMD/BS1) = -1008.11293 au

H (M06-SMD/BS1) = -1007.765456 au

G (M06-SMD/BS1) = -1007.840232 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1008.48581 au

C	1.51838200	-2.02331400	0.21804600
C	0.55386600	-2.95707100	-0.50804200
H	0.63627500	-3.99917400	-0.15414800
C	-0.89368900	-2.51164600	-0.38992400
C	-2.29471800	-0.47617200	-0.14652400
C	-3.06609200	-0.94405400	1.09340200
H	-3.27526200	-2.01721200	1.02133800
H	-4.02083100	-0.41188300	1.19809700
H	-2.46953500	-0.76389200	1.99974000
C	-3.10987500	-0.70285800	-1.42484100
H	-2.56600600	-0.31571000	-2.29789600
H	-4.08421000	-0.20027900	-1.37607900
H	-3.28645700	-1.77304100	-1.57083500
C	-2.03890800	1.02372000	-0.00168400
C	-3.10072100	1.93032300	0.02797300
H	-4.12555800	1.57532500	-0.05727600
C	-2.84526400	3.28596400	0.16856500
H	-3.67005900	3.99597400	0.19145800
C	-1.52943100	3.72689000	0.27844200
H	-1.28670400	4.78082000	0.38820600
C	-0.52424200	2.77763800	0.24827700
H	0.52688300	3.05472200	0.33409400
N	-1.00277000	-1.17722200	-0.23728200
O	-1.83382600	-3.32547800	-0.48242000
N	-0.77223800	1.46590200	0.11462100
H	0.77956300	-2.97962100	-1.58674700
H	2.19427300	0.30826300	-1.64946900
C	1.68990700	-2.38764100	1.67937500
H	2.32184100	-1.66685700	2.21854400
H	0.72058600	-2.43662800	2.20033500
H	2.16231400	-3.38104000	1.78688700

H	2.49818200	-1.98427000	-0.28505100
Pd	0.66642400	-0.16806100	0.14556200
O	2.53052000	0.84891400	0.56269800
C	3.31783500	1.09613900	-0.35586900
O	3.07140100	0.76392900	-1.60817900
C	4.61387400	1.78705500	-0.15535100
H	4.75712400	2.03139600	0.89936400
H	5.42902500	1.14252700	-0.50591000
H	4.63780100	2.70188300	-0.75973800

38

E (M06-SMD/BS1) = -779.1100022 au

H (M06-SMD/BS1) = -778.83203 au

G (M06-SMD/BS1) = -778.892463 au

E (M06-SMD/BS2//M06-SMD/BS1) = -779.3889206 au

C	-2.67880200	-0.93612400	-0.14062700
C	-2.96711500	0.48578300	-0.60759000
H	-3.90770000	0.88162300	-0.18936700
C	-1.83521400	1.43418800	-0.26033100
C	0.62817000	1.48687000	0.08756600
C	0.58203500	2.07876700	1.50143800
H	-0.21782700	2.82461600	1.56865700
H	1.53131000	2.56408100	1.76439900
H	0.38455300	1.28491000	2.23682700
C	0.90014900	2.57211300	-0.96036800
H	0.98961700	2.12467500	-1.95992800
H	1.82658500	3.11845600	-0.74326100
H	0.07686500	3.29256600	-0.97234200
C	1.77220200	0.47351800	0.04589100
C	3.09606200	0.89661700	0.18176400
H	3.32264600	1.95315700	0.30713400
C	4.12341800	-0.03405100	0.16027200
H	5.15663300	0.29203500	0.26447400
C	3.81896500	-1.38287700	0.00376700
H	4.59330300	-2.14548500	-0.02092000
C	2.48738900	-1.73630800	-0.11730600
H	2.18489600	-2.77618800	-0.23721800
N	-0.64104000	0.80341100	-0.21779800
O	-2.02307400	2.65289300	-0.09325000
N	1.49159600	-0.83648900	-0.09433100
H	-3.07566300	0.51995500	-1.70338100

C	-3.12981800	-1.18707200	1.28198800
H	-2.81889700	-2.17437000	1.65376800
H	-2.72875000	-0.42647900	1.97036600
H	-4.23146300	-1.14411900	1.36100700
H	-3.09477000	-1.68952300	-0.82977400
Pd	-0.66402800	-1.18261000	-0.18692000

39

E (M06-SMD/BS1) = -1478.663362 au
H (M06-SMD/BS1) = -1478.172961 au
G (M06-SMD/BS1) = -1478.274095 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1765.613528 au

Pd	-0.05572500	1.21317400	1.04373200
C	1.60306900	2.26614500	0.46441700
C	1.12379300	3.28128600	-0.57329900
H	1.89706400	3.50907000	-1.32593800
C	-0.16029600	2.89035900	-1.27977700
C	-2.25990000	1.61313300	-0.95290700
C	-2.17924800	0.80337500	-2.25475900
H	-1.73516700	1.41288300	-3.04952300
H	-3.17557400	0.47841500	-2.58412500
H	-1.55987400	-0.09490800	-2.11168800
C	-3.19616900	2.81574500	-1.11348400
H	-3.28417400	3.35926300	-0.16234700
H	-4.20146300	2.50809800	-1.42862400
H	-2.79706100	3.49955400	-1.86997900
C	-2.83095000	0.68596100	0.11898300
C	-4.12338500	0.16798300	0.00021000
H	-4.74612000	0.44121300	-0.84920700
C	-4.60888800	-0.70024500	0.96635200
H	-5.61496200	-1.10632200	0.87835700
C	-3.79780600	-1.04591600	2.04391300
H	-4.13870800	-1.72502000	2.82137900
C	-2.52728200	-0.50100000	2.09900400
H	-1.83979400	-0.73766400	2.91230200
N	-0.92508400	2.07482900	-0.53132600
O	-0.44651000	3.34895900	-2.40585400
N	-2.05913300	0.34045800	1.16543000
H	0.90431600	4.24038500	-0.07010400
H	2.24361100	1.50935900	-0.02351000
C	2.35370700	2.91796100	1.60585600

H	2.79342600	2.18434400	2.29566000
H	3.18257900	3.54311900	1.22595100
H	1.69970400	3.57979000	2.19514900
C	2.07411700	-0.99972900	-1.25814700
C	3.40726300	-1.37867700	-1.19214700
C	4.30954600	-0.73819000	-2.03938200
C	3.86796200	0.23791100	-2.92868500
C	2.52036300	0.58469900	-2.98287800
C	1.60388300	-0.03094100	-2.13450100
H	3.74328600	-2.14634400	-0.49818000
H	5.36170300	-1.01446700	-2.00398100
H	4.58075600	0.73159700	-3.58669600
H	2.17214700	1.35066200	-3.67414700
H	0.55528300	0.25971000	-2.15001600
I	0.70546400	-1.88458000	0.11867100
O	-0.40198300	-2.38364700	-1.66627400
C	-1.60872600	-2.77628400	-1.32624500
O	-1.94357500	-2.92896200	-0.15352700
O	2.18392800	-1.26815100	1.72511300
C	1.88915200	-0.48341400	2.70233700
O	0.93456300	0.32156800	2.74436000
C	2.81683000	-0.58727100	3.87718200
H	2.55300600	0.13934100	4.65085900
H	2.77472100	-1.60246300	4.29015800
H	3.84727300	-0.41372000	3.54345700
C	-2.52375100	-3.03773500	-2.48213700
H	-2.60089100	-4.12280300	-2.62872200
H	-3.52376200	-2.66076600	-2.23975300
H	-2.15914200	-2.58167000	-3.40667400

TS₃₉₋₄₀

E (M06-SMD/BS1) = -1478.655863 au
H (M06-SMD/BS1) = -1478.168355 au
G (M06-SMD/BS1) = -1478.264828 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1765.602163 au

Pd	-0.50273900	-1.58511000	-0.24210200
C	0.87375500	-2.70308900	0.77386900
C	0.89109800	-2.17899900	2.20681600
H	1.71932200	-1.46450800	2.34533200
C	-0.36330300	-1.43059800	2.62318000
C	-2.31086900	-0.19051800	1.72297900

C	-1.87573600	1.16366100	2.30549700
H	-1.45510900	1.02482900	3.30718500
H	-2.72417600	1.85655800	2.38137300
H	-1.11023800	1.62912400	1.66647600
C	-3.37931800	-0.85132700	2.60093300
H	-3.71701300	-1.79276900	2.14532300
H	-4.25306500	-0.20063500	2.73476100
H	-2.96270700	-1.07219300	3.58931600
C	-2.91051600	0.07876000	0.34191200
C	-4.06168700	0.85815400	0.20278200
H	-4.55961200	1.26252700	1.08160900
C	-4.56419400	1.12452500	-1.06219700
H	-5.45966500	1.73299100	-1.17480600
C	-3.91161000	0.61381600	-2.18110700
H	-4.26926600	0.80558600	-3.18958500
C	-2.77746900	-0.15087500	-1.97435800
H	-2.21619400	-0.57920500	-2.80586600
N	-1.14608400	-1.08430400	1.58364200
O	-0.56303400	-1.15117400	3.82238600
N	-2.29863800	-0.41498000	-0.74983700
H	1.07384600	-2.98772800	2.93568100
H	1.85278500	-2.58193600	0.28591700
C	0.39857700	-4.13805400	0.68065900
H	0.32646200	-4.49118800	-0.35761800
H	1.09709000	-4.81276100	1.20804800
H	-0.58775800	-4.26942700	1.15244700
C	2.59541800	1.04030900	0.28245200
C	3.80701800	1.09822300	-0.39718000
C	4.97789600	1.09732600	0.35601500
C	4.91899600	1.04700600	1.74708800
C	3.69186400	1.00039900	2.40355700
C	2.50806700	0.99539700	1.67094000
H	3.84033200	1.14092000	-1.48342500
H	5.93976000	1.13986400	-0.15141700
H	5.84072400	1.04648500	2.32601900
H	3.64914300	0.96372300	3.49048100
H	1.54149700	0.95780100	2.17357400
I	0.76918400	1.07035400	-0.79233500
O	0.67477800	3.18433600	-0.17068900
C	-0.54299300	3.60221400	-0.40651600
O	-1.39075000	2.90213900	-0.95822100

O	1.97571500	-0.90647400	-2.03232700
C	1.31949000	-1.85012800	-2.53853000
O	0.18027800	-2.25060700	-2.13532600
C	1.92154400	-2.60740400	-3.69281000
H	1.14382700	-2.93387500	-4.39143400
H	2.67039200	-2.00496600	-4.21543500
H	2.41371900	-3.50633300	-3.29778000
C	-0.81681700	4.98647500	0.10003100
H	0.06060500	5.63136600	-0.00562400
H	-1.67365200	5.41421100	-0.42818800
H	-1.05991400	4.91542300	1.16875300

40

E (M06-SMD/BS1) = -1478.672403 au

H (M06-SMD/BS1) = -1478.185522 au

G (M06-SMD/BS1) = -1478.285741 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1765.612048 au

Pd	0.96978400	0.70921200	0.62575000
C	0.25619100	0.41928900	2.57292100
C	0.56317800	-1.01271300	2.94170100
H	-0.32153600	-1.65466100	2.82250900
C	1.68105900	-1.64039900	2.12774800
C	3.06501800	-1.36297200	0.07341600
C	2.52647200	-2.56687900	-0.70390700
H	2.28316200	-3.38179900	-0.01250800
H	3.26818300	-2.93738400	-1.42337800
H	1.61992700	-2.29173100	-1.26285100
C	4.38010200	-1.70038300	0.78862800
H	4.75137500	-0.82273500	1.33539500
H	5.14535600	-2.00504600	0.06437500
H	4.23178500	-2.52005100	1.49552800
C	3.34984900	-0.23416500	-0.90712100
C	4.33754700	-0.36534700	-1.88452800
H	4.90630400	-1.28830300	-1.96695000
C	4.59474400	0.69098400	-2.74465600
H	5.36454500	0.59528500	-3.50823800
C	3.86835300	1.87157100	-2.61745300
H	4.04851800	2.72601100	-3.26455200
C	2.89126100	1.93017300	-1.64180400
H	2.27785800	2.81833300	-1.50050800
N	2.05942700	-0.90012400	1.05737900

O	2.15460900	-2.73629000	2.45417800
N	2.63531600	0.90147600	-0.81913900
H	0.85272300	-1.07386000	4.00353500
H	-0.81132600	0.66726600	2.56208600
C	1.09173400	1.45716800	3.26338200
H	0.94053600	2.46706000	2.86150600
H	0.78751400	1.48738800	4.32517400
H	2.16342800	1.21436900	3.24105400
C	-2.67198400	0.21831600	0.39850200
C	-3.16966200	1.18380000	-0.46794700
C	-4.29368200	1.90242500	-0.06803400
C	-4.89048900	1.64781900	1.16424200
C	-4.37465200	0.66867000	2.00946300
C	-3.25167800	-0.06327600	1.63092700
H	-2.69318100	1.38154300	-1.42634500
H	-4.69972500	2.66659400	-0.72878500
H	-5.76797400	2.21604600	1.46781200
H	-4.84648000	0.46631500	2.96941900
H	-2.84503300	-0.83713500	2.28045600
I	-0.98999700	-0.93522700	-0.19954700
O	-2.77388100	-2.47871400	-0.92911700
C	-3.26818600	-2.20715300	-2.08851200
O	-2.89025900	-1.29744300	-2.83691900
O	-0.08753100	2.47756200	0.37573400
C	-0.48374900	2.83723300	-0.80075600
O	-0.29259300	2.19282400	-1.84062300
C	-1.19639600	4.16630400	-0.83291900
H	-0.44883000	4.97092700	-0.85805400
H	-1.81847600	4.24513000	-1.73115500
H	-1.81010500	4.31034700	0.06347000
C	-4.40373700	-3.12238500	-2.49855300
H	-5.25732700	-2.97028100	-1.82579600
H	-4.71506200	-2.91615800	-3.52764600
H	-4.10006300	-4.17168000	-2.40621100

TS₄₀₋₄₁

E (M06-SMD/BS1) = -1478.672267 au

H (M06-SMD/BS1) = -1478.183104 au

G (M06-SMD/BS1) = -1478.287105 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1765.611033 au

Pd 0.98264400 -0.50244100 -0.60447600

C	0.33886500	0.03692900	-2.55245700
C	0.57604900	1.51857900	-2.68841800
H	-0.34795100	2.09114800	-2.52934700
C	1.62433200	2.07135400	-1.73467100
C	3.04674900	1.45930700	0.22976200
C	2.40034600	2.30323900	1.33138400
H	2.02560400	3.24393000	0.90728600
H	3.12403900	2.54409700	2.12153200
H	1.55980100	1.76135900	1.78914000
C	4.27473300	2.16340300	-0.35780200
H	4.70475900	1.56775700	-1.17469000
H	5.04375500	2.29849400	0.41172100
H	4.00498900	3.14768500	-0.74575800
C	3.49472200	0.13103200	0.82942900
C	4.55260700	0.05410300	1.73447900
H	5.08207400	0.95462000	2.03731500
C	4.92827800	-1.18010300	2.24423500
H	5.75703800	-1.24746600	2.94642700
C	4.24601100	-2.32667000	1.84716400
H	4.51886500	-3.31130200	2.21738800
C	3.18793100	-2.18127800	0.96930800
H	2.60200600	-3.03492400	0.63078800
N	2.05469900	1.16481600	-0.82614200
O	2.00763900	3.24198200	-1.83860600
N	2.82453100	-0.98425100	0.48639300
H	0.91678100	1.74483300	-3.71237600
H	-0.71148500	-0.27350600	-2.59553300
C	1.25268100	-0.85615600	-3.32994400
H	1.15234500	-1.91433600	-3.05627700
H	0.96522400	-0.77422100	-4.39421500
H	2.30534900	-0.55331100	-3.25086700
C	-2.70844200	-0.23475300	-0.53420900
C	-3.15827700	-1.36416300	0.14038000
C	-4.21436500	-2.08217900	-0.41453100
C	-4.79846900	-1.66472300	-1.60851500
C	-4.33523700	-0.52425900	-2.25877500
C	-3.27717200	0.20769000	-1.72368400
H	-2.70085000	-1.67907300	1.07698200
H	-4.57931400	-2.97231100	0.09547200
H	-5.62419200	-2.23217300	-2.03394300
H	-4.79699400	-0.19486700	-3.18779800

H	-2.91271700	1.10471900	-2.22174600
I	-1.11465100	0.89417500	0.30463500
O	-3.09162600	2.16881500	1.27937400
C	-3.58166900	1.63189800	2.33759100
O	-3.14187600	0.62234500	2.91039200
O	-0.00246700	-2.32671800	-0.57182200
C	-0.30553300	-2.82791000	0.58139600
O	-0.08566200	-2.27422500	1.66719700
C	-0.93677800	-4.19477500	0.51912700
H	-0.13918000	-4.94905500	0.47133000
H	-1.53199600	-4.38312100	1.41893500
H	-1.55889500	-4.30976800	-0.37524700
C	-4.81504600	2.33182200	2.87685900
H	-5.63374100	2.23943800	2.15177500
H	-5.12895000	1.89416400	3.83004500
H	-4.61809900	3.40232700	3.00924900

41

E (M06-SMD/BS1) = -1478.684728 au
H (M06-SMD/BS1) = -1478.194124 au
G (M06-SMD/BS1) = -1478.299778 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1765.621111 au

Pd	0.94236000	0.17569300	0.12181300
C	0.87816700	-0.08922400	2.26591800
C	1.18962100	-1.54574100	2.42687400
H	0.30191400	-2.16605100	2.24796400
C	2.29320500	-1.93162200	1.45297800
C	3.04346400	-1.45210800	-0.87711200
C	2.33125700	-1.43667600	-2.23599300
H	1.84290500	-2.40759100	-2.39650600
H	3.06037700	-1.27281800	-3.04061300
H	1.56669900	-0.65110500	-2.31246000
C	4.03179900	-2.61534900	-0.89860900
H	4.75374500	-2.58040700	-0.07983000
H	4.57521700	-2.60928900	-1.85272600
H	3.47970500	-3.56136100	-0.83729300
C	3.71016300	-0.10175600	-0.66476700
C	5.01951700	0.20369700	-1.01102300
H	5.66495700	-0.56570100	-1.42846100
C	5.48908100	1.49820400	-0.81726700
H	6.51560400	1.74741100	-1.07818800

C	4.64376300	2.46956200	-0.29281000
H	4.97613500	3.49178100	-0.13422600
C	3.34550400	2.11092500	0.02950500
H	2.63007900	2.82325600	0.43787200
N	2.00140800	-1.55580600	0.17256600
O	3.30920700	-2.51464700	1.82588800
N	2.91164800	0.85877000	-0.15059200
H	1.54683600	-1.72965300	3.45071400
H	-0.17378500	0.20267300	2.37041000
C	1.84742300	0.87310600	2.84309600
H	1.68265900	1.90305900	2.50699600
H	1.66432100	0.86257300	3.93334000
H	2.89240300	0.57752200	2.68347100
C	-2.72103200	0.38811100	0.50323100
C	-3.14128200	1.37749400	-0.37779200
C	-4.02277400	2.34731300	0.09518600
C	-4.46675200	2.31069900	1.41522500
C	-4.03559000	1.30345200	2.27505000
C	-3.15104300	0.32569100	1.82353000
H	-2.79214400	1.39554500	-1.40911500
H	-4.36100800	3.13412900	-0.57728000
H	-5.15629400	3.07184000	1.77597000
H	-4.38726300	1.27144900	3.30477500
H	-2.81393800	-0.47032700	2.48567100
I	-1.38444900	-1.11119900	-0.19402100
O	-4.16469000	-2.23274800	-0.39843100
C	-4.76869500	-1.49130900	-1.22822700
O	-4.30633900	-1.08391700	-2.32169000
O	0.05786600	2.05522500	0.18862800
C	-0.05058600	2.47417300	-1.02814800
O	0.30655300	1.79021800	-2.00299000
C	-0.60328300	3.85851500	-1.20268000
H	0.23407700	4.55126300	-1.36313300
H	-1.24325200	3.89877800	-2.09120300
H	-1.16164400	4.18896400	-0.32103600
C	-6.15866100	-1.02066900	-0.82448100
H	-6.05528600	-0.19377400	-0.10554600
H	-6.73030600	-0.65475500	-1.68483200
H	-6.71722000	-1.81850500	-0.32020900

E (M06-SMD/BS1) = -1594.359776 au
 H (M06-SMD/BS1) = -1593.81243 au
 G (M06-SMD/BS1) = -1593.923189 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -1881.344118 au

Pd	-0.66778700	-0.12458800	0.05936500
C	-0.69931700	2.21809700	0.44470100
C	-1.14739000	2.61193800	-0.91623300
H	-0.32007900	2.57029800	-1.63640600
C	-2.30343500	1.71158100	-1.36036600
C	-2.97389400	-0.67428500	-1.47936700
C	-2.26610100	-1.96150300	-1.92492600
H	-1.90882900	-1.83683000	-2.95662800
H	-2.96829200	-2.80530300	-1.89490800
H	-1.40380600	-2.21785400	-1.29205800
C	-4.10989000	-0.41578900	-2.46437100
H	-4.81562600	0.34040700	-2.11437700
H	-4.65216600	-1.35283700	-2.64784900
H	-3.68896200	-0.08250800	-3.42147500
C	-3.44484700	-0.85422800	-0.04639400
C	-4.70768000	-1.28430000	0.33577500
H	-5.46384700	-1.48270500	-0.42015800
C	-4.98663200	-1.45502200	1.68742700
H	-5.97461200	-1.78688900	1.99999500
C	-4.00047600	-1.20145100	2.63424400
H	-4.18331400	-1.32782100	3.69781500
C	-2.75658100	-0.77742600	2.19743100
H	-1.94009600	-0.56310000	2.88543900
N	-1.95180500	0.39940700	-1.42519600
O	-3.41096000	2.18747100	-1.60625000
N	-2.50562300	-0.61045900	0.89387000
H	-1.52788800	3.64219800	-0.86949600
H	0.37165700	2.11740000	0.66023100
C	-1.61164500	2.39152400	1.58542700
H	-1.30583100	1.81365500	2.46453100
H	-1.53649400	3.45949100	1.85829100
H	-2.66388900	2.20698400	1.33374100
C	2.51124700	-1.68351800	-0.72468600
C	2.33055000	-2.93034500	-1.31148300
C	2.95891000	-4.02875300	-0.72881700
C	3.74119900	-3.86608100	0.41169400
C	3.90620700	-2.60429900	0.97754500

C	3.28730800	-1.49113300	0.41143800
H	1.70474800	-3.04850000	-2.19476900
H	2.82963300	-5.01538000	-1.17052400
H	4.22616300	-4.72965200	0.86344100
H	4.51489200	-2.47881400	1.87179900
H	3.38694100	-0.50264700	0.85979300
I	1.50073700	-0.00978100	-1.57663600
O	2.66006000	3.35164900	-0.40598400
C	3.15668600	2.49985500	0.39037600
O	2.53549100	1.92884000	1.32347900
O	0.42946500	-0.59914600	1.75011000
C	0.50236700	-1.87410400	1.96016100
O	0.01870400	-2.72764700	1.20264200
C	1.17432500	-2.25975600	3.24962500
H	0.43187200	-2.19767000	4.05798400
H	1.54334300	-3.28940600	3.20090300
H	1.99245900	-1.57420700	3.49681000
C	4.60583700	2.12012500	0.15352100
H	5.18572200	2.97796300	-0.20667200
H	5.07030500	1.71052000	1.05784500
H	4.64518800	1.34641500	-0.62832800
C	0.92915000	4.76869700	1.99727600
H	1.93301400	5.22244900	2.02862900
H	0.22691000	5.46224300	2.47683400
H	0.95947000	3.84153900	2.59518700
O	0.50234200	4.54178100	0.67388800
H	1.25636700	4.08485300	0.21150200

42

E (M06-SMD/BS1) = -1365.443307 au

H (M06-SMD/BS1) = -1364.961359 au

G (M06-SMD/BS1) = -1365.058313 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1652.328603 au

Pd	-0.29635400	-0.12985400	0.08968900
C	-1.77171800	2.69533800	0.87604500
C	-2.05844300	2.47700700	-0.60770800
H	-1.14205100	2.67952900	-1.17664700
C	-2.60355000	1.10130200	-0.94439500
C	-2.18990500	-1.17233000	-1.72763800
C	-1.02260300	-1.95114900	-2.35145300
H	-0.69595400	-1.44061900	-3.26858400

H	-1.34335600	-2.96911900	-2.61201900
H	-0.15922600	-2.02708200	-1.67544900
C	-3.31577600	-1.15881600	-2.75792200
H	-4.26300500	-0.79973600	-2.34967700
H	-3.46303000	-2.16659500	-3.16861800
H	-3.02515600	-0.50252900	-3.58933700
C	-2.55707000	-1.84333900	-0.42106300
C	-3.57627000	-2.76690900	-0.23326100
H	-4.21440900	-3.04798400	-1.06814900
C	-3.76953900	-3.31588200	1.02967700
H	-4.56819300	-4.03688500	1.19268500
C	-2.94209500	-2.93610800	2.08128400
H	-3.06713000	-3.34184200	3.08157400
C	-1.93684300	-2.01610900	1.83262400
H	-1.25202700	-1.67701800	2.60849300
N	-1.69199700	0.18449500	-1.38802600
O	-3.82301600	0.89908800	-0.83712300
N	-1.75906500	-1.49715700	0.61178500
H	-2.81720100	3.20999800	-0.92052600
H	-1.03169600	1.94178300	1.21890900
C	-3.01006200	2.59497500	1.74313700
H	-2.78064700	2.80701300	2.79500500
H	-3.77924700	3.30296400	1.40301600
H	-3.42987000	1.58133200	1.69750200
C	3.18599100	0.12671700	-0.62791700
C	3.36820700	-0.85595800	-1.59391500
C	4.36309400	-1.80955400	-1.38693100
C	5.14391400	-1.77224900	-0.23436100
C	4.94114000	-0.77727000	0.71809700
C	3.95307500	0.18765900	0.52865300
H	2.74210600	-0.88745900	-2.48445500
H	4.52008600	-2.58779800	-2.13199100
H	5.91548300	-2.52403100	-0.07787000
H	5.54936800	-0.74848800	1.62101300
H	3.77976600	0.96050900	1.27566700
I	1.59759400	1.53508000	-0.88430400
O	0.90072400	-0.52665500	1.73832300
C	1.53482000	-1.65393100	1.73919000
O	1.49651200	-2.48758900	0.82324700
C	2.31277900	-1.92999300	3.00082100
H	1.63066200	-2.37241400	3.74067300

H	3.11870600	-2.64598800	2.80777800
H	2.72180900	-1.01066300	3.43447400
C	-0.44898300	4.18507400	2.15733700
H	0.07187600	5.14444700	2.06493100
H	-1.10656900	4.23118000	3.03970700
H	0.29941800	3.38914300	2.31941500
O	-1.16099900	3.97642800	0.96014700

43

E (M06-SMD/BS1) = -930.4838017 au

H (M06-SMD/BS1) = -930.186073 au

G (M06-SMD/BS1) = -930.251745 au

E (M06-SMD/BS2//M06-SMD/BS1) = -930.8216598 au

C	-2.33569200	2.15883600	-0.23277600
C	-1.38558100	1.15756800	-0.07661900
C	-1.85479200	-0.19380000	0.04774100
C	-3.24359800	-0.48331800	0.01152500
C	-4.17305200	0.56993600	-0.14612900
C	-3.71171500	1.85795700	-0.26384600
H	-2.00767600	3.18721400	-0.33211400
C	-3.63535300	-1.83726900	0.13241600
H	-5.23721500	0.33883400	-0.17428700
H	-4.41779900	2.67804000	-0.38841400
C	-2.68893300	-2.81906800	0.28028500
C	-1.33256900	-2.44689300	0.31052400
H	-4.69754300	-2.08060000	0.10488000
H	-2.96271200	-3.86695700	0.37453200
H	-0.54973700	-3.19743700	0.43109800
N	-0.93158800	-1.19468300	0.20068100
N	-0.00316400	1.32654700	-0.02331400
C	0.66769500	2.51120700	-0.00599200
C	2.14980200	2.30730800	0.21137400
H	2.70592400	3.13490500	-0.25947100
H	2.31187200	2.41675500	1.29896100
C	2.64633700	0.93560300	-0.23514800
H	2.74942100	0.91890100	-1.33482900
C	3.95244000	0.54638000	0.41777100
H	3.83931800	0.41163000	1.50488400
H	4.37363700	-0.37965600	0.00013600
H	4.71576900	1.33201100	0.27225800
O	0.16020800	3.63726300	-0.09702000

Pd	1.08706800	-0.34671900	0.07775200
O	2.23236600	-2.18035500	0.20812200
H	3.05661800	-2.02893600	0.70109700
C	2.55498400	-2.73809700	-1.07063500
H	1.60524100	-2.93905400	-1.57585200
H	3.14713100	-2.03589700	-1.67242200
H	3.10547600	-3.67708800	-0.94036700

44

E (M06-SMD/BS1) = -1502.937736 au
H (M06-SMD/BS1) = -1502.433864 au
G (M06-SMD/BS1) = -1502.524366 au
E (M06-SMD/BS2//M06-SMD/BS1) = -1503.479093 au

C	-4.03933800	0.25381100	0.32207300
C	-2.66899600	0.41114500	0.49274400
C	-1.94720800	-0.66648500	1.11286300
C	-2.62662600	-1.83241700	1.55507300
C	-4.02093800	-1.94801100	1.35332500
C	-4.69680800	-0.91810300	0.74559700
H	-4.60674600	1.04999300	-0.14623400
C	-1.85760800	-2.84827200	2.16996900
H	-4.53204600	-2.85157800	1.68382500
H	-5.77104300	-0.99604700	0.58233500
C	-0.50305400	-2.69102500	2.32330100
C	0.09466400	-1.51128400	1.84367600
H	-2.36154400	-3.75087000	2.51650900
H	0.11110200	-3.45325000	2.79628500
H	1.17168300	-1.35641400	1.94125000
N	-0.59040400	-0.54517800	1.26085600
N	-1.90669000	1.51423400	0.12216200
C	-2.37229600	2.68622700	-0.38555500
C	-1.25245200	3.68498500	-0.57417700
H	-1.53162600	4.40404600	-1.36225500
H	-1.20399900	4.26779500	0.36362400
C	0.10459600	3.03405200	-0.83235900
H	0.14476500	2.68593500	-1.87930300
C	1.25688600	3.96881200	-0.55065700
H	1.29825800	4.25445200	0.51239500
H	2.22662700	3.52695500	-0.81787300
H	1.15410500	4.90649100	-1.12669700
O	-3.55686200	2.96267700	-0.62392400

Pd	0.08893200	1.28077200	0.23764800
C	2.98611400	-1.95531000	-1.72302700
C	2.35322100	-0.82097200	-1.26205300
C	2.82699700	-0.17882900	-0.07807900
C	3.98413700	-0.71252200	0.55946200
C	4.59193000	-1.89014500	0.06580300
C	4.08776900	-2.51196600	-1.04674800
H	2.63589500	-2.40741400	-2.64934400
C	4.49763200	-0.04303900	1.69211900
H	5.46687300	-2.27965000	0.58490300
H	4.55390400	-3.41403100	-1.43732100
C	3.88374200	1.09438900	2.14550800
C	2.72338500	1.53507300	1.48956500
H	5.38340600	-0.44396600	2.18377900
H	4.25545100	1.64625000	3.00473400
H	2.19393200	2.41514600	1.85348900
N	2.19258900	0.92519300	0.43693900
N	1.29425900	-0.25058600	-2.00152800
H	1.36057400	0.74601400	-2.20031900
C	0.06791900	-0.78189100	-2.29588500
C	-0.22194100	-2.19502200	-1.86219600
H	0.34550400	-2.88399900	-2.50817400
H	0.17492800	-2.35197900	-0.84544000
C	-1.70262800	-2.53785700	-1.92050800
H	-2.06220500	-2.43317000	-2.95410300
H	-2.27168400	-1.80702500	-1.32389800
C	-1.96915200	-3.94261400	-1.41169600
H	-1.60691600	-4.06605900	-0.37961800
H	-3.04232700	-4.17466400	-1.41746100
H	-1.45950700	-4.69564800	-2.03012400
O	-0.75891200	-0.09453400	-2.89790300

45

E (M06-SMD/BS1) = -1502.919763 au
 H (M06-SMD/BS1) = -1502.415861 au
 G (M06-SMD/BS1) = -1502.510273 au
 E (M06-SMD/BS2//M06-SMD/BS1) = -1503.461371 au

C	-5.62935000	-0.26338800	0.06070800
C	-4.26184400	-0.09383800	-0.11638800
C	-3.74630000	1.24612300	-0.08131900
C	-4.61514200	2.35058400	0.12071700

C	-6.00057200	2.12765000	0.29129900
C	-6.48037900	0.84159700	0.26003600
H	-6.04420800	-1.26475400	0.04428100
C	-4.03947200	3.64259000	0.14658800
H	-6.66011800	2.98033300	0.44812000
H	-7.54538700	0.65611900	0.39440700
C	-2.68708500	3.79861500	-0.02003100
C	-1.89629400	2.65161000	-0.21559700
H	-4.68942100	4.50394700	0.30097000
H	-2.21919100	4.77982300	-0.00485600
H	-0.81738100	2.73570200	-0.35488300
N	-2.39887000	1.43225200	-0.24627600
N	-3.32154400	-1.09955900	-0.33028600
C	-3.58443700	-2.41792200	-0.53960100
C	-2.33095300	-3.18261500	-0.89726200
H	-2.44000200	-4.23401200	-0.58283500
H	-2.29535600	-3.20107200	-2.00160500
C	-1.05319800	-2.54021100	-0.36479900
H	-0.95231500	-2.76193600	0.71276700
C	0.17666300	-2.99882800	-1.11465500
H	0.17019000	-2.64595100	-2.15765100
H	1.11177600	-2.65343600	-0.65128300
H	0.22544600	-4.10231800	-1.14893600
O	-4.70115000	-2.95398000	-0.50805100
Pd	-1.40280700	-0.52425400	-0.38276300
C	4.40808000	-1.44270100	0.90780000
C	4.13365000	-0.39662700	0.05519600
C	5.18994600	0.43723300	-0.41777900
C	6.51016500	0.19606000	0.04926500
C	6.75422300	-0.85511500	0.96410300
C	5.72077700	-1.65753800	1.37736500
H	3.61324600	-2.12333100	1.20737500
C	7.53334900	1.04087500	-0.43944600
H	7.77158100	-1.01953600	1.31804400
H	5.90520400	-2.48251500	2.06265600
C	7.22131000	2.03217600	-1.33334500
C	5.87811600	2.17517600	-1.74117000
H	8.55686800	0.88552600	-0.09826900
H	7.98192000	2.69949400	-1.73187000
H	5.61643200	2.95453500	-2.45966400
N	4.89110600	1.41928600	-1.30776400

N	2.84875600	-0.13576700	-0.45807200
H	2.83691300	0.24562400	-1.40440600
C	1.63520400	-0.16447300	0.13227100
C	1.50993700	-0.44853800	1.59897500
H	1.26739600	-1.51794000	1.72073800
H	2.48150200	-0.29722200	2.08744700
C	0.45353000	0.40331600	2.29644900
H	-0.53987600	0.18592500	1.87320300
H	0.65355000	1.46812600	2.09910900
C	0.44657200	0.13732800	3.79073100
H	1.41899900	0.37484900	4.24498100
H	-0.31603000	0.74070100	4.29922700
H	0.23207400	-0.92023300	4.00198200
O	0.64992200	0.09159200	-0.59643000

TS^{OMe}₁₈₋₁₉

E (M06-SMD/BS1) = -1360.53033543 au

H (M06-SMD/BS1) = -1360.143034 au

G (M06-SMD/BS1) = -1360.230451 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.41281255 au

C	-3.59499100	1.25130200	1.50901800
C	-2.61915600	0.73667600	0.66745100
C	-2.16198500	1.55457300	-0.41811300
C	-2.70687700	2.85124700	-0.61266700
C	-3.70084500	3.33461600	0.26646600
C	-4.12449600	2.53989700	1.30097600
H	-3.95782500	0.64902200	2.33279800
C	-2.21949000	3.60898000	-1.70378600
H	-4.11400200	4.32913500	0.10441600
H	-4.89143500	2.89726000	1.98612900
C	-1.25934600	3.08989400	-2.53375700
C	-0.77209900	1.79649200	-2.26950900
H	-2.62363800	4.60756700	-1.86844700
H	-0.87109600	3.65058300	-3.38006800
H	-0.01062700	1.34455500	-2.90720500
N	-1.20128200	1.06989400	-1.25840000
N	-2.04673200	-0.53738600	0.80295600
C	-2.24967600	-1.45868900	1.80152600
C	-1.32827000	-2.64915400	1.69655500
H	-1.84272300	-3.53369200	2.10097300
H	-0.46938200	-2.45817600	2.36078100

C	-0.87250400	-2.90379200	0.27872200
H	-1.68982700	-3.33305000	-0.31316000
C	0.42045600	-3.63264600	0.08917300
H	1.24505800	-3.16861400	0.64725000
H	0.69908900	-3.69795000	-0.97263000
H	0.31101400	-4.66758300	0.45760800
O	-3.06786900	-1.31301100	2.70594800
Pd	-0.73542700	-1.04220500	-0.62179800
C	4.86265200	0.81036000	-0.79242200
C	3.82003400	0.73266400	0.13434200
C	2.65359600	0.08876600	-0.26689300
C	2.50868200	-0.48121400	-1.52451100
C	3.56781300	-0.38812700	-2.42577100
C	4.74278100	0.26101200	-2.06144200
H	5.77725400	1.31438700	-0.48509500
H	1.59806600	-0.99967600	-1.82803200
H	3.46331800	-0.83080500	-3.41474000
H	5.56876100	0.33321500	-2.76640800
I	1.02969700	0.00412400	1.14495000
C	4.00715500	1.32115400	1.51367300
O	5.06606200	1.92004600	1.76624900
O	3.04660600	1.14512900	2.32863600
O	-1.47141300	-1.70359300	-2.36946400
C	-2.01365800	-2.95119000	-2.66367700
H	-1.35840700	-3.79640700	-2.38670600
H	-2.19496800	-3.01104400	-3.75012100
H	-2.99258100	-3.09892500	-2.17199700

19^{OMe}

E (M06-SMD/BS1) = -1360.53508673 au

H (M06-SMD/BS1) = -1360.146486 au

G (M06-SMD/BS1) = -1360.235246 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1647.41641234 au

C	-4.16559600	0.39003700	-1.35367700
C	-2.97579600	0.14942600	-0.68253900
C	-2.69406700	-1.18960200	-0.25264300
C	-3.60164400	-2.23711300	-0.56008900
C	-4.78882500	-1.95330100	-1.27120400
C	-5.05553500	-0.66129200	-1.64643100
H	-4.39912000	1.39700600	-1.67840300
C	-3.26920900	-3.54048300	-0.12273000

H	-5.47441700	-2.76712700	-1.50281100
H	-5.97049900	-0.42602400	-2.18743200
C	-2.11065500	-3.75996100	0.57746300
C	-1.27740700	-2.66133100	0.85759400
H	-3.95077900	-4.35910300	-0.35256000
H	-1.83029900	-4.75180000	0.92234200
H	-0.35170300	-2.79380300	1.41995300
N	-1.55988700	-1.43578400	0.46559100
N	-2.01776800	1.13468900	-0.40721700
C	-1.98477000	2.44228600	-0.82884400
C	-0.81078900	3.21280300	-0.27910800
H	-1.10158700	4.26742800	-0.16298000
H	-0.01471400	3.18514300	-1.04071800
C	-0.31589700	2.65734100	1.03182800
H	-1.01238800	2.86092100	1.85437000
C	1.10993500	2.89724000	1.40072900
H	1.80454400	2.69424400	0.57617100
H	1.41222200	2.31818500	2.28485700
H	1.21756000	3.96139400	1.67715000
O	-2.79424800	2.91371900	-1.62106400
Pd	-0.63062200	0.59559800	0.90009400
C	5.06366000	-1.07904200	0.53080800
C	4.06263200	-0.66399100	-0.35422100
C	2.77639900	-0.52947000	0.16273700
C	2.47956100	-0.79825200	1.49499400
C	3.49729700	-1.22055900	2.34652300
C	4.79331900	-1.36108300	1.86236600
H	6.07216300	-1.17936000	0.13387000
H	1.46869600	-0.69694300	1.89304000
H	3.26557300	-1.43898400	3.38758800
H	5.59268700	-1.69140700	2.52317700
I	1.17996300	0.14733800	-1.11641200
C	4.43914600	-0.41233400	-1.80627900
O	5.65482900	-0.31273400	-2.07006700
O	3.48473900	-0.33847000	-2.62855600
O	-1.99450400	0.80846300	2.36479400
C	-1.28700200	0.44311900	3.50759400
H	-0.86529900	-0.58052300	3.43793000
H	-1.98831900	0.43455800	4.36097700
H	-0.47525300	1.15295000	3.76026800

TS^α₁₅₋₁₆

E (M06-SMD/BS1) = -1043.75477998 au

H (M06-SMD/BS1) = -1043.451449 au

G (M06-SMD/BS1) = -1043.521142 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1044.13672027 au

C	2.66119500	-2.26790100	-0.03478000
C	1.78901600	-1.21416100	0.15640000
C	2.28661400	0.11643800	0.08412100
C	3.65918600	0.36673600	-0.14329800
C	4.52893600	-0.73497300	-0.32355200
C	4.02802700	-2.01464400	-0.27815800
H	2.29563600	-3.29044800	0.02191400
C	4.07189300	1.71840000	-0.20164900
H	5.58549400	-0.54793700	-0.50954200
H	4.69584000	-2.86184200	-0.42489500
C	3.15210400	2.72647400	-0.05005600
C	1.79961500	2.39843400	0.15573600
H	5.12419800	1.94310000	-0.37337200
H	3.44295900	3.77263400	-0.09312400
H	1.04021200	3.17114400	0.26743700
N	1.38348300	1.14659900	0.21844700
N	0.44003000	-1.30578300	0.50389800
C	-0.51183400	-2.12512600	-0.05053200
C	-1.85931000	-1.52818500	0.30564000
O	-0.31334000	-3.12138200	-0.74114600
Pd	-0.55290300	0.37252400	0.31196300
O	-1.68473000	2.12309300	0.04531300
C	-2.87030800	1.86414800	-0.32048200
O	-3.31232700	0.68215200	-0.45433200
C	-3.80320100	2.99592100	-0.60476900
H	-4.65352200	2.94313000	0.08607900
H	-4.20247600	2.89350500	-1.62072000
H	-3.30412400	3.96272800	-0.49884000
H	-2.38264600	-0.21932400	-0.04967300
C	-3.02919000	-2.20828000	-0.41199700
H	-3.15370900	-1.79660800	-1.42477300
H	-2.74689000	-3.26256200	-0.54853000
C	-4.33303600	-2.13426200	0.36205800
H	-4.22853700	-2.61487700	1.34518600
H	-5.13771900	-2.65151500	-0.17656500
H	-4.65602000	-1.09878500	0.52861000

H -1.98481200 -1.58918200 1.39731700

TS₁₅₋₁₆

E (M06-SMD/BS1) = -1043.76169994 au

H (M06-SMD/BS1) = -1043.459012 au

G (M06-SMD/BS1) = -1043.525367 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1044.14399250 au

C -3.02646400 1.29846000 -0.74958700

C -1.85571200 0.73534700 -0.26094500

C -1.87608000 -0.65818700 0.01714800

C -3.05417100 -1.43419000 -0.12070700

C -4.22976500 -0.81112000 -0.59338700

C -4.19329200 0.52437600 -0.91243600

H -3.05212800 2.35073000 -1.00658500

C -2.97698500 -2.80507900 0.21394600

H -5.13724600 -1.40226900 -0.70686500

H -5.08640800 1.01402500 -1.29778200

C -1.78991600 -3.34584100 0.64203100

C -0.65569800 -2.52098300 0.72096800

H -3.87163900 -3.42046000 0.12252200

H -1.70344300 -4.39620900 0.90699600

H 0.31199200 -2.91509600 1.02691400

N -0.70383200 -1.23543500 0.41804400

N -0.62946100 1.39504100 -0.04665200

C -0.61538800 2.72032900 0.26433700

C 1.92267100 2.89652200 -0.29014600

C 2.46552800 1.58241200 0.23057700

H 2.43167200 1.53142700 1.33212000

O -1.63822100 3.40725300 0.40783600

Pd 0.89529000 0.05607900 0.26075700

O 2.29810000 -1.49219500 0.45752800

C 3.14854100 -1.47474600 -0.48548200

O 3.24605300 -0.49481600 -1.28667700

C 4.05121400 -2.64822500 -0.66760500

H 5.07818700 -2.30663000 -0.83551800

H 3.73504500 -3.19652000 -1.56445700

H 4.01010300 -3.32020400 0.19357800

H 2.58351100 0.48686000 -0.65447500

H 3.54618100 1.50610800 0.02252100

C 0.71825800 3.39493300 0.48610300

H 0.93386400 3.33835500 1.56712400

H	0.53997900	4.45677500	0.27259500
H	1.67995600	2.82387800	-1.36175700
H	2.70617100	3.66635000	-0.20987400

16^α

E (M06-SMD/BS1) = -1043.78400239 au

H (M06-SMD/BS1) = -1043.475339 au

G (M06-SMD/BS1) = -1043.547544 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1044.16695403 au

C	-2.91889700	2.00765300	-0.15374300
C	-1.92284400	1.10358400	0.16613800
C	-2.21648800	-0.29520600	0.12078800
C	-3.52126400	-0.73495400	-0.21953700
C	-4.51805200	0.22063300	-0.52734200
C	-4.20980000	1.55970900	-0.50031300
H	-2.70430700	3.07373800	-0.11413200
C	-3.75032500	-2.13062300	-0.25982400
H	-5.51560400	-0.12553700	-0.79515100
H	-4.97245100	2.29771500	-0.74413500
C	-2.72757000	-3.00247400	0.01449200
C	-1.45856500	-2.48185300	0.33306200
H	-4.74477600	-2.49471200	-0.51771500
H	-2.87443300	-4.07928100	-0.01301600
H	-0.62292000	-3.14841600	0.54983200
N	-1.20546800	-1.18805900	0.38603900
N	-0.65003400	1.45823400	0.61857500
C	0.22086900	2.30076500	-0.05438400
C	1.56143800	1.89161700	0.44269900
O	-0.04586400	3.06393300	-0.98800200
Pd	0.68319300	-0.01636400	0.57433600
O	2.27075700	-1.49228400	0.52510300
C	2.87882200	-1.78536800	-0.50768800
O	2.62278400	-1.22289100	-1.67274400
C	3.98026700	-2.77711900	-0.54863800
H	4.92336600	-2.24532800	-0.73224000
H	3.83021300	-3.47603400	-1.37885600
H	4.04466600	-3.31607400	0.39905300
H	1.89980600	-0.56302400	-1.56650200
C	2.74915900	2.18116700	-0.43405000
H	2.58334700	1.75690200	-1.43820300
H	2.81932300	3.27363100	-0.58451500

C	4.05471900	1.67114100	0.15050000
H	4.25586100	2.13933200	1.12492400
H	4.90539000	1.89207500	-0.50695400
H	4.02847300	0.58379600	0.31329000
H	1.71546100	2.13065000	1.50475200

16^v

E (M06-SMD/BS1) = -1043.79871674 au

H (M06-SMD/BS1) = -1043.489349 au

G (M06-SMD/BS1) = -1043.559273 au

E (M06-SMD/BS2//M06-SMD/BS1) = -1044.18064468 au

C	-3.22979900	0.74858100	-0.62192500
C	-1.95010800	0.43021100	-0.18799600
C	-1.67128500	-0.94693900	0.07435900
C	-2.68108300	-1.93698000	-0.05782300
C	-3.97490200	-1.55876700	-0.47852200
C	-4.22464200	-0.23808300	-0.76231800
H	-3.47187900	1.77913600	-0.85850600
C	-2.32655300	-3.27589000	0.22849000
H	-4.74570300	-2.32164400	-0.58085200
H	-5.21236300	0.06676400	-1.10568300
C	-1.04506900	-3.58364800	0.60965900
C	-0.10035800	-2.54506400	0.69782500
H	-3.08637000	-4.05199200	0.13590400
H	-0.74563200	-4.60428000	0.83409400
H	0.93139700	-2.75332100	0.98510200
N	-0.39963600	-1.28543900	0.44328200
N	-0.89385900	1.34558300	-0.04936600
C	-1.13618500	2.63298500	0.31386800
C	1.18640000	3.28196500	-0.59915200
C	2.01107900	2.09537200	-0.17152000
H	2.53229100	2.29154300	0.78227100
O	-2.25310000	3.07981200	0.62516100
Pd	0.91798800	0.42968400	0.20175400
O	2.77494300	-0.58737600	0.54044100
C	3.28779900	-1.30948900	-0.32011000
O	2.76634100	-1.47940800	-1.51850500
C	4.53983300	-2.07057200	-0.09478300
H	5.26652600	-1.82594900	-0.87821300
H	4.32652500	-3.14425000	-0.16944600
H	4.95360800	-1.84212100	0.88963900

H	1.93754400	-0.95286300	-1.59888800
H	2.75957200	1.80483700	-0.92709200
C	0.04799800	3.57630900	0.36284200
H	0.43152200	3.57570400	1.39787900
H	-0.36401700	4.58018200	0.19380000
H	0.78280300	3.12813100	-1.61269000
H	1.82696300	4.17947900	-0.65957200