Supporting Information

for

Deciphering the Origin of Stereoinduction in Cooperative Asymmetric Catalysis Involving Pd(II) and Chiral Brønsted Acid

Garima Jindal and Raghavan B. Sunoj*

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076

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

Fax: 91−22−2572−3480 or 91−22−2576−7152

Table of Contents

Page No.		
S3-S4	**Computational Details**	
	List of Tables	
S8	**Table S1**	ρ(r) Values (a.u.) at the Bond Critical Points (bcp) for the C–H···π Interactions for the Stereodetermining Transition States
	List of Figures	
S5	**Figure S1**	Optimized geometries of the diastereomeric TSs for modes **I-III**
S6	**Figure S2**	Space filling model of the lower energy transition state **TS-*re***
S7	**Figure S3**	Optimized geometries of the diastereomeric TSs for model **IV**
S8	**Figure S4**	Topological analysis using Atoms-In-Molecule formalism for the stereocontrolling transition states depicting electron densities at the bond critical points along the bond paths
S10	**Figure S5**	Optimized geometries of stereodetermining TSs on replacing the 3,3' substituents at binol with (a) hydrogens and (b) phenyl groups
S11	**Figure S6**	Overlap between the optimized geometries of the original catalyst (blue) and the modified catalysts (red)
S12	**Figure S7**	Relative electronic energies (kcal/mol) of the TSs of the original and the modified catalysts
S12-S59	**Coordinates of the Optimized Geometries of Transition States at the M06 Level of Theory**	
S59-S70	**Coordinates of the Optimized Geometries of Transition States at the B3LYP Level of Theory**	

I. Computational Details

All computations were carried out using the Gaussian09 suite of quantum chemical program.[1] The geometries were optimized using the M06 density functional theory using Pople's 6-31G** basis set for all atoms except Pd.[2] The LANL2DZ basis set, consisting of an effective core potential (ECP) for 28 core electrons and a double-zeta quality valence basis set for 18 valence electrons, was used for palladium.[3] All the stationary points were characterized, as minima (reactants, intermediates, and products) or a first-order saddle point (transition state) by evaluating the corresponding Hessian indices. The M06 functional has been widely used in the recent literature to account for noncovalent interactions in transition metal systems.[4] The effect of a solvent continuum, toluene in the present reaction, was evaluated using the Cramer-Truhlar continuum solvation model that employs quantum mechanical charge density of solutes, designated as SMD using the 6-311G** triple zeta basis set.[5] The zero-point vibrational energy (ZPVE), thermal, and entropic corrections obtained at 298.15 K and 1 atm pressure derived from the gas phase computations at the M06/6-31G**,LANL2DZ(Pd) level of theory have been applied to the "bottom-of-the-well" energies obtained from the single-point energy evaluations in the solvent phase at the M06 functional to estimate the Gibbs free energies of solutes in the condensed phase.

Topological analysis of the electron densities within Bader's Atoms-in-Molecule (AIM) framework was carried out by using AIM2000 software. AIM analyses were performed on the geometries and the associated wave functions obtained at the M06/6-31G**,LANL2DZ(Pd) level of theory.[6]

(1) Gaussian 09, Revision A.02: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.;Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.;

Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford, CT, 2009.

(2) (a) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257. (b) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta*, **1973**, *28*, 213. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (d) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

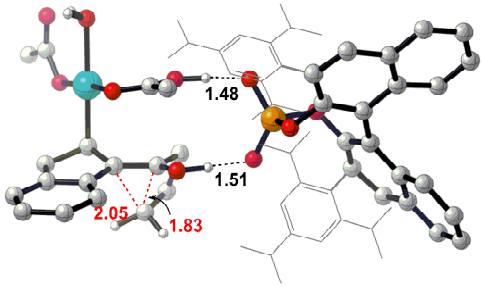
(3) Hay, P. J.; Wadt W. R. *J. Chem. Phys*. **1985**, *82*, 299.

(4) (a) Liu, P.; Xu, X.; Dong, X.; Keitz, B. K.; Herbert, M. B.; Grubbs, R. H.; Houk, K. N. *J. Am. Chem. Soc.* **2012**, *134*, 1464. (b) Komagawa, S.; Wang, C.; Morokuma, K.; Saito, S.; Uchiyama, M. *J. Am. Chem. Soc.* **2013**, *135*, 14508. (c) Wang, Z. J.; Benitez, D.; Tkatchouk, E.; Goddard III, W. A.; Toste, F. D. *J. Am. Chem. Soc.* **2010**, *132*, 13064. (d) Biswas, S.; Huang, Z.; Choliy, Y.; Wang, D. Y.; Brookhart, M.; Krogh-Jespersen, K.; Goldman, A. S. *J. Am. Chem. Soc.* **2012**, *134*, 13276.

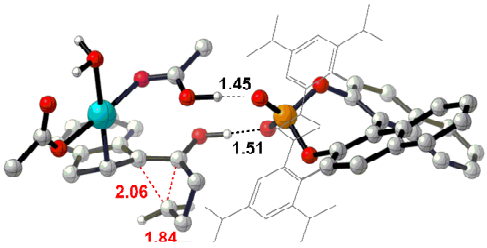
(5) (a) Marenich, A. V. ; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378. (b) Hay, P. J. *J. Chem. Phys.* **1977**, *66*, 4377.

(6) (a) Bader, R. F. W.; *Atoms in Molecules: A Quantum Theory*; Clarendon Press: Oxford, **1990**. (b) *AIM2000 Version 2.0*; Buro fur Innovative Software, SBK-Software: Bielefeld, Germany, **2002**. (c) Biegler-Konig, F.; Schonbohm, J.; Bayles, D. *J. Comput. Chem*. **2001**, *22*, 545. (d) Biegler-Konig, F.; Schonbohm, J. *J. Comput. Chem.* **2002**, *23*, 1489.

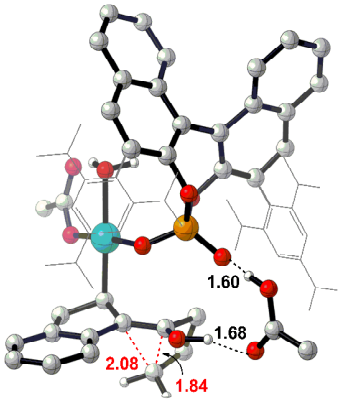
II. Different Ligand Combinations on Palladium in the Enantiocontrolling Transition States



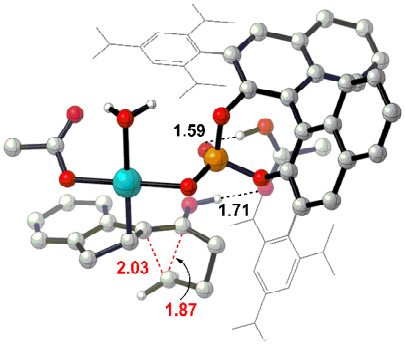
(TS-*si*)$_{I}$ (0.0)



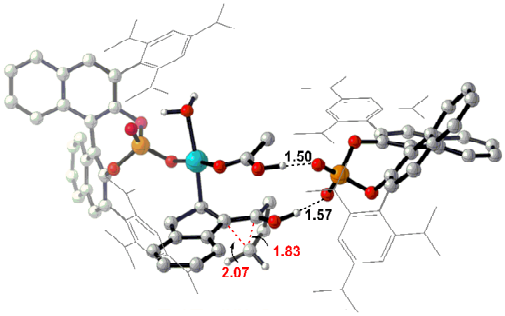
(TS-*re*)$_{I}$ (0.4)



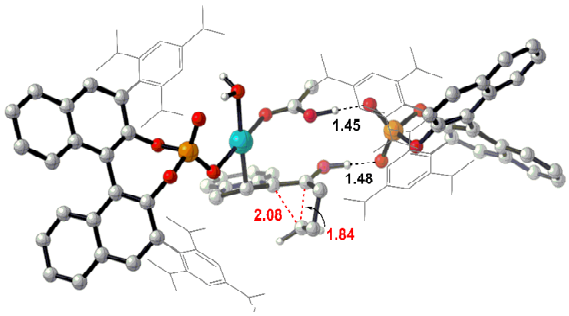
(TS-*si*)$_{II}$ (0.0)



(TS-*re*)$_{II}$ (0.5)

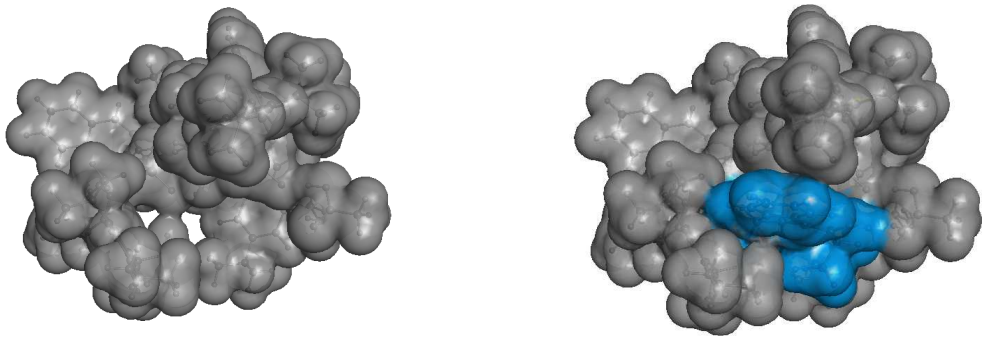


(TS-*si*)$_{III}$ (0.0)



(TS-*re*)$_{III}$ (-7.1)

Figure S1. Optimized geometries of the diastereomeric TSs for modes **I-III** as described in the main text at the M06/6-31G**,LANL2DZ(Pd) level of theory. Relative free energies (kcal/mol) are provided in parentheses. All distances are in Å.



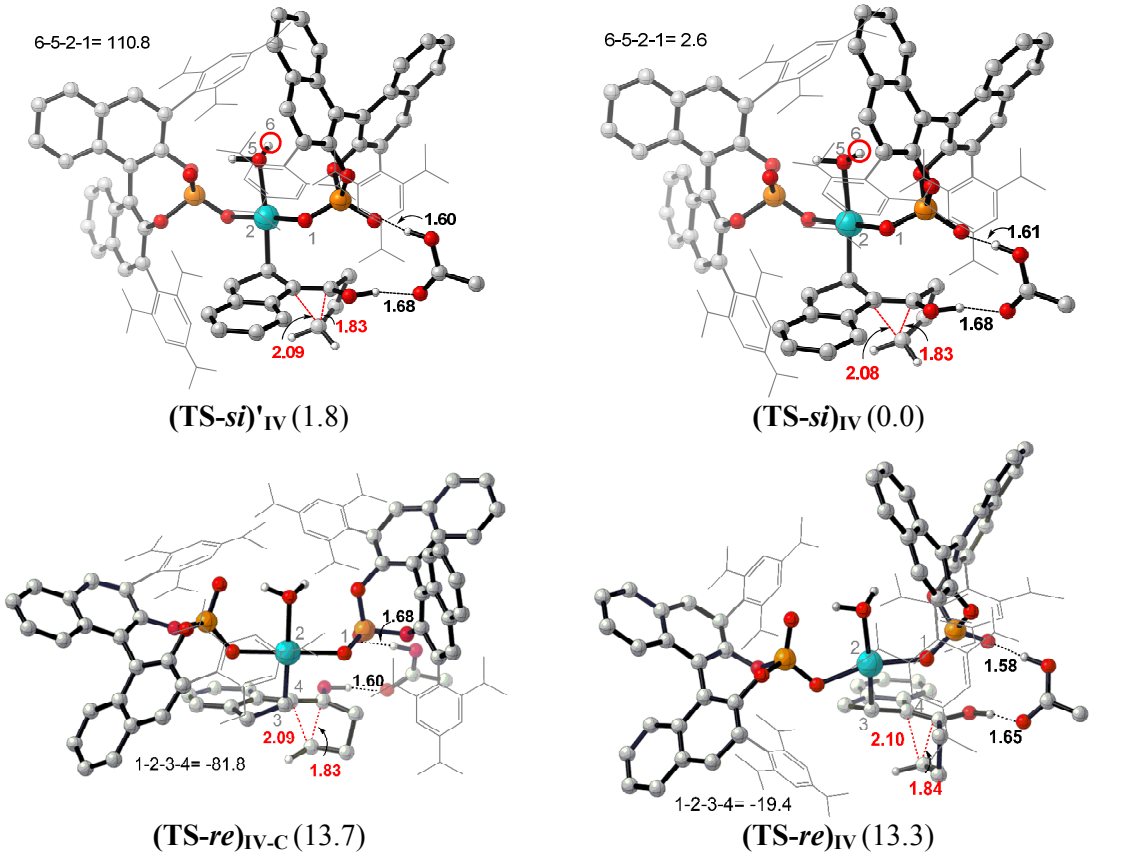
(a) **(b)**

Figure S2. Space filling model of the lower energy **TS-*re*** (a) without the substrate and (b) with substrate. In Figure S2(a), The orthogonal relative orientation of the two chiral phosphates, as shown in Figure S2(a), offers a chiral cavity in which the substrate (indenyl cyclobutanol) can find a good fit (Figure S2(b)).

III. Conformational Sampling of the Enantiocontrolling Transition State

The rich isopropyl decorations on the 3,3' aryl substituents renders large size to the ligand system, making it is difficult to carry out a thorough conformational search. Moreover, since the reaction being examined here is an intramolecular rearrangement, and that all the ligands are bound to Pd, the number of important conformers is severely restricted. However, a small ligand such as water could take different orientations, within the constrained environment near the site of the reactions. We attempted to optimize a few other conformers of the transition state geometry reported in the main text of the manuscript by changing the orientation of the water ligand coordinated to Pd resulting in **(TS-*si*)'$_{IV}$**. For the higher energy diastereomeric TS, **(TS-*re*)$_{IV}$**, the conformation was changed by varying the dihedral resulting in **(TS-*re*)$_{IV\text{-}C}$** as shown in Figure S3.

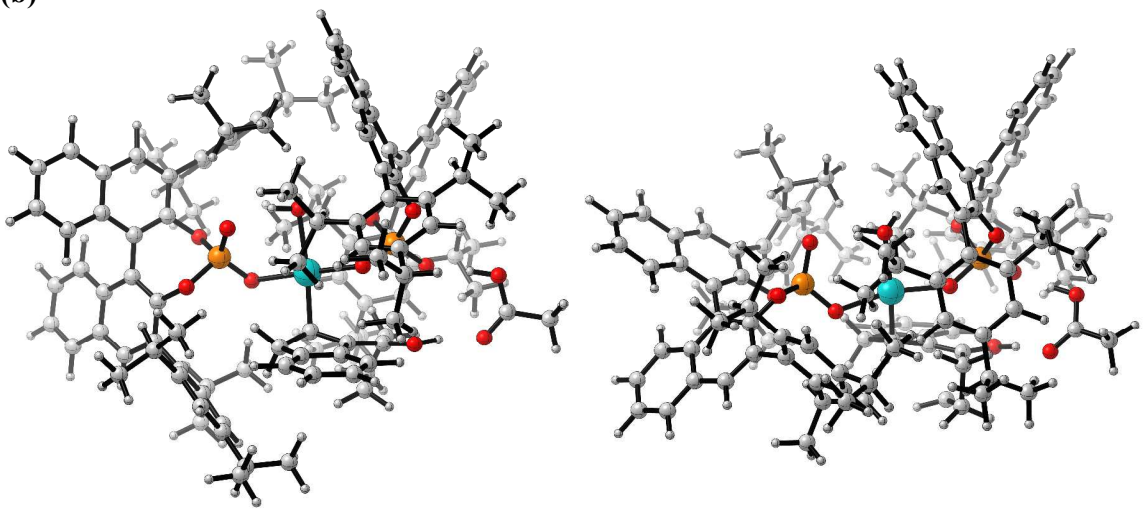
(a)



(TS-*si*)'$_{IV}$ (1.8) **(TS-*si*)$_{IV}$** (0.0)

(TS-*re*)$_{IV-C}$ (13.7) **(TS-*re*)$_{IV}$** (13.3)

(b)



(TS-*si*)$_{IV}$ **(TS-*re*)$_{IV}$**

Figure S3. (a) Optimized geometries of the diastereomeric TSs obtained at the M06/6-31G**,LANL2DZ(Pd) level of theory for mode **IV**. Relative free energies (kcal/mol) are provided in parentheses. All distances are in Å. Select hydrogens have been removed for clarity. (b) Optimized geometries of **(TS-*si*)$_{IV}$** and **(TS-*re*)$_{IV}$** without any modifications in

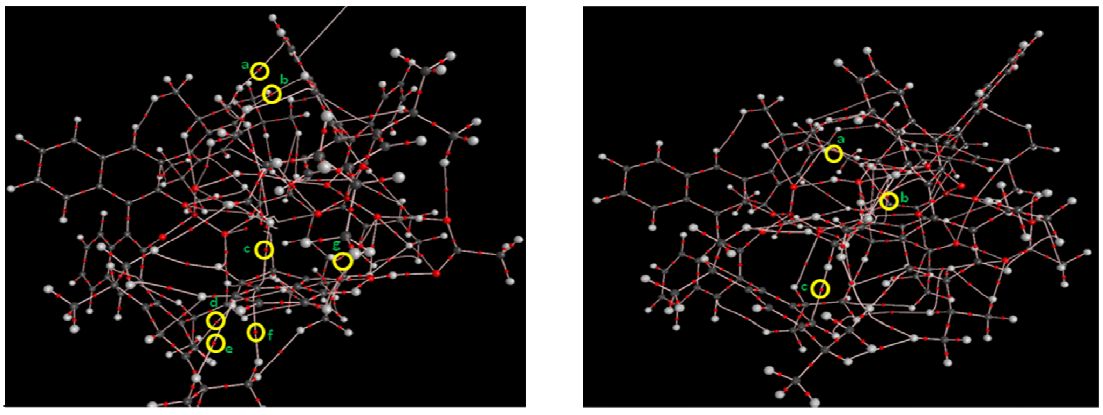
representation of the 3,3' substituents and inclusive of all hydrogens. **(TS-*si*)$_{IV}$** and **(TS-*re*)$_{IV}$** correspond to TSs **(TS-*si*)** and **(TS-*re*)** respectively as given in the main text.

IV. Topological Analysis of the Electron Density using the AIM Formalism

The stabilizing interactions shown in Figure 2 of the main text are further analyzed using the Atoms-in-Molecule (AIM) formalism. The electron density at the bond critical points along the bond paths ρ(r) values for different interactions are summarized in Table S1 and the corresponding images depicting the ρ(r) values are provided in Figure S4.

Table S1. ρ(r) Values (a.u.) at the Bond Critical Points (bcp) for the C–H···π Interactions for the Stereodetermining Transition States as shown in Figure 2 of the Main Text

TS-*si*		**TS-*re***	
Interaction	**ρ(r) × 10^{-2}**	**Interaction**	**ρ(r) × 10^{-2}**
a	0.004	**a**	0.006
b	0.008	**b**	0.010
c	0.009	**c**	0.004
d	0.014		
e	0.007		
f	0.007		
g	0.007		



TS-*si* **TS-*re***

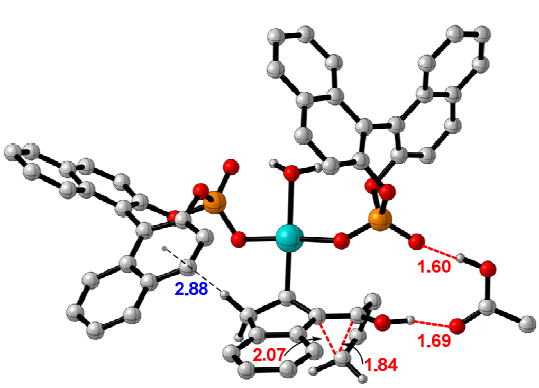
Figure S4. Important bond paths and the corresponding bond critical points (encircled in yellow) obtained using the topological analysis of the electron density using the Atoms-In-Molecule formalism for the stereocontrolling transition states.

V. Analysis of the enantiocontrolling transition states by using modified phosphate ligands

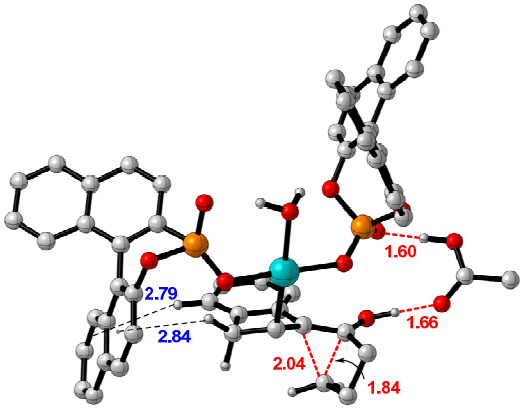
To probe the importance of the 3,3' substituents on the binaphthol framework, the 3,3' groups on the original catalyst (TRIP) are first replaced with hydrogen atoms This is done for both the stereodetermining TSs to evaluate the energy difference between the ring expansion involving the *si* and the *re* face of palladated indenyl framework. Single point energies are first calculated using the frozen geometries. The resulting geometries of these diastereomeric TSs with with the modified phosphates are then allowed to relax by way of geometry optimization at the M06/6-31G**,LANL2DZ(Pd) level of theory. The optimized geometries for the ring expansion to the *si* and the *re* face **(TS-*si*)$_{H}$** and **(TS-*re*)$_{H}$** are given in Figure S5.

In the case of **(TS-*si*)$_{H}$** and **(TS-*re*)$_{H}$** wherein the triisopropylphenyl groups were replaced by simple hydrogen atoms, only a few noncovalent and negligible steric interactions are noticeable (Figure S5). This situation results in a difference of only 0.9 kcal/mol between **(TS-*si*)$_{H}$** and **(TS-*re*)$_{H}$** at the SMD$_{(Toluene)}$/M06/6-311G**,LANL2DZ(Pd)//M06/6-31G**,LANL2DZ(Pd) level of theory. Such diminishing energy differential can come about either by destabilization of the lower energy transition state and stabilization of the higher energy transition state (or vice versa) with the modified phosphates bound to the palladium. The relative energies obtained through the equations shown in Scheme 3 of the main text are provided in Figure S6. It can be seen that both diastereomeric TSs, **(TS-*si*)$_{H}$** and **(TS-*re*)$_{H}$** are destabilized with respect to the TSs with the original catalyst (i.e., **TS-*si*** and **TS-*re***). However, destabilization in the lower energy **(TS-*si*)$_{H}$** is found to be 6.3 kcal/mol more as compared to that in the higher energy TS.

(a)

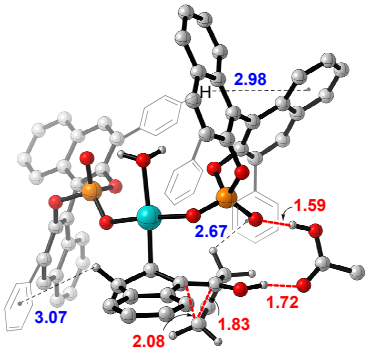


(TS-*si*)$_{H}$ (0.0, *0.0*)

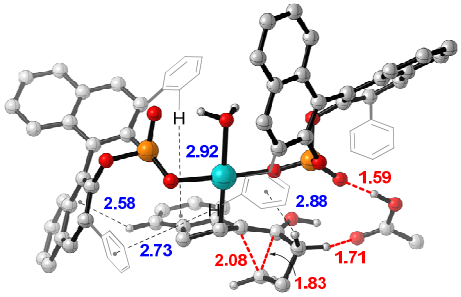


(TS-*re*)$_{H}$ (0.2, *0.9*)

(b)



(TS-*si*)$_{Ph}$ (0.0, *0.0*)



(TS-*re*)$_{Ph}$ (-2.0, *-1.5*)

Figure S5. Optimized geometries of stereodetermining TSs at the M06/6-31G**,LANL2DZ(Pd) level of theory with the modified phosphates obtained by replacing the 3,3' binol substituents with (a) hydrogen atoms, or (b) phenyl groups. Relative electronic energies (kcal/mol) are provided in parentheses. Values in italics correspond to the electronic energies (kcal/mol) at the SMD$_{(Toluene)}$/M06/6-311G**,LANL2DZ(Pd)//M06/6-31G**,LANL2DZ(Pd) level of theory. All distances are in Å.

A similar analysis has been carried out by substituting the 3,3' positions with phenyl groups. The optimized geometries of stereodetermining TSs, namely, **(TS-*si*)$_{Ph}$** and **(TS-*re*)$_{Ph}$**, are provided in Figure S5. The energy difference between the stereodetermining TSs is -1.5 kcal/mol. It can be seen from the optimized geometries, as given in Figure S5, that the number and efficiency of the C–H···π interactions in **(TS-*re*)$_{Ph}$** is better. From Figure S6, it

can be seen that **(TS-*re*)$_{Ph}$** is stabilized by 7.1 kcal/mol as compared to **TS-*re***. On the other hand, **(TS-*si*)$_{Ph}$** is destabilized by 1.6 kcal/mol as compared to **TS-*si***.

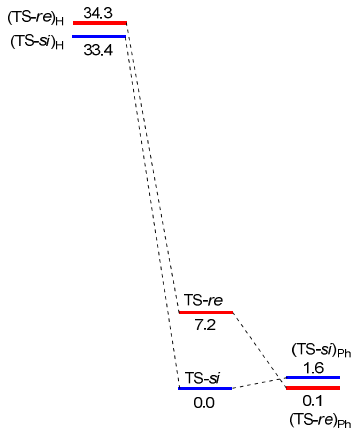


Figure S6. Relative electronic energies (kcal/mol) of the enantiocontrolling TSs for the original and the modified catalysts (optimized geometries) obtained at the SMD$_{(Toluene)}$/M06/6-311G**,LANL2DZ//M06/6-31G**,LANL2DZ(Pd) level of theory.

Such a dramatic lowering in the energy difference between the TSs for the ring expansion to the *si* and *re* faces, in the case of the modified phosphates is interesting. Upon pruning, first all the isopropyl groups and then the triisopropylphenyl altogether, the interactions and hence the geometries are expected to be different. In fact, the geometric deviation between these TSs is captured in Figure S7 wherein overlaid images between unmodified and modified catalysts are given. It can be readily seen that in the cast of **(TS-*re*)$_{Ph}$** both the chiral phosphates show maximum deviation as compared to the corresponding deviation in **(TS-*si*)$_{Ph}$**. In the case of TSs wherein the 3,3' substituents are substituted with hydrogen atoms, **(TS-*si*)$_{H}$** exhibits more deviation than in **(TS-*re*)$_{H}$**.

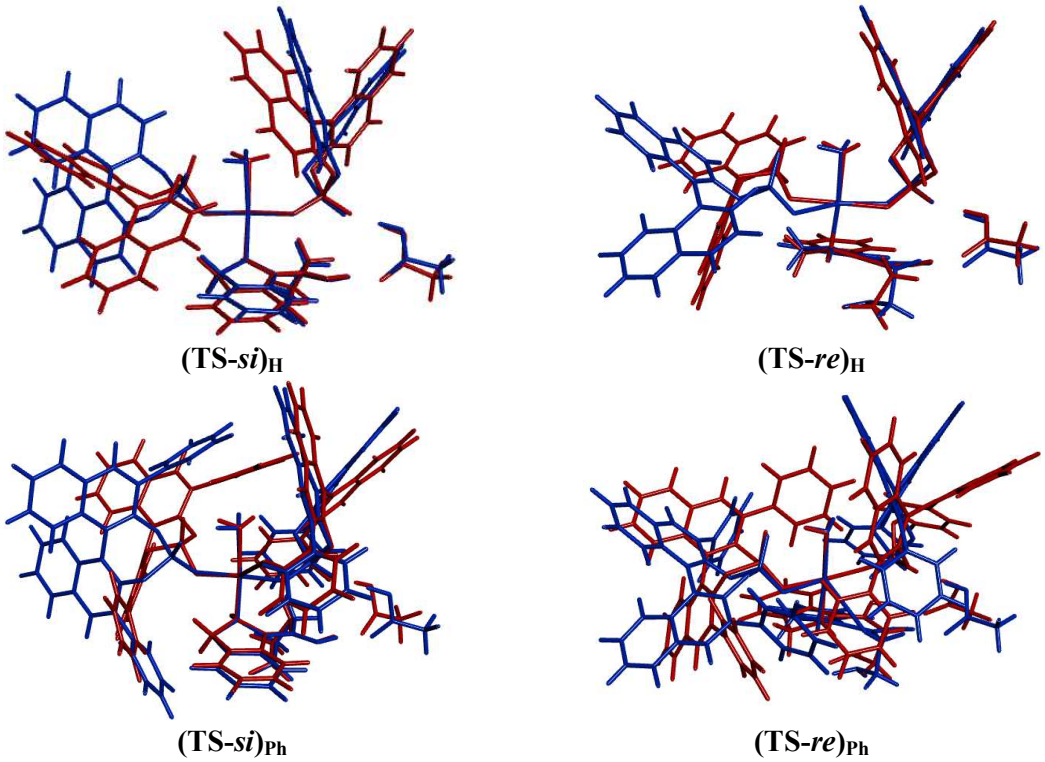


Figure S7. Overlap between the optimized geometries of the original catalyst (blue) and the modified catalysts (red) at the M06/6-31G**,LANL2DZ(Pd) level of theory. In the original catalyst, the isopropyl groups are deleted for clarity.

VI. Coordinates of the Optimized Geometries of Transition States at the M06/6-31G,LANL2DZ(Pd) Level of Theory**

(TS-*si*)I
E0 = -3818.9906197
E0+ZPE = -3817.668256
E298 = -3817.590615
H298 = -3817.589670
G298 = -3817.777045
NImag = -408.6980
C -2.872982 -3.954155 0.882182
C -1.889681 -3.962541 -0.110763
C -2.175998 -4.416990 -1.408448
C -3.446077 -4.875065 -1.725380
C -4.424276 -4.875569 -0.734394
C -4.140626 -4.420019 0.554806
C -0.975195 -4.285132 -2.292074
C -0.035118 -3.402527 -1.476657
C -0.494688 -3.516751 -0.086071
Pd -0.292544 -1.411915 -2.026223

O -0.505749 0.675577 -2.734684
C 0.223421 -3.166460 1.079016
C 1.716451 -2.881734 1.011010
C 2.123968 -4.315631 0.647564
C 0.731114 -4.915998 0.800834
O -0.807571 -0.751590 -0.060805
P 0.012846 0.220575 0.759860
O 0.622911 -0.216560 2.050631
O 1.147657 0.764075 -0.293465
C 1.857712 1.901055 0.034905
C 1.229411 3.127892 -0.071533
C 1.969607 4.295245 0.303647
C 3.353679 4.162355 0.619276
C 3.952048 2.880753 0.610819
C 3.226092 1.739084 0.368331
C 1.382202 5.581372 0.401957
C 2.131692 6.676363 0.752741
C 3.510439 6.548122 1.022826
C 4.103596 5.313874 0.961076
C -0.173065 3.198229 -0.554688
C -1.155977 2.420294 0.034828
C -2.528928 2.491082 -0.315895
C -2.881538 3.373537 -1.307706
C -1.920185 4.122324 -2.023406
C -0.543129 4.022064 -1.669363
C -2.303892 4.950334 -3.105564
C -1.366956 5.627803 -3.841569
C 0.000690 5.493185 -3.524898
C 0.402249 4.714397 -2.467887
C -3.549305 1.661179 0.381737
C -3.905159 1.967969 1.707027
C -4.904996 1.220275 2.327423
C -5.546027 0.168108 1.682973
C -5.159961 -0.134109 0.378998
C -4.177459 0.593202 -0.291641
C -6.645899 -0.603095 2.376014
C -6.348063 -2.098200 2.434705
C -3.284152 3.130893 2.455769
C -4.266516 4.299253 2.521901
C -3.838441 0.221142 -1.722839
C -3.626693 -1.279573 -1.903559
O -0.815074 1.582297 1.076541
C 3.855664 0.390330 0.450388
C 4.128207 -0.338007 -0.722401
C 4.786525 -1.566044 -0.623549
C 5.179228 -2.092120 0.604167
C 4.866520 -1.368929 1.753156
C 4.204574 -0.142556 1.707815
C 3.798840 0.218394 -2.092861

C 5.009868 0.965320 -2.652363
C 5.984187 -3.368069 0.731369
C 5.803629 -4.348488 -0.419515
C 3.879045 0.574504 3.004243
C 3.344055 -0.370603 4.075245
C 3.311569 -0.841286 -3.073505
C 5.097789 1.326870 3.539341
C 7.466535 -3.023918 0.892821
C -2.788011 2.737672 3.843083
C -4.921727 0.714341 -2.682449
C -7.998388 -0.348157 1.713484
O 0.209365 -2.181791 -3.883777
C 0.549447 -1.445642 -4.883227
C 1.065784 -2.233544 -6.064854
O -0.470528 -2.967083 2.182893
O 0.532185 -0.207931 -4.940723
O 0.530330 -2.286467 4.522402
C 0.273601 -1.257266 5.139289
C 0.219383 -1.212837 6.634575
O 0.054903 -0.089230 4.587913
H 2.123720 -2.461799 -5.886351
H 0.534848 -3.182453 -6.173180
H 0.989006 -1.639541 -6.977872
H 1.034135 -3.533492 -1.664639
H -0.520183 -5.274282 -2.475734
H -3.675841 -5.215523 -2.733193
H -2.650435 -3.581489 1.876177
H -5.426629 -5.228112 -0.968499
H -4.921539 -4.426644 1.311284
H 2.084397 -2.549536 1.986462
H 1.993099 -2.109435 0.279283
H 0.462568 -5.265009 1.802235
H 0.371748 -5.625355 0.050685
H 2.867398 -4.761138 1.317858
H 2.503944 -4.405557 -0.375632
H -3.933162 3.479383 -1.574868
H 5.017658 2.797147 0.825712
H 0.191843 -2.224059 7.041743
H 1.113618 -0.697902 7.003404
H -0.646831 -0.634791 6.967280
H 0.069230 -2.648939 2.952352
H 0.201434 -0.124804 3.594299
H 5.161863 5.191426 1.188202
H 1.461116 4.616973 -2.243148
H -1.671179 6.252276 -4.678074
H 1.656423 7.651515 0.829414
H 4.094290 7.424797 1.292971
H 0.746636 6.006208 -4.127372
H -3.362676 5.019166 -3.350959

H 0.319310 5.692863 0.204700
H 5.010900 -2.113695 -1.537807
H 5.151966 -1.785664 2.721209
H -5.198520 1.467604 3.348964
H -5.634837 -0.968867 -0.139593
H 2.985172 0.948133 -1.981104
H 5.860668 0.280438 -2.769616
H 4.784492 1.397294 -3.635071
H 5.322146 1.776493 -1.983299
H 4.123702 -1.507171 -3.396057
H 2.516981 -1.458252 -2.629401
H 2.897671 -0.364971 -3.970741
H 3.083238 1.301564 2.791299
H 4.123738 -1.040778 4.460358
H 2.968059 0.210143 4.927691
H 2.520634 -0.981122 3.689721
H 5.457818 2.086054 2.835416
H 4.859716 1.829550 4.484974
H 5.925354 0.629510 3.728287
H 5.653697 -3.865907 1.658477
H 6.215675 -3.947955 -1.354920
H 6.336683 -5.283017 -0.209339
H 4.749028 -4.592675 -0.596275
H 7.635937 -2.362099 1.749547
H 8.071143 -3.928722 1.032059
H 7.831311 -2.505857 -0.004276
H -2.893801 0.709028 -1.995331
H -6.701961 -0.229980 3.410920
H -2.409375 3.477352 1.890957
H -4.575668 4.608287 1.515384
H -5.171570 4.022937 3.079189
H -3.814504 5.164457 3.023077
H -2.080226 1.902857 3.786738
H -2.278477 3.584066 4.319613
H -3.613026 2.442102 4.504154
H -4.561434 -1.850618 -1.807323
H -3.224692 -1.483393 -2.906886
H -2.915611 -1.666572 -1.163491
H -5.060644 1.800628 -2.625100
H -4.664528 0.461795 -3.718769
H -5.888816 0.246499 -2.451802
H -7.116022 -2.628712 3.011440
H -6.330797 -2.533152 1.426393
H -5.371576 -2.290708 2.895730
H -7.996654 -0.705492 0.675416
H -8.803568 -0.870749 2.245172
H -8.236454 0.721316 1.694576
H 0.147796 1.157068 -2.207954
H -0.107336 0.524728 -3.638871

H -1.194613 -3.863426 -3.279014

(TS-*re*)$_{\mathbf{I}}$
E0 = -3818.9939515
E0+ZPE = -3817.669403
E298 = -3817.592311
H298 = -3817.591367
G298 = -3817.776330
NImag = -419.5159
C 3.406616 2.155699 0.787983
C 2.498939 2.887949 -0.002328
C 2.886512 3.330717 -1.287432
C 4.177442 3.055297 -1.730462
C 5.098992 2.349339 -0.957911
C 4.687610 1.904247 0.292264
C 1.151372 3.268636 0.513117
C -0.036327 2.688507 -0.002464
C -1.306861 3.131386 0.308075
C -1.445284 4.105951 1.345705
C -0.269184 4.657513 1.930868
C 1.002392 4.257308 1.456026
C -0.395243 5.599388 2.980056
C -1.628697 5.965763 3.455260
C -2.793549 5.401660 2.893915
C -2.705064 4.498066 1.863255
O 0.091213 1.608655 -0.869392
P -0.256260 0.185669 -0.141071
O -1.810480 0.383376 0.307327
C -2.677272 1.189816 -0.395485
C -2.475161 2.555379 -0.400725
C -3.386367 3.370361 -1.143292
C -4.523192 2.759782 -1.750879
C -4.703205 1.360206 -1.646004
C -3.787049 0.557478 -1.010461
C -3.193474 4.762857 -1.324932
C -4.093644 5.512615 -2.039581
C -5.236360 4.912392 -2.609946
C -5.441094 3.564143 -2.468831
C -3.963094 -0.919460 -0.902984
C -3.392038 -1.776363 -1.869842
C -3.578952 -3.148935 -1.733764
C -4.322195 -3.703981 -0.688437
C -4.857804 -2.840660 0.258721
C -4.683436 -1.454103 0.174974
C -2.649883 -1.220234 -3.069523
C -1.590927 -2.160234 -3.633614
C -4.554773 -5.200829 -0.670263
C -5.011204 -5.751687 0.673060
C -5.279600 -0.578981 1.261142

C -6.791728 -0.766951 1.362258
C 1.968590 4.148967 -2.176586
C 2.400035 5.614973 -2.172571
C 6.498116 2.130489 -1.492517
C 7.256675 0.999277 -0.811645
C 3.051587 1.627553 2.161980
C 3.304464 0.123772 2.295495
O -0.177475 -0.874430 -1.218737
Pd 1.702035 -1.854997 -1.300357
O 2.583538 0.044820 -2.060081
C 0.892006 -3.620243 -0.532463
C 1.065911 -3.376383 0.909820
C 2.380745 -3.915481 1.283450
C 2.774846 -4.808234 0.275128
C 1.766513 -4.830567 -0.837028
C 3.963877 -5.510837 0.397942
C 4.757929 -5.296573 1.522298
C 4.372402 -4.391937 2.513629
C 3.172479 -3.696320 2.409808
C 0.162750 -2.714885 1.774923
C -1.299734 -2.547385 1.382730
C -1.657035 -4.035276 1.448956
C -0.288679 -4.522601 1.902155
O 3.511165 -2.796065 -1.536995
C 4.565619 -2.180011 -1.127463
C 5.835114 -2.996744 -1.181022
O 4.613719 -1.014676 -0.707587
O 0.610666 -2.219383 2.915430
O 0.524208 0.000451 1.120127
C -3.643363 -0.851581 -4.173997
C -4.595857 -0.821423 2.605647
C -5.566324 -5.578820 -1.754653
C 1.885500 3.599647 -3.597705
C 7.294907 3.433512 -1.398001
C 3.801919 2.389617 3.254085
O -0.354674 1.424443 3.084895
C -1.165094 0.744699 3.856164
O -1.187900 -0.481447 3.932308
C -2.096478 1.625710 4.625819
H 5.678079 -3.979053 -1.632346
H 6.209185 -3.121485 -0.158964
H 6.594622 -2.442000 -1.741507
H -0.133706 -3.628847 -0.917215
H 1.163824 -5.755321 -0.801243
H 4.280398 -6.203193 -0.380389
H 2.858598 -2.991940 3.174145
H 5.699064 -5.833102 1.625016
H 5.015159 -4.230333 3.375447
H -1.820131 -1.926523 2.115922

H -1.441114 -2.099305 0.395258
H -0.118691 -4.588468 2.980709
H 0.146560 -5.391763 1.403922
H -2.459239 -4.269068 2.158530
H -1.948941 -4.440782 0.473907
H -1.548131 2.463284 5.067476
H -2.626138 1.055274 5.389874
H -2.815167 2.060801 3.920703
H -0.053240 -1.595943 3.311006
H 0.087345 0.818446 2.412574
H 2.134379 0.828809 -1.709418
H 3.419227 -0.058087 -1.540665
H 2.238329 -4.789078 -1.824054
H 1.892215 4.736824 1.865029
H -5.589838 0.907440 -2.092275
H -6.307537 3.082023 -2.919627
H -3.607858 4.064938 1.438134
H -1.712424 6.685960 4.265739
H -3.922151 6.578246 -2.172683
H -5.943587 5.518571 -3.170944
H -3.769870 5.684762 3.280845
H 0.513848 6.018220 3.409314
H -2.312250 5.232197 -0.893666
H -5.425686 -3.244705 1.096908
H -3.144590 -3.821564 -2.475409
H 4.484832 3.400214 -2.719605
H 5.369436 1.311421 0.898555
H -5.101783 0.470653 0.991121
H -7.053277 -1.782590 1.685641
H -7.220913 -0.069236 2.091560
H -7.276721 -0.591228 0.394304
H -4.655896 -1.877763 2.902990
H -3.534240 -0.546504 2.567335
H -5.069251 -0.226910 3.397666
H -2.133338 -0.305814 -2.743659
H -2.042424 -3.008435 -4.166524
H -0.966157 -1.621395 -4.355196
H -0.929171 -2.542456 -2.849217
H -4.363225 -0.093961 -3.845224
H -3.116097 -0.459165 -5.052107
H -4.207936 -1.740527 -4.487594
H -3.594592 -5.680494 -0.928349
H -6.012086 -5.382157 0.932546
H -5.071814 -6.845222 0.634730
H -4.331046 -5.478729 1.488952
H -5.242555 -5.244126 -2.746258
H -5.718736 -6.664504 -1.791706
H -6.535106 -5.106295 -1.544549
H 1.981713 1.805115 2.316013

H 6.393341 1.876295 -2.560059
H 0.953502 4.112933 -1.760320
H 2.408512 6.020928 -1.153356
H 3.411952 5.727391 -2.584024
H 1.720845 6.226169 -2.780096
H 1.613002 2.537444 -3.600686
H 1.130416 4.147908 -4.173782
H 2.838683 3.702475 -4.131508
H 4.377367 -0.101333 2.365723
H 2.820115 -0.252590 3.208022
H 2.899477 -0.440486 1.447561
H 3.590890 3.465586 3.221930
H 3.519116 2.017742 4.247011
H 4.887456 2.263301 3.147388
H 8.205613 0.817293 -1.330501
H 7.505668 1.262202 0.226003
H 6.669161 0.073412 -0.796311
H 7.400749 3.732467 -0.346307
H 8.301366 3.310428 -1.817278
H 6.801278 4.256476 -1.928133

(TS-*si*)$_{II}$
E0 = -3818.97884645
E0+ZPE = -3817.657431
E298 = -3817.579087
H298 = -3817.578143
G298 = -3817.770119
NImag = -399.4112

C -3.718030 1.006226 3.473838
C -4.437658 0.206517 2.583320
C -5.841420 0.179883 2.600835
C -6.540856 0.961306 3.509106
C -5.825258 1.763385 4.394400
C -4.428940 1.784674 4.378342
C -6.367697 -0.764337 1.560793
C -5.138732 -1.067740 0.713473
C -3.978911 -0.704743 1.532147
Pd -5.078290 0.245283 -0.892379
O -5.057553 1.582796 -2.648312
C -2.634880 -1.070601 1.286679
O -1.686442 -0.299818 1.789058
O -3.681063 1.586476 -0.044544
C -2.468131 1.512130 -0.312648
C -1.532969 2.535467 0.235213
O -2.017849 0.565253 -1.073523
O -6.544002 -1.037940 -1.566067
C -7.179517 -0.827938 -2.665620
O -7.023204 0.118760 -3.448869

C -8.191126 -1.902094 -2.992212
C -2.320601 -2.187804 0.301913
C -2.918334 -3.309253 1.165214
C -3.233221 -2.426545 2.365124
O 0.492041 0.548343 -1.191408
P 1.296791 -0.123264 -0.115535
O 0.615086 -0.930453 0.953680
O 2.427502 -1.002283 -0.875632
C 3.440101 -1.521437 -0.098685
C 3.396050 -2.909988 0.188345
C 4.448707 -3.439891 0.895318
C 5.485437 -2.629121 1.413514
C 5.481639 -1.227293 1.152828
C 4.461447 -0.683804 0.307524
C 6.475635 -0.430179 1.774103
C 7.442308 -0.994946 2.568275
C 7.470997 -2.388838 2.785199
C 6.507191 -3.184387 2.221837
C 2.244406 -3.748209 -0.246192
C 1.373299 -4.305263 0.716127
C 0.335053 -5.132984 0.285950
C 0.121369 -5.416533 -1.062270
C 0.977371 -4.835060 -1.989871
C 2.034179 -4.007323 -1.613407
C 4.453722 0.733425 -0.129071
C 3.320591 1.510406 0.055097
C 3.255298 2.881572 -0.300951
C 4.382436 3.453074 -0.843690
C 5.544319 2.702193 -1.126532
C 5.576868 1.315201 -0.801357
C 6.716270 0.567439 -1.195412
C 7.775468 1.169924 -1.826625
C 7.758784 2.553659 -2.101816
C 6.659996 3.299227 -1.762669
O 2.221362 0.966220 0.677585
C 2.036044 3.721006 -0.126811
C 1.625831 4.143399 1.150373
C 0.610065 5.096571 1.255505
C -0.006820 5.648194 0.138267
C 0.376054 5.172483 -1.114679
C 1.365606 4.201983 -1.272110
C 1.543870 -4.069998 2.206732
C 2.075868 -5.325191 2.898563
C -0.962218 -6.368339 -1.515212
C -0.636871 -7.800974 -1.095771
C 2.945666 -3.470045 -2.698353
C 2.181457 -2.633743 -3.721888
C 2.259751 3.615944 2.421736
C 1.234558 2.879621 3.283563

C -1.059050 6.724683 0.280023
C -0.583440 8.039910 -0.333883
C 1.646889 3.676279 -2.668043
C 2.312797 4.734938 -3.544495
C 0.256984 -3.606930 2.884635
C 3.708339 -4.610414 -3.371565
C -2.346439 -5.964416 -1.019896
C 2.943294 4.732973 3.207244
C 0.372534 3.148150 -3.326277
C -2.398471 6.304961 -0.321632
H -8.655731 -2.293882 -2.084088
H -8.946326 -1.509566 -3.676475
H -7.674826 -2.731640 -3.487741
H -5.122855 -2.032300 0.202152
H -7.198373 -0.356931 0.973346
H -7.628806 0.950872 3.526444
H -2.632667 1.018231 3.448391
H -6.361207 2.385246 5.108142
H -3.892806 2.421121 5.077919
H -1.238460 -2.280839 0.157261
H -2.785726 -2.017603 -0.676168
H -2.442171 -2.328742 3.116501
H -4.204111 -2.524268 2.858530
H -2.202607 -4.105760 1.398185
H -3.810552 -3.775126 0.736101
H 4.470053 -4.510316 1.101029
H 4.367807 4.513602 -1.096898
H -1.988948 3.031749 1.094271
H -0.565583 2.102486 0.506936
H -1.324561 3.285265 -0.540550
H -0.752987 -0.586053 1.497845
H -0.990067 0.562561 -1.160188
H -6.752322 -1.682882 2.037287
H -5.396080 2.435920 -2.357107
H -5.816374 1.121003 -3.115909
H -0.320260 -5.586560 1.033252
H 0.824342 -5.049791 -3.048795
H 0.302497 5.437138 2.246077
H -0.119693 5.564963 -2.004350
H 6.615027 4.363397 -1.990781
H 8.634209 0.572210 -2.123605
H 6.459803 0.645893 1.622496
H 8.189590 -0.360638 3.039391
H 6.497975 -4.259124 2.398632
H 8.246604 -2.824762 3.410442
H 8.607749 3.019599 -2.596480
H 6.741496 -0.501205 -1.000679
H 3.694270 -2.816319 -2.234699
H 1.642849 -1.812361 -3.236554

H 2.874055 -2.202569 -4.455118
H 1.454430 -3.241011 -4.277095
H 4.410206 -4.220132 -4.118855
H 4.279214 -5.192794 -2.637874
H 3.024571 -5.299037 -3.885084
H 2.278263 -3.266632 2.343093
H 3.021877 -5.664619 2.460686
H 2.243053 -5.141056 3.967148
H 1.359886 -6.153402 2.809988
H -0.520175 -4.384591 2.863691
H 0.449622 -3.372987 3.939070
H -0.124767 -2.702296 2.398879
H -0.978732 -6.335360 -2.615717
H -0.617606 -7.892204 -0.001621
H -1.389043 -8.503621 -1.475541
H 0.344497 -8.111921 -1.471152
H -3.117090 -6.623814 -1.437196
H -2.412094 -6.038301 0.074233
H -2.586693 -4.932342 -1.304234
H 2.333786 2.824261 -2.583155
H 3.264569 5.074689 -3.117325
H 2.513698 4.338554 -4.547254
H 1.666260 5.615340 -3.657882
H -0.358196 3.947157 -3.510430
H 0.607712 2.693116 -4.295901
H -0.095983 2.378969 -2.701969
H -1.211153 6.890861 1.358301
H -0.433136 7.934337 -1.416215
H -1.322774 8.835139 -0.178006
H 0.367990 8.363446 0.102877
H -2.307154 6.123180 -1.400829
H -2.781285 5.387229 0.139983
H -3.150584 7.091422 -0.184130
H 3.034983 2.890438 2.145803
H 0.785708 2.040023 2.738190
H 1.708730 2.477840 4.187413
H 0.426126 3.550987 3.604405
H 3.690796 5.247931 2.591921
H 2.220023 5.483620 3.551689
H 3.448949 4.330032 4.093301

(TS-*re*)$_{II}$
E0 = -3818.9834342
E0+ZPE = -3817.661245
E298 = -3817.583737
H298 = -3817.582793
G298 = -3817.769396
NImag = -409.9455
C 2.796826 0.539443 3.215685

C 2.305475 -0.889909 3.047902
C 1.754461 -0.682874 1.632414
C 2.335888 0.713913 1.439631
C 3.734940 0.926674 1.424629
C 4.397217 2.232275 1.517476
C 5.777949 2.011875 1.648709
C 6.080433 0.543409 1.658377
C 4.772827 -0.077989 1.190966
C 3.868856 3.523596 1.538649
C 4.747768 4.593312 1.659449
C 6.122560 4.376713 1.768961
C 6.646526 3.086022 1.771380
Pd 4.819479 -0.249026 -0.887795
O 4.879096 -0.574635 -3.072237
O 1.565137 1.735684 1.109681
O 3.414817 1.278420 -1.397465
C 2.241803 0.920058 -1.601884
C 1.229022 1.878299 -2.140482
O 1.875887 -0.292390 -1.329076
O 6.288881 -1.618017 -0.397092
C 6.748767 -2.451736 -1.262577
O 6.457943 -2.515462 -2.465454
C 7.734310 -3.450599 -0.702038
O -0.584165 -0.630229 -1.290947
P -1.430093 0.043565 -0.247316
O -2.166833 -1.013882 0.747430
C -3.107281 -1.867445 0.215077
C -4.370977 -1.389165 -0.090067
C -5.310518 -2.312367 -0.656595
C -4.959939 -3.692839 -0.742950
C -3.666259 -4.116889 -0.355724
C -2.714680 -3.224269 0.069597
C -5.897822 -4.618049 -1.261761
C -7.121070 -4.202701 -1.720159
C -7.448651 -2.831292 -1.690114
C -6.568419 -1.912702 -1.174107
C -4.684028 0.045732 0.137122
C -3.810202 1.009717 -0.330785
C -3.981452 2.407268 -0.146704
C -5.141869 2.819137 0.460427
C -6.072055 1.893431 0.991986
C -5.823797 0.491894 0.883648
C -7.217295 2.344477 1.692470
C -8.067915 1.458825 2.302051
C -7.793565 0.076632 2.246135
C -6.702804 -0.393087 1.557580
C -2.862231 3.322964 -0.510192
C -2.098708 3.921999 0.517433
C -0.978953 4.676992 0.171602

C -0.580293 4.849945 -1.151289
C -1.358888 4.269276 -2.146312
C -2.487966 3.503768 -1.854127
C -2.450685 3.779096 1.987779
C -3.165348 5.038429 2.481222
C -3.279570 2.915592 -3.005100
C -2.419672 2.032688 -3.907836
C 0.645699 5.657042 -1.511763
C 0.356154 7.153965 -1.411637
O -2.711449 0.615563 -1.057403
C -1.297647 -3.594053 0.347692
C -0.409471 -3.823562 -0.722587
C 0.939624 -4.045970 -0.439452
C 1.430256 -4.057069 0.862492
C 0.526696 -3.862211 1.905146
C -0.825423 -3.618760 1.673505
C -0.878815 -3.891343 -2.163954
C -1.091203 -5.353711 -2.564186
C 2.888728 -4.312174 1.171587
C 3.114368 -5.798269 1.450773
C -1.760325 -3.433426 2.853143
C -1.281179 -2.360449 3.825909
O -0.825145 1.069695 0.664759
C 0.065371 -3.220557 -3.156985
C 3.844240 -3.822779 0.089576
C -1.980250 -4.768508 3.562773
C -3.958380 4.025151 -3.807367
C 1.864384 5.287632 -0.670737
C -1.249505 3.479378 2.881005
H 7.292290 -4.450366 -0.774318
H 7.986512 -3.238334 0.338805
H 8.637843 -3.454148 -1.318541
H 4.577612 -1.111175 1.487545
H 6.933003 0.251425 1.035741
H 7.718260 2.923344 1.867239
H 2.798237 3.681928 1.456994
H 6.793430 5.228609 1.855948
H 4.358312 5.608966 1.663826
H 0.661022 -0.625456 1.614433
H 2.059951 -1.406617 0.868660
H 2.058553 1.263509 3.577819
H 3.764113 0.726166 3.690360
H 1.555074 -1.188307 3.787649
H 3.125314 -1.615169 3.090685
H 1.716941 2.792453 -2.484288
H 0.508019 2.132357 -1.349486
H 0.661960 1.415836 -2.955432
H 0.595043 1.461455 0.988398
H 0.848151 -0.445348 -1.367775

H 6.322385 0.215223 2.684802
H 5.402811 0.132847 -3.462420
H 5.478215 -1.379380 -3.021449
H -3.414507 -5.174185 -0.439639
H -5.332491 3.884066 0.593942
H 1.630424 -4.203524 -1.266587
H 0.901646 -3.887961 2.931623
H -1.063816 4.407838 -3.188750
H -0.391737 5.137547 0.966747
H -7.394981 3.417541 1.750753
H -8.448700 -0.624378 2.758197
H -6.829626 -0.857801 -1.168924
H -8.404582 -2.495835 -2.085721
H -5.614699 -5.668962 -1.303381
H -7.830231 -4.922083 -2.122825
H -8.940298 1.818004 2.842822
H -6.499355 -1.460114 1.532193
H -2.735429 -3.107347 2.468263
H -1.140903 -1.401073 3.311937
H -2.018143 -2.210857 4.624379
H -0.335947 -2.645554 4.308958
H -2.692795 -4.661419 4.390031
H -2.372571 -5.521278 2.867921
H -1.039492 -5.155590 3.976278
H -1.845722 -3.374678 -2.232459
H -1.801293 -5.864713 -1.903351
H -1.467539 -5.427072 -3.592077
H -0.141977 -5.904308 -2.513147
H 1.021956 -3.752023 -3.242461
H -0.388734 -3.221617 -4.155275
H 0.265030 -2.183444 -2.874656
H 3.117798 -3.761199 2.101574
H 2.860930 -6.388766 0.560184
H 4.162443 -6.000327 1.704982
H 2.483816 -6.152106 2.274815
H 4.876823 -3.828811 0.460009
H 3.810290 -4.464962 -0.800781
H 3.618624 -2.797888 -0.239880
H -3.139837 2.930763 2.091614
H -4.058875 5.264493 1.887072
H -3.470621 4.932034 3.529737
H -2.499816 5.909671 2.412072
H -0.536462 4.313748 2.912257
H -1.588675 3.310622 3.910681
H -0.724990 2.582136 2.538932
H 0.881558 5.430020 -2.564616
H 0.099259 7.425159 -0.378855
H 1.229360 7.748270 -1.708660
H -0.488609 7.439172 -2.048918

H 1.741184 5.618782 0.370173
H 2.043946 4.203821 -0.652152
H 2.767166 5.776034 -1.058514
H -4.075915 2.285526 -2.588157
H -1.936522 1.231599 -3.334757
H -3.036996 1.567550 -4.686128
H -1.641963 2.616783 -4.418832
H -4.610062 4.634070 -3.169350
H -3.217459 4.696013 -4.262034
H -4.567128 3.603335 -4.616621

(TS-*si*)$_{III}$
E0 = -6170.4825231
E0+ZPE = -6168.268180
E298 = -6168.142839
H298 = -6168.141895
G298 = -6168.423839
NImag = -386.6076
C -4.415937 -4.363261 -0.821075
C -5.052764 -3.646079 -1.850052
C -4.425088 -3.506192 -3.108641
C -3.174622 -4.092061 -3.291386
C -2.501471 -4.772887 -2.275221
C -3.143709 -4.897366 -1.045394
C -6.375210 -3.012607 -1.601973
C -6.476781 -1.918442 -0.703596
C -7.646957 -1.237098 -0.447742
C -8.812095 -1.594965 -1.204136
C -8.748520 -2.726153 -2.069874
C -7.527464 -3.424556 -2.224009
C -9.900571 -3.112570 -2.796499
C -11.064440 -2.393811 -2.708071
C -11.115889 -1.245429 -1.891018
C -10.021354 -0.857761 -1.158350
O -5.332748 -1.534728 -0.029180
P -4.616899 -0.213571 -0.654759
O -4.392530 -0.318460 -2.124212
C -7.664355 -0.166881 0.577894
C -6.737767 0.867828 0.560075
C -6.819749 1.976117 1.447474
C -7.843863 1.992022 2.366608
C -8.740786 0.913972 2.515263
C -8.630649 -0.200262 1.636793
C -9.473851 -1.316200 1.874366
C -10.397089 -1.303801 2.889396
C -10.536750 -0.174679 3.724492
C -9.718204 0.908570 3.540574
O -5.761193 0.927131 -0.406704
C -5.860548 3.117199 1.448389

C -5.844879 4.054383 0.400439
C -5.054351 5.203210 0.520001
C -4.293853 5.464958 1.655598
C -4.311462 4.509331 2.672908
C -5.060016 3.337786 2.591812
C -6.725958 3.905242 -0.824569
C -5.933472 3.959345 -2.127588
C -3.452924 6.714589 1.837147
C -1.967856 6.370458 1.984551
C -4.911923 2.307536 3.696493
C -3.581860 1.572771 3.525149
C -5.079922 -2.799779 -4.283193
C -5.617934 -3.834465 -5.273918
C -1.126102 -5.342551 -2.565116
C -0.124924 -4.226660 -2.873961
C -5.122758 -4.674974 0.485381
C -4.314341 -4.308937 1.724461
O -3.424942 0.029441 0.268370
Pd -1.577587 0.329131 -0.733350
O -1.910660 -1.379315 -2.166612
O 0.190711 0.878346 -1.729121
C 1.332065 0.388001 -1.666413
C 1.637565 -0.901917 -0.969466
O 2.299972 1.031973 -2.231031
C -1.461437 1.927425 0.545026
C -0.108050 2.491632 0.433391
C -0.160584 3.637786 -0.462398
C -1.510910 3.918363 -0.731620
C -2.406736 3.001929 0.038596
C -1.847456 4.953434 -1.592127
C -0.823707 5.714257 -2.153177
C 0.518698 5.443302 -1.870742
C 0.867986 4.396144 -1.029245
C 1.050974 1.936484 1.018669
C 0.916895 0.821801 2.042707
C 0.396541 1.728184 3.166898
C 0.444921 3.022801 2.356971
O 2.229590 2.248012 0.510682
C -7.836764 4.954971 -0.807300
C -5.044971 2.901948 5.094413
C -3.630878 7.751355 0.738470
C -4.157107 -1.822121 -5.007673
C -0.578990 -6.243164 -1.467532
C -5.528346 -6.149121 0.503454
O 4.531858 0.238269 -1.365625
P 4.893835 0.001692 0.070090
O 5.106549 -1.614612 0.193882
C 5.890911 -2.150087 1.184902
C 7.266720 -2.011579 1.121702

C 8.051253 -2.571392 2.183148
C 7.411231 -3.381807 3.166789
C 6.007919 -3.547938 3.124865
C 5.232171 -2.908460 2.189307
C 9.442140 -2.331976 2.324085
C 10.160099 -2.900077 3.346405
C 9.531332 -3.742572 4.287290
C 8.182772 -3.970243 4.198357
C 7.887052 -1.265490 0.000397
C 7.434114 0.002343 -0.317714
C 8.037063 0.824131 -1.306962
C 9.137054 0.324380 -1.959701
C 9.593010 -0.998678 -1.755182
C 8.942562 -1.823623 -0.792355
C 10.664339 -1.525371 -2.516512
C 11.059849 -2.829542 -2.368370
C 10.384708 -3.664065 -1.452847
C 9.356601 -3.175290 -0.686007
C 7.516930 2.190003 -1.597710
C 6.781952 2.430446 -2.777616
C 6.346441 3.727359 -3.035922
C 6.591004 4.786862 -2.164473
C 7.309487 4.523136 -1.004197
C 7.778564 3.242234 -0.705270
C 6.467165 1.328200 -3.771925
C 7.510971 1.282050 -4.889226
C 8.585505 3.037900 0.561919
C 7.801192 3.437257 1.808490
C 6.005166 6.146479 -2.476076
C 4.538333 6.186632 -2.040607
O 6.392010 0.540698 0.407641
C 3.744677 -2.960601 2.231733
C 3.033136 -3.744159 1.303418
C 1.641700 -3.754806 1.356036
C 0.921472 -3.011436 2.293300
C 1.650509 -2.266586 3.217323
C 3.049323 -2.226279 3.209717
C 3.740736 -4.638606 0.303855
C 3.369872 -4.311835 -1.138961
C -0.597857 -3.062961 2.276499
C -1.263966 -2.250119 3.378122
C 3.778879 -1.470034 4.307336
C 3.301240 -0.037083 4.515170
O 4.001417 0.509900 1.172031
C 3.469050 -6.108230 0.622864
C -1.145052 -2.611350 0.923362
C 3.689497 -2.252441 5.618795
C 9.918702 3.778023 0.476383
C 6.769788 7.310198 -1.860201

C 5.079179 1.462577 -4.393445
H -1.727851 1.453347 1.492934
H -2.860029 3.540297 0.888479
H -2.892405 5.162270 -1.820042
H 1.906875 4.155003 -0.824827
H -1.071951 6.530481 -2.828356
H 1.299234 6.047518 -2.327310
H 1.884476 0.351784 2.238287
H 0.221195 0.036470 1.722425
H 1.347612 3.633485 2.451172
H -0.443333 3.663113 2.342042
H 1.051370 1.761339 4.044043
H -0.611825 1.473597 3.510328
H 2.970397 1.647368 0.852803
H -2.009708 -2.255151 -1.763591
H -2.832302 -1.118407 -2.405291
H -3.251933 2.611742 -0.541193
H 9.661027 0.954034 -2.678767
H 5.528966 -4.161286 3.889012
H 7.672860 -4.595317 4.930294
H 8.840501 -3.831647 0.009621
H 11.878129 -3.226989 -2.964136
H 11.224105 -2.693026 3.435164
H 10.113374 -4.193635 5.087446
H 10.677557 -4.707189 -1.357732
H 11.153677 -0.871538 -3.237322
H 9.941394 -1.677744 1.614798
H 1.096154 -4.383273 0.648370
H 1.120133 -1.701576 3.983788
H 7.520330 5.332946 -0.305700
H 5.779385 3.927097 -3.946709
H 6.490058 0.374005 -3.227709
H 8.518843 1.079999 -4.511118
H 7.262137 0.501600 -5.619309
H 7.540820 2.242785 -5.421483
H 5.045143 2.267130 -5.140541
H 4.811081 0.535293 -4.913503
H 4.311610 1.668241 -3.642398
H 8.816479 1.968307 0.652703
H 7.573069 4.511311 1.816308
H 6.856542 2.884697 1.863534
H 8.381364 3.218620 2.713621
H 10.495788 3.450948 -0.397599
H 9.766036 4.861619 0.386947
H 10.524059 3.598268 1.373570
H 4.822212 -4.480462 0.408468
H 3.654385 -3.285059 -1.393860
H 3.887158 -4.986381 -1.832430
H 2.291096 -4.423296 -1.312346

H 3.757337 -6.348663 1.653504
H 2.403703 -6.350021 0.509301
H 4.033397 -6.763428 -0.051980
H 4.837121 -1.407376 4.025653
H 2.242920 0.003236 4.809595
H 3.875420 0.430714 5.324380
H 3.452377 0.559291 3.607819
H 4.269125 -1.759482 6.409080
H 2.648000 -2.322578 5.960703
H 4.066674 -3.276091 5.506979
H -0.886677 -4.120999 2.411434
H -1.054424 -1.176149 3.253147
H -2.352593 -2.368299 3.332735
H -0.930321 -2.546982 4.378808
H -0.756467 -3.218140 0.094313
H -2.241445 -2.659788 0.888772
H -0.869152 -1.562901 0.733231
H 3.212820 0.672121 -1.942921
H 2.372662 -1.478746 -1.539363
H 2.091446 -0.705598 0.013381
H 0.725703 -1.485039 -0.826189
H 6.031173 6.264087 -3.571548
H 7.838072 7.268781 -2.101287
H 6.373089 8.265040 -2.224873
H 6.671473 7.318419 -0.766519
H 3.957617 5.389725 -2.521425
H 4.464836 6.042834 -0.953623
H 4.078169 7.152501 -2.287999
H -7.499966 -4.285772 -2.891805
H -7.931906 2.846696 3.039257
H -9.789530 1.780598 4.189176
H -10.072912 0.032412 -0.536637
H -11.940627 -2.694884 -3.277288
H -11.023914 -2.176760 3.055621
H -11.279263 -0.175030 4.518786
H -12.029469 -0.657263 -1.844895
H -9.833782 -3.987248 -3.441976
H -9.375642 -2.196629 1.245423
H -5.068548 5.927093 -0.294122
H -3.712445 4.688980 3.567285
H -2.659531 -5.448826 -0.239815
H -2.691491 -4.006378 -4.266083
H -5.922025 -2.210392 -3.899248
H -6.289798 -4.556876 -4.795209
H -6.166584 -3.345287 -6.088006
H -4.793410 -4.404706 -5.723073
H -3.253449 -2.309699 -5.395066
H -4.682917 -1.388986 -5.867252
H -3.860576 -0.997745 -4.353505

H -6.048358 -4.087006 0.523753
H -3.355511 -4.844393 1.766312
H -4.113080 -3.231438 1.750145
H -4.872208 -4.570230 2.632026
H -6.141181 -6.399280 -0.371402
H -4.646002 -6.802419 0.489556
H -6.106107 -6.385195 1.405591
H -7.209015 2.922102 -0.784919
H -5.167632 3.174872 -2.166621
H -6.601282 3.810629 -2.984377
H -5.442899 4.932986 -2.265498
H -8.425866 4.890074 0.115897
H -7.425275 5.971024 -0.869915
H -8.516238 4.816732 -1.657032
H -5.703707 1.558401 3.583835
H -2.743757 2.287255 3.569258
H -3.435874 0.827799 4.318340
H -3.547859 1.055291 2.555467
H -5.024174 2.107393 5.849523
H -4.224392 3.592139 5.329389
H -5.986228 3.453794 5.206814
H -3.777779 7.170813 2.787557
H -1.578341 5.930703 1.055174
H -1.379973 7.271058 2.198815
H -1.790917 5.657309 2.799616
H -4.679095 8.044200 0.610236
H -3.055947 8.654241 0.972738
H -3.260834 7.370975 -0.223822
H -1.227184 -5.950475 -3.479608
H -1.250213 -7.080280 -1.244083
H 0.391198 -6.658208 -1.765442
H -0.421779 -5.681802 -0.533176
H -0.490931 -3.532460 -3.638211
H 0.082772 -3.634258 -1.970250
H 0.829661 -4.643202 -3.218575

(TS-*re*)$_{III}$
E0 = -6170.4971788
E0+ZPE = -6168.281818
E298 = -6168.157426
H298 = -6168.156482
G298 = -6168.435237
NImag = -378.9847
C -6.256002 -2.463010 -2.591913
C -6.995724 -2.387641 -1.395890
C -6.967902 -3.460171 -0.483280
C -6.210225 -4.586351 -0.787872
C -5.448069 -4.674842 -1.951498
C -5.490252 -3.605671 -2.839792

C -7.733010 -1.141409 -1.040778
C -7.184751 -0.274872 -0.057870
C -7.741509 0.938205 0.303391
C -8.913244 1.369365 -0.399584
C -9.521688 0.484605 -1.339230
C -8.917418 -0.764216 -1.623492
C -10.699948 0.889789 -2.011765
C -11.242072 2.131678 -1.802132
C -10.612638 3.028233 -0.913646
C -9.479748 2.657679 -0.232649
O -6.053544 -0.711852 0.597747
P -4.639722 -0.050438 0.152500
O -4.293388 -0.342984 -1.280006
C -7.073432 1.766213 1.340090
C -7.751933 2.275529 2.493144
C -7.043861 3.131277 3.389265
C -5.673329 3.407130 3.165277
C -4.980583 2.834012 2.126395
C -5.720191 2.027688 1.224834
C -7.714967 3.659880 4.518957
C -9.020562 3.334206 4.782237
C -9.707648 2.450230 3.923739
C -9.090528 1.935620 2.811018
C -3.509958 2.996896 1.939227
C -2.611523 2.385100 2.839274
C -1.239093 2.569493 2.655228
C -0.726966 3.349780 1.622951
C -1.632665 3.913080 0.727887
C -3.009485 3.744168 0.853705
O -5.031900 1.524342 0.146647
C -3.079201 1.577831 4.037956
C -2.338983 0.253273 4.209896
C 0.755159 3.575571 1.423608
C 1.321139 2.564097 0.432858
C -3.908896 4.403280 -0.174748
C -3.755823 5.923291 -0.151381
C -7.779170 -3.435516 0.795998
C -9.042676 -4.278757 0.629217
C -4.572688 -5.891326 -2.164743
C -3.360446 -5.820858 -1.233099
C -6.300366 -1.363949 -3.638652
C -4.954593 -1.075201 -4.298642
O -3.674932 -0.406185 1.248495
C -2.953174 2.408978 5.316843
C 1.563401 3.536265 2.713573
C -3.656031 3.846320 -1.576647
C -6.973269 -3.871836 2.014687
C -4.120966 -6.092302 -3.604299
C -7.332151 -1.712232 -4.713748

O -1.254865 -0.825088 0.854772
C -1.007918 -2.084060 0.704208
C -2.078672 -3.082504 1.003514
O 0.107466 -2.468319 0.301485
Pd 1.617257 -1.018763 -0.037036
C 1.370784 -0.881621 -2.076520
C 0.044717 -1.433732 -2.354724
C 0.214401 -2.798280 -2.847987
C 1.583374 -3.019115 -3.071185
C 2.376629 -1.780998 -2.780332
C 2.021526 -4.254010 -3.528437
C 1.083129 -5.255536 -3.764416
C -0.280385 -5.027464 -3.561580
C -0.730348 -3.795845 -3.105827
C -1.196782 -0.814213 -2.076425
C -0.863493 -0.214071 -3.778440
C -0.858727 1.164596 -3.129140
C -1.273456 0.669043 -1.737167
O 3.182199 0.317745 -0.534639
P 4.278386 0.397482 0.521831
O 3.932017 0.602834 1.956280
O 5.350780 1.543554 0.123115
C 6.236065 1.402509 -0.918221
C 7.268395 0.481457 -0.829768
C 8.150350 0.357293 -1.954323
C 8.049372 1.297153 -3.020452
C 7.030849 2.277254 -2.993042
C 6.082879 2.316804 -1.999489
C 8.942776 1.211010 -4.115933
C 9.878790 0.212127 -4.185313
C 9.947990 -0.751241 -3.157125
C 9.109661 -0.679894 -2.072264
C 7.436487 -0.356947 0.385983
C 6.357357 -1.051341 0.901621
C 6.424699 -1.893828 2.042218
C 7.659223 -2.071502 2.618162
C 8.797570 -1.355423 2.180328
C 8.685218 -0.446576 1.086169
C 10.036510 -1.486873 2.853722
C 11.118798 -0.726208 2.495176
C 10.995401 0.214354 1.451129
C 9.813114 0.350791 0.767292
C 5.191445 -2.486349 2.635550
C 4.733280 -2.020440 3.885613
C 3.589752 -2.601001 4.445887
C 2.873517 -3.605793 3.802797
C 3.331010 -4.028669 2.552161
C 4.473103 -3.494543 1.958909
C 5.427230 -0.915457 4.662737

C 4.463066 0.162724 5.152420
C 4.946874 -4.063588 0.638194
C 5.718634 -5.361321 0.878231
C 1.603555 -4.206691 4.368614
C 0.378880 -3.637598 3.646014
O 5.144990 -0.959368 0.256244
C 4.905689 3.229431 -2.051763
C 3.953818 3.090610 -3.085997
C 2.809282 3.888894 -3.063741
C 2.565495 4.812664 -2.054142
C 3.537657 4.965490 -1.069159
C 4.704332 4.203402 -1.050867
C 4.135700 2.146475 -4.261310
C 2.864398 1.383423 -4.619592
C 1.327978 5.681124 -2.044365
C 0.087755 4.987239 -2.596782
C 5.758348 4.515498 -0.005482
C 6.407925 5.864265 -0.317555
O 1.824775 -0.985145 2.174502
C 4.628830 2.908442 -5.493476
C 1.593797 6.979533 -2.806758
C 5.215839 4.481421 1.419196
C 3.810676 -4.278739 -0.357530
C 1.453291 -4.030962 5.872740
C 6.208543 -1.497143 5.842194
O -2.233969 -1.616920 -1.908029
H 1.498610 0.197541 -2.187288
H 3.280985 -1.955547 -2.182724
H 3.080836 -4.435099 -3.701512
H -1.788794 -3.599845 -2.954965
H 1.416115 -6.229319 -4.116949
H -0.998876 -5.821367 -3.756969
H -2.303762 0.935282 -1.479575
H -0.625176 0.953011 -0.898761
H -1.814153 -0.548914 -4.208552
H -0.035318 -0.499174 -4.434564
H -1.570986 1.861016 -3.585951
H 0.130171 1.637527 -3.150640
H -1.701524 -4.094718 0.848239
H -2.937970 -2.899469 0.347001
H -2.433241 -2.952768 2.031830
H -3.085821 -1.105419 -1.667204
H -2.253516 -0.617746 1.055688
H 2.723661 -1.323316 -3.722335
H 2.172546 -1.840729 2.473239
H 2.565825 -0.344237 2.319215
H -5.151311 4.062655 3.862246
H -9.393694 -1.422789 -2.350265
H -0.549927 2.100305 3.356588

H -1.242616 4.524119 -0.089853
H -6.202802 -5.427027 -0.091077
H -4.911374 -3.652807 -3.760766
H -11.155985 0.194185 -2.715069
H -11.024992 4.024473 -0.770920
H -9.626988 1.246883 2.163466
H -10.733730 2.168671 4.149159
H -7.159988 4.319638 5.184635
H -9.522049 3.740880 5.657287
H -12.143523 2.433208 -2.330371
H -8.998884 3.361153 0.441742
H -4.953447 4.183465 0.082310
H -3.861441 2.769213 -1.613516
H -4.306477 4.338988 -2.310522
H -2.615607 4.015552 -1.889184
H -4.453687 6.394291 -0.854726
H -3.954338 6.326200 0.848820
H -2.740818 6.230357 -0.435579
H -4.140636 1.336935 3.894469
H -3.510789 3.351162 5.252500
H -3.328314 1.851141 6.184125
H -1.902536 2.663651 5.510953
H -1.274107 0.400665 4.430615
H -2.769210 -0.304150 5.051309
H -2.425622 -0.366142 3.312299
H 0.868504 4.581179 0.979491
H 1.584289 2.523775 3.138033
H 2.605174 3.813133 2.513874
H 1.159317 4.217161 3.471873
H 2.384263 2.749746 0.227826
H 1.224058 1.545990 0.839810
H 0.792961 2.593345 -0.532480
H -6.616341 -0.437122 -3.141485
H -8.328941 -1.877655 -4.289292
H -7.408730 -0.910668 -5.459107
H -7.042744 -2.633413 -5.237889
H -4.597324 -1.921567 -4.900834
H -5.053346 -0.219099 -4.977595
H -4.201261 -0.831185 -3.543907
H -5.166906 -6.772771 -1.872468
H -3.443147 -5.289167 -3.928033
H -3.575568 -7.038723 -3.704115
H -4.966597 -6.112661 -4.301165
H -2.776305 -4.911417 -1.437932
H -3.665031 -5.784319 -0.180425
H -2.699952 -6.687412 -1.368144
H -8.100502 -2.401793 0.977759
H -6.057724 -3.276293 2.111137
H -7.564519 -3.739861 2.928741

H -6.691541 -4.931629 1.962574
H -9.647993 -3.915855 -0.210914
H -8.789721 -5.328788 0.429280
H -9.660322 -4.247825 1.535500
H 6.975642 2.991540 -3.813620
H 7.758451 -2.739533 3.474022
H 2.080251 3.780574 -3.866697
H 3.373864 5.710288 -0.286828
H 2.777515 -4.814364 2.034531
H 3.245701 -2.240048 5.413952
H 10.102073 -2.196202 3.677685
H 11.843288 0.842907 1.188986
H 9.172915 -1.431139 -1.289629
H 10.669925 -1.561696 -3.226089
H 8.854286 1.949831 -4.911446
H 10.555152 0.150356 -5.034475
H 12.063700 -0.831023 3.022966
H 9.731248 1.087852 -0.027010
H 6.547950 3.756859 -0.072223
H 4.773204 3.504768 1.647441
H 6.023446 4.663740 2.138536
H 4.455216 5.256898 1.583858
H 7.213201 6.081267 0.395041
H 6.832607 5.875228 -1.328925
H 5.675981 6.680150 -0.254092
H 4.894180 1.399586 -3.992405
H 5.557656 3.456804 -5.300296
H 4.804758 2.223587 -6.332630
H 3.879634 3.645240 -5.812490
H 2.099085 2.034387 -5.063207
H 3.083873 0.600916 -5.357870
H 2.434693 0.913545 -3.728609
H 1.124606 5.941389 -0.991469
H 1.819019 6.760281 -3.859408
H 0.721350 7.643870 -2.777638
H 2.452007 7.518034 -2.388843
H -0.795433 5.626418 -2.469006
H 0.179863 4.785658 -3.672754
H -0.105549 4.031431 -2.088892
H 6.141064 -0.422761 3.990625
H 6.946137 -2.243096 5.522486
H 6.740341 -0.704177 6.382076
H 5.531989 -1.988886 6.554117
H 5.026228 0.966700 5.641617
H 3.907498 0.599789 4.317021
H 3.751166 -0.225176 5.892354
H 1.642264 -5.287138 4.153630
H 1.291508 -2.977085 6.134863
H 0.582218 -4.588797 6.234471

H 2.335647 -4.384584 6.418293
H 0.301879 -2.552675 3.811641
H 0.435317 -3.802610 2.561873
H -0.542842 -4.103393 4.017408
H 5.641889 -3.346974 0.184401
H 4.218221 -4.494047 -1.353750
H 3.171311 -5.128664 -0.084598
H 3.163138 -3.391908 -0.433405
H 6.573509 -5.197044 1.545681
H 5.071861 -6.117073 1.343481
H 6.096785 -5.774285 -0.065341

(TS-*si*)$_{IV}$
E0 = -6170.5033545
E0+ZPE = -6168.288130
E298 = -6168.162423
H298 = -6168.161479
G298 = -6168.442979
NImag = -380.1398
C -3.487118 0.548960 4.425899
C -2.875197 1.425828 3.507713
C -1.480517 1.613940 3.539040
C -0.716293 0.902690 4.465111
C -1.298282 0.025973 5.376197
C -2.682192 -0.122622 5.346268
C -3.696645 2.135268 2.488123
C -3.612648 1.764708 1.118923
C -4.342985 2.368911 0.110337
C -5.347229 3.318233 0.497125
C -5.417289 3.738839 1.857425
C -4.560574 3.150893 2.817183
C -6.302941 3.840737 -0.409945
C -7.233222 4.765777 -0.006179
C -7.259493 5.224758 1.327336
C -6.372028 4.713283 2.238248
C -4.070979 2.037352 -1.312638
C -4.017041 0.720186 -1.740751
C -3.813299 0.350922 -3.095494
C -3.684225 1.355305 -4.022814
C -3.665383 2.716991 -3.653265
C -3.820280 3.067885 -2.281159
C -3.473420 3.730165 -4.623998
C -3.398199 5.050389 -4.263018
C -3.498396 5.401060 -2.900315
C -3.706067 4.438582 -1.942378
O -4.277674 -0.298673 -0.850496
P -3.255597 -0.667212 0.355733
O -2.687677 0.796317 0.792339
C -3.797472 -1.066674 -3.553981

C -5.009968 -1.709762 -3.845077
C -4.973954 -2.976635 -4.429279
C -3.776563 -3.621372 -4.714250
C -2.585170 -2.984204 -4.365605
C -2.567071 -1.714300 -3.789529
C -6.351246 -1.053505 -3.585261
C -7.250381 -1.918605 -2.706491
C -3.777058 -4.957883 -5.421634
C -3.208490 -4.828367 -6.833391
C -1.246465 -1.049300 -3.443635
C -0.667839 -0.255019 -4.614957
C -0.803923 2.662244 2.680416
C 0.587864 2.261754 2.205106
C -0.492401 -0.719671 6.417558
C -0.603546 -0.013605 7.769712
C -4.986658 0.321759 4.464207
C -5.615420 1.091191 5.626245
O -2.052493 -1.421389 -0.182082
Pd -0.076735 -0.835520 0.208775
O 1.951462 -0.289896 0.587328
P 2.725433 0.350810 -0.557963
O 3.365443 1.715996 0.075944
C 4.173720 2.413153 -0.805403
C 5.425864 1.907262 -1.087493
C 6.214104 2.553679 -2.092359
C 5.759494 3.790288 -2.631095
C 4.540450 4.337653 -2.167543
C 3.714146 3.660465 -1.302896
C 7.422499 2.007157 -2.590229
C 8.150734 2.664136 -3.550447
C 7.715567 3.906380 -4.058295
C 6.542753 4.454153 -3.605936
C 5.952578 0.765915 -0.307141
C 5.251389 -0.424231 -0.212881
C 5.789153 -1.569470 0.436332
C 7.030992 -1.453468 1.018412
C 7.736551 -0.233024 1.062890
C 7.181696 0.907191 0.416745
C 7.863116 2.144207 0.553098
C 9.040561 2.229787 1.253101
C 9.609547 1.085772 1.852271
C 8.963942 -0.119381 1.759917
O 4.046651 -0.565655 -0.861710
C 5.109117 -2.892060 0.505501
C 4.739484 -3.419288 1.762402
C 4.288242 -4.735183 1.833378
C 4.161928 -5.548221 0.706005
C 4.505877 -4.995366 -0.523977
C 4.979413 -3.685467 -0.647838

C 4.735501 -2.580468 3.026327
C 5.417745 -3.271143 4.202910
C 3.661745 -6.970920 0.872092
C 3.704037 -7.797808 -0.404774
C 5.420676 -3.193688 -2.012622
C 6.698145 -3.913426 -2.443013
C 2.500723 4.317777 -0.736835
C 2.635193 4.949662 0.513669
C 1.550535 5.660440 1.024678
C 0.335447 5.746607 0.354263
C 0.212262 5.088203 -0.871349
C 1.279536 4.386296 -1.443482
C 3.926685 4.936551 1.311561
C 4.489640 6.349497 1.453277
C -0.758439 6.621433 0.926537
C -2.161669 6.050461 0.772318
C 1.151740 3.808522 -2.844153
C -0.255981 3.354356 -3.222079
C 0.418275 -2.599904 1.135089
C -0.745408 -3.498094 1.079276
C -0.565324 -4.412051 -0.043834
C 0.746369 -4.263060 -0.522022
C 1.499498 -3.273272 0.301457
C 1.179468 -4.997842 -1.617575
C 0.297658 -5.897182 -2.209357
C -0.997124 -6.069370 -1.712093
C -1.448561 -5.323731 -0.632276
C -1.881506 -3.474122 1.920848
O -2.971689 -4.077185 1.474086
O -0.431628 1.068774 -0.909530
C -1.914727 -2.617589 3.177592
C -0.861753 -3.435586 3.938966
C -0.751959 -4.535186 2.890071
O 2.038108 0.620262 -1.855740
C 3.305226 -2.168910 3.378327
C 4.325748 -3.318725 -3.067899
C 2.246023 -7.003346 1.455604
C 3.747774 4.270021 2.673928
C -0.687238 8.012262 0.293775
C 1.591861 4.846567 -3.882348
O -4.078961 -1.289456 1.436446
C -0.746473 3.972915 3.467292
C 0.971560 -0.906526 6.043680
C -5.352795 -1.155742 4.550991
C -7.041946 -0.692008 -4.898841
C -3.030545 -6.030142 -4.636256
C -0.200855 -2.041578 -2.947232
O -6.419776 -2.407047 1.578586
C -6.348047 -3.495389 2.303065

C -7.695428 -4.057255 2.637241
O -5.307137 -4.007071 2.703788
H 0.720500 -2.230570 2.120824
H 2.218881 -3.793617 0.956951
H 2.188754 -4.864847 -2.002660
H -2.458248 -5.433004 -0.252732
H 0.619494 -6.478780 -3.071686
H -1.662012 -6.787253 -2.185330
H -2.907415 -2.666604 3.635455
H -1.681572 -1.557385 3.011777
H -1.438900 -5.380334 2.993250
H 0.240828 -4.891541 2.596400
H -1.189266 -3.799372 4.918900
H 0.084303 -2.903888 4.084402
H -3.576782 1.091165 -5.075397
H -4.621712 3.487678 3.852674
H -8.194267 -3.384879 3.343867
H -8.319827 -4.101592 1.740679
H -7.592181 -5.045399 3.086727
H -3.778473 -3.905269 2.024691
H -5.512540 -1.991298 1.448499
H -6.395796 5.031334 3.279701
H -3.789043 4.730625 -0.901379
H -3.245456 5.820422 -5.015305
H -7.960380 5.144084 -0.720951
H -7.994069 5.966175 1.632513
H -3.411590 6.444827 -2.601065
H -3.371284 3.429178 -5.665843
H -6.300742 3.491181 -1.438818
H 0.361974 1.052647 4.477751
H -3.145872 -0.806296 6.060688
H -5.910644 -3.476141 -4.683841
H -1.636868 -3.489159 -4.554953
H -1.426110 2.839953 1.788553
H -0.198820 3.824388 4.407912
H -0.222854 4.744845 2.890496
H -1.752352 4.337780 3.713668
H 1.332501 2.343076 3.008793
H 0.621876 1.227978 1.841001
H 0.935429 2.928391 1.402422
H -5.415403 0.705425 3.528945
H -5.054514 -1.598673 5.510574
H -6.440742 -1.277342 4.465697
H -4.878785 -1.721408 3.742496
H -5.415202 2.167423 5.562795
H -6.703058 0.948429 5.645068
H -5.214099 0.738474 6.586167
H -0.949335 -1.719305 6.520820
H 1.518329 0.045060 6.083633

H 1.464784 -1.592230 6.742813
H 1.088399 -1.307581 5.028236
H -1.646605 0.079494 8.092393
H -0.049667 -0.554085 8.547428
H -0.186259 0.999646 7.696766
H -1.435163 -0.342136 -2.622711
H -4.827854 -5.276636 -5.509791
H -6.173777 -0.116148 -3.041538
H -6.413025 -0.031340 -5.508391
H -7.253098 -1.590830 -5.493060
H -7.995752 -0.182185 -4.713772
H -6.754446 -2.173304 -1.763058
H -8.180156 -1.386901 -2.469343
H -7.527875 -2.854699 -3.208551
H 0.189112 -2.672955 -3.759011
H 0.658283 -1.495803 -2.528922
H -0.620252 -2.700094 -2.178560
H -1.330703 0.558991 -4.933246
H 0.296294 0.184070 -4.321513
H -0.494911 -0.911065 -5.479712
H -3.113940 -7.007056 -5.128997
H -1.962026 -5.787343 -4.557262
H -3.427687 -6.118542 -3.617969
H -2.154207 -4.523905 -6.801706
H -3.264394 -5.783785 -7.370239
H -3.753052 -4.074751 -7.413287
H -0.435596 1.825396 -0.307387
H 0.416385 1.108189 -1.417216
H 2.105101 -2.574839 -0.287050
H 4.256672 5.335638 -2.500268
H 7.466753 -2.330205 1.500284
H 9.372545 -1.010793 2.234093
H 7.763012 1.046340 -2.211622
H 8.304529 4.419327 -4.814869
H 9.536731 3.192535 1.352116
H 10.547665 1.167286 2.396053
H 9.069721 2.220814 -3.926970
H 6.182617 5.404128 -3.998743
H 7.436441 3.038684 0.106373
H 4.435855 -5.608934 -1.421971
H 4.018116 -5.144765 2.808565
H 1.655653 6.176189 1.981858
H -0.732023 5.148012 -1.414913
H 1.822229 2.937266 -2.905841
H 2.633045 5.157829 -3.760204
H 1.479507 4.442346 -4.895876
H 0.960710 5.742605 -3.805208
H -0.938252 4.207459 -3.336065
H -0.225994 2.845391 -4.193907

H -0.707651 2.662828 -2.502409
H -0.551221 6.733801 2.002872
H -0.862048 7.942712 -0.788936
H -1.447296 8.680523 0.717697
H 0.297741 8.469677 0.442909
H -2.219441 4.987916 1.050009
H -2.878907 6.602266 1.391896
H -2.494125 6.141551 -0.268046
H 4.673856 4.348695 0.762406
H 2.979889 4.776859 3.275451
H 3.450804 3.220911 2.561125
H 4.686483 4.298056 3.241023
H 4.632786 6.817325 0.471393
H 3.817792 6.993766 2.035005
H 5.458075 6.330774 1.968140
H 5.662422 -2.127479 -1.934494
H 3.419467 -2.772922 -2.773897
H 4.668796 -2.900957 -4.021840
H 4.055596 -4.367618 -3.254893
H 7.492359 -3.775773 -1.698648
H 6.529144 -4.992402 -2.555990
H 7.059377 -3.528134 -3.404420
H 5.287675 -1.654758 2.826601
H 2.676010 -3.052868 3.576857
H 3.297915 -1.545272 4.281685
H 2.848129 -1.593241 2.560858
H 5.476563 -2.591436 5.061265
H 4.866644 -4.160906 4.533673
H 6.436903 -3.586568 3.948001
H 4.328515 -7.450910 1.608342
H 1.524535 -6.575287 0.744870
H 1.937354 -8.034923 1.663997
H 2.177705 -6.439468 2.394320
H 4.706083 -7.826972 -0.847479
H 3.398298 -8.829480 -0.197182
H 3.007893 -7.397080 -1.155745

(TS-*re*)$_{IV}$
E0 = -6170.488526
E0+ZPE = -6168.271003
E298 = -6168.146661
H298 = -6168.145716
G298 = -6168.421710
NImag = -377.7521
C -1.698216 4.640397 1.667712
C -2.765303 4.490932 0.764939
C -2.702149 5.096070 -0.507778
C -1.607753 5.900931 -0.819319
C -0.585013 6.142728 0.096721

C -0.641443 5.485319 1.321094
C -4.025016 3.818561 1.186695
C -4.443958 2.584902 0.634704
C -5.692191 2.039203 0.843839
C -6.542044 2.647013 1.822365
C -6.121924 3.864705 2.432672
C -4.884857 4.441878 2.059764
C -6.956110 4.482028 3.395792
C -8.146731 3.911878 3.765710
C -8.549105 2.690010 3.186509
C -7.769592 2.075144 2.238404
O -3.574733 1.928390 -0.210626
P -2.896783 0.584179 0.419830
O -2.242178 0.822945 1.736682
C -6.123628 0.881750 0.026953
C -5.375794 -0.283737 -0.019801
C -5.844533 -1.455620 -0.676447
C -7.043543 -1.383369 -1.346585
C -7.777273 -0.181580 -1.455850
C -7.306617 0.976370 -0.775653
C -8.017741 2.190360 -0.956226
C -9.148288 2.238306 -1.733293
C -9.636005 1.076927 -2.368959
C -8.957715 -0.106668 -2.233844
O -4.197366 -0.379774 0.678672
C -5.168993 -2.785846 -0.607114
C -4.414509 -3.252860 -1.696144
C -4.004285 -4.587647 -1.710760
C -4.298041 -5.464077 -0.670516
C -4.987288 -4.958549 0.431027
C -5.427693 -3.636309 0.483389
C -4.051385 -2.341804 -2.850481
C -2.604674 -2.535682 -3.293598
C -3.882595 -6.916414 -0.744672
C -5.091752 -7.846013 -0.671410
C -6.194542 -3.161192 1.701429
C -7.535850 -3.881269 1.818302
C -3.827773 4.976662 -1.518470
C -3.330702 4.536176 -2.892236
C 0.505685 7.150654 -0.188383
C -0.050889 8.570872 -0.084804
C -1.650275 3.902572 2.992219
C -1.744752 4.860265 4.177452
O -2.091267 0.028356 -0.743650
Pd 0.007577 -0.238021 -0.588160
C -0.175825 0.118823 -2.598255
C -0.675382 1.545141 -2.813935
C 0.542237 2.290296 -3.253851
C 1.624223 1.417229 -3.456373

C 1.166489 0.057489 -3.200281
C 2.887170 1.901679 -3.818194
C 3.030002 3.268451 -4.008502
C 1.944816 4.132420 -3.833533
C 0.699006 3.656011 -3.437082
C 1.922839 -1.114825 -3.390639
O 3.214241 -1.003023 -3.655850
O 1.902736 -1.152060 -0.749964
P 3.290553 -1.026788 -0.164198
O 4.465216 -1.053611 -1.085594
O 3.249515 0.314815 0.759267
C 4.341476 0.497417 1.591822
C 4.411080 -0.245697 2.756199
C 5.574104 -0.110641 3.581254
C 6.547766 0.870883 3.236592
C 6.368554 1.648173 2.071328
C 5.308799 1.459215 1.214235
C 5.829946 -0.936751 4.704978
C 6.961816 -0.769294 5.462646
C 7.902149 0.233322 5.143104
C 7.697053 1.031788 4.048657
C 3.329378 -1.203662 3.090656
C 2.951869 -2.167333 2.172757
C 2.023642 -3.211153 2.462641
C 1.495011 -3.236190 3.730729
C 1.751952 -2.217927 4.677837
C 2.653322 -1.164990 4.352103
C 1.100524 -2.210296 5.935217
C 1.299928 -1.187222 6.826152
C 2.160526 -0.121857 6.488251
C 2.822154 -0.111621 5.285260
C 1.635401 -4.134277 1.359146
C 0.324938 -4.100622 0.834139
C 0.089568 -4.712020 -0.399879
C 1.093536 -5.370939 -1.108508
C 2.340491 -5.511168 -0.499506
C 2.621080 -4.922660 0.733763
C -0.814601 -3.461425 1.597578
C -1.906540 -2.887665 0.712204
C 3.907118 -5.237917 1.473247
C 3.636838 -6.412093 2.418052
C 0.778680 -5.945791 -2.475534
C -0.069574 -7.211270 -2.345161
O 3.572938 -2.184487 0.943278
C 5.250349 2.296127 -0.019433
C 4.375595 3.392619 -0.092732
C 4.585240 4.364249 -1.075112
C 5.606320 4.251565 -2.012620
C 6.363608 3.080238 -2.008258

C 6.212629 2.098773 -1.031835
C 3.177149 3.527428 0.824453
C 1.905363 3.220370 0.025255
C 5.960855 5.349531 -2.994781
C 7.313613 5.957291 -2.614701
C 7.070207 0.848377 -1.095023
C 8.526768 1.132983 -0.732953
C 3.110637 4.889095 1.508818
C 4.923600 6.456678 -3.106167
C 6.983399 0.182449 -2.467681
C 5.107106 -5.535976 0.589292
C 2.006351 -6.224068 -3.334601
C -1.448768 -4.470215 2.562748
O 0.152460 -0.375097 1.657602
C 1.308928 -2.489513 -3.240702
C 0.927408 -2.557606 -4.723419
C 0.988497 -1.040718 -4.978402
C -4.607737 6.287814 -1.606490
C 1.188557 6.942202 -1.535782
C -0.392549 3.040075 3.092860
C -4.994805 -2.535998 -4.036476
C -2.860389 -7.278624 0.329388
C -5.370261 -3.307670 2.978124
O 5.803983 -3.146492 -1.807908
C 5.245119 -3.809730 -2.785345
C 5.829254 -5.169844 -2.997930
O 4.310705 -3.394608 -3.468776
H -0.876070 -0.667166 -2.881939
H -1.468923 1.569930 -3.579156
H -0.132916 4.337012 -3.255660
H 3.727180 1.223758 -3.933976
H 2.080113 5.201442 -3.995357
H 4.003244 3.672428 -4.279000
H 2.017363 -3.236283 -2.871822
H 0.453195 -2.474920 -2.558052
H 1.733691 -0.657733 -5.679309
H 0.025491 -0.542220 -5.106678
H 1.702915 -3.071564 -5.303543
H -0.042199 -3.014302 -4.946517
H 5.644547 -5.504178 -4.020252
H 5.332535 -5.864257 -2.308316
H 6.895960 -5.180270 -2.762417
H 3.678330 -1.872844 -3.534337
H 5.290369 -2.307159 -1.572608
H 0.906216 0.165078 1.929102
H -0.677184 0.093998 1.921529
H -1.125649 1.983601 -1.911984
H 7.111657 2.407980 1.829058
H 0.813392 -4.035466 4.013646

H 0.421081 -3.028766 6.168938
H 5.123444 -1.722085 4.958131
H 8.791568 0.358222 5.756016
H 2.298121 0.701251 7.185592
H 0.786027 -1.186246 7.784401
H 7.139249 -1.421682 6.314474
H 8.421884 1.795591 3.769843
H 3.479488 0.717276 5.033620
H 3.118446 -6.086970 -0.999288
H -0.907114 -4.645109 -0.846043
H 3.932706 5.237243 -1.089873
H 7.121030 2.946867 -2.784107
H -7.436642 -2.285236 -1.818010
H -4.605871 5.407976 2.481952
H -6.622437 5.416930 3.844161
H -7.647835 3.097018 -0.483685
H -10.537740 1.127272 -2.974630
H -9.482678 2.227636 3.498686
H -8.776334 4.391362 4.511470
H -9.669491 3.183790 -1.865074
H -9.305172 -1.010017 -2.733712
H -8.083662 1.127176 1.808916
H -1.580636 6.401245 -1.789188
H 0.167035 5.644371 2.036903
H -5.207684 -5.619806 1.271123
H -3.435175 -4.966735 -2.562125
H 3.260558 2.774559 1.620518
H 1.987783 2.244664 -0.475125
H 1.011409 3.212896 0.663804
H 1.741536 3.975938 -0.755942
H 2.282684 4.919884 2.229017
H 4.038905 5.107143 2.049987
H 2.945059 5.700073 0.786928
H 6.664003 0.128905 -0.370877
H 9.125129 0.215192 -0.788771
H 8.969940 1.861710 -1.425235
H 8.625179 1.536237 0.282124
H 5.938498 0.001468 -2.744624
H 7.456676 0.790857 -3.249721
H 7.503308 -0.783834 -2.448534
H 6.075182 4.881458 -3.988626
H 7.617369 6.728253 -3.333748
H 7.246713 6.423955 -1.622908
H 8.102658 5.198860 -2.570431
H 4.831808 7.003744 -2.158010
H 5.219250 7.180810 -3.873782
H 3.928641 6.075127 -3.365338
H 4.172451 -4.373411 2.095108
H 4.532225 -6.662660 3.000749

H 2.824129 -6.181693 3.117510
H 3.342514 -7.302346 1.845560
H 4.970705 -6.466434 0.019666
H 5.308039 -4.713231 -0.105906
H 6.001319 -5.675817 1.208014
H 0.163213 -5.191444 -2.999240
H 0.471555 -7.972818 -1.767580
H -1.016013 -7.010255 -1.828476
H -0.301968 -7.634141 -3.330834
H 1.701138 -6.519332 -4.345747
H 2.669114 -5.351908 -3.420013
H 2.595095 -7.056084 -2.923239
H -4.143738 -1.303792 -2.495874
H -6.406971 -2.090721 1.575812
H -3.403584 -7.064005 -1.726804
H -2.337930 -1.771040 -4.037228
H -1.921135 -2.456406 -2.436451
H -2.447001 -3.513772 -3.769075
H -6.032635 -2.306930 -3.770030
H -4.711187 -1.886540 -4.874318
H -4.959643 -3.575940 -4.388489
H -8.137688 -3.741985 0.911832
H -7.395599 -4.960547 1.963420
H -8.110159 -3.502446 2.672568
H -5.930581 -2.930408 3.842333
H -5.118988 -4.357569 3.179864
H -4.432719 -2.742390 2.910918
H -4.786547 -8.893230 -0.786443
H -5.597142 -7.754051 0.298891
H -5.825146 -7.613185 -1.451508
H -2.520554 -8.315480 0.210519
H -1.978083 -6.625637 0.286520
H -3.296564 -7.186931 1.333448
H -4.530755 4.207751 -1.174123
H -2.694978 5.299228 -3.361768
H -2.753860 3.604593 -2.822544
H -4.176910 4.361598 -3.567517
H -5.449258 6.196718 -2.304504
H -5.006100 6.575605 -0.625815
H -3.966275 7.106884 -1.957971
H -2.503241 3.212116 3.031151
H -1.728232 4.307870 5.124901
H -0.899620 5.561670 4.186861
H -2.666339 5.453940 4.147664
H -0.419941 2.430121 4.004930
H -0.332593 2.361984 2.232771
H 0.522374 3.649482 3.124793
H 1.267682 7.032937 0.598365
H 0.740496 9.317284 -0.227470

H -0.817329 8.742892 -0.852452
H -0.515688 8.743731 0.892481
H 0.495697 7.123284 -2.369847
H 2.026955 7.640980 -1.655443
H 1.575054 5.920172 -1.642137
H -0.399256 -2.632783 2.182408
H -1.495926 -2.276765 -0.101277
H -2.526379 -3.674325 0.265192
H -2.577469 -2.250398 1.301698
H -0.710318 -5.008836 3.167503
H -2.147730 -3.962319 3.240215
H -2.018728 -5.226331 2.007708

(TS-*re*)$_{IV\text{-}C}$
E0 = -6170.4941213
E0+ZPE = -6168.274555
E298 = -6168.151596
H298 = -6168.150652
G298 = -6168.421224
NImag = -371.0283
C 5.223445 -3.154349 -0.760174
C 5.896818 -2.024665 -0.276286
C 6.798077 -1.320590 -1.109419
C 6.921171 -1.707325 -2.439529
C 6.198442 -2.781591 -2.965916
C 5.390129 -3.510706 -2.102922
C 5.616220 -1.488895 1.081778
C 4.939996 -0.243185 1.167823
C 4.830224 0.477983 2.339153
C 5.146479 -0.194723 3.563036
C 5.740388 -1.490448 3.511384
C 6.019815 -2.079041 2.253529
C 4.833878 0.353340 4.831255
C 5.103312 -0.340067 5.985123
C 5.717478 -1.608879 5.933390
C 6.031357 -2.166989 4.720285
C 4.480422 1.915986 2.282280
C 3.366780 2.360407 1.596541
C 2.999308 3.731912 1.506102
C 3.792407 4.648905 2.148012
C 4.986463 4.272420 2.805461
C 5.364295 2.898326 2.844079
C 5.833403 5.247464 3.385349
C 7.031738 4.895156 3.949562
C 7.435662 3.544141 3.941033
C 6.625865 2.573743 3.405427
O 2.501050 1.435708 1.035292
P 2.907583 0.530589 -0.261603
O 4.500083 0.305243 -0.017214

C 1.772573 4.060371 0.732591
C 0.519482 4.041953 1.378832
C -0.630707 3.976681 0.591174
C -0.563969 3.986036 -0.802210
C 0.676155 4.163078 -1.405070
C 1.855858 4.187753 -0.667631
C 0.406663 4.138697 2.892528
C -0.590533 5.224340 3.297486
C -1.796867 3.692564 -1.615564
C -1.976923 2.176827 -1.638317
C 3.189851 4.384433 -1.365318
C 3.150107 4.123069 -2.867146
C 7.727377 -0.271642 -0.525223
C 8.962201 -0.980009 0.039068
C 6.340489 -3.199137 -4.412262
C 6.303610 -2.024232 -5.385254
C 4.373633 -4.027098 0.137260
C 2.967433 -4.236337 -0.400771
O 2.155183 -0.780673 -0.086101
Pd 0.022493 -0.830813 -0.257968
O -0.093246 0.460821 1.513001
C 0.083075 -2.063387 -1.940740
C -1.290847 -2.648082 -2.244008
C -1.929999 -1.578766 -3.076148
C -0.955920 -0.701179 -3.578475
C 0.338161 -1.107848 -3.029947
C -3.268297 -1.387852 -3.386061
C -3.608071 -0.348073 -4.246118
C -2.629834 0.485247 -4.799235
C -1.292400 0.325116 -4.465003
C 1.608085 -0.666851 -3.478192
O 1.666886 0.473427 -4.147249
O -2.068518 -0.951875 -0.311341
P -3.126912 -0.288087 0.554233
O -4.326402 0.071367 -0.493868
C -5.638857 0.102898 -0.067899
C -6.290360 -1.084333 0.229015
C -7.647898 -1.030100 0.692858
C -8.328998 0.219683 0.688389
C -7.622791 1.383503 0.319681
C -6.287700 1.365038 -0.010563
C -8.344773 -2.155986 1.204812
C -9.648242 -2.055422 1.621933
C -10.335590 -0.825269 1.556230
C -9.680138 0.290651 1.107143
C -5.578131 -2.382768 0.191164
C -4.399935 -2.530206 0.899130
C -3.786326 -3.793734 1.166785
C -4.435086 -4.899211 0.660698

C -5.554259 -4.801941 -0.198667
C -6.118309 -3.526312 -0.476836
C -6.109796 -5.954288 -0.806706
C -7.155470 -5.850603 -1.687849
C -7.686804 -4.580996 -1.999336
C -7.185488 -3.448799 -1.405748
O -3.852222 -1.412094 1.475535
C -2.491010 -3.849130 1.902144
C -1.366792 -4.513670 1.348093
C -0.115047 -4.339982 1.941747
C 0.075959 -3.541242 3.064719
C -1.057579 -2.994802 3.658321
C -2.332974 -3.152847 3.124429
C -5.613740 2.678409 -0.232339
C -5.595972 3.259091 -1.511004
C -5.184830 4.588760 -1.646092
C -4.768020 5.344242 -0.553431
C -4.749831 4.725948 0.697428
C -5.165861 3.410117 0.886977
C -6.106101 2.494782 -2.719791
C -7.586366 2.796857 -2.956244
C -4.312743 6.786779 -0.663619
C -2.818081 6.921901 -0.364625
C -5.204409 2.832275 2.290505
C -3.964337 3.174720 3.108636
C -1.468408 -5.501468 0.197766
C -0.262103 -5.533930 -0.736280
C 1.443212 -3.228224 3.626047
C 2.030408 -2.003522 2.922047
C -3.514421 -2.702465 3.965811
C -3.716005 -3.705510 5.104802
O 2.803306 1.251104 -1.566318
C 2.877893 -1.422575 -3.091742
C 2.639989 -2.608941 -4.032132
C 1.292703 -2.126549 -4.556541
O -2.751435 0.841481 1.451984
C -5.316395 2.769260 -3.994722
C -6.459934 3.295619 3.031098
C -4.627864 7.434424 -2.004163
C -1.670085 -6.914394 0.758009
C 2.426777 -4.390418 3.559868
C -3.383176 -1.284148 4.513260
C 8.145721 0.826418 -1.492400
C 7.615495 -4.019497 -4.607418
C 5.070349 -5.364699 0.386606
C 0.052604 2.819656 3.575999
C -1.775501 4.258957 -3.028203
C 3.695771 5.810885 -1.133065
O 5.108877 1.646167 -2.795340

C 5.144349 1.425553 -4.086661
O 4.193027 1.036269 -4.757035
C 6.492289 1.677336 -4.683468
H 0.888680 -2.766586 -1.711827
H -1.170483 -3.567279 -2.846861
H -4.034375 -2.025107 -2.946271
H -0.527221 0.989842 -4.854896
H -4.654375 -0.177347 -4.494634
H -2.924147 1.284743 -5.476130
H 3.782909 -0.848178 -3.303254
H 2.892691 -1.684038 -2.031349
H 1.284851 -1.587411 -5.508219
H 0.448426 -2.818200 -4.513769
H 3.389229 -2.700830 -4.827776
H 2.578805 -3.572032 -3.512606
H 6.450022 1.568486 -5.767754
H 7.204828 0.957480 -4.263242
H 6.846620 2.675386 -4.407169
H 2.605827 0.712031 -4.356056
H 4.202371 1.486519 -2.390787
H 0.451661 1.248858 1.364150
H -1.033479 0.752701 1.593150
H -1.872736 -2.918255 -1.356889
H 3.510131 5.702079 2.132023
H 6.548123 -3.033180 2.220486
H 6.491664 -3.152639 4.662942
H 6.960104 1.539889 3.399171
H 7.678375 5.652814 4.385622
H 4.835056 0.089962 6.947144
H 5.931622 -2.145180 6.854743
H 8.401285 3.267290 4.357814
H 5.515403 6.288694 3.356039
H 4.348918 1.325537 4.881480
H 7.618835 -1.172647 -3.084859
H 4.864516 -4.385158 -2.493651
H -1.614597 3.891461 1.061568
H 0.729311 4.219118 -2.489208
H 7.219190 0.221742 0.314745
H 9.504215 -1.495847 -0.765248
H 9.647715 -0.260619 0.503781
H 8.691078 -1.729350 0.792194
H 8.766093 0.437072 -2.312265
H 7.272434 1.333331 -1.915484
H 8.752176 1.572510 -0.965759
H 4.266673 -3.523838 1.108584
H 2.963990 -4.703329 -1.396763
H 2.406770 -4.902242 0.265574
H 2.430481 -3.279771 -0.446816
H 6.082105 -5.221435 0.785589

H 4.502060 -5.969882 1.104441
H 5.161115 -5.944538 -0.541676
H 5.482814 -3.853780 -4.641463
H 7.200543 -1.397502 -5.288045
H 6.278671 -2.383422 -6.420991
H 5.429374 -1.377471 -5.227126
H 7.627764 -4.896616 -3.950356
H 7.711843 -4.363777 -5.644589
H 8.500044 -3.413903 -4.369210
H 3.914973 3.679335 -0.925786
H -2.659562 4.118002 -1.084296
H 1.391147 4.444878 3.273192
H -0.377116 6.174578 2.793744
H -1.620938 4.936417 3.049450
H -0.552696 5.392160 4.380816
H 0.799400 2.038238 3.386305
H -0.009221 2.960600 4.662387
H -0.924021 2.443460 3.240595
H 2.569453 4.895450 -3.389486
H 4.168953 4.159173 -3.273109
H 2.713950 3.145963 -3.102781
H 3.836513 6.035732 -0.071077
H 4.654548 5.972195 -1.641950
H 2.972936 6.533390 -1.535897
H -2.875224 1.875171 -2.196678
H -1.098722 1.694566 -2.098077
H -2.070088 1.802425 -0.614195
H -1.065683 3.716166 -3.668404
H -2.767050 4.159514 -3.487816
H -1.499219 5.321986 -3.048749
H -4.069527 -5.895645 0.894239
H -8.142278 2.342322 0.349438
H -10.177701 1.259279 1.079171
H -7.603933 -2.474581 -1.648170
H -7.568476 -6.740917 -2.156267
H -10.153270 -2.934337 2.016139
H -11.371239 -0.762760 1.881699
H -8.499603 -4.498288 -2.717233
H -5.673191 -6.924302 -0.571493
H -7.832775 -3.110442 1.282350
H -5.199973 5.045187 -2.634558
H -4.418148 5.306314 1.560982
H -0.937912 -2.432556 4.585249
H 0.740574 -4.847444 1.501167
H -6.002113 1.420255 -2.499871
H -7.726104 3.868851 -3.150709
H -7.967355 2.243555 -3.823941
H -8.198802 2.530498 -2.087677
H -5.431917 3.806400 -4.336068

H -4.246900 2.570195 -3.857358
H -5.678902 2.126003 -4.807898
H -5.239370 1.736901 2.206267
H -3.938058 4.237211 3.387976
H -3.957801 2.595641 4.040471
H -3.055638 2.919156 2.554493
H -7.379053 2.982188 2.522627
H -6.481253 2.885459 4.048428
H -6.476934 4.391220 3.109444
H -4.855144 7.345282 0.117880
H -2.221897 6.425701 -1.142080
H -2.522514 7.977956 -0.338470
H -2.542180 6.465662 0.593241
H -5.693981 7.376101 -2.252582
H -4.340297 8.492013 -1.991882
H -4.062461 6.953736 -2.815063
H -2.342866 -5.238007 -0.412431
H 1.300846 -2.970420 4.688099
H -4.422847 -2.740571 3.353834
H -3.853722 -4.722764 4.717946
H -2.847594 -3.719090 5.776386
H -4.598450 -3.442244 5.701631
H -3.191869 -0.559114 3.714370
H -4.308787 -0.993460 5.025701
H -2.573216 -1.208412 5.250523
H 0.594704 -6.043644 -0.278139
H -0.511980 -6.092339 -1.647583
H 0.064728 -4.529778 -1.023647
H -2.511706 -6.979788 1.456390
H -1.829723 -7.641821 -0.048610
H -0.774721 -7.219897 1.315715
H 2.990695 -1.726827 3.379414
H 2.206309 -2.207949 1.855531
H 1.360280 -1.135172 2.962792
H 2.691867 -4.629098 2.520332
H 3.361039 -4.121505 4.069764
H 2.027748 -5.299825 4.024713

(TS-*si*)'$_{IV}$
E0 = -6170.5013943
E0+ZPE = -6168.286482
E298 = -6168.160952
H298 = -6168.160008
G298 = -6168.440032
NImag = -382.3160
C -1.382996 -5.346455 -0.694499
C -0.518339 -4.435275 -0.077751
C 0.802097 -4.273566 -0.526615
C 1.260892 -4.990729 -1.623709

C 0.398030 -5.889689 -2.242923
C -0.904527 -6.077890 -1.772072
C 1.536319 -3.297229 0.328925
C 0.439617 -2.647636 1.161864
C -0.726329 -3.539324 1.054853
Pd -0.038915 -0.833949 0.322664
O -0.302517 1.191237 -0.553109
C -1.888343 -3.519601 1.859695
C -1.961436 -2.690125 3.132097
C -0.980328 -3.563392 3.927224
C -0.800723 -4.615307 2.837935
O -2.017832 -1.398328 -0.184834
P -3.251271 -0.696010 0.353477
O -4.064277 -1.334971 1.429316
O -4.273120 -0.333889 -0.858831
C -4.014277 0.695634 -1.737806
C -4.091785 2.014787 -1.308091
C -3.857722 3.050939 -2.277675
C -3.694784 2.703844 -3.649896
C -3.682195 1.342310 -4.019695
C -3.797133 0.334669 -3.094020
C -3.766283 4.423195 -1.937596
C -3.577423 5.388782 -2.895996
C -3.473136 5.041092 -4.259061
C -3.522523 3.720171 -4.621116
C -4.371358 2.345538 0.113866
C -3.631292 1.744683 1.116018
C -3.697605 2.106227 2.486676
C -4.564199 3.117991 2.823074
C -5.431631 3.705355 1.872088
C -5.375045 3.290557 0.509092
C -6.387599 4.673565 2.265991
C -7.287052 5.183729 1.366245
C -7.272435 4.730444 0.030614
C -6.341899 3.811627 -0.386581
C -2.876395 1.380044 3.496256
C -3.499539 0.501606 4.405920
C -2.703848 -0.190705 5.319922
C -1.318597 -0.063187 5.346621
C -0.725373 0.812991 4.442009
C -1.476665 1.547954 3.524255
C -5.002060 0.289097 4.443201
C -5.384578 -1.185026 4.525584
C -0.785599 2.597130 2.676446
C -0.866653 3.940859 3.406866
C -0.517481 -0.832802 6.374074
C 0.940665 -1.038982 5.986631
O -2.710378 0.782389 0.768474
C -3.762363 -1.080653 -3.556819

C -4.966618 -1.731306 -3.865279
C -4.912931 -2.992820 -4.458840
C -3.707154 -3.625700 -4.735545
C -2.525028 -2.982645 -4.367221
C -2.524713 -1.716443 -3.782540
C -6.316668 -1.089586 -3.614376
C -7.001914 -0.732450 -4.932032
C -3.690190 -4.954522 -5.456839
C -2.938200 -6.028524 -4.679527
C -1.210779 -1.044766 -3.423090
C -0.167574 -2.031907 -2.913462
C -7.213165 -1.966939 -2.744852
C -3.114719 -4.803200 -6.863701
C -0.627983 -0.243154 -4.586867
C 0.669347 2.283272 2.353474
C -0.605923 -0.139167 7.734320
C -5.624262 1.058574 5.608781
O 1.995721 -0.319352 0.650561
P 2.702342 0.350481 -0.525116
O 1.970454 0.574279 -1.806778
O 3.318448 1.739288 0.079024
C 4.117303 2.447647 -0.799918
C 5.379316 1.962307 -1.078456
C 6.162499 2.620204 -2.079622
C 5.696101 3.853011 -2.616526
C 4.471211 4.384838 -2.151312
C 3.650065 3.695676 -1.290392
C 6.474198 4.528118 -3.587769
C 7.654377 3.994729 -4.038331
C 8.102102 2.756231 -3.532089
C 7.378708 2.088870 -2.575412
C 5.924352 0.832067 -0.295188
C 5.243916 -0.369941 -0.204212
C 5.801388 -1.507126 0.442849
C 7.039216 -1.369330 1.028836
C 7.722038 -0.136091 1.077876
C 7.148947 0.994972 0.431538
C 7.809007 2.243362 0.569431
C 8.983746 2.348592 1.271215
C 9.571089 1.214083 1.870738
C 8.946190 -0.001854 1.776875
C 2.435816 4.354798 -0.728763
C 2.571885 5.013653 0.506643
C 1.486015 5.731439 1.004442
C 0.269620 5.798754 0.333738
C 0.148978 5.119983 -0.879945
C 1.214776 4.403507 -1.432250
O 4.045873 -0.526728 -0.860266
C 5.150971 -2.845199 0.496499

C 4.794132 -3.398979 1.745828
C 4.373561 -4.725991 1.797439
C 4.263030 -5.525039 0.658847
C 4.593289 -4.946819 -0.563097
C 5.038167 -3.625382 -0.667795
C 4.773162 -2.580901 3.023256
C 3.333486 -2.228574 3.400291
C 3.792197 -6.959520 0.805952
C 2.372664 -7.026545 1.377322
C 5.466366 -3.105568 -2.026222
C 4.369982 -3.237780 -3.078971
C 3.864658 5.015079 1.301671
C 3.680643 4.411206 2.691788
C -0.833002 6.665086 0.902561
C -0.764171 8.061554 0.282620
C 1.078826 3.755200 -2.799442
C 1.526650 4.719383 -3.902528
C 5.493207 -3.266057 4.180670
C 3.863368 -7.771712 -0.479094
C 6.756416 -3.792669 -2.471747
C 4.447121 6.425054 1.374071
C -2.232451 6.088469 0.733164
C -0.336888 3.297996 -3.139511
O -2.970037 -4.106153 1.369768
O -6.422475 -2.440577 1.547676
C -6.342871 -3.538584 2.258624
O -5.296280 -4.055535 2.636236
C -7.686144 -4.101951 2.604584
H 0.724499 -2.318303 2.167972
H 2.252083 -3.828710 0.979660
H 2.277640 -4.848261 -1.984719
H -2.399509 -5.467416 -0.337408
H 0.741496 -6.459881 -3.104515
H -1.553510 -6.797539 -2.264162
H -2.981934 -2.705539 3.524706
H -1.677944 -1.635696 3.007027
H -1.472272 -5.478460 2.865943
H 0.214495 -4.936843 2.584185
H -1.390203 -3.974360 4.856091
H -0.043314 -3.055695 4.176750
H -3.566268 1.081094 -5.072081
H -4.619235 3.453092 3.859318
H -8.320646 -4.140085 1.714806
H -7.578098 -5.093243 3.045830
H -8.176660 -3.434045 3.321128
H -3.781183 -3.956010 1.919639
H -5.516519 -2.025767 1.420681
H -6.402278 4.987823 3.308690
H -3.846712 4.714406 -0.896303

H -3.335712 5.814493 -5.010735
H -8.008648 5.108331 -0.675033
H -8.022156 5.920093 1.682053
H -3.507591 6.433551 -2.596771
H -3.414652 3.421383 -5.662879
H -6.348423 3.465904 -1.416884
H 0.354791 0.940501 4.450299
H -3.176003 -0.874872 6.028161
H -5.842429 -3.497570 -4.728481
H -1.570704 -3.479125 -4.547725
H -1.318590 2.688983 1.717172
H -0.388006 3.859875 4.392823
H -0.334884 4.713027 2.837011
H -1.901984 4.271191 3.562512
H 1.312129 2.414572 3.235991
H 0.810897 1.265290 1.974029
H 1.037123 2.972797 1.583892
H -5.427555 0.679705 3.509059
H -5.094174 -1.632592 5.485265
H -6.473498 -1.294935 4.436235
H -4.913306 -1.755194 3.718740
H -5.413769 2.133075 5.551890
H -6.713239 0.925781 5.627284
H -5.225789 0.696984 6.566537
H -0.989585 -1.825725 6.470642
H 1.503694 -0.097420 6.036343
H 1.427435 -1.743959 6.671190
H 1.045588 -1.424167 4.963388
H -1.644614 -0.033872 8.067295
H -0.053235 -0.695760 8.501511
H -0.174148 0.868402 7.667615
H -1.415238 -0.340314 -2.600964
H -4.737356 -5.281985 -5.554973
H -6.154268 -0.151769 -3.066690
H -6.376078 -0.064570 -5.536822
H -7.200648 -1.632134 -5.529059
H -7.961840 -0.232565 -4.752126
H -6.723215 -2.217743 -1.797318
H -8.151181 -1.446599 -2.515369
H -7.475182 -2.905254 -3.250970
H 0.238412 -2.652250 -3.725218
H 0.678417 -1.485429 -2.472206
H -0.599936 -2.698309 -2.159810
H -1.304344 0.553175 -4.922322
H 0.323150 0.215135 -4.280788
H -0.429829 -0.900745 -5.444454
H -3.010327 -7.000184 -5.184082
H -1.872241 -5.777504 -4.592688
H -3.339717 -6.132688 -3.664415

H -2.063036 -4.490902 -6.822533
H -3.159704 -5.752532 -7.412031
H -3.662202 -4.047345 -7.437923
H -1.209520 1.280828 -0.872483
H 0.321349 1.123763 -1.311410
H 2.145828 -2.581236 -0.234633
H 4.175467 5.381653 -2.478514
H 7.492728 -2.239445 1.506224
H 9.369417 -0.886349 2.251262
H 7.729285 1.131192 -2.197738
H 8.239770 4.516242 -4.791875
H 9.463351 3.319575 1.371557
H 10.506977 1.311220 2.415838
H 9.027198 2.324263 -3.906957
H 6.104702 5.475401 -3.978555
H 7.367523 3.130584 0.122602
H 4.536706 -5.547894 -1.470425
H 4.114669 -5.156171 2.766866
H 1.588478 6.264366 1.952588
H -0.797623 5.160192 -1.420969
H 1.737758 2.873046 -2.813424
H 2.581127 4.996511 -3.818564
H 1.378507 4.265796 -4.890612
H 0.928846 5.640425 -3.861133
H -0.992865 4.150139 -3.363109
H -0.324926 2.662510 -4.034351
H -0.813788 2.735842 -2.329830
H -0.635878 6.768072 1.981823
H -0.928719 7.999642 -0.802228
H -1.531144 8.723110 0.704979
H 0.217273 8.522546 0.443750
H -2.287503 5.024004 1.003745
H -2.956960 6.634083 1.350071
H -2.556897 6.185245 -0.309591
H 4.600188 4.390134 0.777877
H 2.920359 4.949881 3.274347
H 3.367206 3.363552 2.621957
H 4.621805 4.450372 3.254231
H 4.604656 6.835382 0.368800
H 3.775854 7.107273 1.911795
H 5.410219 6.422711 1.899416
H 5.687179 -2.036218 -1.933621
H 3.445554 -2.737934 -2.760259
H 4.689627 -2.775708 -4.020517
H 4.139747 -4.289735 -3.299415
H 7.551138 -3.648138 -1.729260
H 6.609589 -4.873434 -2.598494
H 7.104877 -3.387199 -3.429609
H 5.287877 -1.632090 2.832483

H 2.739426 -3.137726 3.592344
H 3.315783 -1.621101 4.314435
H 2.845917 -1.654527 2.599592
H 5.531073 -2.601705 5.052157
H 4.980894 -4.183851 4.497060
H 6.522292 -3.535259 3.913226
H 4.462791 -7.432893 1.542983
H 1.648465 -6.606763 0.664309
H 2.083727 -8.066256 1.573613
H 2.284684 -6.471894 2.319895
H 4.868439 -7.768874 -0.915941
H 3.583636 -8.813342 -0.284946
H 3.161799 -7.380621 -1.229950

VII. Coordinates of the Optimized Geometries of Transition States at the B3LYP/6-31G**,LANL2DZ(Pd) Level of Theory

(TS-*re*)$_{IV}$
E0 = -6174.3454075
E0+ZPE = -6172.134626
E298 = -6172.002669
H298 = -6172.001725
G298 = -6172.315000
NImag = -355.8548

6	-2.514204	-1.809406	-4.516762
6	-1.359176	-1.174249	-4.032196
6	-0.136432	-1.870775	-3.934185
6	-0.057837	-3.206876	-4.316569
6	-1.205457	-3.835202	-4.806494
6	-2.420802	-3.143093	-4.904781
6	0.950015	-0.970323	-3.411297
6	0.192596	0.290484	-2.957269
6	-1.138872	0.207722	-3.596087
46	0.006905	0.316500	-0.875306
8	-2.001372	0.935286	-0.944592
15	-3.373010	0.735350	-0.317116
8	-4.568025	0.835634	-1.220015
6	-2.079051	1.266976	-3.728180
8	-3.344923	0.948765	-3.963035
8	2.111476	0.010269	-0.891056
15	2.981713	-0.393655	0.303848
8	2.354537	-0.467405	1.665665
8	4.264249	0.636660	0.421005
6	5.462789	0.525660	-0.262170
6	6.222283	-0.632827	-0.158083
6	7.395983	-0.770194	-0.979892

6	7.846143	0.354320	-1.739422
6	7.126767	1.570064	-1.648686
6	5.944119	1.685816	-0.945070
6	8.121384	-1.988807	-1.099188
6	9.233267	-2.078043	-1.907820
6	9.691139	-0.953687	-2.634591
6	9.007434	0.236923	-2.549864
6	5.858215	-1.716229	0.796289
6	4.628659	-2.347824	0.708792
6	4.331267	-3.553277	1.407859
6	5.266916	-4.002133	2.319221
6	6.467951	-3.300257	2.588670
6	6.784680	-2.141938	1.811269
6	7.369302	-3.734760	3.597593
6	8.529110	-3.041073	3.854438
6	8.831932	-1.878258	3.107372
6	7.987006	-1.442748	2.110153
6	3.145133	-4.429530	1.124315
6	3.178462	-5.284285	-0.003653
6	2.189498	-6.263617	-0.143181
6	1.173669	-6.435474	0.799746
6	1.137543	-5.550539	1.880292
6	2.093584	-4.542618	2.061294
6	4.274511	-5.201245	-1.066247
6	3.701816	-4.770850	-2.430725
6	1.974483	-3.609897	3.266167
6	2.256796	-4.347154	4.589683
6	0.172337	-7.580535	0.707550
6	0.783030	-8.878405	1.275819
8	3.675778	-1.814489	-0.158983
6	5.309348	3.043288	-0.857354
6	4.765337	3.647827	-2.013407
6	4.367729	4.989600	-1.955186
6	4.490141	5.756363	-0.796048
6	4.997491	5.127424	0.345030
6	5.416026	3.792384	0.341213
6	4.589611	2.889723	-3.328419
6	3.100763	2.779248	-3.703028
6	4.147452	7.241460	-0.811105
6	5.426796	8.100041	-0.747339
6	6.034234	3.219334	1.617158
6	7.299053	3.996879	2.031849
6	5.405771	3.510354	-4.477712
6	3.161483	7.648767	0.296833
6	5.016135	3.153732	2.770759
6	0.602119	-2.912792	3.315287
6	-0.370793	-7.813179	-0.712091
6	5.069575	-6.515807	-1.182461
8	-0.074443	0.356618	1.331795

8	-3.295358	-0.698435	0.473214
6	-4.321679	-1.004159	1.369613
6	-4.323000	-0.360090	2.597718
6	-5.408640	-0.618587	3.509072
6	-6.364930	-1.627876	3.169083
6	-6.244392	-2.310434	1.933797
6	-5.268621	-2.004941	1.005762
6	-7.431653	-1.915478	4.063503
6	-7.579056	-1.213425	5.236637
6	-6.663312	-0.183359	5.555282
6	-5.607948	0.105386	4.718233
6	-3.266040	0.635002	2.944804
6	-3.048942	1.742262	2.132789
6	-2.334778	2.897557	2.572792
6	-1.715725	2.826061	3.803303
6	-1.721526	1.645362	4.589090
6	-2.507719	0.527558	4.163258
6	-2.484391	-0.652630	4.957005
6	-1.735209	-0.715670	6.112212
6	-0.979724	0.400111	6.543779
6	-0.976399	1.554853	5.795293
6	-5.240490	-2.785272	-0.278530
6	-4.334583	-3.856974	-0.424460
6	-4.460723	-4.716057	-1.524652
6	-5.452427	-4.543537	-2.489560
6	-6.300801	-3.439583	-2.353976
6	-6.219685	-2.553234	-1.276223
8	-3.661577	1.810394	0.893507
6	-2.321451	4.168981	1.775313
6	-3.513257	4.928820	1.650630
6	-3.475985	6.136625	0.948627
6	-2.302825	6.625573	0.366422
6	-1.142235	5.867576	0.513109
6	-1.118843	4.649615	1.206932
6	-4.820197	4.523333	2.333594
6	-5.058788	5.387041	3.589734
6	-2.279926	7.949198	-0.387129
6	-2.602648	9.138438	0.537766
6	0.212552	3.913485	1.350648
6	0.949254	3.744576	0.010209
6	-3.214466	-4.119888	0.577957
6	-1.836991	-3.906211	-0.077990
6	-5.671124	-5.515543	-3.646170
6	-6.933067	-6.370254	-3.401193
6	-7.190609	-1.374234	-1.214481
6	-8.612689	-1.826702	-0.828526
6	-6.037112	4.571164	1.392986
6	1.124694	4.622637	2.373026
6	-3.214428	7.934184	-1.611334

6	-3.330200	-5.512953	1.224951
6	-4.469916	-6.422033	-3.948811
6	-7.218822	-0.578115	-2.533254
6	-1.688207	2.719165	-3.430078
6	-0.786118	2.918812	-4.670488
6	-1.048859	1.549403	-5.302274
8	-6.076001	2.758196	-1.881821
6	-5.830049	3.342134	-3.027553
6	-6.731906	4.521353	-3.299487
8	-4.954504	3.000586	-3.832061
1	0.730309	1.227141	-3.094384
1	1.662680	-0.720252	-4.213116
1	0.878940	-3.751231	-4.237851
1	-3.451415	-1.272847	-4.575402
1	-1.156884	-4.876534	-5.113271
1	-3.301276	-3.653990	-5.280972
1	-2.575223	3.352861	-3.432340
1	-1.193859	2.818492	-2.463332
1	-1.886220	1.481392	-5.996291
1	-0.204620	0.953487	-5.642918
1	-1.094922	3.746000	-5.316703
1	0.265309	3.067036	-4.419161
1	-7.777871	4.220889	-3.193857
1	-6.548669	4.912079	-4.299713
1	-6.542188	5.300696	-2.554868
1	-3.963135	1.731966	-3.863302
1	-5.434653	1.989841	-1.656362
1	-0.757689	-0.240879	1.665058
1	0.822039	0.011188	1.626570
1	1.543203	-1.417514	-2.611637
1	-6.958215	-3.095587	1.702161
1	-1.188779	3.696948	4.180572
1	-0.388991	2.414221	6.107680
1	-4.924678	0.903975	4.977983
1	-8.401590	-1.435623	5.910137
1	-1.722669	-1.631940	6.695342
1	-0.397393	0.338493	7.458343
1	-6.795701	0.390610	6.467904
1	-8.138880	-2.694808	3.791607
1	-3.056403	-1.515752	4.636006
1	-4.388679	6.720565	0.866411
1	-0.220245	6.240390	0.074207
1	-3.765830	-5.544574	-1.614417
1	-7.058532	-3.270462	-3.115690
1	7.520696	2.447218	-2.154491
1	5.076024	-4.930911	2.849517
1	7.116677	-4.622562	4.171583
1	7.782718	-2.862074	-0.554837
1	10.573680	-1.036602	-3.262153

1	9.738094	-1.320288	3.325149
1	9.207697	-3.376429	4.633314
1	9.761968	-3.023310	-1.990768
1	9.338779	1.107110	-3.110803
1	8.230492	-0.545865	1.552989
1	2.232772	-6.926392	-1.002749
1	0.342548	-5.659917	2.614538
1	5.102000	5.700661	1.262338
1	3.965639	5.460259	-2.849673
1	-3.303727	-3.391040	1.387865
1	-1.756972	-2.892853	-0.481956
1	-1.029869	-4.056372	0.645453
1	-1.676021	-4.606460	-0.904850
1	-2.549594	-5.648475	1.981853
1	-4.301343	-5.642664	1.714032
1	-3.219257	-6.315145	0.487475
1	-6.832106	-0.689063	-0.441946
1	-9.290474	-0.966899	-0.779686
1	-9.015776	-2.529769	-1.566582
1	-8.629875	-2.323049	0.146448
1	-6.208606	-0.290549	-2.831860
1	-7.675667	-1.151286	-3.348107
1	-7.808887	0.335575	-2.403934
1	-5.861840	-4.907112	-4.542497
1	-7.131565	-7.028559	-4.254711
1	-6.804996	-6.997064	-2.511531
1	-7.815768	-5.744046	-3.241735
1	-4.291283	-7.136045	-3.136914
1	-4.654316	-7.004427	-4.857568
1	-3.551518	-5.844936	-4.092560
1	-4.725583	3.489929	2.673484
1	-5.973037	5.073529	4.106425
1	-4.224570	5.302895	4.293770
1	-5.166728	6.445392	3.326945
1	-6.265141	5.593810	1.071425
1	-5.879127	3.959376	0.501153
1	-6.924917	4.191513	1.910760
1	-1.255700	8.090081	-0.757542
1	-3.620300	9.065099	0.937001
1	-1.914266	9.175406	1.387802
1	-2.525786	10.086913	-0.005856
1	-3.135443	8.872465	-2.171842
1	-2.966448	7.110214	-2.288002
1	-4.261219	7.815150	-1.310370
1	4.956409	1.870700	-3.181948
1	6.349555	2.193657	1.412930
1	3.662443	7.447736	-1.774786
1	2.977073	2.178901	-4.612395
1	2.546296	2.301612	-2.890914

1	2.659695	3.765404	-3.887804
1	6.472307	3.548999	-4.234326
1	5.290173	2.919965	-5.393654
1	5.080147	4.532720	-4.698830
1	8.037014	4.014479	1.223281
1	7.068796	5.034751	2.295748
1	7.764560	3.529354	2.906635
1	5.476971	2.712053	3.661347
1	4.654315	4.151177	3.044721
1	4.156033	2.537415	2.495801
1	5.184780	9.166037	-0.824524
1	5.957349	7.944194	0.198555
1	6.114398	7.845436	-1.559882
1	2.917618	8.714225	0.221691
1	2.228954	7.081083	0.227856
1	3.582090	7.477359	1.293507
1	4.985526	-4.429013	-0.763323
1	2.976697	-5.500774	-2.808441
1	3.200497	-3.801874	-2.348546
1	4.502905	-4.680325	-3.172975
1	5.885267	-6.406768	-1.905996
1	5.505729	-6.799425	-0.219308
1	4.438349	-7.345259	-1.518985
1	2.721207	-2.819600	3.154436
1	2.187159	-3.655763	5.436827
1	1.535849	-5.155502	4.757209
1	3.258209	-4.788854	4.598022
1	0.571997	-2.188683	4.135990
1	0.413088	-2.375543	2.382235
1	-0.215193	-3.625509	3.473246
1	-0.680414	-7.312853	1.344807
1	0.049808	-9.692963	1.265904
1	1.647202	-9.194087	0.680328
1	1.123328	-8.737291	2.306363
1	0.410832	-8.168609	-1.392627
1	-1.157510	-8.575360	-0.698134
1	-0.791031	-6.895389	-1.133980
1	0.008184	2.907684	1.724735
1	0.316795	3.226605	-0.717438
1	1.255201	4.702270	-0.423422
1	1.856803	3.149016	0.147790
1	0.648689	4.703527	3.355166
1	2.062709	4.072210	2.495408
1	1.371016	5.638125	2.044496

(TS-*si*)$_{IV}$
E0 = -6174.3450907
E0+ZPE = -6172.133965
E298 = -6172.002092

H298 = -6172.001148
G298 = -6172.312616
NImag = -355.0816

6	4.937419	-3.213394	1.957369
6	5.438153	-2.830298	0.691058
6	5.482787	-3.771330	-0.364358
6	5.045135	-5.079724	-0.127343
6	4.565425	-5.490395	1.120678
6	4.508485	-4.535201	2.139145
6	6.083874	-1.486243	0.526658
6	5.508527	-0.388180	-0.183613
6	6.187320	0.811542	-0.357043
6	7.436360	1.015306	0.334108
6	8.024345	-0.078664	1.041966
6	7.334089	-1.312151	1.085658
6	9.268352	0.094661	1.707274
6	9.902214	1.314747	1.710418
6	9.303602	2.414082	1.051200
6	8.108782	2.269905	0.380891
8	4.280300	-0.592891	-0.796086
15	2.940129	0.348310	-0.587612
8	3.574297	1.751528	0.013304
6	4.386544	2.445757	-0.887033
6	5.630969	1.913714	-1.188295
6	6.396305	2.501970	-2.253030
6	5.936832	3.725097	-2.833112
6	4.750961	4.318805	-2.334153
6	3.943671	3.702393	-1.398206
6	7.578014	1.910324	-2.777867
6	8.272098	2.507719	-3.807073
6	7.831479	3.734374	-4.358464
6	6.687022	4.328150	-3.878532
6	2.742947	4.436413	-0.874609
6	2.795999	4.995968	0.425485
6	1.742123	5.812234	0.853682
6	0.645803	6.108388	0.042794
6	0.606186	5.532319	-1.230816
6	1.628635	4.704687	-1.712353
6	3.992864	4.815071	1.360960
6	4.699349	6.159014	1.629724
6	-0.424696	7.081615	0.521002
6	-1.845526	6.501972	0.428487
6	1.527563	4.171976	-3.145074
6	0.153960	3.556091	-3.473649
6	6.063516	-3.420686	-1.734232
6	7.361995	-4.205104	-2.008841
6	4.182484	-6.938318	1.405553
6	5.442242	-7.793152	1.654277

6	4.858882	-2.244098	3.137965
6	5.688639	-2.733171	4.340494
8	2.278847	0.570685	-1.917145
8	2.094788	-0.253310	0.543495
46	0.067777	-0.820056	0.149870
8	-1.951548	-1.274420	-0.157110
15	-3.237828	-0.682749	0.407935
8	-4.320871	-0.421280	-0.791838
6	-4.208868	0.630940	-1.689033
6	-4.328181	1.937488	-1.229901
6	-4.143322	3.009643	-2.174261
6	-4.000272	2.694990	-3.563556
6	-4.026592	1.339529	-3.972476
6	-4.106782	0.298216	-3.071814
6	-4.082745	4.379910	-1.795928
6	-3.925680	5.374462	-2.737288
6	-3.815626	5.059160	-4.112255
6	-3.847335	3.743305	-4.511072
6	-4.677680	2.218724	0.194697
6	-3.926060	1.687107	1.234665
6	-4.134678	2.025791	2.606110
6	-5.152320	2.915296	2.886685
6	-6.033181	3.403261	1.890171
6	-5.822409	3.028827	0.525122
6	-7.139511	4.229271	2.228985
6	-8.034434	4.640422	1.269159
6	-7.859077	4.230399	-0.073490
6	-6.783056	3.450661	-0.436459
8	-2.870182	0.832924	0.920312
6	-3.306226	1.470001	3.729531
6	-1.973363	1.907257	3.919604
6	-1.245985	1.429383	5.014612
6	-1.796016	0.542593	5.943826
6	-3.114580	0.133351	5.743986
6	-3.885666	0.571312	4.659072
6	-4.162078	-1.112227	-3.581879
6	-5.401416	-1.791539	-3.624784
6	-5.459129	-3.050630	-4.233030
6	-4.339119	-3.657413	-4.802455
6	-3.121463	-2.975180	-4.729684
6	-3.004720	-1.715762	-4.130237
6	-6.696654	-1.174347	-3.098017
6	-7.395430	-2.066879	-2.055835
6	-4.459783	-5.010014	-5.493161
6	-4.098941	-4.923953	-6.988208
6	-1.637125	-1.032411	-4.105156
6	-1.206485	-0.577031	-5.513702
6	-1.314517	2.940742	3.009377
6	0.002757	2.426056	2.405026

6	-1.002041	0.054048	7.148710
6	-0.641416	1.210327	8.101102
6	-5.329130	0.076960	4.551038
6	-6.232482	0.754617	5.601860
6	0.529909	-2.675181	0.968253
6	1.631174	-3.306060	0.096840
6	0.884223	-4.272868	-0.778927
6	-0.435960	-4.446460	-0.316768
6	-0.620580	-3.602933	0.868844
6	1.334769	-4.972872	-1.895486
6	0.460311	-5.853478	-2.536769
6	-0.849895	-6.033989	-2.072145
6	-1.313699	-5.333101	-0.962203
6	-1.747639	-3.659454	1.733576
8	-2.831855	-4.264379	1.274585
8	-0.190200	1.069845	-1.017403
6	-1.771267	-2.900837	3.064962
6	-0.697884	-3.754414	3.779053
6	-0.536892	-4.795440	2.669725
8	-3.977839	-1.458366	1.465152
6	-3.627794	-6.096396	-4.787433
6	-7.651332	-0.824704	-4.257682
6	-0.553204	-1.921010	-3.469253
6	-1.099648	4.271524	3.758257
6	0.257553	-0.729434	6.734684
6	-5.439973	-1.452992	4.670096
6	1.836882	5.281279	-4.173914
6	-0.327991	8.422223	-0.234801
6	3.605049	4.116936	2.677358
6	5.044759	-3.618956	-2.870989
6	3.401291	-1.957282	3.546895
6	3.302505	-7.570403	0.314240
8	-6.183255	-2.731401	1.484704
6	-6.115964	-3.876376	2.120357
6	-7.461495	-4.532621	2.310230
8	-5.075313	-4.392476	2.544044
1	0.834727	-2.391773	1.974460
1	2.353592	-3.843002	0.727546
1	2.347267	-4.835224	-2.260260
1	-2.326766	-5.457095	-0.605471
1	0.799346	-6.405089	-3.409495
1	-1.513250	-6.720788	-2.587735
1	-2.758657	-2.978245	3.517959
1	-1.537769	-1.840508	2.953359
1	-1.207056	-5.654376	2.705570
1	0.463361	-5.088734	2.357327
1	-1.031215	-4.190167	4.725813
1	0.227474	-3.208197	3.971951
1	-3.974393	1.113706	-5.033621

1	-5.309583	3.226456	3.915066
1	-7.341939	-5.498421	2.799642
1	-8.104225	-3.884160	2.913224
1	-7.949530	-4.657678	1.339366
1	-3.635146	-4.192915	1.871798
1	-5.281882	-2.251829	1.431193
1	-7.273669	4.514374	3.269314
1	-4.156156	4.643792	-0.748254
1	-3.699244	5.853075	-4.844167
1	-8.583053	4.529245	-0.826071
1	-8.881832	5.263581	1.539694
1	-3.887425	6.412147	-2.418437
1	-3.749136	3.480513	-5.561101
1	-6.670455	3.140612	-1.467965
1	-0.226264	1.778267	5.153629
1	-3.560789	-0.547917	6.464284
1	-6.414442	-3.567858	-4.282984
1	-2.232175	-3.430214	-5.157417
1	-1.995176	3.146496	2.178703
1	-0.434967	4.139206	4.618918
1	-0.643789	5.015766	3.096742
1	-2.047506	4.675661	4.128538
1	0.770053	2.267282	3.169947
1	-0.148708	1.470840	1.893901
1	0.408967	3.153804	1.693622
1	-5.704684	0.345035	3.560469
1	-5.160583	-1.811172	5.667054
1	-6.474862	-1.765719	4.492183
1	-4.804096	-1.945818	3.933758
1	-6.222020	1.844491	5.508868
1	-7.269379	0.417034	5.492866
1	-5.904747	0.507344	6.618000
1	-1.651992	-0.636571	7.702603
1	0.956752	-0.094841	6.179221
1	0.784207	-1.112163	7.616100
1	0.001313	-1.580594	6.095557
1	-1.537289	1.748291	8.426284
1	-0.126989	0.833585	8.992200
1	0.022667	1.932855	7.614145
1	-1.717312	-0.139548	-3.479673
1	-5.514086	-5.310331	-5.427001
1	-6.449364	-0.235082	-2.596971
1	-7.174046	-0.147209	-4.973147
1	-7.960331	-1.722236	-4.805011
1	-8.556277	-0.336382	-3.878468
1	-6.742157	-2.271621	-1.203730
1	-8.296079	-1.570321	-1.677410
1	-7.706605	-3.025133	-2.486966
1	-0.346798	-2.813062	-4.071226

1	0.383003	-1.360653	-3.371569
1	-0.861837	-2.247814	-2.473847
1	-1.937260	0.104362	-5.961251
1	-0.242300	-0.058661	-5.469581
1	-1.095702	-1.432679	-6.189709
1	-3.771358	-7.070900	-5.268184
1	-2.559024	-5.859282	-4.821862
1	-3.914511	-6.187594	-3.734866
1	-3.049073	-4.643891	-7.128165
1	-4.253984	-5.889823	-7.482373
1	-4.713031	-4.176356	-7.499840
1	-0.129357	1.849609	-0.447833
1	0.673539	1.019735	-1.513249
1	2.218373	-2.578087	-0.462325
1	4.467164	5.297643	-2.706763
1	7.792574	-2.147633	1.607764
1	9.700824	-0.756344	2.227296
1	7.922789	0.967983	-2.368097
1	8.392484	4.197673	-5.164805
1	9.788636	3.385632	1.077417
1	10.848935	1.441305	2.227336
1	9.164492	2.030714	-4.201987
1	6.329408	5.263161	-4.301961
1	7.667356	3.128486	-0.108861
1	5.107346	-5.803262	-0.935393
1	4.135749	-4.837519	3.115667
1	1.792079	6.258994	1.844031
1	-0.237322	5.744723	-1.881024
1	2.274121	3.380867	-3.260366
1	2.826505	5.722279	-4.027822
1	1.795083	4.879823	-5.192576
1	1.101160	6.090410	-4.102366
1	-0.640128	4.309805	-3.500695
1	0.187934	3.089321	-4.464029
1	-0.140473	2.788710	-2.755602
1	-0.219387	7.288555	1.579983
1	-0.524524	8.285114	-1.303972
1	-1.059717	9.140661	0.151703
1	0.668989	8.862452	-0.134081
1	-1.933285	5.570105	0.995141
1	-2.578433	7.212128	0.827432
1	-2.120117	6.285572	-0.607983
1	4.722805	4.172236	0.864920
1	2.878750	4.705142	3.249151
1	3.170024	3.133634	2.481273
1	4.490370	3.979749	3.308383
1	5.011493	6.636187	0.695146
1	4.046274	6.860416	2.160258
1	5.591179	6.004203	2.247303

1	6.326948	-2.360139	-1.726034
1	4.149653	-3.012964	-2.704108
1	5.479779	-3.316826	-3.829861
1	4.742917	-4.668761	-2.965070
1	8.106745	-4.025473	-1.226993
1	7.178117	-5.284320	-2.052660
1	7.796735	-3.902420	-2.967844
1	5.287581	-1.291332	2.818581
1	2.882522	-2.875444	3.848973
1	3.373830	-1.267210	4.397865
1	2.853515	-1.496779	2.719995
1	5.670170	-1.988608	5.143781
1	5.297863	-3.670854	4.751082
1	6.733604	-2.903886	4.062020
1	3.600876	-6.936296	2.337802
1	3.846348	-7.675706	-0.630817
1	2.983358	-8.573640	0.616784
1	2.408621	-6.971744	0.116555
1	6.047732	-7.379356	2.466594
1	5.170099	-8.821087	1.919021
1	6.070197	-7.831330	0.757073