Electronic Supplementary Information

For

Mechanism of Catalytic Methylation of 2-Phenylpyridine Using di-*tert*-Butyl Peroxide

Akhilesh K. Sharma, Dipankar Roy, and Raghavan B. Sunoj*

Department of Chemistry

Indian Institute of Technology Bombay

Mumbai 400076,

Fax: (+91) 22-2576-7152

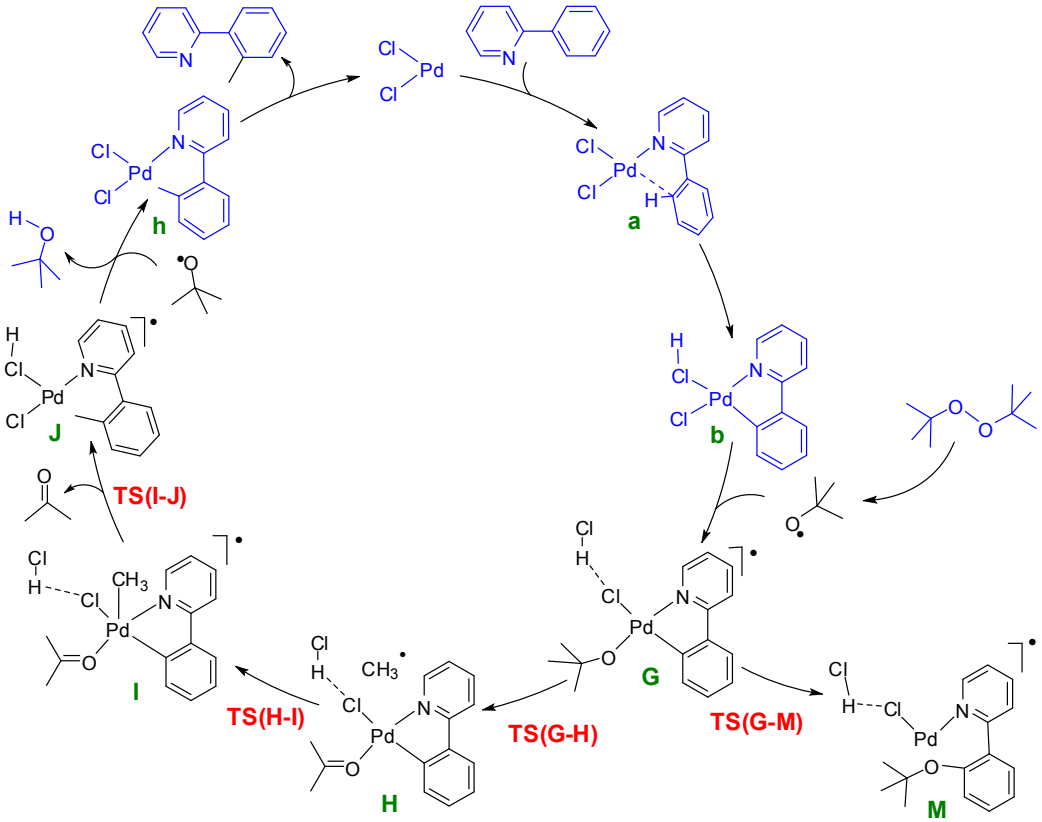
E-mail: sunoj@chem.iitb.ac.in

Gaussian Reference:

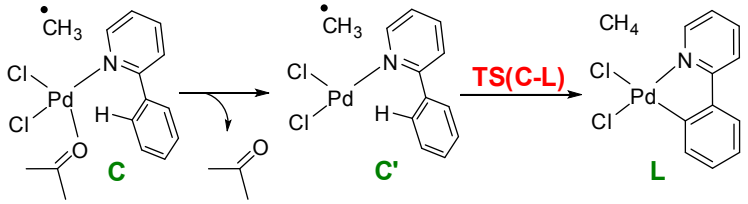
(a) Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

(b) Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

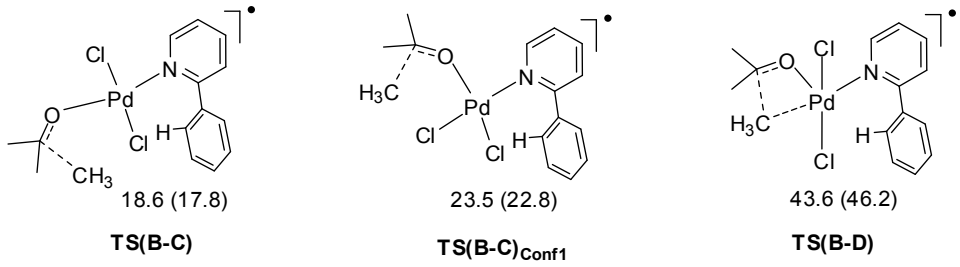
Another possibility through free radical pathway involving reaction through palladacycle **b** is also considered (Scheme S1). The first step in this pathway involves the C–C bond activation. The TS energy for the generation of a methyl radical (**TS(G-H)**) is found to be of lower energy (24.8 kcal/mol) (Figure S1, S3 and Table S2). The uptake of the methyl radical by Pd via a low energy **TS(H-I)** provides a Pd-Me intermediate **I**. The activation barrier for reductive elimination via **TS(I-J)** is also found to be low (~4 kcal/mol). The hydrogen abstraction from intermediate **J** by *tert*-butoxy radical provides the final product complex **h**. Although the energies for most of the steps appear reasonable, the initial conversion of the catalyst-reactant complex **a** to palladacycle **b** exhibits higher activation barrier than the previously discussed radical pathway. That means that the interception by *tert*-butoxy radical is less likely after the palladacycle intermediate is formed. We have also optimized the TS for O–C bond formation (**TS(G-M)**) from intermediate **G**. Interestingly, the radical TS for O–C bond formation is of higher energy than the TS for generation of methyl radical by C–C cleavage.



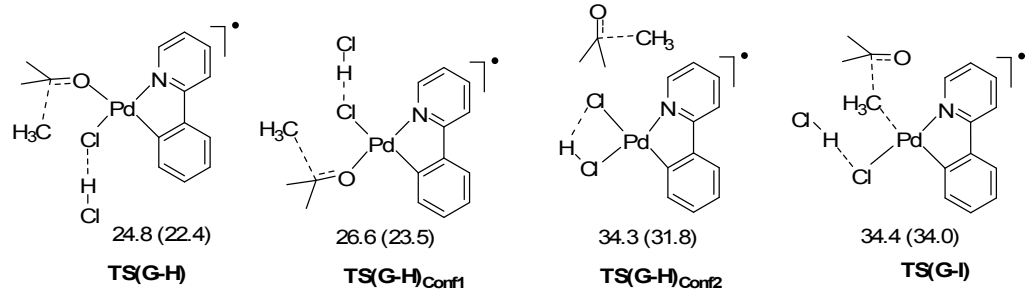
Scheme S1: Mechanism of Pd(II)-catalyzed *ortho*-methylation of 2-phenylpyridine via a radical pathway after (C-H bond activation) involving first C–H bond activation through non-radical pathway.

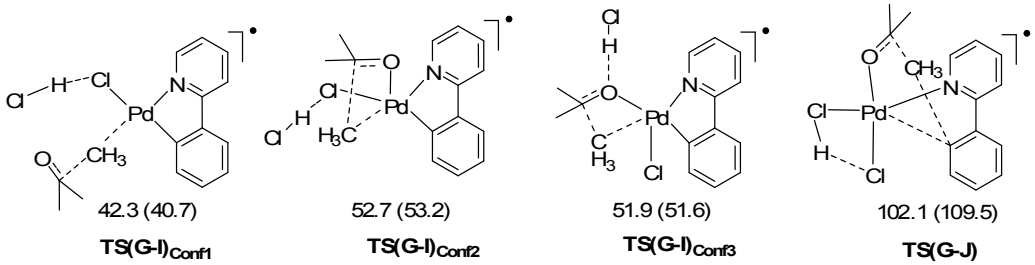


Scheme S2 Formation of side product methane

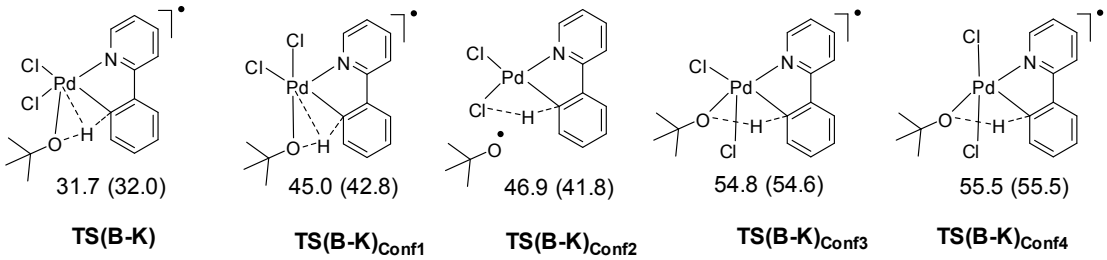


C–C bond activation from intermediate **B**





C–C bond activation from intermediate **G**



C–H bond activation from intermediate **B**

Fig. S1: Different conformers of the TSs for the C–C bond cleavage and C–H bond activation involved in the radical pathway. Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given. The Gibbs free energies obtained using the mPW1K level of theory are given in parenthesis.

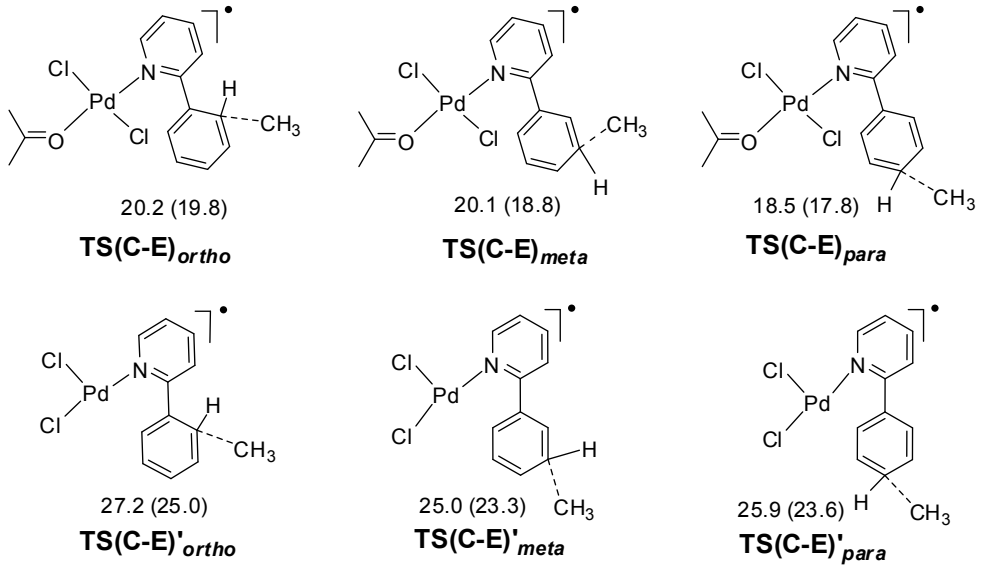
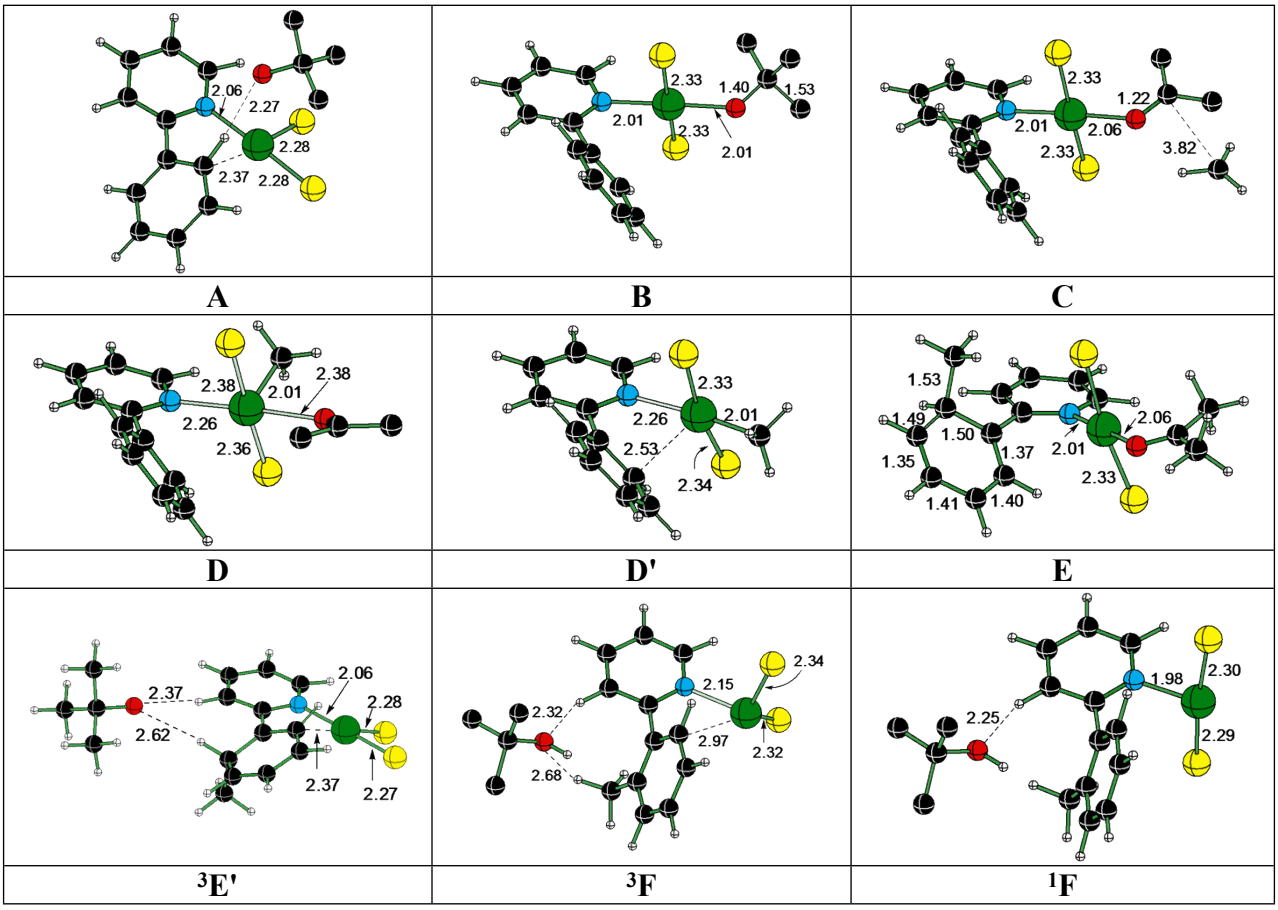
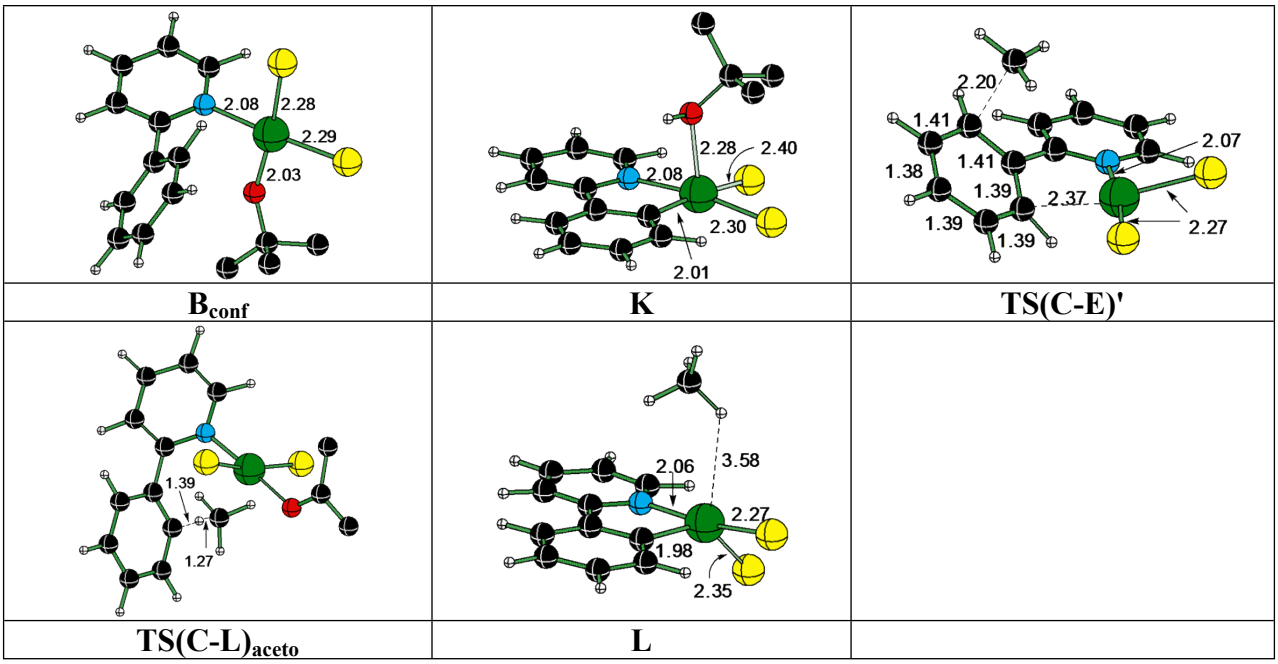


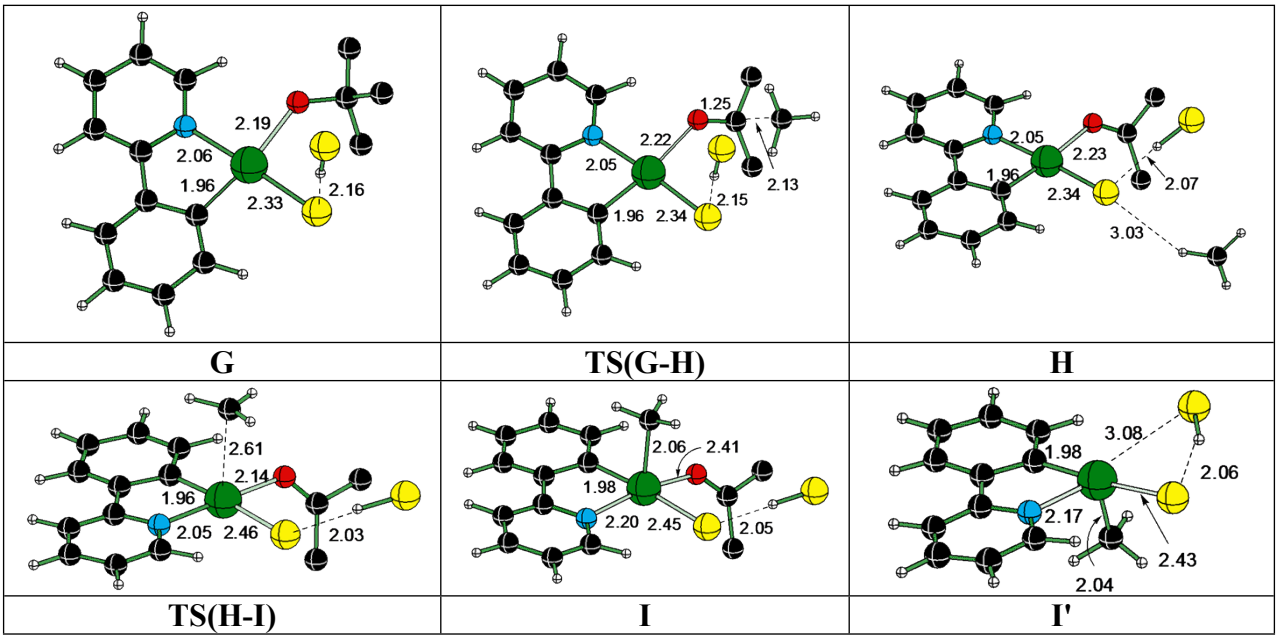
Fig. S2: Energetics of different TSs for methyl radical addition to *ortho*, *meta* and *para* positions of the phenyl ring of 2-phenyl pyridine in the radical pathway.





B_{conf}	K	TS(C-E)'
$TS(C\text{-}L)_{aceto}$	L	

Fig. S3: The mPW1K/LANL2DZ(Pd),6-311+G** optimized geometries of the important transition states and intermediates involved in the radical pathway for $PdCl_2$-catalyzed methylation by *tert*-butyl peroxide. [Only select hydrogen atoms are shown for improved clarity. Atom color code: Pd-Green; Cl-Yellow; O-Red; C-Black; and H-Ivory. Distances in Å]



G	TS(G-H)	H
TS(H-I)	I	I'

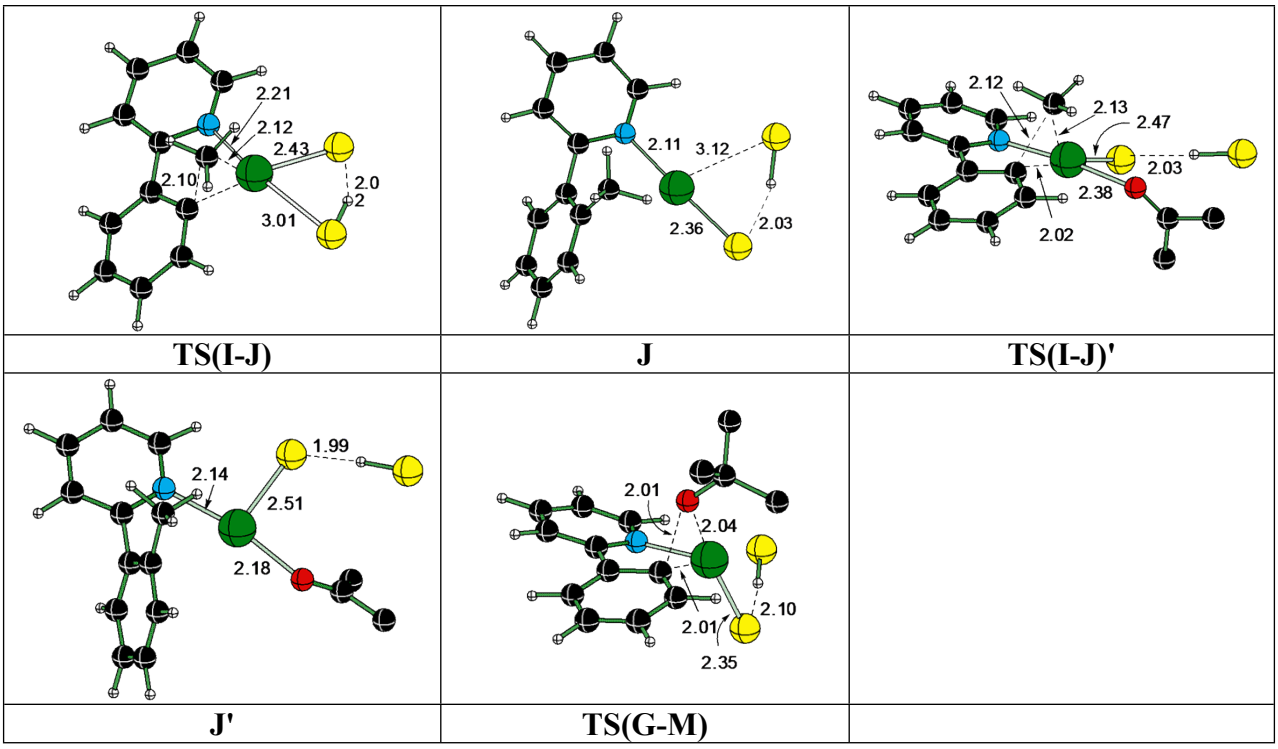


Fig. S4: The mPW1K/LANL2DZ, 6-311+G** optimized geometries of the important transition states and intermediates involved in the radical involving first C–H bond activation through non-radical pathway. [Only select hydrogens are shown for improved clarity. Atom color code: Pd-Green; Cl-Yellow; O-Red; C-Black; and H-Ivory. Distances in Å]

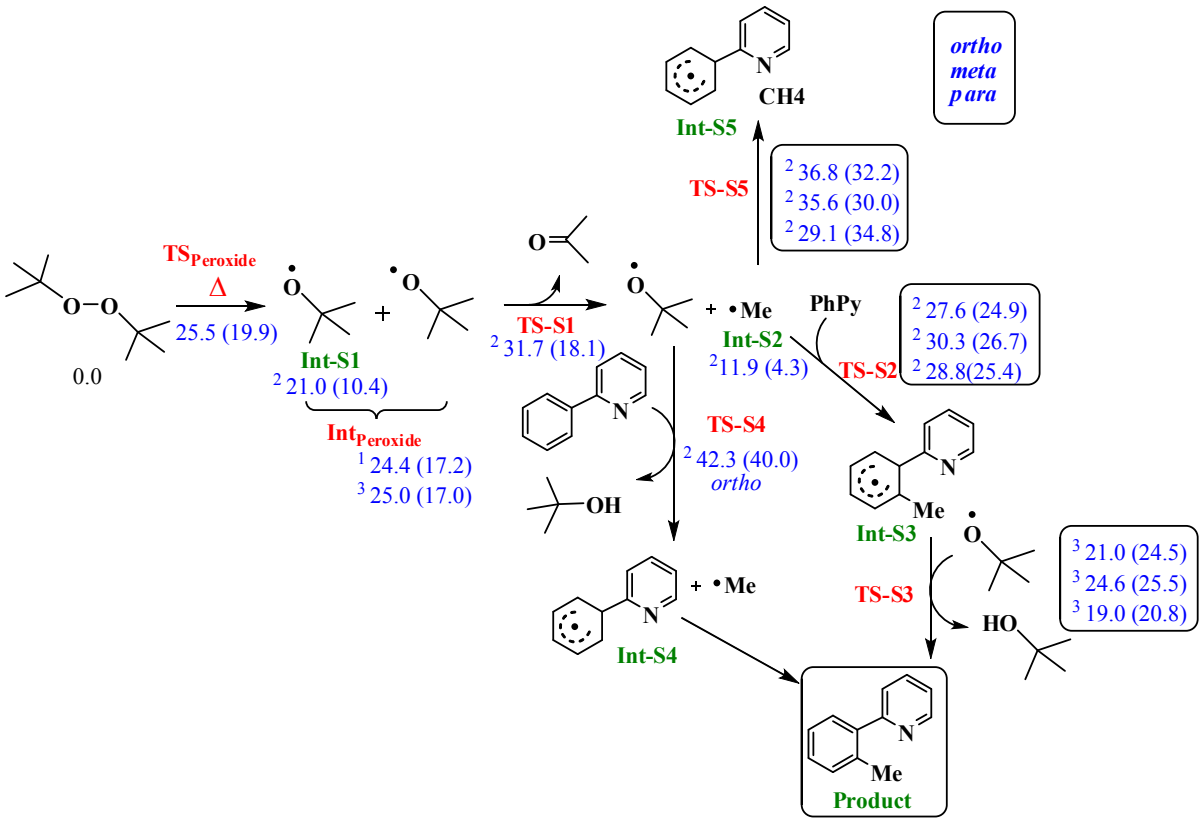
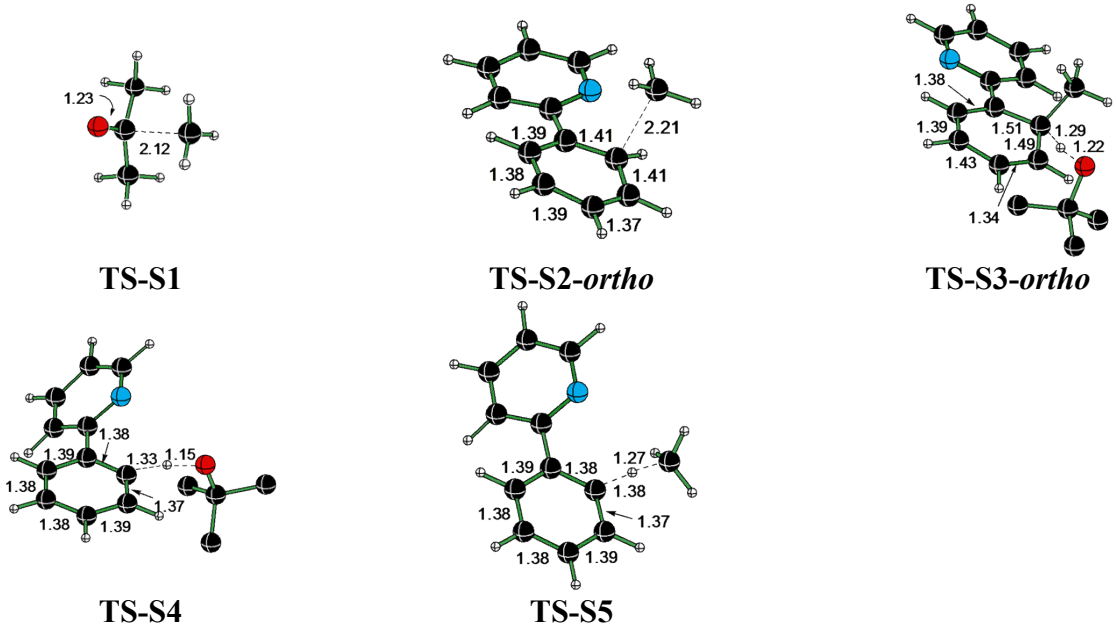


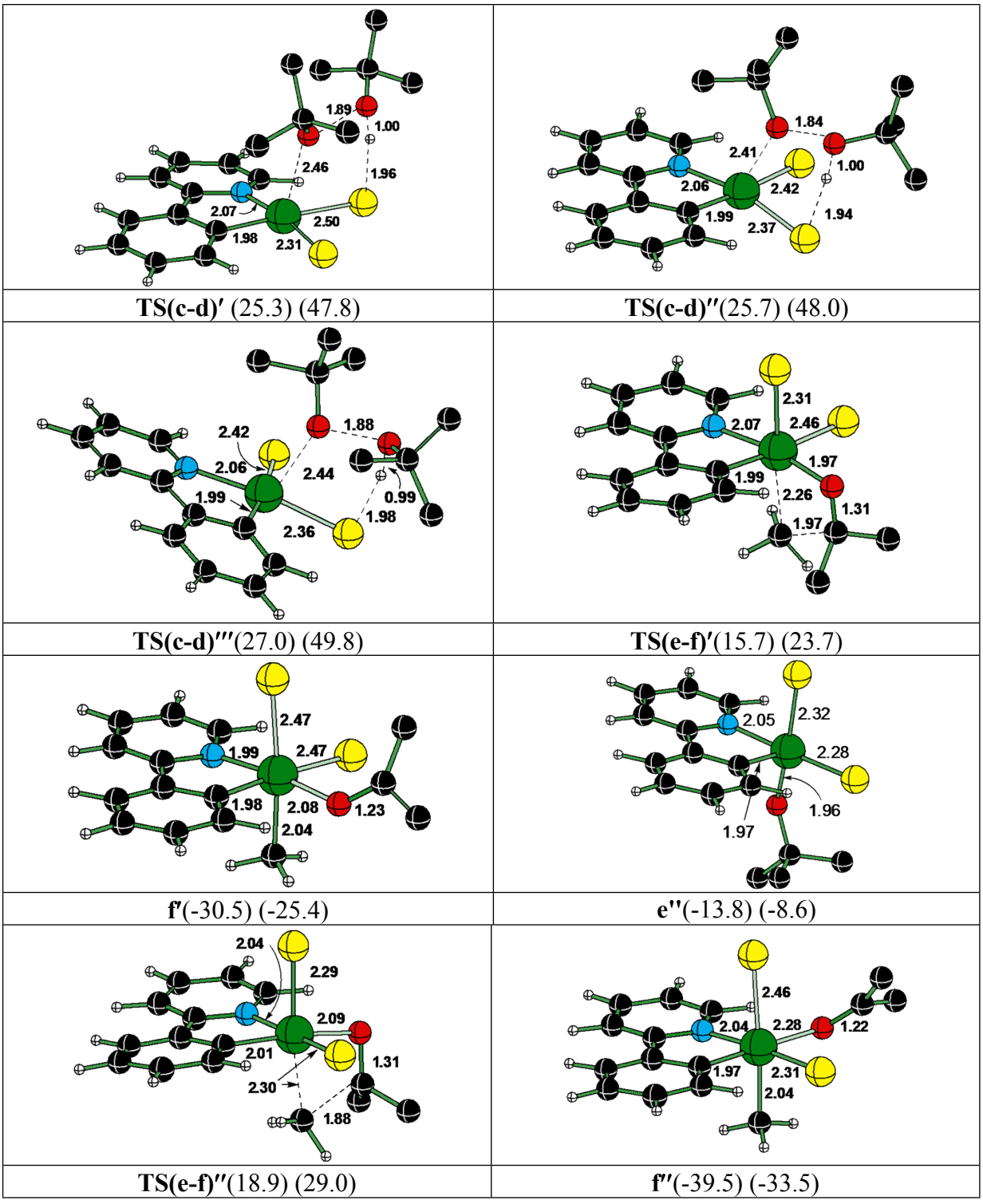
Fig. S5: Uncatalyzed methylation of 2-phenylpyridine through radical pathway. The Gibbs free energies (in kcal/mol) obtained using the M06//mPW1K level of theory are given and mPW1K energies are given in parenthesis.



TS-S1 **TS-S2-*ortho*** **TS-S3-*ortho***

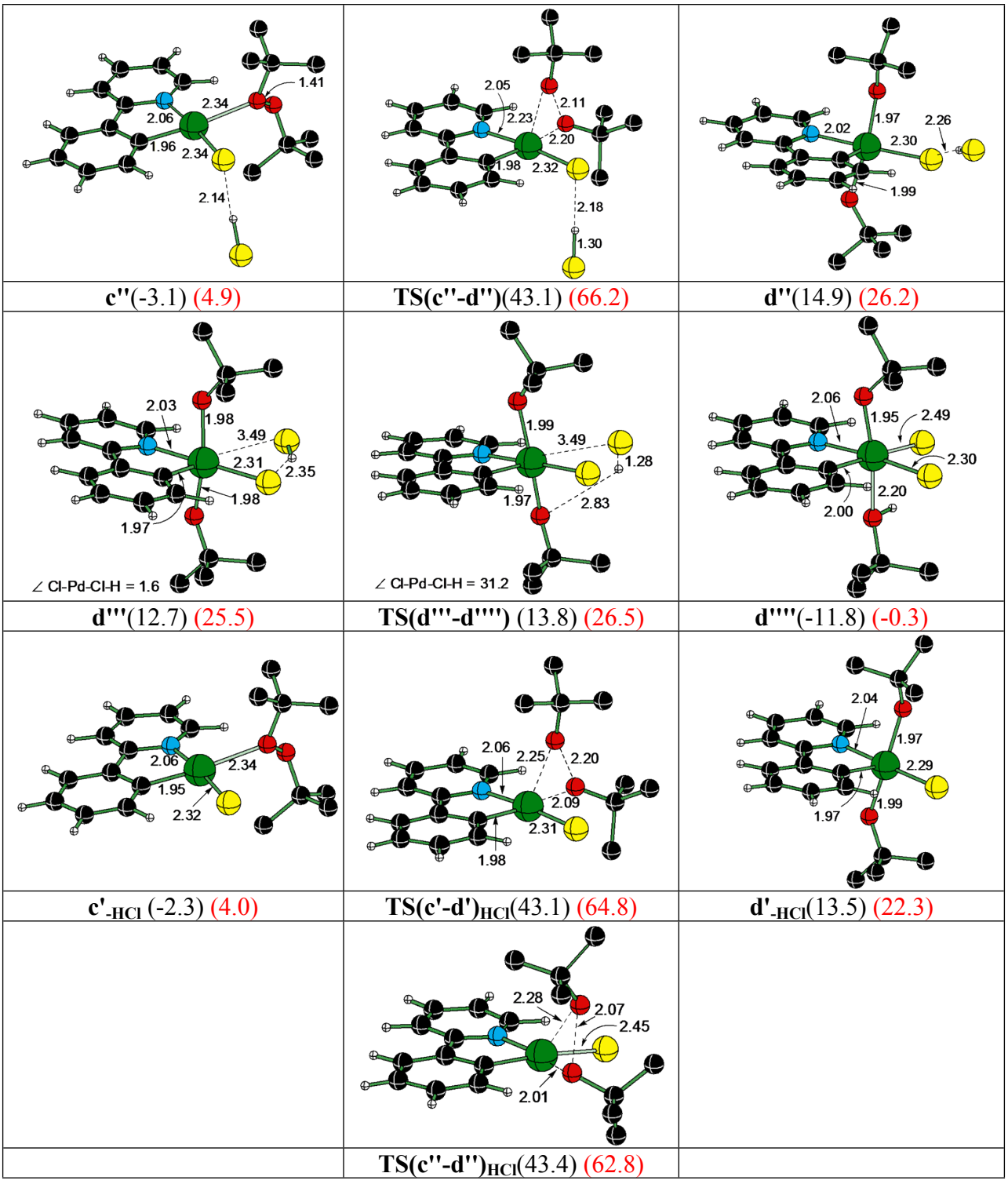
TS-S4 **TS-S5**

Fig. S6: The mPW1K/LANL2DZ(Pd),6-311+G** optimized geometries of the important transition states involved in the uncatalyzed radical pathway. [Only select hydrogens are shown for improved clarity. Atom color code: Pd-Green; Cl-Yellow; O-Red; C-Black; and H-Ivory. Distances in Å]



TS(c-d)′ (25.3) (47.8)	**TS(c-d)″**(25.7) (48.0)
TS(c-d)‴(27.0) (49.8)	**TS(e-f)′**(15.7) (23.7)
f′(-30.5) (-25.4)	**e″**(-13.8) (-8.6)
TS(e-f)″(18.9) (29.0)	**f″**(-39.5) (-33.5)

Fig. S7: The mPW1K/LANL2DZ(Pd), 6-311+G** optimized geometries of the isomeric transition states and intermediates in pathway 1. [Atom color code: Pd– Green, Cl– Yellow, O– Red, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis. The values in red color are the Gibbs free energies obtained using the mPW1K level of theory]



c''(-3.1) (4.9)	**TS(c''-d'')**(43.1) (66.2)	**d''**(14.9) (26.2)
d'''(12.7) (25.5)	**TS(d'''-d'''')** (13.8) (26.5)	**d''''**(-11.8) (-0.3)
c'$_{\text{-HCl}}$ (-2.3) (4.0)	**TS(c'-d')**$_{\text{HCl}}$(43.1) (64.8)	**d'**$_{\text{-HCl}}$(13.5) (22.3)
	TS(c''-d'')$_{\text{HCl}}$(43.4) (62.8)	

Fig. S8: The mPW1K/LANL2DZ(Pd), 6-311+G** optimized geometries of the transition states and intermediates for the addition of peroxide to Pd, followed by proton transfer from chloride to alkoxide in pathway 1.[Atom color code: Pd– Green, Cl– Yellow, O– Red, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis. The values in red color are the Gibbs free energies obtained using the mPW1K level of theory

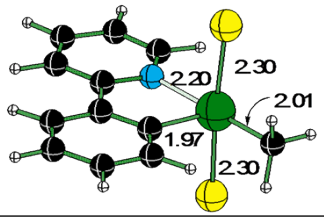
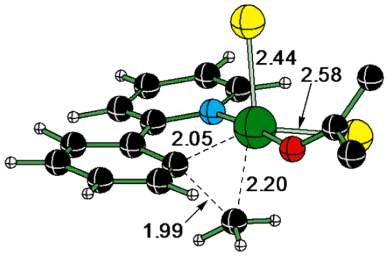
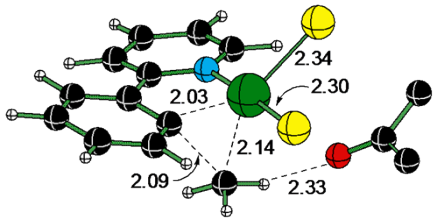
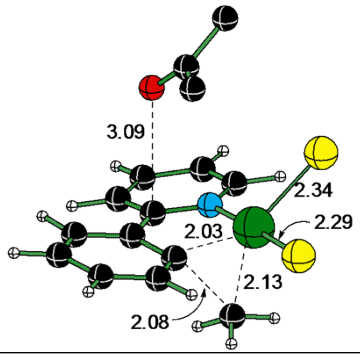
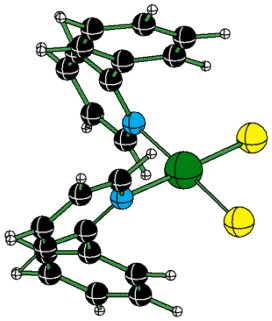
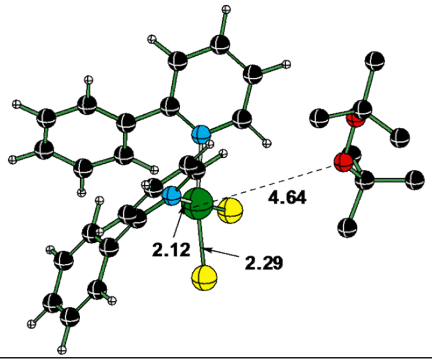
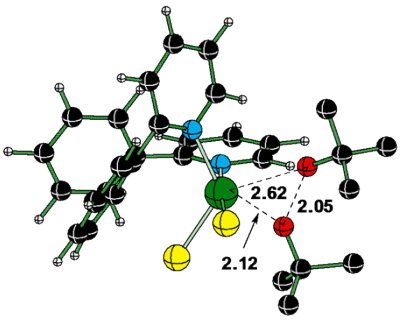
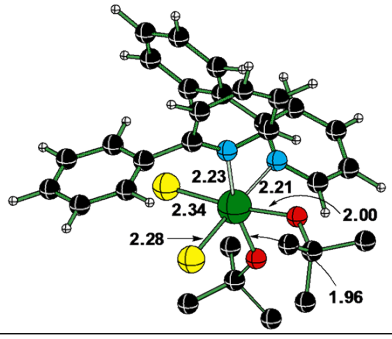
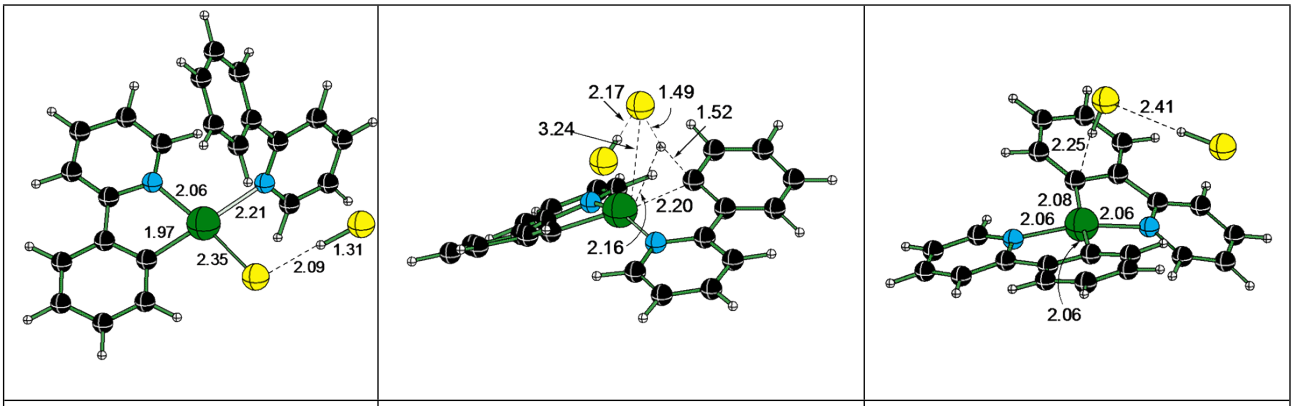
		
	g' (-37.9)(-35.4)	
		
TS(f-h) (-15.0) (-7.9)	**TS(f-h)**$_{\text{Non-Coord}}$ (-36.6) (-28.3)	**TS(f-h)'**$_{\text{Non-Coord}}$ (-37.3) (-28.1)

Fig. S9: The mPW1K/LANL2DZ(Pd), 6-311+G** optimized geometries of the transition states for reductive elimination in the presence of acetone (coordinated either directly to the metal or through hydrogen bonding to an alternative site)and an isomeric intermediate **g** (**g'**) involved in pathway 1.[Atom color code: Pd– Green, Cl– Yellow, O– Red, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis.The values in red color are the Gibbs free energies obtained using the mPW1K level of theory

		
v(-17.5) (-11.8)	**w**(-9.3) (4.8)	**TS(v-x)**(50.3) (91.6)
		

	x(17.8) (48.1)	

Fig. S10: The mPW1K/LANL2DZ(Pd), 6-311+G** optimized geometries of the transition states and intermediate for the peroxyO-O bond cleavage when two molecules of 2-phenylpyridine are bound to the catalyst (Pd). [Atom color code: Pd– Green, Cl– Yellow, O– Red, N– Cyan, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis. The values in red color are the Gibbs free energies obtained using the mPW1K level of theory



y(-10.9) (-6.8)	**TS(y-z)** (33.9) (39.0)	**z**(29.1) (32.8)

Fig. S11: The mPW1K/LANL2DZ(Pd), 6-311+G** optimized geometries of the stationary points for theleading to formation of $[Pd(PhPy)_2]$+2HCl complex formation after C–H on each of 2-phenylpyridine substrate. [Atom color code: Pd– Green, Cl– Yellow, O– Red, N– Cyan, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis.The values in red color are the Gibbs free energies obtained using the mPW1K level of theory

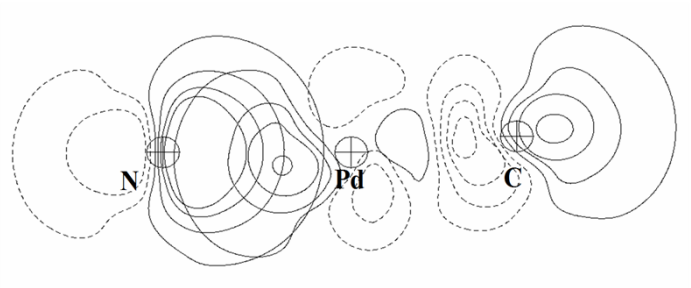


Fig. S12: Contour diagram of $n_N \rightarrow \sigma^*_{Pd-C}$ electron delocalization in the intermediate **o** at the mPW1K/LANL2DZ, 6-311+G** level of theory.

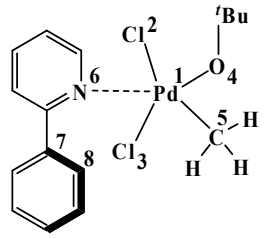
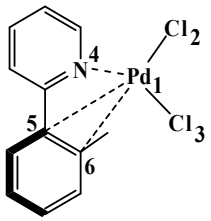
 **o**	 **h**
$E^2[n(N_5) \rightarrow \sigma^*(Pd_1\text{-}Cl_{2,3})] = 2.9$ $E^2[n(N_5) \rightarrow \sigma^*(Pd_1\text{-}C_5)] = 33.2$ $E^2[\ \pi(C_7\text{-}C_8) \rightarrow \sigma^*(Pd_1\text{-}Cl_2)] = 6.4$	$E^2[n(N_4) \rightarrow \sigma^*(Pd_1\text{-}Cl_3)] = 73.0$ $E^2[\ \pi(C_5\text{-}C_6) \rightarrow \sigma^*(Pd_1\text{-}Cl_2)] = 19.1$

Fig. S13: The second order perturbation stabilization energies ($E^{(2)}$, in kcal/mol) of electron delocalization in intermediates for benzene and 2-phenylpyridine substrate.

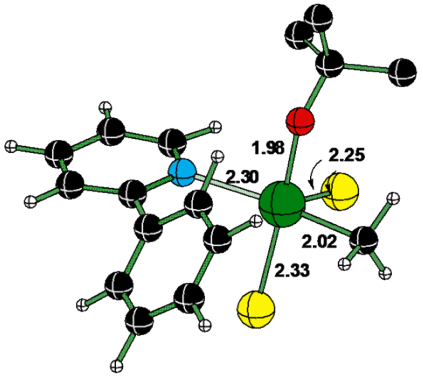
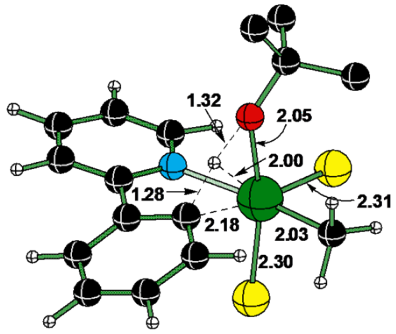
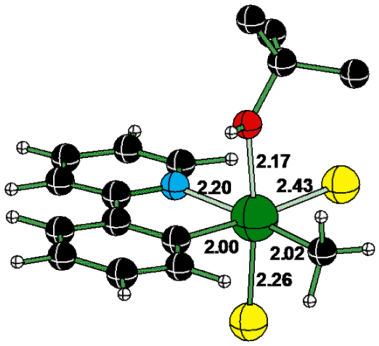
		
o''(-8.1) (5.3)	**TS(o-p')**(7.7) (17.5)	**p'**(-30.3) (-22.0)

Fig. S14: The mPW1K/LANL2DZ, 6-311+G** optimized geometries of the isomerictransition state and intermediates in pathway 2; which differs in *tert*-butyl group orientation. [Atom color code: Pd– Green, Cl– Yellow, O– Red, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis. The values in red color are the Gibbs free energies obtained using the mPW1K level of theory]

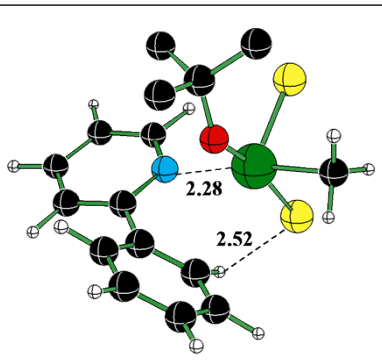
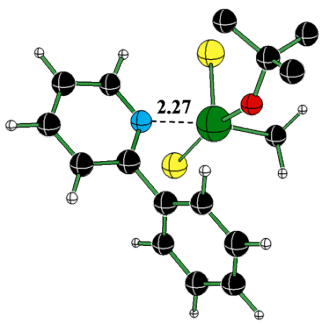
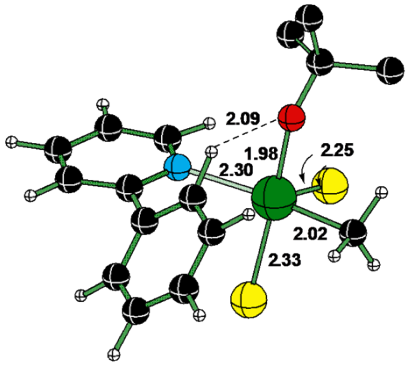
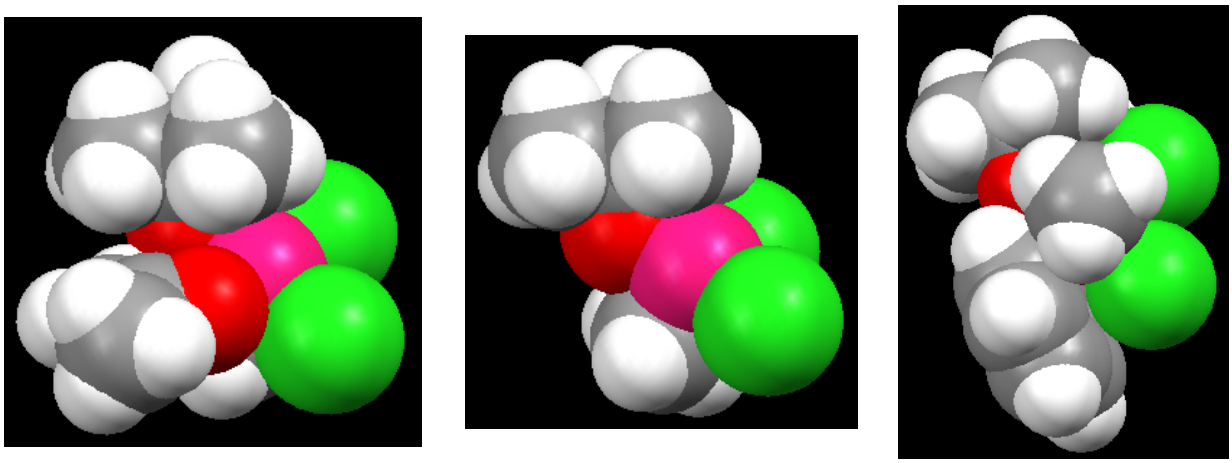
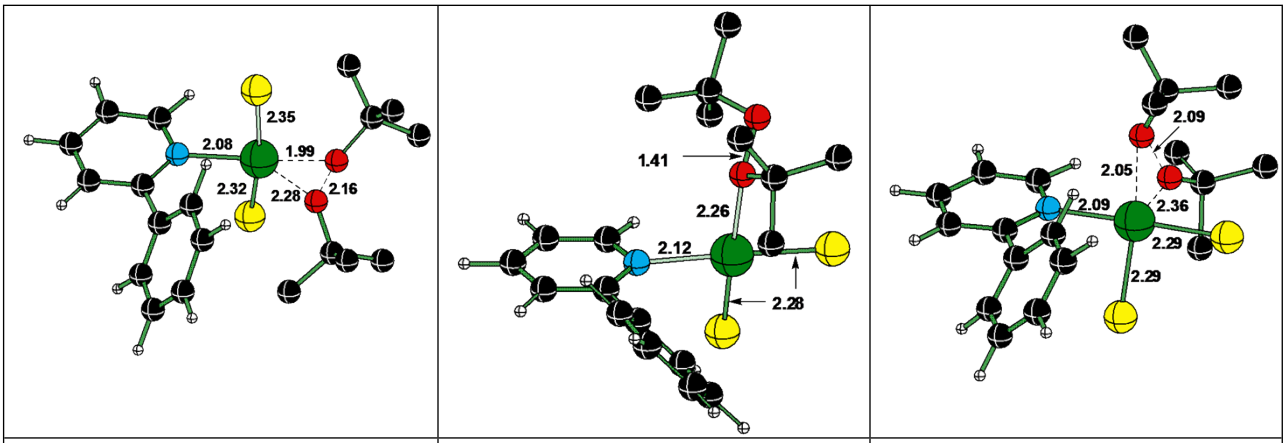
		
o'(-9.9) (4.7)	**TS(o'-o)**(-3.8) (8.7)	**o''**(-8.1) (5.3)

Fig. S15: The mPW1K/LANL2DZ, 6-311+G** optimized geometries of the transition states and intermediates for conformational change to a conformation suitable for proton transfer. [Atom color code: Pd– Green, Cl– Yellow, O– Red, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis. The values in red color are the Gibbs free energies obtained using the mPW1K level of theory.(The change in the inter-ring dihedral angles between **o'** and **o''**are found to be about 93°.)

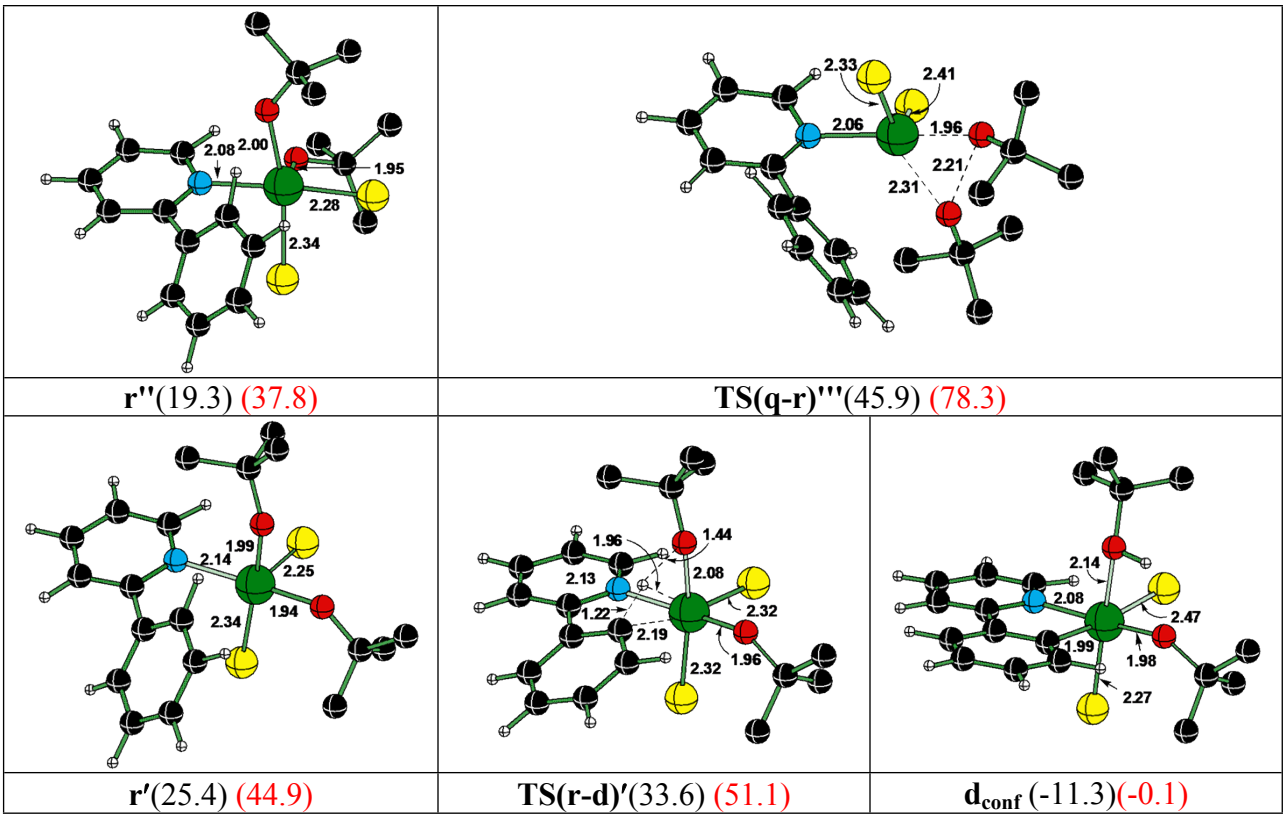


m **n** **o**

Fig. S16: Space filling representation of intermediates equivalent to **m-o** for a model system (benzene) [Atom color code: Pink: Pd, Green: Cl, Red: Oxygen, Gray: C, and White: H]



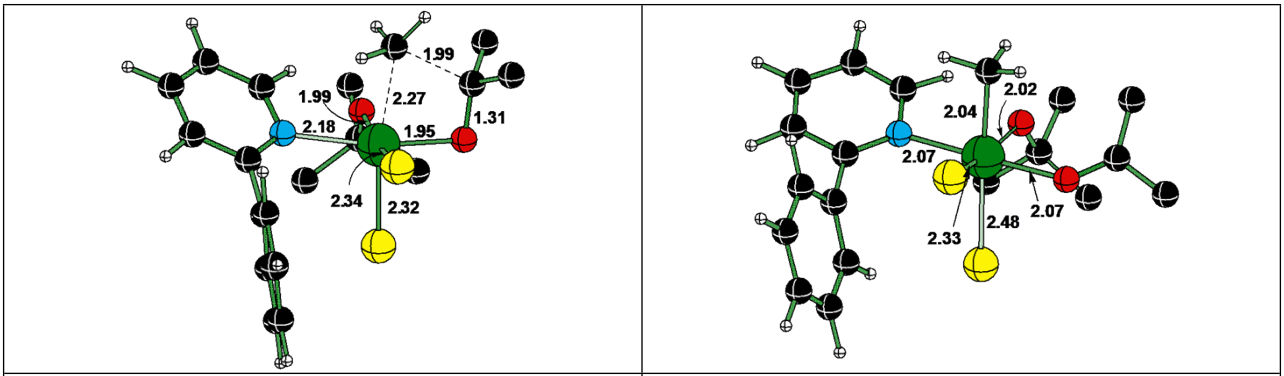
TS(q-r)'(36.6) (63.6)	**q''**(2.6) (14.5)	**TS(q-r)''**(40.9) (67.6)



r''(19.3) (37.8) | **TS(q-r)'''**(45.9) (78.3)

r′(25.4) (44.9) | **TS(r-d)′**(33.6) (51.1) | **d$_{conf}$** (-11.3)(-0.1)

Fig. S17: The mPW1K/LANL2DZ, 6-311+G** optimized geometries of the isomerictransition state and intermediates in pathway 3A. [Atom color code: Pd– Green, Cl– Yellow, O– Red, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis. The values in red color are the Gibbs free energies obtained using the mPW1K level of theory]



TS(r-s)'' (46.2)(66.4) | **s''**(10.2) (28.3)

Fig. S18: The mPW1K/LANL2DZ, 6-311+G** optimized geometries of the isomerictransition state and intermediate in pathway 3B. [Atom color code: Pd– Green, Cl– Yellow, O– Red, C– Black; distances in Å; Relative Gibbs free energies (in kcal/mol) with respect to the Cl_2Pd-2-phenylpyridine complex at the M06//mPW1K level of theory are given in parenthesis. The values in red color are the Gibbs free energies obtained using the mPW1K level of theory]

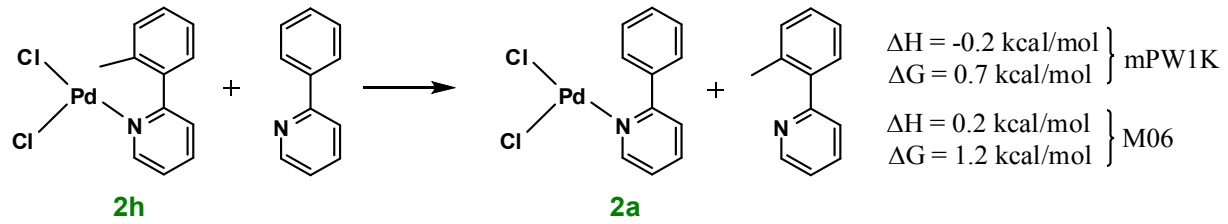


Fig. S19: The energy change during the product removal with simultaneous coordination of substrate (2-phenylpyridine).

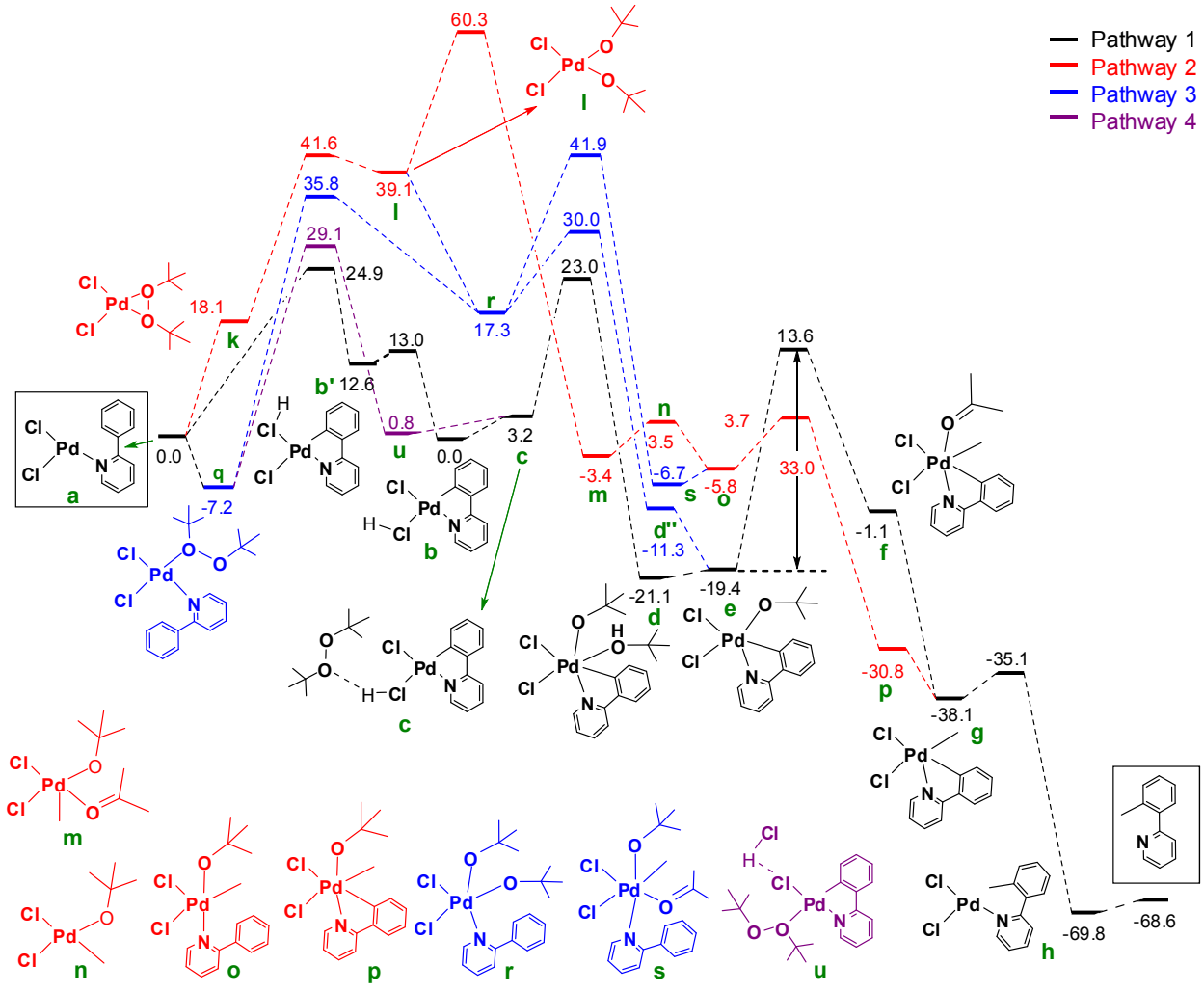


Fig. S20: Gibbs free energy profile obtained at the M06//mPW1K/LANL2DZ(Pd),6-311+G** level of theory for non-radical mechanism depicted as **pathways 1** (black), **pathway 2** (red) **pathway 3** (blue) and **pathway 4** (violet) for methylation of 2-phenyl pyridine.

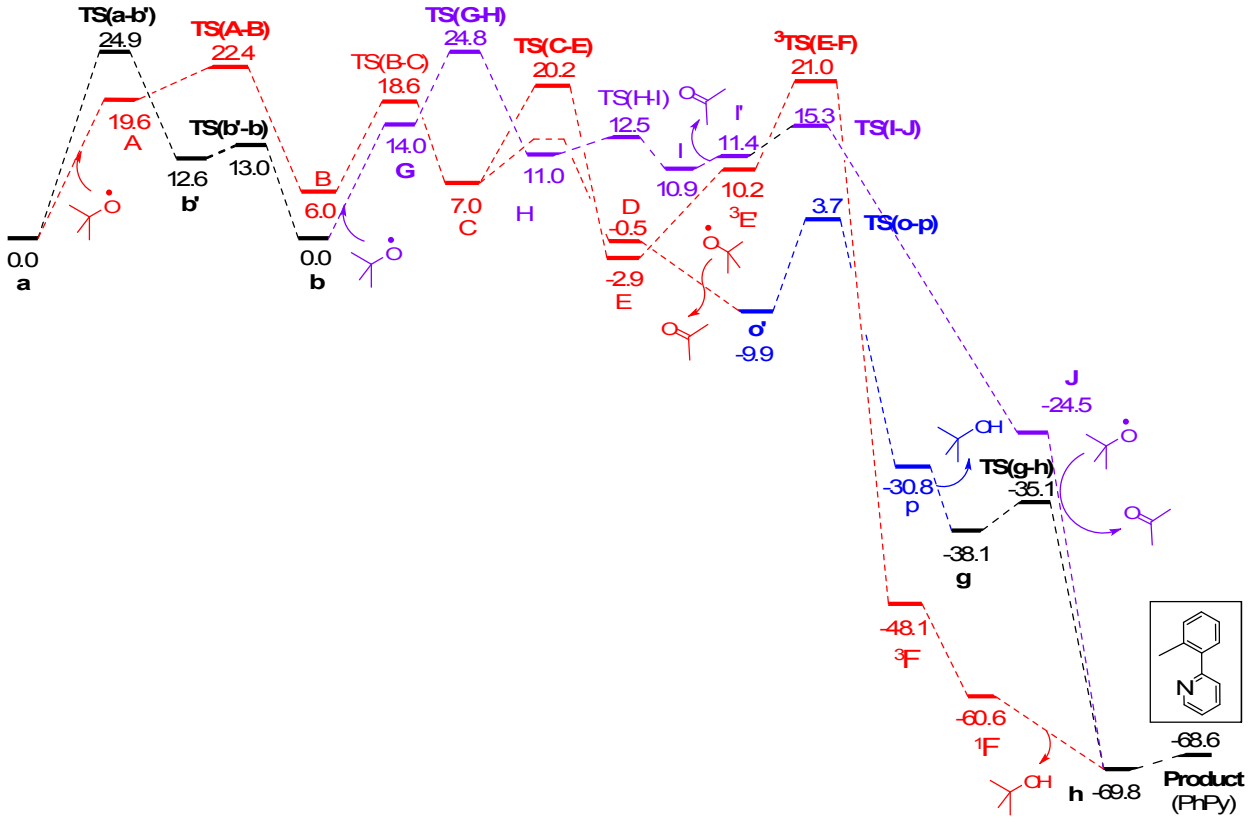


Fig. S21: Gibbs free energy profile obtained at the M06//mPW1K/LANL2DZ(Pd),6-311+G** level of theory for the two radical pathways. (The combination of red and blue pathway is radical pathway discussed in main text whereas the violet colored lines correspond to another alternative wherein C–H activation occurs first by a non-radical pathway as shown in Scheme S1 in the ESI)

Table S1: Energies[a] of Stationary Points with respect to $PdCl_2$-Substrate Complex for Different Substrates at the mPW1K and M06 Functional

	M06		mPW1K	
	ΔH	ΔG	ΔH	ΔG
a	0.0	0.0	0.0	0.0
TS**(a-b)**	33.6	34.9	33.2	34.5
b	-0.1	0.0	-2.0	-1.8
TS(a-b′)	23.8	24.9	24.2	25.3
b′	12.9	12.6	11.3	11.0
TS(b′-b)	12.5	13.0	11.1	11.6
c	-8.5	3.2	-3.6	8.1
TS(c-d)	7.6	23.0	30.3	45.8
d	-36.1	-21.1	-24.3	-9.2
e	-19.4	-19.4	-14.5	-14.5
TS(e-f)	10.9	13.6	20.4	23.1
f	-1.4	-1.1	5.9	6.2
g	-25.4	-38.1	-24.7	-37.3
TS(g-h)	-23.4	-35.1	-20.0	-31.6
h	-55.5	-69.8	-55.3	-69.7
Product	-55.2	-68.6	-55.5	-68.9
k	18.5	18.1	22.5	22.1
TS(k-l)	42.5	41.6	66.5	65.6
l	40.0	39.1	51.8	50.9
TS(l-m)	59.6	60.3	72.1	72.8
m	-1.7	-3.4	6.6	4.8
n	18.9	3.5	24.4	9.0
o	-5.2	-5.8	9.0	8.5
TS(o-p)	2.8	3.7	14.9	15.8
p	-30.6	-30.8	-22.3	-22.5
q	-20.6	-7.2	-11.1	2.3
TS(q-r)	21.3	35.8	46.8	61.3
r	2.5	17.3	21.0	35.8
TS(r-s)	26.5	41.9	47.4	62.9
s	-17.7	-6.7	1.0	12.1
TS(r-d)	13.2	30.0	29.4	46.2
TS(q-t)	37.2	53.5	48.2	64.5
t	36.2	52.3	46.6	62.8
TS(t-u)	36.9	52.4	50.1	65.6
u	-10.9	0.8	-4.0	7.7

[a]The energies (in kcal/mol) are taken with respect to $PdCl_2$-substrate complex.

Table S2: Relative Energies[a] of the Transition States and Intermediates Involved in the Methylation of 2-Phenyl Pyridine in the Radical Pathway

TS / Intermediates	Spin Multiplicity	M06//mPW1K		mPW1K	
		ΔH	ΔG	ΔH	ΔG
$TS_{Peroxide}$ [b]	1	28.1	25.5	22.5	19.9
$Int_{Peroxide}$ [b]	1	30.0	24.4	22.8	17.2
A	2	24.1	19.6	19.0	14.5
TS(A-B)	2	24.6	22.4	21.9	19.6
B	2	8.6	6.0	4.8	2.2
TS(B-C)	2	20.9	18.6	20.1	17.8
C	2	15.8	7.0	11.6	2.9
D	2	5.2	-0.5	5.4	-0.3
TS(C-E)	2	23.9	20.2	23.5	19.8
E	2	0.4	-2.9	-2.5	-5.8
^{3}E' [c]	3	17.8	10.2	13.1	5.6
^{3}TS(E-F) [c]	3	23.5	21.0	26.9	24.5
^{3}F [c]	3	-39.2	-48.1	-44.3	-53.2
^{1}F	1	-54.6	-60.6	-53.5	-59.5
TS(B-K)	2	30.9	31.7	31.2	32.0
K	2	5.6	4.9	0.1	-0.6
TS(C-L)	2	42.0	26.8	39.3	24.1
L	2	15.8	-5.1	-8.6	12.3
G	2	18.3	14.0	12.6	8.3
TS(G-H)	2	29.0	24.8	26.5	22.4
H	2	21.8	11.0	16.9	6.0
TS(H-I)	2	18.7	12.5	17.9	11.7
I	2	17.5	10.9	14.6	8.0
I' [d]	2	28.5	11.4	23.0	5.9
TS(I-J)	2	31.4	15.3	27.3	11.2
J	2	-5.7	-24.5	-17.4	-36.2
TS(G-M)	2	-	-	36.9	39.0

[a] Energies (in kcal/mol) are with respect to $PdCl_2$-2-phenylpyridine and *tert*-butyl peroxide. [b] The energies are with respect to *tert*-butyl peroxide. [c] TS is optimized in triplet state. **E'** intermediate is formed by the addition of *tert*-butoxy radical to **E**. [d] Intermediate **I'** is formed by the removal of acetone from **I**.

Table S3: Relative Energies[a] of the Transition States and Intermediates Involved in the Non-Radical Pathway for Methylation of 2-Phenyl Pyridine Computed at Higher Temperature (130°C) and its Comparison with that at Standard Temperature (25°C)

	M06//mPW1K				mPW1K			
	298.15 K		403.15 K		298.15 K		403.15 K	
	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG
a	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS(a-b)	33.6	34.9	33.5	35.4	33.2	34.5	33.1	35.0
b	-0.1	0.0	0.0	0.1	-2.0	-1.8	-1.9	-1.8
TS(a-b′)	23.8	24.9	23.7	25.3	24.2	25.3	24.2	25.7
b′	12.9	12.6	13.1	12.5	11.3	11.0	11.5	10.9
TS(b′-b)	12.5	13.0	12.5	13.2	11.1	11.6	11.1	11.8
c	-8.5	3.2	-8.1	7.3	-3.6	8.1	-3.2	12.2
TS(c-d)	7.6	23.0	7.9	28.4	30.3	45.8	30.6	51.2
d	-36.1	-21.1	-35.7	-15.9	-24.3	-9.2	-23.8	-4.0
e	-19.4	-19.4	-19.2	-19.4	-14.5	-14.5	-14.3	-14.5
TS(e-f)	10.9	13.6	11.1	14.5	20.4	23.1	20.6	24.0
f	-1.4	-1.1	-0.9	-1.0	5.9	6.2	6.4	6.3
g	-25.4	-38.1	-25.4	-42.5	-24.7	-37.3	-24.6	-41.7
TS(g-h)	-23.4	-35.1	-23.6	-39.1	-20.0	-31.6	-20.1	-35.6
h	-55.5	-69.8	-55.5	-74.9	-55.3	-69.7	-55.3	-74.7
Product	-55.2	-68.6	-55.3	-73.4	-55.5	-68.9	-55.6	-73.7
k	18.5	18.1	18.6	18.0	22.5	22.1	22.5	22.0
TS(k-l)	42.5	41.6	42.5	41.3	66.5	65.6	66.5	65.3
l	40.0	39.1	40.2	38.7	51.8	50.9	52.0	50.5
TS(l-m)	59.6	60.3	59.7	60.5	72.1	72.8	72.2	73.0
m	-1.7	-3.4	-1.4	-4.1	6.6	4.8	6.9	4.2
n	18.9	3.5	18.9	-2.0	24.4	9.0	24.4	3.5
o	-5.2	-5.8	-4.9	-6.1	9.0	8.5	9.4	8.2
TS(o-p)	2.8	3.7	3.0	3.9	14.9	15.8	15.1	16.0
p	-30.6	-30.8	-30.2	-30.9	-22.3	-22.5	-21.9	-22.6
q	-20.6	-7.2	-20.3	-2.6	-11.1	2.3	-10.8	6.9
TS(q-r)	21.3	35.8	21.7	40.8	46.8	61.3	47.2	66.4
r	2.5	17.3	3.0	22.4	21.0	35.8	21.5	40.9
TS(r-s)	26.5	41.9	26.9	47.3	47.4	62.9	47.8	68.2
s	-17.7	-6.7	-17.0	-2.9	1.0	12.1	1.7	15.9
TS(r-d)	13.2	30.0	13.6	35.9	29.4	46.2	29.7	52.0

[a] Energies (in kcal/mol) are with respect to $PdCl_2$-substrate complex (**a**).

Table S4: Relative Energies[a] of the Transition States and Intermediates Involved in the Radical Pathway at High Temperature (130°C) for Methylation of 2-Phenyl Pyridine

TS / Intermediates	M06//mPW1K				mPW1K			
	298.15 K		403.15 K		298.15 K		403.15 K	
	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG
$TS_{Peroxide}$ [b]	28.1	25.5	28.2	24.5	22.5	19.9	22.6	18.9
$Int_{Peroxide}$ [b]	30.0	24.4	30.3	22.3	22.9	17.5	23.1	15.2
A	24.1	19.6	24.5	18.0	19.0	14.5	19.3	12.8
TS(A-B)	24.6	22.4	24.7	21.5	21.9	19.6	22.0	18.8
B	8.6	6.0	8.9	5.0	4.8	2.2	5.1	1.2
TS(B-C)	20.9	18.6	21.3	17.7	20.1	17.8	20.5	16.9
C	15.8	7.0	16.6	3.8	11.6	2.9	12.5	-0.3
D	5.2	-0.5	5.7	-2.7	5.4	-0.3	5.9	-2.4
D'	16.7	0.7	16.8	-5.0	14.2	-1.8	14.4	-7.5
TS(C-E)	23.9	20.2	24.3	18.8	23.5	19.8	24.0	18.4
E	0.4	-2.9	0.8	-4.1	-2.5	-5.8	-2.2	-7.1
^{3}E' [c]	17.8	10.2	18.2	7.5	13.1	5.6	13.6	2.9
^{3}TS(E-F) [c]	23.5	21.0	23.7	20.2	26.9	24.5	27.2	23.6
^{3}F [c]	-39.2	-48.1	-38.8	-51.3	-44.3	-53.2	-44.0	-56.4
^{1}F	-54.6	-60.6	-54.3	-62.8	-53.5	-59.5	-53.2	-61.7
TS(B-K)	30.9	31.7	31.0	31.9	31.2	32.0	31.3	32.3
K	5.6	4.9	5.9	4.7	0.1	-0.6	0.4	-0.9
TS(C-L)	42.0	26.8	42.2	21.4	39.3	24.1	39.5	18.7
L	15.8	-5.1	16.2	-12.5	-8.6	12.3	12.6	-16.0
G	18.3	14.0	18.8	12.5	12.6	8.3	13.1	6.8
TS(G-H)	29.0	24.8	29.5	23.2	26.5	22.4	27.1	20.8
H	21.8	11.0	22.9	7.0	16.9	6.0	17.9	2.0
TS(H-I)	18.7	12.5	19.4	10.2	17.9	11.7	18.6	9.4
I	17.5	10.9	18.2	8.4	14.6	8.0	15.3	5.5
I' [d]	28.5	11.4	28.8	5.3	23.0	5.9	23.3	-0.2
TS(I-J)	31.4	15.3	31.5	9.6	27.3	11.2	27.4	5.5
J	-5.7	-24.5	-5.6	-31.1	-17.4	-36.2	-17.3	-42.8
TS(G-M)	42.0	39.9	42.2	39.1	36.9	39.0	39.3	36.1

[a] Energies (in kcal/mol) are with respect to $PdCl_2$-2-phenylpyridine and *tert*-butyl peroxide. [b] The energies are with respect to *tert*-butyl peroxide. [c] TS is optimized in the triplet state. **E'** intermediate is formed by the addition of *tert*-butoxy radical to **E**. [d] The **I'** is formed by removal of acetone from **I**.

Optimized Coordinates, Total electronic Energy (E_0), ZPE-Corrected Total electronic Energy (E_{0+ZPE}), Enthalpy (H_{298}), and Gibbs Free Energy (G_{298}) (All energy values given are in a.u.)at the mPW1K/LANL2DZ(Pd), 6-311+G** level of theory. The total electronic Energy at the M06 functional ($E_{0\text{-}M06}$) obtained using mPW1K optimized geometries is also given. Number of imaginary frequencies (N_{Imag}) and its value in cm^{-1} is also provided.

Phenyl Pyridine E_0 = -479.3147996 E_{0+ZPE} = -479.140545 H_{298} = -479.131011 G_{298} = -479.175154 N_{Imag} = 0 E_0(M06) =-479.0840939 C 2.785489 -1.187470 0.241063 H 3.302484 -2.115621 0.430862 C 3.505890 -0.027467 0.011715 H 4.584806 -0.047091 0.019469 C 2.833676 1.156227 -0.234642 C 1.404788 -1.163927 0.227218 C 1.451340 1.181228 -0.242888 C 0.719106 0.023216 -0.006099 H 0.944391 2.108249 -0.461293 H 3.386160 2.062515 -0.429432 C -0.758314 0.024541 -0.003153 C -1.489319 1.179714 0.261801 C -2.867101 1.121617 0.245610 C -3.484047 -0.085080 -0.023879 C -2.675888 -1.182986 -0.255300 N -1.356536 -1.137473 -0.246320 H -0.986938 2.102943 0.498108 H -3.451265 2.005763 0.450737 H -4.557622 -0.179102 -0.046986 H -3.114766 -2.149942 -0.460584 H 0.834791 -2.063083 0.394683	**Product** E_0 = -518.6300875 E_{0+ZPE} = -518.427625 H_{298} = -518.416501 G_{298} = -518.463891 N_{Imag} = 0 E_0(M06) =-518.3756515 N 1.426573 0.823309 -0.691009 C 0.831255 -0.163114 -0.029370 C 1.559299 -1.139017 0.646616 C 2.937618 -1.090882 0.616091 C 3.553662 -0.071118 -0.084148 C 2.747593 0.858983 -0.714035 C -0.647673 -0.213937 -0.046031 C -1.436297 0.917390 0.196458 C -2.816489 0.770879 0.164610 C -3.418353 -0.444124 -0.106563 C -2.635574 -1.556729 -0.346045 C -1.260188 -1.434012 -0.308842 H -3.433260 1.635199 0.363199 H -4.494812 -0.518937 -0.127757 H -0.642583 -2.296107 -0.512251 H -3.088710 -2.511151 -0.564475 H 1.043762 -1.908419 1.198402 H 3.521778 -1.834239 1.136989 H 4.627379 0.009137 -0.138120 H 3.189161 1.675969 -1.268504 C -0.851272 2.259634 0.508721 H -0.426286 2.716139 -0.380724 H -1.616744 2.918970 0.908842 H -0.047178 2.186563 1.236685	***tert*-Butylperoxide** E_0 = -466.0643493 E_{0+ZPE} = -465.807538 H_{298} = -465.793494 G_{298} = -465.846060 N_{Imag} = 0 E_0(M06) =-465.8627018 O 0.472680 0.525569 -0.279498 O -0.472675 -0.525467 -0.279715 C -1.784237 0.647825 1.379401 C -1.755528 0.027044 -0.005164 H -1.503534 -0.086078 2.131369 H -1.097471 1.486482 1.438693 H -2.785419 1.007297 1.607604 C -2.128462 1.037912 -1.074560 C -2.656069 -1.190610 -0.073646 H -2.079426 0.579671 -2.059445 H -3.141319 1.400205 -0.911097 H -1.451961 1.886702 -1.055866 H -3.685673 -0.899135 0.118690 H -2.604588 -1.649525 -1.057658 H -2.362083 -1.928206 0.669053 C 1.784156 -0.648506 1.379099 C 1.755533 -0.027051 -0.005167 H 1.503394 0.085008 2.131427 H 1.097388 -1.487195 1.437912 H 2.785319 -1.008096 1.607190 C 2.128576 -1.037373 -1.075040 C 2.656030 1.190674 -0.073003 H 2.079539 -0.578657 -2.059703 H 3.141457 -1.399671 -0.911722 H 1.452138 -1.886219 -1.056773 H 3.685623 0.899147 0.119308 H 2.604642 1.650044 -1.056808 H 2.361943 1.927922 0.670003
$PdCl_2$ E_0 = -1047.1924565 E_{0+ZPE} = -1047.190326 H_{298} = -1047.184868 G_{298} = -1047.217055 N_{Imag} = 0 E_0(M06) =-1047.1008795 Pd 0.000000 0.0000000.000000 Cl 0.000000 0.000000 2.270000 Cl 0.000000 0.000000 -2.270000 **HCl** E_0 = -460.8373098 E_{0+ZPE} = -460.830750 H_{298} = -460.827445 G_{298} = -460.848647 N_{Imag} = 0 E_0(M06) =-460.7926529 H 0.000000 0.000000 -1.220599 Cl 0.000000 0.000000 0.071800	**Acetone** E_0 = -193.1507439 E_{0+ZPE} = -193.065053 H_{298} = -193.058822 G_{298} = -193.092992 N_{Imag} = 0 E_0(M06) =-193.078573 C 0.000008 0.183947 -0.000036 O -0.000056 1.382869 0.000009 C -1.277242 -0.607118 -0.002598 H -1.258215 -1.369681 -0.778713 H -1.383378 -1.124471 0.950279 H -2.123986 0.053234 -0.148237 C 1.277291 -0.607044 0.002604 H 1.383279 -1.124802 -0.950064 H 2.124043 0.053376 0.147845 H 1.258359 -1.369319 0.779002	***tert*-butanol** E_0 = -233.683983 E_{0+ZPE} = -233.545253 H_{298} = -233.537648 G_{298} = -233.574181 N_{Imag} = 0 E_0(M06) =-233.5777767 C 1.477855 -0.000333 -0.337276 C 0.005778 -0.000002 0.017730 H 1.963404 0.880386 0.075466 H 1.963071 -0.881172 0.075605 H 1.614971 -0.000441 -1.416069 C -0.676599 -1.250291 -0.512444 C -0.676015 1.250629 -0.512390 H -1.729932 -1.265313 -0.231944 H -0.623016 -1.297669 -1.598276 H -0.202781 -2.139030 -0.102877 H -0.621710 1.298432 -1.598167 H -1.729527 1.265725 -0.232571 H -0.202317 2.139124 -0.102155 O -0.034237 -0.000021 1.435301 H -0.944384 0.000107 1.714859
a	**b**	**b'**

E_0 = -1526.5983938 E_{0+ZPE} = -1526.419652 H_{298} = -1526.404946 G_{298} = -1526.462451 N_{Imag} = 0 E_0(M06) =-1526.2872709 N 0.934663 -1.088091 -0.132488 C 1.899094 -0.159212 -0.127025 C 3.234965 -0.517692 -0.147345 C 3.568577 -1.856955 -0.172304 C 2.561926 -2.802807 -0.174117 C 1.250334 -2.377249 -0.150586 C 1.431426 1.232997 -0.074649 C 0.245239 1.579894 -0.727165 C -0.295095 2.848850 -0.592171 C 0.367226 3.795130 0.164104 C 1.558381 3.465661 0.790751 C 2.085503 2.191465 0.683914 H -0.173088 0.919549 -1.500816 Pd -0.994138 -0.337015 -0.090170 Cl -1.893130 -2.282806 0.671296 Cl -3.027623 0.672909 -0.165540 H -1.230759 3.076374 -1.075815 H -0.045781 4.785031 0.274133 H 2.982270 1.933038 1.224986 H 2.069662 4.201971 1.391246 H 3.993353 0.247238 -0.159032 H 4.604293 -2.157972 -0.195457 H 2.778709 -3.857669 -0.192592 H 0.416411 -3.060486 -0.129737	E_0 = -1526.5974327 E_{0+ZPE} = -1526.422929 H_{298} = -1526.408153 G_{298} = -1526.465370 N_{Imag} = 0 E_0(M06) =-1526.2833323 N -0.618981 1.317888 -0.000872 C -1.851119 0.781012 0.000887 C -2.967765 1.604589 0.003720 C -2.803477 2.972108 0.004681 C -1.526277 3.505099 0.002742 C -0.459329 2.635057 -0.000073 C -1.856097 -0.672296 -0.000260 C -0.596818 -1.285111 -0.001431 C -0.507882 -2.663890 -0.002736 C -1.665729 -3.426550 -0.003061 C -2.913393 -2.824694 -0.001905 C -3.009126 -1.448535 -0.000472 H 3.341587 0.133500 0.002874 Pd 0.907493 -0.043356 -0.002345 Cl 3.081636 1.467346 -0.004871 Cl 2.655267 -1.627171 0.010418 H 0.456254 -3.143841 -0.003422 H -1.589106 -4.503458 -0.004150 H -3.983287 -0.983480 0.000281 H -3.807667 -3.427651 -0.002158 H -3.953387 1.171631 0.005292 H -3.665791 3.620542 0.006883 H -1.354054 4.568009 0.003351 H 0.558351 2.990195 -0.001806	E_0 = -1526.5775456 E_{0+ZPE} = -1526.402092 H_{298} = -1526.386910 G_{298} = -1526.444917 N_{Imag} = 0 E_0(M06) =-1526.2638752 N -0.662610 -1.258549 -0.024766 C -1.856467 -0.643633 0.042839 C -3.019192 -1.395512 0.098552 C -2.940080 -2.771749 0.079373 C -1.701626 -3.380363 0.004330 C -0.577935 -2.583572 -0.044071 C -1.772333 0.809176 0.030060 C -0.472370 1.333841 -0.040971 C -0.337087 2.709606 -0.130106 C -1.445317 3.543626 -0.114333 C -2.719062 3.013675 -0.014270 C -2.881416 1.644192 0.048976 H 2.406095 2.525202 0.568093 Pd 0.957548 -0.046085 -0.029734 Cl 2.602443 -1.786358 -0.078121 Cl 2.906030 1.418915 0.158568 H 0.633620 3.169383 -0.244162 H -1.310528 4.612493 -0.186344 H -3.877623 1.232702 0.107204 H -3.580020 3.662976 0.000824 H -3.974640 -0.902664 0.155192 H -3.840263 -3.365167 0.122058 H -1.595381 -4.451775 -0.014487 H 0.423049 -2.982619 -0.097135
c E_0 = -1992.6675984 E_{0+ZPE} = -1992.233574 H_{298} = -1992.204215 G_{298} = -1992.295581 N_{Imag} = 0 E_0(M06) =-1992.1625828 N -1.705044 1.508706 -0.271847 C -2.897955 1.664107 0.327428 C -3.351909 2.933918 0.660720 C -2.574126 4.032878 0.374463 C -1.348358 3.853485 -0.241699 C -0.955358 2.569263 -0.545394 C -3.609602 0.420145 0.569245 C -2.965324 -0.752991 0.153067 C -3.592891 -1.971007 0.353376 C -4.838382 -2.018633 0.958011 C -5.474985 -0.859247 1.370739 C -4.860302 0.358935 1.175896 H 2.027559 -0.276228 -0.919597 Pd -1.219922 -0.461341 -0.685824 Cl 1.086947 0.093391 -1.816423 Cl -0.804824 -2.703602 -1.074337 H -3.108333 -2.877730 0.034485 H -5.316658 -2.975380 1.106726 H -5.358972 1.260758 1.497132 H -6.445061 -0.906666 1.840183 H -4.308270 3.052454 1.140151 H -2.920113 5.022687 0.629226 H -0.707532 4.684272 -0.484653 H -0.010994 2.368435 -1.023206 O 3.414176 0.564917 0.796428 O 3.232517 -0.603425 0.029867 C 3.010885 -1.746812 0.907998 C 4.227356 -1.963456 1.780288 H 4.393590 -1.117312 2.439592 H 4.064114 -2.844672 2.395765 H 5.117391 -2.130456 1.180035	**c'** E_0 = -1992.664949 E_{0+ZPE} = -1992.231522 H_{298} = -1992.201910 G_{298} = -1992.292928 N_{Imag} = 0 E_0(M06) =-1992.1646236 C -0.666449 1.630210 0.432798 C -2.023182 1.965246 0.339392 C -2.477275 3.212706 0.749348 C -1.587349 4.141896 1.249098 C -0.242876 3.822559 1.336264 C 0.211930 2.576935 0.931206 C -2.879008 0.930889 -0.219490 N -2.219034 -0.184668 -0.582671 C -2.873856 -1.207956 -1.119403 C -4.236845 -1.177175 -1.321252 C -4.933590 -0.043595 -0.950222 C -4.250301 1.018340 -0.397481 Pd -0.216547 -0.184524 -0.207151 Cl 0.154704 -2.428560 -1.082887 H -3.523900 3.467462 0.678538 H -1.938675 5.110976 1.566632 H 0.457765 4.548151 1.722217 H 1.262369 2.346243 1.005691 H -4.772606 1.911807 -0.101099 H -6.002018 0.013819 -1.089578 H -4.729040 -2.030796 -1.755394 H -2.269614 -2.058966 -1.387672 O 2.790462 -0.349508 -0.682534 O 1.889461 0.033721 0.336003 C 3.039441 0.696380 -1.631316 C 2.382073 -0.556579 1.591951 C 3.694715 1.898688 -0.984302 C 4.004156 -0.012097 -2.565598 C 1.775885 1.081818 -2.374265 C 3.602803 0.226490 2.023416 C 1.245205 -0.385803 2.574786	**c''** E_0 = -1992.6727896 E_{0+ZPE} = -1992.239028 H_{298} = -1992.209405 G_{298} = -1992.300691 N_{Imag} = 0 E_0(M06) =-1992.1727525 C 2.269819 0.683199 0.367743 C 3.114927 -0.343994 -0.076344 C 4.492285 -0.156483 -0.113694 C 5.036092 1.046240 0.284482 C 4.201260 2.062394 0.719331 C 2.827286 1.886897 0.763309 C 2.458320 -1.569049 -0.498940 N 1.120591 -1.539449 -0.375669 C 0.384926 -2.569202 -0.777019 C 0.946798 -3.712395 -1.301047 C 2.324889 -3.773835 -1.411551 C 3.084464 -2.696208 -1.014130 Pd 0.372007 0.211301 0.400029 Cl -0.369718 2.300972 1.145607 H 5.143894 -0.946779 -0.454409 H 6.104241 1.193223 0.254740 H 4.622250 3.007181 1.029167 H 2.192492 2.685727 1.105651 H 4.156685 -2.719068 -1.106934 H 2.802959 -4.653563 -1.813880 H 0.315590 -4.527079 -1.613756 H -0.682539 -2.451367 -0.681238 O -1.840937 -0.507072 0.614863 O -2.496707 -1.105560 -0.480600 C -2.349607 -1.107782 1.837937 C -2.885526 -0.128425 -1.471572 C -2.095840 -2.602212 1.817325 C -1.557907 -0.442885 2.942766 C -3.824968 -0.800613 1.981401 C -3.640485 1.028585 -0.855297 C -1.669716 0.355500 -2.235908

C 1.766765 -1.513147 1.738175	C 2.702674 -2.022571 1.396064	C -3.782938 -0.961131 -2.367081
H 1.591324 -2.377164 2.374445	H 2.928720 -2.456926 2.367371	H -4.128729 -0.351947 -3.198022
H 1.882559 -0.638037 2.370919	H 1.858305 -2.548901 0.964402	H -3.244038 -1.814477 -2.772183
H 0.889983 -1.391205 1.107390	H 3.560501 -2.158962 0.747289	H -4.649330 -1.322546 -1.819261
C 2.829318 -2.884346 -0.074463	H 3.970868 -0.175100 2.964461	H -3.924434 1.723457 -1.641788
H 2.697592 -3.809736 0.480307	H 4.396288 0.138375 1.288623	H -4.544362 0.687845 -0.358381
H 1.944008 -2.748411 -0.689576	H 3.367468 1.277634 2.171372	H -3.018495 1.565597 -0.145815
H 3.706257 -2.987509 -0.709380	H 1.580098 -0.740314 3.546585	H -1.980808 0.996117 -3.057442
C 4.483207 1.354737 0.252411	H 0.945675 0.652693 2.675574	H -1.009594 0.946971 -1.606528
C 4.491115 2.541282 1.196284	H 0.380183 -0.979731 2.287277	H -1.111829 -0.483301 -2.645987
H 5.267096 3.240699 0.896036	H 4.298635 0.665192 -3.363217	H -1.898660 -0.837291 3.897434
H 3.534136 3.055827 1.174465	H 4.897376 -0.327736 -2.032753	H -0.494134 -0.652207 2.851263
H 4.690499 2.222098 2.215928	H 3.532831 -0.886497 -3.005021	H -1.694800 0.633304 2.934511
C 5.801814 0.610209 0.300603	H 3.907437 2.647447 -1.744012	H -2.450099 -3.040029 2.747594
H 6.594835 1.253024 -0.074603	H 3.041324 2.352891 -0.246378	H -2.622325 -3.080395 0.996710
H 6.050993 0.320532 1.317497	H 4.630953 1.625561 -0.505515	H -1.032347 -2.811938 1.732750
H 5.768136 -0.279120 -0.321477	H 2.032648 1.722486 -3.215573	H -4.186516 -1.217291 2.918609
C 4.157370 1.789255 -1.162853	H 1.275940 0.194941 -2.755716	H -3.992535 0.272061 1.997748
H 4.115237 0.938195 -1.836520	H 1.085839 1.633721 -1.741351	H -4.398481 -1.240678 1.171814
H 3.202523 2.306531 -1.197844	Cl -1.349660 -3.867899 1.579758	Cl -0.802647 4.268208 -1.647306
H 4.928367 2.465071 -1.525833	H -0.735036 -3.376887 0.524343	H -0.603633 3.528152 -0.589538
d	**d'**	**d''**
E_0 = -1992.7037339	E_0 = -1992.6489239	E_0 = -1992.6370572
E_{0+ZPE} = -1992.265929	E_{0+ZPE} = -1992.217485	E_{0+ZPE} = -1992.205666
H_{298} = -1992.237099	H_{298} = -1992.187626	H_{298} = -1992.175615
G_{298} = -1992.323210	G_{298} = -1992.278341	G_{298} = -1992.266796
N_{Imag} = 0	N_{Imag} = 0	N_{Imag} = 0
E_0(M06) =-1992.2098826	E_0(M06) =-1992.1547291	E_0(M06) =-1992.1422116
N -0.489463 1.533041 0.316445	C -0.220478 0.392466 1.442241	C -0.022575 0.158868 1.220324
C -1.801812 1.728170 0.152496	C -1.517931 0.873325 1.356148	C 1.208941 -0.068456 1.826077
C -2.374980 2.922483 0.559737	C -2.086017 1.377242 2.521022	C 1.280595 0.008584 3.210346
C -1.579092 3.887085 1.138369	C -1.366625 1.378135 3.699504	C 0.152277 0.304228 3.948890
C -0.226612 3.649627 1.307217	C -0.077528 0.871997 3.736641	C -1.055415 0.522457 3.311733
C 0.285532 2.444586 0.879531	C 0.516352 0.357515 2.592519	C -1.156236 0.459546 1.927585
C -2.493372 0.599516 -0.444403	C -2.164393 0.819383 0.052319	C 2.310897 -0.430072 0.953253
C -1.722107 -0.517028 -0.760458	N -1.405294 0.273773 -0.904010	N 1.956073 -0.537756 -0.328936
C -2.271809 -1.633618 -1.342505	C -1.838684 0.179325 -2.149283	C 2.808095 -0.920055 -1.262024
C -3.637817 -1.647652 -1.582798	C -3.089546 0.623995 -2.515030	C 4.119765 -1.205515 -0.952722
C -4.429900 -0.559396 -1.261072	C -3.896160 1.183309 -1.541032	C 4.523406 -1.085659 0.365464
C -3.859341 0.562122 -0.696912	C -3.433129 1.285392 -0.246955	C 3.615512 -0.702110 1.329520
H 2.311616 -0.380935 0.991456	Pd 0.473549 -0.335252 -0.242329	Pd 0.064431 0.051257 -0.747488
Pd 0.201808 -0.260927 -0.373969	Cl -0.449618 -2.404191 0.408206	Cl -2.091947 0.662249 -1.278866
Cl 0.329174 0.648354 -2.514289	H -3.092778 1.764904 2.507978	H 2.218777 -0.170275 3.712461
Cl 0.852637 -2.330205 -1.125319	H -1.816863 1.768662 4.598191	H 0.214055 0.360681 5.023860
H -1.654294 -2.472164 -1.610707	H 0.473697 0.866173 4.664336	H -1.940163 0.750170 3.885738
H -4.079742 -2.521906 -2.035731	H 1.508752 -0.063944 2.579243	H -2.093977 0.649187 1.439364
H -4.477983 1.412276 -0.454832	H -4.046946 1.718927 0.523811	H 3.911290 -0.614691 2.360975
H -5.490025 -0.583160 -1.457098	H -4.884721 1.536191 -1.789278	H 5.544373 -1.297829 0.641855
H -3.430161 3.088208 0.426444	H -3.418931 0.525855 -3.535332	H 4.800532 -1.513513 -1.727892
H -2.012539 4.821575 1.459098	H -1.161242 -0.263441 -2.861908	H 2.416842 -1.004383 -2.263069
H 0.423516 4.378628 1.760485	O 1.211497 1.176304 -1.224482	O -0.260859 -1.796964 -1.334768
H 1.324834 2.176136 0.972697	O 2.208746 -0.739855 0.555145	O 0.942040 1.833404 -0.637492
O 0.432274 -0.832687 1.517528	C 1.595351 2.466276 -0.844060	C -0.800742 -2.916641 -0.700765
O 2.356353 0.276628 0.290067	C 3.050473 -1.618322 -0.156765	C 0.459177 3.138388 -0.810951
C 3.668802 0.383250 -0.288879	C 2.551803 2.470313 0.335927	C -0.845669 -3.983862 -1.791061
C 3.690535 1.718190 -1.002959	C 2.305633 3.008264 -2.083253	C 0.099127 -3.384954 0.436093
H 3.550628 2.536262 -0.298661	C 0.378947 3.330161 -0.540250	C -2.205741 -2.660574 -0.181919
H 4.646344 1.860676 -1.501389	C 4.430442 -0.974850 -0.177611	C 1.694401 4.008172 -0.583108
H 2.901491 1.756586 -1.749021	C 3.103361 -2.952146 0.574064	C -0.052720 3.359428 -2.227462
C 4.674962 0.352761 0.846611	C 2.569087 -1.822154 -1.590897	C -0.602168 3.506441 0.215077
H 5.684276 0.475028 0.460770	H 3.272123 -2.444309 -2.141171	H -0.869616 4.558157 0.124544
H 4.480949 1.152125 1.558749	H 1.609265 -2.342130 -1.611493	H -1.502917 2.917598 0.072154
H 4.636045 -0.599420 1.374674	H 2.487946 -0.866969 -2.107504	H -0.224508 3.335535 1.221092
C 3.909325 -0.750914 -1.263353	H 5.164915 -1.646306 -0.620516	H 1.451602 5.062438 -0.708905
H 4.899756 -0.654498 -1.704589	H 4.411509 -0.052710 -0.752845	H 2.078512 3.855334 0.422625
H 3.845334 -1.715052 -0.765537	H 4.745757 -0.741728 0.836696	H 2.473945 3.743555 -1.293581
H 3.167221 -0.735160 -2.055649	H 3.780770 -3.646104 0.077361	H -0.318687 4.403708 -2.385455
C -0.382727 -1.551502 2.397836	H 3.455616 -2.799523 1.592011	H 0.723047 3.094428 -2.943890
C -0.797305 -2.904814 1.845791	H 2.114228 -3.397223 0.619811	H -0.931067 2.753363 -2.425747

H -1.330815 -3.475284 2.604942	H 2.631892 4.033666 -1.916691	H -0.272304 -4.309365 0.875492
H -1.453561 -2.789040 0.988025	H 3.175515 2.398931 -2.314006	H 1.108537 -3.561700 0.069260
H 0.074535 -3.467231 1.526272	H 1.635278 2.990049 -2.939089	H 0.139813 -2.635506 1.224221
C 0.506794 -1.756903 3.623393	H 2.897756 3.483410 0.535952	H -1.249741 -4.916763 -1.400847
H -0.033147 -2.292441 4.402779	H 2.062721 2.095218 1.229909	H -1.471944 -3.646698 -2.612591
H 1.387086 -2.334800 3.352702	H 3.408791 1.836062 0.136699	H 0.154338 -4.170888 -2.175535
H 0.828870 -0.797080 4.020710	H 0.669366 4.366676 -0.376952	H -2.633330 -3.569359 0.238591
C -1.609304 -0.743336 2.797797	H -0.322537 3.297163 -1.371421	H -2.195810 -1.904775 0.599916
H -1.310244 0.236175 3.166050	H -0.125595 2.982593 0.358007	H -2.848376 -2.312340 -0.985171
H -2.277691 -0.610500 1.951052	Cl -3.801810 -2.558725 -0.396364	Cl -4.968034 0.069646 0.700429
H -2.167648 -1.249501 3.583685	H -2.535932 -2.514699 -0.084701	H -3.954908 0.167396 -0.097063
c'-HCl	**d'''**	**d''''**
E_0 = -1531.8225711	E_0 = -1992.6381539	E_0 = -1992.6899173
E_{0+ZPE} = -1531.397667	E_{0+ZPE} = -1992.206628	E_{0+ZPE} = -1992.252071
H_{298} = -1531.370944	H_{298} = -1992.176563	H_{298} = -1992.223278
G_{298} = -1531.453538	G_{298} = -1992.267904	G_{298} = -1992.308943
N_{Imag} = 0	N_{Imag} = 0	N_{Imag} = 0
E_0(M06) =-1531.3644947	E_0(M06) =-1992.1457364	E_0(M06) =-1992.1954897
C -2.268591 -0.896275 -0.101847	C 1.147587 -0.389586 -1.112246	C 0.116758 0.774015 1.354683
C -3.048624 0.268301 -0.047659	C 2.236005 -0.834584 -0.371592	C 0.138563 2.103775 0.940670
C -4.436716 0.191400 -0.099018	C 3.374876 -1.230880 -1.061204	C 0.140256 3.110076 1.900476
C -5.056217 -1.035352 -0.205870	C 3.406651 -1.176739 -2.439781	C 0.136575 2.790062 3.242208
C -4.286312 -2.186225 -0.263297	C 2.302205 -0.728484 -3.142346	C 0.136817 1.462407 3.632704
C -2.903391 -2.122487 -0.211435	C 1.150490 -0.325134 -2.480555	C 0.129280 0.445116 2.689975
C -2.316813 1.520652 0.042530	C 2.084276 -0.859284 1.073136	C 0.180209 2.352998 -0.492572
N -0.982429 1.370209 0.087256	N 0.886835 -0.443934 1.487286	N 0.151765 1.249747 -1.249632
C -0.187124 2.432748 0.112380	C 0.556724 -0.411445 2.763871	C 0.228739 1.311028 -2.569422
C -0.679004 3.719389 0.126519	C 1.450164 -0.803895 3.737163	C 0.317023 2.521202 -3.223839
C -2.051684 3.895567 0.109262	C 2.703235 -1.235089 3.341499	C 0.331074 3.679323 -2.470096
C -2.874613 2.792634 0.061379	C 3.027429 -1.266554 2.001148	C 0.264192 3.597806 -1.095593
Pd -0.344130 -0.587911 0.041222	Pd -0.376779 0.140990 0.014226	Pd 0.073452 -0.507424 -0.179347
Cl 0.261185 -2.818908 -0.186641	Cl -3.286341 1.229671 1.605198	Cl -0.180343 -1.887570 -2.233287
H -5.037490 1.087314 -0.055983	H 4.238157 -1.583331 -0.518267	H 0.149170 4.147032 1.602170
H -6.132510 -1.096309 -0.245403	H 4.294273 -1.485418 -2.968485	H 0.140347 3.574328 3.982559
H -4.767610 -3.149154 -0.349189	H 2.326522 -0.686738 -4.220294	H 0.143441 1.208180 4.681792
H -2.315512 -3.023231 -0.256352	H 0.292044 0.025707 -3.024306	H 0.129144 -0.585931 2.998466
H -3.944291 2.909926 0.031367	H 3.997360 -1.603027 1.676980	H 0.287098 4.488731 -0.492169
H -2.476488 4.887424 0.123639	H 3.427007 -1.548668 4.077451	H 0.400234 4.643191 -2.950153
H 0.000215 4.554976 0.148958	H 1.164044 -0.770014 4.774547	H 0.376954 2.542689 -4.298810
H 0.871516 2.228006 0.107308	H -0.438244 -0.067053 2.995803	H 0.213364 0.360669 -3.081492
O 1.920087 -0.141091 0.437870	O -1.097586 -1.674749 0.316156	O -2.089000 -0.440792 -0.571411
O 2.607237 0.790857 -0.366398	O 0.472954 1.888226 0.409507	O 2.005588 -0.253794 -0.221204
C 2.494575 -0.119004 1.772550	C -1.873068 -2.563472 -0.439785	C -3.338454 -0.709260 0.106938
C 2.906725 0.252427 -1.671654	C 0.462798 3.142786 -0.213742	C 3.004518 -1.175453 0.142373
C 2.393407 1.277718 2.353863	C -1.351492 -2.724824 -1.858940	C -3.192097 -0.231327 1.531560
C 1.645601 -1.094825 2.557804	C -1.732129 -3.892409 0.299978	C -4.400680 0.087202 -0.628706
C 3.933420 -0.586516 1.717917	C -3.338841 -2.150804 -0.450606	C -3.626747 -2.195918 0.045724
C 3.825642 1.325351 -2.224505	C 1.497053 3.942685 0.576719	C 4.248821 -0.445400 -0.378037
C 3.605849 -1.086468 -1.582823	C 0.895736 3.070031 -1.669671	C 3.115140 -1.341205 1.647588
C 1.645053 0.145852 -2.506100	C -0.893326 3.823350 -0.088066	C 2.873977 -2.508954 -0.569282
H 1.909206 -0.086224 -3.535821	H -0.842137 4.853108 -0.439482	H 3.756526 -3.116793 -0.376259
H 0.996179 -0.651058 -2.150647	H -1.646615 3.305455 -0.672797	H 2.000929 -3.055041 -0.227501
H 1.096448 1.084853 -2.499515	H -1.207684 3.831549 0.953209	H 2.778024 -2.356728 -1.640383
H 4.122652 1.061643 -3.236181	H 1.570173 4.961215 0.197603	H 5.133923 -1.036729 -0.150091
H 3.322083 2.288718 -2.257534	H 1.214125 3.981661 1.625908	H 4.183710 -0.309444 -1.453688
H 4.720864 1.419994 -1.615296	H 2.473109 3.469327 0.500888	H 4.344555 0.527916 0.095527
H 3.829127 -1.433811 -2.589111	H 0.976577 4.069732 -2.093829	H 3.994168 -1.933247 1.896548
H 4.541544 -1.009346 -1.036467	H 1.865478 2.583353 -1.749372	H 3.207349 -0.368751 2.126229
H 2.964948 -1.823854 -1.108267	H 0.172620 2.512227 -2.256987	H 2.242505 -1.848973 2.043929
H 2.046343 -1.170484 3.566242	H -2.321535 -4.670411 -0.183569	H -5.374896 -0.067052 -0.169420
H 0.614151 -0.755919 2.627241	H -0.689640 -4.201988 0.316705	H -4.168344 1.148793 -0.600539
H 1.647978 -2.076811 2.095791	H -2.074957 -3.784309 1.326218	H -4.465788 -0.223877 -1.669456
H 2.804300 1.277862 3.360712	H -1.914362 -3.493443 -2.386299	H -4.142750 -0.337262 2.049108
H 2.953822 1.993299 1.759465	H -1.451962 -1.795367 -2.411786	H -2.444928 -0.817419 2.057176
H 1.356236 1.597238 2.417011	H -0.303335 -3.016049 -1.844623	H -2.901729 0.816008 1.560117
H 4.341598 -0.603080 2.725877	H -3.954722 -2.923650 -0.909097	H -4.571675 -2.411257 0.539945
H 3.994867 -1.589920 1.307724	H -3.684963 -1.995273 0.568789	H -3.705653 -2.533238 -0.986995
H 4.540988 0.084370 1.118549	H -3.479847 -1.230671 -1.008255	H -2.836478 -2.759955 0.530362
	Cl -1.855479 0.810099 -1.623665	Cl -0.140595 -2.365729 1.161620

	H -3.107733 1.186148 0.326713	H -2.010882 -1.004722 -1.354445
d'-HCl E_0 = -1531.7920334 E_{0+ZPE} = -1531.369048 H_{298} = -1531.342227 G_{298} = -1531.424280 N_{Imag} = 0 E_0(M06) =-1531.3380212 C -0.083438 0.043587 1.329071 C 0.093216 1.416440 1.469621 C 0.070634 1.951881 2.750910 C -0.122645 1.131694 3.844055 C -0.291758 -0.229756 3.666984 C -0.280035 -0.793214 2.397906 C 0.347191 2.176483 0.257318 N 0.412665 1.419966 -0.839598 C 0.690488 1.931356 -2.023919 C 0.908343 3.282355 -2.184461 C 0.831546 4.095282 -1.067477 C 0.555203 3.542793 0.165128 Pd -0.065987 -0.541108 -0.550227 Cl -0.548122 -2.751252 -0.220669 H 0.211220 3.011926 2.895087 H -0.138035 1.554051 4.836070 H -0.440568 -0.872186 4.521170 H -0.425366 -1.849114 2.256048 H 0.501359 4.160390 1.045282 H 0.992692 5.158229 -1.157100 H 1.131249 3.679929 -3.159938 H 0.744393 1.236108 -2.846132 O 1.799375 -0.939569 -1.033792 O -1.895003 0.215459 -0.719230 C 2.947545 -1.241107 -0.302154 C -3.173191 -0.348303 -0.613515 C 3.988427 -1.592285 -1.362570 C 3.419614 -0.027732 0.490399 C 2.752064 -2.427554 0.627799 C -4.109538 0.840714 -0.822550 C -3.419502 -1.377857 -1.707464 C -3.429770 -0.946004 0.761881 H -4.467001 -1.265981 0.850547 H -2.793502 -1.808953 0.932154 H -3.232899 -0.204413 1.533480 H -5.150952 0.523063 -0.788013 H -3.945363 1.586539 -0.048263 H -3.918286 1.300604 -1.789291 H -4.448051 -1.735542 -1.680576 H -3.241419 -0.927523 -2.682558 H -2.758810 -2.231212 -1.592708 H 4.370297 -0.225541 0.983442 H 3.549015 0.826107 -0.172194 H 2.694246 0.234089 1.258113 H 4.944695 -1.834600 -0.900958 H 3.651488 -2.447721 -1.941959 H 4.131098 -0.753193 -2.039693 H 3.688075 -2.681717 1.123707 H 2.014509 -2.199102 1.393016 H 2.399424 -3.291514 0.072691	**e** E_0 = -1759.0010014 E_{0+ZPE} = -1758.705518 H_{298} = -1758.683952 G_{298} = -1758.757461 N_{Imag} = 0 E_0(M06) =-1758.602222 C 0.584947 1.359277 -0.000148 C 1.956980 1.184502 -0.000136 C 2.734401 2.337951 -0.000298 C 2.132201 3.579919 -0.000474 C 0.751289 3.692877 -0.000514 C -0.055290 2.563236 -0.000348 C 2.461123 -0.180468 -0.000029 N 1.504854 -1.114812 0.000108 C 1.806797 -2.401967 0.000154 C 3.112340 -2.839247 0.000081 C 4.119950 -1.890995 -0.000049 C 3.796043 -0.551610 -0.000105 Pd -0.423581 -0.322999 0.000146 C -2.941434 -1.689733 0.001435 O -2.132327 0.603681 0.000337 C -3.288077 -0.201857 -0.000015 C -4.080673 0.138115 1.253727 Cl -0.398486 -0.405624 -2.306751 Cl -0.397874 -0.404369 2.307069 C -4.078986 0.136162 -1.255374 H -3.494937 -0.099081 -2.141025 H -5.016644 -0.417631 -1.289362 H -4.307182 1.199294 -1.271136 H -2.382924 -1.960206 0.898608 H -3.850997 -2.287035 0.000819 H -2.381285 -1.961509 -0.894418 H -5.018463 -0.415487 1.287185 H -3.497896 -0.095940 2.140536 H -4.308726 1.201298 1.267608 H 0.977588 -3.091437 0.000256 H 3.327153 -3.894316 0.000116 H 5.154719 -2.195833 -0.000112 H 4.566352 0.200353 -0.000216 H 2.743545 4.468167 -0.000596 H 0.289051 4.667892 -0.000661 H -1.132318 2.602221 -0.000352 H 3.810759 2.264377 -0.000287	**e'** E_0 = -1759.0010009 E_{0+ZPE} = -1758.705492 H_{298} = -1758.683959 G_{298} = -1758.756057 N_{Imag} = 0 E_0(M06) =-1758.6022867 O 2.133288 0.603745 -0.026186 Pd 0.424039 -0.322914 -0.009368 Cl 0.410326 -0.418583 2.297273 Cl 0.382275 -0.392105 -2.316317 C 4.143840 0.202229 -1.183359 C 3.288023 -0.202148 0.008395 H 4.372414 1.264015 -1.129515 H 5.082129 -0.351270 -1.197681 H 3.606243 0.015992 -2.109249 C 4.013289 0.068921 1.318256 C 2.944051 -1.687083 -0.092840 H 3.387420 -0.212376 2.160679 H 4.949847 -0.485410 1.370235 H 4.236693 1.129888 1.401247 H 3.850829 -2.286807 -0.046217 H 2.319623 -2.001791 0.746752 H 2.451664 -1.911114 -1.038391 N -1.504490 -1.114615 -0.002179 C -1.806453 -2.401750 -0.005483 C -3.111987 -2.839013 0.000957 C -4.119544 -1.890761 0.011130 C -3.795603 -0.551391 0.014349 C -2.460699 -0.180261 0.007376 H -0.977269 -3.091202 -0.013617 H -3.326828 -3.894071 -0.001986 H -5.154303 -2.195591 0.016473 H -4.565874 0.200576 0.022068 C -1.956516 1.184689 0.008919 C -2.733853 2.338160 0.017239 C -2.131584 3.580099 0.016154 C -0.750701 3.692987 0.006525 C 0.055776 2.563300 -0.001781 C -0.584504 1.359353 0.000246 H -2.742855 4.468375 0.022495 H -0.288414 4.667977 0.005245 H 1.132769 2.602292 -0.009879 H -3.810193 2.264640 0.024263
e'' E_0 = -1758.9948464 E_{0+ZPE} = -1758.698655 H_{298} = -1758.677320 G_{298} = -1758.748057 N_{Imag} = 0 E_0(M06) =-1758.5965617 O 1.115877 -1.308612 0.501923 Pd 0.431214 -0.048906 -0.830920	**f** E_0 = -1758.9668397 E_{0+ZPE} = -1758.673701 H_{298} = -1758.651329 G_{298} = -1758.724390 N_{Imag} = 0 E_0(M06) =-1758.5719132 C 0.386644 1.449525 -0.033719 C 1.775367 1.396118 -0.112688	**f'** E_0 = -1759.0182366 E_{0+ZPE} = -1758.724446 G_{298} = -1758.774846 N_{Imag} = 0 E_0(M06) =-1758.61969 O -2.272793 0.619903 -0.446379 Pd -0.419646 -0.301123 -0.228039 Cl -1.437637 -2.519937 -0.575306

Cl 2.383204 1.002128 -1.364992 Cl -0.644212 0.970105 -2.616731 C 3.497354 -1.689310 0.566915 C 2.244331 -1.303919 1.338232 H 3.733112 -0.944749 -0.185580 H 4.349558 -1.785417 1.238371 H 3.344361 -2.646277 0.071793 C 2.424188 0.028912 2.045571 C 1.928909 -2.384902 2.370200 H 1.511485 0.301513 2.571328 H 3.233197 -0.033561 2.771293 H 2.667515 0.810912 1.332774 H 2.760596 -2.508028 3.062425 H 1.039066 -2.117981 2.935304 H 1.749234 -3.334444 1.871900 N -1.322409 -1.005269 -0.390779 C -1.644293 -2.196020 -0.862785 C -2.817392 -2.817613 -0.496467 C -3.655699 -2.164536 0.389468 C -3.302735 -0.925086 0.878896 C -2.108904 -0.354796 0.469257 H -0.944432 -2.650613 -1.545055 H -3.060681 -3.786506 -0.897978 H -4.582997 -2.621359 0.697810 H -3.942974 -0.404119 1.569927 C -1.584276 0.937434 0.875360 C -2.215958 1.817600 1.746090 C -1.642987 3.038032 2.037624 C -0.439002 3.397279 1.457480 C 0.219878 2.540257 0.587094 C -0.365940 1.328096 0.336193 H -2.140661 3.716134 2.712178 H 0.001410 4.358018 1.674810 H 1.149648 2.816632 0.124220 H -3.161152 1.548807 2.191386	C 2.533552 2.561199 -0.204949 C 1.897858 3.783750 -0.218115 C 0.513299 3.841736 -0.136622 C -0.236693 2.681049 -0.043546 C 2.345173 0.062700 -0.098291 N 1.466261 -0.953897 0.003070 C 1.865923 -2.220524 -0.014852 C 3.192724 -2.558333 -0.112993 C 4.125896 -1.539244 -0.199527 C 3.700699 -0.233672 -0.194879 Pd -0.448914 -0.453979 0.138059 C -1.206015 -2.419984 0.407088 O -2.343775 0.375397 0.333299 C -3.454002 0.159175 -0.115404 C -4.554641 1.076136 0.299391 Cl -0.583859 -0.653008 -2.189885 Cl -0.247094 -0.350612 2.449422 C -3.793989 -0.946663 -1.043556 H -2.909593 -1.393520 -1.476731 H -4.355439 -1.693653 -0.481843 H -4.453573 -0.572979 -1.823364 H -0.622993 -2.908814 1.181252 H -2.226559 -2.334333 0.767445 H -1.176871 -2.965068 -0.532863 H -5.453332 0.511519 0.534755 H -4.248347 1.680998 1.143837 H -4.793625 1.724409 -0.543596 H 1.095055 -2.965443 0.050198 H 3.477174 -3.596516 -0.122329 H 5.178023 -1.765500 -0.275781 H 4.407708 0.573793 -0.271488 H 2.475723 4.691892 -0.288732 H 0.019170 4.802538 -0.143508 H -1.311762 2.745533 0.032229 H 3.611089 2.525993 -0.264227	Cl -0.444942 -0.324171 2.246302 C -4.501915 1.262067 -0.352906 C -3.359746 0.411850 0.081481 H -4.206041 1.952804 -1.132763 H -5.307451 0.618644 -0.702849 H -4.884951 1.805669 0.509452 C -0.235404 -0.109379 -2.254951 C -3.600355 -0.620347 1.103361 H -0.591588 -1.054895 -2.639891 H -0.877880 0.721447 -2.517705 H 0.798031 0.087515 -2.509225 H -4.596425 -0.542269 1.523767 H -3.452435 -1.594371 0.634269 H -2.826533 -0.553377 1.869035 N 1.458915 -0.963640 -0.145831 C 1.758329 -2.256312 -0.110269 C 3.059642 -2.678466 0.043290 C 4.056108 -1.728859 0.173235 C 3.727713 -0.391252 0.149578 C 2.403651 -0.016668 -0.007203 H 0.922313 -2.930985 -0.209373 H 3.273685 -3.733374 0.065907 H 5.084510 -2.029760 0.299112 H 4.484724 0.365275 0.265128 C 1.890153 1.338740 -0.028916 C 2.665453 2.488953 0.057552 C 2.058839 3.727554 0.037538 C 0.679931 3.821295 -0.066000 C -0.104420 2.681373 -0.148690 C 0.506643 1.449424 -0.130469 H 2.658136 4.621630 0.104189 H 0.208175 4.792250 -0.079381 H -1.175791 2.760113 -0.226700 H 3.739307 2.421612 0.141936
f″ E_0 = -1759.0293532 E_{0+ZPE} = -1758.736012 H_{298} = -1758.713244 G_{298} = -1758.787696 N_{Imag} = 0 E_0(M06) =-1758.6324198 O 2.419396 0.534299 -0.519238 Pd 0.356992 -0.395113 -0.209698 Cl 1.259684 -2.514331 -0.356285 Cl 0.572522 -0.126010 2.230532 C 3.777786 -0.692288 0.997515 C 3.520927 0.333527 -0.041718 H 3.754345 -1.668222 0.513898 H 4.741626 -0.546854 1.474235 H 2.965427 -0.689650 1.721608 C 0.115791 -0.481324 -2.232051 C 4.678925 1.144996 -0.521588 H 1.102809 -0.226612 -2.600922 H -0.169118 -1.484993 -2.511410 H -0.629700 0.249569 -2.521320 H 5.484413 0.482301 -0.832848 H 4.389662 1.795022 -1.338795 H 5.062925 1.736628 0.308712 N -0.528885 1.440862 -0.189250 C 0.138921 2.584101 -0.217209 C -0.505011 3.795697 -0.116100 C -1.882037 3.798097 0.027938 C -2.564733 2.603304 0.064898 C -1.859777 1.413232 -0.044561 H 1.207372 2.501460 -0.324990 H 0.063140 4.709958 -0.143362 H -2.419258 4.729527 0.116080 H -3.633952 2.585182 0.187490	**g** E_0 = -1565.8635331 E_{0+ZPE} = -1565.657464 H_{298} = -1565.641262 G_{298} = -1565.700735 N_{Imag} = 0 E_0(M06) =-1565.5303985 Pd -0.963991 -0.026133 -0.088999 Cl -2.563387 -1.637619 -0.213388 Cl -2.601663 1.699065 -0.315269 C -0.952243 -0.229682 1.929304 H -1.080169 -1.276629 2.153096 H -0.008345 0.175426 2.264676 H -1.812299 0.378363 2.174217 C 0.471817 -2.701859 -0.077844 H -0.493308 -3.180553 -0.070971 C 1.630925 -3.461462 -0.118606 H 1.557978 -4.538240 -0.139903 C 2.874500 -2.853174 -0.136003 C 0.558205 -1.324618 -0.054375 C 2.965442 -1.476959 -0.111422 C 1.810786 -0.703250 -0.067539 H 3.938202 -1.010357 -0.130776 H 3.771548 -3.451026 -0.169753 C 1.819809 0.753720 -0.045434 C 2.950530 1.555137 -0.033549 C 2.809828 2.926385 -0.017273 C 1.544167 3.482372 -0.014113 C 0.455404 2.638463 -0.026460 N 0.600154 1.318229 -0.039136 H 3.928411 1.105687 -0.039111 H 3.684636 3.557947 -0.007863 H 1.392151 4.548343 -0.004436 H -0.565459 2.990555 -0.034217	**g'** E_0 = -1565.8590584 E_{0+ZPE} = -1565.653857 H_{298} = -1565.637460 G_{298} = -1565.697805 N_{Imag} = 0 E_0(M06) =-1565.5285458 C -0.715679 1.050355 0.000237 C 0.575213 1.567499 -0.000091 C 0.705081 2.952820 -0.000014 C -0.404740 3.771425 0.000316 C -1.670974 3.217481 0.000495 C -1.836341 1.840852 0.000420 C 1.718460 0.653123 -0.000712 N 1.398139 -0.640137 -0.001703 C 2.340241 -1.566043 -0.002471 C 3.682127 -1.250598 -0.002280 C 4.034256 0.086540 -0.001186 C 3.048088 1.049592 -0.000386 Pd -0.785673 -0.913625 0.000107 C -2.786632 -1.142392 0.004174 Cl -0.808723 -1.016959 -2.298985 Cl -0.800956 -1.017615 2.299386 H -2.899391 -2.224382 0.006122 H -3.181823 -0.709335 0.912750 H -3.185192 -0.712121 -0.904259 H 2.004975 -2.591780 -0.003262 H 4.423720 -2.031593 -0.002942 H 5.072961 0.378219 -0.000941 H 3.310178 2.093424 0.000534 H -0.281096 4.842536 0.000352 H -2.543831 3.851737 0.000644 H -2.824130 1.417510 0.000454 H 1.687524 3.397327 -0.000297

C -2.420694 0.075478 -0.009836 C -3.777822 -0.201175 0.113250 C -4.216093 -1.507233 0.155199 C -3.299927 -2.543208 0.079774 C -1.942581 -2.289792 -0.040329 C -1.514646 -0.982386 -0.089517 H -5.269099 -1.719481 0.250566 H -3.640692 -3.566676 0.118475 H -1.233460 -3.097023 -0.089868 H -4.492719 0.604269 0.181024		
h E_0 = -1565.9136334 E_{0+ZPE} = -1565.706869 H_{298} = -1565.690142 G_{298} = -1565.752360 N_{Imag} = 0 E_0(M06) =-1565.5794667 Pd -0.378133 0.854327 -0.040896 Cl -2.598453 1.314595 -0.157320 Cl 0.210132 3.044374 -0.170939 C -0.210816 -1.173522 2.366902 H -0.869285 -0.468227 2.866333 H -0.167581 -2.076484 2.974960 H 0.783433 -0.742712 2.339686 C -2.070940 -1.929929 0.888110 H -2.708861 -1.862380 1.755537 C -2.575671 -2.408463 -0.294632 H -3.610341 -2.706703 -0.352387 C -1.763648 -2.499059 -1.419537 C -0.740792 -1.515940 1.005115 C -0.456556 -2.088955 -1.346944 C 0.065222 -1.587274 -0.146835 H 0.179969 -2.129390 -2.217357 H -2.162817 -2.867337 -2.350926 C 1.477884 -1.125336 -0.112000 C 2.606828 -1.908288 -0.216748 C 3.839882 -1.278453 -0.188832 C 3.904645 0.096697 -0.063477 C 2.729084 0.816784 0.023288 N 1.559291 0.199403 -0.000974 H 2.516772 -2.977792 -0.311845 H 4.745543 -1.860066 -0.263776 H 4.850283 0.612081 -0.039258 H 2.692705 1.892103 0.100985	**i** E_0 = -1759.0905844 E_{0+ZPE} = -1758.795611 H_{298} = -1758.772655 G_{298} = -1758.848810 N_{Imag} = 0 E_0(M06) =-1758.6895772 O 0.680305 -0.959953 -1.598135 Pd 1.337727 0.310352 -0.035498 Cl 3.210038 -0.990847 0.221249 Cl 2.031427 1.793183 1.553179 C 0.544652 -2.972011 -0.345726 C 0.512280 -2.165588 -1.589879 H 0.119439 -2.410926 0.480763 H 0.041415 -3.925223 -0.469180 H 1.594482 -3.138833 -0.101799 C -3.435620 -0.838144 -1.082725 C 0.291598 -2.869079 -2.884113 H -0.681050 -3.358238 -2.871752 H 0.354428 -2.176841 -3.714525 H 1.039190 -3.653378 -2.992533 N -0.293753 1.543583 -0.367781 C -0.025223 2.705376 -0.959980 C -1.004854 3.613821 -1.288528 C -2.314267 3.309298 -0.970574 C -2.585910 2.115419 -0.338696 C -1.552095 1.237400 -0.044363 H 1.015238 2.902147 -1.158775 H -0.736815 4.539321 -1.769651 H -3.111492 4.000641 -1.195550 H -3.589165 1.860423 -0.041602 C -1.813750 -0.015302 0.696290 C -1.159095 -0.201392 1.910484 C -1.411551 -1.320016 2.680412 C -2.315476 -2.265982 2.232402 C -2.952252 -2.090638 1.018017 C -2.722495 -0.969400 0.230329 H -0.899985 -1.449064 3.620911 H -2.519315 -3.145753 2.823348 H -3.643571 -2.842372 0.665639 H -0.452589 0.541568 2.249755 H -3.713736 -1.818584 -1.459861 H -2.823391 -0.346176 -1.833400 H -4.355264 -0.262657 -0.984729	**j** E_0 = -1759.0612142 E_{0+ZPE} = -1758.767962 H_{298} = -1758.743978 G_{298} = -1758.825475 N_{Imag} = 0 E_0(M06) =-1758.6605023 C 3.513279 -1.267961 0.176525 C 2.351467 -0.536217 -0.045555 C 1.189089 -1.173352 -0.502091 C 1.218362 -2.538404 -0.734019 C 2.382391 -3.256260 -0.509745 C 3.529263 -2.627360 -0.053740 C 2.252233 0.897953 0.173646 N 1.044657 1.414527 -0.111687 C 0.814699 2.708804 0.072247 C 1.780185 3.574104 0.535934 C 3.032698 3.062317 0.822851 C 3.269439 1.717815 0.643044 Pd -0.330759 0.028135 -0.786867 Cl -1.804599 -1.641308 -1.434091 Cl -2.220305 1.769581 -1.266918 H 0.335099 -3.037266 -1.094565 H 2.391476 -4.319708 -0.697103 H 4.410025 -0.780219 0.527340 H 4.431163 -3.193935 0.116913 H 4.235370 1.299100 0.867197 H 3.817478 3.706540 1.187906 H 1.547813 4.617118 0.669060 H -0.180129 3.053018 -0.156273 O -2.405127 0.440058 2.478812 C -2.017972 -0.697341 2.564425 C -0.627645 -1.022374 3.019314 C -2.890250 -1.855782 2.190397 C -3.697973 1.108492 -0.498511 H -4.514847 1.749804 -0.800514 H -3.541484 1.119094 0.571856 H -3.810192 0.100734 -0.874356 H -0.124523 -1.623758 2.263979 H -0.068315 -0.111912 3.199848 H -0.669212 -1.616338 3.931427 H -2.635720 -2.147415 1.169834 H -2.718484 -2.714325 2.834491 H -3.934414 -1.564171 2.218996
j' E_0 = -1565.9007034 E_{0+ZPE} = -1565.694349 E_{298} = -1565.678370 H_{298} = -1565.677426 G_{298} = -1565.740528 N_{Imag} = 0 E_0(M06) =-1565.5649887 Pd -0.704125 -0.278015 -0.067853 Cl -1.968809 -2.217416 -0.100791 Cl -2.952871 1.100967 -0.255543 C -4.214896 0.215579 0.651418 H -4.158916 0.528909 1.684618 H -5.164118 0.483428 0.208473		

H -3.992353 -0.837763 0.539675 C 1.237915 -2.555082 0.023431 H 0.396520 -3.225766 0.004241 C 2.529352 -3.055012 0.063836 H 2.680842 -4.124058 0.076820 C 3.622485 -2.204150 0.086233 C 1.026367 -1.187274 0.006355 C 3.422567 -0.840536 0.069776 C 2.130772 -0.325175 0.030833 H 4.275899 -0.179827 0.088056 H 4.624112 -2.603318 0.116478 C 1.835316 1.097506 0.020955 C 2.776300 2.118928 0.048252 C 2.359921 3.430592 0.047094 C 1.005015 3.711050 0.022127 C 0.124034 2.653859 -0.005111 N 0.523248 1.387727 -0.010751 H 3.825491 1.879839 0.071356 H 3.084699 4.229586 0.067614 H 0.633063 4.721649 0.024340 H -0.940563 2.819823 -0.018682		

k	**l**	**m**
E_0 = -1513.3119884 E_{0+ZPE} = -1513.050862 H_{298} = -1513.031597 G_{298} = -1513.098144 N_{Imag} = 0 E_0(M06) =-1513.0362251 O -0.968606 0.579393 -0.300197 O -1.324885 -0.526217 0.507416 Pd 1.044091 -0.161929 0.057173 C -3.236146 -1.134536 -0.881781 C -1.923307 -1.591436 -0.287630 H -3.927760 -0.810327 -0.110017 H -3.082906 -0.325195 -1.589239 H -3.690468 -1.964158 -1.417576 C -0.961336 -2.049041 -1.362743 C -2.125461 -2.658045 0.768382 H -0.021799 -2.396886 -0.934145 H -1.401229 -2.881352 -1.906997 H -0.754629 -1.255770 -2.075821 H -2.573747 -3.534826 0.308743 H -1.176821 -2.950534 1.210268 H -2.787128 -2.305840 1.555068 C -2.873099 1.861714 0.517330 C -1.374671 1.847258 0.328965 H -3.392618 1.729125 -0.426504 H -3.190870 1.094687 1.216412 H -3.158918 2.827640 0.925904 C -0.646199 2.013959 1.643937 C -0.929017 2.858673 -0.703242 H 0.430866 2.051854 1.495811 H -0.953559 2.949856 2.104122 H -0.886371 1.206665 2.330364 H -1.151601 3.856371 -0.333175 H 0.139382 2.787675 -0.884515 H -1.458584 2.713913 -1.641147 Cl 2.417233 1.290095 -0.972744 Cl 2.745940 -1.446615 0.722476	E_0 = -1513.262947 E_{0+ZPE} = -1513.004704 H_{298} = -1512.984910 G_{298} = -1513.052310 N_{Imag} = 0 E_0(M06) =-1512.9996807 O -1.273039 0.976888 -0.309780 O 1.317942 0.635059 -0.832940 Pd -0.081369 -0.551273 -0.271996 C 1.645603 2.228364 0.944149 C 2.264567 1.244979 -0.027664 H 0.960430 2.893048 0.426840 H 1.090647 1.697524 1.712552 H 2.423766 2.815633 1.425976 C 3.192765 0.248842 0.635875 C 3.028593 2.014474 -1.138818 H 3.591128 -0.447893 -0.095105 H 4.015319 0.770147 1.119805 H 2.656459 -0.319740 1.391216 H 3.832449 2.559882 -0.648943 H 3.447657 1.323054 -1.861390 H 2.368466 2.713599 -1.640058 C -3.353296 1.571008 -1.154227 C -2.633100 0.670219 -0.156064 H -3.131530 2.612382 -0.938422 H -3.027619 1.352013 -2.167565 H -4.429713 1.422140 -1.087412 C -2.893206 -0.794136 -0.497126 C -3.087145 0.983996 1.260793 H -2.369159 -1.473001 0.186334 H -3.949105 -1.033702 -0.392116 H -2.605295 -1.020703 -1.524060 H -4.161339 0.840766 1.363936 H -2.583316 0.345251 1.980217 H -2.850839 2.017644 1.498908 Cl 0.020420 -0.788901 1.947420 Cl 1.104088 -2.482365 -0.670870	E_0 = -1513.3344753 E_{0+ZPE} = -1513.077463 H_{298} = -1513.056907 G_{298} = -1513.125632 N_{Imag} = 0 E_0(M06) =-1513.065613 O -0.629125 1.113164 0.583954 O 1.810916 0.136270 -0.490878 Pd -0.092486 -0.684850 -0.034987 Cl 0.768080 -2.725728 -0.697746 Cl -2.153041 -1.553583 0.192670 C -2.867105 1.929115 0.292097 C -1.434909 1.939256 -0.219536 H -3.286044 0.930527 0.226792 H -2.885942 2.238251 1.334848 H -3.493967 2.611351 -0.281000 C -0.848928 3.341000 -0.083398 C -1.387396 1.511142 -1.681991 H 0.161760 3.374671 -0.486423 H -1.455691 4.069955 -0.618254 H -0.813704 3.628319 0.964982 H -1.935236 2.212057 -2.308675 H -0.358936 1.480544 -2.042977 H -1.845148 0.531920 -1.817942 C 2.323774 1.511996 1.380488 C 2.569814 0.927326 0.036419 H 1.256682 1.542024 1.576663 H 2.823748 0.882068 2.117720 H 2.762257 2.502622 1.455502 C 0.220977 -1.197084 1.894737 C 3.805670 1.319824 -0.694792 H -0.255616 -2.152966 2.040610 H 1.299929 -1.243608 1.941873 H -0.245184 -0.366002 2.404298 H 4.665628 1.270405 -0.030415 H 3.953539 0.689380 -1.562675 H 3.704879 2.358959 -1.007952

n	**o**	**o'**
E_0 = -1320.1527057 E_{0+ZPE} = -1319.984393 H_{298} = -1319.969738 G_{298} = -1320.026091 N_{Imag} = 0 E_0(M06) =-1319.9515385	E_0 = -1799.4946885 E_{0+ZPE} = -1799.149423 H_{298} = -1799.125209 G_{298} = -1799.202041 N_{Imag} = 0 E_0(M06) =-1799.0768053	E_0 = -1799.4990913 E_{0+ZPE} = -1799.154269 H_{298} = -1799.129754 G_{298} = -1799.208058 N_{Imag} = 0 E_0(M06) =-1799.0817002

O 1.211996 -0.271516 0.771833 Pd -0.590411 -0.254957 0.069467 Cl -2.695471 -0.810107 -0.645223 Cl -0.770747 1.934308 -0.297475 C 2.826609 1.248415 -0.139695 C 2.304348 -0.178131 -0.105396 H 2.073318 1.922826 -0.536164 H 3.079637 1.573098 0.866280 H 3.717355 1.320033 -0.761292 C 3.355393 -1.111867 0.486837 C 1.915655 -0.648402 -1.500852 H 2.987758 -2.134503 0.508376 H 4.265714 -1.077017 -0.108984 H 3.592128 -0.807663 1.502540 H 2.776001 -0.652098 -2.166207 H 1.518549 -1.663783 -1.473081 H 1.175650 0.018290 -1.949148 C -1.222561 0.043974 1.959857 H -2.128834 0.626136 1.904327 H -1.374876 -0.989122 2.252472 H -0.370396 0.528585 2.412078	N -0.423898 1.451100 -0.222668 C -1.620019 1.471106 0.365295 C -2.344033 2.646583 0.490202 C -1.817831 3.812759 -0.027088 C -0.591970 3.774564 -0.663508 C 0.068919 2.565246 -0.739152 C -2.130243 0.169814 0.825024 C -1.254999 -0.753179 1.401376 C -1.695364 -2.031083 1.719023 C -3.003600 -2.393956 1.471242 C -3.877609 -1.469405 0.921469 C -3.447685 -0.195298 0.601599 Pd 0.460430 -0.642677 -0.571956 Cl 1.968930 -0.176051 -2.180434 C 0.986357 -2.575605 -0.869713 O 1.795259 -0.738816 0.902950 C 2.584304 0.222607 1.543166 C 3.420285 1.047336 0.578714 Cl -1.222167 -0.956055 -2.147743 C 1.752719 1.140716 2.432019 C 3.518167 -0.609098 2.422972 H -0.263357 -0.450390 1.708382 H -1.008585 -2.728451 2.173225 H -3.347378 -3.388827 1.706507 H -4.123983 0.495421 0.123153 H -4.898608 -1.752170 0.717057 H -3.296176 2.640364 0.994730 H -2.361084 4.740719 0.062343 H -0.153900 4.657407 -1.098504 H 1.018710 2.472078 -1.243247 H 4.169714 0.036265 3.010590 H 2.938759 -1.230168 3.101763 H 4.131821 -1.257300 1.803285 H 4.092808 1.702200 1.130767 H 4.007762 0.401096 -0.066239 H 2.790839 1.664609 -0.055344 H 2.390431 1.835997 2.975292 H 1.049694 1.725062 1.844270 H 1.195377 0.559721 3.165211 H 1.946318 -2.653821 -0.382416 H 0.989024 -2.768258 -1.930853 H 0.177878 -3.078441 -0.351735	O 0.406174 -1.304787 0.701531 Pd 0.898238 0.048892 -0.623469 Cl 1.153764 1.463045 -2.473505 Cl 2.804003 0.852183 0.276536 C 0.787101 -0.405934 2.912396 C 0.863143 -1.610220 1.984232 H 1.475065 0.370553 2.591622 H -0.222058 0.000507 2.914784 H 1.044733 -0.690398 3.931233 C -0.121235 -2.678052 2.466000 C 2.266551 -2.200071 1.972238 H -0.106855 -3.530710 1.792245 H 0.148254 -3.014501 3.466001 H -1.129898 -2.274697 2.489636 H 2.564834 -2.500589 2.975321 H 2.295168 -3.082761 1.335785 H 2.990577 -1.477894 1.607630 C 2.079020 -1.305077 -1.538801 H 2.474792 -1.940716 -0.762723 H 1.338086 -1.797711 -2.160172 H 2.825584 -0.770944 -2.105790 C -2.203925 -0.136551 -0.376476 C -1.647773 -0.367703 -1.634557 H -1.125936 0.428675 -2.148504 C -1.865910 -1.575060 -2.281271 C -3.002942 -1.107624 0.203400 C -2.639643 -2.550928 -1.684247 C -3.214479 -2.309360 -0.446700 H -3.426500 -0.941976 1.182063 H -3.819672 -3.069861 0.022204 H -2.806255 -3.493267 -2.182175 H -1.443649 -1.736313 -3.261193 C -1.884365 1.117684 0.324234 N -0.609889 1.501912 0.278696 C -0.244058 2.639946 0.845790 C -1.137593 3.453067 1.513386 C -2.459009 3.054982 1.586080 C -2.841994 1.874393 0.981531 H 0.802321 2.892284 0.762865 H -0.799431 4.371444 1.963739 H -3.187950 3.664852 2.097108 H -3.869705 1.550053 0.989829
o'' E_0 = -1799.4988057 E_{0+ZPE} = -1799.153735 H_{298} = -1799.129335 G_{298} = -1799.207014 N_{Imag} = 0 E_0(M06) =-1799.079637 O 1.588753 -0.421528 1.065103 Pd 0.449557 -0.485288 -0.549686 Cl -1.149113 -0.854318 -2.199459 Cl 1.897581 0.310914 -2.083333 C 2.937940 1.587217 1.053014 C 2.855205 0.096739 1.349208 H 2.870307 1.768629 -0.015500 H 2.127283 2.110763 1.555253 H 3.882390 1.997585 1.406646 C 3.000842 -0.122057 2.855874 C 3.963509 -0.656443 0.627005 H 2.905467 -1.179187 3.091052 H 3.974512 0.224863 3.198903 H 2.227936 0.422669 3.392682 H 4.939643 -0.269037 0.914592 H 3.933655 -1.712802 0.888736 H 3.864504 -0.556417 -0.449556 C 1.189676 -2.314184 -0.976709 H 2.136591 -2.362640 -0.462525 H 0.419726 -2.941897 -0.542895	**p** E_0 = -1799.545918 E_{0+ZPE} = -1799.199218 H_{298} = -1799.175147 G_{298} = -1799.251312 N_{Imag} = 0 E_0(M06) =-1799.1185484 N -0.726666 1.420347 0.148277 C -1.883953 0.993004 0.656521 C -2.802687 1.897860 1.168990 C -2.504056 3.244660 1.138706 C -1.305438 3.666601 0.594767 C -0.441824 2.710401 0.099915 C -2.082428 -0.461230 0.598704 C -1.157526 -1.237951 -0.108765 C -1.322167 -2.605237 -0.193079 C -2.399171 -3.216660 0.429946 C -3.315608 -2.460459 1.137490 C -3.155405 -1.092548 1.221068 Pd 0.405115 -0.214022 -0.824602 Cl 2.209591 1.251782 -1.521672 C 1.293075 -1.778871 -1.747481 O 1.335690 -0.828425 1.052828 C 2.469370 -0.380483 1.849393 C 3.709112 -0.722474 1.056742 Cl -0.794594 0.064430 -2.725504 C 2.351338 1.107596 2.095029	**p'** E_0 = -1799.5453041 E_{0+ZPE} = -1799.198662 H_{298} = -1799.174554 G_{298} = -1799.250615 N_{Imag} = 0 E_0(M06) =-1799.117835 O 1.220852 -0.622139 1.160214 Pd 0.395869 -0.239468 -0.810846 Cl -0.744832 -0.095405 -2.760942 Cl 2.230982 1.164834 -1.559455 C 2.524236 1.178322 2.001624 C 2.456105 -0.325360 1.872392 H 2.565542 1.638461 1.019105 H 1.656594 1.552688 2.539520 H 3.420051 1.456603 2.552271 C 2.332204 -0.987141 3.230682 C 3.627514 -0.877229 1.089764 H 2.237126 -2.069433 3.135791 H 3.223371 -0.789988 3.820675 H 1.471706 -0.603133 3.773970 H 4.556931 -0.647674 1.606718 H 3.556813 -1.959399 0.992632 H 3.661826 -0.429956 0.100681 C 1.308051 -1.869966 -1.587899 H 1.640245 -2.448050 -0.732150 H 0.602382 -2.404261 -2.207897

H 1.253683 -2.411342 -2.049103	C 2.413247 -1.164401 3.146179	H 2.135178 -1.479262 -2.164152
C -2.245961 -0.055808 0.828905	H 0.602842 -1.032542 1.629857	C -2.093424 -0.410499 0.606711
C -3.496404 -0.541843 0.485148	H -0.620874 -3.209346 -0.744342	C -3.173551 -1.006637 1.247621
H -4.214933 0.108002 0.010928	H -2.519861 -4.286840 0.356623	H -3.884729 -0.400681 1.786989
C -3.797354 -1.876441 0.681498	H -3.873177 -0.513461 1.780925	C -3.353671 -2.375211 1.209039
C -1.306780 -0.917296 1.401743	H -4.153737 -2.934760 1.623266	C -1.180967 -1.223492 -0.074842
C -2.859244 -2.739891 1.225761	H -3.744018 1.559736 1.566984	C -2.452613 -3.166286 0.522562
C -1.619885 -2.257104 1.594198	H -3.210743 3.961748 1.527265	C -1.368359 -2.588895 -0.123353
H -0.374639 -0.526208 1.785888	H -1.045394 4.710571 0.541024	H 0.863534 -1.454166 1.459753
H -0.891027 -2.909995 2.049160	H 0.503623 2.959794 -0.359659	H -0.686048 -3.219259 -0.669606
H -3.101438 -3.781795 1.364612	H 3.256329 -0.896251 3.777547	H -2.591893 -4.235812 0.477952
H -4.764179 -2.252637 0.384994	H 1.503222 -0.941973 3.704633	H -4.198333 -2.820819 1.710399
C -1.853855 1.326736 0.513089	H 2.456495 -2.234369 2.956061	C -1.875430 1.041641 0.613117
N -0.640704 1.473707 -0.018531	H 4.591745 -0.408770 1.609437	N -0.739655 1.440666 0.038854
C -0.226503 2.678174 -0.375045	H 3.772115 -1.795288 0.890526	C -0.439439 2.723903 -0.057851
C -0.998558 3.809783 -0.204005	H 3.700579 -0.209490 0.099854	C -1.269399 3.705487 0.445174
C -2.252826 3.669611 0.358216	H 3.187364 1.449517 2.701586	C -2.446275 3.314793 1.055666
C -2.690609 2.411821 0.720802	H 2.367527 1.640487 1.149160	C -2.758191 1.973348 1.140563
H 0.751813 2.727274 -0.827044	H 1.430189 1.343134 2.625381	H 0.491093 2.945779 -0.559917
H -0.622407 4.771300 -0.511700	H 1.709924 -2.353502 -0.928330	H -0.999406 4.743971 0.350105
H -2.884226 4.530808 0.513132	H 2.050522 -1.336500 -2.379241	H -3.125298 4.051750 1.456224
H -3.658480 2.265379 1.171459	H 0.550941 -2.316338 -2.320173	H -3.681197 1.659688 1.597084
q	**q'**	**q″**
E_0 = -1992.6834917	E_0 = -1992.6815687	E_0 = -1992.6633164
E_{0+ZPE} = -1992.245305	E_{0+ZPE} = -1992.243421	E_{0+ZPE} = -1992.225687
H_{298} = -1992.216168	H_{298} = -1992.214290	H_{298} = -1992.196342
G_{298} = -1992.304920	G_{298} = -1992.303211	G_{298} = -1992.285424
N_{Imag} = 0	N_{Imag} = 0	N_{Imag} = 0
E_0(M06) =-1992.185843	E_0(M06) =-1992.1851668	E_0(M06) =-1992.1694726
C 2.565312 1.317139 1.090484	C 2.185511 1.588492 1.176240	C 2.900948 -0.623585 0.571189
C 2.987316 0.581832 -0.009775	C 2.735767 1.023527 0.033182	C 2.647416 -0.089800 -0.686766
C 3.644935 1.216572 -1.054446	C 3.227550 1.841639 -0.975102	C 3.098713 -0.757818 -1.820138
C 3.871927 2.578460 -1.003978	C 3.166887 3.215375 -0.842833	C 3.772772 -1.957849 -1.699764
C 3.462007 3.309199 0.097972	C 2.636786 3.778110 0.305781	C 4.016258 -2.490798 -0.445043
C 2.811880 2.676980 1.143148	C 2.148978 2.964081 1.312337	C 3.584707 -1.820014 0.685598
C 2.813348 -0.880487 -0.026401	C 2.897036 -0.437108 -0.054279	C 1.987269 1.220064 -0.817438
N 1.602078 -1.411807 0.155222	N 1.847333 -1.243394 0.116963	N 0.875906 1.493136 -0.125085
C 1.453451 -2.732575 0.227507	C 2.016601 -2.564168 0.147718	C 0.395865 2.737683 -0.148477
C 2.509348 -3.601447 0.089668	C 3.243393 -3.156233 -0.031340	C 0.938091 3.745189 -0.910300
C 3.767016 -3.075180 -0.134761	C 4.337561 -2.342152 -0.253700	C 2.047460 3.457346 -1.681240
C 3.917162 -1.707393 -0.184443	C 4.160874 -0.977057 -0.254945	C 2.578507 2.189668 -1.620869
Pd -0.102101 -0.345628 0.095511	Pd -0.078188 -0.652405 0.072263	Pd -0.237173 0.193629 1.130341
Cl 0.187637 -0.226358 -2.203097	Cl -0.207012 -1.027280 2.361781	Cl 0.793387 1.286462 2.844647
Cl -0.336367 -0.613182 2.406937	Cl 0.164006 -0.326236 -2.225102	Cl -1.446836 -1.025096 2.626304
H 3.948376 0.647612 -1.919607	H 3.630647 1.399914 -1.873318	H 2.898835 -0.348870 -2.799350
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H 2.054512 0.821618 1.902561	H 1.799862 0.950315 1.957163	H 2.575954 -0.095769 1.454876
H 2.493739 3.242149 2.005477	H 1.735661 3.399167 2.208965	H 3.779975 -2.226486 1.665539
H 4.885473 -1.255221 -0.318554	H 4.993579 -0.305524 -0.380184	H 3.479973 1.940201 -2.154890
H 4.622042 -3.722262 -0.253504	H 5.318299 -2.765399 -0.405002	H 2.509912 4.215846 -2.293478
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H 0.451370 -3.087386 0.397422	H 1.130156 -3.149849 0.321078	H -0.455729 2.927133 0.481571
O -1.994834 0.635225 0.068349	O -2.168369 -0.269695 -0.170163	O -2.756180 -0.581819 -0.691531
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C -2.100906 2.097600 0.002569	C -3.117183 -1.390569 -0.208733	C -3.052845 0.732075 -1.177211
C -3.609893 -1.055632 -0.260694	C -2.542820 2.055887 -0.043152	C -1.202076 -2.251000 -0.873514
C -1.945087 2.561956 -1.428623	C -3.538735 -1.758463 1.197082	C -3.080618 1.703952 -0.012072
C -3.438485 2.499634 0.583974	C -4.297828 -0.978350 -1.060379	C -2.107517 1.154330 -2.281667
C -0.966850 2.589043 0.871545	C -2.351755 -2.517010 -0.866837	C -4.457851 0.541800 -1.720773
C -4.690660 -1.277627 -1.302497	C -3.470113 2.919916 0.791068	C -1.296666 -2.374458 -2.379667
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H -3.251285 -3.154244 -0.034543 H -2.133847 -2.347995 -1.145056 H -1.964809 -2.150617 0.612971 H -3.514429 3.584391 0.572808 H -4.255891 2.099712 -0.007012 H -3.535049 2.159110 1.611038 H -1.927705 3.649872 -1.441791 H -1.021132 2.186940 -1.857412 H -2.771755 2.222082 -2.043518 H -1.046440 3.669931 0.961551 H -1.011145 2.147531 1.862985 H -0.001751 2.361286 0.426370	H -0.995559 3.537072 -0.109210 H -0.803739 2.343867 1.178983 H -0.430049 1.926045 -0.500915 H -4.995063 -1.810667 -1.121536 H -4.818944 -0.135644 -0.618181 H -3.980913 -0.719342 -2.066532 H -4.162164 -2.649106 1.150880 H -2.671676 -1.964091 1.816733 H -4.111814 -0.960397 1.656691 H -3.039458 -3.340567 -1.043938 H -1.922966 -2.204629 -1.814468 H -1.557175 -2.880007 -0.218414	H 0.386894 -3.635719 -0.638067 H 0.937446 -1.982018 -0.841624 H 0.236723 -2.506220 0.703838 H -2.428810 2.113990 -2.679940 H -1.089798 1.255742 -1.922989 H -2.116135 0.429570 -3.091238 H -3.273516 2.716803 -0.360332 H -3.857814 1.420946 0.691918 H -2.143060 1.695303 0.536167 H -4.869185 1.504418 -2.015394 H -4.455611 -0.116796 -2.585255 H -5.103280 0.114506 -0.957877
r E_0 = -1992.6301793 E_{0+ZPE} = -1992.193990 H_{298} = -1992.164967 G_{298} = -1992.251508 N_{Imag} = 0 E_0(M06) =-1992.1469188 C 2.191045 -1.239393 0.261807 C 2.719395 0.052974 0.243785 C 3.820433 0.335789 -0.547054 C 4.366056 -0.653147 -1.342535 C 3.821262 -1.927838 -1.354881 C 2.740624 -2.221917 -0.548764 Pd -0.234950 -0.210950 -0.316492 C 2.046609 1.109761 1.011438 N 0.715677 1.159358 0.925693 C 0.013982 2.019427 1.645555 C 0.628627 2.936252 2.470010 C 2.008937 2.937574 2.543225 C 2.725513 2.011652 1.814038 H 4.212942 1.339848 -0.586476 H 5.206696 -0.422127 -1.978108 H 4.242261 -2.687160 -1.994777 H 1.411404 -1.494851 0.969845 H 2.317549 -3.213632 -0.540794 H 3.799461 1.955311 1.878249 H 2.522636 3.641882 3.179003 H 0.032022 3.628099 3.040472 H -1.055059 1.946842 1.530666 O -1.921599 0.763879 -0.157400 O -0.654567 -1.019130 1.452188 C -1.616204 -1.864559 3.351053 C -1.588265 -1.996624 1.826055 H -0.621488 -2.019136 3.761992 H -1.958887 -0.872986 3.635114 H -2.289167 -2.605834 3.779915 C -2.983934 -1.734007 1.283940 C -1.109554 -3.393407 1.456260 H -3.001829 -1.806614 0.201846 H -3.679700 -2.465571 1.692267 H -3.316938 -0.739363 1.566294 H -1.788897 -4.149960 1.846213 H -1.050676 -3.509141 0.379352 H -0.124554 -3.573745 1.884992 C -2.751938 0.873155 -2.460771 C -2.519957 1.574687 -1.137972 H -1.806154 0.654593 -2.946300 H -3.287144 -0.059003 -2.311370 H -3.337610 1.517704 -3.113415 C -3.880281 1.816939 -0.454710 C -1.804626 2.901143 -1.318524 H -3.750631 2.290238 0.514622 H -4.467922 2.477074 -1.089859 H -4.411369 0.879946 -0.324409 H -2.368594 3.537104 -1.997906 H -1.715255 3.423848 -0.368008 H -0.814345 2.752126 -1.736096	**r′** E_0 = -1992.6139974 E_{0+ZPE} = -1992.178251 H_{298} = -1992.148975 G_{298} = -1992.236975 N_{Imag} = 0 E_0(M06) =-1992.1322502 N 1.738161 -0.208096 -0.624192 C 2.412695 0.830635 -0.121919 C 3.768728 0.978400 -0.369107 C 4.418270 0.055481 -1.160636 C 3.697503 -0.994187 -1.696473 C 2.355171 -1.087137 -1.402644 C 1.650445 1.820624 0.653010 C 0.689653 1.408910 1.575282 C -0.110601 2.346657 2.211804 C 0.057634 3.691070 1.952019 C 1.031351 4.102043 1.054381 C 1.822243 3.174597 0.405116 Pd -0.371522 -0.248289 -0.284431 Cl -0.827329 -1.797409 -1.853998 O -2.221468 -0.205616 0.309663 C -3.352858 0.421436 -0.232798 C -3.305492 1.933074 -0.076705 O -0.295921 -1.485317 1.274480 C 0.441843 -2.620680 1.616197 C 0.376038 -3.726935 0.575892 Cl -0.444422 1.455393 -1.893878 C -3.639619 0.020344 -1.669925 C -4.455826 -0.144654 0.671857 C 1.891951 -2.300342 1.962857 C -0.274402 -3.097649 2.884296 H 0.611541 0.369501 1.863078 H -0.855988 2.011545 2.915264 H -0.566764 4.421422 2.442125 H 2.536445 3.499883 -0.334888 H 1.157151 5.151914 0.840048 H 4.296441 1.809055 0.069045 H 5.473977 0.155860 -1.359191 H 4.157370 -1.731752 -2.332483 H 1.739381 -1.873844 -1.805713 H 0.211618 -3.987900 3.282284 H -0.253955 -2.318828 3.642253 H -1.310808 -3.326833 2.655770 H 0.830893 -4.634702 0.968891 H -0.656040 -3.934927 0.310413 H 0.905071 -3.450700 -0.331014 H 2.387049 -3.176385 2.378569 H -4.581729 0.462307 -1.989804 H -2.852700 0.368641 -2.330814 H -3.713482 -1.059814 -1.755290 H -4.265349 2.369218 -0.349819 H -3.098428 2.191537 0.959837 H -2.539206 2.370993 -0.706742 H -5.417563 0.271952 0.376442 H -4.491895 -1.226216 0.584183 H -4.264484 0.113947 1.709783	**r″** E_0 = -1992.6271411 E_{0+ZPE} = -1992.190737 H_{298} = -1992.161777 G_{298} = -1992.248300 N_{Imag} = 0 E_0(M06) =-1992.1437527 C 3.821968 -0.308275 -0.785024 C 2.752186 -0.050896 0.056019 C 2.177916 1.219522 0.075753 C 2.648300 2.207597 -0.775334 C 3.699361 1.938910 -1.628741 C 4.290591 0.685171 -1.622996 C 2.162770 -1.114291 0.879835 N 0.831471 -1.208021 0.887866 C 0.212182 -2.100257 1.641173 C 0.913104 -2.992853 2.423299 C 2.293466 -2.939267 2.411422 C 2.925027 -1.988780 1.636542 Pd -0.272407 0.098225 -0.304091 Cl 0.607692 -0.986664 -2.183967 Cl -1.230279 1.671336 -1.652693 H 1.426465 1.454530 0.819094 H 2.189652 3.183394 -0.761505 H 4.060849 2.701816 -2.299983 H 4.249997 -1.297585 -0.826636 H 5.107046 0.473147 -2.295633 H 3.998224 -1.895818 1.626101 H 2.873803 -3.623063 3.011263 H 0.379800 -3.710413 3.023816 H -0.863934 -2.083971 1.584137 O -1.748414 -1.162502 -0.090807 O -0.636872 0.901751 1.485799 C -2.877475 -1.357004 -0.905243 C -1.250464 2.096060 1.885472 C -2.566476 -1.588306 -2.369417 C -3.386461 -2.674477 -0.283620 C -3.932678 -0.284866 -0.727996 C -1.112374 2.045116 3.409563 C -0.522551 3.328259 1.363638 C -2.724554 2.149814 1.526497 H -3.190240 3.029660 1.967855 H -2.859698 2.194907 0.451731 H -3.229005 1.266363 1.908757 H -1.541590 2.940172 3.858066 H -1.628984 1.173188 3.801921 H -0.064268 1.981662 3.691535 H -0.990571 4.236228 1.740072 H 0.513783 3.328960 1.699535 H -0.546955 3.362043 0.278458 H -4.299925 -2.961962 -0.800200 H -2.648525 -3.461387 -0.404679 H -3.608780 -2.541877 0.771405 H -3.482914 -1.865851 -2.887145 H -2.173286 -0.684353 -2.824555 H -1.832823 -2.377111 -2.494244 H -4.847348 -0.585049 -1.235584

Cl 0.732706 0.803576 -2.201049 Cl -1.053753 -1.863933 -1.658043	H 2.457512 -1.989152 1.089767 H 1.937337 -1.507141 2.706886	H -4.155293 -0.135525 0.323966 H -3.601824 0.655256 -1.156219
s E_0 = -1992.6608278 E_{0+ZPE} = -1992.227608 H_{298} = -1992.196831 G_{298} = -1992.289278 N_{Imag} = 0 E_0(M06) =-1992.1779297 O 2.318369 -0.540412 1.060256 Pd 0.783300 -0.475262 -0.474030 Cl 0.294345 -2.721638 0.048649 Cl -0.809597 -0.451829 -2.070519 C 3.643367 -2.501069 0.727195 C 3.209795 -1.270682 1.441620 H 2.853568 -2.886371 0.095391 H 4.514514 -2.243810 0.122754 H 3.960415 -3.257460 1.439641 C 2.037631 -1.075083 -1.935245 C 3.938070 -0.917833 2.695507 H 1.806615 -0.483489 -2.805108 H 3.006274 -0.835361 -1.518555 H 1.849087 -2.129668 -2.072479 H 5.010031 -1.043388 2.563047 H 3.706390 0.093349 3.006065 H 3.627189 -1.615124 3.473490 N -0.606739 0.583668 1.276429 C 0.189181 1.379061 1.986064 C -0.266080 2.353727 2.848181 C -1.629722 2.535315 2.967269 C -2.463985 1.723915 2.232760 C -1.927196 0.745452 1.398999 H 1.244653 1.239766 1.829374 H 0.437593 2.958860 3.396212 H -2.036172 3.288402 3.625061 H -3.535147 1.810568 2.310693 C -2.860262 -0.129540 0.664869 C -3.914026 0.428769 -0.049620 C -4.817680 -0.381913 -0.708335 C -4.685492 -1.758722 -0.645564 C -3.645544 -2.317993 0.074185 C -2.735411 -1.508184 0.726680 H -5.620209 0.060812 -1.278084 H -5.389497 -2.393012 -1.162236 H -3.531186 -3.389608 0.120737 H -4.006562 1.502592 -0.115490 H -1.916811 -1.945209 1.272099 O 1.528131 1.333200 -0.698833 C 1.355597 2.174412 -2.974765 C 1.157242 2.428618 -1.486699 H 2.375716 1.846716 -3.167070 H 0.663317 1.420125 -3.336727 H 1.183112 3.087466 -3.542402 C -0.265624 2.893745 -1.210657 C 2.135223 3.515715 -1.036516 H -0.387365 3.135737 -0.157335 H -0.491781 3.786099 -1.792782 H -0.980215 2.121569 -1.477365 H 1.954756 4.439666 -1.584245 H 2.014738 3.710563 0.026222 H 3.159155 3.196939 -1.215685	**s''** E_0 = -1992.6397052 E_{0+ZPE} = -1992.204872 H_{298} = -1992.175239 G_{298} = -1992.263348 N_{Imag} = 0 E_0(M06) =-1992.1558968 O -1.841189 -1.842855 -0.264863 Pd -0.488165 -0.280723 -0.322148 Cl 0.994469 -1.922271 -1.064889 Cl -0.192160 -0.825167 2.080499 C -3.773213 -1.094029 -1.455384 C -2.978149 -2.048953 -0.641669 H -3.397125 -0.086025 -1.321470 H -3.681863 -1.393373 -2.500377 H -4.825652 -1.161189 -1.194221 C -0.775337 0.013178 -2.322774 C -3.598426 -3.350046 -0.268032 H 0.178171 0.277016 -2.757045 H -1.124003 -0.932178 -2.714415 H -1.513831 0.803898 -2.361669 H -4.122254 -3.781081 -1.117921 H -2.847953 -4.029950 0.115200 H -4.340096 -3.156936 0.507189 N 0.878050 1.264288 -0.429200 C 0.299130 2.408954 -0.813160 C 0.991948 3.570462 -1.043833 C 2.360023 3.564261 -0.872458 C 2.954876 2.392765 -0.471601 C 2.212338 1.234440 -0.246949 H -0.774083 2.356121 -0.906521 H 0.453682 4.451753 -1.349949 H 2.951241 4.451397 -1.038885 H 4.016658 2.338103 -0.302299 C 3.008210 0.060595 0.173095 C 2.929618 -0.459527 1.453012 C 3.787389 -1.476287 1.833608 C 4.727314 -1.968464 0.949289 C 4.822923 -1.432461 -0.324519 C 3.976789 -0.412544 -0.705780 H 3.708195 -1.886889 2.827895 H 5.387103 -2.768107 1.249427 H 5.552497 -1.813346 -1.022257 H 2.186891 -0.095697 2.140553 H 4.040568 -0.003741 -1.702949 O -1.982948 1.061823 -0.113339 C -3.357309 0.456125 1.802992 C -2.618599 1.550494 1.045606 H -4.105278 -0.007533 1.160420 H -2.662174 -0.297291 2.159883 H -3.878598 0.876481 2.661673 C -1.658585 2.286035 1.970345 C -3.640340 2.548197 0.496878 H -1.187819 3.119151 1.450576 H -2.196904 2.692089 2.825411 H -0.891430 1.612763 2.338928 H -4.205187 2.997580 1.312138 H -3.141806 3.342979 -0.054261 H -4.339459 2.052755 -0.173571	**d_{conf}** E_0 = -1992.6898782 E_{0+ZPE} = -1992.252047 H_{298} = -1992.223359 G_{298} = -1992.308619 N_{Imag} = 0 E_0(M06) =-1992.1949884 N 1.766908 -0.431290 -0.756054 C 2.598197 0.462691 -0.202109 C 3.963898 0.360251 -0.412071 C 4.449882 -0.653664 -1.209653 C 3.568215 -1.545776 -1.790235 C 2.220836 -1.397454 -1.541545 C 1.937059 1.498002 0.578703 C 0.547690 1.491326 0.586603 C -0.179166 2.415460 1.292423 C 0.502325 3.387243 2.009789 C 1.886844 3.419315 2.017094 C 2.603181 2.477760 1.307285 Pd -0.244962 -0.049114 -0.402505 Cl -0.908315 -2.113629 -1.574628 O -2.059114 0.400250 0.242013 C -3.220561 0.812144 -0.445733 C -3.176691 2.305802 -0.733707 O -0.456700 -0.948274 1.529838 C -0.278123 -2.258589 2.119328 C -1.488801 -3.114673 1.810827 Cl -0.152514 1.243101 -2.266027 C -3.469731 0.029079 -1.721041 C -4.339179 0.519369 0.552671 C 0.980653 -2.847344 1.528222 C -0.125477 -2.026696 3.611318 H -1.383819 -0.662851 1.566515 H -1.253586 2.369046 1.285904 H -0.056502 4.123234 2.567806 H 3.681775 2.505299 1.325248 H 2.407966 4.178422 2.578713 H 4.631973 1.077616 0.032563 H 5.510905 -0.739814 -1.385939 H 3.906713 -2.341638 -2.431841 H 1.465111 -2.044654 -1.961624 H 0.014919 -2.975242 4.125380 H 0.731871 -1.390019 3.813494 H -1.012878 -1.549066 4.021606 H -1.364823 -4.101660 2.251205 H -2.391056 -2.674827 2.234962 H -1.616593 -3.216041 0.737518 H 1.202493 -3.793439 2.015896 H -4.420287 0.335236 -2.155321 H -2.684541 0.207772 -2.448616 H -3.497994 -1.036306 -1.518716 H -4.078654 2.617906 -1.257287 H -3.116787 2.876766 0.191495 H -2.320184 2.552528 -1.352614 H -5.293931 0.857670 0.153775 H -4.403985 -0.548731 0.744924 H -4.156776 1.036124 1.492625 H 0.847570 -3.028009 0.465786 H 1.825308 -2.179330 1.681439
t E_0 = -1992.5885837 E_{0+ZPE} = -1992.152252 H_{298} = -1992.124128 G_{298} = -1992.208457 N_{Imag} = 0 E_0(M06) =-1992.0924655	**u** E_0 = -1992.6680872 E_{0+ZPE} = -1992.234243 H_{298} = -1992.204754 G_{298} = -1992.296242 N_{Imag} = 0 E_0(M06) =-1992.1663398	

C 2.772848 2.881592 0.119298 C 2.217437 1.615928 -0.019273 C 0.848367 1.433257 0.163652 C 0.034883 2.507070 0.444745 C 0.599783 3.766993 0.577613 C 1.963086 3.955496 0.423599 C 2.962183 0.421684 -0.353748 N 2.201005 -0.676686 -0.492135 C 2.727625 -1.863995 -0.769064 C 4.083421 -2.006468 -0.956155 C 4.894323 -0.893575 -0.834133 C 4.332162 0.326132 -0.529822 Pd 0.278865 -0.475492 -0.032462 Cl 1.096304 -1.016027 2.253990 Cl -0.359013 -2.707607 -0.810397 H 0.062265 -0.054089 -1.444434 H -1.027743 2.378242 0.543166 H -0.036726 4.609552 0.802482 H 3.833702 3.031551 -0.009582 H 2.390562 4.939409 0.534041 H 4.944474 1.203582 -0.413348 H 5.961574 -0.977814 -0.967300 H 4.483557 -2.979625 -1.183632 H 2.027880 -2.681470 -0.836860 O -2.419332 0.883275 -0.399376 O -1.888369 -0.247196 0.244495 C -2.970486 0.597439 -1.712542 C -2.537561 -0.421252 1.583535 C -1.879328 0.376541 -2.742324 C -3.914850 -0.584358 -1.713485 C -3.701379 1.898437 -1.986795 C -1.984509 0.614866 2.533647 C -4.038364 -0.273262 1.459435 C -2.202148 -1.839756 1.982075 H -2.694616 -2.038778 2.932123 H -2.570235 -2.542176 1.241030 H -1.138202 -1.992135 2.117407 H -2.376187 0.417358 3.528912 H -0.902055 0.562101 2.591007 H -2.300036 1.614504 2.245105 H -4.447121 -0.350349 2.463986 H -4.324850 0.691242 1.055321 H -4.472867 -1.068706 0.865352 H -4.219021 -0.779554 -2.739175 H -3.413981 -1.473847 -1.341620 H -4.808562 -0.390966 -1.130762 H -2.323502 0.401337 -3.735675 H -1.130498 1.164385 -2.693238 H -1.412334 -0.598225 -2.620403 H -4.179887 1.844029 -2.961231 H -4.466941 2.078323 -1.236821 H -3.010762 2.738086 -1.991245	C -4.391046 -0.582577 -0.018184 C -3.007768 -0.665664 -0.013338 N -2.269582 0.387802 0.382744 C -2.855502 1.515254 0.769798 C -4.226322 1.656330 0.782016 C -5.003188 0.585998 0.381447 C -2.216447 -1.813588 -0.424263 C -2.755488 -2.993582 -0.921345 C -1.920306 -4.010676 -1.337276 C -0.547768 -3.839199 -1.270825 C -0.003882 -2.664684 -0.772104 C -0.828932 -1.646765 -0.326694 Pd -0.257175 0.098645 0.385076 O 1.873042 -0.324372 0.547149 C 2.467728 -0.869023 1.770407 C 1.572838 -0.376250 2.885092 Cl 0.313057 2.369870 1.135902 Cl -0.403613 4.329152 -1.548317 O 2.594668 -0.813175 -0.556601 C 2.835858 0.213207 -1.545637 C 3.786857 -0.514404 -2.476951 C 1.551844 0.569796 -2.267921 C 3.480359 1.439034 -0.937574 C 2.472589 -2.381872 1.710324 C 3.865858 -0.311327 1.919191 H -0.086232 3.597612 -0.506086 H 1.066166 -2.539155 -0.751252 H 0.108156 -4.625869 -1.613361 H -3.824852 -3.122061 -0.994636 H -2.336380 -4.927671 -1.723940 H -4.976835 -1.428369 -0.335253 H -6.079589 0.661047 0.378668 H -4.662306 2.588807 1.097935 H -2.190069 2.307029 1.073062 H 1.977152 -0.731713 3.830120 H 1.523577 0.707433 2.906154 H 0.563432 -0.771503 2.784176 H 2.897404 -2.768956 2.633561 H 1.462929 -2.770052 1.611362 H 3.075018 -2.742292 0.882452 H 4.294042 -0.674094 2.850610 H 4.505339 -0.635769 1.104676 H 3.844431 0.773701 1.950829 H 3.650595 2.173386 -1.721454 H 2.828668 1.889542 -0.194751 H 4.438202 1.199239 -0.484242 H 1.781581 1.189560 -3.131765 H 1.038043 -0.324909 -2.609721 H 0.880838 1.146508 -1.636058 H 4.054842 0.141745 -3.300837 H 4.695890 -0.801899 -1.954978 H 3.321156 -1.406609 -2.888272	

TS(a-b)	**TS(a-b′)**	**TS(b′-b)**
E_0 = -1526.5408452 E_{0+ZPE} = -1526.366259 H_{298} = -1526.352111 G_{298} = -1526.407448 N_{Imag} = 1 (-599.8483) E_0(M06) =-1526.2290345 N 0.517246 1.324795 -0.050958	E_0 = -1526.5533031 E_{0+ZPE} = -1526.380600 H_{298} = -1526.366376 G_{298} = -1526.422094 N_{Imag} = 1 (-1128.5003) E_0(M06) =-1526.2428669 N 0.069643 1.417068 -0.083483	E_0 = -1526.5769483 E_{0+ZPE} = -1526.401909 H_{298} = -1526.387309 G_{298} = -1526.443964 N_{Imag} = 1 (-156.5922) E_0(M06) =-1526.2635448 Pd 0.959597 -0.098765 -0.032596

C 1.752461 0.796400 -0.008753	C 1.380370 1.244935 0.157447	N -0.718388 -1.233160 -0.016517
C 2.858837 1.631152 -0.001768	C 2.190954 2.346404 0.381308	C -0.699010 -2.560909 -0.027361
C 2.680147 2.997213 -0.038820	C 1.649457 3.613340 0.328226	C -1.861075 -3.301196 0.011510
C 1.399574 3.516558 -0.081622	C 0.305224 3.764864 0.050022	C -3.068888 -2.631944 0.066015
C 0.337240 2.640506 -0.082925	C -0.458725 2.634049 -0.141121	C -3.080394 -1.253359 0.076524
C 1.785601 -0.658681 0.023863	C 1.849286 -0.139476 0.098088	C -1.881562 -0.559520 0.032603
C 0.551651 -1.319221 0.003725	C 0.894298 -1.170214 -0.002474	C -1.726464 0.887045 0.020444
C 0.510144 -2.698433 0.041810	C 1.334921 -2.454389 -0.286709	C -2.792036 1.777371 0.037162
C 1.692559 -3.420609 0.093525	C 2.687229 -2.740392 -0.400970	C -2.558023 3.137107 -0.010292
C 2.915879 -2.773721 0.109715	C 3.619726 -1.735206 -0.254023	C -1.257292 3.602591 -0.086519
C 2.963278 -1.395381 0.075858	C 3.197648 -0.438334 -0.026111	C -0.190816 2.715613 -0.102148
H -1.439501 0.212368 1.309138	H -0.347252 -1.734576 0.685100	C -0.402354 1.347583 -0.037599
Pd -1.008895 -0.064702 -0.086813	Pd -1.008130 -0.305778 -0.078996	H 0.282307 -3.007789 -0.066320
Cl -2.723567 1.579724 0.258298	Cl -3.063866 0.741324 -0.377491	H -1.807275 -4.376630 0.000300
Cl -2.531513 -1.748341 -0.137643	Cl -1.743782 -2.456509 0.653159	H -3.997768 -3.180043 0.099604
H -0.437738 -3.208774 0.030693	H 0.618631 -3.253616 -0.397799	H -4.011064 -0.713790 0.117142
H 1.652863 -4.498908 0.121654	H 3.002325 -3.750697 -0.610773	H -3.808675 1.417303 0.082831
H 3.921053 -0.898664 0.090931	H 3.933729 0.348762 0.015742	H -3.384834 3.829539 0.002712
H 3.831366 -3.342456 0.151157	H 4.672991 -1.949016 -0.344097	H -1.068361 4.664457 -0.139508
H 3.848800 1.210459 0.031447	H 3.235723 2.210477 0.600742	H 0.807590 3.115748 -0.186489
H 3.536522 3.653506 -0.033677	H 2.274306 4.475215 0.503373	Cl 2.501654 -1.931514 -0.051888
H 1.216882 4.577301 -0.109287	H -0.157589 4.735588 -0.005898	H 2.668639 1.909718 1.221926
H -0.689651 2.969688 -0.100725	H -1.518718 2.668832 -0.336672	Cl 2.928592 1.375895 0.087230

TS(c-d)	**TS(c-d)′**	**TS(c-d)″**
E_0 = -1992.6141416	E_0 = -1992.6098546	E_0 = -1992.6093041
E_{0+ZPE} = -1992.178572	E_{0+ZPE} = -1992.174259	E_{0+ZPE} = -1992.173868
H_{298} = -1992.150088	H_{298} = -1992.145691	H_{298} = -1992.145208
G_{298} = -1992.235563	G_{298} = -1992.232261	G_{298} = -1992.231970
N_{Imag} = 1 (-310.0681)	N_{Imag} = 1 (-285.6389)	N_{Imag} = 1 (-289.5721)
E_0(M06) =-1992.1376707	E_0(M06) =-1992.1330484	E_0(M06) =-1992.1320462
N 1.778106 -1.241453 -0.396214	N -0.931766 1.679408 -0.307100	C 4.351436 -0.650640 0.604284
C 2.949252 -0.722192 0.011037	C -2.008640 1.808345 0.484771	C 3.109394 -0.198516 0.182151
C 4.035372 -1.554601 0.242890	C -2.331695 3.045626 1.024965	N 2.156936 -1.079728 -0.169795
C 3.905144 -2.911924 0.046096	C -1.566042 4.146130 0.708096	C 2.395609 -2.385953 -0.133046
C 2.694997 -3.423212 -0.385777	C -0.495712 4.001622 -0.155232	C 3.608670 -2.892254 0.281197
C 1.653208 -2.547800 -0.601612	C -0.212252 2.743191 -0.639878	C 4.600364 -2.004848 0.656091
C 2.939516 0.724999 0.168040	C -2.789816 0.589231 0.630301	C 2.705028 1.195316 0.072274
C 1.746487 1.380971 -0.165490	C -2.328059 -0.531064 -0.074305	C 3.522667 2.259421 0.439853
C 1.670674 2.754748 -0.015328	C -3.105532 -1.677740 -0.083855	C 3.064823 3.554798 0.322164
C 2.764101 3.464553 0.454263	C -4.295733 -1.722595 0.623302	C 1.788966 3.786058 -0.165744
C 3.945320 2.817367 0.778361	C -4.729402 -0.627436 1.352597	C 0.969437 2.731689 -0.536049
C 4.032350 1.448988 0.634612	C -3.980518 0.529919 1.348275	C 1.414067 1.425032 -0.423841
H -2.491270 -1.049297 -0.420629	H 2.570436 -0.209010 -0.760523	Pd 0.417220 -0.232250 -0.887627
Pd 0.329891 0.174211 -0.844754	Pd -0.594662 -0.246987 -0.997331	O -1.270011 0.050381 0.806724
Cl -1.205701 -1.546675 -1.832336	Cl 1.463337 0.408741 -2.249265	C -1.169182 -0.174463 2.183826
Cl -0.941286 1.930448 -1.638110	Cl -0.535416 -2.376832 -1.882312	C 0.348706 -0.252304 2.446504
H 0.763200 3.270373 -0.280301	H -2.779804 -2.535984 -0.647917	Cl -0.554342 -2.386107 -1.409143
H 2.691872 4.536550 0.562833	H -4.889723 -2.624252 0.603016	Cl -1.251383 0.955671 -2.075368
H 4.953609 0.947720 0.889620	H -4.335398 1.390984 1.893946	O -2.890522 0.791669 0.338759
H 4.793084 3.377644 1.140320	H -5.653575 -0.671769 1.907244	C -4.109077 0.068197 0.008777
H 4.973669 -1.136764 0.564817	H -3.187511 3.143459 1.670372	C -4.986247 0.100637 1.238862
H 4.745079 -3.566283 0.221611	H -1.813961 5.113384 1.117377	C -4.742431 0.888682 -1.111136
H 2.553913 -4.476238 -0.562076	H 0.110349 4.840471 -0.453723	C -3.801814 -1.333929 -0.462831
H 0.686341 -2.869021 -0.957828	H 0.601565 2.552334 -1.322475	C -1.715545 1.016642 2.956353
O -1.264443 -0.069892 0.837878	O 1.210452 -0.825711 0.577430	C -1.799099 -1.494281 2.582384
O -2.959685 -0.716136 0.392892	O 2.996258 -0.431208 0.115650	H -2.400285 0.965031 -0.511794
C -4.069001 0.157582 0.031571	C 3.741999 0.718351 0.577224	H -0.013151 2.929215 -0.930820
C -5.274813 -0.471221 0.707917	C 2.802742 1.798900 1.066006	H 1.427308 4.798969 -0.263950
H -5.139202 -0.516866 1.785645	H 2.170874 1.422843 1.865210	H 4.517323 2.082476 0.820173
H -6.158993 0.128620 0.502415	H 3.379632 2.639981 1.444004	H 3.698481 4.380271 0.606430
H -5.446768 -1.477444 0.335168	H 2.169410 2.146088 0.258219	H 5.114589 0.056602 0.880224
C -3.818989 1.558675 0.548589	C 4.680270 0.260375 1.672364	H 5.564124 -2.365105 0.981713
H -4.624079 2.204045 0.205118	H 5.413106 1.041319 1.860973	H 3.763917 -3.957863 0.298634
H -3.808125 1.584961 1.633575	H 4.159612 0.071293 2.605320	H 1.575679 -3.010732 -0.454954
H -2.878944 1.938513 0.161548	H 5.212946 -0.637796 1.370865	H 0.474430 -0.353121 3.522646
C -4.214726 0.159060 -1.476490	C 4.545513 1.189859 -0.629949	H 0.772299 -1.118969 1.955207
H -5.091286 0.745480 -1.743131	H 5.141360 2.053172 -0.340917	H 0.845863 0.647492 2.103988
H -3.342639 0.599057 -1.950777	H 5.216840 0.406854 -0.972715	H -1.520858 0.877863 4.017030
H -4.349971 -0.849861 -1.859139	H 3.891718 1.473115 -1.449141	H -1.237893 1.934560 2.626592

C -1.014432 -0.504973 2.150479	C 1.249119 -1.956460 1.386017	H -2.785209 1.111040 2.805543
C 0.326647 0.133441 2.547046	C 1.892004 -3.130404 0.675742	H -1.542526 -1.736763 3.611283
H 0.479425 -0.066369 3.605879	H 1.811303 -4.023158 1.292125	H -2.881103 -1.455987 2.511929
H 1.141653 -0.300115 1.982980	H 1.398145 -3.306894 -0.274762	H -1.438650 -2.286124 1.931174
H 0.310767 1.204828 2.382032	H 2.942729 -2.925099 0.494937	H -4.726700 -1.814040 -0.775290
C -2.072547 0.037107 3.100028	C 1.909081 -1.647322 2.720054	H -3.106814 -1.328339 -1.296513
H -1.829127 -0.267273 4.115108	H 1.752546 -2.475247 3.406259	H -3.356559 -1.928717 0.327318
H -2.106336 1.121393 3.061615	H 2.976647 -1.523615 2.580896	H -5.707900 0.451799 -1.357064
H -3.046956 -0.364491 2.843849	H 1.492288 -0.746285 3.162415	H -4.898711 1.918303 -0.799636
C -0.929237 -2.017506 2.206929	C -0.241023 -2.273652 1.673164	H -4.120728 0.874222 -2.001208
H -1.883352 -2.459310 1.936116	H -0.756108 -1.410007 2.077959	H -5.945341 -0.355421 1.006631
H -0.173683 -2.380397 1.516897	H -0.723186 -2.602029 0.762982	H -4.551588 -0.453866 2.064630
H -0.667735 -2.343289 3.211395	H -0.241579 -3.074967 2.409174	H -5.163681 1.124139 1.559892
TS(c-d)‴	**TS(c'-d')**	**TS(c''-d'')**
E_0 = -1992.6072639	E_0 = -1992.57868	E_0 = -1992.5681698
E_{0+ZPE} = -1992.171683	E_{0+ZPE} = -1992.148356	E_{0+ZPE} = -1992.139194
H_{298} = -1992.143197	H_{298} = -1992.118990	H_{298} = -1992.109102
G_{298} = -1992.229083	G_{298} = -1992.208910	G_{298} = -1992.203093
N_{Imag} = 1 (-309.8643)	N_{Imag} = 1 (-416.2622)	N_{Imag} = 1 (-145.1618)
E_0(M06) =-1992.1309632	E_0(M06) =-1992.0994407	E_0(M06) =-1992.0921653
N 2.385651 -0.294117 0.029749	C -0.304988 -1.500642 -0.893113	C 1.935975 0.487211 0.445017
C 2.683950 0.868191 0.634499	C -1.601428 -1.999484 -0.725098	C 2.792731 -0.466970 -0.129222
C 3.845615 0.982453 1.384994	C -1.967508 -3.201989 -1.319001	C 4.161254 -0.411726 0.101646
C 4.702352 -0.092472 1.479328	C -1.055721 -3.906904 -2.077630	C 4.687218 0.578706 0.905915
C 4.394331 -1.265874 0.816187	C 0.223511 -3.406261 -2.252229	C 3.843679 1.512723 1.482583
C 3.218618 -1.325886 0.100049	C 0.598691 -2.207811 -1.665951	C 2.476786 1.468789 1.258592
C 1.735244 1.939652 0.368204	C -2.503327 -1.183955 0.075469	C 2.157457 -1.490751 -0.944922
C 0.660671 1.612696 -0.470114	N -1.964124 -0.029388 0.505823	N 0.827194 -1.352090 -1.042965
C -0.187388 2.626914 -0.881845	C -2.679098 0.807519 1.248210	C 0.090291 -2.217968 -1.721596
C -0.002027 3.926010 -0.434544	C -3.984207 0.538837 1.601467	C 0.660439 -3.288892 -2.377118
C 1.032231 4.233756 0.433425	C -4.556221 -0.640376 1.166495	C 2.032340 -3.448740 -2.304265
C 1.906587 3.241705 0.825921	C -3.810112 -1.509724 0.399283	C 2.787797 -2.548612 -1.582404
H -2.520413 -0.352326 -0.751198	Pd 0.007435 0.260484 -0.051520	Pd 0.037559 0.259788 -0.054629
Pd 0.601835 -0.304303 -1.003438	Cl -0.025145 2.590012 0.814152	Cl -0.644311 2.187904 1.051173
Cl -1.340335 -0.058089 -2.317490	H -2.967382 -3.589809 -1.198251	H 4.821567 -1.139839 -0.344401
Cl 0.865273 -2.597279 -1.728031	H -1.343624 -4.838338 -2.539086	H 5.750296 0.622018 1.083370
H -0.986321 2.404155 -1.569679	H 0.935784 -3.949461 -2.855221	H 4.251266 2.289209 2.112179
H -0.670703 4.704619 -0.771079	H 1.591349 -1.817219 -1.811999	H 1.834914 2.204545 1.712158
H 2.731937 3.491733 1.475206	H -4.235247 -2.435563 0.051694	H 3.855936 -2.662510 -1.511401
H 1.168386 5.244656 0.784454	H -5.576220 -0.882655 1.421679	H 2.512814 -4.274863 -2.805424
H 4.078109 1.911798 1.875849	H -4.530243 1.249352 2.198475	H 0.039045 -3.976863 -2.925268
H 5.610242 -0.011001 2.056970	H -2.172866 1.709712 1.550923	H -0.970247 -2.015169 -1.711642
H 5.045291 -2.123309 0.846649	O 1.743376 0.015539 1.399966	O -1.317037 -1.121202 1.049233
H 2.906893 -2.206192 -0.442452	O 1.920882 0.121019 -0.662685	O -1.946894 -0.334896 -0.801088
O -1.143268 -0.803730 0.620521	C 2.114347 -1.199778 1.910497	C -1.548454 -1.664089 2.281203
O -2.930658 -0.501205 0.141019	C 2.758814 1.176927 -1.081167	C -3.090639 0.302008 -1.222622
C -3.692091 0.659763 0.561658	C 3.243999 -1.870857 1.152018	C -2.150725 -3.059336 2.122885
C -4.883584 0.121159 1.327237	C 2.657642 -0.667053 3.275489	C -0.135316 -1.797848 2.907354
H -4.581805 -0.389588 2.236759	C 0.955521 -2.140408 2.167457	C -2.409974 -0.760147 3.147313
H -5.533474 0.945758 1.611541	C 3.857439 0.457357 -1.865268	C -3.956250 -0.673431 -2.007940
H -5.453905 -0.569675 0.712346	C 2.000942 2.125406 -1.995787	C -3.864859 0.873013 -0.036978
C -2.840086 1.569526 1.421553	C 3.381737 1.937791 0.082898	C -2.633809 1.458563 -2.131115
H -3.415944 2.453797 1.685096	H 4.027850 2.713049 -0.323786	H -3.511401 1.968225 -2.525449
H -2.544201 1.070335 2.338341	H 2.613428 2.401099 0.690717	H -2.037996 2.169852 -1.568057
H -1.946280 1.880488 0.891499	H 3.979834 1.279020 0.704889	H -2.048137 1.078504 -2.964286
C -4.154561 1.374815 -0.697842	H 4.569424 1.187780 -2.244717	H -4.875751 -0.201135 -2.348421
H -4.799230 2.204620 -0.417685	H 4.387072 -0.246475 -1.229754	H -3.419232 -1.044500 -2.878761
H -3.313066 1.762350 -1.262664	H 3.436328 -0.079890 -2.711640	H -4.221037 -1.521628 -1.379581
H -4.720845 0.704032 -1.339398	H 2.686330 2.852540 -2.427553	H -4.734948 1.427148 -0.383763
C -1.133119 -1.914952 1.462972	H 1.533994 1.571784 -2.807612	H -4.202956 0.055487 0.596092
C 0.364342 -2.152114 1.770178	H 1.236584 2.663886 -1.445955	H -3.228728 1.528155 0.547812
H 0.397712 -2.923793 2.536508	H 3.009520 -1.536798 3.827806	H -0.244969 -2.262647 3.885463
H 0.865422 -2.500674 0.875862	H 3.479095 0.021912 3.116897	H 0.497943 -2.416294 2.279726
H 0.832690 -1.250802 2.150588	H 1.871682 -0.173423 3.835674	H 0.314573 -0.816820 3.018304
C -1.820905 -1.594172 2.780313	H 3.590536 -2.744854 1.698677	H -2.299111 -3.519209 3.097638
H -1.722950 -2.441072 3.454547	H 2.891041 -2.186215 0.175822	H -3.114282 -2.988836 1.624232
H -1.376680 -0.722044 3.251921	H 4.076372 -1.187355 1.017171	H -1.497442 -3.691222 1.527664
H -2.877492 -1.415581 2.613471	H 1.280193 -2.996567 2.754636	H -2.492985 -1.151041 4.159594
C -1.715726 -3.133557 0.776823	H 0.164107 -1.627053 2.707194	H -1.981343 0.237513 3.183813

H -2.773762 -2.981888 0.585677 H -1.204699 -3.310960 -0.165440 H -1.598117 -4.007631 1.413743	H 0.554589 -2.507403 1.226177 Cl -2.417900 3.834626 -1.238447 H -1.445194 3.409518 -0.463148	H -3.410451 -0.682847 2.728816 Cl 0.406849 4.698537 -1.124330 H 0.027229 3.763438 -0.304182
TS(c'-d')$_{\cdot HCl}$ E_0 = -1531.7198549 E_{0+ZPE} = -1531.299512 H_{298} = -1531.272472 G_{298} = -1531.356612 N_{Imag} = 1 (-136.5535) E_0(M06) =-1531.2863299 C -1.924656 -0.959946 -0.367096 C -2.831346 0.097343 -0.178862 C -4.194926 -0.152927 -0.081172 C -4.668256 -1.446212 -0.162338 C -3.776797 -2.491040 -0.340949 C -2.415572 -2.253506 -0.441832 C -2.254598 1.430603 -0.084859 N -0.920477 1.452239 -0.216888 C -0.237666 2.582899 -0.123465 C -0.867610 3.790881 0.089602 C -2.245134 3.799186 0.215599 C -2.945185 2.614176 0.131901 Pd -0.041203 -0.381623 -0.521041 Cl 0.737669 -2.519044 -0.927618 H -4.892099 0.659295 0.058570 H -5.726816 -1.639510 -0.085823 H -4.143496 -3.504613 -0.405501 H -1.732444 -3.073341 -0.586031 H -4.016725 2.603169 0.235125 H -2.772476 4.725755 0.382924 H -0.287830 4.695996 0.157897 H 0.831932 2.474074 -0.223071 O 1.281510 -0.027456 1.262016 O 1.899220 0.647003 -0.614875 C 1.526835 -0.414893 2.546779 C 3.054842 0.494174 -1.347941 C 1.870716 0.785898 3.419881 C 0.159122 -1.003795 2.994608 C 2.584081 -1.506699 2.616922 C 3.865881 1.781192 -1.295283 C 3.880468 -0.682062 -0.833356 C 2.608513 0.199772 -2.791572 H 3.489855 0.102936 -3.423919 H 2.043216 -0.726857 -2.826032 H 1.994694 1.012257 -3.172941 H 4.789662 1.691363 -1.863912 H 3.292016 2.611103 -1.703360 H 4.122212 2.015089 -0.263798 H 4.758809 -0.828763 -1.459246 H 4.209118 -0.472145 0.181826 H 3.283425 -1.587422 -0.829253 H 0.258139 -1.315822 4.032956 H -0.618903 -0.252324 2.910789 H -0.093089 -1.855835 2.372674 H 2.013718 0.481633 4.454707 H 2.791510 1.244763 3.067069 H 1.077344 1.527271 3.376572 H 2.664165 -1.904043 3.626882 H 2.330547 -2.311661 1.933122 H 3.553719 -1.106294 2.330836	**TS(c''-d'')$_{\cdot HCl}$** E_0 = -1531.7270248 E_{0+ZPE} = -1531.305565 H_{298} = -1531.279099 G_{298} = -1531.359708 N_{Imag} = 1 (-425.9925) E_0(M06) =-1531.2898715 C 0.808479 1.307508 -0.524537 C 2.200067 1.323336 -0.372201 C 2.905701 2.514700 -0.500413 C 2.238098 3.688174 -0.784964 C 0.863200 3.670852 -0.952618 C 0.151879 2.488372 -0.825925 C 2.827322 0.037389 -0.101206 N 1.971510 -0.999990 -0.085492 C 2.412089 -2.232600 0.137395 C 3.746372 -2.499644 0.360896 C 4.641798 -1.447643 0.351557 C 4.180047 -0.169660 0.118680 Pd -0.010930 -0.491226 -0.377002 Cl -0.664861 -2.852817 -0.451312 H 3.979006 2.531400 -0.387162 H 2.787614 4.610884 -0.886074 H 0.339366 4.585369 -1.188312 H -0.916258 2.478717 -0.964092 H 4.860569 0.664357 0.106452 H 5.693125 -1.619859 0.523548 H 4.064060 -3.513752 0.535617 H 1.653772 -3.000786 0.122010 O -1.532472 -0.362240 1.314842 O -1.804031 0.399604 -0.590251 C -1.487645 0.603917 2.284987 C -2.946977 -0.134213 -1.222491 C -2.379410 1.800425 2.010929 C -2.117546 -0.255602 3.426852 C -0.084959 1.012171 2.684983 C -3.798918 1.104387 -1.503661 C -2.560042 -0.810220 -2.528409 C -3.726605 -1.096047 -0.333844 H -4.597843 -1.439540 -0.888133 H -3.113851 -1.950257 -0.069547 H -4.064348 -0.603516 0.572765 H -4.718208 0.806442 -2.004588 H -4.056398 1.613602 -0.579380 H -3.266867 1.797953 -2.150573 H -3.455596 -1.092609 -3.079439 H -1.979734 -0.126472 -3.144983 H -1.975746 -1.705146 -2.339094 H -2.156776 0.381306 4.309066 H -3.119279 -0.570906 3.158884 H -1.506291 -1.126886 3.633197 H -2.411559 2.447741 2.884542 H -1.986171 2.365321 1.172341 H -3.389409 1.481466 1.772894 H -0.103672 1.605716 3.596488 H 0.529403 0.131678 2.853794 H 0.370290 1.609491 1.899828	**TS(d'''-d'''')** E_0 = -1992.6373144 E_{0+ZPE} = -1992.206197 H_{298} = -1992.176609 G_{298} = -1992.266223 N_{Imag} = 1 (-158.9808) E_0(M06) =-1992.1448183 C 1.081299 -0.642671 -1.086722 C 1.889182 -1.470801 -0.316445 C 2.902571 -2.171792 -0.957555 C 3.090601 -2.033692 -2.317763 C 2.269834 -1.194146 -3.049635 C 1.250201 -0.478941 -2.436427 C 1.585357 -1.555737 1.102079 N 0.526670 -0.828905 1.462207 C 0.072377 -0.815269 2.700876 C 0.693950 -1.544198 3.691861 C 1.804612 -2.296304 3.354498 C 2.254988 -2.309694 2.050835 Pd -0.301296 0.277232 -0.025305 Cl -2.835930 1.942303 1.695248 H 3.544710 -2.828641 -0.391437 H 3.879028 -2.581375 -2.808815 H 2.417545 -1.084572 -4.112919 H 0.616418 0.180233 -3.001690 H 3.112826 -2.896821 1.770689 H 2.316566 -2.876329 4.106384 H 0.311389 -1.518669 4.697959 H -0.803949 -0.214257 2.884016 O -1.776386 -1.024036 0.144187 O 1.160581 1.511084 0.507283 C -2.621382 -1.686969 -0.755291 C 1.522465 2.791706 0.066477 C -1.913872 -2.044757 -2.052071 C -3.032219 -2.966724 -0.032036 C -3.862298 -0.850523 -1.043427 C 2.727034 3.135477 0.941657 C 1.951553 2.804402 -1.393072 C 0.417280 3.806897 0.317732 H 0.758772 4.814935 0.085831 H -0.454232 3.595886 -0.293610 H 0.119867 3.777747 1.363793 H 3.102862 4.129791 0.703922 H 2.444991 3.111670 1.991482 H 3.523436 2.412467 0.782266 H 2.340114 3.784344 -1.666419 H 2.734138 2.067084 -1.559622 H 1.112530 2.581888 -2.044727 H -3.734032 -3.546829 -0.630001 H -2.156719 -3.579363 0.171087 H -3.505403 -2.720516 0.915698 H -2.569503 -2.628806 -2.695872 H -1.624886 -1.145149 -2.587906 H -1.022101 -2.633352 -1.846626 H -4.574563 -1.405113 -1.653156 H -4.353384 -0.586353 -0.108569 H -3.597673 0.059782 -1.573235 Cl -1.308602 1.496635 -1.693133 H -2.883516 1.564086 0.468905
TS(e-f) E_0 = -1758.9422407 E_{0+ZPE} = -1758.649505 H_{298} = -1758.628307 G_{298} = -1758.697587 N_{Imag} = 1 (-311.4117)	**TS(e-f)′** E_0 = -1758.9429402 E_{0+ZPE} = -1758.649090 H_{298} = -1758.628249 G_{298} = -1758.696609 N_{Imag} = 1 (-479.8845)	**TS(e-f)″** E_0 = -1758.934654 E_{0+ZPE} = -1758.640884 H_{298} = -1758.620198 G_{298} = -1758.688167 N_{Imag} = 1 (-558.0210)

E_0(M06) =-1758.5507801	E_0(M06) =-1758.5491462	E_0(M06) =-1758.5441288
C -0.812438 1.367522 -0.000086	O -2.282496 0.571645 0.517818	O 2.331899 0.629042 0.452043
C -2.103562 0.866931 0.000044	Pd -0.553617 -0.332500 0.265378	Pd 0.522304 -0.395243 0.276724
C -3.174758 1.755617 0.000064	Cl -1.510107 -2.599100 0.295112	Cl 1.406298 -2.508677 0.442084
C -2.932257 3.113374 -0.000053	Cl 0.059086 -0.333047 2.490529	Cl -0.047116 -0.418498 2.494343
C -1.629270 3.590820 -0.000199	C -2.849861 1.874276 -1.386924	C 3.797799 -0.519567 -1.016218
C -0.554902 2.715335 -0.000215	C -2.686068 0.526487 -0.729388	C 2.690162 0.490691 -0.801697
C -2.225282 -0.581592 0.000089	H -1.962352 2.486146 -1.273355	H 3.509246 -1.498900 -0.653604
N -1.064670 -1.257913 0.000016	H -3.097311 1.779591 -2.440101	H 4.100469 -0.585060 -2.059541
C -1.039225 -2.580940 -0.000068	H -3.676596 2.373725 -0.883243	H 4.648242 -0.179501 -0.428127
C -2.192720 -3.328781 -0.000031	C -1.227178 -0.128993 -1.882613	C 1.281067 -0.134343 -1.877567
C -3.405384 -2.661975 0.000093	C -3.805751 -0.446977 -0.981882	C 2.951990 1.802841 -1.516090
C -3.421234 -1.286811 0.000145	H -0.689522 -1.073489 -1.917607	H 0.737605 0.720031 -2.257875
Pd 0.588528 -0.079998 -0.000009	H -2.067388 -0.305806 -2.540677	H 2.034237 -0.466309 -2.581610
C 2.070192 -1.811278 0.000157	H -0.640512 0.711275 -2.227570	H 0.624906 -1.009810 -1.858231
O 2.175121 1.144951 -0.000054	H -4.125653 -0.441274 -2.021136	H 3.173270 1.659479 -2.570549
C 3.114590 0.281363 0.000035	H -3.520210 -1.447845 -0.676822	H 2.111216 2.482852 -1.419230
C 3.843176 0.071097 -1.286776	H -4.639754 -0.125087 -0.359970	H 3.817348 2.262129 -1.040503
Cl 0.465793 -0.046727 2.329804	N 1.320132 -1.036773 -0.245805	N -0.450635 1.398138 0.160222
Cl 0.465844 -0.047003 -2.329823	C 1.644345 -2.320476 -0.320541	C 0.112186 2.537873 0.533502
C 3.843185 0.071418 1.286895	C 2.921703 -2.718421 -0.652448	C -0.594431 3.719270 0.506734
H 3.141494 -0.027680 2.107569	C 3.872985 -1.747866 -0.902988	C -1.914123 3.686604 0.090575
H 4.520918 -0.774834 1.250264	C 3.529238 -0.416247 -0.803037	C -2.492754 2.486584 -0.261936
H 4.431025 0.976111 1.452525	C 2.231642 -0.074452 -0.460145	C -1.736918 1.324675 -0.205792
H 1.679964 -2.247999 -0.914498	H 0.843329 -3.012746 -0.107641	H 1.140953 2.453475 0.849612
H 3.141678 -1.948718 0.000531	H 3.154738 -3.768356 -0.705839	H -0.119518 4.635518 0.814061
H 1.679378 -2.248110 0.914508	H 4.882193 -2.025857 -1.164487	H -2.496787 4.594158 0.057598
H 4.520749 -0.775276 -1.250008	H 4.261514 0.354198 -0.972975	H -3.526199 2.442672 -0.559654
H 3.141492 -0.027983 -2.107458	C 1.738622 1.278396 -0.245797	C -2.209398 -0.026414 -0.463772
H 4.431199 0.975654 -1.452512	C 2.504924 2.430860 -0.387539	C -3.500240 -0.322170 -0.888348
H -0.067041 -3.044788 -0.000173	C 1.972820 3.659819 -0.056114	C -3.887536 -1.634562 -1.058413
H -2.133185 -4.403761 -0.000100	C 0.682035 3.747274 0.440350	C -2.990171 -2.655985 -0.796923
H -4.332611 -3.213437 0.000135	C -0.099017 2.610492 0.580669	C -1.698327 -2.378083 -0.375921
H -4.353124 -0.748467 0.000218	C 0.427585 1.398303 0.203097	C -1.307354 -1.066271 -0.222075
H -3.759522 3.805394 -0.000037	H 2.572018 4.550048 -0.163594	H -4.889273 -1.862164 -1.386885
H -1.449669 4.655513 -0.000298	H 0.281206 4.706014 0.732506	H -3.295382 -3.684275 -0.918487
H 0.461173 3.077241 -0.000318	H -1.093013 2.660034 0.992294	H -1.008153 -3.177675 -0.167863
H -4.192953 1.397635 0.000168	H 3.521947 2.370314 -0.743184	H -4.206741 0.470343 -1.081931
TS(g-h)	**TS(f-h)**	**TS(f-h)$_{\text{Non-Coord}}$**
E_0 = -1565.8548532	E_0 = -1758.989448	E_0 = -1759.018417
E_{0+ZPE} = -1565.649332	E_{0+ZPE} = -1758.696734	E_{0+ZPE} = -1758.726139
H_{298} = -1565.633792	H_{298} = -1758.674696	H_{298} = -1758.703392
G_{298} = -1565.691661	G_{298} = -1758.746964	G_{298} = -1758.779367
N_{Imag} = 1 (-301.1747)	N_{Imag} = 1 (-445.4879)	N_{Imag} = 1 (-286.9805)
E_0(M06) =-1565.5260029	E_0(M06) =-1758.5941681	E_0(M06) =-1758.6251959
Pd 0.873298 -0.500022 0.078745	Pd -0.450299 -0.231803 -0.141281	Pd 0.143079 -0.537831 0.302194
Cl 3.091825 0.063824 0.102536	Cl -0.535494 -0.631654 2.261209	Cl 1.748138 0.014379 1.912357
Cl 1.334343 -2.504031 -1.004535	Cl -1.535923 -2.363498 -1.108389	Cl 0.732195 -2.754738 0.398407
C 0.661436 0.481166 1.962321	C 0.011384 0.623023 -2.118606	C -0.295468 -0.771183 -1.777732
H 1.412302 1.224283 2.174307	H -0.686546 1.402173 -2.384205	H -0.434852 -1.803318 -2.054989
H -0.321866 0.750479 2.317658	H 0.993465 0.791987 -2.534169	H -0.969403 -0.095996 -2.282850
H 0.965598 -0.484364 2.364612	H -0.360310 -0.346995 -2.444909	H 0.738221 -0.448763 -1.906762
C 0.920485 2.539983 0.000809	C 0.145008 2.769142 -0.363562	C -2.399990 -2.075032 -0.337374
H 1.980045 2.505031 0.193949	H -0.888999 2.954814 -0.605426	H -1.811420 -2.973614 -0.420805
C 0.313343 3.706459 -0.430213	C 0.974805 3.806700 0.011413	C -3.780098 -2.133185 -0.250905
H 0.912303 4.593057 -0.569934	H 0.578385 4.809197 0.065329	H -4.270464 -3.094178 -0.273158
C -1.047142 3.741593 -0.686548	C 2.307250 3.573372 0.321748	C -4.530268 -0.975340 -0.130010
C 0.157086 1.402445 0.172162	C 0.645856 1.479372 -0.438879	C -1.770580 -0.846989 -0.301529
C -1.806504 2.600015 -0.527796	C 2.802097 2.287057 0.283699	C -3.898850 0.251298 -0.083230
C -1.215054 1.418684 -0.100222	C 1.979603 1.231085 -0.086100	C -2.515430 0.330069 -0.167193
H -2.858176 2.622495 -0.767975	H 3.822978 2.099125 0.578683	H -4.484436 1.148140 0.047277
H -1.512383 4.653758 -1.024604	H 2.947458 4.389768 0.614980	H -5.604926 -1.029862 -0.059170
C -1.934092 0.155834 0.018388	C 2.378905 -0.162449 -0.044545	C -1.768477 1.578583 -0.074062
C -3.312028 0.012071 0.035116	C 3.675124 -0.642014 0.061981	C -2.301761 2.850566 -0.197749
C -3.856117 -1.251588 0.129336	C 3.889247 -2.001011 0.125835	C -1.466081 3.942947 -0.091672
C -3.019711 -2.349986 0.202138	C 2.811042 -2.867103 0.082769	C -0.116234 3.750011 0.132715
C -1.657386 -2.142984 0.178974	C 1.543394 -2.343492 -0.028898	C 0.354889 2.459948 0.251395
N -1.142461 -0.923083 0.100298	N 1.355503 -1.030384 -0.102288	N -0.456057 1.416710 0.147844
H -3.945301 0.880945 -0.020228	H 4.498985 0.050267 0.093513	H -3.354521 2.978516 -0.383374

H -4.927447 -1.378219 0.145772 H -3.406475 -3.352721 0.269617 H -0.943812 -2.950779 0.199667	H 4.894047 -2.384936 0.209340 H 2.938915 -3.934830 0.134046 H 0.649369 -2.944874 -0.080370 O -2.238959 0.785022 -0.243031 C -3.351752 0.495460 0.183757 C -4.462065 1.444488 -0.099170 H -4.890554 1.777492 0.844755 H -4.119513 2.293439 -0.677676 H -5.248784 0.915217 -0.634290 C -3.642681 -0.729780 0.944405 H -2.960410 -0.785620 1.793081 H -4.678585 -0.772794 1.259897 H -3.382193 -1.583532 0.313576	H -1.866621 4.939954 -0.189557 H 0.567417 4.577659 0.216609 H 1.389627 2.232400 0.442750 O 2.745539 0.692231 -1.634239 C 3.667349 0.220282 -1.015386 C 3.910422 -1.254154 -0.963326 H 3.485952 -1.626950 -0.030514 H 3.410509 -1.752866 -1.785655 H 4.972450 -1.486018 -0.964423 C 4.607063 1.082209 -0.229340 H 4.583701 0.773652 0.814013 H 5.625632 0.946980 -0.589653 H 4.325020 2.125562 -0.312256
TS(f-h)'$_{\text{Non-Coord}}$ E_0 = -1759.0167923 E_{0+ZPE} = -1758.724668 H_{298} = -1758.701777 G_{298} = -1758.779096 N_{Imag} = 1 (-295.9128) E_0(M06) =-1758.6248361 Pd -0.729476 -0.779446 -0.613490 Cl -2.662275 -1.868006 -0.033795 Cl 0.519178 -2.731145 -0.313042 C -1.855525 0.428093 -1.960262 H -2.908325 0.490567 -1.739624 H -1.436954 1.354958 -2.322375 H -1.664929 -0.382356 -2.663265 C -2.498722 1.340009 0.665224 H -3.323133 0.647241 0.628693 C -2.569137 2.491690 1.429637 H -3.467124 2.698646 1.991166 C -1.498960 3.368950 1.483132 C -1.347505 1.073356 -0.048382 C -0.345601 3.092661 0.777111 C -0.256135 1.944871 0.002405 H 0.502178 3.754173 0.859510 H -1.558322 4.260499 2.086948 C 0.947483 1.552267 -0.718580 C 2.023426 2.378171 -0.995255 C 3.106806 1.865461 -1.674146 C 3.099544 0.539867 -2.067367 C 1.999387 -0.230572 -1.763780 N 0.955065 0.275232 -1.120992 H 2.009687 3.405796 -0.675515 H 3.954226 2.495897 -1.893846 H 3.930288 0.100719 -2.593335 H 1.937025 -1.277720 -2.010232 O 2.223678 0.422106 1.852856 C 1.936522 -0.606686 2.409352 C 2.903725 -1.747494 2.503150 H 2.523603 -2.568910 1.897378 H 3.878282 -1.445243 2.137255 H 2.981313 -2.105988 3.527582 C 0.586600 -0.825255 3.022271 H 0.101162 -1.669119 2.533824 H 0.689612 -1.076907 4.076745 H -0.026393 0.062026 2.912890	**TS(e-i)** E_0 = -1758.8737734 E_{0+ZPE} = -1758.582797 H_{298} = -1758.561056 G_{298} = -1758.631438 N_{Imag} = 1 (-837.3638) E_0(M06) =-1758.4940982 O 1.281724 -1.694759 0.197262 Pd 0.559843 -0.163355 -0.904955 Cl 2.629726 0.539411 -1.583308 Cl -0.445366 1.293775 -2.355067 C 2.942708 -0.551823 1.556765 C 1.848295 -1.542324 1.316497 H 2.802670 0.362559 1.002257 H 3.063457 -0.352556 2.616119 H 3.861736 -1.010756 1.184477 C 0.340713 -0.586390 2.556935 C 2.012818 -2.843960 2.058267 H 2.427109 -2.710923 3.052479 H 1.067940 -3.373873 2.114785 H 2.705352 -3.448876 1.474142 N -1.309361 -0.902178 -0.448342 C -1.773557 -2.037515 -0.946155 C -3.050974 -2.475775 -0.678577 C -3.853065 -1.698190 0.139541 C -3.354116 -0.529582 0.671850 C -2.058463 -0.144579 0.362192 H -1.101496 -2.591717 -1.581590 H -3.404854 -3.397010 -1.109229 H -4.859638 -2.010374 0.370428 H -3.946349 0.074412 1.338386 C -1.381214 1.039446 0.854084 C -2.024126 2.203006 1.257652 C -1.293978 3.322764 1.594611 C 0.089319 3.293397 1.504140 C 0.760901 2.146007 1.115198 C 0.009568 1.032121 0.830697 H -1.798222 4.227748 1.892148 H 0.665247 4.176555 1.735832 H 1.834225 2.143035 1.046278 H -3.103276 2.240070 1.255543 H 0.874594 -1.240987 3.242022 H -0.627647 -1.011123 2.325569 H 0.275020 0.387675 3.018760	**TS(e-j)** E_0 = -1758.9175024 E_{0+ZPE} = -1758.625430 H_{298} = -1758.603600 G_{298} = -1758.675417 N_{Imag} = 1 (-577.1304) E_0(M06) =-1758.5387418 C -3.204353 1.665116 0.559974 C -2.173689 0.814612 0.171932 C -0.981160 1.342548 -0.332828 C -0.839025 2.711462 -0.452288 C -1.875285 3.547510 -0.067713 C -3.055297 3.030261 0.441068 C -2.262163 -0.634746 0.240641 N -1.172090 -1.277290 -0.209016 C -1.130288 -2.604212 -0.229534 C -2.180745 -3.376162 0.214272 C -3.309475 -2.734971 0.692893 C -3.352331 -1.358972 0.704682 Pd 0.367382 -0.033685 -0.802496 Cl 1.954123 1.501243 -1.515333 Cl 1.792099 -1.850629 -1.637649 H 0.074017 3.124828 -0.845017 H -1.756617 4.616176 -0.168149 H -4.127681 1.265131 0.950574 H -3.855869 3.689207 0.738551 H -4.223992 -0.842527 1.067922 H -4.153094 -3.305184 1.050118 H -2.110015 -4.450138 0.176824 H -0.225186 -3.036673 -0.625242 O 0.953766 0.384729 1.534006 C 2.103446 0.203142 2.008258 C 3.071010 1.363428 1.984604 C 2.195202 -0.753086 3.198124 C 2.856189 -0.981796 0.711577 H 3.822923 -1.311953 1.071758 H 2.055070 -1.690621 0.772255 H 2.850172 -0.217720 -0.054225 H 4.090316 1.057563 2.202655 H 3.025829 1.861350 1.020874 H 2.756407 2.073590 2.749382 H 3.209196 -1.082869 3.398472 H 1.843686 -0.195363 4.066209 H 1.541767 -1.607353 3.059649
TS(j'-g) E_0 = -1565.832735 E_{0+ZPE} = -1565.628151 H_{298} = -1565.612097 G_{298} = -1565.671701 N_{Imag} = 1 (-393.2474) E_0(M06) =-1565.5070128 Pd -0.894930 -0.147768 -0.165144 Cl -2.309690 -1.960947 -0.307375 Cl -2.758805 1.364651 -0.202644 C -2.060361 0.387231 1.802631		

H -1.229361 -0.236473 2.103019 H -2.027266 1.397773 2.167307 H -3.014959 -0.106614 1.823944 C 0.793771 -2.668397 -0.022892 H -0.116492 -3.240345 -0.084861 C 2.016464 -3.313389 0.072647 H 2.045733 -4.392657 0.085889 C 3.195561 -2.590889 0.147917 C 0.736378 -1.286007 -0.043292 C 3.152285 -1.213058 0.125509 C 1.930299 -0.554883 0.029527 H 4.074361 -0.655133 0.182163 H 4.143596 -3.100091 0.222140 C 1.809073 0.894313 -0.010136 C 2.866757 1.793446 0.025325 C 2.614968 3.145631 -0.034503 C 1.308323 3.589208 -0.131940 C 0.302200 2.650137 -0.162192 N 0.545861 1.345928 -0.096815 H 3.877364 1.429838 0.093903 H 3.432187 3.849729 -0.009071 H 1.066218 4.637005 -0.188335 H -0.735532 2.929773 -0.243055		
TS(k-l) E_0 = -1513.2380767 E_{0+ZPE} = -1512.980717 G_{298} = -1513.028761 N_{Imag} = 1 (-91.6656) E_0(M06) =-1512.994349 O -1.208211 0.578865 0.458742 O 0.792390 1.055398 -0.472536 Pd 0.211981 -0.743004 -0.144260 C 1.041148 2.938013 0.944629 C 1.719256 1.743580 0.298794 H 0.567541 3.561725 0.192528 H 0.278701 2.587119 1.634229 H 1.769774 3.533471 1.489255 C 2.427326 0.866307 1.311424 C 2.711922 2.209518 -0.796933 H 2.900113 0.013561 0.833073 H 3.188503 1.445711 1.827839 H 1.717696 0.503496 2.052678 H 3.467262 2.819090 -0.304363 H 3.184240 1.354702 -1.268592 H 2.201768 2.806089 -1.545495 C -2.352142 2.264573 -0.737561 C -2.364084 0.806190 -0.277730 H -2.251095 2.926278 0.117819 H -1.515856 2.431277 -1.410341 H -3.278478 2.500173 -1.257122 C -2.502775 -0.130129 -1.463357 C -3.517576 0.591787 0.715152 H -2.521822 -1.167347 -1.137197 H -3.424638 0.074183 -2.003112 H -1.674643 0.005195 -2.158805 H -4.462905 0.819427 0.225429 H -3.523795 -0.438738 1.055591 H -3.395204 1.244413 1.574135 Cl -0.815250 -2.169622 1.238776 Cl 1.837005 -2.163012 -0.835115	**TS(l-m)** E_0 = -1513.2282812 E_{0+ZPE} = -1512.971775 H_{298} = -1512.952545 G_{298} = -1513.017369 N_{Imag} = 1 (-407.6285) E_0(M06) =-1512.9661583 O 1.285445 0.500078 -0.608697 O -0.845582 0.771582 1.177827 Pd -0.378272 -0.475789 -0.226814 Cl -2.456567 -1.549768 -0.274354 Cl 0.532640 -2.384044 0.638103 C 3.324843 -0.792504 -0.626988 C 2.575530 0.402212 -0.061460 H 2.858767 -1.723584 -0.326460 H 3.331566 -0.742175 -1.713943 H 4.356514 -0.795513 -0.279150 C 3.253903 1.689415 -0.535608 C 2.540723 0.380656 1.458584 H 2.759576 2.563363 -0.118099 H 4.294693 1.698545 -0.217054 H 3.223961 1.754074 -1.620347 H 3.553509 0.404332 1.855715 H 2.000238 1.244744 1.837243 H 2.052072 -0.518124 1.820560 C -0.634052 2.971094 0.340105 C -1.415688 1.695514 0.452528 H 0.396147 2.753243 0.082019 H -1.075515 3.653942 -0.378865 H -0.657622 3.441751 1.322438 C -1.219203 1.168245 -1.511483 C -2.904582 1.779991 0.616960 H -1.467675 0.248650 -2.041036 H -2.087758 1.804494 -1.586861 H -0.284145 1.619420 -1.801709 H -3.338773 2.544786 -0.020502 H -3.367643 0.816298 0.431481 H -3.088349 2.051829 1.655404	**TS(o'-o)** E_0 = -1799.493185 E_{0+ZPE} = -1799.148610 H_{298} = -1799.124809 G_{298} = -1799.201734 N_{Imag} = 1 (-53.7554) E_0(M06) =-1799.072434 O 1.190836 -1.004549 0.783412 Pd 0.613020 -0.058355 -0.819000 Cl -0.501082 0.704692 -2.712585 Cl 2.414271 1.214978 -1.261209 C 2.384295 0.489654 2.254157 C 2.278686 -0.904059 1.651032 H 2.625317 1.220352 1.487400 H 1.441991 0.768074 2.720702 H 3.165620 0.521700 3.011643 C 1.952993 -1.909405 2.757007 C 3.585663 -1.304591 0.981828 H 1.822537 -2.902079 2.334258 H 2.762098 -1.941027 3.484704 H 1.036860 -1.626427 3.268964 H 4.405930 -1.278896 1.697174 H 3.512590 -2.317826 0.591092 H 3.827475 -0.627667 0.167767 C 1.503221 -1.455270 -1.963879 H 2.376351 -1.794269 -1.429323 H 0.691856 -2.179087 -1.973491 H 1.706469 -1.032136 -2.935254 C -2.256445 -0.422405 0.492065 C -2.975603 -0.694818 -0.665616 H -3.203008 0.104008 -1.352883 C -3.374504 -1.989537 -0.945447 C -1.939246 -1.458303 1.361364 C -3.061783 -3.016561 -0.072791 C -2.341977 -2.750075 1.079119 H -1.365705 -1.251122 2.249820 H -2.088613 -3.549365 1.757962 H -3.374447 -4.025843 -0.292604 H -3.926028 -2.193616 -1.849834 C -1.853903 0.971693 0.806076 N -0.645099 1.368089 0.415374 C -0.254759 2.612289 0.651619 C -1.050795 3.527121 1.308439 C -2.305035 3.125556 1.725326 C -2.714199 1.831938 1.468875

		H 0.727757 2.874879 0.290134 H -0.692553 4.528723 1.479466 H -2.959515 3.812230 2.239744 H -3.686771 1.479756 1.771071
TS(o-p) E_0 = -1799.480083 E_{0+ZPE} = -1799.139258 H_{298} = -1799.115809 G_{298} = -1799.190364 N_{Imag} = 1 (-941.3414) E_0(M06) =-1799.0587653 N -0.378320 1.398980 -0.476252 C -1.577866 1.409217 0.105466 C -2.294963 2.589934 0.229121 C -1.763506 3.753712 -0.289392 C -0.536528 3.715969 -0.922695 C 0.125177 2.505496 -0.992501 C -2.067250 0.104916 0.580391 C -1.152478 -0.946189 0.772333 C -1.619363 -2.200540 1.152372 C -2.964189 -2.420694 1.368975 C -3.857981 -1.380165 1.179201 C -3.416538 -0.127822 0.789266 Pd 0.529615 -0.652912 -0.619259 Cl 2.330534 -0.083836 -1.949745 C 1.143860 -2.583251 -0.717930 O 1.376882 -0.654270 1.283986 C 2.042972 0.345920 2.032118 C 3.043493 1.103901 1.183292 Cl -0.757541 -1.057548 -2.479099 C 1.048652 1.305679 2.669124 C 2.772794 -0.429259 3.123652 H -0.014230 -0.725207 1.244189 H -0.909879 -2.999396 1.306209 H -3.318204 -3.393087 1.673084 H -4.140731 0.651523 0.613439 H -4.914388 -1.547025 1.323906 H -3.247886 2.601647 0.730406 H -2.306377 4.681973 -0.201131 H -0.095850 4.599251 -1.354066 H 1.083445 2.401393 -1.479852 H 3.314774 0.249560 3.780499 H 2.063534 -0.997815 3.720542 H 3.480966 -1.122562 2.677964 H 3.621409 1.786005 1.804927 H 3.722518 0.417049 0.687559 H 2.545449 1.685239 0.412930 H 1.563314 2.008454 3.321516 H 0.520026 1.880546 1.913584 H 0.320337 0.762050 3.268447 H 1.707665 -2.699051 0.198076 H 1.739985 -2.674109 -1.612867 H 0.236427 -3.168580 -0.767978	**TS(o-p')** E_0 = -1799.4759823 E_{0+ZPE} = -1799.135926 H_{298} = -1799.112326 G_{298} = -1799.187579 N_{Imag} = 1 (-1282.9640) E_0(M06) =-1799.0510018 O 1.184798 -0.150047 1.200842 Pd 0.465222 -0.392342 -0.700666 Cl -0.795658 -0.781413 -2.579562 Cl 2.116291 0.620881 -1.964667 C 2.860502 1.483277 1.591670 C 2.450923 0.036140 1.807903 H 2.970892 1.686143 0.530245 H 2.101191 2.147600 1.998086 H 3.807039 1.696711 2.086440 C 2.245617 -0.241107 3.288889 C 3.499736 -0.897927 1.235171 H 1.928241 -1.270176 3.444310 H 3.170580 -0.081078 3.840469 H 1.483571 0.420546 3.693664 H 4.467288 -0.699051 1.692371 H 3.247381 -1.937974 1.431902 H 3.594561 -0.750033 0.162766 C 1.342669 -2.196113 -0.980155 H 1.645884 -2.510836 0.009423 H 0.585797 -2.824707 -1.427363 H 2.180476 -2.034697 -1.642510 C -2.115733 -0.198695 0.697180 C -3.412012 -0.629475 0.921986 H -4.230123 0.073224 0.927202 C -3.678607 -1.977233 1.090505 C -1.068998 -1.143265 0.652495 C -2.662096 -2.917012 1.036027 C -1.369993 -2.496352 0.802013 H 0.028948 -0.796925 1.211047 H -0.571856 -3.221576 0.758160 H -2.883368 -3.964853 1.163745 H -4.696692 -2.298343 1.250174 C -1.815165 1.221387 0.446434 N -0.705264 1.460993 -0.249772 C -0.363283 2.695835 -0.562692 C -1.121959 3.785770 -0.178880 C -2.265549 3.559156 0.560920 C -2.621129 2.263136 0.878934 H 0.542841 2.799677 -1.140800 H -0.815025 4.781550 -0.452496 H -2.877627 4.384267 0.890702 H -3.502032 2.065617 1.466290	
TS(q-r) E_0 = -1992.5870621 E_{0+ZPE} = -1992.152772 H_{298} = -1992.123782 G_{298} = -1992.210799 N_{Imag} = 1 (-418.8163) E_0(M06) =-1992.1149757 C 2.499921 1.007086 1.267588 C 2.924282 0.347805 0.120017 C 3.690330 1.024386 -0.820119 C 4.018143 2.350837 -0.621295 C 3.596006 3.006663 0.523309 C 2.840636 2.333414 1.465479	**TS(q-r)'** E_0 = -1992.5832922 E_{0+ZPE} = -1992.149226 H_{298} = -1992.120145 G_{298} = -1992.207172 N_{Imag} = 1 (-366.8566) E_0(M06) =-1992.113519 C -2.078262 1.211678 -1.342215 C -2.714900 0.642429 -0.246970 C -3.504377 1.435496 0.578273 C -3.658740 2.782400 0.311768 C -3.044092 3.342708 -0.795430 C -2.257265 2.555719 -1.617813	**TS(q-r)'''** E_0 = -1992.5577501 E_{0+ZPE} = -1992.124283 H_{298} = -1992.094908 G_{298} = -1992.183704 N_{Imag} = 1 (-225.4423) E_0(M06) =-1992.0966606 C -2.838344 2.320623 0.336381 C -2.144456 1.206430 0.794072 C -1.040594 1.380293 1.616337 C -0.643784 2.653731 1.985080 C -1.337317 3.758246 1.528824 C -2.431711 3.589390 0.696478

C 2.612632 -1.079002 -0.073293	C -2.668827 -0.814137 -0.026098	C -2.636286 -0.140172 0.455782
N 1.345146 -1.491731 0.007117	N -1.509839 -1.472919 0.008512	N -1.802586 -1.055973 -0.053927
C 1.056511 -2.783825 -0.102618	C -1.509666 -2.799612 0.133733	C -2.264729 -2.266309 -0.366097
C 2.019221 -3.740048 -0.326139	C -2.659768 -3.541421 0.251423	C -3.577005 -2.630044 -0.169379
C 3.334062 -3.331806 -0.441085	C -3.869060 -2.874127 0.245995	C -4.448509 -1.702753 0.363518
C 3.630243 -1.993301 -0.307003	C -3.868621 -1.505850 0.101109	C -3.969522 -0.450307 0.678843
Pd -0.213473 -0.154452 0.111027	Pd 0.425380 -0.726077 0.094885	Pd 0.093481 -0.527467 -0.676411
Cl 0.282329 0.271912 -2.140005	Cl 0.472010 -1.052598 -2.236537	O 1.920246 -0.061161 -1.197337
Cl -0.455568 -0.696480 2.368259	Cl 0.208130 -0.822473 2.404583	O 1.688833 -0.312735 0.981861
H 3.996410 0.519853 -1.723382	H -3.983403 0.997815 1.440930	C 2.356797 -0.757605 2.083162
H 4.595913 2.876845 -1.365202	H -4.261503 3.393035 0.965841	C 2.814408 0.403050 2.960143
H 3.855520 4.042654 0.677897	H -3.178700 4.390823 -1.014848	Cl -1.027889 0.497278 -2.442857
H 1.921965 0.479451 2.010601	H -1.462806 0.599682 -1.983582	Cl 0.833029 -2.805136 -0.442522
H 2.515724 2.836796 2.362701	H -1.783742 2.984455 -2.487702	C 1.345001 -1.625999 2.880714
H 4.645735 -1.637354 -0.355042	H -4.790924 -0.951836 0.052148	C 3.528678 -1.647798 1.668527
H 4.120194 -4.049005 -0.618837	H -4.799032 -3.413221 0.337896	C 2.426851 1.200124 -1.489101
H 1.735205 -4.775359 -0.411124	H -2.597247 -4.611808 0.350365	C 3.886909 1.182622 -1.056656
H 0.016634 -3.045274 -0.011557	H -0.542631 -3.275092 0.146736	C 2.360300 1.348527 -3.019953
O -1.713138 1.131953 0.416735	O 2.339696 -0.292079 0.449682	C 1.677436 2.324073 -0.803821
O -2.308271 -0.545588 -0.725663	O 1.206208 1.366834 -0.339394	H -0.498987 0.522335 1.980002
C -1.936502 2.348549 -0.250939	C 3.441522 -0.698567 -0.320946	H 0.210181 2.780167 2.631667
C -3.232867 -1.291926 -0.045459	C 1.289358 2.365768 0.582560	H -1.024010 4.750174 1.815265
C -2.658451 2.176212 -1.582527	C 3.667405 0.182793 -1.544293	H -3.677209 2.189510 -0.329233
C -2.845136 3.098783 0.728445	C 4.611207 -0.531522 0.654332	H -2.965269 4.448888 0.321794
C -0.640383 3.121822 -0.437132	C 3.329101 -2.162950 -0.719909	H -4.608501 0.300031 1.113204
C -4.183539 -1.563643 -1.257658	C 1.267168 3.533888 -0.479406	H -5.484624 -1.950214 0.534740
C -2.692249 -2.609254 0.471402	C 0.088566 2.503300 1.489831	H -3.895947 -3.622351 -0.440248
C -3.993551 -0.533314 1.026532	C 2.595323 2.434422 1.349230	H -1.543343 -2.948198 -0.782225
H -4.797977 -1.156328 1.410862	H 2.624306 3.349202 1.936621	H 3.330301 0.040169 3.846993
H -3.311322 -0.285757 1.833881	H 2.657368 1.580278 2.015049	H 3.499013 1.042941 2.407684
H -4.413487 0.383200 0.627073	H 3.447081 2.420193 0.677264	H 1.964650 1.002807 3.277750
H -4.970919 -2.216852 -0.885352	H 1.361902 4.446059 0.107322	H 1.860969 -2.017868 3.755041
H -4.612886 -0.637129 -1.619720	H 2.100743 3.445011 -1.165435	H 0.503967 -1.023932 3.212956
H -3.652978 -2.059692 -2.062950	H 0.330171 3.538828 -1.021094	H 0.992713 -2.440839 2.259293
H -3.494374 -3.215618 0.886198	H 0.137291 3.443686 2.034504	H 4.021586 -2.060175 2.546976
H -2.227991 -3.167839 -0.338766	H -0.833068 2.476904 0.917873	H 3.172897 -2.451814 1.034220
H -1.965990 -2.425937 1.259607	H 0.077137 1.687755 2.208462	H 4.250963 -1.060648 1.106904
H -3.063251 4.087694 0.328703	H 5.531228 -0.852736 0.168937	H 2.817050 2.295787 -3.302406
H -3.780234 2.567351 0.875252	H 4.721433 0.504676 0.956997	H 2.903802 0.535649 -3.492063
H -2.354487 3.210523 1.691209	H 4.452345 -1.138331 1.541353	H 1.330002 1.328805 -3.355317
H -2.832106 3.162445 -2.008633	H 4.557095 -0.164368 -2.066158	H 1.721237 2.184456 0.273236
H -2.057091 1.592651 -2.269866	H 2.818366 0.126646 -2.215368	H 2.130525 3.280645 -1.055622
H -3.616608 1.684994 -1.444322	H 3.819775 1.217835 -1.253986	H 0.635418 2.348620 -1.111945
H -0.858828 4.125519 -0.798041	H 4.267082 -2.501388 -1.156774	H 4.398969 0.331927 -1.497209
H -0.117756 3.205978 0.512928	H 3.124599 -2.767781 0.161328	H 4.386435 2.097851 -1.367105
H 0.009208 2.633227 -1.155077	H 2.540460 -2.312656 -1.449081	H 3.940448 1.098583 0.026197
TS(r-d)	**TS(r-d)′**	**TS(q-d)**
E_0 = -1992.6115093	E_0 = -1992.6033602	E_0 = -1992.5470745
E_{0+ZPE} = -1992.179796	E_{0+ZPE} = -1992.171635	E_{0+ZPE} = -1992.117833
H_{298} = -1992.151657	H_{298} = -1992.143432	H_{298} = -1992.088826
G_{298} = -1992.234961	G_{298} = -1992.227138	G_{298} = -1992.175284
N_{Imag} = 1 (-1250.7024)	N_{Imag} = 1 (-641.1324)	N_{Imag} = 1 (-1346.3859)
E_0(M06) =-1992.1244258	E_0(M06) =-1992.1184555	E_0(M06) =-1992.081219
C 1.885730 -0.737094 -0.339745	N 1.700488 -0.164107 -0.798058	N -2.012839 -0.936157 0.272659
C 2.603817 0.443202 -0.080505	C 2.342226 0.904056 -0.308493	C -2.700265 0.207071 0.239028
C 3.874823 0.608144 -0.599995	C 3.685767 1.099383 -0.580641	C -4.011419 0.236821 0.698684
C 4.423916 -0.388584 -1.388881	C 4.349206 0.195797 -1.385578	C -4.607912 -0.921523 1.141206
C 3.713333 -1.543866 -1.673717	C 3.657251 -0.877758 -1.910000	C -3.886739 -2.100935 1.124418
C 2.439262 -1.707779 -1.166066	C 2.322134 -1.020730 -1.591269	C -2.580293 -2.059065 0.700202
Pd -0.235916 -0.141596 -0.355307	C 1.526376 1.819440 0.493997	C -2.050962 1.377447 -0.355313
C 1.926793 1.478047 0.704120	C 0.322080 1.330636 1.026937	C -0.671901 1.575495 -0.348840
N 0.592193 1.398250 0.729795	C -0.555898 2.188029 1.679102	C -0.109507 2.581704 -1.116793
C -0.143249 2.229404 1.443735	C -0.213431 3.511216 1.870548	C -0.909356 3.447755 -1.837082
C 0.437601 3.246529 2.172496	C 0.989652 3.982250 1.368336	C -2.283383 3.295874 -1.809406
C 1.813080 3.372953 2.148274	C 1.855641 3.149474 0.676896	C -2.841532 2.266281 -1.083543
C 2.566626 2.479688 1.414014	Pd -0.372342 -0.244147 -0.325582	Pd -0.026258 -0.936981 -0.121742
H 4.427588 1.519467 -0.432925	Cl -0.796761 -2.060416 -1.702362	Cl -0.565209 -0.950893 -2.398747
H 5.410537 -0.251152 -1.804116	O -2.178437 -0.182470 0.425669	O 1.509646 0.995157 0.738677
H 4.149174 -2.303402 -2.303595	C -3.395649 0.197492 -0.164261	C 2.043815 1.664449 1.826959

H 1.146262 -1.151552 0.620209	C -3.532715 1.709768 -0.273556	C 0.913920 2.004568 2.804165
H 1.863723 -2.590016 -1.397772	O -0.080993 -1.195724 1.499259	Cl 0.175641 -1.521709 2.156861
H 3.641655 2.540533 1.404636	C 0.804885 -2.201181 1.937511	C 3.007017 0.692609 2.529582
H 2.299726 4.155347 2.709572	C 0.843521 -3.375032 0.979314	C 2.785570 2.915154 1.380642
H -0.181575 3.914948 2.746664	Cl -0.642899 1.213198 -2.107181	H 0.241071 1.173362 0.410666
H -1.204629 2.038495 1.404536	C -3.675862 -0.469459 -1.499041	H 0.960332 2.698874 -1.119654
O -2.060953 0.470762 0.152130	C -4.400219 -0.324823 0.869349	H -0.457734 4.240460 -2.413541
O 0.067154 -1.126277 1.442421	C 2.207564 -1.663026 2.186498	H -3.906642 2.104771 -1.134625
C -0.181505 -2.227622 3.465659	C 0.192936 -2.644503 3.265332	H -2.918362 3.955918 -2.379031
C -0.514780 -2.305460 1.979766	H 0.281170 0.194051 1.471789	H -4.543948 1.172159 0.716278
H 0.895601 -2.196719 3.613281	H -1.488667 1.783304 2.037838	H -5.624656 -0.904564 1.501413
H -0.616211 -1.331651 3.900854	H -0.880504 4.180144 2.390920	H -4.311200 -3.033119 1.456118
H -0.578050 -3.097449 3.987236	H 2.757578 3.560491 0.251866	H -1.952407 -2.933034 0.709428
C -2.018105 -2.299769 1.784573	H 1.249447 5.022236 1.494535	H 3.252765 3.412233 2.228510
C 0.114723 -3.549245 1.374233	H 4.203030 1.944711 -0.159623	H 3.563943 2.658345 0.665279
H -2.269197 -2.338275 0.729839	H 5.396851 0.332584 -1.603800	H 2.104150 3.622001 0.911695
H -2.458941 -3.161995 2.282647	H 4.133048 -1.597996 -2.554096	H 1.327366 2.486535 3.687182
H -2.447450 -1.392783 2.199796	H 1.716301 -1.826525 -1.975700	H 0.207523 2.688334 2.337341
H -0.279552 -4.443053 1.853881	H 0.789948 -3.436929 3.715036	H 0.393706 1.098732 3.099668
H -0.099383 -3.609740 0.311990	H 0.145932 -1.807031 3.957011	H 3.369678 1.163304 3.441263
H 1.193976 -3.539446 1.521900	H -0.816296 -3.009846 3.100763	H 2.487979 -0.229309 2.764102
C -3.406932 0.238955 -1.879288	H 1.420306 -4.191870 1.410446	H 3.851359 0.471510 1.886047
C -3.105155 1.016540 -0.610071	H -0.162611 -3.723192 0.767747	O 1.909855 -1.121143 -0.188125
H -2.570503 0.283855 -2.569251	H 1.300194 -3.098820 0.033880	C 2.843165 -1.077188 -1.223114
H -3.605258 -0.803760 -1.651674	H 2.824860 -2.421962 2.663433	C 2.647627 -2.362539 -2.044192
H -4.282453 0.664023 -2.367606	H -4.682491 -0.214602 -1.827150	H 3.404437 -2.401663 -2.825679
C -4.301640 0.897993 0.340502	H -2.972959 -0.139344 -2.257024	H 2.760720 -3.230912 -1.400947
C -2.865052 2.486342 -0.931211	H -3.598665 -1.548221 -1.408412	H 1.663084 -2.374001 -2.497992
H -4.105132 1.426357 1.270708	H -4.514397 1.972578 -0.664722	C 2.692104 0.147512 -2.113257
H -5.187054 1.330138 -0.123606	H -3.431601 2.172640 0.706566	H 2.822110 1.040781 -1.508693
H -4.496586 -0.145680 0.569322	H -2.780427 2.123982 -0.936445	H 3.459916 0.126642 -2.883961
H -3.718050 2.903542 -1.463889	H -5.411654 -0.059627 0.564829	H 1.718109 0.172535 -2.588840
H -2.734101 3.064044 -0.016894	H -4.323938 -1.404936 0.950884	C 4.220351 -1.092092 -0.579927
H -1.983395 2.608319 -1.551783	H -4.203267 0.111021 1.845536	H 4.295591 -1.909106 0.132317
Cl 0.040708 1.089374 -2.284156	H 2.696703 -1.378459 1.258869	H 4.991129 -1.213717 -1.338219
Cl -0.930899 -1.945426 -1.593031	H 2.173298 -0.796792 2.845132	H 4.402576 -0.157127 -0.057483

TS(q-r)"

E_0 = -1992.5739524
E_{0+ZPE} = -1992.140653
H_{298} = -1992.111212
G_{298} = -1992.200833
N_{Imag} = 1 (-134.6104)
E_0(M06) =-1992.103602

C -4.199441 0.426825 -0.526262		
C -3.047929 0.264925 0.231603		
C -2.735157 -0.991434 0.733549		
C -3.551691 -2.073481 0.465558		
C -4.689133 -1.908755 -0.302992		
C -5.011910 -0.656508 -0.796829		
C -2.183201 1.419404 0.518966		
N -0.856119 1.296864 0.407158		
C -0.062008 2.311922 0.735915		
C -0.552286 3.525300 1.162128		
C -1.921708 3.683354 1.256837		
C -2.738588 2.619982 0.943037		
Pd 0.106843 -0.369830 -0.397792		
Cl -1.015632 -0.040124 -2.364626		
Cl 1.034139 -2.284491 -1.253680		
H -1.862320 -1.119232 1.354657		
H -3.295786 -3.045871 0.855792		
H -5.320999 -2.755373 -0.521851		
H -4.433746 1.393225 -0.945127		
H -5.890574 -0.526525 -1.409062		
H -3.808298 2.690089 1.047649		
H -2.347860 4.617615 1.588366		
H 0.129651 4.321427 1.409947		
H 0.993529 2.115571 0.641033		
O 2.275901 0.572049 -0.361413		
O 1.285236 -0.267652 1.278448		

TS(r-s)

E_0 = -1992.5852802
E_{0+ZPE} = -1992.151539
H_{298} = -1992.122873
G_{298} = -1992.208351
N_{Imag} = 1 (-563.7106)
E_0(M06) =-1992.1058223

O 2.121274 -0.584536 1.336887		
Pd 0.720515 -0.500170 -0.061145		
Cl 0.021445 -2.622544 0.672992		
Cl -0.673722 -0.680372 -1.934187		
C 3.558438 -2.452879 1.089539		
C 3.093885 -1.100393 0.614938		
H 2.709125 -3.109047 1.243445		
H 4.265384 -2.899486 0.395535		
H 4.060460 -2.303155 2.044652		
C 2.393731 -1.575486 -1.086733		
C 4.190277 -0.113581 0.303813		
H 1.659470 -1.234301 -1.827895		
H 3.324843 -1.242177 -1.523543		
H 2.270743 -2.640805 -0.981065		
H 4.969209 -0.552345 -0.315257		
H 3.764200 0.764511 -0.168450		
H 4.632109 0.184062 1.253622		
N -0.568336 0.584649 1.219462		
C 0.173081 1.298074 2.068786		
C -0.364653 2.188434 2.967320		
C -1.732057 2.367660 2.975657		
C -2.493177 1.633228 2.096046		
C -1.900951 0.729967 1.218727		
H 1.236469 1.142593 2.005868		
H 0.289000 2.727914 3.631883		
H -2.199925 3.059964 3.658433		

TS(r-s)'

E_0 = -1992.5795266
E_{0+ZPE} = -1992.145728
H_{298} = -1992.116958
G_{298} = -1992.203058
N_{Imag} = 1 (-509.9239)
E_0(M06) =-1992.0998816

O 1.326919 1.550525 1.132676		
Pd 0.655671 0.107429 -0.071812		
Cl -0.175319 -1.708943 -1.245838		
Cl 1.163796 1.232182 -2.050012		
C -0.019843 1.616793 3.071161		
C 1.079317 0.962642 2.268925		
H -0.931239 1.695407 2.488893		
H -0.217722 1.093088 4.002279		
H 0.315957 2.624973 3.310422		
C 0.350442 -0.869512 1.963612		
C 2.298045 0.552386 3.046553		
H -0.300852 -1.410403 1.276038		
H 1.246051 -1.448532 2.114306		
H -0.245783 -0.694852 2.847048		
H 2.045551 -0.027089 3.929845		
H 2.968066 -0.005737 2.402941		
H 2.797865 1.468742 3.360657		
N -1.255942 1.252141 -0.162264		
C -0.980090 2.546744 -0.343375		
C -1.908251 3.466427 -0.772966		
C -3.182716 3.026262 -1.063066		
C -3.481018 1.698234 -0.853880		
C -2.507714 0.827759 -0.378942		
H 0.033153 2.840143 -0.134935		
H -1.616532 4.495707 -0.897306		
H -3.937398 3.706296 -1.426962		

C 3.382900 0.900832 -1.062002	H -3.566228 1.722557 2.075697	H -4.474461 1.315448 -1.018537
C 1.727113 -1.160681 2.242538	C -2.816590 -0.018318 0.331710	C -2.938565 -0.543844 -0.040148
C 2.751821 1.080626 -2.494839	C -3.583986 0.694078 -0.581371	C -3.505242 -1.361063 -1.008572
C 3.991739 2.220457 -0.609776	C -4.511892 0.040984 -1.367823	C -3.991785 -2.606860 -0.667815
C 4.396632 -0.231012 -1.127109	C -4.698210 -1.323362 -1.227556	C -3.935295 -3.041419 0.645711
C 2.081918 -0.372130 3.493723	C -3.957258 -2.027664 -0.297011	C -3.395143 -2.221336 1.618499
C 0.565877 -2.123380 2.527271	C -3.018427 -1.380021 0.483908	C -2.900339 -0.975472 1.276146
C 2.926735 -1.957995 1.745892	H -5.086203 0.596372 -2.092987	H -4.407262 -3.245758 -1.431329
H 3.222999 -2.693143 2.491535	H -5.422233 -1.835407 -1.842559	H -4.315851 -4.015846 0.909828
H 2.684930 -2.458929 0.815451	H -4.101480 -3.090263 -0.180257	H -3.365028 -2.547197 2.646811
H 3.760969 -1.282004 1.576442	H -3.431423 1.756721 -0.695390	H -3.526861 -1.032626 -2.035914
H 2.431348 -1.032296 4.285216	H -2.433549 -1.933246 1.197412	H -2.502537 -0.324048 2.038158
H 2.872719 0.340646 3.270173	O 1.558294 1.258428 -0.470987	O 2.330688 -0.867747 0.195661
H 1.216720 0.178307 3.855703	C 1.597245 1.756816 -2.843534	C 3.178094 -1.551812 -1.989837
H 0.878442 -2.842135 3.282162	C 1.247733 2.223261 -1.438319	C 3.466122 -0.951699 -0.625967
H -0.293303 -1.577690 2.909535	H 2.637407 1.436908 -2.878952	H 2.668843 -2.504683 -1.880945
H 0.292925 -2.659402 1.622176	H 0.962846 0.930911 -3.147337	H 2.548146 -0.895922 -2.580112
H 4.831488 2.496272 -1.243414	H 1.468963 2.566518 -3.560063	H 4.113092 -1.708825 -2.525639
H 3.253330 3.017368 -0.645620	C -0.194547 2.699516 -1.354853	C 4.203352 0.372984 -0.723778
H 4.353611 2.127125 0.412223	C 2.172686 3.383388 -1.054622	C 4.320016 -1.945470 0.176078
H 3.570054 1.380119 -3.148058	H -0.410680 3.068907 -0.353911	H 4.416266 0.759455 0.270498
H 2.318444 0.142016 -2.818481	H -0.364274 3.511907 -2.059524	H 5.146398 0.240102 -1.251329
H 1.986257 1.847304 -2.476004	H -0.878682 1.891692 -1.594368	H 3.611420 1.107370 -1.258113
H 5.168209 -0.013825 -1.862177	H 2.028348 4.216634 -1.740628	H 5.256817 -2.116570 -0.351145
H 4.876055 -0.355262 -0.158633	H 1.957302 3.720032 -0.043899	H 4.546304 -1.551776 1.163822
H 3.895470 -1.157499 -1.389638	H 3.213624 3.073511 -1.102635	H 3.797039 -2.891361 0.282649

TS(r-s)''	**TS(q-u)**	**TS(q-u)'**
E_0 = -1992.5787983	E_0 = -1992.6074678	E_0 = -1992.6213964
E_{0+ZPE} = -1992.145116	E_{0+ZPE} = -1992.178507	E_{0+ZPE} = -1992.191372
H_{298} = -1992.116370	H_{298} = -1992.149125	H_{298} = -1992.161685
G_{298} = -1992.202771	G_{298} = -1992.238918	G_{298} = -1992.256311
N_{Imag} = 1 (-485.2991)	N_{Imag} = 1 (-871.1022)	N_{Imag} = 1 (-1151.9418)
E_0(M06) =-1992.0981247	E_0(M06) =-1992.1178545	E_0(M06) =-1992.1159703
O -1.965739 -1.797301 0.306147	C -1.867412 -1.229100 0.237109	C -2.166156 0.716650 -0.820784
Pd -0.607322 -0.434212 -0.024941	C -2.935399 -0.368158 -0.044252	C -2.321863 1.293648 0.454860
Cl 0.950338 -2.089277 -0.600334	C -4.174769 -0.913620 -0.345114	C -3.045986 2.467924 0.593531
Cl 0.067977 -0.523365 2.193051	C -4.363097 -2.283649 -0.369938	C -3.621816 3.081257 -0.503851
C -3.809090 -1.379427 -1.123053	C -3.313509 -3.137307 -0.084350	C -3.511449 2.497070 -1.748024
C -2.426312 -1.929804 -0.909788	C -2.073234 -2.606519 0.211410	C -2.798118 1.317377 -1.899648
H -3.862153 -0.363364 -0.749900	C -2.789053 1.099804 0.007373	C -1.858713 0.543910 1.622112
H -4.108052 -1.421754 -2.166489	N -2.136274 1.594264 1.050665	N -1.494245 -0.726133 1.379376
H -4.489677 -2.001376 -0.542391	C -2.043324 2.907400 1.164050	C -1.132588 -1.531649 2.370849
C -1.483278 -0.650829 -2.111837	C -2.576378 3.794638 0.247275	C -1.109848 -1.104066 3.680582
C -2.130612 -3.268647 -1.529701	C -3.229989 3.275802 -0.854470	C -1.453620 0.205489 3.952526
H -0.435974 -0.474272 -2.341490	C -3.343189 1.906722 -0.978761	C -1.832184 1.034265 2.917819
H -1.789622 -1.387643 -2.841136	Pd 0.074223 -0.657024 0.080099	Pd -1.306867 -1.172689 -0.593734
H -2.094509 0.238051 -2.130041	Cl -0.250026 -0.454705 -2.182980	Cl -0.551649 -3.347485 -0.239146
H -2.533373 -3.349218 -2.536346	Cl -0.077787 -0.890263 2.522796	Cl -0.691538 -0.901391 -2.880319
H -1.064015 -3.462848 -1.525766	H -5.007349 -0.255134 -0.540804	H -3.199426 2.898360 1.570398
H -2.613986 -4.015911 -0.902219	H -5.338465 -2.683968 -0.600628	H -4.177860 3.996730 -0.377164
N 0.732301 1.138975 -0.725919	H -3.457901 -4.206250 -0.094977	H -3.982536 2.949064 -2.607036
C 0.035905 2.074169 -1.378399	H -1.215149 -0.967870 1.539933	H -1.112328 0.119421 -1.754389
C 0.609861 3.058816 -2.145964	H -1.250864 -3.268737 0.437023	H -2.717070 0.875698 -2.880682
C 1.984876 3.082374 -2.258763	H -3.823745 1.462590 -1.834979	H -2.098651 2.058720 3.111709
C 2.708969 2.144024 -1.561990	H -3.641323 3.927943 -1.609627	H -1.428119 0.581186 4.963564
C 2.074296 1.183576 -0.777694	H -2.470875 4.857925 0.390923	H -0.813052 -1.786891 4.458607
H -1.032827 2.011576 -1.244192	H -1.515130 3.271267 2.034591	H -0.854968 -2.531230 2.076589
H -0.018735 3.779724 -2.641624	O 2.298085 -0.290009 0.014480	O 2.973512 1.135818 -0.660416
H 2.484735 3.826841 -2.858994	O 2.752334 0.798954 -0.755093	O 2.746790 0.154452 0.330175
H 3.785872 2.147119 -1.578283	C 3.166383 -1.426044 -0.273869	C 2.808759 2.420789 -0.075614
C 2.965351 0.301746 0.004180	C 2.688354 2.022568 -0.011509	C 3.550927 -0.987521 0.029935
C 2.995366 0.378123 1.386059	C 3.154370 -1.717976 -1.759311	C 1.404871 2.564436 0.484575
C 3.930812 -0.350484 2.099027	C 4.562033 -1.118843 0.226065	C 3.855814 2.665942 0.995370
C 4.839039 -1.153779 1.437603	C 2.559461 -2.566281 0.515010	C 3.013921 3.346158 -1.259165
C 4.822048 -1.220380 0.053929	C 3.267421 2.999616 -1.017275	C 5.023810 -0.636563 0.129773
C 3.898101 -0.486242 -0.659877	C 1.251070 2.375670 0.309301	C 3.147960 -1.964628 1.116470
H 3.941952 -0.290327 3.175955	C 3.533777 1.957998 1.244023	C 3.200892 -1.534472 -1.340792
H 5.561437 -1.727853 1.997190	H 3.481028 2.911495 1.764663	H 3.769773 -2.442132 -1.531899
H 5.525173 -1.850652 -0.467989	H 3.168485 1.187711 1.916832	H 2.143814 -1.778613 -1.395754

H 2.290599 1.004736 1.904050 H 3.873799 -0.549213 -1.737063 O -2.023671 0.959123 0.128844 C -3.206750 0.608738 2.225035 C -2.576750 1.593935 1.253459 H -3.965162 0.013958 1.722030 H -2.461640 -0.063996 2.634286 H -3.680106 1.144522 3.046397 C -1.566508 2.494573 1.948764 C -3.679558 2.467015 0.647086 H -1.153825 3.213254 1.242366 H -2.042764 3.049911 2.755125 H -0.755549 1.909464 2.367739 H -4.181989 3.029156 1.432502 H -3.261029 3.172994 -0.066966 H -4.418539 1.853428 0.137414	H 4.575227 1.757050 1.007691 H 3.279535 3.998342 -0.588247 H 4.285570 2.724893 -1.281242 H 2.664908 3.016268 -1.921283 H 1.201645 3.394481 0.688527 H 0.634003 2.305223 -0.582627 H 0.837263 1.722635 1.073710 H 5.201948 -1.979109 0.044222 H 4.983180 -0.268439 -0.299537 H 4.558949 -0.914437 1.293443 H 3.723279 -2.626193 -1.947504 H 2.138180 -1.853641 -2.117264 H 3.605820 -0.905455 -2.318832 H 3.199901 -3.438982 0.414353 H 2.475187 -2.319779 1.569664 H 1.574702 -2.829990 0.134218	H 3.435418 -0.812233 -2.116815 H 5.629954 -1.522259 -0.047846 H 5.290997 0.112268 -0.609854 H 5.261425 -0.252184 1.119322 H 3.730466 -2.877610 1.019941 H 3.332963 -1.541607 2.101761 H 2.096762 -2.223551 1.025698 H 3.750719 3.670663 1.399830 H 3.744207 1.955083 1.808426 H 4.856158 2.565878 0.581230 H 1.248485 3.578053 0.848843 H 0.667817 2.356172 -0.286930 H 1.250094 1.872643 1.307091 H 2.909662 4.381480 -0.943331 H 4.006529 3.212913 -1.682186 H 2.278469 3.143240 -2.033277
TS(q-t) E_0 = -1992.5840312 E_{0+ZPE} = -1992.149729 H_{298} = -1992.121645 G_{298} = -1992.205741 N_{Imag} = 1 (-701.8928) E_0(M06) =-1992.088755 C 2.798048 2.874672 0.171224 C 2.211713 1.632141 -0.030395 C 0.830441 1.488046 0.108620 C 0.041254 2.580731 0.405539 C 0.638803 3.814519 0.601986 C 2.012035 3.961987 0.490688 C 2.939344 0.422028 -0.355906 N 2.169913 -0.672852 -0.464722 C 2.688716 -1.870837 -0.712743 C 4.041271 -2.023893 -0.912717 C 4.859066 -0.912499 -0.830429 C 4.306826 0.316668 -0.547199 Pd 0.254334 -0.452938 -0.008236 Cl 1.077118 -1.314108 2.209088 Cl -0.408823 -2.606734 -0.979109 H 0.170350 0.528898 -1.175152 H -1.027478 2.474672 0.467019 H 0.024074 4.668711 0.841747 H 3.866710 2.996167 0.087259 H 2.467415 4.926787 0.648186 H 4.925320 1.193192 -0.461022 H 5.923728 -1.004983 -0.977752 H 4.433870 -3.004373 -1.121124 H 1.984963 -2.685884 -0.753544 O -2.401135 0.899393 -0.394756 O -1.876437 -0.213341 0.280210 C -2.914769 0.575933 -1.718591 C -2.530470 -0.377440 1.616083 C -1.785613 0.460526 -2.724580 C -3.748258 -0.685633 -1.731842 C -3.753255 1.808608 -1.998840 C -1.891333 0.588040 2.586411 C -4.016665 -0.116224 1.506487 C -2.288335 -1.828330 1.962292 H -2.751177 -2.022890 2.927906 H -2.740329 -2.476973 1.218202 H -1.232976 -2.061499 2.042179 H -2.293693 0.404601 3.580102 H -0.816138 0.444148 2.635182 H -2.121559 1.616578 2.318951 H -4.428463 -0.212270 2.508203 H -4.235619 0.882752 1.146826 H -4.507542 -0.850168 0.878216 H -4.026588 -0.900450 -2.760863 H -3.172125 -1.528710 -1.361406 H -4.661411 -0.573629 -1.157165	**TS(t-u)** E_0 = -1992.580306 E_{0+ZPE} = -1992.146998 H_{298} = -1992.118581 G_{298} = -1992.203902 N_{Imag} = 1 (-617.9001) E_0(M06) =-1992.0885722 C 4.321830 0.437488 -0.557329 C 2.953747 0.470178 -0.343105 N 2.236707 -0.659317 -0.451990 C 2.812388 -1.822455 -0.728075 C 4.168038 -1.911012 -0.947239 C 4.929735 -0.759443 -0.865132 C 2.163745 1.617990 0.041261 C 2.655701 2.907304 0.202275 C 1.818329 3.913006 0.636459 C 0.492947 3.629806 0.922639 C -0.013094 2.347884 0.767298 C 0.820898 1.355653 0.308528 Pd 0.291285 -0.535634 0.031706 O -1.912416 -0.328338 0.179553 C -2.649648 -0.809983 1.378692 C -2.128149 -2.208580 1.615559 Cl 1.033378 -0.988842 2.411383 Cl -0.335508 -2.567736 -1.390245 O -2.464671 0.904732 -0.206949 C -2.815140 0.980616 -1.610691 C -3.701102 2.213451 -1.601991 C -1.591582 1.229696 -2.475088 C -3.565228 -0.240197 -2.094678 C -2.361673 0.123697 2.531741 C -4.129310 -0.862154 1.067499 H 0.012687 -0.694828 -1.454447 H -1.044877 2.142680 0.988026 H -0.159330 4.413321 1.277767 H 3.692793 3.123944 -0.003248 H 2.198186 4.914304 0.763097 H 4.897862 1.342180 -0.464859 H 5.995156 -0.797174 -1.030204 H 4.606629 -2.867452 -1.174827 H 2.155554 -2.673906 -0.783362 H -2.681923 -2.629008 2.452398 H -2.287775 -2.833795 0.742819 H -1.076344 -2.214066 1.882938 H -2.852679 -0.257593 3.424201 H -1.295264 0.172757 2.733534 H -2.755357 1.117326 2.332745 H -4.639652 -1.221441 1.957799 H -4.529055 0.116419 0.824726 H -4.338123 -1.556409 0.260098 H -3.737097 -0.138147 -3.163908 H -2.980628 -1.141737 -1.934921 H -4.529585 -0.340456 -1.607736	

H -2.207954 0.417443 -3.726658 H -1.133520 1.331436 -2.679175 H -1.209907 -0.448262 -2.570375 H -4.188445 1.728853 -2.991725 H -4.559012 1.903367 -1.275938 H -3.144612 2.709229 -1.965970	H -1.913790 1.608544 -3.443026 H -0.933582 1.964096 -2.019919 H -1.034607 0.316618 -2.663332 H -4.053252 2.412385 -2.610862 H -4.563253 2.064659 -0.957659 H -3.150451 3.084143 -1.254270	

v E_0 = -2005.9549427 E_{0+ZPE} = -2005.599706 H_{298} = -2005.574725 G_{298} = -2005.656341 N_{Imag} = 0 E_0(M06) =-2005.42223 C -3.029563 0.381561 -1.897577 C -2.379006 0.950512 -0.809426 C -2.914041 0.798752 0.465680 C -4.076588 0.070722 0.643156 C -4.712578 -0.507663 -0.442199 C -4.188466 -0.349884 -1.713773 C -1.150784 1.740508 -1.014563 N -0.085900 1.502753 -0.242912 C 1.006163 2.250884 -0.377327 C 1.106696 3.256709 -1.311789 C 0.024233 3.499479 -2.134225 C -1.114049 2.738012 -1.979623 Pd 0.000814 -0.001202 1.194785 Cl -0.108735 1.654009 2.789872 Cl 0.110459 -1.675949 2.770338 N 0.083072 -1.496737 -0.251168 C 1.149638 -1.735052 -1.020279 C 1.114154 -2.731118 -1.986809 C -0.025214 -3.489904 -2.146555 C -1.110111 -3.245715 -1.327665 C -1.010373 -2.241940 -0.391013 C 2.378659 -0.946421 -0.812786 C 3.027480 -0.373682 -1.900004 C 4.187298 0.356226 -1.715567 C 4.713880 0.508508 -0.444292 C 4.079574 -0.073892 0.639923 C 2.916194 -0.800490 0.461793 H 2.431690 -1.265233 1.307698 H 4.490120 0.032219 1.631798 H 5.620480 1.075792 -0.299367 H 2.609294 -0.479684 -2.889948 H 4.677538 0.808164 -2.564075 H 1.995225 -2.916779 -2.578229 H -0.058482 -4.273386 -2.887758 H -2.018576 -3.819425 -1.400409 H -1.823533 -2.014858 0.278330 H 1.817377 2.024617 0.294630 H 2.014029 3.832735 -1.380283 H 0.058179 4.284286 -2.874018 H -1.993708 2.923521 -2.573187 H -2.428909 1.260829 1.312654 H -4.485246 -0.039454 1.635359 H -5.618499 -1.076153 -0.297862 H -4.679846 -0.798939 -2.563091 H -2.613248 0.491218 -2.887854		
w E_0 = -2472.012872 E_{0+ZPE} = -2471.399592 H_{298} = -2471.359609 G_{298} = -2471.476040 N_{Imag} = 0 E_0(M06) =-2471.2917906 C -2.938445 2.959401 1.489084	**TS(w-x)** E_0 = -2471.8744309 E_{0+ZPE} = -2471.265150 H_{298} = -2471.225436 G_{298} = -2471.337753 N_{Imag} = 1 (-178.9202) E_0(M06) =-2471.1967685 C -2.663763 1.856083 1.425820	**x** E_0 = -2471.9497131 E_{0+ZPE} = -2471.336860 H_{298} = -2471.298028 G_{298} = -2471.406961 N_{Imag} = 0 E_0(M06) =-2471.254562 C -1.129485 2.848944 1.335950

C	-2.052433	2.663849	0.459799	C	-1.843599	2.457711	0.481007	C	-0.064092	3.110733	0.490797
C	-2.517005	2.587726	-0.848187	C	-2.403195	2.963993	-0.683726	C	-0.226882	4.030572	-0.537791
C	-3.853815	2.819900	-1.116747	C	-3.762478	2.845328	-0.907736	C	-1.446810	4.642168	-0.742772
C	-4.734848	3.108097	-0.088940	C	-4.574435	2.232383	0.030173	C	-2.515256	4.360097	0.092084
C	-4.277624	3.167832	1.216481	C	-4.023498	1.739326	1.198629	C	-2.350634	3.469281	1.135956
C	-0.608572	2.544449	0.730708	C	-0.418857	2.712627	0.811362	C	1.283872	2.558471	0.759958
N	0.078992	1.499576	0.262656	N	0.537833	1.785684	0.670674	N	1.574005	1.248056	0.730991
C	1.406197	1.478946	0.401922	C	1.772262	2.051978	1.105594	C	2.800311	0.852914	1.076123
C	2.108441	2.468855	1.050868	C	2.121959	3.259203	1.668696	C	3.798027	1.723084	1.455697
C	1.403146	3.529600	1.584742	C	1.161172	4.242499	1.773831	C	3.528537	3.074142	1.450766
C	0.036478	3.566995	1.416424	C	-0.117895	3.957067	1.347585	C	2.260558	3.485707	1.104167
Pd	-0.642473	-0.226525	-0.697342	Pd	0.414218	-0.061828	-0.334106	Pd	0.524699	-0.462108	-0.197070
Cl	-1.066130	-2.213773	-1.754401	Cl	0.359369	-2.079533	-1.377728	Cl	-0.393792	-2.216641	-1.321236
N	-1.103699	-1.165616	1.131690	N	-0.924925	-0.880740	1.269696	N	-1.173232	-0.427722	1.247760
C	-2.220181	-1.842417	1.430314	C	-2.038397	-1.615691	1.165360	C	-2.471240	-0.724739	1.109355
C	-2.305307	-2.566856	2.616823	C	-2.644270	-2.141515	2.307041	C	-3.279329	-0.902824	2.231292
C	-1.241690	-2.611579	3.486620	C	-2.102782	-1.920011	3.550591	C	-2.769593	-0.746645	3.498128
C	-0.093926	-1.914937	3.161183	C	-0.950993	-1.161442	3.642964	C	-1.437244	-0.409282	3.626081
C	-0.077322	-1.211442	1.980825	C	-0.406338	-0.669836	2.479679	C	-0.685903	-0.277029	2.482368
C	-3.385217	-1.831482	0.531275	C	-2.671886	-1.870508	-0.138200	C	-3.152882	-0.862944	-0.197771
C	-3.878647	-0.651788	-0.003125	C	-2.831266	-0.860753	-1.073018	C	-3.393514	0.242604	-0.995597
C	-5.001595	-0.672648	-0.808329	C	-3.460904	-1.119864	-2.275004	C	-4.151306	0.112612	-2.146034
C	-5.636593	-1.867599	-1.091033	C	-3.935726	-2.387434	-2.554258	C	-4.671775	-1.116242	-2.503858
C	-5.148167	-3.048377	-0.559493	C	-3.780322	-3.402049	-1.624362	C	-4.443665	-2.221403	-1.701045
C	-4.033401	-3.029318	0.253306	C	-3.157036	-3.143706	-0.420743	C	-3.697913	-2.092418	-0.546817
O	3.980768	-0.558233	-0.558854	O	2.441812	0.186082	-0.916290	O	2.232999	-0.756435	-1.116108
C	4.310373	-0.330741	-1.939429	C	3.228059	0.551715	-2.005520	C	2.674211	-0.353927	-2.387947
C	3.376164	-1.285203	-2.655288	C	2.922383	-0.322680	-3.209508	C	1.831812	-0.898448	-3.528258
O	4.780149	0.266750	0.264248	O	2.616557	-0.821733	0.861908	O	1.396857	-1.504791	1.271956
C	5.176315	-0.474123	1.417600	C	3.399151	-1.848036	1.325450	C	1.600333	-2.880379	1.448450
C	5.975890	0.544901	2.205504	C	2.600564	-2.457916	2.496605	C	0.297106	-3.618065	1.726123
Cl	-0.005003	0.764835	-2.677598	Cl	-0.333374	1.069871	-2.345232	Cl	-0.439258	0.969311	-1.770177
C	3.951622	-0.923748	2.195522	C	3.597714	-2.926880	0.266224	C	2.361517	-3.520098	0.297838
C	6.038933	-1.662880	1.040167	C	4.734347	-1.333242	1.853896	C	2.471979	-2.937283	2.706791
C	4.015911	1.109141	-2.315316	C	3.034183	2.035762	-2.311430	C	2.861011	1.152015	-2.496575
C	5.760482	-0.680113	-2.210863	C	4.682857	0.342386	-1.560823	C	4.052955	-1.026865	-2.432200
H	-2.580508	3.010604	2.506662	H	-2.240684	1.488627	2.347924	H	-1.002999	2.178945	2.169050
H	-4.963147	3.379553	2.022278	H	-4.650735	1.265568	1.937632	H	-3.171134	3.259952	1.805012
H	-5.777933	3.284486	-0.302697	H	-5.634084	2.138041	-0.150145	H	-3.468706	4.840010	-0.066274
H	-1.829508	2.357570	-1.648638	H	-1.769169	3.427135	-1.420899	H	0.598814	4.237597	-1.200785
H	-4.203156	2.774461	-2.136607	H	-4.185889	3.230058	-1.822461	H	-1.566231	5.335977	-1.560364
H	-0.545661	4.400986	1.771722	H	-0.911046	4.680862	1.434409	H	1.989521	4.528139	1.118171
H	1.911195	4.329323	2.101340	H	1.395803	5.209121	2.192351	H	4.282980	3.796156	1.723207
H	3.180783	2.390584	1.112635	H	3.134291	3.413204	2.003776	H	4.764535	1.333319	1.728667
H	1.927638	0.638210	-0.030644	H	2.482468	1.248413	0.985160	H	2.955113	-0.211693	1.036710
H	0.804629	-0.667709	1.689173	H	0.500090	-0.089555	2.509320	H	0.366455	-0.070994	2.546654
H	0.775909	-1.914600	3.796389	H	-0.474814	-0.957285	4.587615	H	-0.972259	-0.264870	4.587249
H	-1.308725	-3.173650	4.405190	H	-2.574923	-2.323266	4.433301	H	-3.399390	-0.877676	4.364661
H	-3.227839	-3.073985	2.843641	H	-3.557516	-2.701104	2.193868	H	-4.316796	-1.145325	2.072638
H	-3.633665	-3.955252	0.637013	H	-3.007782	-3.945482	0.286552	H	-3.511933	-2.954436	0.075680
H	-5.626810	-3.987181	-0.790665	H	-4.131188	-4.398620	-1.843716	H	-4.843086	-3.185128	-1.976629
H	-6.506126	-1.880818	-1.729927	H	-4.416341	-2.590042	-3.499152	H	-5.255431	-1.215195	-3.406261
H	-5.376563	0.251457	-1.217767	H	-3.559480	-0.326943	-2.998934	H	-4.326994	0.977689	-2.766313
H	-3.392915	0.284943	0.216451	H	-2.457117	0.128112	-0.872835	H	-2.988247	1.200941	-0.719916
H	6.429761	-0.034394	-1.649654	H	4.895868	0.926490	-0.670078	H	4.677612	-0.672759	-1.615906
H	5.965657	-1.715247	-1.950638	H	4.867805	-0.705461	-1.352823	H	3.948441	-2.104672	-2.351777
H	5.971648	-0.548888	-3.269632	H	5.341716	0.665960	-2.363680	H	4.542253	-0.788370	-3.375324
H	2.334990	-1.048721	-2.455918	H	1.892376	-0.177693	-3.520019	H	0.839935	-0.460806	-3.527487
H	3.534415	-1.206210	-3.728101	H	3.584194	-0.071791	-4.037435	H	2.311806	-0.670523	-4.479120
H	3.570854	-2.312023	-2.354934	H	3.052254	-1.370522	-2.954452	H	1.729872	-1.975896	-3.437302
H	4.257301	1.270334	-3.363583	H	3.669920	2.325690	-3.146637	H	3.317241	1.405282	-3.452352
H	2.961646	1.336088	-2.182397	H	1.998782	2.227935	-2.571327	H	1.907640	1.663827	-2.427015
H	4.615112	1.793335	-1.720263	H	3.303309	2.640749	-1.448121	H	3.516818	1.508578	-1.704130
H	5.481362	-2.358632	0.421198	H	5.307618	-0.881161	1.048444	H	3.414705	-2.421659	2.539477
H	6.923138	-1.341054	0.496713	H	4.572663	-0.581199	2.623714	H	1.961821	-2.467403	3.544726
H	6.360736	-2.185961	1.938210	H	5.326342	-2.142165	2.278976	H	2.686519	-3.972522	2.967805
H	5.360826	1.402570	2.467421	H	1.641239	-2.820619	2.141100	H	-0.364900	-3.559856	0.869426
H	6.344822	0.095567	3.124226	H	3.164325	-3.290242	2.915406	H	0.490934	-4.667907	1.941146
H	6.827386	0.893974	1.626994	H	2.441806	-1.716982	3.275886	H	-0.204399	-3.182749	2.588940
H	4.255111	-1.436015	3.106241	H	4.133942	-3.780809	0.677605	H	2.574623	-4.563468	0.527833

H 3.341156 -0.066597 2.472658 H 3.354147 -1.607526 1.599574	H 2.635710 -3.250407 -0.117586 H 4.172922 -2.534642 -0.568169	H 1.787433 -3.473310 -0.619999 H 3.300617 -2.998680 0.133539
y E_0 = -2005.9408944 E_{0+ZPE} = -2005.589991 H_{298} = -2005.564617 G_{298} = -2005.648375 N_{Imag}= 0 E_0(M06) =-2005.4056092 N -1.374010 1.083910 -0.817447 C -2.700935 1.092376 -0.599282 C -3.445084 2.230598 -0.885569 C -2.820175 3.344628 -1.397391 C -1.454839 3.313682 -1.621482 C -0.773821 2.158095 -1.313497 C -3.227251 -0.155598 -0.072458 C -2.287465 -1.177524 0.127809 C -2.732960 -2.394872 0.618591 C -4.074716 -2.588603 0.903792 C -4.997621 -1.573675 0.706730 C -4.573145 -0.356627 0.217913 Pd -0.434041 -0.683226 -0.329672 Cl 0.453486 -2.788952 0.203308 N 1.601173 -0.084147 -0.933812 C 2.399563 0.782789 -0.304463 C 3.650225 1.103674 -0.817615 C 4.079012 0.515406 -1.987053 C 3.253883 -0.394956 -2.618773 C 2.029710 -0.666672 -2.050577 C 1.934282 1.388342 0.956789 C 1.354456 0.603542 1.946915 C 0.937746 1.179401 3.132532 C 1.091738 2.538547 3.341301 C 1.674732 3.324530 2.362552 C 2.099182 2.750928 1.178803 H 1.255859 -0.460621 1.799889 H 0.496763 0.559313 3.897128 H 0.762541 2.984451 4.267181 H 2.545218 3.368758 0.413359 H 1.796569 4.385147 2.519291 H 4.284680 1.782307 -0.272226 H 5.053954 0.746054 -2.387571 H 3.551269 -0.898905 -3.522999 H 1.356724 -1.384623 -2.492508 H -2.029436 -3.194933 0.778094 H -4.402807 -3.544469 1.284773 H -5.294096 0.432065 0.063741 H -6.040508 -1.732623 0.932319 H -4.506608 2.233701 -0.707385 H -3.392344 4.231301 -1.622798 H 0.288857 2.077054 -1.467885 H -0.925347 4.160902 -2.023429 H 2.518629 -2.669528 0.477795 Cl 3.814557 -2.549483 0.651608	**TS(y-z)** E_0 = -2005.8626513 E_{0+ZPE} = -2005.518556 H_{298} = -2005.493670 G_{298} = -2005.575468 N_{Imag} = 1 (-669.9648) E_0(M06) =-2005.3289187 N -2.018054 1.285320 -0.024073 C -3.143272 0.599787 -0.299242 C -4.345709 1.270210 -0.483921 C -4.386966 2.642204 -0.387848 C -3.220063 3.332671 -0.116311 C -2.059609 2.610629 0.049224 C -2.971082 -0.843214 -0.348624 C -1.648136 -1.296818 -0.250702 C -1.457435 -2.657546 -0.057514 C -2.523602 -3.544055 -0.068434 C -3.816181 -3.087137 -0.258763 C -4.040915 -1.731203 -0.375559 Pd -0.269831 0.162754 -0.095231 Cl 1.212784 0.054692 2.787437 N 1.428586 -0.776256 -0.900169 C 2.511286 0.013394 -1.025272 C 3.671627 -0.475080 -1.611649 C 3.705448 -1.755548 -2.114833 C 2.567369 -2.531769 -2.034207 C 1.458312 -1.998726 -1.417318 C 2.388370 1.383920 -0.520220 C 1.283817 1.675392 0.292257 C 1.219192 2.957065 0.833913 C 2.159100 3.928557 0.543355 C 3.206622 3.632891 -0.312881 C 3.326289 2.361472 -0.836335 H 1.095419 0.745454 1.477740 H 0.442368 3.191615 1.549476 H 2.083768 4.910005 0.987184 H 4.148887 2.148354 -1.501169 H 3.937802 4.386922 -0.560126 H 4.545546 0.150273 -1.662568 H 4.606650 -2.139481 -2.566961 H 2.530533 -3.534382 -2.425352 H 0.551040 -2.568087 -1.341902 H -0.476206 -3.050571 0.161056 H -2.342227 -4.596831 0.089948 H -5.055214 -1.370480 -0.456652 H -4.644273 -3.778197 -0.273928 H -5.237500 0.711662 -0.710542 H -5.317465 3.169329 -0.531342 H -1.122196 3.101904 0.236995 H -3.198440 4.406738 -0.040422 H 1.714772 -1.996317 2.291288 Cl 2.020655 -3.222961 1.973323	**z** E_0 = -2005.8710389 E_{0+ZPE} = -2005.525072 H_{298} = -2005.498661 G_{298} = -2005.585324 N_{Imag} = 0 E_0(M06) =-2005.3351254 N -2.157783 1.171809 -0.233453 C -3.223741 0.352415 -0.160771 C -4.509461 0.880836 -0.203906 C -4.692256 2.236103 -0.351957 C -3.584943 3.056865 -0.470731 C -2.338611 2.476424 -0.411009 C -2.905268 -1.066208 -0.065225 C -1.551390 -1.400450 -0.239618 C -1.217903 -2.736280 -0.042309 C -2.172723 -3.698747 0.247106 C -3.507300 -3.349339 0.364586 C -3.870738 -2.026555 0.221329 Pd -0.322898 0.247200 -0.388666 Cl 1.199935 0.125320 3.032085 N 1.427317 -0.592252 -1.085983 C 2.516779 0.197682 -1.053733 C 3.704059 -0.230505 -1.633466 C 3.758837 -1.449131 -2.270952 C 2.617486 -2.225176 -2.336227 C 1.474876 -1.752602 -1.731625 C 2.326255 1.496819 -0.411781 C 1.002497 1.820190 -0.058739 C 0.828159 3.022831 0.621903 C 1.881739 3.882875 0.892902 C 3.166449 3.553346 0.499412 C 3.389056 2.353151 -0.145096 H 0.974459 0.689971 1.885684 H -0.150378 3.303155 0.986597 H 1.701537 4.805297 1.425374 H 4.399280 2.087001 -0.417076 H 3.991390 4.215085 0.712555 H 4.572975 0.403460 -1.599984 H 4.678851 -1.783425 -2.724874 H 2.602599 -3.176336 -2.840959 H 0.556426 -2.310894 -1.763557 H -0.185699 -3.054010 -0.075409 H -1.870731 -4.725300 0.395824 H -4.905831 -1.750192 0.356429 H -4.251897 -4.096308 0.591521 H -5.357621 0.221025 -0.143939 H -5.688788 2.648210 -0.391766 H -1.444181 3.064338 -0.517390 H -3.676313 4.120494 -0.612964 H 2.009627 -1.999211 2.222915 Cl 2.532990 -3.093423 1.795277
TS(e-e_{oc}) E_0 = -1758.9809593 E_{0+ZPE} = -1758.685498 H_{298} = -1758.664903 G_{298} = -1758.733229 N_{Imag}= 1 (-315.2140) E_0(M06) = -1758.5854233 C -0.213181 1.077590 -0.699535 C 1.078388 1.560335 -0.527555 C 1.393258 2.767209 -1.136484 C 0.449643 3.444000 -1.883630 C -0.815449 2.906462 -2.046694 C -1.170913 1.704986 -1.450753	**TS(e-e_{oc})'** E_0 = -1758.938422 E_{0+ZPE} = -1758.646202 H_{298} = -1758.624201 G_{298} = -1758.696567 N_{Imag}= 1 (-614.9395) E_0(M06) = -1758.548365 C 3.019771 1.932851 0.408371 C 2.062913 0.979111 0.076226 C 0.804106 1.366592 -0.406050 C 0.544479 2.718706 -0.561875 C 1.503722 3.663108 -0.231707 C 2.739767 3.275126 0.259066	**e_{oc}** E_0 = -1759.0794577 E_{0+ZPE} = -1758.781158 H_{298} = -1758.760141 G_{298} = -1758.830442 N_{Imag}= 0 E_0(M06) = -1758.6757888 C -1.628193 -0.527491 -0.385804 C -1.744821 0.847882 -0.580089 C -2.722814 1.307808 -1.455532 C -3.557849 0.432032 -2.118744 C -3.410938 -0.929618 -1.927947 C -2.439483 -1.411029 -1.071751

C 2.022741 0.722140 0.191167	C 2.299120 -0.454903 0.176712	C -0.858284 1.822334 0.084504
N 1.630056 -0.547802 0.341267	N 1.260676 -1.214725 -0.208295	N 0.456642 1.579074 0.173125
C 2.406945 -1.442537 0.929460	C 1.344510 -2.538948 -0.192271	C 1.263498 2.493100 0.704728
C 3.646093 -1.104502 1.427260	C 2.485901 -3.190307 0.224716	C 0.801834 3.694352 1.197646
C 4.069641 0.206105 1.298053	C 3.565391 -2.429598 0.634213	C -0.552354 3.951485 1.139466
C 3.256132 1.127946 0.674898	C 3.473454 -1.054816 0.610247	C -1.386271 3.007642 0.577643
Pd -0.280108 -0.931672 -0.303405	Pd -0.409055 -0.160895 -0.804468	Pd 1.238208 -0.282049 -0.316902
C -2.330051 -0.801362 2.424147	Cl -2.133113 1.204574 -1.548370	C 0.341360 -1.468294 2.527990
O -0.698361 0.413312 1.130926	Cl -1.702584 -2.169697 -1.230453	O -0.636521 -0.971799 0.441579
C -1.881821 0.555449 1.911934	O -1.043269 -0.279650 1.422175	C -0.907255 -1.687051 1.705104
C -1.402835 1.420793 3.072479	C -2.220444 0.202458 1.674856	C -2.117195 -1.064673 2.365716
Cl -2.401032 -1.392549 -1.038523	C -3.414817 -0.551066 1.226498	Cl 1.956565 -2.409841 -0.731567
Cl 0.570873 -2.458455 -1.785406	C -2.339599 1.668100 1.882547	Cl 3.150544 0.626179 -1.131448
C -3.012200 1.263155 1.187541	C -1.511259 -0.596563 3.159803	C -1.099986 -3.160412 1.414530
H -3.384280 0.667332 0.361222	H -0.407243 3.033389 -0.957709	H -0.292230 -3.520459 0.783806
H -3.834056 1.425428 1.882382	H 1.284852 4.712304 -0.365991	H -1.082081 -3.711796 2.352104
H -2.687856 2.233524 0.820175	H 3.989522 1.633737 0.776654	H -2.055009 -3.361961 0.937960
H -1.510936 -1.294312 2.944167	H 3.483426 4.014312 0.513104	H 0.512582 -0.407855 2.696010
H -3.156498 -0.687162 3.123762	H 4.306701 -0.446374 0.917420	H 0.224794 -1.955279 3.493158
H -2.662398 -1.431983 1.605256	H 4.476203 -2.904321 0.965730	H 1.207597 -1.894632 2.028618
H -2.216588 1.588320 3.776194	H 2.519164 -4.266870 0.219827	H -2.292573 -1.564333 3.315126
H -0.584813 0.933056 3.596215	H 0.458348 -3.057195 -0.527829	H -1.956210 -0.007361 2.562847
H -1.055947 2.383914 2.706792	H -1.449325 2.083920 2.341082	H -3.012555 -1.176950 1.759827
H 2.024158 -2.449020 0.975968	H -2.428007 2.077321 0.871671	H 2.311212 2.240002 0.704162
H 4.258617 -1.854624 1.897807	H -3.232117 1.928423 2.442697	H 1.498079 4.401303 1.616613
H 5.032169 0.507725 1.680697	H -1.469667 -1.668255 3.062841	H -0.957479 4.873346 1.526923
H 3.564449 2.154090 0.569272	H -0.625911 -0.119227 3.545611	H -2.449539 3.171123 0.526587
H 0.707242 4.376685 -2.358522	H -2.410214 -0.261744 3.676408	H -4.300499 0.810106 -2.802843
H -1.546259 3.417634 -2.654314	H -3.248930 -1.621147 1.234684	H -4.036696 -1.624438 -2.465561
H -2.145852 1.274262 -1.582532	H -4.301516 -0.265758 1.784482	H -2.286304 -2.469178 -0.953427
H 2.394634 3.160608 -1.051149	H -3.542588 -0.263086 0.177403	H -2.803347 2.367344 -1.642437
TS(o-o$_{oc}$)	**TS(o-o$_{oc}$)'**	
E_0 = -1799.4905904	E_0 = -1799.4864958	
E_{0+ZPE} = -1799.145319	E_{0+ZPE} = -1799.141315	
H_{298} = -1799.121791	H_{298} = -1799.117681	
G_{298} = -1799.197598	G_{298} = -1799.193771	
N_{Imag}= 1 (-425.2026)	N_{Imag}= 1 (-470.2122)	
E_0(M06) = -1799.0712428	E_0(M06) = -1799.0674635	
O 1.250350 0.334605 1.163488	O -1.999136 0.690649 0.372782	
Pd 0.732114 -0.351770 -0.661831	Pd -0.530680 -0.244113 -0.654285	
Cl -0.017336 -0.845171 -2.790319	Cl 1.069850 -0.865159 -2.195813	
Cl 2.396863 -1.918333 -0.895854	Cl -1.681118 -2.192380 -1.059468	
C 3.430516 1.145946 0.471364	C -2.264767 -0.875523 2.191839	
C 2.575793 0.598812 1.602483	C -2.929861 0.170601 1.314497	
H 3.589169 0.394887 -0.296743	H -1.947774 -1.728660 1.598873	
H 2.949552 2.015443 0.026170	H -1.402175 -0.445527 2.697041	
H 4.402964 1.458283 0.848521	H -2.957304 -1.225934 2.955433	
C 2.369118 1.679057 2.659820	C -3.306750 1.386121 2.153751	
C 3.244836 -0.608203 2.240167	C -4.181479 -0.403896 0.669020	
H 1.738379 1.305468 3.462687	H -3.772019 2.147176 1.531409	
H 3.325696 1.983529 3.081655	H -4.008712 1.106209 2.937586	
H 1.888639 2.549989 2.221308	H -2.421335 1.813858 2.617156	
H 4.225764 -0.325178 2.616523	H -4.871154 -0.726947 1.446063	
H 2.663855 -0.971918 3.086465	H -4.695850 0.347576 0.072081	
H 3.379379 -1.407520 1.517992	H -3.945434 -1.264116 0.050202	
C 0.318134 -1.525687 1.223481	C -2.335950 0.693192 -1.660288	
H 1.194781 -1.898560 1.716940	H -3.197285 0.062797 -1.550260	
H -0.386147 -0.981025 1.823319	H -2.490414 1.740146 -1.479940	
H -0.103239 -2.210991 0.497823	H -1.722775 0.449160 -2.520907	
C -2.498225 -0.010587 0.443556	C 2.410674 -0.071852 0.666228	
C -2.576977 -1.135921 -0.367569	C 1.643163 -0.891957 1.482147	
H -2.150541 -1.112390 -1.359250	H 0.683840 -0.549795 1.836869	
C -3.196265 -2.280128 0.101335	C 2.115465 -2.133028 1.864678	
C -3.056611 -0.039324 1.716334	C 3.664277 -0.501601 0.252273	
C -3.734495 -2.312387 1.376238	C 3.358044 -2.562157 1.437046	
C -3.663650 -1.190027 2.184084	C 4.131552 -1.743617 0.631584	
H -2.992398 0.832747 2.349846	H 4.252018 0.117505 -0.407549	
H -4.079802 -1.210656 3.179313	H 5.095032 -2.081768 0.283668	
H -4.212053 -3.209292 1.739389	H 3.722718 -3.535521 1.725996	
H -3.258159 -3.148460 -0.536045	H 1.509536 -2.764267 2.495272	

C -1.884027 1.230932 -0.060562 N -0.666763 1.206799 -0.607046 C -0.158094 2.323658 -1.122962 C -0.817738 3.529713 -1.097474 C -2.066012 3.578919 -0.507961 C -2.601218 2.419603 0.006263 H 0.816340 2.236611 -1.575603 H -0.357119 4.400804 -1.531971 H -2.621785 4.502679 -0.466457 H -3.588442 2.405874 0.437109	C 1.917421 1.259727 0.282807 N 0.658765 1.405061 -0.150179 C 0.182214 2.623400 -0.382148 C 0.941643 3.762637 -0.254267 C 2.258304 3.628067 0.142819 C 2.740024 2.370242 0.425939 H -0.852153 2.677164 -0.670016 H 0.505389 4.724633 -0.464393 H 2.893120 4.493394 0.253350 H 3.743451 2.227522 0.790390	

Optimized Coordinates of Radical Pathway

Me·
E0 = -39.8426447
E0+ZPE = -39.812347
E298 = -39.809291
H298 = -39.808347
G298 = -39.831085
NImag = 0
E_0(M06) = -39.8107365
C 0.000000 -0.000000 0.000038
H -0.000000 1.075707 -0.000077
H -0.931590 -0.537853 -0.000077
H 0.931590 -0.537853 -0.000077

***tert*-butyl Radical**
E0 = -233.010569
E0+ZPE = -232.885334
E298 = -232.878923
H298 = -232.877979
G298 = -232.914769
NImag = 0
E_0(M06) = -232.9012411
O -0.000053 0.249029 1.422077
C 1.260861 -0.781266 -0.314824
C 0.000011 -0.021334 0.073332
H 2.144427 -0.217538 -0.027721
H 1.290883 -1.744202 0.189994
H 1.291024 -0.960328 -1.387666
C -1.260134 -0.782478 -0.314743
C -0.000696 1.374108 -0.566319
H -2.144176 -0.220410 -0.025866
H -1.291131 -0.959896 -1.387832
H -1.288331 -1.746250 0.188589
H 0.000118 1.259271 -1.647675
H -0.885727 1.930771 -0.272135
H 0.883075 1.932161 -0.270980

$TS_{Peroxide}$
E0 = -466.0242176
E0+ZPE = -465.772623
E298 = -465.758580
H298 = -465.757636
G298 = -465.814388
NImag = 1 (-31.1836)
E_0(M06) = -465.8136531
C -3.284002 -0.000118 -0.943465
C -2.099908 0.000005 0.034447
C -2.115928 1.259894 0.887106
O -1.008077 -0.000047 -0.806463
O 1.008032 -0.000009 0.806381
C 2.099908 0.000005 -0.034455
C 2.116010 1.259893 -0.887105
C -2.115843 -1.259738 0.887320
C 2.115859 -1.259743 -0.887316
C 3.283943 -0.000148 0.943530
H -4.206173 -0.000097 -0.367086
H -3.264189 0.884677 -1.573425
H -3.264132 -0.885022 -1.573271
H -2.114740 -2.143871 0.254717
H -1.231977 -1.287163 1.518212
H -2.999413 -1.284289 1.522206
H -2.114833 2.143922 0.254355
H -2.999530 1.284515 1.521945
H -1.232093 1.287472 1.518040
H 1.232020 -1.287155 -1.518251
H 2.999461 -1.284324 -1.522157
H 2.114704 -2.143870 -0.254703
H 4.206148 -0.000146 0.367206
H 3.264112 0.884647 1.573491
H 3.264015 -0.885053 1.573332
H 2.114927 2.143915 -0.254346
H 2.999629 1.284490 -1.521921
H 1.232189 1.287500 -1.518060

$^{1}Int_{Peroxide}$
E0 = -466.0242582
E0+ZPE = -465.773194
E298 = -465.758054
H298 = -465.757110
G298 = -465.818638
NImag = 0
E_0(M06) = -465.811227
O -1.298786 -0.000088 -1.001556
O 1.298789 0.000056 1.001561
C 2.214999 -0.000002 -0.026911
C -2.215000 -0.000001 0.026912
C 3.563057 0.000352 0.708202
H 4.358485 0.000406 -0.033251
H 3.662277 0.885363 1.330131
H 3.662616 -0.884452 1.330371
C 2.066366 -1.260096 -0.867496
H 2.180199 -2.144347 -0.245408
H 1.082269 -1.284555 -1.328516
H 2.816273 -1.287777 -1.655633
C 2.065945 1.259716 -0.867986
H 2.179716 2.144250 -0.246290
H 2.815677 1.287231 -1.656297
H 1.081736 1.283758 -1.328787
C -2.065955 -1.259696 0.868021
H -1.081739 -1.283744 1.328806
H -2.815676 -1.287174 1.656344
H -2.179752 -2.144248 0.246354
C -3.563053 -0.000368 -0.708202
H -4.358482 -0.000401 0.033250
H -3.662604 0.884421 -1.330395
H -3.662274 -0.885395 -1.330108
C -2.066362 1.260120 0.867457
H -2.180216 2.144351 0.245344
H -2.816252 1.287819 1.655611
H -1.082255 1.284601 1.328454

$^{3}Int_{Peroxide}$
E0 = -466.02399
E0+ZPE = -465.772994
E298 = -465.757856
H298 = -465.756912
G298 = -465.818926
NImag = 0
E_0(M06) = -465.8096779
O -1.386711 -0.000331 -1.048689
O 1.386719 0.000313 1.048695
C 2.251103 -0.000026 -0.023643
C -2.251103 0.000024 0.023643
C 3.633894 0.000948 0.643365
H 4.391678 0.000828 -0.136549
H 3.763477 0.886238 1.259258
H 3.764254 -0.883526 1.260269
C 2.061119 -1.260649 -0.855426
H 2.201594 -2.144438 -0.238184
H 1.057744 -1.284623 -1.273235
H 2.774016 -1.290784 -1.677121
C 2.060077 1.259457 -0.856928
H 2.200033 2.144101 -0.240797
H 2.772814 1.289075 -1.678783
H 1.056608 1.282189 -1.274580
C -2.060089 -1.259455 0.856938
H -1.056616 -1.282210 1.274580
H -2.772818 -1.289053 1.678800
H -2.200071 -2.144099 0.240814
C -3.633906 -0.000936 -0.643375
H -4.391695 -0.000803 0.136535
H -3.764261 0.883535 -1.260283
H -3.763505 -0.886226 -1.259264
C -2.061099 1.260650 0.855421
H -2.201583 2.144436 0.238177
H -2.773983 1.290791 1.677126
H -1.057718 1.284627 1.273215

A
E0 = -1759.6181467
E0+ZPE = -1759.313678
E298 = -1759.291180
H298 = -1759.290236
G298 = -1759.370714

TS(A-B)
E0 = -1759.6128313
E0+ZPE = -1759.308150
E298 = -1759.286555
H298 = -1759.285611
G298 = -1759.362483

B
E0 = -1759.641975
E0+ZPE = -1759.335629
E298 = -1759.313758
H298 = -1759.312813
G298 = -1759.390261

NImag = 0 E_0(M06) = -1759.206473 N 1.047623 1.352066 0.177508 C 2.072391 0.968821 -0.592648 C 2.917892 1.897754 -1.171200 C 2.687891 3.240496 -0.947929 C 1.624342 3.619396 -0.152210 C 0.823918 2.640517 0.398654 C 2.223305 -0.484699 -0.748312 C 1.072478 -1.275576 -0.832911 C 1.172090 -2.659019 -0.847401 C 2.415334 -3.258478 -0.820319 C 3.557211 -2.474831 -0.767399 C 3.467153 -1.095504 -0.721704 Pd -0.084806 -0.200580 0.929761 Cl -0.956627 1.062045 2.615940 O -1.729732 0.415872 -1.588311 C -3.091327 0.183534 -1.582180 C -3.397995 -1.303145 -1.661815 Cl -1.296176 -2.021198 1.570658 C -3.691060 0.815707 -0.331437 C -3.589246 0.913533 -2.836753 H 0.107463 -0.814487 -1.084241 H 0.271509 -3.250069 -0.876763 H 2.498492 -4.333522 -0.832211 H 4.360994 -0.499293 -0.623324 H 4.528351 -2.944171 -0.735797 H 3.728421 1.564722 -1.797879 H 3.329496 3.983167 -1.395956 H 1.409459 4.656167 0.045429 H -0.008577 2.864129 1.045887 H -4.665992 0.780524 -2.909471 H -3.366534 1.974836 -2.777275 H -3.129020 0.503096 -3.731892 H -4.471642 -1.475551 -1.702838 H -2.947139 -1.734566 -2.553314 H -3.003890 -1.812546 -0.786048 H -4.769575 0.671486 -0.327993 H -3.278030 0.355320 0.561980 H -3.476830 1.880538 -0.302163	NImag = 1 (-63.1440) E_0(M06) = -1759.2050189 C -0.988312 2.872547 0.259914 C -1.306381 1.694832 -0.403505 C -0.752431 1.444675 -1.658949 C 0.144646 2.344117 -2.215539 C 0.464763 3.505511 -1.542612 C -0.113441 3.773790 -0.311751 C -2.180571 0.691927 0.226796 N -1.755721 -0.575825 0.175962 C -2.484961 -1.544667 0.718237 C -3.681864 -1.286385 1.351777 C -4.129127 0.018665 1.422979 C -3.370754 1.020476 0.852345 Pd 0.114591 -0.822112 -0.674009 Cl -0.062615 -3.104106 -0.725364 H -1.397529 3.063225 1.240083 Cl 2.140509 -0.894853 -1.701002 O 1.360517 0.680169 1.012889 C 2.350162 0.243774 1.873855 C 3.708797 0.699588 1.361920 C 2.291961 -1.261979 2.067630 C 2.003473 0.970497 3.183014 H 2.485972 -1.770574 1.127282 H 3.036324 -1.581285 2.794612 H 1.309051 -1.563879 2.421555 H 2.744208 0.697346 3.930558 H 2.024520 2.047603 3.043859 H 1.021554 0.674038 3.541934 H -2.076888 -2.538611 0.625777 H -4.244216 -2.100115 1.778164 H -5.063593 0.253595 1.908507 H -3.695365 2.047717 0.865622 H 0.583905 2.127718 -3.175759 H 1.163854 4.204237 -1.974339 H 0.138566 4.680952 0.215192 H -1.082085 0.593845 -2.241966 H 3.724390 1.779344 1.237523 H 4.491325 0.413201 2.061822 H 3.910774 0.236303 0.400687	NImag = 0 E_0(M06) = -1759.23249 O 2.282022 0.856804 0.090322 Pd 0.590346 -0.235920 0.052913 Cl 0.311530 0.259897 -2.204449 Cl 0.980641 -0.908238 2.253687 C 3.971659 1.279582 -1.428923 C 3.560261 0.400349 -0.246124 H 3.951236 2.329042 -1.151915 H 4.982625 1.006778 -1.722368 H 3.298446 1.118637 -2.265422 C 4.417452 0.699668 0.982227 C 3.572438 -1.069806 -0.605877 H 4.060631 0.130103 1.835267 H 5.444629 0.414461 0.767600 H 4.384899 1.757792 1.222963 H 4.581668 -1.377284 -0.870547 H 3.239456 -1.668202 0.238696 H 2.919934 -1.255224 -1.455820 N -1.135369 -1.272175 0.021265 C -1.042098 -2.596784 -0.064672 C -2.142299 -3.400940 -0.242502 C -3.384316 -2.801348 -0.334179 C -3.475358 -1.432059 -0.221526 C -2.328370 -0.672686 -0.033375 H -0.048933 -3.005542 0.012581 H -2.018724 -4.468509 -0.309413 H -4.273251 -3.396126 -0.475493 H -4.428527 -0.931316 -0.248527 C -2.418149 0.786407 0.138905 C -3.146823 1.547018 -0.765244 C -3.261846 2.912265 -0.588861 C -2.663532 3.523166 0.499359 C -1.945565 2.766431 1.408278 C -1.816941 1.401626 1.230782 H -3.810772 3.500746 -1.307296 H -2.754947 4.589544 0.636897 H -1.482708 3.237348 2.261332 H -3.591666 1.073725 -1.627004 H -1.264484 0.811584 1.946377
TS(B-C) E0 = -1759.6137076 E0+ZPE = -1759.311486 E298 = -1759.289345 H298 = -1759.288401 G298 = -1759.365352 NImag = 1 (-391.3925) E_0(M06) = -1759.2090111 O 2.296684 0.877283 -0.035521 Pd 0.584253 -0.245338 0.016392 Cl 0.254237 0.246454 -2.235232 Cl 0.999922 -0.959786 2.204801 C 4.344281 1.582676 -0.926669 C 3.399760 0.501433 -0.485009 H 4.224203 2.467348 -0.312021 H 5.378781 1.256118 -0.927045 H 4.066228 1.839404 -1.949600 C 4.336138 0.057375 1.375764 C 3.531970 -0.846774 -1.126003 H 3.579324 -0.588272 1.793649 H 5.253107 -0.385470 1.017672 H 4.398991 1.051596 1.787808 H 4.567457 -1.106838 -1.319637 H 3.060722 -1.610622 -0.515048 H 2.988600 -0.796880 -2.070557 N -1.154688 -1.264278 0.021472 C -1.080959 -2.589633 -0.065375 C -2.193890 -3.380800 -0.222809 C -3.430161 -2.766664 -0.290779	**TS(B-C)$_{conf1}$** E0 = -1759.6051984 E0+ZPE = -1759.303290 E298 = -1759.281105 H298 = -1759.280161 G298 = -1759.357428 NImag = 1 (-371.5266) E_0(M06) = -1759.2006895 O -0.958049 0.755727 1.024431 Pd -0.725031 -0.772990 -0.402986 Cl -2.778708 -0.430686 -1.385601 Cl -0.253662 -2.466974 -1.858961 C -1.518265 1.986453 2.937371 C -1.874594 1.040998 1.820949 H -0.794743 2.719358 2.598811 H -2.389123 2.479754 3.355580 H -1.058135 1.392530 3.728544 C -2.910463 2.458355 0.599792 C -3.009695 0.090471 2.059886 H -3.123470 1.793635 -0.223835 H -3.716926 2.729734 1.263880 H -2.122852 3.181625 0.461482 H -3.836496 0.567966 2.575398 H -3.344386 -0.353800 1.128426 H -2.626387 -0.704329 2.702556 N 1.114938 -1.112204 0.483115 C 1.252990 -2.260155 1.142371 C 2.373897 -2.561356 1.881068 C 3.399614 -1.635871 1.920774	**TS(B-D)** E0 = -1759.5716822 E0+ZPE = -1759.268200 E298 = -1759.246907 H298 = -1759.245962 G298 = -1759.320057 NImag = 1 (-671.6273) E_0(M06) = -1759.1724254 O -2.509791 0.874842 -0.337699 Pd -0.700783 -0.223728 0.100847 Cl -0.158168 -0.727872 -2.111005 Cl -1.011522 0.053270 2.408730 C -3.713807 -0.539880 -1.799521 C -3.273836 -0.175976 -0.402531 H -2.852535 -0.657753 -2.448425 H -4.328069 -1.436237 -1.817885 H -4.311824 0.292173 -2.169005 C -4.349071 -0.229677 0.655240 H -4.874884 -1.180255 0.658016 H -3.923518 -0.028700 1.632739 H -5.065957 0.556739 0.420557 N 0.639780 1.323701 0.079577 C 0.095343 2.536471 0.050251 C 0.858311 3.671976 -0.093852 C 2.227532 3.532794 -0.215400 C 2.780925 2.271598 -0.170760 C 1.961865 1.162543 -0.013552 H -0.979459 2.570578 0.131314 H 0.380149 4.636569 -0.115359

C -3.501666 -1.396494 -0.175839 C -2.341472 -0.651626 -0.010376 H -0.092081 -3.010984 -0.005038 H -2.084401 -4.449827 -0.291698 H -4.328928 -3.350435 -0.414958 H -4.448882 -0.883884 -0.183594 C -2.411883 0.808154 0.166175 C -3.155450 1.578198 -0.717568 C -3.254048 2.943868 -0.534649 C -2.623776 3.546177 0.540232 C -1.890021 2.780251 1.428550 C -1.778029 1.414936 1.244107 H -3.814976 3.539380 -1.237918 H -2.702066 4.612967 0.682912 H -1.400909 3.244516 2.270550 H -3.624954 1.111548 -1.569812 H -1.211999 0.817740 1.942964	C 3.268700 -0.464098 1.208868 C 2.109311 -0.219874 0.482596 H 0.431382 -2.951795 1.055167 H 2.436490 -3.502930 2.400140 H 4.300486 -1.835424 2.480131 H 4.067573 0.257643 1.173928 C 1.984901 1.001313 -0.331698 C 2.347408 2.233658 0.197622 C 2.260149 3.376659 -0.573888 C 1.819406 3.295404 -1.883922 C 1.470251 2.068623 -2.419616 C 1.551593 0.922808 -1.650194 H 2.531936 4.331724 -0.151439 H 1.751531 4.187646 -2.487114 H 1.133386 1.997372 -3.441750 H 2.675008 2.300823 1.224286 H 1.295022 -0.034508 -2.078382	H 2.859841 4.399291 -0.331470 H 3.846593 2.126245 -0.229199 C 2.532944 -0.191167 0.075497 C 3.447371 -0.623305 -0.875454 C 3.994656 -1.888189 -0.786202 C 3.643183 -2.724860 0.259397 C 2.742516 -2.292735 1.215889 C 2.185060 -1.029780 1.128048 H 4.687923 -2.225775 -1.540659 H 4.071928 -3.712751 0.327143 H 2.475289 -2.935485 2.040187 H 3.699375 0.017469 -1.706272 H 1.500299 -0.686156 1.889061 C -2.269905 -1.778249 0.150323 H -2.673843 -1.934729 1.137169 H -1.234153 -2.170937 0.144529 H -2.735048 -2.344600 -0.642413
C E0 = -1759.6265303 E0+ZPE = -1759.328105 E298 = -1759.302892 H298 = -1759.301948 G298 = -1759.389166 NImag = 0 E_0(M06) = -1759.2164819 O 2.187927 1.052779 -0.317347 Pd 0.532854 -0.165133 -0.146607 Cl -0.048009 0.334992 -2.342524 Cl 1.262785 -0.890789 1.946782 C 4.327956 1.745641 -0.938433 C 3.234507 0.744751 -0.856021 H 4.021242 2.686654 -0.499460 H 5.200940 1.353064 -0.418994 H 4.606961 1.886263 -1.981463 C 5.226745 -0.423903 2.188312 C 3.438769 -0.609239 -1.434100 H 4.153368 -0.511180 2.229333 H 5.827877 -1.265842 1.889462 H 5.710854 0.466979 2.550808 H 4.428047 -0.733955 -1.859548 H 3.275009 -1.343448 -0.647014 H 2.675173 -0.766132 -2.195629 N -1.126658 -1.288824 0.023546 C -0.986183 -2.606383 -0.096509 C -2.062951 -3.459030 -0.148984 C -3.332348 -2.917739 -0.071651 C -3.469439 -1.555948 0.078254 C -2.342739 -0.746386 0.132704 H 0.026052 -2.969034 -0.150617 H -1.900944 -4.518766 -0.250147 H -4.204325 -3.551890 -0.110259 H -4.439586 -1.100022 0.183186 C -2.475079 0.703740 0.347567 C -3.348731 1.443919 -0.437092 C -3.502462 2.798669 -0.215208 C -2.796250 3.418856 0.800623 C -1.931869 2.682139 1.590861 C -1.765829 1.328290 1.366797 H -4.166337 3.372311 -0.842919 H -2.917539 4.477042 0.973826 H -1.382939 3.160101 2.387056 H -3.879078 0.964909 -1.245674 H -1.098669 0.752897 1.990833	**D** E0 = -1759.6393692 E0+ZPE = -1759.336579 E298 = -1759.312853 H298 = -1759.311909 G298 = -1759.394250 NImag = 0 E_0(M06) = -1759.2361788 O 2.808446 -0.736008 -0.017237 Pd 0.435019 -0.842587 0.018210 Cl 0.418854 -0.000180 -2.202295 Cl 0.537569 -1.724070 2.209141 C 3.170399 1.567908 -0.433029 C 3.596216 0.147910 -0.257839 H 2.171923 1.610000 -0.855679 H 3.156322 2.034768 0.552052 H 3.868205 2.121366 -1.054362 C 5.054761 -0.156924 -0.370625 H 5.635788 0.544154 0.225169 H 5.255947 -1.175351 -0.061278 H 5.358418 -0.021905 -1.408485 N -1.823188 -0.756443 0.082451 C -2.560298 -1.848618 -0.041603 C -3.915298 -1.805730 -0.292798 C -4.517357 -0.568036 -0.418469 C -3.753127 0.569239 -0.262181 C -2.396711 0.442768 0.000088 H -2.040021 -2.787262 0.064731 H -4.476359 -2.720422 -0.387975 H -5.574829 -0.489557 -0.618061 H -4.195913 1.550409 -0.310824 C -1.543967 1.616452 0.252917 C -1.608315 2.741266 -0.557901 C -0.809122 3.835297 -0.290396 C 0.055322 3.820675 0.792321 C 0.121652 2.704019 1.604786 C -0.673356 1.601534 1.339119 H -0.852799 4.699350 -0.935096 H 0.673039 4.680715 1.000759 H 0.779849 2.688863 2.459776 H -2.256854 2.743517 -1.420070 H -0.648130 0.746390 2.000006 C 0.634961 -2.693364 -0.745901 H 0.389614 -3.363592 0.065642 H -0.033112 -2.727038 -1.594924 H 1.679027 -2.726350 -1.025610	**D'** <witout-acetone> E0 = -1566.4721071 E0+ZPE = -1566.256546 E298 = -1566.239923 H298 = -1566.238979 G298 = -1566.303662 NImag = 0 E_0(M06) = -1566.1368837 Pd -0.786351 -0.881890 0.277778 Cl -0.708186 0.251604 2.312685 Cl -0.904371 -2.382756 -1.511000 N 1.437888 -0.597605 -0.016941 C 2.402172 -1.480349 0.180963 C 3.737899 -1.133112 0.144299 C 4.068084 0.184222 -0.111389 C 3.061004 1.102821 -0.333237 C 1.746781 0.670986 -0.282303 H 2.087848 -2.494166 0.374683 H 4.494938 -1.880324 0.314811 H 5.101559 0.491817 -0.149128 H 3.281973 2.132195 -0.563097 C 0.588663 1.548346 -0.516504 C 0.473236 2.787133 0.090034 C -0.683900 3.526735 -0.066799 C -1.737765 3.042175 -0.828104 C -1.624304 1.820199 -1.456708 C -0.462938 1.066213 -1.310543 H -0.776491 4.479608 0.430569 H -2.639084 3.625077 -0.933267 H -2.421406 1.446827 -2.080069 H 1.263072 3.147199 0.730060 H -0.317378 0.188075 -1.926134 C -2.788070 -0.986066 0.480110 H -3.195034 -1.205554 -0.497263 H -2.933343 -1.805450 1.177269 H -3.111435 -0.041387 0.894801
TS(C-E) E0 = -1759.6074709 E0+ZPE = -1759.306817 E298 = -1759.283966 H298 = -1759.283022	**TS(C-E)meta** E0 = -1759.6085547 E0+ZPE = -1759.308044 E298 = -1759.285163 H298 = -1759.284219	**TS(C-E)para** E0 = -1759.6101768 E0+ZPE = -1759.309642 E298 = -1759.286778 H298 = -1759.285834

G298 = -1759.362178 NImag = 1 (-505.0016) E_0(M06) = -1759.2034503 C -3.352187 -0.997271 0.419864 C -2.280414 -0.444689 -0.321920 C -1.621652 -1.234114 -1.252738 C -2.050694 -2.524967 -1.511759 C -3.180233 -3.027509 -0.872526 C -3.848313 -2.262023 0.051941 C -1.934154 0.971616 -0.150637 N -0.657132 1.376632 -0.126645 C -0.363376 2.673527 -0.048267 C -1.324094 3.649921 0.040437 C -2.650336 3.258666 0.045061 C -2.949673 1.921129 -0.056763 Pd 0.935396 0.145501 -0.055582 Cl 1.386604 0.533777 -2.313948 Cl 0.773042 0.063634 2.262745 H -0.808222 -0.820978 -1.829084 H -1.534408 -3.117234 -2.250342 H -3.544898 -4.012905 -1.119626 H -3.983468 -0.340562 0.996942 H -4.729224 -2.645033 0.543321 H -3.972806 1.589634 -0.104485 H -3.441260 3.989771 0.107768 H -1.032282 4.684302 0.104710 H 0.684873 2.918494 -0.052899 O 2.516498 -1.173872 0.020462 C 3.675630 -0.867852 0.225512 C 4.709272 -1.933972 0.257861 C 4.076729 0.546461 0.443796 H 5.465168 -1.721640 -0.496653 H 5.209246 -1.916139 1.225096 H 4.264863 -2.905490 0.082330 H 3.519573 0.925777 1.299749 H 5.142443 0.655634 0.610646 H 3.771439 1.121549 -0.429593 C -2.442411 -1.523881 2.370035 H -3.312248 -1.889500 2.895385 H -2.028852 -0.580392 2.689365 H -1.728764 -2.260020 2.038030	G298 = -1759.363721 NImag = 1 (-537.2879) E_0(M06) = -1759.2031266 C 3.129599 -0.972237 -0.377442 C 2.229978 -0.237159 0.368430 C 1.669985 -0.778390 1.527715 C 2.054293 -2.046826 1.943654 C 2.940424 -2.791784 1.201049 C 3.413848 -2.308529 -0.036334 C 1.917294 1.147860 -0.020070 N 0.642287 1.542032 -0.085725 C 0.342388 2.807431 -0.368813 C 1.306121 3.749719 -0.636030 C 2.631707 3.358812 -0.603024 C 2.935636 2.054524 -0.284876 Pd -0.890253 0.249646 0.071304 Cl -1.540142 1.230147 2.081406 Cl -0.446911 -0.537802 -2.074680 H 0.988034 -0.192724 2.124645 H 1.666036 -2.437670 2.871512 H 3.243697 -3.770353 1.540155 H 3.553039 -0.551385 -1.276441 H 4.259648 -2.792447 -0.498363 H 3.956763 1.720851 -0.208385 H 3.419558 4.067618 -0.805384 H 1.015998 4.761583 -0.862902 H -0.705726 3.053124 -0.373411 O -2.417024 -1.127117 0.242866 C -3.541856 -0.977506 -0.194252 C -4.538607 -2.063947 -0.013655 C -3.937010 0.266220 -0.905955 H -5.398276 -1.673973 0.529088 H -4.896203 -2.384653 -0.990978 H -4.103862 -2.899435 0.520315 H -3.276888 0.384989 -1.764661 H -4.972757 0.251385 -1.226206 H -3.761814 1.108478 -0.237974 C 2.178779 -3.402543 -1.474038 H 2.270779 -4.412786 -1.103576 H 2.686973 -3.189302 -2.402932 H 1.231274 -2.908031 -1.329847	G298 = -1759.365373 NImag = 1 (-514.8178) E_0(M06) = -1759.2055529 C -3.151862 1.113209 -0.536039 C -2.264844 0.372293 0.246702 C -1.639717 0.985185 1.336851 C -1.845860 2.317992 1.593773 C -2.616531 3.104185 0.715120 C -3.352087 2.448637 -0.291666 C -2.045288 -1.047382 -0.037618 N -0.798524 -1.534482 -0.035316 C -0.582064 -2.834600 -0.222578 C -1.600937 -3.723780 -0.464327 C -2.896055 -3.239398 -0.507094 C -3.116277 -1.900143 -0.284260 Pd 0.821620 -0.345881 0.074589 Cl 1.419252 -1.316749 2.104441 Cl 0.407470 0.451948 -2.074221 H -1.020285 0.398444 1.998830 H -1.375999 2.776368 2.449843 H -2.913463 4.094934 1.020826 H -3.659165 0.638023 -1.361789 H -4.027346 3.014396 -0.914447 H -4.114410 -1.496045 -0.264696 H -3.725862 -3.903745 -0.692024 H -1.376858 -4.766258 -0.614085 H 0.445365 -3.151976 -0.170324 O 2.445898 0.922924 0.205192 C 3.550136 0.689238 -0.247145 C 4.622751 1.706256 -0.099152 C 3.846822 -0.588701 -0.946112 H 5.462977 1.265722 0.435267 H 4.984287 1.987540 -1.087113 H 4.256015 2.577413 0.428831 H 3.164116 -0.675883 -1.790842 H 4.874979 -0.648504 -1.285088 H 3.628890 -1.407462 -0.261714 C -1.033690 4.066380 -0.493926 H -1.618853 4.704923 -1.138748 H -0.599875 3.185354 -0.941090 H -0.457849 4.560659 0.274016
TS(C-E)'$_{ortho}$ E0 = -1566.4264611 E0+ZPE = -1566.214277 E298 = -1566.197942 H298 = -1566.196998 G298 = -1566.260886 NImag = 1 (-522.1504) E_0(M06) = -1566.0917838 C -2.845745 -0.695014 0.370889 C -1.730082 -0.218709 -0.351796 C -0.879084 -1.140236 -0.958580 C -1.147052 -2.501846 -0.928003 C -2.328468 -2.948936 -0.350149 C -3.189397 -2.056402 0.245878 C -1.368296 1.199792 -0.343375 N -0.055543 1.462117 -0.268314 C 0.377449 2.716232 -0.239826 C -0.491770 3.785446 -0.290164 C -1.849145 3.534908 -0.362106 C -2.294360 2.229263 -0.385957 Pd 1.144162 -0.216205 -0.150596 Cl 2.874337 0.908568 0.806594 Cl 2.297672 -2.173476 -0.144574 H -0.102351 -0.792418 -1.658360 H -0.450978 -3.187924 -1.380683 H -2.576418 -3.998180 -0.380603 H -3.595375 0.005313 0.702515 H -4.110350 -2.405811 0.686105	**TS(C-E)'$_{meta}$** E0 = -1566.4301275 E0+ZPE = -1566.217456 E298 = -1566.201138 H298 = -1566.200194 G298 = -1566.263580 NImag = 1 (-445.9424) E_0(M06) = -1566.0961263 C -0.759553 2.500278 0.561070 C -0.071204 1.678216 -0.305096 C -0.757816 0.970400 -1.313510 C -2.142133 1.143061 -1.449911 C -2.828201 1.947853 -0.584779 C -2.159257 2.574023 0.488399 C 1.373033 1.421859 -0.157980 N 1.658827 0.117542 -0.151363 C 2.908818 -0.298730 -0.011336 C 3.948724 0.600078 0.116977 C 3.667548 1.953399 0.116551 C 2.358518 2.377765 -0.019361 Pd -0.090743 -0.976325 -0.187094 Cl 0.927458 -2.846528 0.653712 Cl -2.141271 -1.976541 -0.212353 H -0.201278 0.507958 -2.118788 H -2.658408 0.634566 -2.247276 H -3.893740 2.073831 -0.691124 H -0.232571 3.018751 1.346703 H -2.669714 3.337506 1.053300	**TS(C-E)'$_{para}$** E0 = -1566.4281604 E0+ZPE = -1566.216094 E298 = -1566.199635 H298 = -1566.198691 G298 = -1566.263176 NImag = 1 (-490.0146) E_0(M06) = -1566.0932676 C -0.864315 2.844914 0.406936 C -0.211413 1.806986 -0.252498 C -0.981624 0.892072 -0.995594 C -2.355909 0.955738 -0.999712 C -3.014630 1.912676 -0.209854 C -2.237952 2.922843 0.392593 C 1.229238 1.586131 -0.139159 N 1.607734 0.299405 -0.109991 C 2.891536 -0.018229 0.003810 C 3.873315 0.945733 0.090575 C 3.501186 2.277094 0.067795 C 2.166118 2.603055 -0.046910 Pd 0.047871 -1.058949 -0.183772 Cl 1.269728 -2.726808 0.770085 Cl -1.780934 -2.402210 -0.377849 H -0.492580 0.247099 -1.737206 H -2.917862 0.236470 -1.572204 H -4.070576 2.073465 -0.352670 H -0.293345 3.574749 0.959948 H -2.730739 3.732443 0.908049

H -3.344770 2.001337 -0.457404 H -2.555264 4.349455 -0.405275 H -0.103156 4.789692 -0.269373 H 1.445430 2.837798 -0.154828 C -2.058197 -0.646353 2.428751 H -2.898523 -1.032014 2.985905 H -1.838371 0.402795 2.558364 H -1.211824 -1.304882 2.311521	H 2.101129 3.423933 -0.031684 H 4.462897 2.675271 0.218261 H 4.957314 0.236884 0.222330 H 3.045553 -1.368216 0.014272 C -2.753793 1.185614 2.149380 H -2.156670 1.578128 2.958035 H -2.453129 0.245631 1.712241 H -3.812267 1.393183 2.184060	H 1.844370 3.630408 -0.084988 H 4.245705 3.055319 0.131531 H 4.904999 0.649271 0.177935 H 3.107569 -1.073770 0.043433 C -3.578972 0.627364 1.524874 H -2.600907 0.479387 1.953232 H -4.010550 -0.225045 1.023995 H -4.251256 1.291075 2.047247
E E0 = -1759.6523075 E0+ZPE = -1759.347878 E298 = -1759.325426 H298 = -1759.324482 G298 = -1759.403045 NImag = 0 E_0(M06) = -1759.2442129 C -3.322506 -1.121014 0.431514 C -2.209240 -0.483988 -0.353914 C -1.526432 -1.180848 -1.317012 C -1.825318 -2.511772 -1.615437 C -2.863997 -3.173625 -0.925047 C -3.580770 -2.531655 0.021756 C -1.921391 0.931368 -0.141840 N -0.653528 1.374156 -0.156666 C -0.390969 2.676880 -0.084623 C -1.373884 3.625856 0.054806 C -2.686745 3.195185 0.127721 C -2.955896 1.851537 0.028176 Pd 0.948889 0.156988 -0.068592 Cl 1.577707 0.771054 -2.229358 Cl 0.538610 -0.223772 2.190399 H -0.763166 -0.680178 -1.894556 H -1.272035 -3.020690 -2.387541 H -3.090395 -4.201463 -1.165822 H -4.249883 -0.562266 0.244099 H -4.377538 -3.044443 0.541261 H -3.972346 1.497498 0.045666 H -3.492898 3.902770 0.244289 H -1.109279 4.667803 0.113816 H 0.649557 2.948634 -0.137837 O 2.547851 -1.143587 0.019579 C 3.671396 -0.842397 0.373993 C 4.726746 -1.887415 0.398446 C 4.008520 0.547006 0.780678 H 5.552041 -1.577929 -0.240888 H 5.120333 -1.971494 1.410357 H 4.331665 -2.840088 0.069041 H 3.347861 0.829375 1.599569 H 5.045367 0.653420 1.079315 H 3.790093 1.204466 -0.060161 C -3.070275 -1.047657 1.943668 H -3.903823 -1.492524 2.483821 H -2.957836 -0.018068 2.273600 H -2.157516 -1.575214 2.202235	**^{3}TS(E-F)** E0 = -1799.4580003 E0+ZPE = -1799.120977 E298 = -1799.097641 H298 = -1799.096697 G298 = -1799.176428 NImag = 1 (-2113.5382) E_0(M06) = -1799.0229467 C 1.170441 -3.051695 0.361828 C 1.982555 -2.202080 1.015684 C 1.695326 -0.742707 1.121088 C 0.611355 -0.257640 0.191241 C -0.153429 -1.190592 -0.476827 C 0.064380 -2.567968 -0.386553 H 1.371533 -4.111851 0.376240 H 2.837029 -2.567847 1.564384 H 2.815764 -0.154978 0.790977 H -0.805081 -0.857013 -1.312821 H -0.591786 -3.238983 -0.913819 C 1.484275 -0.320518 2.558908 H 0.566686 -0.769413 2.943769 H 2.311631 -0.655174 3.179100 H 1.394388 0.758267 2.652425 O 3.825644 0.458082 0.584657 C 3.643473 -0.049232 -1.767465 C 4.540779 0.011301 -0.542098 H 2.860670 -0.794039 -1.633795 H 3.175909 0.915415 -1.949995 H 4.218077 -0.324042 -2.649206 C 5.612785 1.082877 -0.724988 C 5.190732 -1.335412 -0.274458 H 6.232355 1.154924 0.164697 H 6.246306 0.826572 -1.571302 H 5.156609 2.051407 -0.910963 H 5.841280 -1.620456 -1.098619 H 5.784799 -1.292039 0.635143 H 4.437846 -2.112135 -0.162195 C 0.262085 1.150297 0.115459 C 1.176749 2.181062 0.304388 C 0.747712 3.487517 0.199867 H 2.208393 1.942955 0.508233 C -1.446893 2.683277 -0.222841 C -0.581631 3.748536 -0.074431 H 1.449119 4.296701 0.331827 H -2.502790 2.815328 -0.396093 H -0.956232 4.754595 -0.161300 N -1.035115 1.427907 -0.129624 Pd -2.273308 -0.214691 -0.229312 Cl -3.431766 -2.161704 -0.429323 Cl -4.147283 0.952026 0.311615	**^{3}F** E0 = -1799.5822029 E0+ZPE = -1799.236427 E298 = -1799.211251 H298 = -1799.210307 G298 = -1799.300346 NImag = 0 E_0(M06) = -1799.1334154 C -1.004948 -3.192069 -0.474427 C -1.361794 -2.323039 -1.490372 C -1.091104 -0.961607 -1.420731 C -0.441501 -0.485682 -0.277709 C -0.078735 -1.361593 0.743793 C -0.357802 -2.713114 0.648716 H -1.224137 -4.244492 -0.568069 H -1.847033 -2.710365 -2.374110 H -3.430256 -0.563688 0.019469 H 0.400769 -0.975198 1.632046 H -0.070189 -3.378050 1.447424 C -1.479116 -0.066165 -2.556984 H -0.712306 0.674898 -2.766257 H -1.638920 -0.649210 -3.459042 H -2.403432 0.463846 -2.334454 O -3.876211 0.272067 -0.094267 C -5.114967 -0.160522 1.918904 C -5.191824 0.168523 0.438024 H -4.633361 -1.125056 2.077344 H -4.540481 0.597359 2.445906 H -6.108237 -0.209945 2.360135 C -5.821272 1.528112 0.220183 C -5.956862 -0.907013 -0.314132 H -5.835681 1.772659 -0.839198 H -6.842991 1.542081 0.591571 H -5.255333 2.295516 0.743087 H -6.979783 -0.984643 0.047980 H -5.982997 -0.679413 -1.377073 H -5.484215 -1.880237 -0.183983 C -0.078011 0.939702 -0.122490 C -1.015047 1.959680 -0.119264 C -0.582552 3.259121 0.057420 H -2.060884 1.716239 -0.224831 C 1.640901 2.449162 0.213252 C 0.766318 3.513169 0.223557 H -1.296227 4.068382 0.071261 H 2.704848 2.578357 0.330645 H 1.141191 4.513579 0.361139 N 1.219271 1.201380 0.046369 Pd 2.650069 -0.407698 0.042650 Cl 3.173170 -0.679843 2.302573 Cl 4.219841 0.413096 -1.459030
^{3}E' (**E** with *tert*-butoxy group) E0 = -1799.4862798 E0+ZPE = -1799.144173 E298 = -1799.119561 H298 = -1799.118617 G298 = -1799.206592 NImag = 0 E_0(M06) = -1799.038329 C 0.326059 -3.412696 -0.168373 C 1.330800 -2.735685 0.431140	**B_{Conf}** E0 = -1759.632789 E0+ZPE = -1759.326481 E298 = -1759.304797 H298 = -1759.303853 G298 = -1759.379505 NImag = 0 E_0(M06) = -1759.2290691 C -2.160908 2.300526 -0.072821 C -1.820515 1.028827 -0.519618	

C 1.326425 -1.255204 0.624317 C 0.218379 -0.582691 -0.133018 C -0.759379 -1.330848 -0.752705 C -0.762094 -2.727725 -0.747682 H 0.358918 -4.489968 -0.222488 H 2.165783 -3.273780 0.856186 H 2.285764 -0.858474 0.276346 H -1.440836 -0.843262 -1.478063 H -1.577060 -3.255882 -1.212201 C 1.234545 -0.936901 2.127331 H 0.297899 -1.307437 2.535717 H 2.053710 -1.413108 2.661446 H 1.289236 0.133902 2.305533 O 4.476632 0.531318 -0.094731 C 5.898453 -1.302938 0.456146 C 5.783369 0.095855 -0.131295 H 5.609735 -1.298175 1.504889 H 5.251349 -1.993792 -0.078044 H 6.921966 -1.665172 0.391287 C 6.100810 0.074850 -1.634482 C 6.684933 1.089909 0.586736 H 6.001298 1.067498 -2.063218 H 7.126491 -0.262727 -1.761877 H 5.439378 -0.608184 -2.159334 H 7.725479 0.780200 0.520709 H 6.585379 2.078574 0.147151 H 6.417748 1.152503 1.639146 C 0.130275 0.869438 -0.144686 C 1.242046 1.701242 -0.087480 C 1.060697 3.067384 -0.124850 H 2.231866 1.279107 -0.032025 C -1.284352 2.705635 -0.227962 C -0.220202 3.582973 -0.200055 H 1.915864 3.724534 -0.095879 H -2.309955 3.037514 -0.248794 H -0.403301 4.643980 -0.227549 N -1.108924 1.391978 -0.202844 Pd -2.624139 -0.001213 -0.158633 Cl -4.134501 -1.700824 -0.228444 Cl -4.168527 1.466588 0.638883	C -1.242870 0.876045 -1.775687 C -1.001661 1.985736 -2.564400 C -1.331861 3.250564 -2.110232 C -1.912327 3.407019 -0.862947 C -2.127049 -0.150746 0.308435 N -1.200340 -1.099217 0.466455 C -1.489167 -2.202021 1.152599 C -2.709825 -2.401915 1.755127 C -3.672660 -1.419558 1.625143 C -3.380742 -0.292195 0.889289 Pd 0.771210 -0.937337 -0.180913 Cl 0.332753 -2.597776 -1.675000 H -2.604680 2.424487 0.903712 Cl 2.965197 -0.904070 -0.838966 O 0.947126 0.479251 1.261817 C 1.755777 1.594209 1.493656 C 2.064554 2.315983 0.193604 C 3.029618 1.017913 2.128529 C 1.026602 2.490650 2.481018 H 3.530917 0.353407 1.434081 H 3.681839 1.853326 2.373522 H 2.791832 0.481605 3.043073 H 1.652492 3.338763 2.748614 H 0.107878 2.870910 2.041605 H 0.781083 1.940588 3.385586 H -0.707293 -2.941572 1.205702 H -2.893576 -3.310064 2.303981 H -4.646279 -1.539624 2.074287 H -4.121268 0.473081 0.727188 H -0.556578 1.856898 -3.538350 H -1.139556 4.113991 -2.728138 H -2.168753 4.391591 -0.503641 H -1.003123 -0.110549 -2.142647 H 1.142831 2.648055 -0.278869 H 2.673128 3.191763 0.408536 H 2.601853 1.666517 -0.488683	
^{1}F E0 = -1799.597091 E0+ZPE = -1799.250383 E298 = -1799.225826 H298 = -1799.224882 G298 = -1799.310326 NImag = 0 E_0(M06) = -1799.1582586 C -1.219413 -3.095703 0.452514 C -1.355801 -2.526613 -0.801788 C -0.909687 -1.239464 -1.070873 C -0.308821 -0.530769 -0.026836 C -0.157091 -1.104802 1.229098 C -0.615667 -2.385564 1.472857 H -1.573675 -4.100329 0.626041 H -1.803619 -3.098348 -1.600926 H -3.232692 -0.478550 -0.041734 H 0.322188 -0.542460 2.016193 H -0.494116 -2.822729 2.451214 C -1.046060 -0.665101 -2.445827 H -0.097990 -0.256738 -2.787067 H -1.350106 -1.435596 -3.147709 H -1.793967 0.124985 -2.475762 O -3.657745 0.360834 -0.205436 C -4.886384 0.130455 1.846571 C -4.969071 0.333930 0.343365 H -4.419650 -0.825268 2.082202 H -4.293676 0.919393 2.303221 H -5.876672 0.137528 2.297386 C -5.569351 1.684642 0.015078	**G** E0 = -1759.6254903 E0+ZPE = -1759.323672 E298 = -1759.301326 H298 = -1759.300381 G298 = -1759.380444 NImag = 0 E_0(M06) = -1759.2129585 O 1.879745 1.187695 -0.008688 Pd 0.137431 -0.110065 -0.243931 Cl 2.223278 -2.828223 2.485881 Cl 1.417652 -1.989158 -0.774543 C 3.585067 2.768344 -0.442374 C 3.116471 1.332902 -0.620946 H 3.618253 3.030877 0.611849 H 4.580041 2.895564 -0.862011 H 2.915237 3.456072 -0.954441 C 4.021793 0.367269 0.164483 C 3.043547 0.932595 -2.085451 H 5.028420 0.468609 -0.234783 H 4.033755 0.621089 1.220190 H 3.682292 -0.654413 0.040507 H 4.025570 1.040463 -2.540501 H 2.717038 -0.097047 -2.186138 H 2.350698 1.578892 -2.620315 N -1.107556 1.436432 0.297821 C -0.702959 2.641605 0.678408 C -1.585543 3.632112 1.046197 C -2.938953 3.344489 1.017526 C -3.356599 2.090525 0.631867	**TS(G-H)** E0 = -1759.5995076 E0+ZPE = -1759.301771 E298 = -1759.279053 H298 = -1759.278109 G298 = -1759.358087 NImag = 1 (-377.0251) E_0(M06) = -1759.192258 O 1.857742 1.277998 -0.019302 Pd 0.118304 -0.083320 -0.260426 Cl 2.319511 -2.766251 2.428573 Cl 1.464425 -1.922835 -0.808758 C 3.651796 2.770889 -0.316634 C 2.889001 1.520430 -0.674303 H 3.634412 2.935959 0.755122 H 4.675283 2.752104 -0.675546 H 3.146127 3.608516 -0.799866 C 4.201684 0.130306 0.269595 C 3.032686 1.015786 -2.082132 H 5.134244 0.398540 -0.202820 H 4.070716 0.415768 1.300710 H 3.712841 -0.775873 -0.049906 H 4.062096 1.046895 -2.424157 H 2.632672 0.012389 -2.176096 H 2.447348 1.680934 -2.719640 N -1.162605 1.424219 0.277553 C -0.782708 2.643374 0.636431 C -1.686307 3.615996 1.001960 C -3.032397 3.293592 0.993151 C -3.423284 2.024334 0.629754

C -5.766589 -0.782839 -0.308450 H -5.590448 1.836952 -1.061354 H -6.585870 1.756660 0.394339 H -4.978593 2.479887 0.463851 H -6.786802 -0.806508 0.068875 H -5.799460 -0.644291 -1.386418 H -5.313402 -1.751923 -0.101773 C 0.140780 0.864821 -0.215334 C -0.773340 1.884492 -0.438900 C -0.330365 3.183331 -0.560800 H -1.822334 1.633323 -0.482915 C 1.881368 2.406505 -0.219864 C 1.021150 3.452624 -0.447132 H -1.035704 3.981914 -0.730359 H 2.941840 2.551881 -0.110433 H 1.412474 4.452736 -0.526604 N 1.441757 1.152871 -0.118927 Pd 2.783644 -0.280363 0.139560 Cl 3.086737 0.260195 2.350476 Cl 2.706227 -0.897387 -2.064366	C -2.416230 1.133633 0.273607 H 0.363574 2.796239 0.689513 H -1.216611 4.597542 1.348757 H -3.663291 4.092968 1.299131 H -4.404687 1.846148 0.612164 C -2.699985 -0.232522 -0.132717 C -3.986168 -0.751026 -0.234027 C -4.173339 -2.062435 -0.616806 C -3.073429 -2.855591 -0.898239 C -1.787274 -2.348952 -0.802199 C -1.584809 -1.033932 -0.419419 H -5.170705 -2.465720 -0.694868 H -3.215264 -3.883624 -1.196318 H -0.943107 -2.978802 -1.024122 H -4.845171 -0.135345 -0.014637 H 1.871716 -2.561741 1.259402	C -2.462864 1.086565 0.273259 H 0.281008 2.817734 0.629922 H -1.339585 4.594618 1.288226 H -3.772130 4.027508 1.273378 H -4.465105 1.753454 0.625703 C -2.711621 -0.292436 -0.111730 C -3.982998 -0.850768 -0.187610 C -4.135359 -2.172454 -0.549422 C -3.014528 -2.935015 -0.834657 C -1.743621 -2.387675 -0.763479 C -1.573977 -1.061247 -0.402332 H -5.120651 -2.607608 -0.607764 H -3.128592 -3.971300 -1.116129 H -0.883856 -2.995067 -0.989188 H -4.857161 -0.258061 0.035953 H 1.924731 -2.492928 1.215282
TS(G-H)$_{Conf1}$ E0 = -1759.5982704 E0+ZPE = -1759.300245 E298 = -1759.277745 H298 = -1759.276801 G298 = -1759.356302 NImag = 1 (-361.1076) E_0(M06) = -1759.1899411 O 1.704155 1.313067 0.094809 Pd 0.137143 -0.043315 -0.165586 Cl 2.840311 -2.648021 2.303978 Cl 1.631419 -1.890263 -0.805221 C 3.254645 3.006472 -0.367400 C 2.569780 1.711096 -0.711894 H 3.405584 3.085468 0.703340 H 4.195615 3.133252 -0.891301 H 2.587251 3.812277 -0.677493 C 4.188354 0.427749 -0.137264 C 2.499217 1.326484 -2.159151 H 3.749737 -0.508636 -0.443566 H 4.979972 0.843815 -0.741354 H 4.213470 0.632471 0.920803 H 3.428483 1.532506 -2.680070 H 2.229578 0.281065 -2.267826 H 1.713242 1.933521 -2.611829 N -1.575613 -1.132280 -0.338153 C -1.615121 -2.414744 -0.680320 C -2.803826 -3.101902 -0.800327 C -3.983980 -2.425067 -0.556476 C -3.939041 -1.094524 -0.200086 C -2.713354 -0.456074 -0.092368 H -0.658197 -2.878501 -0.858233 H -2.792458 -4.142215 -1.078255 H -4.933465 -2.930608 -0.641685 H -4.845861 -0.548799 -0.002930 C -2.503842 0.932169 0.288127 C -3.526019 1.815531 0.612949 C -3.224674 3.107695 0.993404 C -1.901419 3.512440 1.058002 C -0.878104 2.635181 0.733480 C -1.165448 1.341519 0.335813 H -4.016690 3.794656 1.247014 H -1.663879 4.519159 1.368705 H 0.148333 2.957180 0.806124 H -4.558218 1.501251 0.576543 H 2.342532 -2.397281 1.119764	**TS(G-H)$_{Conf2}$** E0 = -1759.578892 E0+ZPE = -1759.282909 E298 = -1759.259616 H298 = -1759.258672 G298 = -1759.343124 NImag = 1 (-505.5449) E_0(M06) = -1759.1714687 O -5.155525 0.743521 2.386604 Pd 0.448800 -0.655801 -0.655924 Cl -1.570132 -0.568992 -1.870346 Cl -0.254366 -3.218177 -0.779739 C -4.730891 1.326124 0.119175 C -4.669306 0.392237 1.307935 H -4.624223 2.355730 0.444282 H -3.988609 1.088224 -0.636642 H -5.717607 1.216016 -0.332575 C -2.645677 0.711584 1.828978 C -4.570377 -1.080648 0.975795 H -2.550928 0.037249 2.664519 H -2.173758 0.423683 0.901813 H -2.664824 1.762457 2.067494 H -3.826741 -1.285297 0.211694 H -4.361134 -1.655324 1.871986 H -5.541561 -1.395973 0.592192 N 2.181431 -0.698361 0.430787 C 2.741090 -1.796777 0.921800 C 3.902313 -1.763611 1.660293 C 4.494680 -0.534341 1.890428 C 3.913275 0.605121 1.379763 C 2.741869 0.504527 0.643259 H 2.234386 -2.724266 0.710755 H 4.324366 -2.678026 2.041196 H 5.405171 -0.465871 2.465101 H 4.359655 1.570035 1.548685 C 2.011352 1.604889 0.037158 C 2.404831 2.935778 0.109044 C 1.652136 3.912054 -0.510288 C 0.506856 3.559430 -1.204392 C 0.101628 2.235593 -1.282421 C 0.848157 1.254351 -0.659215 H 1.957280 4.944947 -0.454431 H -0.081080 4.321613 -1.693171 H -0.789415 1.974660 -1.827922 H 3.298939 3.214885 0.645434 H -1.125675 -2.413537 -1.408664	**TS(G-I)** E0 = -1759.578144 E0+ZPE = -1759.281344 E298 = -1759.258124 H298 = -1759.257179 G298 = -1759.339630 NImag = 1 (-539.3542) E_0(M06) = -1759.1740514 O -3.205160 2.307867 -0.138940 Pd 0.219844 -0.450834 -0.333595 Cl -0.429548 -2.624763 -0.835988 Cl -2.563122 -2.941017 1.832001 C -4.684363 1.205580 -1.637574 C -3.958422 1.337343 -0.318981 H -4.063950 1.564800 -2.451590 H -5.011240 0.189674 -1.836410 H -5.571758 1.837066 -1.585594 C -2.436366 -0.045426 -0.649372 C -4.615983 0.677161 0.869167 H -1.987168 -0.000705 0.337734 H -2.982048 -0.949383 -0.866457 H -1.933189 0.426031 -1.481398 H -4.907198 -0.349676 0.672744 H -3.964383 0.713127 1.735252 H -5.518375 1.244944 1.098783 N 0.823500 1.462988 0.107890 C 0.017652 2.511206 0.240378 C 0.497259 3.768785 0.537192 C 1.860201 3.931518 0.700071 C 2.693403 2.842051 0.562441 C 2.151632 1.601862 0.264015 H -1.040997 2.345097 0.107623 H -0.192316 4.589770 0.636193 H 2.272070 4.901163 0.933113 H 3.757522 2.947676 0.686291 C 2.895596 0.364271 0.092917 C 4.276838 0.262699 0.209924 C 4.898437 -0.956254 0.033990 C 4.141481 -2.077873 -0.259062 C 2.762582 -1.994888 -0.379070 C 2.139246 -0.774866 -0.203953 H 5.970343 -1.032740 0.125560 H 4.625652 -3.032955 -0.396229 H 2.182246 -2.872041 -0.606289 H 4.871098 1.133960 0.439280 H -1.702100 -2.922028 0.848319
TS(G-I)$_{Conf1}$ E0 = -1759.568594	**TS(G-I)$_{Conf2}$** E0 = -1759.5532946	**TS(G-I)$_{Conf3}$** E0 = -1759.5587853

E0+ZPE = -1759.271256
E298 = -1759.248538
H298 = -1759.247594
G298 = -1759.328912
NImag = 1 (-641.0513)
E_0(M06) = -1759.1625857

O	-3.202808	2.477604	-0.105180
Pd	0.097279	-0.309210	-0.352506
Cl	-0.726430	-2.528541	-0.923017
Cl	-2.578284	-2.941681	1.894502
C	-4.655569	1.196625	-1.484352
C	-3.800703	1.391777	-0.253196
H	-4.190712	1.654332	-2.351029
H	-4.869823	0.150865	-1.682043
H	-5.603462	1.703300	-1.303227
C	-2.144316	0.350666	-0.838633
C	-4.208867	0.602631	0.966844
H	-1.679571	0.386687	0.162371
H	-2.618297	-0.576010	-1.113819
H	-1.775624	0.986856	-1.626482
H	-4.328710	-0.456805	0.764838
H	-3.493237	0.741375	1.770100
H	-5.171093	0.992499	1.299651
N	2.067638	-0.819525	-0.211261
C	2.522555	-2.052863	-0.397524
C	3.863107	-2.353697	-0.291363
C	4.744905	-1.334415	0.016487
C	4.265653	-0.056264	0.208245
C	2.906486	0.187802	0.090244
H	1.777056	-2.794742	-0.635090
H	4.196572	-3.365619	-0.447187
H	5.801277	-1.534251	0.107733
H	4.935919	0.750660	0.450229
C	2.244151	1.469346	0.266852
C	2.901709	2.651335	0.580908
C	2.182741	3.819935	0.735090
C	0.807931	3.805947	0.578081
C	0.140441	2.630050	0.263571
C	0.852826	1.455230	0.103547
H	2.692422	4.738658	0.978930
H	0.241320	4.716479	0.701487
H	-0.933181	2.658270	0.154632
H	3.973712	2.666960	0.706550
H	-1.838577	-2.870864	0.813857

E0+ZPE = -1759.254578
E298 = -1759.232835
H298 = -1759.231891
G298 = -1759.309040
NImag = 1 (-650.4025)
E_0(M06) = -1759.1506481

O	-0.769307	1.071897	-1.890366
Pd	-0.444375	-0.054660	-0.019091
Cl	-2.537995	-1.988104	2.895642
Cl	-2.109998	-1.794548	-0.466174
C	-3.127844	1.254686	-2.059565
C	-1.809931	1.717888	-1.491493
H	-3.230007	0.180474	-1.952375
H	-3.974095	1.762895	-1.606301
H	-3.112739	1.497989	-3.122003
C	-2.154424	1.290735	0.465862
C	-1.637259	3.216425	-1.411190
H	-1.680648	0.760230	1.321733
H	-2.152960	2.332447	0.748698
H	-3.134770	0.858326	0.347542
H	-2.488737	3.710857	-0.952411
H	-0.721629	3.472892	-0.889706
H	-1.548972	3.576301	-2.436010
N	1.186800	-1.250990	-0.439346
C	1.101510	-2.465943	-0.965086
C	2.225556	-3.191409	-1.297095
C	3.465740	-2.623146	-1.075811
C	3.546407	-1.359215	-0.530797
C	2.380998	-0.680170	-0.214223
H	0.101411	-2.843275	-1.108336
H	2.119749	-4.176551	-1.718814
H	4.366642	-3.161411	-1.326478
H	4.503491	-0.899417	-0.353576
C	2.297882	0.646837	0.378135
C	3.403946	1.392703	0.764787
C	3.237082	2.628020	1.357627
C	1.961531	3.117578	1.573179
C	0.851109	2.382568	1.184192
C	1.008576	1.152746	0.578176
H	4.098403	3.202529	1.659441
H	1.824688	4.076252	2.050303
H	-0.130803	2.784728	1.373202
H	4.401279	1.009485	0.612438
H	-2.441577	-2.025374	1.588066

E0+ZPE = -1759.258510
E298 = -1759.237178
H298 = -1759.236234
G298 = -1759.311443
NImag = 1 (-480.5443)
E_0(M06) = -1759.1549589

O	2.284831	0.214832	0.193120
Pd	0.312929	-0.436653	0.046859
Cl	2.948748	2.456380	-1.554365
Cl	-0.164939	-1.058490	2.369474
C	3.299672	-1.577168	1.348337
C	2.804226	-0.975624	0.062336
H	2.515066	-1.571591	2.097739
H	3.681394	-2.585206	1.215910
H	4.111700	-0.940595	1.698504
C	1.382207	-2.342223	-0.421671
C	3.691942	-1.142363	-1.143080
H	1.012203	-2.375220	-1.444489
H	2.277620	-2.945999	-0.397516
H	0.712057	-2.812109	0.293619
H	4.069202	-2.155258	-1.241774
H	3.177103	-0.854485	-2.054163
H	4.539581	-0.469856	-1.014449
N	-0.709576	1.337824	0.234536
C	-0.143144	2.463465	0.642663
C	-0.875300	3.616792	0.816428
C	-2.234334	3.572351	0.563441
C	-2.816267	2.391861	0.152654
C	-2.025550	1.264873	-0.008254
H	0.917994	2.424560	0.827603
H	-0.386289	4.519466	1.140590
H	-2.840861	4.455408	0.691742
H	-3.874987	2.339416	-0.034840
C	-2.479630	-0.058103	-0.415616
C	-3.788914	-0.349317	-0.777016
C	-4.138100	-1.635288	-1.136505
C	-3.180272	-2.634313	-1.130898
C	-1.871386	-2.353195	-0.769420
C	-1.512638	-1.068654	-0.421488
H	-5.155105	-1.859407	-1.416869
H	-3.451971	-3.642570	-1.404884
H	-1.145064	-3.150821	-0.762472
H	-4.540598	0.425124	-0.781263
H	2.674781	1.399038	-0.783546

TS(G-J)
E0 = -1759.4649744
E0+ZPE = -1759.167687
E298 = -1759.146082
H298 = -1759.145137
G298 = -1759.219213
NImag = 1 (-958.2888)
E_0(M06) = -1759.0733774

O	1.265062	-0.268198	1.639368
Pd	0.747836	-0.895791	-0.166685
Cl	2.983277	-0.976628	-1.211129
Cl	0.217112	-1.893985	-2.245448
C	2.419143	1.764149	1.071542
C	1.466804	0.989416	1.939833
H	2.169919	1.665692	0.021836
H	2.434322	2.817688	1.338997
H	3.423073	1.362047	1.220200
C	-0.273139	1.985590	1.952215
C	1.758322	1.120812	3.415272
H	1.885845	2.157254	3.716939
H	0.966188	0.669728	4.005401
H	2.682033	0.584266	3.626368
N	-1.146797	-0.999862	0.515681
C	-1.518673	-2.049437	1.240094

H
E0 = -1759.6140873
E0+ZPE = -1759.320369
E298 = -1759.294540
H298 = -1759.293596
G298 = -1759.384191
NImag = 0
E_0(M06) = -1759.202726

O	-1.375850	1.628013	-0.068421
Pd	0.098046	-0.046896	-0.054701
Cl	-4.239860	-0.191412	-1.764450
Cl	-1.621222	-1.633294	-0.180403
C	-3.319433	2.926868	0.113927
C	-2.412891	1.820860	0.535797
H	-2.942244	3.408245	-0.779808
H	-4.310386	2.520799	-0.077047
H	-3.414576	3.651533	0.921284
C	-4.977327	-2.322254	1.886507
C	-2.830917	0.995197	1.699733
H	-5.279673	-2.509576	2.902502
H	-5.718905	-2.097806	1.139492
H	-3.942907	-2.411591	1.601743
H	-3.657864	0.355691	1.391788
H	-2.022052	0.362260	2.043058

TS(H-I)
E0 = -1759.6120126
E0+ZPE = -1759.316870
E298 = -1759.292908
H298 = -1759.291964
G298 = -1759.375094
NImag = 1 (-82.2990)
E_0(M06) = -1759.2073287

O	1.723855	1.289619	0.048577
Pd	0.102574	-0.108552	0.042379
Cl	4.814830	-1.047135	0.603609
Cl	1.678660	-1.990445	-0.095217
C	3.733272	2.347417	-0.514048
C	2.590808	1.435902	-0.793789
H	3.690045	2.713005	0.504160
H	4.665715	1.811930	-0.677788
H	3.706620	3.181517	-1.214305
C	0.249502	-0.002250	2.642046
C	2.563706	0.730830	-2.101200
H	-0.787799	0.052371	2.927052
H	0.759845	-0.948578	2.707556
H	0.835652	0.900853	2.673735
H	2.992643	1.347529	-2.885909
H	3.173190	-0.167393	-2.003232

C -2.820252 -2.230893 1.646486 C -3.759039 -1.283339 1.280866 C -3.359065 -0.187575 0.548071 C -2.027630 -0.054040 0.176598 H -0.744924 -2.758365 1.483075 H -3.084211 -3.098732 2.226828 H -4.790713 -1.391435 1.577800 H -4.054614 0.588829 0.276664 C -1.535396 1.111502 -0.563371 C -2.191364 1.522640 -1.719053 C -1.736667 2.614977 -2.430392 C -0.628394 3.309145 -1.972323 C 0.017150 2.918722 -0.811230 C -0.414938 1.806895 -0.106196 H -2.234427 2.916145 -3.338324 H -0.264655 4.165027 -2.522050 H 0.857278 3.496568 -0.456981 H -3.035789 0.954582 -2.082355 H -0.686910 1.207065 2.588186 H -1.143708 2.528067 1.572332 H 0.225673 2.758143 2.540649 H 2.114452 -1.502521 -2.101410	H -3.196415 1.634516 2.500447 N 1.681222 1.250449 0.000936 C 1.573614 2.572546 -0.013762 C 2.674140 3.399269 0.017334 C 3.928432 2.815269 0.062404 C 4.037770 1.442737 0.067604 C 2.889021 0.663104 0.032468 H 0.568582 2.958999 -0.059080 H 2.546369 4.468496 0.003524 H 4.815937 3.428420 0.088277 H 5.005288 0.971489 0.094345 C 2.837048 -0.789176 0.013225 C 3.966754 -1.599425 0.044083 C 3.832394 -2.971214 0.010555 C 2.567184 -3.532034 -0.055217 C 1.434765 -2.733852 -0.084825 C 1.554311 -1.354867 -0.050313 H 4.707618 -3.601259 0.034152 H 2.457774 -4.605947 -0.083688 H 0.458453 -3.184962 -0.136962 H 4.953270 -1.163862 0.093861 H -3.190923 -0.783656 -1.235437	H 1.554808 0.420448 -2.351836 N -1.590361 -1.252127 -0.155983 C -1.591106 -2.575763 -0.253573 C -2.760636 -3.296925 -0.362771 C -3.960318 -2.609445 -0.367198 C -3.954457 -1.234975 -0.263299 C -2.745669 -0.563521 -0.158572 H -0.619357 -3.043972 -0.242932 H -2.721223 -4.370212 -0.441944 H -4.895587 -3.141229 -0.449869 H -4.877931 -0.681407 -0.261933 C -2.572080 0.875833 -0.036118 C -3.617169 1.792033 -0.023778 C -3.352106 3.139516 0.113675 C -2.042230 3.571936 0.245852 C -0.994928 2.664172 0.236359 C -1.246765 1.311795 0.087728 H -4.162717 3.851028 0.122375 H -1.834605 4.625443 0.360933 H 0.018641 3.013577 0.353566 H -4.640129 1.460514 -0.120029 H 3.577220 -1.464558 0.403671
I E0 = -1759.620165 E0+ZPE = -1759.322203 E298 = -1759.298127 H298 = -1759.297183 G298 = -1759.381024 NImag = 0 E_0(M06) = -1759.2120913 O 1.934114 1.392453 -0.170602 Pd 0.090298 -0.129638 0.145735 Cl 4.763921 -1.269340 0.719449 Cl 1.580993 -2.071084 -0.039837 C 4.060233 2.317806 -0.549751 C 2.919377 1.410890 -0.874260 H 3.764081 3.056143 0.185872 H 4.860149 1.702769 -0.138342 H 4.445687 2.798306 -1.445807 C 0.090908 0.170093 2.182809 C 3.052640 0.558512 -2.091335 H -0.912531 0.186892 2.585145 H 0.656904 -0.698159 2.499727 H 0.617270 1.100333 2.356159 H 2.882225 1.190086 -2.964252 H 4.059843 0.158089 -2.168379 H 2.335182 -0.253226 -2.079346 N -1.752805 -1.269353 -0.212355 C -1.852833 -2.582894 -0.342095 C -3.075130 -3.213224 -0.448773 C -4.216360 -2.432777 -0.405800 C -4.104120 -1.065425 -0.264002 C -2.842224 -0.493528 -0.170906 H -0.917113 -3.121912 -0.359077 H -3.124585 -4.283624 -0.558446 H -5.191992 -2.888322 -0.478187 H -4.985697 -0.449247 -0.216460 C -2.573033 0.939384 -0.019806 C -3.567163 1.908425 -0.112787 C -3.254604 3.246065 0.022360 C -1.942960 3.627314 0.251258 C -0.944263 2.671574 0.347135 C -1.247947 1.330130 0.206693 H -4.031758 3.990312 -0.053651 H -1.696716 4.673203 0.358190 H 0.076858 2.970409 0.527171 H -4.590927 1.625332 -0.304578 H 3.517446 -1.615041 0.463903	**TS(I-J)'** E0 = -1759.6127916 E0+ZPE = -1759.315065 E298 = -1759.291724 H298 = -1759.290780 G298 = -1759.372982 NImag = 1 (-284.9970) E_0(M06) = -1759.2064445 O -1.996764 1.325780 0.326510 Pd -0.125143 -0.133372 0.162589 Cl -4.771631 -1.576945 0.359791 Cl -1.573751 -2.001051 -0.538311 C -4.164991 2.217441 0.190362 C -2.977404 1.501399 -0.363099 H -3.906406 2.734220 1.107011 H -4.584410 2.907093 -0.537997 H -4.924721 1.466583 0.406352 C -3.061333 1.033927 -1.776105 H -4.026055 0.568423 -1.961117 H -2.988461 1.906354 -2.426649 H -2.267053 0.333883 -2.004322 N 1.742840 -1.309157 -0.115962 C 1.860401 -2.626138 -0.152867 C 3.092426 -3.249135 -0.156527 C 4.225390 -2.457613 -0.106336 C 4.095969 -1.084323 -0.067036 C 2.824683 -0.526942 -0.084651 H 0.931300 -3.175477 -0.190093 H 3.155468 -4.323922 -0.194039 H 5.206051 -2.907810 -0.092341 H 4.966591 -0.452808 -0.009159 C 2.543150 0.912215 -0.073332 C 3.481776 1.856233 -0.471141 C 3.160326 3.198877 -0.508211 C 1.886984 3.608938 -0.151328 C 0.943789 2.681593 0.256074 C 1.258227 1.333573 0.296532 H 3.895929 3.920511 -0.826573 H 1.626860 4.656122 -0.185658 H -0.042942 3.003533 0.550426 H 4.463567 1.538266 -0.787739 H -3.506062 -1.784688 0.034812 C 0.487714 0.524170 2.096795 H 0.030891 1.455717 2.396301 H -0.084408 -0.324979 2.473464 H 1.513531 0.452607 2.427965	**J'** (acetone coordinated to Pd in **J**) E0 = -1759.6864664 E0+ZPE = -1759.385983 E298 = -1759.362044 H298 = -1759.361100 G298 = -1759.446679 NImag = 0 E_0(M06) = -1759.2711743 O -1.856473 1.386901 -0.152709 Pd -0.317941 -0.161870 -0.192769 Cl -4.657141 -0.925263 1.196773 Cl -1.861023 -2.135600 -0.120219 C -3.875483 2.567113 -0.270526 C -2.924771 1.510193 -0.717063 H -3.377261 3.283255 0.371842 H -4.338614 3.062593 -1.120144 H -4.666740 2.071002 0.291334 C -3.332593 0.650478 -1.861111 H -4.388079 0.402542 -1.793711 H -3.186209 1.225963 -2.776685 H -2.738913 -0.256058 -1.897114 N 1.484639 -1.317880 -0.153470 C 1.484638 -2.643277 -0.248767 C 2.653689 -3.374582 -0.310741 C 3.859024 -2.702145 -0.278132 C 3.855553 -1.323777 -0.175173 C 2.644144 -0.658339 -0.109210 H 0.508974 -3.104964 -0.276350 H 2.608613 -4.448369 -0.386544 H 4.792049 -3.242094 -0.328084 H 4.773344 -0.760140 -0.137454 C 2.565565 0.817654 0.002364 C 2.877860 1.594480 -1.105515 C 2.807229 2.973336 -1.042745 C 2.428659 3.579244 0.140233 C 2.129697 2.808280 1.248619 C 2.190847 1.422028 1.208085 H 3.045582 3.567119 -1.911184 H 2.370268 4.654884 0.204321 H 1.847335 3.290094 2.172772 H 3.168303 1.107859 -2.024584 H -3.536163 -1.455864 0.712901 C 1.895231 0.613891 2.435142 H 1.796583 1.259715 3.302102 H 0.970166 0.049498 2.330624 H 2.688404 -0.103836 2.635109

I' (I without acetone)	TS(I-J)	J
E0 = -1566.4540503	E0 = -1566.4460366	E0 = -1566.5207854
E0+ZPE = -1566.242977	E0+ZPE = -1566.235425	E0+ZPE = -1566.307461
E298 = -1566.225921	E298 = -1566.219050	E298 = -1566.290360
H298 = -1566.224977	H298 = -1566.218106	H298 = -1566.289415
G298 = -1566.291394	G298 = -1566.282879	G298 = -1566.358368
NImag = 0	NImag = 1 (-288.5789)	NImag = 0
E_0(M06) = -1566.1139485	E_0(M06) = -1566.1082757	E_0(M06) = -1566.170887
Pd -0.826765 -0.186457 0.072985	Pd -0.849718 -0.294048 0.091751	Pd 0.995974 -0.371715 -0.142390
Cl -3.623820 0.860819 -0.675562	Cl -3.741962 0.538057 -0.003495	Cl 2.371625 -2.289257 -0.223600
Cl -2.312052 -2.107207 -0.083642	Cl -2.103939 -2.180922 -0.779857	Cl 3.963842 0.597220 -0.016171
N 1.084577 -1.202828 -0.112307	N 1.178333 -1.156192 -0.026734	N -0.162222 1.383993 -0.039063
C 1.265497 -2.513673 -0.143094	C 1.504314 -2.437700 0.000226	C 0.424771 2.578440 -0.020144
C 2.526737 -3.070461 -0.175123	C 2.818860 -2.854086 0.057735	C -0.290057 3.756016 -0.010025
C 3.615384 -2.216867 -0.166821	C 3.808362 -1.888649 0.098745	C -1.670120 3.687500 -0.021968
C 3.416138 -0.852286 -0.132518	C 3.461018 -0.553565 0.066894	C -2.278780 2.448793 -0.037259
C 2.120393 -0.355330 -0.107618	C 2.118955 -0.208319 -0.008958	C -1.496419 1.305041 -0.041383
H 0.366073 -3.111083 -0.145127	H 0.679536 -3.133376 -0.037308	H 1.503797 2.573660 -0.019032
H 2.645544 -4.140488 -0.204359	H 3.053807 -3.905242 0.071903	H 0.229976 4.699232 0.004084
H 4.618812 -2.613354 -0.185283	H 4.847218 -2.174403 0.157714	H -2.265305 4.587411 -0.014187
H 4.256591 -0.179633 -0.117765	H 4.217889 0.211397 0.111274	H -3.351798 2.351002 -0.035423
C 1.753137 1.062938 -0.082019	C 1.610232 1.164634 -0.093297	C -2.101715 -0.044399 -0.081951
C 2.682375 2.088639 -0.216690	C 2.397401 2.224515 -0.524320	C -2.823632 -0.401599 -1.216539
C 2.271608 3.406792 -0.216179	C 1.858318 3.487568 -0.675686	C -3.392888 -1.653026 -1.326508
C 0.927598 3.710665 -0.082463	C 0.518058 3.699781 -0.405072	C -3.249456 -2.555906 -0.287932
C -0.007072 2.696654 0.058510	C -0.277504 2.656951 0.038621	C -2.551353 -2.197194 0.847212
C 0.395428 1.374698 0.055805	C 0.258497 1.391647 0.197370	C -1.965666 -0.943444 0.979541
H 2.998359 4.196339 -0.324837	H 2.478982 4.299568 -1.019806	H -3.938162 -1.923355 -2.216845
H 0.604084 4.740565 -0.086162	H 0.087381 4.680613 -0.536145	H -3.685716 -3.540001 -0.360333
H -1.052571 2.943637 0.166172	H -1.318752 2.830268 0.263040	H -2.456673 -2.902558 1.659432
H 3.731281 1.865396 -0.338209	H 3.432120 2.056525 -0.781386	H -2.917690 0.307865 -2.025021
H -3.435722 -0.433427 -0.490074	H -3.396221 -0.680470 -0.405534	H 3.590740 -0.675248 -0.101954
C -1.003399 0.306796 2.048151	C -0.473441 0.577550 1.991815	C -1.252722 -0.601805 2.254791
H -1.607917 1.204832 2.094996	H -1.072079 1.448063 2.216178	H -1.819952 -0.966190 3.107897
H -1.524480 -0.567064 2.421439	H -0.939190 -0.322107 2.399070	H -0.271254 -1.073991 2.296722
H -0.034038 0.448326 2.504876	H 0.529911 0.675480 2.380114	H -1.111927 0.467242 2.377136
TS(B-K)	**TS(B-K)$_{Conf1}$**	**TS(B-K)$_{Conf2}$**
E0 = -1759.5938073	E0 = -1759.5766514	E0 = -1759.5691738
E0+ZPE = -1759.292376	E0+ZPE = -1759.274716	E0+ZPE = -1759.270734
E298 = -1759.271661	E298 = -1759.253979	E298 = -1759.248730
H298 = -1759.270717	H298 = -1759.253035	H298 = -1759.247786
G298 = -1759.342748	G298 = -1759.325497	G298 = -1759.327066
NImag = 1 (-1766.9924)	NImag = 1 (-1211.4480)	NImag = 1 (-1135.6150)
E_0(M06) = -1759.1908937	E_0(M06) = -1759.1698175	E_0(M06) = -1759.1576434
N 1.318735 -1.142649 -0.037888	N 0.236061 1.406758 -0.049385	N 1.395434 -1.239396 0.107934
C 2.244733 -0.248745 0.339214	C 1.387713 1.279936 -0.710238	C 2.438318 -0.474952 0.471777
C 3.429820 -0.670694 0.917768	C 1.934040 2.374482 -1.362687	C 3.586457 -1.066928 0.974504
C 3.649265 -2.020179 1.101894	C 1.287502 3.591756 -1.290076	C 3.639025 -2.436776 1.119562
C 2.683104 -2.922704 0.703390	C 0.112740 3.700238 -0.569866	C 2.543585 -3.198755 0.762670
C 1.523554 -2.440461 0.132857	C -0.386427 2.568978 0.042849	C 1.436632 -2.558845 0.248720
C 1.899096 1.152369 0.086366	C 1.999356 -0.054568 -0.668722	C 2.224897 0.966268 0.350331
C 0.546791 1.450658 -0.147414	C 1.187756 -1.153547 -0.344921	C 1.057870 1.419090 -0.293909
C 0.175087 2.747095 -0.471497	C 1.765713 -2.406719 -0.176183	C 0.733031 2.764295 -0.210323
C 1.127044 3.748809 -0.529936	C 3.122155 -2.587114 -0.366517	C 1.571288 3.664317 0.429802
C 2.457775 3.451865 -0.288525	C 3.910851 -1.501053 -0.706263	C 2.737916 3.222658 1.018417
C 2.848104 2.159103 0.012847	C 3.357915 -0.239992 -0.855003	C 3.048945 1.875834 0.995785
Pd -0.410034 -0.327152 -0.835026	Pd -0.462000 -0.415946 0.907441	H 0.322334 1.299839 -1.619931
Cl -1.107040 -2.329160 -1.757956	Cl -2.291814 0.368864 2.091609	Pd -0.077924 -0.228435 -0.868925
O -0.811246 -0.008982 1.540933	O -1.360253 -1.325551 -0.719494	Cl -1.376785 -2.123287 -1.301849
C -2.128538 0.144742 2.017536	C -2.182966 -0.837860 -1.762091	Cl -0.998667 1.286144 -2.482666
C -2.663851 1.537715 1.746471	C -3.263545 0.072879 -1.216804	H -0.174918 3.122777 -0.669090
Cl -2.181971 0.776110 -1.781492	Cl 0.905697 -0.045844 2.720459	H 1.301827 4.708326 0.469243
C -3.026866 -0.930464 1.433656	C -1.351536 -0.113579 -2.810036	H 3.926776 1.534965 1.521411
C -1.952990 -0.075892 3.524376	C -2.807329 -2.087615 -2.369938	H 3.393330 3.916682 1.520505
H -0.258748 0.838861 0.696177	H 0.001371 -1.253911 -0.785958	H 4.432205 -0.458760 1.244768
H -0.861989 2.960036 -0.675442	H 1.136004 -3.245596 0.079442	H 4.529994 -2.904806 1.508302
H 0.834531 4.757779 -0.775514	H 3.566428 -3.562098 -0.242380	H 2.540458 -4.270965 0.862856

H 3.894827 1.941691 0.157725 H 3.202158 4.230713 -0.349255 H 4.162327 0.053526 1.231012 H 4.565739 -2.362518 1.556698 H 2.813361 -3.984294 0.829735 H 0.732170 -3.085588 -0.214728 H -2.923026 0.011460 4.009215 H -1.550381 -1.065458 3.720033 H -1.283095 0.668248 3.946835 H -3.642934 1.658105 2.204756 H -1.999115 2.292551 2.162597 H -2.770462 1.699588 0.677282 H -4.008403 -0.890340 1.901967 H -3.147665 -0.787735 0.363462 H -2.598498 -1.914665 1.603018	H 4.003919 0.596226 -1.071698 H 4.973952 -1.631129 -0.838283 H 2.846898 2.269479 -1.924199 H 1.700811 4.452357 -1.792587 H -0.411571 4.636718 -0.479961 H -1.292859 2.573421 0.628693 H -3.470329 -1.824552 -3.192682 H -2.033193 -2.752297 -2.745951 H -3.380266 -2.619695 -1.615645 H -3.942094 0.372991 -2.013704 H -3.830635 -0.429506 -0.439257 H -2.832864 0.968672 -0.777635 H -1.973226 0.188021 -3.650596 H -0.897865 0.783206 -2.394580 H -0.562496 -0.760372 -3.189838	H 0.553801 -3.086249 -0.075724 O -1.938582 0.443920 1.392282 C -3.267796 0.101350 1.516889 C -4.013204 0.352837 0.214746 H -3.901730 1.390192 -0.090694 H -3.614725 -0.283889 -0.570846 H -5.072942 0.133439 0.331536 C -3.764008 1.054177 2.614768 H -3.646399 2.089757 2.308095 H -4.819248 0.857623 2.788809 H -3.218578 0.893294 3.540472 C -3.398628 -1.345674 1.970449 H -2.857747 -1.499815 2.901155 H -4.444288 -1.604836 2.125601 H -2.988270 -2.007108 1.211917
TS(B-K)$_{Conf3}$ E0 = -1759.5587367 E0+ZPE = -1759.256183 E298 = -1759.235466 H298 = -1759.234522 G298 = -1759.306788 NImag = 1 (-1526.0494) E_0(M06) = -1759.154941 N 1.688273 -0.870390 -0.305385 C 2.382333 0.203891 0.103266 C 3.692148 0.043609 0.525880 C 4.274300 -1.206051 0.492976 C 3.543848 -2.285462 0.038463 C 2.235543 -2.076873 -0.337059 C 1.707844 1.509494 0.015270 C 0.318958 1.617772 -0.177974 C -0.229916 2.855529 -0.480716 C 0.548744 4.000163 -0.503453 C 1.904583 3.903680 -0.271225 C 2.475114 2.666796 -0.040636 Pd -0.309862 -0.489554 -0.423819 Cl -0.199759 -1.010418 2.012471 O -2.048728 0.520281 -0.456915 C -3.246620 0.300862 0.286910 C -3.520600 -1.175665 0.478196 Cl -0.849991 -2.598256 -1.201013 C -3.163383 1.021322 1.620773 C -4.326242 0.925096 -0.587313 H -0.863404 1.095705 0.050046 H -1.289419 2.915933 -0.678397 H 0.094115 4.954791 -0.717440 H 3.546537 2.605454 0.058472 H 2.528803 4.782757 -0.301151 H 4.246174 0.888431 0.895306 H 5.291534 -1.334677 0.828435 H 3.959623 -3.277862 -0.001504 H 1.585610 -2.873558 -0.660570 H -5.298390 0.837044 -0.105507 H -4.119814 1.979721 -0.755577 H -4.366410 0.423452 -1.550325 H -4.483302 -1.310167 0.968230 H -3.541072 -1.687403 -0.479249 H -2.755012 -1.636703 1.095346 H -4.099078 0.917083 2.166660 H -2.365217 0.608163 2.230593 H -2.979886 2.084281 1.470364	**TS(B-K)$_{Conf4}$** E0 = -1759.5560532 E0+ZPE = -1759.254335 E298 = -1759.233537 H298 = -1759.232593 G298 = -1759.305311 NImag = 1 (-1607.5719) E_0(M06) = -1759.1526441 N -1.689915 -0.931702 0.239165 C -2.275526 0.141596 -0.310013 C -3.580247 0.016265 -0.772475 C -4.259438 -1.171013 -0.613395 C -3.637796 -2.238228 0.007110 C -2.331389 -2.078580 0.402573 C -1.538607 1.425176 -0.340718 C -0.148214 1.552834 -0.186221 C 0.418065 2.804003 0.000989 C -0.349559 3.951615 -0.078277 C -1.710407 3.843756 -0.281495 C -2.292188 2.597264 -0.387304 Pd 0.300776 -0.695341 0.378795 Cl 0.334380 -1.611719 -1.777214 O 2.082444 0.265799 0.243467 C 3.298033 -0.109673 -0.392695 C 3.532540 -1.598058 -0.216263 Cl 0.163567 -0.246069 2.637109 C 3.286504 0.284271 -1.859476 C 4.364919 0.678488 0.356155 H 0.991110 0.905976 -0.280265 H 1.478501 2.870502 0.188446 H 0.114713 4.918653 0.038146 H -3.365824 2.541351 -0.458250 H -2.329492 4.726091 -0.320110 H -4.053169 0.842491 -1.272570 H -5.270249 -1.264215 -0.978416 H -4.135937 -3.180624 0.157927 H -1.767931 -2.878239 0.853658 H 5.352121 0.459691 -0.047669 H 4.184378 1.746726 0.261247 H 4.350240 0.421464 1.411688 H 4.514520 -1.874592 -0.595284 H 3.488012 -1.857844 0.839465 H 2.785375 -2.172206 -0.756708 H 4.247241 0.054217 -2.316416 H 2.510521 -0.248755 -2.398603 H 3.114780 1.354594 -1.961924	**TS(B-K)$_{Conf5}$** E0 = -1759.5864488 E0+ZPE = -1759.285736 E298 = -1759.264668 H298 = -1759.263724 G298 = -1759.337357 NImag = 1 (-1795.9743) E_0(M06) = -1759.1853738 N -0.732152 1.298075 -0.490408 C -1.940183 0.876327 -0.083432 C -2.955308 1.788423 0.157156 C -2.718366 3.132969 -0.037102 C -1.473812 3.544234 -0.474156 C -0.503835 2.589540 -0.693531 C -2.076281 -0.572791 0.068135 C -0.898775 -1.334590 0.102178 C -0.973331 -2.718580 0.155041 C -2.204948 -3.346090 0.209118 C -3.365286 -2.591019 0.185326 C -3.306308 -1.210910 0.109208 Pd 0.653019 -0.215361 -0.840825 Cl 2.019337 1.155617 -2.107204 O 1.217244 -0.713678 1.504678 C 1.448631 0.332000 2.410909 C 2.387667 1.353923 1.795411 Cl 1.956052 -2.029107 -1.316036 C 0.158251 0.965154 2.900534 C 2.150256 -0.390353 3.566844 H 0.106969 -0.937958 0.863271 H -0.057086 -3.287885 0.158261 H -2.261047 -4.422442 0.256448 H -4.223457 -0.645963 0.050347 H -4.326578 -3.080494 0.211102 H -3.915769 1.444617 0.501042 H -3.499489 3.852976 0.151277 H -1.248296 4.583276 -0.645736 H 0.482424 2.833996 -1.056521 H 2.415010 0.336589 4.331920 H 1.495643 -1.138973 4.004421 H 3.052974 -0.877455 3.211936 H 2.656214 2.111173 2.529464 H 3.290640 0.867891 1.438649 H 1.920668 1.844169 0.945205 H 0.366515 1.669309 3.702866 H -0.338044 1.510828 2.102774 H -0.520901 0.205791 3.281877
K E0 = -1759.6507442 E0+ZPE = -1759.342546 E298 = -1759.321262 H298 = -1759.320318 G298 = -1759.394661 NImag = 0	**TS(C-L)** E0 = -1566.4244488 E0+ZPE = -1566.216327 E298 = -1566.199895 H298 = -1566.198951 G298 = -1566.262300 NImag = 1 (-1374.7740)	**L** E0 = -1566.4749411 E0+ZPE = -1566.261319 E298 = -1566.242911 H298 = -1566.241967 G298 = -1566.314455 NImag = 1

E_0(M06) = -1759.23851 N 1.282666 -1.226374 -0.106099 C 2.307439 -0.463923 0.305657 C 3.447108 -1.057031 0.824842 C 3.512551 -2.431390 0.916662 C 2.443462 -3.194440 0.487699 C 1.337710 -2.548713 -0.023137 C 2.091052 0.970561 0.152107 C 0.866164 1.373266 -0.392762 C 0.599267 2.715455 -0.575096 C 1.548636 3.659899 -0.213542 C 2.760881 3.270281 0.329200 C 3.032367 1.929966 0.510988 Pd -0.354219 -0.163662 -0.836021 Cl -1.435005 -2.148686 -1.633773 O -1.034330 0.032034 1.333981 C -2.365377 0.094538 1.912136 C -2.905052 1.500851 1.753575 Cl -1.947490 1.189627 -1.806922 C -3.209978 -0.912466 1.171459 C -2.214307 -0.280078 3.375018 H -0.529025 0.772602 1.664757 H -0.339021 3.021711 -1.006995 H 1.336444 4.707805 -0.362758 H 3.981995 1.634753 0.929849 H 3.495353 4.009960 0.606438 H 4.271673 -0.447748 1.152483 H 4.395376 -2.903379 1.319338 H 2.457050 -4.269998 0.539262 H 0.468008 -3.070778 -0.392968 H -3.183908 -0.264339 3.867571 H -1.793629 -1.277452 3.471012 H -1.565235 0.422712 3.896512 H -3.901752 1.568041 2.183533 H -2.273999 2.223697 2.272162 H -2.959616 1.769786 0.702931 H -4.201398 -0.947038 1.617328 H -3.308158 -0.646468 0.123320 H -2.769245 -1.903721 1.227034	E_0(M06) = -1566.0888898 N 0.893545 -1.176919 0.002730 C 1.930131 -0.324959 0.012532 C 3.229180 -0.796128 0.107271 C 3.449726 -2.155906 0.179942 C 2.370331 -3.017791 0.155112 C 1.100992 -2.486261 0.064773 C 1.569322 1.088186 -0.102039 C 0.247308 1.450283 0.185135 C -0.183379 2.755491 0.015517 C 0.701265 3.708341 -0.454638 C 2.010622 3.358463 -0.743021 C 2.443229 2.055799 -0.574937 Pd -0.978181 -0.289849 -0.082254 Cl -2.024645 -2.238899 -0.742214 Cl -2.958604 0.863086 -0.056375 H -0.301637 0.891761 1.278879 H -1.207836 3.004203 0.242609 H 0.367950 4.723687 -0.602325 H 3.452543 1.791624 -0.849918 H 2.696802 4.102580 -1.116165 H 4.052068 -0.102065 0.132915 H 4.455674 -2.538102 0.257031 H 2.498272 -4.086021 0.205117 H 0.212789 -3.097351 0.023740 C -0.647191 0.721439 2.675286 H 0.078710 1.395883 3.107266 H -1.672496 1.059729 2.646587 H -0.505311 -0.327342 2.889227	E_0(M06) = -1566.1380876 N 1.328013 -0.689799 0.121397 C 1.878650 0.522160 -0.040126 C 3.249545 0.684179 0.071909 C 4.036910 -0.412859 0.351369 C 3.448394 -1.654243 0.507254 C 2.080080 -1.751006 0.378660 C 0.912888 1.564543 -0.352325 C -0.427334 1.177053 -0.429607 C -1.410252 2.070690 -0.798363 C -1.053739 3.387137 -1.049664 C 0.264474 3.796866 -0.947279 C 1.246224 2.889306 -0.604637 Pd -0.731354 -0.729528 0.002321 Cl -0.632352 -2.734943 -1.218348 Cl -2.992492 -0.610898 0.166038 H -0.712689 1.933398 3.115575 H -2.435647 1.754381 -0.873139 H -1.819379 4.095448 -1.326660 H 2.273555 3.213641 -0.544147 H 0.528821 4.823540 -1.145138 H 3.691113 1.656999 -0.059702 H 5.106022 -0.300338 0.442111 H 4.030586 -2.535590 0.716067 H 1.559289 -2.690762 0.460937 C -1.232105 1.160262 3.673384 H -1.718433 1.603799 4.536653 H -1.977414 0.694293 3.036850 H -0.519679 0.412843 4.009847
TS(C-L)$_{aceto}$ E0 = -1759.591539 E0+ZPE = -1759.296012 E298 = -1759.272479 H298 = -1759.271535 G298 = -1759.353674 NImag = 1 (-1608.3073) E_0(M06) = -1759.1845708 O 2.519048 0.948221 0.252774 Pd 0.832379 -0.204257 -0.014400 Cl 0.594458 0.695082 -2.152122 Cl 1.393888 -1.415306 1.900602 C 4.751226 1.607972 0.108156 C 3.630955 0.667886 -0.152784 H 4.407713 2.468547 0.668165 H 5.535472 1.087745 0.655820 H 5.179456 1.922457 -0.842425 C -1.760299 -0.187655 3.305049 C 3.890576 -0.590736 -0.898449 H -0.797367 -0.680654 3.325510 H -1.895376 0.546395 4.090395 H -2.598198 -0.869099 3.220076 H 4.923744 -0.680724 -1.214652 H 3.622084 -1.424819 -0.250893 H 3.224743 -0.616381 -1.760345 N -0.860068 -1.269192 -0.256161 C -0.733848 -2.584231 -0.421177 C -1.797574 -3.388333 -0.757446 C -3.037044 -2.802706 -0.927604 C -3.165429 -1.444827 -0.731201	**TS(G-M)** E0 = -1759.5818717 E0+ZPE = -1759.280784 E298 = -1759.259264 H298 = -1759.258319 G298 = -1759.334931 NImag = 1 (-295.3394) E_0(M06) = -1759.1736757 C -1.440753 0.148928 -0.642349 C -1.430889 1.522157 -0.409588 C -2.456953 2.272970 -0.965101 C -3.443495 1.676845 -1.727793 C -3.402461 0.314257 -1.960523 C -2.398251 -0.468631 -1.411220 C -0.303799 2.100515 0.316760 N 0.789407 1.333788 0.366191 C 1.888025 1.758866 0.965777 C 1.959441 3.002214 1.560439 C 0.835437 3.806419 1.531384 C -0.309188 3.354533 0.908076 Pd 0.371335 -0.680253 -0.397926 C -0.961582 -2.067648 3.006522 O -0.987480 -0.696590 1.123049 C -1.531905 -1.912517 1.602438 C -3.046164 -1.789099 1.673384 Cl 1.858200 -0.937687 -2.205139 Cl 4.520517 -0.856899 -0.086242 C -1.120178 -3.104375 0.753483 H -0.034842 -3.206854 0.728405 H -1.522563 -4.027147 1.166669	**TS(G-M)$_{conf}$** E0 = -1759.5817383 E0+ZPE = -1759.281007 E298 = -1759.259731 H298 = -1759.258787 G298 = -1759.332808 NImag = 1 (-417.8938) E_0(M06) = -1759.1791746 C 0.495875 1.209405 -0.527031 C 1.861611 0.903118 -0.529544 C 2.747940 1.842605 -1.037090 C 2.291378 3.044017 -1.540284 C 0.930034 3.302281 -1.558637 C 0.018143 2.392680 -1.051691 C 2.255015 -0.415265 -0.060993 N 1.268992 -1.323147 -0.059821 C 1.498525 -2.562835 0.344596 C 2.743681 -2.982319 0.759620 C 3.775008 -2.059421 0.763468 C 3.531343 -0.766001 0.356320 Pd -0.617709 -0.469438 -0.512324 C -2.086204 0.067131 2.411683 O -0.069722 0.691506 1.257282 C -1.087620 1.174358 2.116563 C -0.317187 1.536411 3.383373 Cl -2.718975 0.310859 -1.382599 Cl -2.209887 -2.811368 -0.802701 C -1.806019 2.402109 1.586485 H -2.375514 2.163384 0.692464 H -2.505356 2.765468 2.337198

C -2.057075 -0.687473 -0.383161 H 0.254109 -2.983332 -0.267681 H -1.646292 -4.447138 -0.883057 H -3.895697 -3.398468 -1.195748 H -4.118927 -0.952083 -0.822376 C -2.194913 0.760008 -0.130828 C -2.619029 1.609032 -1.147731 C -2.762638 2.962101 -0.908643 C -2.494867 3.482585 0.346269 C -2.091160 2.642912 1.372302 C -1.941013 1.300404 1.114375 H -3.071846 3.614855 -1.709765 H -2.605977 4.541179 0.527122 H -1.901733 3.035026 2.360429 H -2.793772 1.210278 -2.135234 H -1.752584 0.482805 2.221064	H -1.487273 -3.020842 -0.267703 H -1.220801 -1.200876 3.608548 H -1.358965 -2.959042 3.489905 H 0.122279 -2.146242 2.968633 H -3.481963 -2.666162 2.148577 H -3.315472 -0.912451 2.257163 H -3.485158 -1.683529 0.685679 H 2.733335 1.087589 0.954291 H 2.873534 3.322163 2.031625 H 0.848307 4.780081 1.996155 H -1.201343 3.957449 0.890993 H -4.227630 2.277595 -2.159191 H -4.153391 -0.154425 -2.577790 H -2.372939 -1.529119 -1.594656 H -2.461706 3.344005 -0.831511 H 3.577245 -0.918986 -0.995583	H -1.101594 3.199855 1.365998 H -1.567688 -0.824108 2.758320 H -2.789094 0.377811 3.183264 H -2.659425 -0.182191 1.521357 H -1.001025 1.897781 4.149717 H 0.207826 0.665717 3.767654 H 0.411457 2.314359 3.170770 H 0.654396 -3.234071 0.324117 H 2.893900 -4.001857 1.072253 H 4.762082 -2.345759 1.091992 H 4.312362 -0.024917 0.377463 H 2.987562 3.762811 -1.941055 H 0.561949 4.224512 -1.982095 H -1.036991 2.593316 -1.082193 H 3.802439 1.613209 -1.070901 H -2.786311 -1.662180 -1.159848
Stationary Points for Reaction in Absence of Catalyst		
TS-S1 E0 = -232.9767788 E0+ZPE = -232.856117 E298 = -232.849066 H298 = -232.848122 G298 = -232.886536 NImag = 1 (-511.8265) E_0(M06) = -232.878624 O -0.128563 -0.000024 1.430114 C -0.706542 -1.282346 -0.484954 C -0.301780 0.000024 0.209388 H -0.228554 -2.133475 -0.012058 H -1.784888 -1.393467 -0.367280 H -0.487751 -1.274278 -1.548700 C -0.706051 1.282591 -0.484895 C 1.749206 -0.000269 -0.320296 H -0.228024 2.133637 -0.011878 H -0.487047 1.274533 -1.548566 H -1.784400 1.393958 -0.367536 H 1.674803 0.000454 -1.396973 H 2.072735 0.914208 0.148949 H 2.072630 -0.915376 0.147671		
TS-S2$_{ortho}$ E0 = -519.1433815 E0+ZPE = -518.935584 E298 = -518.924492 H298 = -518.923548 G298 = -518.973779 NImag = 1 (-507.1554) E_0(M06) = -518.8882391 C 2.618889 -1.514661 0.257579 C 3.348371 -0.488129 -0.337780 C 2.704279 0.644299 -0.772416 C 1.322072 0.806559 -0.562181 C 0.564276 -0.295489 -0.100790 C 1.241757 -1.419963 0.352302 C 1.347670 2.114786 1.224754 H 4.415472 -0.588378 -0.464996 H 3.261923 1.442159 -1.238507 H 0.791873 1.601872 -1.058725 C -0.902532 -0.201889 -0.079666 H 0.696780 -2.243832 0.785650 H 3.121302 -2.398565 0.618155 H 1.812733 1.445947 1.931053 H 1.942814 2.947225 0.881920 H 0.284967 2.273753 1.308341 N -1.427997 1.006347 -0.277764 C -2.741528 1.141447 -0.274289 C -3.621821 0.094962 -0.075249 C -3.084906 -1.164822 0.119804	**TS-S2$_{meta}$** E0 = -519.1401561 E0+ZPE = -518.932424 E298 = -518.921311 H298 = -518.920367 G298 = -518.970860 NImag = 1 (-545.5660) E_0(M06) = -518.8835969 C 1.880585 1.038296 0.578609 C 1.097666 0.096083 -0.083349 N 1.630011 -1.003143 -0.609139 C 2.933535 -1.186910 -0.513856 C 3.791677 -0.298725 0.108504 C 3.241969 0.837260 0.670815 C -0.365899 0.257096 -0.216696 C -0.973338 1.512992 -0.130970 C -2.343399 1.644957 -0.319573 C -3.129727 0.539458 -0.545966 C -2.555605 -0.748788 -0.513030 C -1.152839 -0.853737 -0.457128 C -3.123366 -1.440302 1.474351 H -2.787534 2.628771 -0.312492 H -4.190915 0.649326 -0.708134 H -3.119202 -1.581328 -0.904516 H -0.674408 -1.814224 -0.556523 H -0.376548 2.398524 0.018418 H -2.638658 -0.688308 2.076390 H -4.201443 -1.395769 1.429632	**TS-S2$_{para}$** E0 = -519.1419625 E0+ZPE = -518.934253 E298 = -518.923087 H298 = -518.922143 G298 = -518.973028 NImag = 1 (-524.9928) E_0(M06) = -518.8857144 N 1.729373 -1.162833 0.082293 C 1.182814 0.042721 -0.067942 C 1.967343 1.196317 -0.063632 C 3.329075 1.086143 0.117570 C 3.886506 -0.167775 0.284555 C 3.034214 -1.256511 0.251962 C -0.276409 0.086136 -0.251006 C -1.008371 1.272902 -0.139373 C -2.370595 1.287806 -0.312776 C -3.076574 0.090380 -0.537757 C -2.326555 -1.081480 -0.760489 C -0.966795 -1.086229 -0.578634 C -3.914605 -0.301713 1.474052 H -0.507779 2.200680 0.088534 H -2.911519 2.217864 -0.228834 H -4.098363 0.137445 -0.879730 H -2.833981 -1.993250 -1.036402 H -0.398420 -1.993246 -0.702663 H -2.992145 -0.392622 2.024360 H -4.498035 0.589513 1.649202

C -1.716362 -1.319212 0.114089 H -3.114359 2.143379 -0.439498 H -4.686452 0.263068 -0.080954 H -3.726661 -2.020326 0.266109 H -1.285406 -2.298064 0.238856	H -2.688908 -2.428318 1.501856 H 3.317687 -2.094171 -0.960225 H 4.849947 -0.498462 0.154507 H 3.864130 1.555534 1.182758 H 1.428218 1.904345 1.032034	H -4.468603 -1.212609 1.305181 H 1.522770 2.165042 -0.216708 H 3.949067 1.969746 0.121058 H 4.945967 -0.302822 0.429789 H 3.425147 -2.258092 0.370985
TS-S3$_{ortho}$ E0 = -752.1749137 E0+ZPE = -751.842097 E298 = -751.824051 H298 = -751.823107 G298 = -751.889160 NImag = 1 (-2062.8679) E_0(M06) = -751.8203843 C -1.309650 3.115157 -0.282670 C -1.555220 2.059855 0.510292 C -0.487063 1.080575 0.856178 C 0.726304 1.135509 -0.036839 C 0.922522 2.268259 -0.799034 C -0.042764 3.259597 -0.921274 H -2.079896 3.851138 -0.459803 H -2.511674 1.935846 0.995325 H -1.073053 -0.064115 0.758095 H 1.849407 2.344854 -1.344752 H 0.145033 4.115112 -1.549948 C -0.142764 1.171560 2.332189 H 0.285200 2.152953 2.542531 H -1.035633 1.051822 2.941162 H 0.584351 0.419281 2.624069 O -1.668673 -1.127154 0.840514 C -1.422372 -1.372979 -1.549138 C -2.339829 -1.481573 -0.342154 H -1.116165 -0.340439 -1.707550 H -0.528943 -1.975678 -1.408027 H -1.932375 -1.714266 -2.447777 C -2.726449 -2.939274 -0.105033 C -3.589053 -0.636623 -0.534254 H -3.355808 -3.026176 0.776809 H -3.275181 -3.320105 -0.964051 H -1.838405 -3.548191 0.041240 H -4.170569 -0.992701 -1.382668 H -4.213347 -0.681515 0.355265 H -3.325753 0.401826 -0.721512 C 1.738121 0.090536 -0.016855 C 1.539381 -1.131023 0.636285 C 2.546090 -2.074175 0.620279 H 0.601701 -1.346606 1.119858 C 3.830699 -0.561773 -0.671414 C 3.725862 -1.793604 -0.041299 H 2.405370 -3.021671 1.118133 H 4.733832 -0.302253 -1.208012 H 4.539714 -2.499471 -0.077173 N 2.882669 0.348205 -0.665268	**TS-S3$_{ortho}$-Conf1** E0 = -752.1702097 E0+ZPE = -751.837962 E298 = -751.819710 H298 = -751.818766 G298 = -751.886107 NImag = 1 (-2125.7111) E_0(M06) = -751.8162343 C -1.601586 3.020827 -0.314493 C -1.749282 1.928388 0.453802 C -0.586454 1.082978 0.841844 C 0.624325 1.258749 -0.037090 C 0.721866 2.425375 -0.767522 C -0.335274 3.320340 -0.892298 H -2.444168 3.664522 -0.518271 H -2.703406 1.676140 0.891328 H -1.031535 -0.132207 0.773969 H 1.640679 2.654013 -1.285705 H -0.209534 4.216315 -1.478712 C -0.296706 1.243527 2.324308 H 0.055166 2.257826 2.521645 H -1.204017 1.080631 2.901466 H 0.460556 0.534961 2.639164 O -1.668101 -1.161869 0.877111 C -0.922037 -1.813570 -1.324003 C -2.082027 -1.699833 -0.348562 H -0.558406 -0.826269 -1.602683 H -0.101297 -2.365303 -0.874069 H -1.233744 -2.325650 -2.232599 C -2.581615 -3.091804 0.032195 C -3.217122 -0.887736 -0.953352 H -3.390332 -3.019154 0.754672 H -2.948244 -3.609186 -0.852270 H -1.776212 -3.673243 0.472361 H -3.602952 -1.367076 -1.851462 H -4.030795 -0.789308 -0.238154 H -2.874789 0.109037 -1.223509 C 1.689832 0.269489 -0.024459 C 2.732286 0.279009 -0.961868 C 3.709786 -0.685946 -0.892470 H 2.760566 1.015540 -1.746854 C 2.563334 -1.598207 0.967436 C 3.636233 -1.653308 0.096382 H 4.516345 -0.692551 -1.609806 H 2.456715 -2.338505 1.749113 H 4.378503 -2.429783 0.185356 N 1.621767 -0.676497 0.915575	**TS-S3$_{ortho}$-Conf2** E0 = -752.1687765 E0+ZPE = -751.836517 E298 = -751.818262 H298 = -751.817318 G298 = -751.884277 NImag = 1 (-2131.6667) E_0(M06) = -751.8143167 C -0.274502 3.532494 -0.368684 C -0.973207 2.464064 0.050710 C -0.289986 1.225797 0.522887 C 1.120597 1.083582 0.015354 C 1.787550 2.228418 -0.363046 C 1.139299 3.451014 -0.513461 H -0.782414 4.448858 -0.629647 H -2.048625 2.501006 0.133925 H -0.941099 0.282982 -0.075438 H 2.844754 2.181311 -0.577251 H 1.701133 4.321276 -0.812459 C -0.404812 1.092790 2.030361 H 0.176924 1.885655 2.504318 H -1.437533 1.206250 2.353448 H -0.019458 0.134776 2.360250 O -1.540935 -0.394969 -0.896868 C -3.661420 -0.098931 0.212111 C -2.628844 -1.074206 -0.334191 H -3.261279 0.451960 1.060805 H -3.950205 0.612200 -0.558270 H -4.552263 -0.625242 0.549658 C -3.216408 -1.837496 -1.518150 C -2.176317 -2.048461 0.741661 H -2.472944 -2.509522 -1.938148 H -4.074289 -2.423125 -1.192694 H -3.536005 -1.146898 -2.294036 H -3.023541 -2.603423 1.141309 H -1.459207 -2.752880 0.329061 H -1.691716 -1.521178 1.559136 C 1.769923 -0.217809 0.008489 C 2.922793 -0.460894 -0.748703 C 3.506655 -1.705655 -0.707663 H 3.331454 0.307224 -1.383309 C 1.780646 -2.373114 0.768939 C 2.931952 -2.694116 0.073221 H 4.392160 -1.909438 -1.290288 H 1.290181 -3.118577 1.380980 H 3.351819 -3.685066 0.132692 N 1.212302 -1.183322 0.743127
TS-S3$_{meta}$ E0 = -752.1701115 E0+ZPE = -751.838203 E298 = -751.819768 H298 = -751.818823 G298 = -751.887603 NImag = 1 (-2031.8981) E_0(M06) = -751.8113386 C -0.182268 2.484968 -1.128414 C -1.253267 2.166829 -0.366915 C -1.112878 1.218148 0.773921 C 0.132357 0.404254 0.733080 C 1.188880 0.756094 -0.041027 C 1.059541 1.831044 -0.967131 H -0.278585 3.232735 -1.902159	**TS-S3$_{meta}$-Conf1** E0 = -752.1694453 E0+ZPE = -751.837470 E298 = -751.819061 H298 = -751.818116 G298 = -751.886968 NImag = 1 (-2036.2270) E_0(M06) = -751.8107328 C -0.207783 2.575677 -1.049032 C -1.271858 2.204007 -0.303128 C -1.109159 1.211406 0.796356 C 0.142609 0.413481 0.712532 C 1.186971 0.803351 -0.059311 C 1.043344 1.929972 -0.920528 H -0.313748 3.362134 -1.782096	**TS-S3$_{para}$** E0 = -752.1785406 E0+ZPE = -751.845846 E298 = -751.827503 H298 = -751.826558 G298 = -751.895105 NImag = 1 (-2046.9128) E_0(M06) = -751.8211325 C -0.653962 0.791759 1.212111 C 0.612321 1.235292 1.178641 C 1.330570 1.486840 -0.095914 C 0.596890 1.007168 -1.293408 C -0.666945 0.563914 -1.229011 C -1.372070 0.456010 0.017218 H -1.124919 0.659801 2.173217

H -2.209543 2.644357 -0.517967 H -2.100728 0.391075 0.729199 H 1.899920 2.077176 -1.592429 C -1.335064 1.879963 2.119890 H -0.553264 2.618136 2.305964 H -2.297203 2.386202 2.145768 H -1.312033 1.144727 2.920986 O -3.048310 -0.355712 0.854870 C -2.068135 -2.045756 -0.557421 C -3.264132 -1.148599 -0.281911 H -1.192367 -1.451459 -0.811229 H -1.835611 -2.642876 0.321440 H -2.271428 -2.718424 -1.388488 C -4.476498 -1.993265 0.101525 C -3.588714 -0.288871 -1.492947 H -5.328788 -1.355147 0.319155 H -4.737156 -2.659188 -0.718639 H -4.257612 -2.591246 0.982120 H -3.848583 -0.907527 -2.349838 H -4.427479 0.367623 -1.272953 H -2.732743 0.324579 -1.767386 C 2.463382 0.006901 0.003155 C 2.857021 -0.697969 1.137550 C 4.044523 -1.397776 1.113643 H 2.251088 -0.678335 2.028109 C 4.358277 -0.617245 -1.099131 C 4.817600 -1.366238 -0.032062 H 4.368453 -1.950874 1.982048 H 4.937448 -0.552178 -2.010135 H 5.754787 -1.894971 -0.096574 N 3.219474 0.052377 -1.088438 H 0.177846 -0.460215 1.378285	H -2.237668 2.667854 -0.434218 H -2.107346 0.396634 0.720422 H 1.878794 2.282164 -1.501830 C -1.318865 1.819646 2.169398 H -0.545949 2.563371 2.369535 H -2.288909 2.307735 2.229132 H -1.266819 1.056023 2.941550 O -3.112582 -0.275816 0.771513 C -2.085037 -2.170916 -0.306662 C -3.222453 -1.162111 -0.309524 H -1.131985 -1.676115 -0.483290 H -2.035190 -2.678202 0.653957 H -2.225962 -2.917816 -1.085823 C -4.550732 -1.869466 -0.053221 C -3.277285 -0.408234 -1.628580 H -5.364222 -1.149343 -0.029551 H -4.743962 -2.591597 -0.844013 H -4.522954 -2.392094 0.899130 H -3.440534 -1.091429 -2.459984 H -4.086592 0.318174 -1.613471 H -2.343583 0.122765 -1.804750 C 2.446909 0.027971 -0.029073 C 3.351985 0.065006 -1.085724 C 4.509866 -0.681984 -1.007144 H 3.144548 0.650953 -1.965383 C 3.772216 -1.436044 1.110480 C 4.735445 -1.451194 0.117088 H 5.222365 -0.667541 -1.817802 H 3.903681 -2.028119 2.006044 H 5.625657 -2.049340 0.225214 N 2.664889 -0.721649 1.047650 H 0.249767 -0.451539 1.348027	H 1.136100 1.454774 2.097465 H 2.429532 0.829863 -0.026096 C 1.854999 2.900017 -0.226959 H 1.023676 3.604862 -0.279969 H 2.474481 3.163898 0.626829 H 2.452073 3.007441 -1.129185 O 3.566512 0.376470 0.065356 C 3.064575 -1.580675 -1.247696 C 3.595578 -1.024572 0.063920 H 2.008958 -1.344654 -1.364901 H 3.608878 -1.150621 -2.085324 H 3.173967 -2.662957 -1.283000 C 5.081740 -1.346154 0.206169 C 2.823717 -1.586168 1.247220 H 5.472443 -0.931489 1.131477 H 5.225042 -2.424818 0.216674 H 5.640950 -0.926546 -0.625710 H 2.914071 -2.669900 1.289933 H 3.205490 -1.169844 2.176613 H 1.767298 -1.337706 1.168204 C -2.732652 -0.011651 0.033911 C -3.488926 -0.103044 1.214740 C -4.782783 -0.566781 1.156615 H -3.070996 0.191536 2.161741 C -4.503517 -0.803820 -1.185650 C -5.315716 -0.932331 -0.067693 H -5.372524 -0.640282 2.057607 H -4.881562 -1.073093 -2.163089 H -6.324527 -1.299850 -0.160854 N -3.266253 -0.362792 -1.149146 H 1.102706 1.070724 -2.245908 H -1.192377 0.261837 -2.119839
TS-S5$_{ortho}$ E0 = -519.1254511 E0+ZPE = -518.922512 E298 = -518.910866 H298 = -518.909922 G298 = -518.962095 NImag = 1 (-1642.1025) E_0(M06) = -518.8673162 C -0.491784 3.200327 0.443356 H -0.105162 3.535380 -0.509797 H -1.365567 3.749058 0.774477 H 0.273943 3.120126 1.204186 N 1.381280 0.734963 -0.590673 C 2.700092 0.807789 -0.608420 C 3.532294 -0.165687 -0.086674 C 2.944005 -1.270842 0.498285 C 1.567804 -1.356847 0.526506 C 0.813866 -0.333144 -0.041165 H 3.118835 1.692874 -1.068067 H 4.603434 -0.053340 -0.133030 H 3.548130 -2.051168 0.935509 H 1.079185 -2.192190 1.000888 C -0.661456 -0.391492 -0.049678 C -1.330377 -1.608382 -0.170094 C -2.712319 -1.663106 -0.181243 C -3.458032 -0.502928 -0.068304 C -2.810301 0.717965 0.052309 C -1.437105 0.750053 0.052098 H -3.207773 -2.615726 -0.287699 H -4.536717 -0.547020 -0.076089 H -3.378602 1.631717 0.146817 H -0.762995 -2.520132 -0.285138 H -0.875782 2.003441 0.230806	**TS-S5**$_{meta}$ E0 = -519.1278641 E0+ZPE = -518.925067 E298 = -518.913299 H298 = -518.912355 G298 = -518.965712 NImag = 1 (-1666.0508) E_0(M06) = -518.8680008 C 4.329945 -2.106153 0.255812 H 3.779474 -3.032813 0.150810 H 5.030893 -1.938167 -0.552340 H 4.772840 -1.985411 1.236534 N -1.517940 -1.185843 -0.346021 C -2.781747 -1.566963 -0.331067 C -3.831103 -0.734331 0.012286 C -3.529173 0.564935 0.372763 C -2.211711 0.972572 0.364718 C -1.223995 0.067745 -0.015533 H -2.969689 -2.594881 -0.609990 H -4.845701 -1.098276 0.003974 H -4.308944 1.251081 0.666336 H -1.950224 1.972152 0.669626 C 0.204133 0.445098 -0.049611 C 0.609610 1.768623 -0.188721 C 1.951386 2.104410 -0.209154 C 2.919717 1.119047 -0.089950 C 2.502669 -0.186008 0.038533 C 1.178980 -0.546156 0.055906 H 2.242712 3.137342 -0.327240 H 3.969080 1.373419 -0.104103 H -0.125507 2.549007 -0.308273 H 3.449671 -1.174434 0.152551 H 0.868716 -1.575026 0.148365	**TS-S5**$_{para}$ E0 = -519.1275763 E0+ZPE = -518.924847 E298 = -518.913001 H298 = -518.912057 G298 = -518.967048 NImag = 1 (-1660.8429) E_0(M06) = -518.8676853 C -5.518024 -0.037650 -0.016103 H -5.793191 -0.832226 -0.698533 H -5.816827 -0.233495 1.006052 H -5.820137 0.941340 -0.367018 N 1.967490 -1.140004 0.248644 C 3.286574 -1.193139 0.255525 C 4.100749 -0.100668 0.019749 C 3.490225 1.108641 -0.252573 C 2.112790 1.174605 -0.267067 C 1.375282 0.024653 0.002941 H 3.720258 -2.162059 0.462639 H 5.173779 -0.200986 0.041594 H 4.078997 1.988832 -0.461521 H 1.615555 2.099866 -0.506360 C -0.102184 0.031950 0.008897 C -0.824569 1.196320 0.249378 C -2.210259 1.183964 0.245193 C -2.858423 -0.002982 -0.002118 C -2.176109 -1.174821 -0.236418 C -0.792269 -1.153833 -0.224290 H -2.762172 2.090861 0.442719 H -0.309134 2.119165 0.468003 H -4.233821 -0.020562 -0.007433 H -0.224968 -2.054901 -0.393712 H -2.703457 -2.098041 -0.425622

TS-S4 E0 = -712.2919669 E0+ZPE = -711.997181 E298 = -711.981038 H298 = -711.980093 G298 = -712.042624 NImag = 1 (-2111.8247) E_0(M06) = -711.9653514 N -1.341772 -0.987210 -1.040359 C -1.972411 -2.146906 -1.067337 C -2.954477 -2.508782 -0.162488 C -3.284418 -1.606287 0.830509 C -2.630737 -0.391767 0.870655 C -1.665277 -0.116658 -0.092675 H -1.680110 -2.825335 -1.857211 H -3.437985 -3.469652 -0.234722 H -4.034179 -1.847305 1.568561 H -2.845274 0.325528 1.646366 C -0.947876 1.172759 -0.103435 C -1.604976 2.361460 0.210194 C -0.944927 3.575504 0.167841 C 0.390612 3.633057 -0.188672 C 1.069258 2.463172 -0.497861 C 0.387984 1.272382 -0.447616 H -1.480830 4.482216 0.402094 H 0.904266 4.581516 -0.228039 H 2.111946 2.482234 -0.773513 H -2.655883 2.333396 0.457395 H 1.127705 0.207572 -0.749365 O 1.989226 -0.527006 -0.969847 C 2.544794 -1.064006 0.203860 C 1.481015 -1.735460 1.056595 H 1.931651 -2.232965 1.913506 H 0.768763 -1.002078 1.429606 H 0.936741 -2.471070 0.470715 C 3.284626 0.000160 0.999451 H 3.796333 -0.441153 1.852806 H 4.023955 0.492639 0.371786 H 2.593727 0.752472 1.373654 C 3.529906 -2.102847 -0.321165 H 4.034164 -2.590365 0.510740 H 3.008441 -2.855434 -0.906212 H 4.276590 -1.630380 -0.954017		