Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

for

Deciphering the Origin of Cooperative Catalysis by Dirhodium Acetate and Chiral Spiro Phosphoric Acid in an Asymmetric Amination Reaction

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Computational Methods

All the stationary points along the potential energy surface such as reactants, intermediates and transition states were fully optimized in the gas phase at the B3LYP levels of theory[1] using Gaussian09 suite of quantum chemical programs.[2] The most important transition states, particularly the stereocontrolling transition states, were further optimized using the M06 and B3LYP-D functional.[3] The Lanl2DZ basis set, consisting of effective core potential for 28 inner electrons for rhodium (Rh) and Pople's 6-31G* basis set for the remaining elements were used.[4] The effect of continuum solvation was incorporated by using the SMD solvation model.[5] Since the experimental studies employed chloroform ($CHCl_3$) as a solvent, we used the continuum dielectric of chloroform (ε=4.81) in our computations in the condensed phase. All the stationary points thus obtained in the gas phase at the B3LYP/6-31G* level of theory were subjected to single-point energy calculations at the $SMD_{(CHCl3)}$/M06/Lanl2DZ(Rh),6-31G**(C,H,N,O,F,P,Cl) level of theory. The Gibbs free energies and enthalpies for all stationary points in the condensed phase were obtained by adding the corresponding ZPVE and thermal energies obtained in the gas phase computations. The energetic quantity employed for the discussions in the text therefore is Gibbs free energies in the solvent. Most of transition states were also optimized at the B3LYP level of theory in the condensed phase using a DGDZVP basis set for rhodium (Rh) and 6-31G** for the rest of the atoms.[6] Further optimization of the stereodetermining transition states were carried out at M06 and B3LYP-D level of theory both in the gas phase and the condensed phase by using Lanl2DZ basis set for rhodium (Rh) and 6-31G** for rest of atoms. The stereodetermining transition states were again optimized in the solvent phase at the B3LYP-D level of theory by using one and only one basis set DGDZVP for all atoms. The use of these functionals for mechanism and stereoselctivity studies have been documented wherein weak non-covalent interactions are found to be important.[7,3b]

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1 (a) A. D. Becke, *Phys. Rev. A* 1988, ***38***, 3098. (b) A. D. Becke, *J. Chem. Phys.* 1993, ***98***, 5648. (c) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1998, ***37***, 785.

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

3 (a) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* 2008, ***120***, 215. (b) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.* 2008, ***41***, 157. (b) S. Grimme, *J. Comput. Chem.* 2006, ***27***, 1787.

4 (a) P. J. Hay and W. R. Wadt, *J. Chem. Phys*. 1985, ***82***, 299. (b) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, ***56***, 2257. (c) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, ***28***, 213.

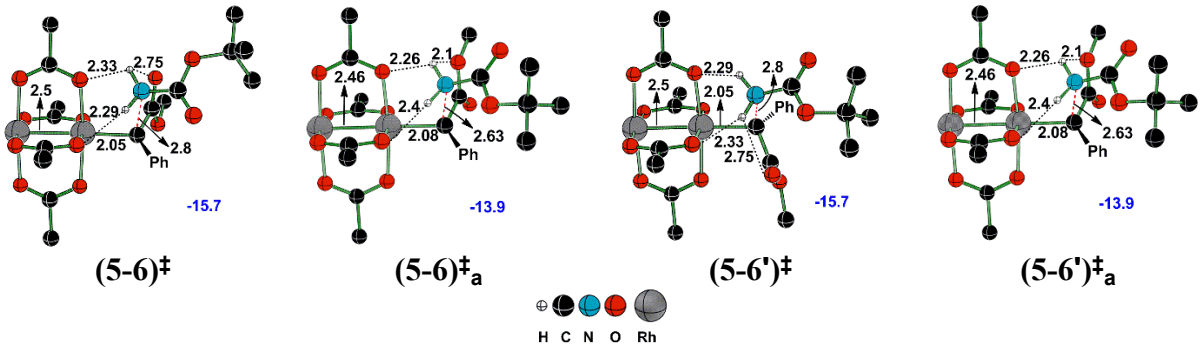
5 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.* 2009, ***113***, 6378.

6 N. Godbout, D. R. Salahub, J. Andzelm and E. Wimmer, *Can. J. Chem.* 1992, ***70***, 560.

All the optimized stationary points were characterized by frequency calculations to authenticate the nature of the transition states (TSs) as having one and only one imaginary frequency representing the desired reaction coordinate. All other minima were characterized by a Hessian index of zero. Topological analysis of the electron densities within Bader's Atoms-in-Molecule (AIM) framework was carried out by using AIM2000 software.[8] The electron density (ρ_{bcp}) at the bond critical point (bcp) correspond either to the strength of the bond or the interactions between two atoms in a given molecule. Natural bond orbital (NBO) analysis was carried out at same level of theory as the one used for optimization.[9]

$\mathbf{3}_{\mathbf{N\ site}}$ **3**

Figure S1. Computed Gibbs Free Energies (in kcal/mol) of a series possible adducts between the catalyst and substrates. The relative Gibbs free energies are with respect to the separated reactants.



(5-6)‡ **$(5\text{-}6)^{‡}_{a}$** **(5-6')‡** **$(5\text{-}6')^{‡}_{a}$**

Figure S2: The optimized geometries of transition states for the C–N bond formation that differ in the mode of attack of *tert*-butyl carbamate to dirhodium cabenoid **5**. The subscript 'a' is used when *tert*-butyl carbamate attacks *anti* to the carbonyl oxygen of the ester (-CO_2Me) group. The relative Gibbs free energy with respect to the separated reactants are provided. Only select atoms are shown for clarity.

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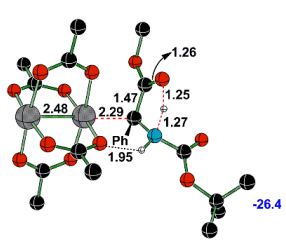
7 (a) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.* 2008, ***41***, 157. (b) Y. Zhao and D. G. Truhlar, *Org. Lett*. 2007, ***9***, 1967.

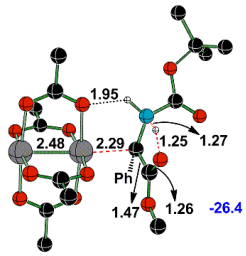
8 (a) Bader, R. F. W. *Atoms in Molecules: A Quantum Theory*; Clarendon Press: Oxford, 1990. (b) *AIM2000 Version 2.0*; Buro fur Innovative Software, SBK-Software: Bielefeld, Germany, 2002. (c) F. Biegler-Konig, J. Schonbohm and D. Bayles, *J. Comput. Chem*. 2001, ***22***, 545. (d) F. Biegler-Konig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

9 (a) A. E. Reed, R. B. Weinstock and F. Weinhold, *J. Chem. Phys.* 1985, ***83***, 735. (b) A. E. Reed, L. A. Curtiss and F. Weinhold, *Chem. Rev.* 1988, ***88***, 899. (c) E. D. Glendening, A. E. Reed, J. E. Carpenter, F. Weinhold, NBO Version 3.1; Gaussian, Inc.: Wallingford, CT, 2009.

Generation of enol (7 and 7') and dirhodium enolate (8 and 8') from 1,3-dipolar intermediate 6 and 6'

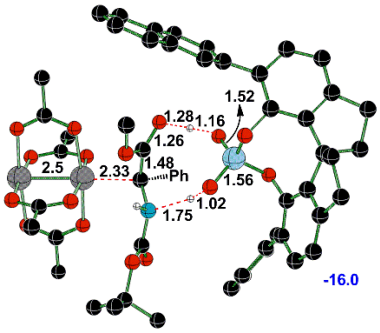


(6-7)‡

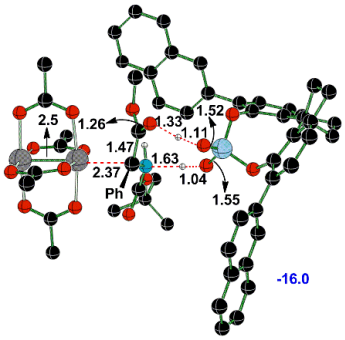


(6'-7)‡

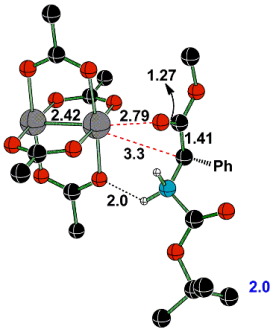
Figure S3(a): The optimized geometries of transition states for enolization of the 1,3-dipolar intermediate (**6**/**6'**). The relative Gibbs free energies with respect to the separated reactants are provided. Only select atoms are shown for clarity.



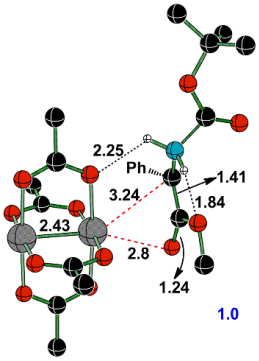
(6-7')‡



(6'-7')‡



(6-8)‡



(6'-8')‡

Figure S3(b): The optimized geometries of transition states for enolization of the 1,3-dipolar intermediate (**6**/**6'**). The relative Gibbs free energies with respect to the separated reactants are provided. Only select atoms are shown for clarity.

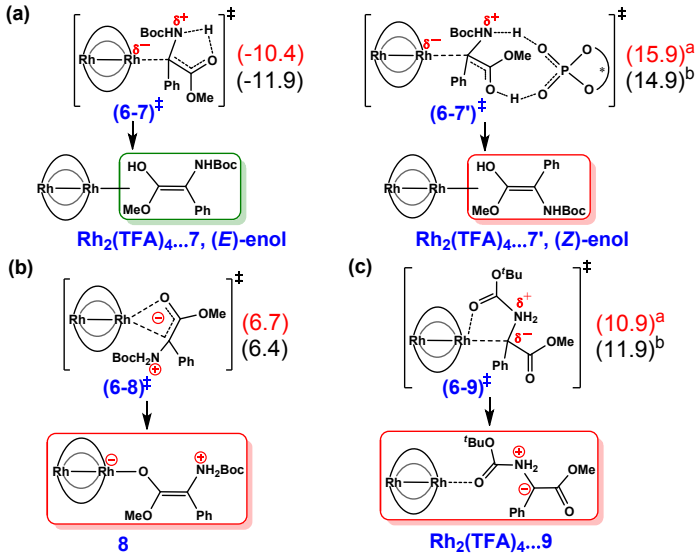
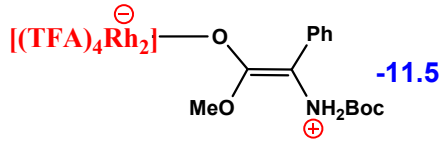
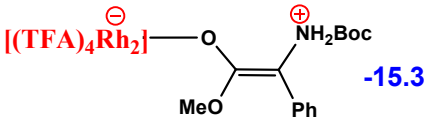
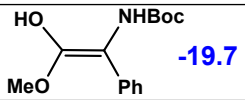
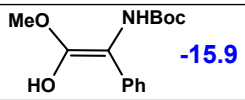
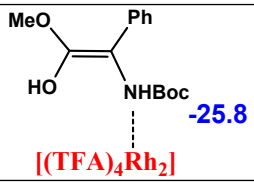
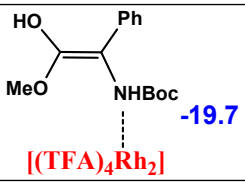
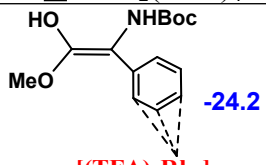
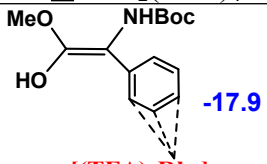
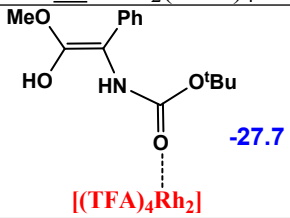
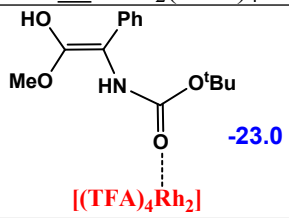
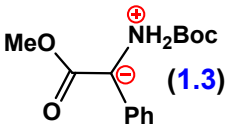
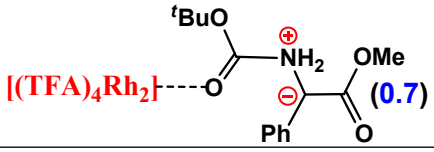


Figure S3(c): Different transition states for enolization (**7**/**7'** or **8**) and for the generation ylide (**9**) from the 1,3-dipolar intermediate (**6**). The relative Gibbs free energies values (kcal/mol) computed with respect to the separated reactants are provided in parenthesis. The values in red and black colors respectively indicate optimisations in the condensed phase at the $B3LYP_{(chloroform)}$/DGDZVP(Rh),6-31G**(C,H,N,O,F) and $B3LYP_{(chloroform)}$/Lanl2DZ(Rh),6-31G**(C,H,N,O,F) level of theories. The superscripts 'a' and 'b' represent values obtained at the $B3LYP_{(chloroform)}$DGDZVP (Rh),6-31G**(C, H, N, O, F, P)//B3LYP/Lanl2DZ (Rh),6-31G*(C,H,N,O,F,P) and $B3LYP_{(chloroform)}$//B3LYP/Lanl2DZ(Rh),6-31G**(C,H,N,O,F) level of theory respectively

Table S1: Computed Gibbs Free Energies (in kcal/mol) of the enolate (**8** and **8'**), enol (**7** and **7'**), ylide (**10**) and interaction of enol and ylide to $Rh_2(TFA)_4$ through various site. The value in blue are relative Gibbs free energy with respect to separated reactants.

	
8'	**8**
	
7	**7'**
	
7N ···$Rh_2(TFA)_4$	**7'**N···$Rh_2(TFA)_4$
	
7Ph···$Rh_2(TFA)_4$	**7'**Ph···$Rh_2(TFA)_4$
	
7O···$Rh_2(TFA)_4$	**7'**O···$Rh_2(TFA)_4$
	
9	**9**O···$Rh_2(TFA)_4$

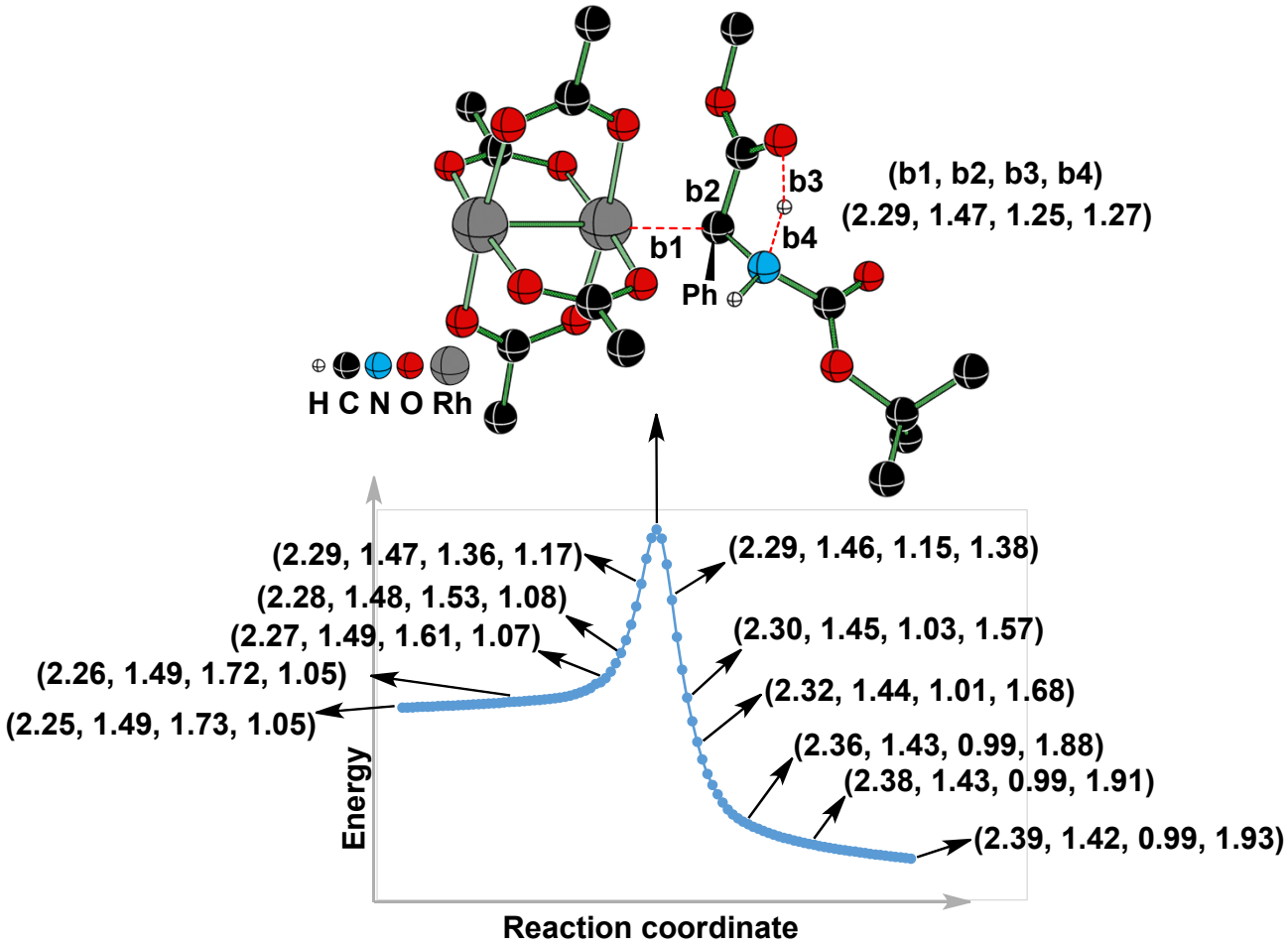


Figure S4: The reaction profile along the intrinsic reaction coordinate (IRC) for the enolization transition state (**6-7**)‡. Along the forward direction the Rh-C (b1) and H-N (b4) distances gradually increase, whereas the O-H distance (b3) decreases. This shows that dirhodium carboxylate departs as the proton transfer gets completed. In the reverse direction toward the reactant, not much change in Rh-C bond distance (b1) is noticed. However H-N distance (b4) decreases and O-H distance (b3) increase. Fluorine are not shown in figures and only selected hydrogens are shown.

Table S2: Various Modes of Protonation of the *α*-Carbon (leading to major *R*-enantiomer **10**) and the Corresponding Relative Gibbs Free Energies (in kcal/mol) at the $SMD_{(CHCl3)}$/M06/Lanl2DZ(Rh), 6-31G**//B3LYP/Lanl2DZ(Rh),6-31G* Level of Theory. Direct Intramolecular protonation (**I**), Double Protonation via Relay Proton Transfer Catalyzed by (*R*)-SPA in the Dirhodium (trifluro)acetate bound Enol (**II**), and in Enolate (**III**)

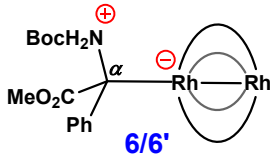
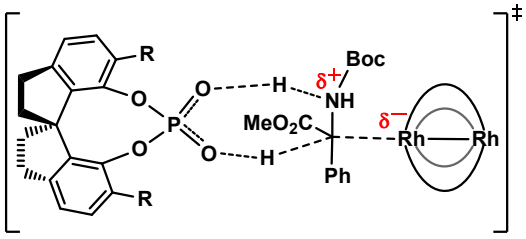
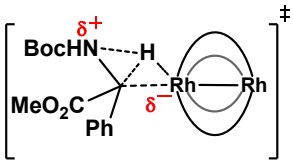
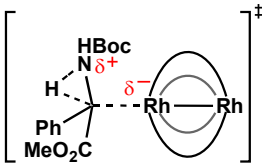
I. Zwitterionic **6/6'** [Describe the difference between n/n']			
Sr.No.	Type of Intermediate	Transition State	ΔG_{rel}
1.			−1.4
2.			12.8
3.			30.1

Table S2..*Continued…*

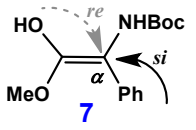
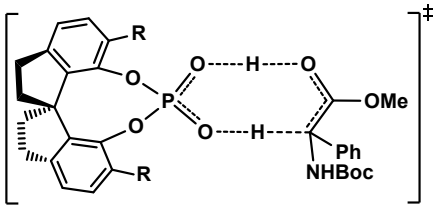
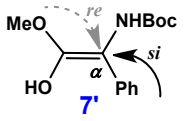
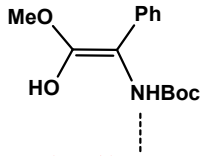
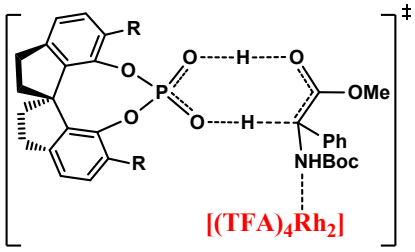
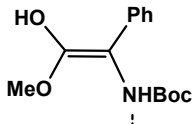
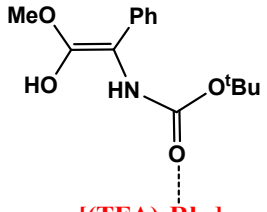
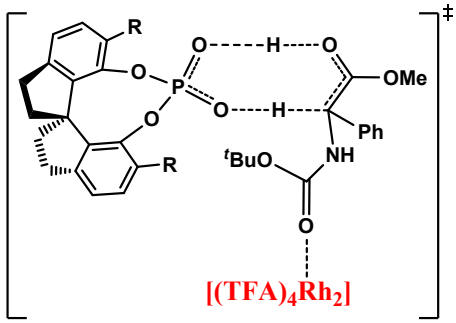
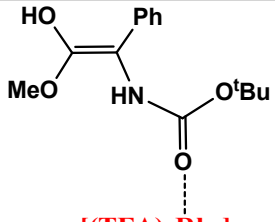
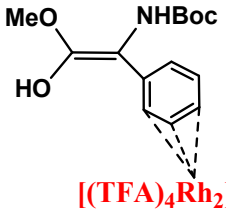
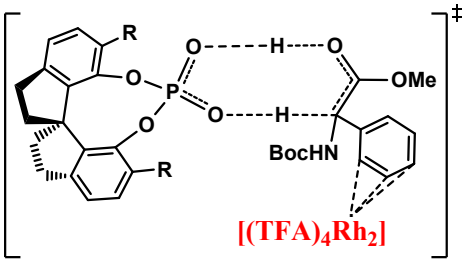
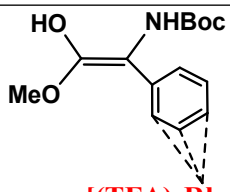
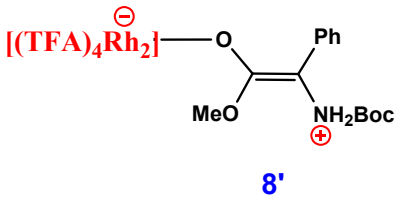
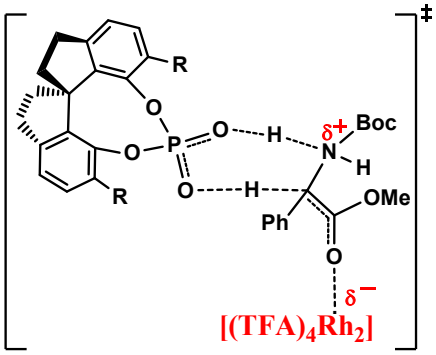
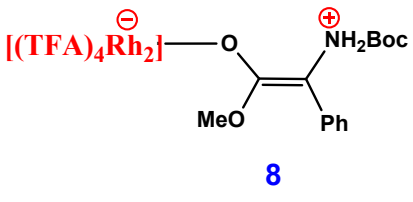
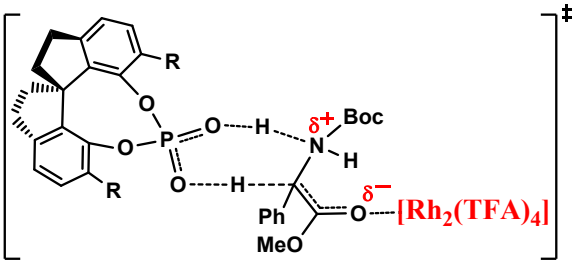
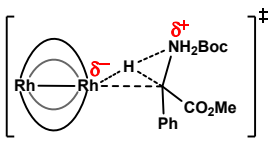
II. (*R*)-SPA Catalyzed Double Proton Transfer in Enol (7/7')			
4.	 **7**		−17.3
5.	 **7'**		−10.6
6.	 **[(TFA)$_4$Rh$_2$]** **7N···Rh$_2$(TFA)$_4$**		−9.4
7.	 **[(TFA)$_4$Rh$_2$]** **9'N···Rh$_2$(TFA)$_4$**		−15.9
8.	 **[(TFA)$_4$Rh$_2$]** **7O···Rh$_2$(TFA)$_4$**		−24.4
9.	 **[(TFA)$_4$Rh$_2$]** **7'O···Rh$_2$(TFA)$_4$**		−20.8

Table S2..*Continued…*

10.			−20.9
11.			−14.7
III. (*R*)-SPA Catalyzed Double Proton Transfer in Dirhodium Enolate (**8**/**8'**)			
12.			−12.1
13.			−14.2

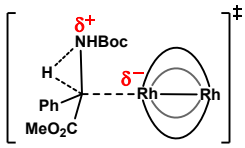
Direct and relay proton transfer (via (R)-SPA) leading to *R* and *S*-enantiomers (10 or 10' respectively) from 1,3-dipolar intermediates 6 and 6'



((6-10))‡ 12.8

((6'-10'))‡ 12.4

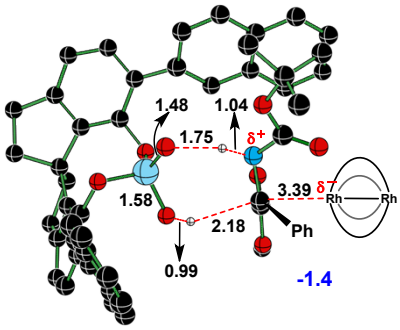
Transition States Leading to *R*-enantiomer **10**



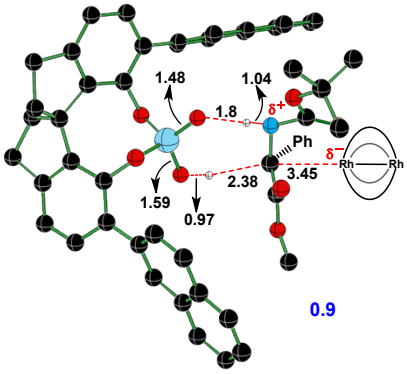
((6'-10)")‡ 30.1

((6-10')")‡ 30.2

Transition States leading to *S*-enantiomer **10'**



(A(6'-10))‡

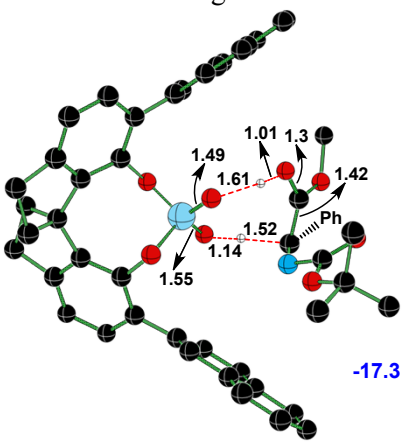


(A(6-10'))‡

Figure S5: The optimized geometries for the direct and relay proton transfer to the *α*-carbon (designated as **A)**. Distances are in Å. Fluorine are not shown in figures and only selected hydrogens and carbons are shown. The value in blue are relative Gibbs free energy with respect to separated reactants.

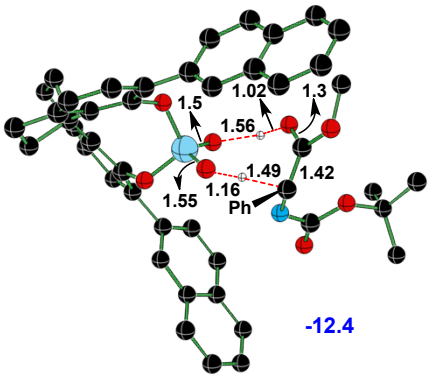
Double proton transfer relay mechanism via (*R*)-SPA in the stereocontrolling step wherein *α*-carbon of enol (7 and 7') or of the enol intermediate bound to [$Rh_2(TFA)_4$] (7···$Rh_2(TFA)_4$ and 7'···$Rh_2(TFA)_4$) is protonated

Transition States Leading to *R*-enantiomer (**10**)



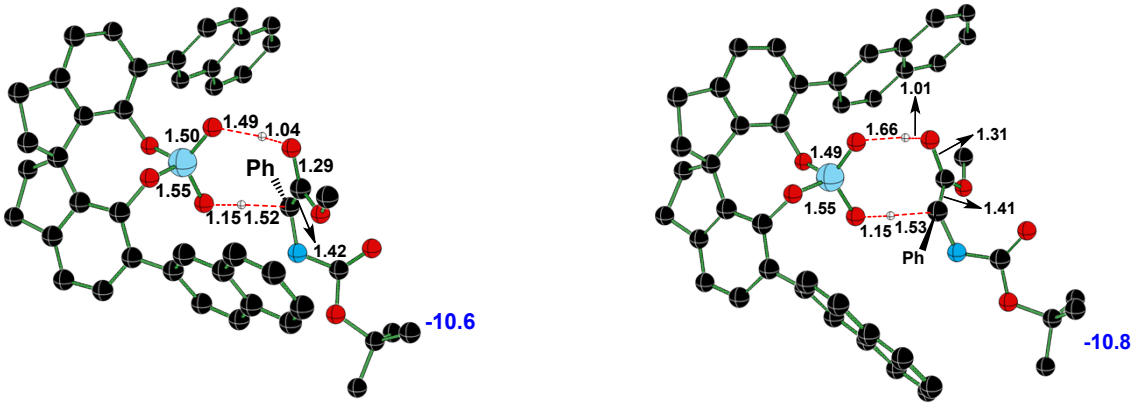
(B(7-10))‡

Transition States leading to *S*-enantiomer (**10'**)



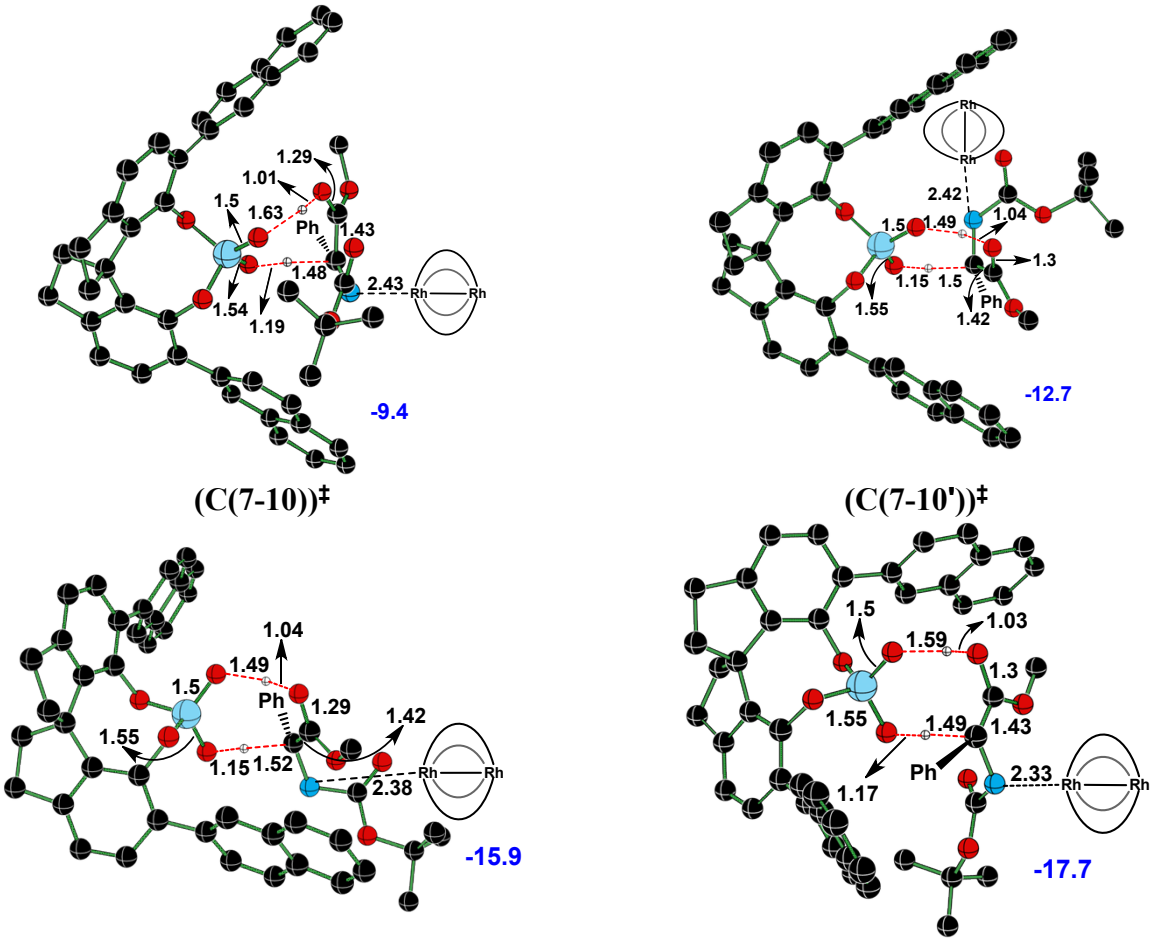
(B(7-10'))‡

Figure S6..*Continued…*



(B(7'-10))‡ **(B(7'-10'))‡**

Figure S6(a): The optimized transition state geometries for double relay proton transfer via (*R*)-SPA leading to *R* or *S*-enantiomer (**10** or **10'** respectively) from enol (**7** and **7'**) intermediate (designated as **B)**. Only selected hydrogens and carbons are shown. The relative Gibbs free energy with respect to the separated reactants are also provided.

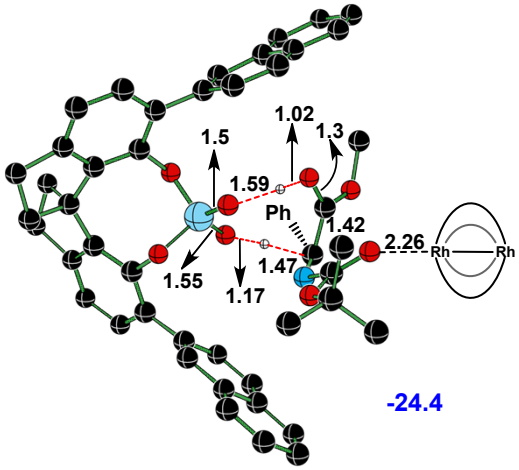


(C(7-10))‡ **(C(7-10'))‡**

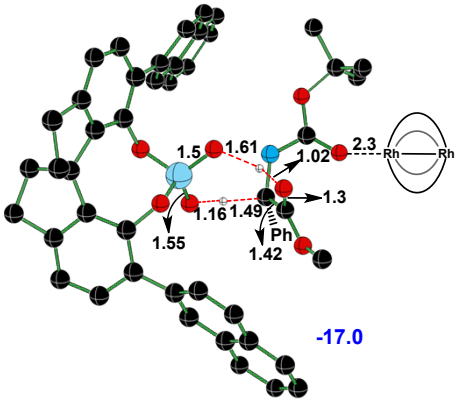
(C(7'-10))‡ **(C(7'-10'))‡**

Figure S6(b): The optimized transition state geometries for double relay proton transfer via (*R*)-SPA leading to *R* or *S*-enantiomer (**10** or **10'** respectively) from dirhodium bound to –$\underline{N}H_2$Boc of enol (**7** and **7'**) intermediate (designated as **C)**. Only selected hydrogens and carbons are shown. The relative Gibbs free energy with respect to the separated reactants are also provided.

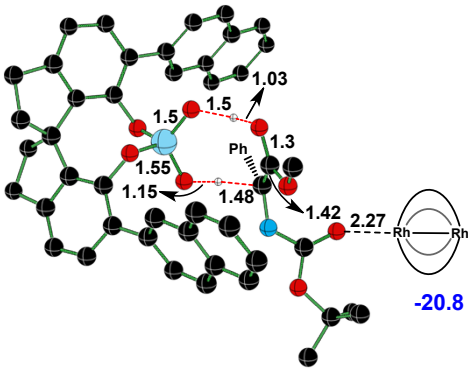
Figure S6(c)..*Continued…*



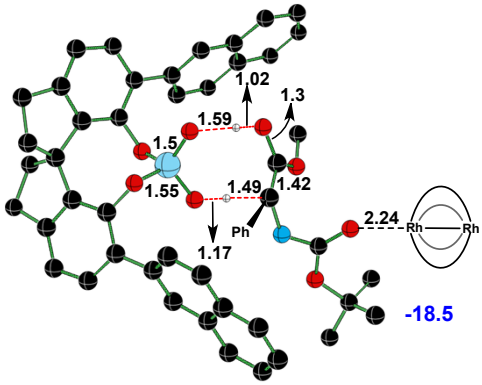
(D(7-10))‡



(D(7-10'))‡

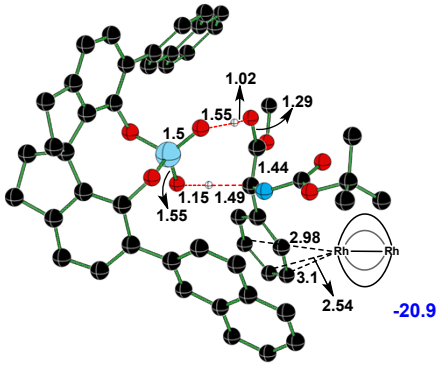


(D(7'-10))‡

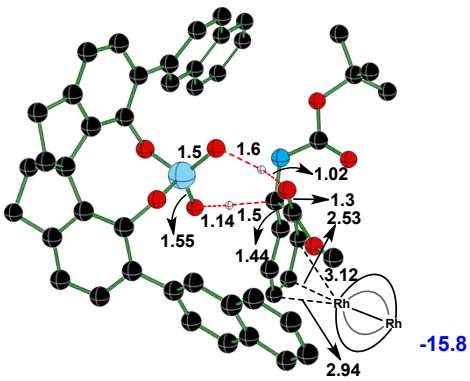


(D(7'-10'))‡

Figure S6(c): The optimized transition state geometries for double relay proton transfer via (*R*)-SPA leading to *R* or *S*-enantiomer (**10** or **10'** respectively) from dirhodium bound to O=C(ᵗBoc) of enol (**7** and **7'**) intermediate (designated as **D)**. Only selected hydrogens and carbons are shown. The relative Gibbs free energy with respect to the separated reactants are also provided.

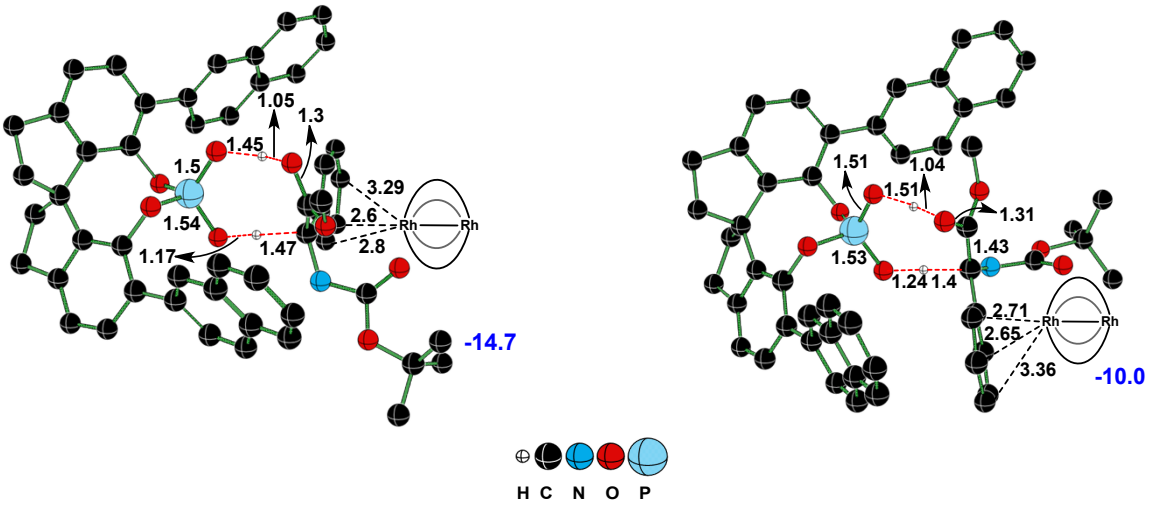


(E(7-10))‡



(E(7-10'))‡

Figure S6(d)..*Continued…*

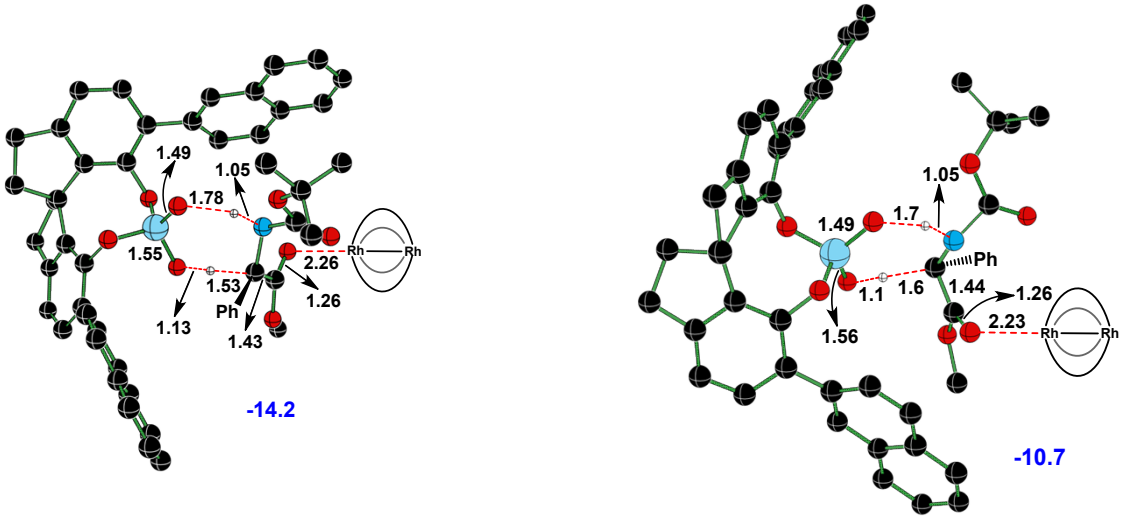


(E(7'-10))‡ **(E(7'-10'))‡**

Figure S6(d): The optimized transition state geometries for double relay proton transfer via (*R*)-SPA leading to *R* or *S*-enantiomer (**10** or **10'** respectively) from dirhodium bound to Ph group of enol (**7** and **7'**) intermediate (designated as **E**). Only selected hydrogens and carbons are shown. The relative Gibbs free energy with respect to the separated reactants are also provided.

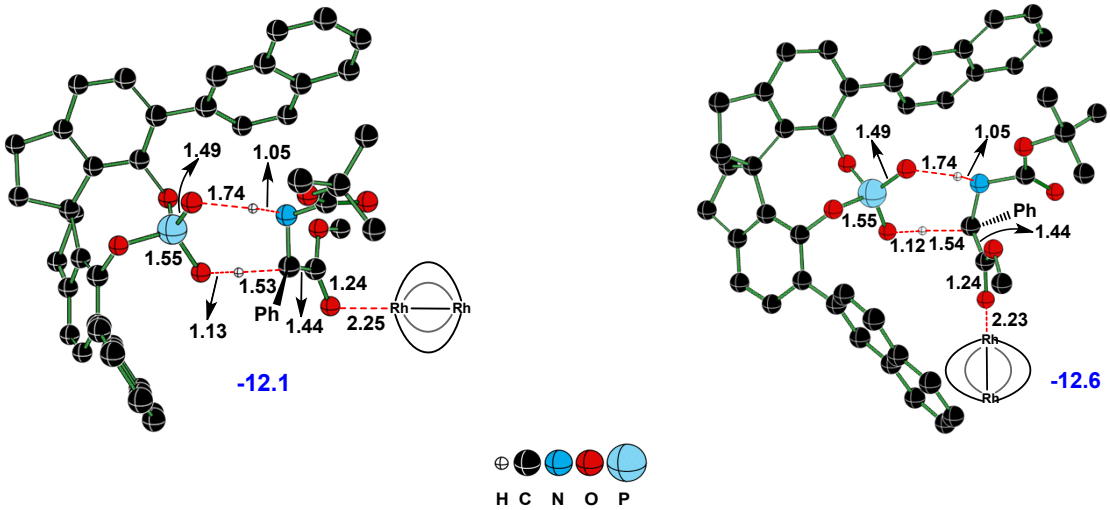
Double proton transfer relay via (*R*)-SPA in the stereocontrolling step wherein the *α*-carbon of dirhodium enolate (8 and 8') gets protonated

Transition States Leading to *R*-enantiomer (**10**) Transition States Leading to *S*-enantiomer (**10'**)



(8-10)‡ **(8-10')‡**

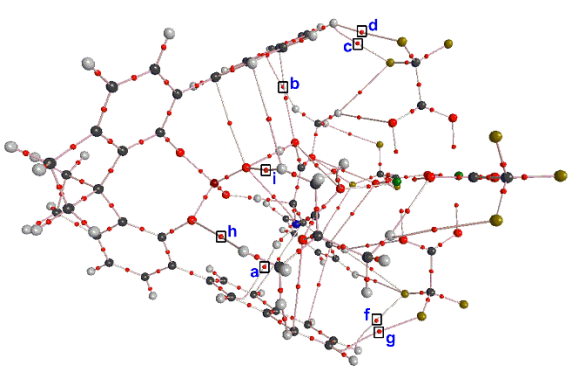
Figure S7..*Continued…*



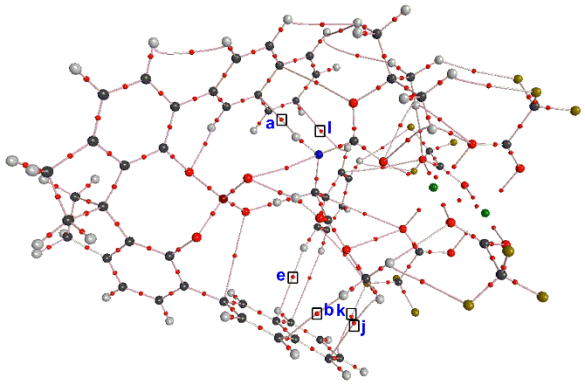
(8'-10)‡ **(8'-10')‡**

Figure S7: The optimized transition state geometries for double relay proton transfer via (*R*)-SPA leading to *R* or *S*-enantiomer (**10** or **10'** respectively) from dirhodium enolate (**8'** and **8**) intermediate. Only selected hydrogens and carbons are shown. The relative Gibbs free energy with respect to the separated reactants are also provided.

Table S3: Topological Analysis of Electron Densities using Atoms-in-Molecule Formalism using the Wave Function of Fully Optimized Geometries in the Condensed Phase at the $SMD_{(CHCl3)}$/M06/Lanl2DZ(Rh),6-31G**(C,H,N,O,F,P,Cl) level of theory. The Bond Critical Points along the Bond Paths of Key Weak Interactions (a to l) in the Stereocontrolling Transition States are Shown in Square Shape



(7-10)‡

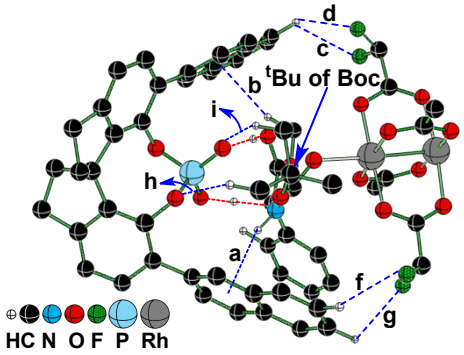


(7-10')‡

Bond path[i]	Type of Interaction	ρ_{bcp} x 10^{-2} (a.u.)	
		(7-10)‡	**(7-10')‡**
a	(NH_2Boc)N-H•••π of *β*-naphthyl	1.2685	0.8116
b	(Methoxy)C-H···π of *β*-naphthyl	0.8471	0.8411
c	(CF_3)C-F···H of *β*-naphthyl	0.5052	*no bcp*
d	(CF_3)C-F···H of *β*-naphthyl	0.4497	*no bcp*
e	(phenyl)C-H···π of *β*-naphthyl	*no bcp*	0.4693
f	(CF_3)C-F···H of *β*-naphthyl	0.3844	*no bcp*
g	(CF_3)C-F···H of *β*-naphthyl	0.3587	*no bcp*
h[j]	(^{t}Boc methyl)C-H···O of P-O	0.1235	*no bcp*
i[j]	(^{t}Boc Methyl)C-H···O of P=O	0.8462	*no bcp*
j[j]	(Methoxy)C-H···π of *β*-naphthyl ring	*no bcp*	0.4879
k[j]	(CF_3)C-F···π of *β*-naphthyl ring	*no bcp*	0.8036
l[j]	(phenyl)C-H···π of *β*-naphthyl ring	*no bcp*	0.4415

[i] the descriptors a-g are as shown in Figure 2 of the main manuscript. [j] these interactions are not shown in Figure 2 in the lowest energy stereodetermining transition state **((7-10))‡**.

Additional interactions in the lowest energy stereocontrolling transition state



	Gas phase		Solvent phase	
	M06	B3LYP-D	M06	B3LYP-D
h	3.13	3.42	3.37	4.53
i	2.47	2.57	2.51	3.35

((7-10))‡

Figure S8: The transition state geometry optimized in solvent phase at M06 to get major *R*-enantiomer, Distances are in Å. There is two additional interaction h and i due to ^{t}Boc C-H···O(P-O) and ^{t}Boc C-H···O(P=O) respectively. These interaction keep the ^{t}Boc group properly in the center of the chiral cavity and keep the enol-$Rh_2(TFA)_4$ i.e **7**···$Rh_2(TFA)_4$···O(C=O) in proper proximity for chiral induction.

Table S4: The Total Electronic Energy ($E_{0(gas)}$ in a.u) and Gibbs Free Energy ($G_{298(gas)}$ in a.u) of Different Stationary Points Obtained at the B3LYP/Lanl2DZ(Rh),6-31G*(C,H,N,O,F,P,Cl) Level of Theory. The Gibbs Free Energy of Different Stationary Points in the Condensed Phase ($G_{298(in\ solvent)}$ in a.u) are Obtained at the $SMD_{(CHCl3)}$/M06/Lanl2DZ(Rh), 6-31G**//B3LYP/Lanl2DZ(Rh),6-31G* Level of Theory by including thermal and entropic corrections as derived from the gas phase geometries

Stationary Points	$E_{0(gas)}$	$G_{298(gas)}$	$G_{298(in\ solvent)}$
1	-607.6703228	-607.550957	-607.1740469
2	-402.3814791	-402.250728	-402.0267871
(*R*)-SPA	-2068.5397173	-2068.057559	-2066.906658
$[Rh_2(TFA)_4]$	-2323.9091792	-2323.856788	-2323.067601
$CHCl_3$	-1419.268307	-1419.276530	-1419.163453
N_2	-109.5207184	-109.533568	-109.4626795
3	-2931.6089769	-2931.414581	-2930.24595
(3-4)‡	-2931.5873838	-2931.393304	-2930.231775
4	-2931.5973978	-2931.402759	-2930.246022
(4-5)‡	-2931.5846443	-2931.390946	-2930.232915
5	-2822.0914573	-2821.903993	-2820.808575
(5-6)‡	-3224.4831815	-3224.144164	-3222.830867
6	-3224.5097603	-3224.164690	-3222.85468
6'	-3224.5109192	-3224.163866	-3222.854652
(6-8)‡	-3224.469373	-3224.127208	-3222.808957

(6'-8')‡	-3224.4607988	-3224.119023	-3222.804085
(6-7)‡	-3224.501073	-3224.157839	-3222.847879
(6-7')‡	-5293.0367082	-5292.184451	-5289.73794
(6'-7')‡	-5293.0384211	-5292.187012	-5289.738036
7	-900.5736181	-900.305025	-899.7695832
7'	-900.5631036	-900.295929	-899.7636068
8	-3224.4958623	-3224.152817	-3222.830187
8'	-3224.4830051	-3224.138635	-3222.824217
7N ···$Rh_2(TFA)_4$	-3224.514361	-3224.166090	-3222.846952
7'N ···$Rh_2(TFA)_4$	-3224.5043926	-3224.157057	-3222.837226
7O···$Rh_2(TFA)_4$	-3224.5129873	-3224.170222	-3222.84998
7'O···$Rh_2(TFA)_4$	-3224.5028202	-3224.158818	-3222.842502
7Ph···$Rh_2(TFA)_4$	-3224.5084917	-3224.164122	-3222.844455
7'Ph···$Rh_2(TFA)_4$	-3224.4898967	-3224.149783	-3222.834395
(6-9)‡	-3224.4591086	-3224.114982	-3222.804416
9	-900.5277486	-900.261224	-899.7360001
9O···$Rh_2(TFA)_4$	-3224.5115806	-3224.165646	-3222.846129
(6-10)‡	-3224.4343586	-3224.094207	-3222.785321
(A(6'-10))‡	-5293.031427	-5292.178651	-5289.71476
(A(6-10'))‡	-5293.0194804	-5292.168480	-5289.710937
(B(7-10))‡	-2969.1190299	-2968.348677	-2966.67248
(B(7-10'))‡	-2969.1145022	-2968.344824	-2966.664597
(B(7'-10))‡	-2969.1102746	-2968.340208	-2966.661809
(B(7'-10'))‡	-2969.1078111	-2968.339339	-2966.662145
(C(7-10))‡	-5293.0381305	-5292.180363	-5289.727472
(C(7-10'))‡	-5293.0444009	-5292.192070	-5289.732733
(C(7'-10))‡	-5293.0493094	-5292.194631	-5289.737895
(C(7'-10'))‡	-5293.0525221	-5292.202112	-5289.740777
(D(7-10))‡	-5293.0639203	-5292.214607	-5289.751401
(D(7-10'))‡	-5293.0564507	-5292.207404	-5289.739662
(D(7'-10))‡	-5293.0574959	-5292.212190	-5289.745615
(D(7'-10'))‡	-5293.0538562	-5292.203194	-5289.742017
(E(7-10))‡	-5293.0565261	-5292.210354	-5289.745751
(E(7-10'))‡	-5293.0534497	-5292.204832	-5289.737709
(E(7'-10))‡	-5293.0505057	-5292.198597	-5289.735882
(E(7'-10'))‡	-5293.040671	-5292.191482	-5289.728351
(8-10)‡	-5293.0557275	-5292.205737	-5289.735118
(8-10')‡	-5293.0563183	-5292.199585	-5289.729603
(8'-10)‡	-5293.0544765	-5292.202633	-5289.731761
(8'-10')‡	-5293.0525004	-5292.199182	-5289.732613

Table S5: The Total Electronic Energies ($E_{0(gas)}$ and $E_{0(sol)}$ in a.u) and Gibbs Free Energies ($G_{298(gas)}$ and $G_{298(sol)}$ in a.u) of Stereodetermining Transition States obtained using different DFT Functionals (M06 and B3LYP-D) in the Gas phase and in the Condensed phase

DFT functional		**(7-10)‡**	**(7-10')‡**
M06	$E_{0(gas)}$	-5290.5672462	-5290.5538598
	$E_{0(sol)}$	-5290.6177984	-5290.6068097
	$G_{298(gas)}$	-5289.688271	-5289.678568
	$G_{298(sol)}$	-5289.740306	-5289.736173
B3LYP-D	$E_{0(gas)}$	-5293.42957	-5293.4140197
	$E_{0(sol)}$	-5293.4785682	-5293.4652229
	$G_{298(gas)}$	-5292.568516	-5292.553282
	$G_{298(sol)}$	-5292.618314	-5292.605419

Table S6(a): The Total Electronic Energies ($E_{0(gas)}$ in a.u), Gibbs Free Energies ($G_{298(gas)}$ in a.u) and Optimized Cartesian Coordinates of Different Stationary Points obtained at B3LYP/ Lanl2DZ(Rh),6-31G*(C,H,N,O,F,P,Cl) Level of Theory. The Number of Imaginary Frequencies, along with their Values (in cm^{-1}) as Applicable, is Provided

1

E_0 = -607.6703228
G_{298} = -607.550957
NImag =0

C	-0.500610	0.401813	-0.000054
C	-1.621395	-0.551105	-0.000106
N	-0.849127	1.672984	-0.000034
N	-1.121461	2.778226	-0.000020
O	-1.517426	-1.763135	-0.000020
O	-2.815731	0.094003	0.000005
C	-3.970750	-0.758727	0.000104
H	-4.827263	-0.084042	0.000180
H	-3.980939	-1.393180	-0.890092
H	-3.980786	-1.393186	0.890297
C	0.942972	0.078759	-0.000021
C	1.387635	-1.256160	-0.000036
C	1.904662	1.107251	0.000027
C	2.753225	-1.539497	-0.000007
H	0.662424	-2.058602	-0.000074
C	3.265244	0.811581	0.000056
H	1.595189	2.148846	0.000040
C	3.700363	-0.515085	0.000039
H	3.074620	-2.577789	-0.000021
H	3.986021	1.624877	0.000092
H	4.762020	-0.745319	0.000062

2

E_0 = -402.3814791
G_{298} = -402.250728
NImag = 0

N	-2.516937	0.807339	0.056185
H	-2.385182	1.778511	-0.185688
H	-3.408878	0.388567	-0.160695
C	-1.434187	-0.036719	-0.001204
O	-1.520075	-1.251691	-0.005278
O	-0.295435	0.697001	-0.015614
C	1.022200	0.045124	-0.000108
C	1.203891	-0.804731	-1.263044
H	2.226140	-1.198451	-1.298624
H	0.503607	-1.641281	-1.276721
H	1.044588	-0.193599	-2.158674
C	1.983258	1.237353	-0.006544
H	1.822618	1.867677	0.874173
H	3.020134	0.885254	0.002832
H	1.833298	1.849912	-0.901720
C	1.187291	-0.777500	1.282760
H	2.209123	-1.169713	1.340096
H	1.015075	-0.147591	2.162642
H	0.487389	-1.614293	1.305057

(*R*)-SPA

E_0 = -2068.5397173
G_{298} = -2068.057559
NImag = 0

C	-1.279937	4.763889	-1.622725
C	0.168937	4.392714	-1.235389
C	0.016798	3.462562	0.014400
C	-1.276299	2.734035	-0.344878
C	-2.056805	3.539372	-1.189520
C	-3.344252	3.151954	-1.547011
C	-3.853135	1.948470	-1.059752
C	-3.080743	1.083540	-0.265373
C	-1.773262	1.496599	0.057571
C	1.320525	2.746471	0.351963
C	2.071923	3.509897	1.260031
C	1.275586	4.708244	1.728214
C	-0.161817	4.335396	1.303758
C	3.347471	3.107727	1.643743
C	3.870426	1.920672	1.130226
C	3.126460	1.102823	0.264226
C	1.837859	1.538557	-0.104492
O	1.046132	0.711779	-0.905251
P	0.006482	-0.326745	-0.189088
O	0.813818	-1.022542	1.014543
O	-0.923524	0.617967	0.750214
O	-0.636136	-1.177977	-1.202810
C	3.682412	-0.196911	-0.200481
H	4.871360	1.604723	1.409495
H	3.930620	3.703057	2.341685
H	-3.951654	3.776957	-2.196823
H	-4.868873	1.652899	-1.304732
C	-3.651863	-0.208733	0.196836
H	-1.390137	4.973648	-2.692703
H	-1.618595	5.662773	-1.088344
H	0.633120	3.820000	-2.046297
H	0.802666	5.262546	-1.034930
H	1.612743	5.628770	1.231011
H	1.368029	4.880010	2.806543
H	-0.628825	3.722117	2.082744
H	-0.804922	5.204404	1.133383
H	1.522534	-1.602227	0.683644
C	-4.364314	-1.012024	-0.676281
C	-4.973427	-2.220646	-0.251230
C	-4.848284	-2.617922	1.119232
C	-4.107950	-1.783626	1.999652
C	-3.526339	-0.620089	1.556722

$[Rh_2(TFA)_4]$

E_0 = -2323.9091792
G_{298} = -2323.856788
NImag = 0

Rh	-0.007705	-0.017414	-1.196535
Rh	-0.015952	-0.009410	1.206219
O	1.439584	1.451953	1.142981
C	1.833615	1.837409	0.006567
O	1.445323	1.446114	-1.130528
C	2.963305	2.893865	-0.008152
O	-1.471048	-1.471402	1.142497
C	-1.858594	-1.862776	0.005919
O	-1.462434	-1.479522	-1.131105
C	-2.992204	-2.914992	-0.008266
O	-1.478537	1.443820	1.130736
C	-1.862895	1.831639	-0.009044
O	-1.470552	1.437506	-1.142827
C	-2.918049	2.962549	-0.001169
O	1.453624	-1.471720	-1.121607
C	1.843199	-1.854547	0.017831
O	1.447363	-1.464081	1.151937
C	2.977694	-2.905960	0.009784
F	-3.826789	2.744436	0.956092
F	-3.539889	3.049563	-1.178783
F	-2.297438	4.128528	0.249417
F	2.736091	3.803348	-0.962792
F	4.128297	2.275948	-0.267957
F	3.057671	3.514726	1.169498
F	4.141450	-2.282947	-0.242875
F	2.760457	-3.816723	-0.945955
F	3.067539	-3.526417	1.188168
F	-3.081809	-3.542141	1.166523
F	-4.156374	-2.290258	-0.256803
F	-2.775696	-3.819996	-0.969343

H -4.443844 -0.731207 -1.723269
H -4.009720 -2.078401 3.041935
H -2.970453 0.004070 2.248281
C -5.464413 -3.824601 1.544873
C -6.171074 -4.606705 0.658005
C -6.291598 -4.216951 -0.699180
C -5.705542 -3.052311 -1.142111
H -5.794052 -2.752020 -2.183623
H -6.848718 -4.843623 -1.390512
H -6.637646 -5.528307 0.995713
H -5.367804 -4.122164 2.586591
C 3.643614 -0.566870 -1.578959
C 4.195555 -1.750370 -2.008144
C 4.817367 -2.648729 -1.098687
C 4.857049 -2.295401 0.289192
C 4.278529 -1.065177 0.702082
H 3.174802 0.102777 -2.291403
H 4.161749 -2.013259 -3.062665
H 4.301472 -0.807917 1.758530
C 5.470059 -3.190255 1.208419
C 6.021060 -4.375667 0.775552
C 5.983316 -4.723467 -0.597738
C 5.394134 -3.878852 -1.512468
H 5.361718 -4.143484 -2.566675
H 6.420929 -5.662237 -0.925996
H 6.487786 -5.050777 1.487640
H 5.498007 -2.921433 2.261866

$CHCl_3$

E_0 = -1419.268307
G_{298} = -1419.276530
NImag = 0
Cl 0.000000 1.703769 -0.083800
C 0.000000 0.000000 0.455356
H 0.000000 0.000000 1.541681
Cl 1.475508 -0.851885 -0.083800
Cl -1.475508 -0.851885 -0.083800

N_2

E_0 = -109.5207184
G_{298} = -109.533568
NImag = 0
N 0.000000 0.000000 0.552659
N 0.000000 0.000000 -0.552659

3

E_0 = -2931.6089769
G_{298} = -2931.414581
NImag = 0
Rh -2.007061 0.266910 1.340123
Rh -0.388254 -0.071887 -0.442795
O -1.953080 -0.705269 -1.639971
C -3.108882 -0.716374 -1.132983
O -3.465188 -0.377532 0.028904
C -4.232261 -1.269959 -2.040094
O 1.075782 0.580616 0.878045
C 0.714843 0.921469 2.040716
O -0.437032 0.899409 2.546576
C 1.839897 1.490803 2.935852
O -0.731825 1.883118 -1.023764
C -1.571451 2.553257 -0.360456
O -2.248554 2.198134 0.643061
C -1.842653 3.991714 -0.859262
O -1.663650 -1.697127 1.915781
C -0.823215 -2.365008 1.257725
O -0.137734 -2.007322 0.258033
C -0.550235 -3.799662 1.765004
F -0.888009 4.406431 -1.696767
F -1.907089 4.839817 0.175716
F -3.021811 4.013740 -1.505831
F -5.402705 -0.686007 -1.763195
F -4.350250 -2.593627 -1.820316
F -3.948440 -1.077176 -3.332243
F -0.154144 -4.594410 0.760102
F -1.640387 -4.328819 2.326885
F 0.431545 -3.755990 2.684476
F 3.018123 0.909043 2.651137
F 1.955415 2.810699 2.703880
F 1.574524 1.303093 4.229941
C 3.300761 0.220706 -1.580230
C 2.300245 -0.750837 -1.962650
N 2.825243 1.445917 -1.409146
N 2.444781 2.502686 -1.263704
O 1.087172 -0.499014 -2.089569
O 2.804312 -1.960867 -2.197825
C 1.854038 -3.010419 -2.496720
H 2.466457 -3.886167 -2.708837

(3-4)‡

E_0 = -2931.5873838
G_{298} = -2931.393304
NImag = 1 (-69.8336 cm^{-1})
C -2.015133 -2.200015 -0.364190
O -1.181867 -1.888775 0.530521
Rh -0.245956 -0.052409 0.387161
O -1.801483 0.839459 1.412237
C -2.794789 1.243686 0.748160
O -2.983425 1.179483 -0.500158
Rh -1.498223 0.321062 -1.643472
O 0.056404 -0.558717 -2.683162
C 1.049258 -0.967283 -2.018404
O 1.230188 -0.919515 -0.770316
O 0.618024 1.804910 0.109100
C 0.271035 2.470608 -0.907422
O -0.555178 2.155324 -1.806043
O -2.370843 -1.530927 -1.374316
C 2.244610 -0.115461 2.462804
C 1.369506 -1.248677 2.823549
O 0.272421 -1.107898 3.345390
O 1.902514 -2.438191 2.498547
N 1.782490 1.038614 2.927367
C -2.728625 -3.558686 -0.175580
C -3.900492 1.949085 1.567891
C 0.924851 3.866758 -1.026441
C 2.215813 -1.556853 -2.844882
F 3.048049 -0.557302 -3.188298
F 1.762593 -2.138875 -3.960363
F 2.897750 -2.458878 -2.132856
F 0.817916 4.350645 -2.264751
F 2.226658 3.799540 -0.700348
F 0.315339 4.708142 -0.175824
F -1.975119 -4.397894 0.548066
F -2.989296 -4.126340 -1.357321
F -3.887629 -3.355371 0.472573
F -5.071882 1.909962 0.926001
F -3.549052 3.235196 1.746911
F -4.042155 1.371688 2.764719
C 3.562443 -0.088520 1.781085
C 4.486893 -1.135192 1.937853
C 3.916102 1.017377 0.987052

H 1.208881 -3.185967 -1.633658
H 1.249265 -2.737894 -3.364026
C 4.745448 0.001671 -1.309326
C 5.553393 -0.676988 -2.234559
C 5.317118 0.491136 -0.124356
C 6.908678 -0.867580 -1.970809
H 5.117181 -1.056137 -3.152413
C 6.677503 0.312214 0.124977
H 4.690761 0.988906 0.610853
C 7.476007 -0.368798 -0.795662
H 7.525048 -1.398251 -2.691159
H 7.109073 0.694228 1.045818
H 8.534356 -0.513349 -0.597589

C 5.727359 -1.075484 1.304636
H 4.231166 -1.991780 2.548538
C 5.164406 1.074833 0.370545
H 3.207218 1.825072 0.832416
C 6.075334 0.027942 0.523363
H 6.429193 -1.895070 1.433146
H 5.418386 1.936834 -0.240220
H 7.045711 0.070638 0.036870
N 1.401080 2.032192 3.319231
C 1.061910 -3.583139 2.756216
H 1.668016 -4.445169 2.477647
H 0.157174 -3.532381 2.147416
H 0.790722 -3.624901 3.813582

4

E_0 = -2931.5973978
G_{298} = -2931.402759
NImag = 0
C -1.586414 -2.146821 -0.888766
O -0.864488 -1.901182 0.118876
Rh -0.032327 -0.007380 0.300631
O -1.746919 0.666442 1.243028
C -2.692105 1.094365 0.518165
O -2.750030 1.172930 -0.736094
Rh -1.111930 0.525645 -1.835785
O 0.591492 -0.163480 -2.787983
C 1.536979 -0.577466 -2.065106
O 1.606867 -0.637131 -0.805257
O 0.672082 1.943759 0.322495
C 0.400181 2.687439 -0.664582
O -0.271098 2.416524 -1.691835
O -1.888927 -1.393153 -1.849607
C 1.080549 -0.471963 2.398479
C 0.295488 -1.686554 2.840778
O -0.689525 -1.610095 3.544159
O 0.795352 -2.816064 2.332555
N 0.572192 0.605983 3.075371
C -2.138682 -3.590393 -0.934815
C -3.917783 1.611292 1.307261
C 0.932780 4.134580 -0.552712
C 2.793157 -1.104702 -2.797384
F 3.885674 -0.470257 -2.343966
F 2.707522 -0.920913 -4.117036
F 2.931499 -2.419496 -2.554203
F 1.100095 4.684678 -1.757274
F 2.106681 4.157120 0.098355
F 0.048283 4.872472 0.141894
F -1.121115 -4.448634 -1.127066
F -3.028803 -3.751196 -1.913357
F -2.728029 -3.894387 0.237338
F -4.952763 1.854055 0.499922
F -3.584152 2.752956 1.936012
F -4.288759 0.710238 2.227319
C 2.574138 -0.381220 2.218006
C 3.404026 -1.502772 2.372467
C 3.161162 0.861225 1.916197
C 4.785053 -1.378855 2.219445
H 2.976465 -2.468995 2.600703
C 4.542018 0.975603 1.777010
H 2.542095 1.737358 1.757533
C 5.362436 -0.143788 1.926473
H 5.410309 -2.259375 2.338094
H 4.973604 1.944287 1.541460
H 6.438928 -0.054040 1.812712
N 0.133828 1.518070 3.558611
C 0.022947 -4.007300 2.601297
H 0.607802 -4.823543 2.178575
H -0.947972 -3.932721 2.110334
H -0.111066 -4.137420 3.677232

(4-5)‡

E_0 = -2931.5846443
G_{298} = -2931.390946
NImag = 1 (-379.0200 cm^{-1})
C 2.472640 1.317305 -0.836259
O 1.544880 0.681242 -1.418389
Rh -0.019027 -0.046160 -0.265922
O 1.079305 -1.766520 0.140238
C 1.878613 -1.759494 1.121366
O 2.126196 -0.839822 1.939335
Rh 1.122250 0.956062 1.697094
O 0.030964 2.690255 1.321223
C -0.741339 2.701290 0.334679
O -0.974315 1.783140 -0.510855
O -1.495729 -0.672952 1.055668
C -1.361622 -0.395127 2.283112
O -0.434627 0.226219 2.861518
O 2.595864 1.600083 0.381586
C -1.020084 -0.985538 -1.952584
C -0.150656 -2.120945 -2.442142
O 0.739038 -2.018343 -3.259470
O -0.464822 -3.237165 -1.772398
C 0.452861 -4.341441 -1.933150
H 0.008479 -5.162823 -1.372162
H 0.555876 -4.598497 -2.989596
H 1.425040 -4.072666 -1.517971
N -0.613788 0.182527 -3.215965
N -0.458496 1.160248 -3.713570
C -2.491376 -1.105368 -2.033993
C -3.321775 -0.142556 -1.423856
C -3.095157 -2.174539 -2.732150
C -4.706887 -0.256662 -1.499220
H -2.878021 0.698494 -0.906869
C -4.479561 -2.292081 -2.789026
H -2.478692 -2.924516 -3.214387
C -5.288613 -1.332876 -2.173494
H -5.333427 0.492462 -1.024363
H -4.928028 -3.127373 -3.318814
H -6.370262 -1.423496 -2.222268
C 3.633660 1.760405 -1.757695
C -2.543922 -0.839462 3.176195
C 2.625390 -3.097516 1.330733
C -1.530147 4.003519 0.065846
F -3.061891 -1.998101 2.748593
F -3.505933 0.103421 3.117369
F -2.166088 -0.982225 4.449685
F 1.742848 -4.054369 1.671079
F 3.550667 -3.007027 2.285144
F 3.226534 -3.472486 0.184176
F 3.190805 2.026664 -2.993778
F 4.534728 0.763903 -1.831397
F 4.240523 2.850092 -1.276371
F -1.086481 4.568389 -1.070983
F -2.836808 3.718966 -0.085967
F -1.396262 4.879533 1.061627

5

E_0 = -2822.0914573
G_{298} = -2821.903993
NImag = 0
C -0.638019 -1.692563 -1.499225
C 0.499929 -2.381610 -2.164678
O 0.978020 -1.967572 -3.201417
Rh -0.042966 -0.217342 -0.232722
O -1.058817 -1.033679 1.388718

(5-6)‡

E_0 = -3224.4831815
G_{298} = -3224.144164
NImag = 1 (-30.2283 cm^{-1})
C -1.154496 0.372647 -1.225118
C -1.603130 -0.859738 -1.946430
O -2.242002 -1.759441 -1.445715
Rh 0.534086 0.021085 -0.114124
O 1.544719 1.562715 -1.065455

C -0.968636 -0.453085 2.514125 O -0.321608 0.572552 2.829224 Rh 0.734673 1.565902 1.332732 O 1.717411 2.424981 -0.277175 C 1.644150 1.842923 -1.387708 O 1.026796 0.781357 -1.698917 O 1.685835 -1.249910 0.283474 C 2.489507 -0.716365 1.105347 O 2.403067 0.380641 1.706279 O -1.680734 0.998451 -0.624972 C -1.774886 2.101985 -0.004954 O -0.994417 2.611861 0.832061 O 0.911201 -3.443658 -1.467003 C 2.168364 -4.033715 -1.870454 H 2.205170 -5.001658 -1.371802 H 2.209292 -4.149351 -2.954865 H 2.984979 -3.395755 -1.525737 C 2.418925 2.479878 -2.566139 C -3.063618 2.888903 -0.339146 C -1.817216 -1.118373 3.622925 C 3.735836 -1.583690 1.401204 C -1.960984 -2.082055 -1.844934 C -2.199849 -2.953530 -2.950613 C -3.078672 -1.627341 -1.088021 C -3.488113 -3.329760 -3.287895 H -1.361698 -3.291797 -3.550850 C -4.362495 -2.037176 -1.417133 H -2.912300 -0.982391 -0.237304 C -4.569207 -2.876924 -2.517272 H -3.661370 -3.977177 -4.141918 H -5.206800 -1.698677 -0.824874 H -5.578780 -3.183275 -2.777772 F 1.586092 2.705220 -3.594139 F 3.383918 1.638095 -2.973465 F 2.984038 3.637079 -2.211600 F -3.091042 4.075798 0.267856 F -3.160471 3.078043 -1.664240 F -4.132764 2.174010 0.065567 F 4.319067 -1.959657 0.245371 F 4.634446 -0.926691 2.134536 F 3.364341 -2.693190 2.063528 F -3.122459 -0.986851 3.312940 F -1.533577 -2.427364 3.706134 F -1.603749 -0.555640 4.813058	C 2.762874 1.759987 -0.769820 O 3.491532 1.150090 0.047884 Rh 2.657618 -0.418158 1.133377 O 1.656656 -1.954012 2.118730 C 0.453923 -2.153986 1.823042 O -0.278470 -1.549995 0.982595 O 1.229140 -1.333007 -1.524476 C 2.349547 -1.893122 -1.329095 O 3.161919 -1.743438 -0.386036 O 0.018920 1.300571 1.451588 C 0.853907 1.466080 2.397666 O 1.978874 0.944644 2.559946 O -1.132115 -0.847800 -3.206739 C -1.225214 -2.096735 -3.926896 H -0.920451 -1.862186 -4.946417 H -2.247492 -2.479357 -3.902417 H -0.542372 -2.823083 -3.481547 N -2.789704 0.026294 1.031135 C -4.060389 0.366052 0.651525 O -4.434281 1.520488 0.504817 O -4.785456 -0.752533 0.435452 C -6.151875 -0.689169 -0.098174 H -2.529371 -0.941061 1.168021 H -2.209521 0.740021 1.449397 C -0.252239 -3.325424 2.545892 C 0.371305 2.474430 3.465097 C 3.401257 2.943407 -1.534187 C 2.751391 -2.882072 -2.448507 C -1.752226 1.624271 -1.542067 C -2.794789 1.712093 -2.511806 C -1.311801 2.828607 -0.922352 C -3.342600 2.935540 -2.858401 H -3.151209 0.809320 -2.994545 C -1.870869 4.047443 -1.271501 H -0.541290 2.782695 -0.166091 C -2.880725 4.103605 -2.239092 H -4.130674 2.988132 -3.603114 H -1.526067 4.958244 -0.792147 H -3.314140 5.062664 -2.509705 C -7.068070 0.056302 0.878728 H -6.781864 1.106024 0.960809 H -8.105309 -0.003281 0.529487 H -7.017237 -0.403318 1.871862 C -6.539373 -2.167685 -0.191491 H -6.508357 -2.637132 0.797012 H -7.553939 -2.267815 -0.591772 H -5.847686 -2.705069 -0.848067 C -6.142164 -0.043752 -1.488791 H -5.848511 1.005796 -1.429040 H -5.444223 -0.576950 -2.144542 H -7.142104 -0.106362 -1.933061 F -1.545836 -3.033036 2.763949 F -0.189395 -4.423579 1.772978 F 0.326844 -3.592731 3.719268 F 1.221823 2.564168 4.486453 F -0.832224 2.098004 3.932969 F 0.243067 3.689782 2.899274 F 1.752024 -3.759384 -2.669067 F 3.851950 -3.564769 -2.133531 F 2.973386 -2.203985 -3.588086 F 2.781308 4.086070 -1.181725 F 3.251191 2.771286 -2.856976 F 4.701651 3.063510 -1.262007
6 E_0 = -3224.5097603 G_{298} = -3224.164690 NImag = 0 C 3.192653 -0.149701 -1.147836 O 2.009881 0.081235 -1.531943 Rh 0.500116 0.023759 -0.113494 O 0.297847 -2.033446 -0.370035 C 1.048658 -2.795561 0.312615 O 1.927520 -2.495978 1.155173 Rh 2.264752 -0.475212 1.570049 O 2.449700 1.572951 1.843977 C 1.709982 2.327740 1.161268 O 0.832216 2.030334 0.300193 O -0.885995 -0.174747 1.439425 C -0.450155 -0.400261 2.614659 O 0.729718 -0.532477 3.001566	**6'** E_0 = -3224.5109192 G_{298} = -3224.163866 NImag = 0 N 2.269127 -0.961854 0.451611 C 3.751513 -0.914106 0.716093 O 4.385774 -1.035850 -0.419213 C 5.887914 -0.961864 -0.497086 C 1.692094 -0.134802 -0.694296 C 1.650835 -1.096310 -1.839233 O 1.382558 -0.548163 -3.024638 C 1.080220 -1.465782 -4.096074 O 4.138819 -0.808621 1.848827 O 1.775112 -2.306784 -1.665274 H 2.015853 -1.932758 0.156605 H 0.120254 -1.946794 -3.902431 H 1.020899 -0.846799 -4.991106

O 3.627401 -0.388294 0.007892 C -1.214640 0.411272 -1.502058 C -0.707952 -0.109022 -2.810099 O -0.853486 -1.286991 -3.128509 O -0.017213 0.769890 -3.535617 N -2.173286 -0.676491 -1.031337 H -2.112717 -0.803307 -0.012207 C -3.613359 -0.537554 -1.447326 O -3.907965 -0.253802 -2.572378 O -4.346453 -0.809019 -0.388573 C -5.850953 -0.772936 -0.446125 C 4.259522 -0.191750 -2.266831 C 0.849828 -4.300805 0.019887 C -1.570012 -0.555772 3.667428 C 1.857473 3.847666 1.406562 F 0.732043 4.319829 1.974720 F 2.886227 4.120933 2.214161 F 2.045236 4.489435 0.242298 F -2.461907 0.445745 3.550252 F -2.219433 -1.717692 3.447476 F -1.091960 -0.560887 4.910121 F 3.813561 0.378338 -3.397138 F 5.375616 0.440353 -1.884885 F 4.563651 -1.474889 -2.535274 F 1.368557 -5.062889 0.985891 F -0.461328 -4.584412 -0.089290 F 1.447355 -4.612365 -1.143049 C -1.784933 1.782800 -1.311642 C -1.653149 2.807545 -2.266166 C -2.479077 2.083284 -0.119961 C -2.201017 4.069910 -2.040947 H -1.120556 2.618379 -3.187273 C -3.031140 3.344701 0.095338 H -2.558291 1.345725 0.671221 C -2.897774 4.348006 -0.865226 H -2.083408 4.839453 -2.799217 H -3.551732 3.545593 1.028121 H -3.323046 5.333174 -0.695596 H -1.785879 -1.517666 -1.518189 C -6.329530 -1.843883 -1.425927 H -7.423444 -1.889762 -1.397298 H -6.022482 -1.617686 -2.449255 H -5.942607 -2.828800 -1.144173 C -6.296713 0.636712 -0.834342 H -7.384618 0.706454 -0.728482 H -5.839334 1.381598 -0.175692 H -6.034356 0.872267 -1.867490 C -6.230963 -1.111269 0.993895 H -5.847616 -2.096205 1.278006 H -5.829997 -0.367339 1.689187 H -7.321189 -1.123500 1.090791 C 0.660069 0.240724 -4.693763 H -0.045673 -0.282034 -5.342390 H 1.082859 1.110258 -5.196211 H 1.453212 -0.437580 -4.376771	H 1.866151 -2.217503 -4.191440 Rh -0.454656 -0.027315 -0.066099 Rh -2.777723 0.072387 0.829793 O -0.639222 2.001342 -0.460152 O -0.448221 -2.050240 0.433951 O 0.205712 0.324397 1.880933 O -1.912750 0.477571 2.696221 O -2.591869 -1.973813 1.204217 O -2.758400 2.099772 0.379735 O -1.302510 -0.448250 -1.911874 O -3.431203 -0.349100 -1.095801 C -2.564125 -0.513929 -1.989371 C -1.720809 2.577343 -0.147978 C -0.667771 0.491124 2.793248 C -1.504960 -2.539261 0.937550 H 1.800592 -0.736678 1.340734 C -0.059022 0.714424 4.195495 C -1.422911 -4.057006 1.222165 C -3.081167 -0.833503 -3.411232 C -1.732914 4.100202 -0.418827 C 2.312142 1.225761 -0.769358 C 2.639669 1.853848 -1.985743 C 2.579098 1.930222 0.424040 C 3.220998 3.121475 -2.002343 H 2.434138 1.353429 -2.921516 C 3.167059 3.193690 0.400416 H 2.300157 1.513300 1.385778 C 3.495282 3.798484 -0.813373 H 3.461047 3.580094 -2.958038 H 3.356734 3.708526 1.338289 H 3.947751 4.785939 -0.832410 C 6.128473 -1.076693 -2.000557 H 5.735340 -2.022072 -2.386994 H 5.643890 -0.251869 -2.531836 H 7.203469 -1.038174 -2.203437 C 6.474334 -2.147982 0.267296 H 6.267760 -2.077206 1.337432 H 6.071653 -3.091791 -0.114826 H 7.560465 -2.160953 0.126655 C 6.347348 0.390846 0.046476 H 5.835133 1.209916 -0.467826 H 6.166483 0.476450 1.119838 H 7.423480 0.493760 -0.130448 F -2.386458 -4.454331 2.056781 F -0.232175 -4.365340 1.766163 F -1.547834 -4.733925 0.066741 F -2.491474 -1.956577 -3.870940 F -2.766378 0.173705 -4.244779 F -4.402366 -1.011801 -3.434998 F 0.870989 1.684448 4.144017 F -0.983677 1.052182 5.093009 F 0.542296 -0.422400 4.598358 F -1.144255 4.381421 -1.589834 F -2.978729 4.584629 -0.440814 F -1.049751 4.724736 0.560756
(6-8)‡ E_0 = -3224.469373 G_{298} = -3224.127208 NImag = 1 (-201.6245 cm^{-1}) C 3.556286 -0.299190 -1.057448 O 2.428796 -0.061160 -1.570506 Rh 0.775048 -0.094050 -0.329853 O 0.556834 -2.145689 -0.578290 C 1.205725 -2.905894 0.193129 O 1.996169 -2.596027 1.126713 Rh 2.289235 -0.583068 1.505686 O 2.500280 1.452990 1.781625 C 1.858859 2.217926 1.007024 O 1.078326 1.909946 0.064723 O -0.779627 -0.181132 1.050233 C -0.495592 -0.401525 2.264859 O 0.635300 -0.589388 2.777933 O 3.836046 -0.553892 0.147273 C -2.027692 1.176716 -1.521183 C -0.999124 0.988904 -2.478182 O -0.579891 -0.174557 -2.771296 O -0.488042 2.084527 -3.066927 N -2.529248 -0.155914 -1.137983 H -2.379561 -0.380027 -0.142408 C -3.939120 -0.503902 -1.533848	**(6'-8')‡** E_0 = -3224.4607988 G_{298} = -3224.119023 NImag = 1 (-262.7992 cm^{-1}) C -1.921358 -2.622878 0.435555 O -1.190579 -2.108025 -0.455551 Rh -0.902562 -0.052608 -0.408537 O -2.616025 0.228791 -1.518864 C -3.713466 0.311708 -0.905561 O -3.927651 0.266641 0.340092 Rh -2.308274 -0.002655 1.575298 O -0.601892 -0.271396 2.732453 C 0.497741 -0.369910 2.130168 O 0.724692 -0.356986 0.888051 O -0.720051 1.993089 -0.206394 C -1.300651 2.556350 0.759245 O -2.018817 2.034663 1.660720 O -2.526738 -2.055997 1.385125 C 2.054871 -0.042514 -1.735883 C 1.083935 -0.722773 -2.501933 O 0.069807 -0.241374 -3.033646 O 1.364008 -2.091060 -2.595910 C 0.396741 -2.922875 -3.253802 H 0.959504 -3.654262 -3.838721 H -0.224445 -3.427952 -2.510133

O -4.406409 -0.141979 -2.574034
O -4.434981 -1.253277 -0.565859
C -5.823377 -1.817731 -0.651086
C 4.739951 -0.325781 -2.051582
C 0.963782 -4.415452 -0.037537
C -1.697193 -0.401901 3.238076
C 2.105986 3.730288 1.214820
F 1.099453 4.458066 0.727076
F 2.254010 4.009859 2.515343
F 3.238085 4.072719 0.570959
F -1.792885 0.797674 3.828838
F -2.843910 -0.644321 2.575619
F -1.545573 -1.337959 4.179405
F 4.570302 0.596910 -3.007677
F 5.899597 -0.094512 -1.429843
F 4.794316 -1.538218 -2.630371
F 1.763203 -5.164825 0.723846
F -0.316231 -4.704550 0.268374
F 1.173452 -4.725560 -1.323859
C -2.624920 2.340149 -0.908928
C -2.312229 3.659616 -1.322772
C -3.550830 2.203357 0.155636
C -2.898681 4.759872 -0.709439
H -1.608798 3.805188 -2.131600
C -4.134031 3.315380 0.760309
H -3.810244 1.220705 0.540861
C -3.817173 4.604809 0.334486
H -2.636254 5.756495 -1.055986
H -4.837901 3.166722 1.575739
H -4.272309 5.471202 0.805578
H -1.864991 -0.756134 -1.711455
C -5.908972 -2.746265 -1.862888
H -6.882537 -3.248011 -1.860248
H -5.808403 -2.194818 -2.799843
H -5.131619 -3.516174 -1.815029
C -6.824207 -0.663403 -0.712623
H -7.840634 -1.069783 -0.674540
H -6.694319 0.008066 0.142282
H -6.716656 -0.088430 -1.634407
C -5.933129 -2.592054 0.661255
H -5.186495 -3.391181 0.706686
H -5.783811 -1.927823 1.518216
H -6.927393 -3.043053 0.740247
C 0.594377 1.864597 -3.989557
H 0.265653 1.240443 -4.824001
H 0.868539 2.859378 -4.342831
H 1.440795 1.387404 -3.491105
H -0.230220 -2.309884 -3.902217
N 2.923983 -0.945447 -0.954518
C 4.415669 -0.897734 -1.234608
O 4.835230 -0.901118 -2.353929
O 5.026087 -0.891175 -0.066201
C 6.525362 -0.820842 0.033201
H 2.765019 -0.846411 0.059902
H 2.594076 -1.886147 -1.242755
C 1.736793 -0.498793 3.046531
C -2.036457 -4.163526 0.382487
C -4.974415 0.431762 -1.792319
C -1.063766 4.079075 0.889891
F 1.964196 0.664433 3.669151
F 1.551286 -1.453998 3.963034
F 2.840670 -0.813096 2.330164
F -0.983653 -4.696777 1.033950
F -3.159345 -4.590334 0.963240
F -2.012721 -4.601220 -0.885177
F -5.918984 1.154371 -1.178957
F -4.687927 1.000777 -2.965428
F -5.459263 -0.804062 -2.018643
F 0.002422 4.283448 1.685100
F -0.825793 4.634271 -0.300530
F -2.126781 4.678404 1.441385
C 2.250774 1.383864 -1.579468
C 1.640542 2.308351 -2.462413
C 3.068300 1.912640 -0.553052
C 1.847251 3.674389 -2.319866
H 0.994322 1.933465 -3.246794
C 3.270601 3.287617 -0.422594
H 3.540637 1.256564 0.173443
C 2.665497 4.181790 -1.303804
H 1.362624 4.355141 -3.015417
H 3.902123 3.656879 0.382349
H 2.822259 5.251722 -1.201271
C 7.115466 -2.091456 -0.578198
H 6.920798 -2.145848 -1.651421
H 8.199880 -2.092325 -0.424633
H 6.704781 -2.982885 -0.092177
C 7.011583 0.454619 -0.655416
H 8.083643 0.573897 -0.464939
H 6.854603 0.414989 -1.734950
H 6.493525 1.332333 -0.256349
C 6.740908 -0.765994 1.544261
H 6.266477 0.121618 1.974005
H 6.324040 -1.653325 2.030919
H 7.813042 -0.724232 1.760819

(6-7)‡

E_0 = -3224.501073
G_{298} = -3224.157839
NImag = 1 (-1197.7059 cm^{-1})

C -1.280767 0.459966 -1.505770
C -0.753562 -0.124992 -2.751822
O -1.128276 -1.304538 -3.022735
Rh 0.451756 -0.017030 -0.077836
O 1.720407 1.421353 -0.857098
C 2.864476 1.548713 -0.333590
O 3.374756 0.927090 0.633729
Rh 2.250184 -0.555036 1.552688
O 0.953214 -1.994659 2.345709
C -0.178733 -2.129056 1.830300
O -0.682701 -1.506813 0.843605
O 1.328379 -1.421881 -1.342018
C 2.350650 -2.044883 -0.928356
O 2.955715 -1.943618 0.166130
O -0.256943 1.321794 1.348088
C 0.380522 1.448859 2.432723
O 1.424039 0.862045 2.817970
O 0.110449 0.518794 -3.491083
C 0.719576 -0.211434 -4.587109
H 1.342674 0.522323 -5.095999
H -0.053553 -0.598858 -5.252912
H 1.322962 -1.025317 -4.184495
N -2.339544 -0.537214 -1.134343
C -3.727561 -0.254257 -1.460141
O -4.051248 0.248088 -2.505907
O -4.480226 -0.699451 -0.459759
C -5.971513 -0.682638 -0.535111
H -1.910075 -1.331442 -2.038937
H -2.230614 -0.930876 -0.195443

(6-7')‡

E_0 = -5293.0367082
G_{298} = -5292.184451
NImag = 1 (-710.3832 cm^{-1})

C 5.285520 2.185861 -0.123823
C 6.563877 1.636258 -0.135812
C 7.539520 2.193189 -0.977074
C 7.253638 3.312416 -1.751378
C 5.988209 3.889601 -1.664107
C 4.977957 3.348739 -0.850355
C 8.823779 1.398494 -0.900278
C 8.363610 0.088945 -0.227287
C 7.161837 0.508236 0.689979
C 6.375406 -0.723144 1.117031
C 6.925194 -1.248185 2.297426
C 7.942677 -0.290765 2.880711
C 7.693599 1.004309 2.074518
C 6.514110 -2.487433 2.777263
C 5.580267 -3.221197 2.046988
C 4.973520 -2.710452 0.885347
C 5.344523 -1.413167 0.487345
O 4.610131 -0.768546 -0.549432
P 3.508883 0.303196 -0.088008
O 2.651026 -0.240751 1.103431
O 4.275131 1.524918 0.624922
O 2.748475 0.717516 -1.344276
N 0.016650 -0.990925 1.053019
C -0.433251 -2.279311 1.467613
O -0.503436 -2.234555 2.813932
C -0.898645 -3.413240 3.614848
C -0.404991 -0.238683 -0.166321
C 0.047242 1.148283 0.090849
O -0.258876 1.604292 1.296381

C 2.890005 -3.092107 -1.930024	C 0.144768 2.940719 1.661633
C -0.257907 2.444787 3.428753	O -0.625229 -3.241465 0.764519
C 3.772796 2.588289 -1.030740	O 0.717580 1.873115 -0.693743
C -1.082600 -3.231320 2.428259	H 5.758874 4.784484 -2.235013
C -6.368272 -1.296458 0.807658	H 8.004949 3.739727 -2.410206
H -5.967144 -2.309970 0.907256	H 6.933408 -2.896518 3.692752
H -7.459194 -1.346473 0.883549	H 5.307810 -4.221459 2.369820
H -5.990979 -0.691566 1.638222	H 7.811882 -0.146874 3.959114
C -6.455484 0.763566 -0.654281	H 8.965998 -0.663505 2.734968
H -6.150931 1.210051 -1.602420	H 6.913925 1.601314 2.561022
H -6.060140 1.370168 0.167146	H 8.583669 1.633463 1.976149
H -7.549156 0.782181 -0.593976	H 9.573773 1.921071 -0.290045
C -6.425031 -1.557511 -1.705439	H 9.277412 1.231897 -1.883528
H -7.517477 -1.636089 -1.693727	H 7.998050 -0.608035 -0.989801
H -6.012610 -2.568055 -1.613303	H 9.155796 -0.416838 0.332802
H -6.120110 -1.132931 -2.664055	H 1.750219 -0.711479 0.971424
F -0.864569 -4.384489 1.769199	H -0.431732 3.663981 1.086136
F -2.380030 -2.908677 2.292286	H -0.089551 3.019246 2.722791
F -0.824096 -3.422575 3.723860	H 1.210700 3.077271 1.481944
F 1.996451 -4.087241 -2.064650	H 1.731035 1.258481 -1.180044
F 4.052599 -3.610160 -1.533793	Rh -2.711143 0.110151 -0.120669
F 3.069180 -2.523308 -3.141563	Rh -5.187530 0.462717 0.072695
F 4.764349 2.989471 -0.230553	O -2.559968 2.200135 -0.237653
F 4.312646 2.024774 -2.131191	O -3.126361 -1.924916 -0.040417
F 3.067557 3.662373 -1.411906	O -2.657443 0.151578 1.968143
F -0.627694 3.570479 2.801569	O -4.901085 0.526611 2.140967
F -1.358278 1.879830 3.967504	O -5.377170 -1.599984 0.152853
F 0.582188 2.761558 4.417398	O -4.812370 2.512840 -0.058465
C -1.619076 1.900397 -1.341864	O -3.045577 0.070398 -2.177406
C -1.029086 2.908056 -2.127575	O -5.298565 0.375200 -1.996856
C -2.522793 2.293657 -0.336187	C -4.220230 0.202523 -2.620823
C -1.350322 4.248665 -1.922484	C -3.622664 2.884739 -0.196511
H -0.314086 2.647647 -2.895986	C -3.741713 0.345222 2.587224
C -2.843410 3.634100 -0.138800	C -4.328935 -2.291853 0.063201
H -2.965811 1.549479 0.318281	C -3.387355 4.407731 -0.327914
C -2.260935 4.622229 -0.933346	C -3.630568 0.307429 4.129185
H -0.882599 5.005569 -2.546392	C -4.572792 -3.818837 0.108862
H -3.542786 3.905124 0.647426	C -4.326376 0.101637 -4.160409
H -2.507971 5.668772 -0.778987	C -0.028234 -0.780838 -1.511426
	C -0.270323 0.011736 -2.655378
	C 0.540894 -2.050128 -1.707776
	C 0.042655 -0.443540 -3.930548
	H -0.726403 0.987102 -2.548197
	C 0.840944 -2.508157 -2.992867
	H 0.717054 -2.705228 -0.866762
	C 0.598245 -1.711943 -4.109589
	H -0.172007 0.189818 -4.787140
	H 1.260884 -3.500568 -3.114735
	H 0.830094 -2.076888 -5.106769
	C 3.675239 4.068967 -0.769785
	C 3.309436 4.718972 0.394849
	C 2.859977 4.206771 -1.928304
	C 2.139567 5.520913 0.458065
	H 3.940431 4.643413 1.277463
	C 1.709703 4.959688 -1.891936
	H 3.149774 3.692472 -2.839968
	C 1.312753 5.635125 -0.707024
	C -0.857643 -2.865234 5.043656
	H -1.142948 -3.650442 5.751678
	H 0.149869 -2.518777 5.297614
	H -1.551444 -2.027677 5.154559
	C -2.315257 -3.849833 3.234201
	H -3.011995 -3.014080 3.345322
	H -2.357276 -4.218789 2.209558
	H -2.640645 -4.651196 3.907201
	C 0.125516 -4.536359 3.429484
	H 0.113471 -4.912005 2.404913
	H 1.133035 -4.179049 3.671688
	H -0.112192 -5.362758 4.108478
	C 4.065714 -3.584069 0.097784
	C 4.278569 -3.772800 -1.257718
	C 3.057169 -4.350959 0.748667
	C 3.538021 -4.727359 -1.999192
	H 5.052944 -3.207231 -1.768559
	C 2.307817 -5.269770 0.051955
	H 2.875064 -4.193876 1.807801
	C 2.528023 -5.495085 -1.333114
	H 1.531077 -5.836499 0.557826
	C 3.773688 -4.955322 -3.383130
	H 4.540944 -4.372001 -3.886398
	C 1.784134 -6.448778 -2.078361

	H 1.009873 -7.020042 -1.572476 C 2.033932 -6.643808 -3.418601 C 3.040310 -5.891943 -4.076250 H 1.457695 -7.374661 -3.979006 H 3.227506 -6.056249 -5.133864 H 1.083541 5.042465 -2.776651 C 1.757278 6.209524 1.642237 H 2.391387 6.130639 2.522498 C 0.125359 6.412154 -0.634725 H -0.516392 6.471401 -1.509496 C -0.223171 7.058505 0.530474 C 0.604207 6.962148 1.677255 H -1.138723 7.640968 0.576682 H 0.321200 7.482527 2.588209 F -5.495981 -4.170056 -0.799761 F -3.456403 -4.516400 -0.129058 F -5.030987 -4.162277 1.330626 F -4.216913 -1.186436 -4.533736 F -5.495219 0.574250 -4.607671 F -3.336655 0.796435 -4.748514 F -3.947123 -0.932899 4.567312 F -2.383784 0.582832 4.545266 F -4.468950 1.178505 4.701428 F -2.653699 4.846905 0.719259 F -2.701220 4.677896 -1.455099 F -4.529719 5.096257 -0.353896 H -0.139286 -0.375600 1.850466
(6'-7')‡ E_0 = -5293.0384211 G_{298} = -5292.187012 NImag = 1 (-344.6385 cm^{-1}) N -0.001278 -0.352060 1.115360 C -0.475703 -0.020914 2.423777 O -0.347548 -1.118406 3.194825 C -0.569929 -1.026241 4.662345 C -0.356809 0.398665 -0.120945 C -0.019206 -0.476654 -1.257780 O -0.424231 -1.736277 -1.138801 C -0.251808 -2.594066 -2.291750 O -0.831670 1.072413 2.784550 O 0.639136 -0.134265 -2.276875 H 1.629348 -0.318019 1.068785 H -0.801703 -3.500121 -2.050947 H 0.808496 -2.807478 -2.440452 H -0.672936 -2.111141 -3.172154 H 1.845012 0.269336 -1.887666 Rh -2.714483 0.433642 -0.384964 Rh -5.219998 0.442902 -0.402679 O -2.866192 -0.981342 -1.926513 O -2.860577 1.900966 1.070022 O -2.851186 -1.105439 1.037239 O -5.129764 -1.157864 0.930902 O -5.134671 1.776495 1.182350 O -5.144322 -0.906922 -1.991230 O -2.855379 1.916105 -1.836818 O -5.130804 2.022441 -1.744069 C -3.991148 2.371907 -2.145698 C -4.009545 -1.295682 -2.361873 C -4.000890 -1.549862 1.314312 C -3.996901 2.193036 1.529648 C -3.970700 -2.346093 -3.495485 C -4.054032 -2.781545 2.248705 C -3.978119 3.164607 2.732443 C -3.975316 3.563433 -3.131246 C 0.146472 1.809557 -0.217153 C -0.078251 2.544156 -1.400468 C 0.811905 2.465683 0.833515 C 0.296130 3.879408 -1.504589 H -0.577801 2.079591 -2.237395 C 1.187364 3.804645 0.726141 H 1.019919 1.953002 1.760869 C 0.919322 4.525261 -0.435855 H 0.080682 4.417088 -2.424288 H 1.686816 4.283782 1.562961 H 1.196044 5.572701 -0.506807 C -0.332587 -2.464728 5.127134 H -0.452939 -2.525935 6.213739 H 0.679502 -2.798015 4.874301 H -1.052507 -3.144802 4.662848 C -2.006362 -0.589813 4.969711	**7** E_0 = -900.5736181 G_{298} = -900.305025 NImag = 0 N -0.279195 -0.166643 -0.596409 C -1.465451 0.148986 -0.019652 O -2.420571 -0.714119 -0.413941 C -3.831291 -0.547247 -0.013614 C 1.020063 0.365703 -0.303856 O -1.640188 1.112226 0.739721 H -0.303633 -0.968045 -1.215108 C -4.512403 -1.720987 -0.722619 H -5.585281 -1.718427 -0.503983 H -4.091960 -2.673801 -0.385105 H -4.379293 -1.649087 -1.806976 C -4.372686 0.788853 -0.532687 H -4.211402 0.872113 -1.613166 H -3.890598 1.632172 -0.035846 H -5.451051 0.842544 -0.345866 C -3.959844 -0.680260 1.507220 H -3.456119 0.141272 2.019001 H -3.526164 -1.628114 1.844426 H -5.019376 -0.672966 1.787037 C 2.073144 -0.654808 -0.128688 C 3.428160 -0.425301 -0.446774 C 1.724548 -1.939814 0.338585 C 4.381966 -1.427693 -0.283750 H 3.728628 0.541552 -0.828785 C 2.681723 -2.941489 0.492728 H 0.692687 -2.148428 0.606037 C 4.019618 -2.692729 0.184685 H 5.418194 -1.219809 -0.539377 H 2.378274 -3.917777 0.862850 H 4.767417 -3.472034 0.304132 C 1.189449 1.719426 -0.229652 O 0.203660 2.623277 -0.304258 O 2.421737 2.247527 -0.071323 C 2.509188 3.544932 0.532402 H 3.578102 3.732484 0.646648 H 2.022709 3.557357 1.513444 H 2.058775 4.310074 -0.104308 H -0.609740 2.228703 0.122250

H -2.723492 -1.275471 4.511136 H -2.208103 0.422850 4.619571 H -2.160580 -0.621047 6.054413 C 0.468723 -0.077692 5.269613 H 0.304837 0.951299 4.944838 H 1.481672 -0.385895 4.986837 H 0.396617 -0.111597 6.362286 F -5.122145 3.856538 2.817650 F -2.962620 4.029815 2.649277 F -3.836853 2.449261 3.870834 F -4.122305 4.710590 -2.442359 F -4.980032 3.467732 -4.013415 F -2.820556 3.625476 -3.810391 F -4.836571 -2.539224 3.309938 F -2.833296 -3.126321 2.707211 F -4.550870 -3.841034 1.583049 F -3.566123 -3.531733 -2.990602 F -3.086992 -1.980242 -4.444344 F -5.162438 -2.516509 -4.070159 H -0.154717 -1.350394 0.964982 C 4.596709 -2.627696 0.109044 C 5.974514 -2.456506 0.221354 C 6.672970 -3.184111 1.198526 C 6.019347 -4.119910 1.992433 C 4.660518 -4.349967 1.783760 C 3.920831 -3.616549 0.841698 C 8.132565 -2.787701 1.217393 C 8.137150 -1.488642 0.385817 C 6.952993 -1.657564 -0.627729 C 6.624849 -0.321627 -1.278393 C 7.415908 -0.148015 -2.424699 C 8.138998 -1.431330 -2.771969 C 7.431734 -2.472427 -1.875442 C 7.455620 1.083324 -3.069499 C 6.731229 2.149484 -2.539836 C 5.885714 2.005240 -1.423138 C 5.805338 0.718888 -0.856167 O 4.841380 0.452938 0.156462 P 3.495756 -0.287661 -0.290896 O 2.879917 0.419294 -1.497064 O 3.872489 -1.781356 -0.768783 O 2.676250 -0.350630 1.028612 H 4.142373 -5.110753 2.360047 H 6.559001 -4.679216 2.752119 H 8.065680 1.227777 -3.957301 H 6.820901 3.132173 -2.991473 H 8.068633 -1.676781 -3.837618 H 9.209756 -1.359667 -2.535709 H 6.553740 -2.874308 -2.393749 H 8.071916 -3.316177 -1.600005 H 8.756865 -3.563991 0.753450 H 8.515925 -2.640991 2.233323 H 7.924653 -0.632262 1.035733 H 9.089030 -1.295372 -0.117642 C 2.492220 -3.996360 0.621234 C 2.177667 -4.884843 -0.390759 C 1.470551 -3.574989 1.515922 C 0.860216 -5.389134 -0.554089 H 2.956291 -5.229291 -1.067441 C 0.180456 -4.037656 1.377860 H 1.714359 -2.879478 2.312874 C -0.164118 -4.954192 0.348115 C 5.227148 3.211495 -0.859875 C 5.216517 3.447349 0.505174 C 4.732713 4.226254 -1.731484 C 4.757789 4.676278 1.044491 H 5.598870 2.696106 1.189862 C 4.288511 5.429188 -1.239443 H 4.697838 4.034607 -2.799721 C 4.297150 5.699924 0.155092 H 3.914614 6.190555 -1.919692 C 4.759058 4.932167 2.443317 H 5.110474 4.154323 3.117191 C 3.855043 6.935769 0.697364 H 3.505956 7.710863 0.018999 C 3.864082 7.151732 2.058037 C 4.320386 6.139743 2.939356 H 3.520782 8.100284 2.461526 H 4.322547 6.321970 4.010489 H -0.593084 -3.695335 2.056694 C 0.523449 -6.305797 -1.587289	

H 1.303308 -6.638492 -2.268391
C -1.488817 -5.441138 0.175050
H -2.268084 -5.098613 0.849646
C -1.784427 -6.321381 -0.842627
C -0.768609 -6.760886 -1.728830
H -2.800984 -6.682173 -0.970796
H -1.016199 -7.457869 -2.524714

7'

E_0 = -900.5631036
G_{298} = -900.295929
NImag = 0

N -0.133565 -0.195694 -0.712570
C -1.289509 -0.095246 0.020839
O -2.261893 -0.799660 -0.615886
C -3.615145 -0.897100 -0.055764
C 1.084573 0.451508 -0.379917
O -1.411133 0.518953 1.067298
H -0.195506 -0.725070 -1.572544
C -4.341914 -1.763981 -1.088573
H -5.381531 -1.922715 -0.782953
H -3.855656 -2.740410 -1.184390
H -4.339042 -1.279548 -2.070567
C -4.254908 0.493505 0.028710
H -4.225818 0.984290 -0.950501
H -3.733309 1.120106 0.753588
H -5.304044 0.398983 0.331660
C -3.571617 -1.599118 1.306703
H -3.030783 -0.997082 2.038616
H -3.079563 -2.574158 1.216188
H -4.592068 -1.766365 1.669974
C 2.275389 -0.399114 -0.182837
C 3.577596 0.042928 -0.502826
C 2.134891 -1.710306 0.315309
C 4.687942 -0.776781 -0.295857
H 3.717740 1.018899 -0.960289
C 3.244731 -2.528131 0.510979
H 1.141474 -2.076956 0.554127
C 4.530427 -2.065488 0.215220
H 5.677662 -0.410327 -0.556533
H 3.106053 -3.532586 0.903111
H 5.394514 -2.705448 0.370309
C 1.079998 1.799648 -0.193599
O 2.094472 2.509660 0.364642
O 0.037669 2.557806 -0.552696
C -0.404233 3.550550 0.391714
H -1.255694 4.039045 -0.084049
H 0.382690 4.281884 0.591517
H -0.722987 3.062276 1.316463
H 2.728584 1.883740 0.756796

8

E_0 = -3224.4958623
G_{298} = -3224.152817
NImag = 0

C 3.660246 -0.371351 -1.240501
O 2.522788 -0.079839 -1.707514
Rh 0.938065 0.007435 -0.387495
O 0.581714 -2.025423 -0.632530
C 1.220839 -2.825627 0.110430
O 2.072387 -2.573601 1.002223
Rh 2.515284 -0.581250 1.395276
O 2.843983 1.451680 1.656965
C 2.218341 2.248904 0.910703
O 1.376989 1.993192 0.001004
O -0.554169 0.034314 1.074638
C -0.225841 -0.231431 2.269230
O 0.906347 -0.504370 2.733752
O 3.989035 -0.624072 -0.050315
C -2.516604 1.346325 -1.223091
C -1.294366 1.468010 -1.874580
O -0.504245 0.446183 -1.994895
O -0.962232 2.658037 -2.399586
N -2.684161 -0.049127 -0.766702
H -2.610183 -0.164823 0.253287
C -3.881925 -0.797598 -1.297440
O -4.222804 -0.686078 -2.438311
O -4.347133 -1.532980 -0.308062
C -5.518443 -2.457184 -0.511461
C 4.788217 -0.417366 -2.297295
C 0.870041 -4.314131 -0.117173
C -1.389080 -0.172842 3.286142
C 2.476601 3.757507 1.128654
F 1.392563 4.316757 1.694075
F 3.530002 3.967793 1.921202
F 2.698661 4.359846 -0.051469
F -1.453426 1.050337 3.830914
F -2.567919 -0.420637 2.668853
F -1.231369 -1.073411 4.258066
F 4.882637 0.776055 -2.908137
F 5.968811 -0.709755 -1.746387
F 4.502485 -1.347616 -3.222789
F 1.598347 -5.120941 0.656219
F -0.433876 -4.508712 0.169887
F 1.072123 -4.646414 -1.400829
C -3.546422 2.308263 -0.870813
C -3.601336 3.595510 -1.453979
C -4.535185 1.987338 0.087554
C -4.592317 4.501082 -1.090643
H -2.861812 3.872828 -2.193178
C -5.526358 2.901526 0.441742
H -4.527095 1.023338 0.589473
C -5.565068 4.166043 -0.144032
H -4.607105 5.481932 -1.559058
H -6.265612 2.621295 1.187922
H -6.336292 4.879295 0.132030
C -5.133922 -3.513726 -1.547353
H -5.941776 -4.249362 -1.622824
H -4.979239 -3.072052 -2.533978
H -4.223547 -4.041179 -1.243592
C -6.736542 -1.630311 -0.923218
H -7.613786 -2.284981 -0.960630
H -6.933394 -0.839705 -0.191938
H -6.602013 -1.177192 -1.907190
C -5.690639 -3.065362 0.878649
H -4.786263 -3.599122 1.186683
H -5.908711 -2.290608 1.620262
H -6.523378 -3.775662 0.865806
C 0.319865 2.775287 -3.044569
H 0.504065 1.923894 -3.702199
H 0.261810 3.700311 -3.619730
H 1.111154 2.846938 -2.295561
H -1.821662 -0.488846 -1.175979

8'

E_0 = -3224.4830051
G_{298} = -3224.138635
NImag = 0

Rh	-1.012706	-0.030197	-0.493510
Rh	-2.239956	-0.204308	1.619970
O	-3.952012	-0.530399	0.494940
C	-3.834810	-0.564967	-0.759670
O	-2.801724	-0.411439	-1.469147
O	-0.438462	0.122276	2.604553
C	0.587305	0.293607	1.892873
O	0.691331	0.316055	0.637077
O	-1.838066	-2.244094	1.593979
C	-1.152852	-2.691103	0.637724
O	-0.657992	-2.071248	-0.345209
O	-1.473442	1.993550	-0.491879
C	-2.112131	2.448996	0.494702
O	-2.560350	1.838174	1.502941
O	0.085561	0.164638	-2.412297
C	1.287637	-0.214990	-2.493398
O	1.579701	-1.463116	-3.026646
C	0.475046	-2.282948	-3.447586
H	-0.256161	-1.685366	-3.995007
H	0.911324	-3.044760	-4.096312
H	0.000306	-2.746824	-2.581113
C	2.424701	0.511248	-2.151889
N	3.669096	-0.277981	-2.285002
H	4.420299	0.240543	-2.757812
H	3.384732	-1.088145	-2.865958
C	4.229191	-0.861961	-0.980164
O	5.519614	-0.612258	-0.964733
O	3.509567	-1.438010	-0.223183
C	6.376292	-1.026826	0.214282
C	-2.391973	3.969712	0.488398
C	1.921803	0.446734	2.658798
C	-5.121528	-0.856242	-1.566113
C	-0.825219	-4.201188	0.682330
F	-3.715692	4.191886	0.516905
F	-1.886662	4.564030	-0.601385
F	-1.841012	4.536215	1.574674
F	-6.203115	-0.881508	-0.782308
F	-5.005294	-2.052702	-2.172460
F	-5.298144	0.081000	-2.510400
F	-1.747933	-4.882049	1.368608
F	-0.754025	-4.710618	-0.558721
F	0.369214	-4.377613	1.278600
F	2.794973	1.198320	1.972405
F	2.472452	-0.775425	2.833355
F	1.736595	0.999056	3.862123
C	6.357429	-2.551002	0.316786
H	6.685234	-3.008882	-0.622642
H	7.052986	-2.861341	1.103688
H	5.364164	-2.925398	0.572649
C	5.853483	-0.332169	1.470253
H	6.552606	-0.523359	2.291663
H	5.794085	0.750434	1.319956
H	4.869390	-0.698332	1.765778
C	7.750305	-0.502900	-0.195713
H	7.734746	0.584522	-0.318006
H	8.480131	-0.750849	0.581294
H	8.080002	-0.957893	-1.135078
C	2.562969	1.885135	-1.699133
C	3.812080	2.406848	-1.293269
C	1.456121	2.765799	-1.684441
C	3.945474	3.735607	-0.886414
H	4.701286	1.782227	-1.269480
C	1.597645	4.083091	-1.264310
H	0.486753	2.402692	-1.995483
C	2.840788	4.583713	-0.862284
H	4.922677	4.100530	-0.579563
H	0.718269	4.720891	-1.245773
H	2.942729	5.614365	-0.534776

7N ···$Rh_2(TFA)_4$

E_0 = -3224.514361
G_{298} = -3224.166090
NImag = 0

N	-0.687245	1.927083	-0.657461
C	0.337649	2.613896	-1.376091
O	1.058070	3.341353	-0.543697
C	2.283012	4.084553	-0.983770
C	-2.033534	1.809947	-1.207971
C	-2.246405	1.115182	-2.367445
O	-3.504410	0.891970	-2.772416
C	-3.706535	0.177179	-4.000471
O	0.490479	2.484673	-2.580916
O	-1.305606	0.615408	-3.170188
O	1.939739	0.701131	0.808063
C	2.733561	-0.070572	1.420126
O	2.625246	-1.301745	1.649991
Rh	0.924386	-2.276846	0.962864
O	-0.819654	-3.121865	0.225594
C	-1.619481	-2.355427	-0.371426
O	-1.518417	-1.115683	-0.590625
Rh	0.180250	-0.120920	0.065278
O	-0.734901	0.240819	1.886271
C	-0.650893	-0.656518	2.773712
O	-0.063777	-1.768783	2.719405
O	1.171183	-0.605851	-1.691135
C	1.766700	-1.720124	-1.742948
O	1.850636	-2.615966	-0.861989
H	-0.751876	2.312959	0.284605
H	-3.358181	-0.854279	-3.904191
H	-4.785462	0.196006	-4.158381
H	-3.192647	0.664128	-4.833015
C	-3.102656	2.320345	-0.323430
C	-2.976444	3.588513	0.276074
C	-4.235921	1.547085	-0.008251
C	-3.946662	4.069257	1.155077
H	-2.120196	4.215805	0.034880
C	-5.210617	2.036671	0.858621
H	-4.334748	0.555141	-0.433577
C	-5.071900	3.296931	1.446213
H	-3.827786	5.052879	1.601732
H	-6.075981	1.421457	1.090988
H	-5.831368	3.670550	2.127437
C	2.536153	-1.982908	-3.058269
C	-1.412679	-0.366399	4.087860
C	4.026844	0.615000	1.917759
C	-2.909164	-2.988396	-0.942025
F	4.704004	-0.155679	2.767859
F	4.817410	0.887683	0.859317
F	3.734088	1.777215	2.529477
F	2.748297	-3.288337	-3.246552
F	1.860688	-1.499946	-4.109406
F	3.728546	-1.358861	-2.995362
F	-3.985871	-2.314011	-0.502077
F	-2.886622	-2.912618	-2.288186
F	-3.033497	-4.268641	-0.591617
F	-2.633749	-0.927244	4.016089
F	-0.765590	-0.885965	5.137806
F	-1.558858	0.949393	4.282355
C	2.799174	4.655064	0.336919
H	3.053050	3.850646	1.032889
H	3.697650	5.252813	0.151835
H	2.046665	5.298950	0.803596
C	1.854875	5.191151	-1.949070
H	1.453910	4.777309	-2.876662
H	1.097911	5.834367	-1.487470
H	2.723264	5.812320	-2.193807
C	3.291728	3.114899	-1.600985
H	2.920317	2.682830	-2.531655
H	4.215083	3.662959	-1.818916
H	3.531406	2.310074	-0.901698
H	-0.468026	1.130389	-3.058182

7'N ···$Rh_2(TFA)_4$

E_0 = -3224.5043926
G_{298} = -3224.157057
NImag = 0

N	0.176604	1.731097	-1.334912
C	-0.708560	2.843923	-1.057546
O	-1.954763	2.417033	-1.233327

7O···$Rh_2(TFA)_4$

E_0 = -3224.5129873
G_{298} = -3224.170222
NImag = 0

N	-2.322898	2.083151	-1.931564
C	-0.987960	2.218610	-2.019517
O	-0.649632	3.471335	-2.317059

C -3.127210 3.319634 -1.077462 C 1.560720 2.010905 -1.671886 C 1.929655 1.684926 -2.935748 O 1.011539 1.288724 -3.840824 C 1.423660 0.297317 -4.803836 O -0.332498 3.946281 -0.737261 O 3.186359 1.739288 -3.422936 O -1.480889 -0.763038 -1.363100 C -2.005610 -1.901402 -1.189811 O -1.807896 -2.730363 -0.265466 Rh -0.435114 -2.230318 1.220069 O 0.950251 -1.586085 2.613057 C 1.446154 -0.436750 2.456260 O 1.217632 0.411017 1.549831 Rh -0.117329 -0.099296 0.047830 O 1.390703 -1.032364 -1.038051 C 1.644971 -2.245132 -0.782686 O 1.105757 -3.007768 0.057121 O -1.657689 0.662058 1.216723 C -2.208052 -0.115950 2.045834 O -1.952374 -1.323500 2.294933 H -0.238951 1.219533 -2.118698 H 1.785909 -0.600735 -4.294499 H 0.525247 0.067336 -5.377117 H 2.199226 0.695958 -5.460943 C 2.585866 2.398032 -0.658519 C 3.621483 1.485483 -0.367934 C 2.602796 3.650793 -0.021776 C 4.639773 1.815824 0.528569 H 3.601772 0.497741 -0.820042 C 3.614771 3.970621 0.883603 H 1.815755 4.361289 -0.238123 C 4.636714 3.059815 1.159996 H 5.421047 1.092736 0.745862 H 3.607835 4.942607 1.369733 H 5.422955 3.317155 1.864548 C -3.397865 0.497313 2.819590 C 2.786964 -2.836254 -1.640010 C -3.018066 -2.300657 -2.287619 C 2.525419 -0.021397 3.483425 F -3.596063 -3.474225 -2.026782 F -3.974671 -1.362060 -2.389014 F -2.382680 -2.386497 -3.470952 F -3.677546 -0.194639 3.924781 F -3.139141 1.769331 3.162657 F -4.486355 0.490314 2.020855 F 2.356326 -0.658031 4.647402 F 3.738459 -0.345963 2.991907 F 2.496108 1.296756 3.706414 F 3.021821 -4.114637 -1.350346 F 2.467530 -2.743874 -2.946939 F 3.917396 -2.132266 -1.436389 C -4.302218 2.350124 -1.217638 H -4.314205 1.639102 -0.386695 H -5.244601 2.907752 -1.209955 H -4.236156 1.789330 -2.155226 C -3.097646 4.339559 -2.218509 H -2.223935 4.991628 -2.142370 H -3.080728 3.832092 -3.189130 H -3.996984 4.963605 -2.175856 C -3.128368 3.982563 0.302107 H -2.314142 4.700678 0.405932 H -4.079851 4.509742 0.436258 H -3.041414 3.231186 1.091003 H 3.783110 1.992340 -2.694110	C 0.739136 3.927958 -2.594625 C -3.097644 0.919325 -1.627355 C -2.828195 -0.248080 -2.285018 O -3.594916 -1.332364 -2.086982 C -3.069742 -2.611580 -2.478458 O -0.176189 1.261401 -1.904318 O -1.826870 -0.422451 -3.163614 H -2.840561 2.947791 -2.049103 H -2.070120 -2.774458 -2.070544 H -3.767401 -3.337940 -2.060937 H -3.036506 -2.700839 -3.567430 C -4.149954 1.133463 -0.615364 C -5.375120 0.437310 -0.629598 C -3.956842 2.101774 0.391136 C -6.350718 0.691125 0.331915 H -5.559277 -0.302077 -1.398640 C -4.939420 2.356938 1.346689 H -3.015826 2.642663 0.440058 C -6.143391 1.652007 1.324420 H -7.286917 0.139649 0.297203 H -4.756732 3.103698 2.115242 H -6.909946 1.848668 2.068950 C 0.504452 5.370969 -3.048470 H 0.013078 5.950688 -2.260669 H 1.463017 5.845653 -3.280680 H -0.122995 5.400403 -3.945077 C 1.359818 3.096093 -3.719808 H 1.548362 2.068507 -3.406242 H 0.706844 3.089431 -4.599662 H 2.313718 3.548831 -4.011486 C 1.555808 3.883785 -1.303245 H 1.756583 2.860513 -0.986421 H 2.518210 4.380873 -1.469644 H 1.033292 4.412958 -0.499485 O 0.797633 -1.624001 -1.430598 C 1.316422 -2.677964 -0.964920 O 1.748973 -2.898402 0.197762 Rh 1.541117 -1.394768 1.608251 O 1.255624 0.198358 2.902529 C 0.737644 1.249328 2.437526 O 0.344534 1.484255 1.259964 Rh 0.548482 -0.024900 -0.140861 O 2.467243 0.637921 -0.577853 C 3.421391 0.203840 0.127615 O 3.385806 -0.617874 1.081082 O -1.281476 -0.824239 0.421021 C -1.302800 -1.679249 1.349461 O -0.343028 -2.111720 2.043901 C 0.510838 2.393352 3.452922 C 1.371939 -3.860445 -1.958478 C -2.685381 -2.315330 1.625784 C 4.804648 0.784030 -0.246071 F 4.796704 2.114729 -0.046313 F 5.059713 0.551927 -1.543728 F 5.781326 0.247133 0.486859 F 1.775635 -3.444926 -3.165456 F 2.194086 -4.822010 -1.534657 F 0.131216 -4.378489 -2.078567 F -2.717841 -2.901587 2.826104 F -2.915587 -3.257419 0.685805 F -3.655864 -1.402094 1.561576 F 0.539635 3.586282 2.843640 F 1.444594 2.377739 4.409404 F -0.695949 2.236357 4.026263 H -1.028718 0.067905 -2.851315
7'O···$Rh_2(TFA)_4$ E_0 = -3224.5028202 G_{298} = -3224.158818 NImag = 0 N 2.261401 2.195317 1.778413 C 0.918444 2.298086 1.914861 O 0.597493 3.552864 2.253464 C -0.786883 4.082264 2.281953 C 3.037152 1.001806 1.693991 C 2.882619 0.066848 2.660300 O 2.166055 0.308114 3.782851 C 1.155714 -0.661157 4.137784 O 0.100238 1.370941 1.786646 O 3.435301 -1.170312 2.544702 H 2.761390 3.071924 1.870195	**7Ph···$Rh_2(TFA)_4$** E_0 = -3224.5084917 G_{298} = -3224.164122 NImag = 0 N -4.777368 0.332219 -1.569889 C -5.668140 -0.093798 -0.633438 O -6.477587 -1.027404 -1.153962 C -7.609359 -1.598601 -0.388676 C -3.620871 1.155360 -1.385576 C -3.707628 2.318812 -0.653343 O -2.655199 3.143338 -0.578349 C -2.547144 4.000906 0.574486 O -5.725211 0.348529 0.521659 O -4.778254 2.709488 0.031713 H -4.887660 -0.089748 -2.483658

H 1.603263 -1.617534 4.431566 H 0.635358 -0.232771 4.994938 H 0.457228 -0.814933 3.313359 C 3.982819 0.926548 0.558818 C 5.248475 0.324358 0.675165 C 3.637680 1.514971 -0.671093 C 6.125932 0.295709 -0.406230 H 5.540930 -0.128431 1.616021 C 4.517521 1.483077 -1.752713 H 2.665958 1.982672 -0.786086 C 5.766692 0.873264 -1.626891 H 7.099181 -0.174863 -0.292415 H 4.216381 1.932167 -2.695374 H 6.453832 0.848668 -2.468332 C -0.563622 5.512402 2.782433 H 0.092363 6.063953 2.101267 H -1.521631 6.038621 2.842209 H -0.106911 5.508966 3.777390 C -1.649046 3.290807 3.269226 H -1.842361 2.278595 2.913308 H -1.158414 3.238593 4.247438 H -2.607544 3.805868 3.398351 C -1.359664 4.084177 0.863732 H -1.529941 3.072638 0.495172 H -2.322101 4.608083 0.861784 H -0.684964 4.610337 0.179521 O -1.164064 -1.478328 1.475455 C -1.755298 -2.491891 1.005955 O -1.988632 -2.784250 -0.197101 Rh -1.333551 -1.468750 -1.656355 O -0.612191 -0.062854 -3.001202 C -0.040731 0.956881 -2.532843 O 0.163466 1.266550 -1.324766 Rh -0.471948 -0.057672 0.133277 O -2.333012 0.861855 0.170401 C -3.206032 0.478032 -0.658390 O -3.124233 -0.430561 -1.526258 O 1.299522 -1.126153 -0.020963 C 1.355554 -2.070122 -0.855916 O 0.480955 -2.441142 -1.687487 C 0.433405 2.004543 -3.566709 C -2.290447 -3.475072 2.072130 C 2.639078 -2.931488 -0.808360 C -4.546980 1.241785 -0.567892 F -4.326814 2.559784 -0.720976 F -5.098351 1.042148 0.641250 F -5.409346 0.841103 -1.503722 F -3.390530 -2.949777 2.641520 F -2.607372 -4.656128 1.537475 F -1.369891 -3.668826 3.030183 F 2.861397 -3.528258 -1.985483 F 2.471063 -3.887891 0.128037 F 3.706913 -2.200899 -0.486103 F -0.519999 2.944684 -3.702345 F 0.658379 1.446554 -4.758317 F 1.561635 2.607947 -3.155782 H 3.650432 -1.493475 3.435888	H -2.610054 3.416923 1.496104 H -1.559790 4.455779 0.488684 H -3.325689 4.766646 0.565294 C -2.378389 0.623606 -1.942762 C -1.337173 1.449097 -2.420763 C -2.189923 -0.783278 -2.005207 C -0.139066 0.900025 -2.858719 H -1.469175 2.522049 -2.438447 C -0.990342 -1.329576 -2.421707 H -2.983388 -1.439034 -1.661295 C 0.080240 -0.493409 -2.814833 H 0.646073 1.553534 -3.225703 H -0.852694 -2.406389 -2.414603 H 0.976261 -0.921870 -3.254653 C -8.232836 -2.560150 -1.403317 H -7.507236 -3.318122 -1.715241 H -9.093216 -3.067979 -0.955782 H -8.573566 -2.019629 -2.292315 C -8.596014 -0.490866 -0.007870 H -8.158121 0.202235 0.712200 H -8.906649 0.067769 -0.897645 H -9.490232 -0.938935 0.439177 C -7.075731 -2.357252 0.829685 H -6.604288 -1.679630 1.543404 H -7.903184 -2.873275 1.329136 H -6.344036 -3.111129 0.519229 O 1.149502 -2.250895 -0.319134 C 1.699035 -2.761201 0.697617 O 2.356015 -2.195328 1.610926 Rh 2.629586 -0.147937 1.473491 O 2.826446 1.898654 1.236924 C 2.262304 2.421695 0.238955 O 1.617085 1.864337 -0.690956 Rh 1.323305 -0.200053 -0.597313 O -0.360256 0.115202 0.575240 C -0.204389 0.236199 1.820154 O 0.857004 0.165546 2.498703 O 3.102029 -0.499077 -1.616022 C 4.168462 -0.549054 -0.938891 O 4.320161 -0.451549 0.307792 C 2.310989 3.965242 0.162012 C 1.527687 -4.293795 0.808968 C 5.456336 -0.714754 -1.778525 C -1.481234 0.537114 2.639775 F -1.615762 -0.349233 3.635261 F -1.383523 1.770643 3.176816 F -2.580488 0.499880 1.878410 F 0.219436 -4.600815 0.853832 F 2.118635 -4.780102 1.902069 F 2.065072 -4.886200 -0.271292 F 6.495331 -1.069323 -1.018427 F 5.279613 -1.645199 -2.727849 F 5.741433 0.456315 -2.377933 F 3.340061 4.459989 0.853505 F 2.403646 4.379852 -1.107574 F 1.167734 4.459971 0.686900 H -5.267339 1.892144 0.349480
7'Ph···Rh$_2$(TFA)$_4$ E_0 = -3224.4898967 G_{298} = -3224.149783 NImag = 0 N 4.873090 -0.282076 -1.664566 C 5.665622 0.189787 -0.644756 O 6.494896 1.132481 -1.152348 C 7.470689 1.828105 -0.297479 C 3.826743 -1.227556 -1.514058 C 4.129126 -2.446884 -0.988289 O 5.397519 -2.862260 -0.819397 C 5.779494 -3.267609 0.516425 O 5.617818 -0.187176 0.513648 O 3.155664 -3.303934 -0.587608 H 5.011753 0.147774 -2.569565 H 5.221541 -4.152490 0.843571 H 6.839008 -3.515311 0.448469 H 5.624544 -2.435774 1.204654 C 2.481549 -0.794866 -1.920133 C 1.476356 -1.698613 -2.333775 C 2.182435 0.587557 -1.948800 C 0.230405 -1.242194 -2.736099 H 1.678982 -2.761341 -2.337154	**(6-9))‡** E_0 = -3224.4591086 G_{298} = -3224.114982 NImag = 1 (-36.3973 cm^{-1}) N -2.902764 -0.301781 2.393224 C -2.900699 0.963377 1.551129 O -4.013786 1.610825 1.794058 C -4.29551 2.941861 1.119415 C -2.204599 -1.478291 1.84474 C -1.137052 -1.926536 2.680581 O -0.947795 -1.027263 3.7554 C 0.122708 -1.305536 4.664514 O -1.972235 1.234167 0.847364 O -0.447801 -2.926205 2.559336 O 0.185858 -1.870148 -0.480436 C 1.102645 -2.376057 -1.18151 O 2.131848 -1.818897 -1.657213 Rh 2.382023 0.192061 -1.281081 O 2.530438 2.215669 -0.844811 C 1.622966 2.720865 -0.128643 O 0.60931 2.166413 0.374938

C 0.933560 1.045389 -2.339043 H 2.939664 1.297910 -1.635871 C -0.076129 0.135676 -2.718787 H -0.523018 -1.953149 -3.062045 H 0.719269 2.109800 -2.334042 H -1.000362 0.495498 -3.161316 C 8.160247 2.773826 -1.284938 H 7.435963 3.463794 -1.730259 H 8.926446 3.361841 -0.768891 H 8.640311 2.209546 -2.091192 C 8.472848 0.823037 0.281028 H 7.983967 0.136641 0.973970 H 8.939092 0.244531 -0.524255 H 9.264176 1.359476 0.816591 C 6.743034 2.619311 0.794919 H 6.232143 1.952285 1.491118 H 7.466092 3.224946 1.352842 H 6.006646 3.296340 0.348040 O -1.694051 2.107176 -0.780534 C -2.453450 2.696168 0.039895 O -3.054355 2.222953 1.040894 Rh -2.812792 0.205268 1.444584 O -2.489164 -1.814562 1.741925 C -1.739569 -2.411521 0.921594 O -1.140564 -1.948600 -0.087543 Rh -1.353229 0.077053 -0.509631 O 0.224574 0.502134 0.766476 C -0.029222 0.680814 1.990308 O -1.141321 0.633342 2.583164 O -3.044428 -0.343469 -1.639897 C -4.154853 -0.401816 -1.038485 O -4.400250 -0.235301 0.185254 C -1.483335 -3.906979 1.220396 C -2.692607 4.192971 -0.265231 C -5.358156 -0.725786 -1.953746 C 1.208989 1.001198 2.859565 F 0.873305 1.214437 4.134885 F 2.075136 -0.022176 2.807391 F 1.817729 2.102112 2.386638 F -1.535186 4.795530 -0.577447 F -3.237728 4.825540 0.776517 F -3.524714 4.299128 -1.317502 F -6.503140 -0.765400 -1.269328 F -5.460912 0.209578 -2.912657 F -5.166659 -1.918865 -2.542864 F -2.549433 -4.470499 1.799633 F -1.199593 -4.581294 0.098347 F -0.434740 -4.013334 2.057832 H 3.513159 -4.207432 -0.613888	Rh 0.311862 0.133743 0.000296 O 1.461577 -0.292926 1.674452 C 2.710739 -0.383901 1.521519 O 3.391988 -0.254157 0.468179 O -0.684933 0.601975 -1.755061 C -0.000033 0.747186 -2.804694 O 1.247703 0.641895 -2.957577 H -2.362723 -0.100516 3.26377 H -0.300419 -1.502434 5.654876 H 0.778375 -0.433399 4.700178 H 0.675266 -2.176109 4.310056 C 1.783346 4.217852 0.22181 C 3.498866 -0.701159 2.813649 C 0.918702 -3.875705 -1.514967 C -0.825457 1.074859 -4.070015 C -2.920811 -2.234985 0.838698 C -2.434754 -3.48061 0.368816 C -4.139513 -1.767616 0.291001 C -3.133255 -4.199623 -0.592381 H -1.504108 -3.858074 0.769223 C -4.833895 -2.502498 -0.670751 H -4.565898 -0.814816 0.599584 C -4.33849 -3.724035 -1.122418 H -2.724928 -5.145864 -0.937854 H -5.766938 -2.109711 -1.067659 H -4.875132 -4.293101 -1.876097 H -3.884347 -0.486928 2.652378 F 2.565982 4.84913 -0.657449 F 2.334629 4.32803 1.445038 F 0.586048 4.827499 0.243801 F -0.05003 1.515543 -5.064387 F -1.742048 2.018193 -3.792271 F -1.467424 -0.031374 -4.482195 F 0.746271 -4.584264 -0.389307 F -0.169661 -4.031077 -2.288804 F 1.97828 -4.363733 -2.167465 F 4.816704 -0.619712 2.622129 F 3.200142 -1.940808 3.237037 F 3.153924 0.170365 3.781968 C -5.659344 3.302209 1.702337 H -5.607863 3.399192 2.791357 H -6.405362 2.541466 1.452269 H -5.991216 4.258894 1.287133 C -3.215644 3.940254 1.535215 H -2.235171 3.678781 1.131335 H -3.149918 4.008305 2.626476 H -3.488934 4.93008 1.154172 C -4.361215 2.719548 -0.390796 H -4.67131 3.65495 -0.868912 H -5.101926 1.952482 -0.639278 H -3.393906 2.428447 -0.805616
9 E_0 = -900.5277486 G_{298} = -900.261224 NImag = 0 C -1.3126424012 0.4957531484 -1.6709914942 C -0.3487710131 -0.0674122712 -2.5368381163 O 0.6275671243 0.4531585672 -3.0638027548 O -0.6188348856 -1.4477750277 -2.7550691264 C 0.3468023924 -2.1325248545 -3.5497844687 H -0.0518691874 -3.1369006448 -3.7099698543 H 1.312240261 -2.1884356733 -3.0357872054 H 0.490081513 -1.622307154 -4.50547293 N -2.3369932655 -0.4638746449 -1.2251688673 C -3.7404284673 -0.303595637 -1.8044138803 O -3.9080682565 -0.0767669958 -2.9648922549 O -4.5940213499 -0.4899355287 -0.8136977851 C -6.0771734308 -0.3679149685 -1.0343501536 H -2.4347421822 -0.5165829435 -0.2009561287 C -6.631912862 -0.6085685756 0.3682215677 H -6.3455801567 -1.5982402845 0.7382304688 H -7.7248708156 -0.5525971908 0.34455621 H -6.263245594 0.1470563968 1.0689086324 C -6.3908380161 1.0437309829 -1.5306288673 H -5.9820253031 1.2203836681 -2.5271999662	**9O···Rh_2(TFA)$_4$** E_0 = -3224.5115806 G_{298} = -3224.165646 NImag = 0 N 3.5337082826 -0.6341497024 0.6006600535 C 2.6839913574 -0.8691507853 1.6523407369 O 3.3001565582 -1.612007116 2.5746974312 C 2.6286509409 -2.1617506558 3.7835964968 C 3.4917497324 0.5664642723 -0.1966791265 C 3.3735280199 0.3414424931 -1.538020066 O 3.5145025554 1.3157661807 -2.4417360319 C 3.2947770811 1.0068647078 -3.8264313989 O 1.5236883258 -0.4540301742 1.7517585601 O 3.1547923842 -0.874789436 -2.0758523814 O 0.259007378 1.4244513308 -0.6458047943 C -0.5676133699 1.8857530875 -1.4798201451 O -1.6998883125 1.4356360368 -1.8061493201 Rh -2.3627649167 -0.2621521256 -0.8444652221 O -2.93246805 -1.9615515389 0.1911635406 C -2.1298732965 -2.4155197445 1.049668328 O -0.9986464479 -1.9669415263 1.3867200008 Rh -0.2807251626 -0.2778944336 0.4201200657 O 0.5195322862 -1.5003820964 -1.0589409681 C -0.215866949 -1.7780275584 -2.0506467323

H -5.9853495491 1.7941164412 -0.8444877932 H -7.4778174738 1.172010572 -1.5739417008 C -6.5200339174 -1.4569274257 -2.0116414595 H -7.6113479637 -1.4344178978 -2.101403754 H -6.2312997914 -2.4477508809 -1.6449427028 H -6.0902808377 -1.3026845622 -3.0034703195 C -1.3861119792 1.837344332 -1.145345223 C -0.4331439561 2.8232664002 -1.5115676104 C -2.3935722933 2.2284421599 -0.2295656074 C -0.4968546813 4.1069893606 -0.9863487035 H 0.3479068362 2.5491126361 -2.2099355612 C -2.4427122217 3.5227451719 0.2923814866 H -3.1599627487 1.5257147971 0.0909690246 C -1.4982137 4.4763602244 -0.0787541734 H 0.250741515 4.8359437176 -1.2914132821 H -3.2323235456 3.7800407571 0.9953918941 H -1.5384309195 5.4841877646 0.3248344178 H -1.9684133964 -1.3690295265 -1.5815751375	O -1.4118995845 -1.4489358554 -2.2602665322 O -1.2196285633 0.9185819838 1.8166674996 C -2.4285539352 1.2229701369 1.617306811 O -3.1710069538 0.9183535116 0.6432288703 H 2.8295623078 -1.4615780594 -1.368247978 H 2.3283462207 0.5213482394 -3.9770100181 H 3.3177654089 1.9704470133 -4.3353272581 H 4.0892337855 0.35938224 -4.2088545913 C -2.5661042928 -3.7258823613 1.7447645166 C 0.4514105394 -2.5937374119 -3.1820466819 C -0.1106553546 3.1728942056 -2.2058736193 C -3.0910339844 2.0371075948 2.7526531751 C 3.7315573551 1.8612596236 0.4679860173 C 3.3692331124 3.0931337284 -0.114136177 C 4.3325699627 1.8956811134 1.7426158523 C 3.6099664405 4.2947221502 0.547424231 H 2.8888422755 3.106500492 -1.0824395806 C 4.5689290961 3.1015226167 2.401400906 H 4.6241287117 0.9692485602 2.2290480808 C 4.2120766488 4.3120615559 1.8076675027 H 3.3116316209 5.2270789429 0.0745651713 H 5.0372857627 3.0904127298 3.3824807672 H 4.3939657051 5.2528293193 2.319851573 H 4.4514973241 -1.0402030479 0.7640867641 F -3.8866832034 -3.739303535 1.9525617175 F -2.2448448963 -4.7649682944 0.9512040815 F -1.9429100653 -3.882007423 2.919872648 F -4.1945847662 2.6581928596 2.3265739282 F -3.4295086564 1.1933098777 3.746255415 F -2.2418307126 2.9495450482 3.239603053 F 0.9475059503 2.8893106708 -2.9944143303 F 0.2662068637 4.0996380251 -1.3141282598 F -1.0807500822 3.6788947273 -2.9695229787 F -0.3978110671 -3.4971838171 -3.6811988176 F 0.8146381217 -1.7554706487 -4.171373834 F 1.5453805538 -3.232161709 -2.7410683811 C 3.7913614847 -2.8568823914 4.4966483668 H 4.2279612677 -3.6348718442 3.8620663756 H 4.5758615057 -2.1383118709 4.7551108905 H 3.4329338295 -3.3243800709 5.4192522525 C 1.5615337642 -3.1709184487 3.3597362181 H 0.7306559269 -2.6935511652 2.8397881951 H 1.9973636546 -3.9389492351 2.71070087 H 1.1640262439 -3.669972617 4.2505074187 C 2.0656486973 -1.0241298242 4.6391021617 H 1.7198329639 -1.4350261001 5.5941146203 H 2.8425541514 -0.2817170091 4.8511608857 H 1.2277449149 -0.5262954871 4.1496033108

Optimized Cartesian Coordinates for the stereodetermining transition states at the B3LYP level of theory in gas phase

(6-10)‡	**(A(6'-10))‡**
E_0 = -3224.4343586 G_{298} = -3224.094207 NImag = 1 (-1628.0033 cm^{-1}) C -1.018598 1.413391 -1.531814 C -0.289737 1.249325 -2.844948 O -0.689812 0.530217 -3.745827 Rh 0.428968 -0.015096 -0.066514 O 2.028268 1.301778 -0.159587 C 3.079576 1.028077 0.487851 O 3.337676 0.018380 1.190905 Rh 1.876260 -1.441907 1.327194 O 0.324778 -2.824020 1.386346 C -0.750860 -2.523605 0.815456 O -1.035515 -1.482647 0.151488 O 1.195239 -1.016686 -1.716185 C 2.085925 -1.895041 -1.521120 O 2.580265 -2.295936 -0.437374 O -0.213441 0.877777 1.685216 C 0.233156 0.431164 2.779344 O 1.071025 -0.489483 2.979628 O 0.830004 1.967378 -2.885102 C 1.660229 1.767397 -4.047245	E_0 = -5293.031427 G_{298} = -5292.178651 NImag = 1 (-97.9650 cm^{-1}) C 4.969480 -2.702713 -0.193729 C 6.303903 -2.653478 -0.597114 C 7.213263 -3.590202 -0.080254 C 6.782464 -4.601407 0.769658 C 5.437721 -4.659102 1.121739 C 4.497718 -3.709987 0.674096 C 8.617215 -3.298664 -0.556811 C 8.491240 -1.850883 -1.068189 C 7.015934 -1.737564 -1.589564 C 6.657856 -0.272079 -1.806126 C 7.052387 0.121457 -3.095101 C 7.453920 -1.085058 -3.917475 C 6.939315 -2.264767 -3.059813 C 7.008077 1.460535 -3.468403 C 6.561317 2.408780 -2.548045 C 6.081627 2.043877 -1.278090 C 6.110160 0.674747 -0.947740 O 5.479979 0.242774 0.239762 P 3.961795 -0.302190 0.096761

H 2.494136 2.457119 -3.922197	O 3.278820 0.573155 -1.049585
H 1.101492 1.992309 -4.958504	O 4.092240 -1.716517 -0.678674
H 2.012375 0.734028 -4.073993	O 3.257688 -0.324023 1.406564
N -2.308855 0.585537 -1.731650	N 0.465403 -0.289296 1.093973
C -3.411232 0.552007 -0.841637	C -0.499608 -0.234424 2.241216
O -3.356571 0.959940 0.293578	O 0.148326 -0.585818 3.326660
O -4.429627 -0.019075 -1.488808	C -0.541555 -0.636694 4.663740
C -5.692128 -0.358828 -0.774099	C 0.231451 0.680687 0.003261
H -2.398908 0.213437 -2.679396	C 0.245462 -0.038612 -1.235870
H -1.300426 0.188595 -1.087093	O 0.154047 0.716070 -2.352999
C -1.920721 -3.524239 0.962444	C 0.216087 0.001991 -3.596377
C 4.194757 2.090250 0.352492	O -1.643248 0.091654 2.084124
C -0.375844 1.085407 4.042031	O 0.380189 -1.276191 -1.277613
C 2.618219 -2.545372 -2.819349	O -2.697277 1.676397 -1.697670
C -1.244089 2.817367 -1.045477	C -3.564411 1.981215 -2.559716
C -0.255624 3.526953 -0.350208	O -4.756473 1.581574 -2.663307
C -2.432595 3.478511 -1.395444	Rh -5.411633 0.186673 -1.279303
C -0.462546 4.862265 -0.004642	O -5.949722 -1.226537 0.135169
H 0.677818 3.046210 -0.091479	C -5.057605 -1.596351 0.948281
C -2.633287 4.813270 -1.050979	O -3.868783 -1.197778 1.058472
H -3.203610 2.954625 -1.952758	Rh -3.185498 0.260844 -0.269523
C -1.649563 5.510335 -0.347967	O -2.657019 -1.263991 -1.579462
H 0.312388 5.396061 0.538584	C -3.539754 -1.714591 -2.357969
H -3.560087 5.306015 -1.331824	O -4.735403 -1.340980 -2.507104
H -1.806826 6.549289 -0.071690	O -3.899976 1.766526 0.966641
F 5.182077 1.882965 1.225357	C -5.097642 2.131732 0.820984
F 3.688809 3.317735 0.556471	O -5.966132 1.705396 0.009782
F 4.702649 2.042301 -0.893063	H 5.090165 -5.461015 1.765093
F 0.418809 0.919726 5.105072	H 7.481377 -5.336934 1.159554
F -1.563315 0.508576 4.301024	H 7.319121 1.771104 -4.462605
F -0.569375 2.396083 3.851133	H 6.559196 3.460432 -2.818380
F -2.768727 -3.073145 1.904937	H 7.012475 -1.070028 -4.920446
F -2.596890 -3.630381 -0.195151	H 8.543184 -1.134037 -4.054370
F -1.488241 -4.734902 1.317195	H 5.892814 -2.476667 -3.306407
F 1.610441 -3.140938 -3.475368	H 7.510610 -3.187339 -3.203028
F 3.564003 -3.451378 -2.568325	H 8.913397 -3.984655 -1.363011
F 3.140660 -1.592614 -3.618282	H 9.363551 -3.405331 0.238440
C -6.366197 0.929134 -0.295640	H 8.623464 -1.152960 -0.233626
H -5.767420 1.432136 0.465743	H 9.224870 -1.592037 -1.837439
H -6.524540 1.614004 -1.135910	H 2.472612 1.030499 -0.734396
H -7.344987 0.687162 0.133031	H 0.363746 -1.203340 0.581010
C -6.511058 -1.038887 -1.871965	H -0.465387 -0.849502 -3.586494
H -7.486342 -1.337868 -1.474536	H -0.079312 0.726575 -4.356084
H -6.674106 -0.358344 -2.713789	H 1.234605 -0.353220 -3.780995
H -5.998672 -1.932819 -2.241163	C 3.095659 -3.855348 1.157300
C -5.385951 -1.329134 0.369023	C 1.988389 -3.763674 0.329200
H -4.836726 -2.199735 -0.001989	C 2.894455 -4.225218 2.522662
H -4.798068 -0.852111 1.155241	C 0.681729 -4.078902 0.800463
H -6.328180 -1.679434 0.804814	H 2.101268 -3.467673 -0.708557
	C 1.648001 -4.539372 3.005041
	H 3.750295 -4.250157 3.190319
	C 0.506725 -4.497131 2.161007
	H 1.523233 -4.831730 4.045609
	C 5.559342 3.084816 -0.355378
	C 4.734545 4.131318 -0.864039
	C 5.895365 3.100606 0.988419
	C 4.285854 5.142997 -0.049174
	H 4.439909 4.108725 -1.909083
	C 5.449460 4.130956 1.855132
	H 6.524792 2.316891 1.398830
	C 4.630169 5.180916 1.328108
	H 3.644439 5.922558 -0.451787
	C -5.458495 -2.738887 1.909363
	C -3.127712 -2.935842 -3.211899
	C -3.069659 2.929832 -3.675644
	C -5.543041 3.262505 1.776619
	C 0.381538 2.097024 0.306866
	C 0.032591 3.107257 -0.624609
	C 0.878714 2.523276 1.564047
	C 0.156018 4.452927 -0.298378
	H -0.359211 2.824570 -1.590102
	C 0.997860 3.875338 1.877919
	H 1.202594 1.797887 2.304824
	C 0.632057 4.853875 0.953671
	H -0.138392 5.198180 -1.033414
	H 1.393384 4.161947 2.848597
	H 0.716813 5.907624 1.203511
	H 1.450620 -0.291635 1.452786
	F -6.773236 -2.745330 2.145117
	F -5.120988 -3.919911 1.345707
	F -4.813608 -2.636384 3.080796

	F -5.336080 2.888253 3.050993 F -4.820465 4.369215 1.536101 F -6.837484 3.556623 1.625359 F -2.425226 2.199635 -4.610634 F -2.212523 3.840614 -3.191500 F -4.084400 3.568568 -4.263680 F -3.702672 -2.898628 -4.418365 F -1.798408 -3.002880 -3.373353 F -3.531330 -4.059346 -2.581582 C -0.461983 -4.019870 -0.046840 H -0.341589 -3.678254 -1.069030 C -0.791499 -4.849707 2.617608 H -0.911654 -5.180546 3.647189 C -1.709191 -4.359818 0.431203 C -1.877985 -4.780267 1.773301 H -2.571505 -4.306105 -0.225273 H -2.870010 -5.036901 2.131930 C 5.797431 4.158579 3.233963 H 6.419530 3.360131 3.631503 C 4.189135 6.212858 2.199061 H 3.567438 7.008308 1.794772 C 4.541745 6.210396 3.530627 C 5.354394 5.172701 4.052864 H 4.199880 7.006550 4.186563 H 5.627026 5.182089 5.104787 C 0.587265 -1.111838 5.576622 H 0.965017 -2.084861 5.248131 H 1.418011 -0.399316 5.573184 H 0.214500 -1.207299 6.601512 C -1.684270 -1.649615 4.602113 H -2.482763 -1.327275 3.931513 H -1.318345 -2.623912 4.265019 H -2.103374 -1.768546 5.607519 C -1.011083 0.771958 5.027555 H -1.410761 0.759618 6.047443 H -0.175917 1.479446 4.998945 H -1.797086 1.121694 4.355036
(A(6-10'))‡ E_0 = -5293.0194804 G_{298} = -5292.168480 NImag = 1 (-126.5574 cm^{-1}) C 5.774990 -1.988028 -0.518410 C 7.080359 -1.542720 -0.339688 C 7.980540 -2.340822 0.384133 C 7.602210 -3.597372 0.845918 C 6.314507 -4.063353 0.572450 C 5.375694 -3.270885 -0.104799 C 9.295702 -1.614156 0.570440 C 8.932660 -0.160863 0.190972 C 7.785772 -0.301304 -0.866839 C 7.083468 1.030463 -1.112088 C 7.726299 1.722099 -2.151200 C 8.765396 0.844013 -2.813086 C 8.401213 -0.559620 -2.283798 C 7.369836 3.031120 -2.456749 C 6.371150 3.654108 -1.710809 C 5.661029 2.978134 -0.701950 C 6.018461 1.637827 -0.452060 O 5.276167 0.890402 0.479410 P 4.104934 -0.108781 -0.013666 O 3.148943 0.713982 -0.977292 O 4.822409 -1.113847 -1.072491 O 3.463253 -0.760110 1.158863 N 0.728794 -1.121619 0.972040 C -0.062286 -1.283304 2.262675 O 0.815534 -1.552304 3.207403 C 0.402622 -1.598155 4.644742 C 0.263628 -0.067780 0.030420 C 0.143434 1.165913 0.744381 O -1.256415 -1.245206 2.285239 O -3.165701 2.050731 -1.173461 C -4.295324 2.594644 -1.299214 O -5.433360 2.137366 -0.997867 Rh -5.508650 0.249884 -0.157902 O -5.464685 -1.644382 0.677334 C -4.344871 -2.228167 0.708614 O -3.223407 -1.806188 0.326346 Rh -3.093236 0.131150 -0.399402 O -3.427216 -0.637601 -2.294529 C -4.615836 -0.821066 -2.665204	**(B(7-10))‡** E_0 = -2969.1190299 G_{298} = -2968.348677 NImag = 1 (-731.7761 cm^{-1}) C -3.477010 -0.893442 0.511321 C -3.738981 -2.226541 0.815369 C -4.545336 -2.534938 1.921886 C -5.151271 -1.523098 2.659541 C -4.946132 -0.195279 2.285730 C -4.101751 0.153830 1.217696 C -4.585073 -4.031119 2.147792 C -3.414076 -4.531853 1.272794 C -3.334202 -3.505971 0.093102 C -2.037030 -3.648291 -0.695170 C -2.215494 -4.548463 -1.757388 C -3.669159 -4.952024 -1.872989 C -4.378391 -3.885013 -1.011620 C -1.141452 -4.925482 -2.556797 C 0.121114 -4.398711 -2.287530 C 0.330376 -3.464592 -1.259007 C -0.783069 -3.077343 -0.489045 O -0.642153 -2.067978 0.472582 P -0.975711 -0.534803 0.020483 O -0.208108 -0.203982 -1.291096 O -2.529719 -0.598130 -0.480017 O -0.739270 0.356850 1.199639 N 2.215436 0.958158 0.413883 C 2.807328 1.685685 1.418228 O 3.146051 0.859534 2.433038 C 3.787148 1.382097 3.647705 C 1.724342 1.563799 -0.792785 C 0.866324 2.668141 -0.543209 O 0.842257 3.670544 -1.394429 C -0.179307 4.680922 -1.249465 O 2.972404 2.895823 1.377942 O 0.015086 2.736902 0.445502 H -5.441082 0.600598 2.834622 H -5.778491 -1.757905 3.515809 H -1.278573 -5.620238 -3.381596 H 0.973504 -4.705429 -2.887022 H -4.022974 -4.962373 -2.910187 H -3.834128 -5.962656 -1.472876 H -4.584247 -2.997400 -1.620600

O -5.687704 -0.577164 -2.040025	H -5.328036 -4.226392 -0.587731
O -2.964162 0.960355 1.494307	H -5.542472 -4.458944 1.818036
C -4.032497 1.229814 2.102119	H -4.468093 -4.299763 3.203881
O -5.225191 1.071340 1.716116	H -2.480001 -4.485052 1.843969
H 6.013014 -5.053932 0.900615	H -3.540743 -5.561375 0.922980
H 8.296640 -4.213953 1.410864	H 0.614808 0.576122 -1.153344
H 7.871286 3.571963 -3.255259	H 2.170619 -0.045551 0.536024
H 6.125554 4.693694 -1.903978	H -0.078480 5.182737 -0.285612
H 8.731845 0.904828 -3.906762	H 0.004655 5.377509 -2.066726
H 9.781766 1.134995 -2.512111	H -1.172561 4.238152 -1.335701
H 7.633419 -1.007972 -2.924471	H -0.158745 1.830565 0.873216
H 9.251452 -1.247997 -2.249170	C 2.660635 1.633264 -1.967056
H 10.070861 -2.019848 -0.094738	C 2.156794 1.608634 -3.277337
H 9.682016 -1.699493 1.592365	C 4.050825 1.686016 -1.789677
H 8.540320 0.363676 1.069588	C 3.013471 1.649991 -4.376815
H 9.782049 0.414967 -0.189458	H 1.082725 1.547545 -3.433419
H 2.196288 0.604086 -0.720655	C 4.909818 1.720487 -2.889072
H 0.732136 -2.034031 0.498765	H 4.459655 1.706506 -0.785234
O 0.425765 1.266736 1.946548	C 4.396568 1.703759 -4.187968
O -0.312856 2.213882 0.008117	H 2.600402 1.628839 -5.382290
H 1.724951 -0.946238 1.249184	H 5.984248 1.770117 -2.728822
C -0.576416 3.417995 0.743828	H 5.066476 1.731366 -5.043549
H -1.231363 3.209695 1.592113	C 1.704060 -2.941877 -1.027179
H 0.352759 3.863404 1.104687	C 2.312108 -3.028720 0.214117
H -1.069940 4.083171 0.034884	C 2.451872 -2.420376 -2.122564
C 4.013076 -3.806522 -0.392522	C 3.666826 -2.645267 0.404686
C 3.665025 -4.159902 -1.727862	H 1.759388 -3.427424 1.060417
C 3.094392 -4.012458 0.618161	C 3.757971 -2.021015 -1.965785
C 2.441585 -4.716751 -2.016423	H 1.964001 -2.317768 -3.087060
H 4.387752 -3.991170 -2.520751	C 4.409510 -2.131627 -0.708401
C 1.807628 -4.554213 0.347762	H 4.304704 -1.601673 -2.806054
H 3.341175 -3.720775 1.635277	C -3.912478 1.587296 0.872849
C 1.476657 -4.929702 -0.995738	C -3.682987 2.540637 1.907864
H 2.192226 -4.987704 -3.039266	C -4.022400 2.038263 -0.431190
C 4.618782 3.706476 0.068293	C -3.583790 3.883093 1.630404
C 3.756421 4.580890 -0.571917	H -3.563746 2.187326 2.927741
C 4.549130 3.598893 1.489691	C -3.928087 3.417456 -0.751284
C 2.833903 5.383461 0.147553	H -4.199471 1.330110 -1.235239
H 3.772493 4.657928 -1.656113	C -3.709619 4.366296 0.300543
C 3.664900 4.361308 2.214117	H -3.399643 4.594165 2.432301
H 5.215841 2.914391 2.002185	C 3.949233 0.124503 4.506049
C 2.790036 5.281097 1.575816	H 4.559281 -0.618834 3.984013
H 3.631199 4.272093 3.297167	H 4.435329 0.376820 5.454692
C -0.044444 -0.450570 -1.356500	H 2.972995 -0.321492 4.723199
C -0.021192 0.506441 -2.403378	C 2.866604 2.393012 4.341624
C -0.311778 -1.789090 -1.723657	H 2.738645 3.290035 3.734316
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H 0.171089 1.545559 -2.165235	H 3.296940 2.676980 5.309046
C -0.516001 -2.153323 -3.054157	C 5.153655 1.981818 3.296929
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C -0.484679 -1.199560 -4.069451	H 5.682234 2.262057 4.215389
H -0.221332 0.899109 -4.496285	H 5.763233 1.244288 2.762863
H -0.722015 -3.195164 -3.285799	C -4.055423 3.892370 -2.086645
H -0.653646 -1.483598 -5.103955	H -4.223794 3.171203 -2.883034
C -4.327227 -3.667911 1.272794	C -3.622868 5.746818 -0.024627
C -4.773769 -1.476308 -4.056584	H -3.457393 6.463401 0.776763
C -3.855968 1.794088 3.530480	C -3.968702 5.237769 -2.369644
C -4.254877 4.014992 -1.908087	C -3.749600 6.174921 -1.328443
F -5.514415 -4.024380 1.766678	H -4.069383 5.586508 -3.393949
F -3.408182 -3.771852 2.250134	H -3.685927 7.234091 -1.563239
F -3.994411 -4.530082 0.292143	C 4.321046 -2.779507 1.660704
F -2.827501 2.651156 3.584270	H 3.758685 -3.174376 2.503336
F -3.604709 0.774714 4.377111	C 5.766694 -1.756817 -0.517792
F -4.959098 2.423921 3.946113	H 6.320309 -1.357055 -1.363795
F -4.561065 -2.801175 -3.941051	C 5.643271 -2.424234 1.808584
F -6.002187 -1.285666 -4.549461	C 6.372439 -1.902009 0.710377
F -3.882101 -0.975813 -4.920445	H 6.134591 -2.544321 2.770602
F -5.474158 4.551884 -1.995998	H 7.413816 -1.620581 0.842012
F -3.490106 4.814061 -1.140794	
F -3.715876 3.965248 -3.136506	
C -0.533456 -2.787732 4.867106	
H -1.457162 -2.683581 4.294348	
H -0.043724 -3.727227 4.587419	
H -0.790361 -2.847316 5.930540	
C -0.233842 -0.259278 5.021568	
H -0.345280 -0.214586 6.110836	
H 0.402617 0.568334 4.696456	
H -1.218444 -0.133268 4.569320	
C 1.742313 -1.796799 5.352819	
H 1.582334 -1.856189 6.434280	
H 2.224498 -2.722902 5.023160	

H 2.416668 -0.961429 5.142785 C 0.821611 -4.706293 1.363898 H 1.073863 -4.416380 2.381057 C 0.186918 -5.464499 -1.261732 H -0.056072 -5.759168 -2.279937 C -0.432668 -5.195142 1.066148 C -0.750988 -5.583728 -0.259301 H -1.188141 -5.273725 1.841841 H -1.744347 -5.962382 -0.479730 C 1.955471 6.293351 -0.502416 H 1.986339 6.365974 -1.587048 C 1.878093 6.097642 2.297023 H 1.847879 6.016934 3.381065 C 1.082489 7.071910 0.224506 C 1.044114 6.974476 1.638085 H 0.417847 7.764984 -0.284085 H 0.350995 7.594271 2.200455	
(B(7-10'))‡ E_0 = -2969.1145022 G_{298} = -2968.344824 NImag = 1 (-954.7057 cm^{-1}) C -2.702794 -2.359678 -0.264560 C -4.008278 -2.046658 -0.627039 C -4.675838 -2.855732 -1.558652 C -4.077722 -4.016412 -2.039770 C -2.811058 -4.372004 -1.574297 C -2.089942 -3.555646 -0.685943 C -6.019047 -2.253311 -1.913182 C -5.908897 -0.821554 -1.338006 C -4.946009 -0.962470 -0.112407 C -4.468208 0.390499 0.405225 C -5.333062 0.854036 1.409842 C -6.356268 -0.202990 1.761372 C -5.746955 -1.474301 1.134448 C -5.173125 2.121999 1.958329 C -4.145100 2.937822 1.488925 C -3.233989 2.494624 0.514990 C -3.396951 1.189151 0.009853 O -2.459910 0.679788 -0.894512 P -1.229784 -0.247699 -0.346333 O -0.436462 0.525700 0.738199 O -1.969574 -1.433293 0.492209 O -0.454779 -0.730051 -1.537151 N 2.369045 -0.870779 -0.074149 C 3.460630 -1.415210 -0.715952 O 4.242576 -0.440155 -1.237566 C 5.473245 -0.765564 -1.971353 C 2.156122 0.534808 0.167860 C 2.089761 1.263944 -1.057487 O 2.582916 2.479348 -1.131472 C 2.344419 3.254004 -2.325903 O 3.661769 -2.615236 -0.798580 O 1.507150 0.817592 -2.134630 H -2.356108 -5.300187 -1.907730 H -4.589712 -4.648252 -2.761273 H -5.843883 2.480555 2.734969 H -4.036659 3.946913 1.875339 H -6.513249 -0.296052 2.842004 H -7.334723 0.031625 1.318500 H -5.044575 -1.932834 1.839684 H -6.492096 -2.230356 0.868031 H -6.843267 -2.809788 -1.444949 H -6.209940 -2.259309 -2.992456 H -5.443560 -0.160130 -2.077709 H -6.875779 -0.388045 -1.062563 H 0.705182 0.585367 0.506380 H 1.764875 -1.561564 0.352930 H 1.279565 3.273400 -2.560748 H 2.703264 4.253574 -2.085011 H 2.905591 2.828579 -3.161180 H 0.841597 0.060789 -1.932149 C 2.838018 1.141282 1.361992 C 2.502192 2.432410 1.807471 C 3.771691 0.408338 2.109910 C 3.106797 2.980747 2.936205 H 1.759022 3.012378 1.269549 C 4.369266 0.955245 3.246958 H 4.023990 -0.603397 1.810605 C 4.047044 2.246673 3.663604 H 2.832809 3.984282 3.252440	**(B(7'-10))‡** E_0 = -2969.1102746 G_{298} = -2968.340208 NImag = 1 (-935.3179 cm^{-1}) C -3.636829 -0.935905 0.126054 C -3.991313 -2.282745 0.079123 C -5.033825 -2.749959 0.894186 C -5.761611 -1.869033 1.687060 C -5.452457 -0.510321 1.647041 C -4.389844 -0.010267 0.873927 C -5.171990 -4.252037 0.772595 C -3.850859 -4.653824 0.081157 C -3.470291 -3.414912 -0.797689 C -2.029748 -3.496722 -1.283287 C -1.973578 -4.145331 -2.526544 C -3.368993 -4.395073 -3.056404 C -4.233401 -3.477191 -2.164166 C -0.749152 -4.442566 -3.115788 C 0.424973 -4.093820 -2.448836 C 0.405281 -3.407137 -1.223102 C -0.849868 -3.082292 -0.671843 O -0.925041 -2.289428 0.479944 P -1.075978 -0.671585 0.258150 O 0.004036 -0.214362 -0.753682 O -2.481139 -0.513136 -0.551845 O -1.077648 -0.012552 1.605834 N 2.908805 1.241643 -0.638181 C 4.043870 2.015562 -0.590967 O 4.984008 1.460075 -1.406196 C 6.282584 2.112557 -1.604074 C 1.789596 1.457949 0.242170 C 2.001339 1.035896 1.585027 O 3.193967 0.602138 1.936183 C 3.361830 0.012510 3.243812 O 4.165918 3.035428 0.061324 O 1.079678 0.974743 2.509768 H -6.042150 0.194147 2.226366 H -6.567765 -2.227501 2.322227 H -0.701369 -4.942428 -4.079896 H 1.387506 -4.351727 -2.881630 H -3.463531 -4.159503 -4.122549 H -3.654182 -5.450281 -2.939776 H -4.267072 -2.469922 -2.594479 H -5.264660 -3.826095 -2.050022 H -6.042866 -4.522464 0.158558 H -5.307179 -4.742775 1.743260 H -3.070060 -4.804005 0.835462 H -3.928352 -5.573943 -0.507050 H 0.795646 0.478429 -0.257291 H 3.011534 0.327146 -1.058921 H 2.646431 -0.796861 3.394085 H 4.379505 -0.373251 3.243992 H 3.231607 0.774662 4.015332 H 0.144977 0.763170 2.132056 C 0.983692 2.704206 -0.034737 C 0.645812 2.995571 -1.366390 C 0.578194 3.599507 0.965607 C -0.059921 4.152355 -1.688398 H 0.952359 2.311302 -2.151596 C -0.138732 4.751329 0.641613 H 0.832482 3.410549 2.003364 C -0.458212 5.037935 -0.685241 H -0.306851 4.358123 -2.726910

H 5.090130 0.364805 3.807162	H -0.439069 5.432995 1.433033
H 4.513340 2.672592 4.548117	H -1.021360 5.932379 -0.932296
C -2.181519 3.427998 0.033464	C 1.693849 -3.081067 -0.556382
C -1.432220 4.169144 0.930454	C 1.941496 -3.460330 0.750796
C -2.002900 3.662022 -1.362202	C 2.739721 -2.452242 -1.295040
C -0.516137 5.163993 0.498555	C 3.213351 -3.271338 1.353160
H -1.537436 3.986635 1.996813	H 1.159232 -3.944865 1.328371
C -1.135036 4.629431 -1.812271	C 3.976737 -2.232002 -0.733039
H -2.582625 3.080670 -2.071515	H 2.540582 -2.138413 -2.316059
C -0.371552 5.414237 -0.904778	C 4.257855 -2.644614 0.598250
H -1.036721 4.817258 -2.879513	H 4.756988 -1.734954 -1.304861
C 6.460863 -1.484635 -1.045342	C -4.158443 1.458754 0.843654
H 6.077477 -2.462185 -0.749054	C -4.117864 2.196856 2.061868
H 7.417867 -1.620767 -1.562040	C -4.110543 2.149365 -0.354543
H 6.641290 -0.885642 -0.145868	C -4.062106 3.570279 2.057561
C 6.005157 0.617716 -2.357772	H -4.120379 1.654249 3.002732
H 6.180985 1.226916 -1.465549	C -4.071196 3.567024 -0.393453
H 6.948110 0.518673 -2.905824	H -4.142719 1.604449 -1.293948
H 5.287597 1.142217 -2.998078	C -4.056602 4.298737 0.838027
C 5.138965 -1.587705 -3.220985	H -4.028918 4.118370 2.996443
H 4.753752 -2.571706 -2.950329	C 6.987122 1.170583 -2.585425
H 4.386866 -1.068095 -3.825141	H 6.415341 1.083018 -3.515159
H 6.040631 -1.713479 -3.831409	H 7.984804 1.552796 -2.826532
C -0.749681 -3.977149 -0.203143	H 7.096880 0.170146 -2.152492
C 0.205015 -4.517261 -1.113035	C 7.047339 2.181849 -0.276717
C -0.424793 -3.916331 1.142395	H 6.540753 2.840310 0.430263
C 1.424491 -4.972980 -0.672917	H 7.127790 1.182457 0.166356
H -0.031320 -4.534783 -2.172927	H 8.061268 2.559712 -0.452115
C 0.821528 -4.388760 1.629622	C 6.087824 3.497543 -2.232702
H -1.139917 -3.514691 1.854230	H 5.564609 4.166402 -1.547805
C 1.769997 -4.931728 0.704051	H 7.063454 3.932776 -2.478442
H 2.154246 -5.352890 -1.382454	H 5.508328 3.415301 -3.158995
C 0.254326 5.932036 1.415050	C -4.087608 4.288380 -1.618621
H 0.142521 5.740316 2.479678	H -4.099754 3.730774 -2.552144
C 0.525590 6.429340 -1.333421	C -4.054160 5.718651 0.795185
H 0.621962 6.627410 -2.398921	H -4.043030 6.270409 1.732596
C 1.121321 6.904289 0.967790	C -4.097196 5.665323 -1.627620
C 1.256491 7.157794 -0.420013	C -4.079048 6.388487 -0.408411
H 1.937558 7.933108 -0.760473	H -4.118319 6.204038 -2.571341
H 1.702968 7.484646 1.678736	H -4.088074 7.475178 -0.427642
C 1.157144 -4.346316 3.011868	C 3.494393 -3.713622 2.675850
H 0.434579 -3.934897 3.712934	H 2.702990 -4.196951 3.244046
C 3.019547 -5.396635 1.192614	C 5.534875 -2.476274 1.197650
H 3.743364 -5.788037 0.482566	H 6.323787 -1.997786 0.622030
C 3.314674 -5.343430 2.536363	C 4.746868 -3.547821 3.224911
C 2.373134 -4.814817 3.455282	C 5.777404 -2.920971 2.479621
H 2.617969 -4.777218 4.513538	H 4.950629 -3.899588 4.232747
H 4.274337 -5.702843 2.898324	H 6.762294 -2.797701 2.922081
(B(7'-10'))‡	**(C(7-10))‡**
E_0 = -2969.1078111	E_0 = -5293.0381305
G_{298} = -2968.339339	G_{298} = -5292.180363
NImag = 1 (-841.8244 cm^{-1})	NImag = 1 (-1145.1054 cm^{-1})
C -3.773425 -0.211230 -0.106391	C -5.925113 0.481649 0.294277
C -4.430031 -1.388714 0.238419	C -6.596749 -0.473469 1.051138
C -5.508797 -1.345605 1.134399	C -7.286101 -0.076102 2.208068
C -5.989389 -0.126480 1.600544	C -7.387424 1.269558 2.543632
C -5.397162 1.051605 1.145316	C -6.807024 2.221060 1.705431
C -4.277815 1.041361 0.295260	C -6.055044 1.855955 0.575675
C -5.973449 -2.747437 1.469886	C -7.817600 -1.284225 2.949692
C -4.823691 -3.625750 0.922895	C -7.067151 -2.452392 2.270896
C -4.239613 -2.807321 -0.275069	C -6.816762 -1.959906 0.807071
C -2.896615 -3.345678 -0.748653	C -5.834746 -2.859640 0.063733
C -3.086724 -4.270631 -1.787684	C -6.537303 -3.880918 -0.593958
C -4.542872 -4.326146 -2.193023	C -8.029045 -3.651139 -0.508983
C -5.111325 -3.041352 -1.556875	C -8.108983 -2.180689 -0.052407
C -2.012613 -4.972641 -2.322311	C -5.854372 -4.922549 -1.210089
C -0.740018 -4.756369 -1.797053	C -4.463878 -4.930703 -1.173838
C -0.507756 -3.819002 -0.776497	C -3.713352 -3.889444 -0.591341
C -1.606788 -3.087575 -0.285703	C -4.440695 -2.839776 0.015957
O -1.411094 -2.077296 0.666131	O -3.774071 -1.759526 0.609721
P -1.245481 -0.530568 0.157521	P -3.552185 -0.350051 -0.182434
O -0.040398 -0.450711 -0.822819	O -2.717372 -0.588568 -1.465219
O -2.555282 -0.287027 -0.803290	O -5.043381 0.058159 -0.717421
O -1.204310 0.383488 1.341810	O -2.975874 0.629309 0.797063
N 3.052110 0.918040 -0.570315	N 0.308737 0.016257 -0.014446
C 4.171245 1.698524 -0.414740	C -0.131709 0.400021 1.311130
O 5.188470 1.163022 -1.137392	O -0.179638 -0.691866 2.076067
C 6.513151 1.792084 -1.154980	C -0.452369 -0.599531 3.543206
C 1.874488 1.105667 0.238352	C -0.309188 0.555183 -1.270734
C 1.126519 2.272428 -0.046578	C -0.820929 1.895142 -1.316415

O 1.460888 3.048313 -1.050855	O -0.631022 2.579428 -2.422890
C 0.545474 4.085871 -1.463310	C -1.453959 3.743530 -2.678515
O 4.215621 2.721145 0.249119	O -0.327714 1.545362 1.638003
O 0.028153 2.594494 0.594690	O -1.617999 2.458341 -0.460410
H -5.799608 2.012209 1.453061	O 2.792741 -1.294104 1.554108
H -6.824667 -0.084454 2.294974	C 3.907946 -1.581070 2.074506
H -2.158301 -5.683889 -3.131345	O 5.028127 -1.034176 1.907968
H 0.107191 -5.320371 -2.176251	Rh 5.127811 0.572453 0.594629
H -4.678716 -4.357299 -3.280063	O 5.079339 2.169041 -0.719034
H -5.031377 -5.223733 -1.787452	C 3.956887 2.512843 -1.173399
H -4.964913 -2.197079 -2.240091	O 2.825596 1.983316 -0.985514
H -6.179718 -3.101982 -1.327052	Rh 2.708210 0.320522 0.252326
H -6.926282 -2.980985 0.974171	O 3.176695 -1.016549 -1.279275
H -6.136106 -2.888635 2.544526	C 4.393773 -1.243048 -1.513392
H -4.046320 -3.737158 1.687209	O 5.414835 -0.747680 -0.960151
H -5.146653 -4.628572 0.624879	O 2.486771 1.638924 1.841584
H 0.810488 0.191751 -0.378859	C 3.515136 2.098177 2.408560
H 3.191671 0.023097 -1.019977	O 4.727868 1.879869 2.144953
H 0.390422 4.803207 -0.655652	H -6.925476 3.277953 1.924862
H 1.035277 4.563615 -2.311420	H -7.922326 1.582625 3.436659
H -0.411340 3.652901 -1.758028	H -6.392364 -5.729441 -1.701062
H -0.375576 1.799054 1.079099	H -3.930725 -5.771870 -1.603555
C 2.010403 0.733321 1.701686	H -8.537476 -3.827406 -1.463778
C 2.298446 1.713395 2.666231	H -8.493688 -4.324860 0.224998
C 1.927698 -0.602778 2.111728	H -8.066613 -1.519991 -0.925789
C 2.476656 1.365897 4.005503	H -9.022715 -1.942980 0.500878
H 2.405030 2.748095 2.357352	H -8.905334 -1.381327 2.825489
C 2.115615 -0.952592 3.448731	H -7.628502 -1.230324 4.027883
H 1.706883 -1.376268 1.384729	H -6.099184 -2.607346 2.760927
C 2.385687 0.030445 4.401816	H -7.614314 -3.399755 2.304971
H 2.698540 2.139253 4.736660	H -1.651293 -0.062793 -1.384641
H 2.038309 -1.995318 3.743885	H 0.295207 -1.003697 -0.077631
H 2.525502 -0.241650 5.445021	H -1.276140 4.508333 -1.921476
C 0.877671 -3.697047 -0.242554	H -1.137901 4.088967 -3.661902
C 1.161699 -4.083207 1.099275	H -2.507437 3.463012 -2.681276
C 1.924615 -3.338183 -1.071196	H -2.011773 1.813230 0.215939
C 2.456792 -4.126858 1.561324	C 0.361357 0.002801 -2.514805
H 0.339144 -4.365488 1.749622	C 0.035165 -1.305275 -2.908230
C 3.270888 -3.350115 -0.618358	C 1.260507 0.728669 -3.312895
H 1.716952 -3.035647 -2.094503	C 0.586653 -1.869835 -4.058744
C 3.547711 -3.763723 0.725480	H -0.675354 -1.886239 -2.328335
H 2.662355 -4.445019 2.580786	C 1.798835 0.169314 -4.471250
C -3.723285 2.332075 -0.189481	H 1.537264 1.734741 -3.036447
C -3.532881 2.545505 -1.587282	C 1.465250 -1.131726 -4.850169
C -3.496779 3.384984 0.679040	H 0.322715 -2.886562 -4.333249
C -3.174515 3.780627 -2.072844	H 2.483555 0.757943 -5.077039
H -3.702600 1.721167 -2.272545	H 1.888093 -1.566060 -5.752296
C -3.104842 4.667242 0.212330	C 3.253552 3.009671 3.630031
H -3.612876 3.232649 1.749097	C 4.721617 -2.281451 -2.611867
C -2.956207 4.879580 -1.196822	C 3.854640 -2.737337 3.098407
H -3.062904 3.933332 -3.144257	C 3.931908 3.768070 -2.076140
C -2.862196 5.752813 1.097564	F 5.055632 -3.276916 3.304850
H -2.968906 5.588397 2.167143	F 3.387099 -2.260468 4.270345
C -2.584591 6.168835 -1.663834	F 3.014443 -3.703807 2.681913
H -2.481630 6.328556 -2.735032	F 4.200029 3.948869 3.739398
C -2.497007 6.990181 0.614965	F 2.060667 3.608216 3.546778
C -2.359318 7.201618 -0.779566	F 3.272440 2.251321 4.745212
H -2.313967 7.810839 1.303250	F 3.356216 3.475243 -3.258683
H -2.075748 8.183522 -1.148896	F 3.205644 4.731143 -1.482844
C 4.355947 -2.977726 -1.459194	F 5.158400 4.237476 -2.308320
H 4.145262 -2.668643 -2.480631	F 5.535877 -1.732546 -3.527856
C 4.895640 -3.792527 1.172141	F 5.361427 -3.327949 -2.050337
H 5.101916 -4.105037 2.193111	F 3.629709 -2.734469 -3.225451
C 5.652404 -3.015824 -0.995099	C -5.480790 2.920495 -0.287613
C 5.925084 -3.427898 0.332849	C -5.703887 2.901890 -1.696702
H 6.951899 -3.453375 0.687364	C -4.818119 4.002733 0.264799
H 6.472377 -2.732364 -1.649314	C -5.309818 3.953557 -2.489828
C 7.313533 0.857775 -2.067628	H -6.215827 2.052495 -2.137178
H 6.868985 0.819874 -3.067750	C -4.379652 5.094975 -0.528711
H 8.346116 1.211310 -2.159465	H -4.615096 4.020811 1.332554
H 7.327424 -0.157570 -1.657769	C -4.645408 5.083010 -1.936727
C 7.108183 1.807484 0.258140	H -5.512285 3.935024 -3.558469
H 6.526900 2.452027 0.919265	C -0.343290 -2.057515 3.993516
H 7.121308 0.794162 0.674688	H 0.657677 -2.453655 3.801086
H 8.140048 2.175512 0.220901	H -0.535262 -2.120922 5.069837
C 6.424545 3.197220 -1.762433	H -1.077506 -2.685502 3.479746
H 5.957379 3.153395 -2.752755	C -1.864640 -0.058044 3.771772
H 5.838004 3.860322 -1.124892	H -1.951723 0.980229 3.450410
H 7.431534 3.614324 -1.878864	H -2.601855 -0.647796 3.221076
	H -2.094382 -0.117296 4.842078
	C 0.617006 0.254086 4.227335

	H 0.586895 1.288144 3.884889 H 0.438592 0.239387 5.308537 H 1.612778 -0.158824 4.045170 C -3.685298 6.203629 0.028453 H -3.477994 6.207713 1.095827 C -4.219560 6.184345 -2.727292 H -4.430902 6.176077 -3.794351 C -3.278485 7.253391 -0.765318 C -3.550789 7.245550 -2.156310 H -2.747846 8.093927 -0.326574 H -3.230083 8.082206 -2.771140 C -2.228335 -3.989875 -0.628014 C -1.410429 -3.552161 0.456851 H -1.872406 -3.055383 1.300307 C -0.049432 -3.762492 0.455043 H 0.552144 -3.428541 1.295628 C 0.593189 -4.432610 -0.620995 C -0.208592 -4.861226 -1.726251 C -1.603944 -4.610730 -1.701657 H -2.189861 -4.919268 -2.562983 C 1.989608 -4.690839 -0.638311 H 2.587973 -4.369473 0.209736 C 0.421237 -5.533009 -2.810810 H -0.189463 -5.864436 -3.647901 C 2.569955 -5.342780 -1.703589 C 1.777805 -5.768254 -2.799304 H 3.640949 -5.521563 -1.713834 H 2.248107 -6.282903 -3.632826
(C(7-10'))‡ E_0 = -5293.0444009 G_{298} = -5292.192070 NImag = 1 (-909.2314 cm^{-1}) C 3.777595 -2.991085 -0.224064 C 5.018803 -3.007398 -0.854853 C 5.946170 -4.006735 -0.520853 C 5.610776 -5.011064 0.380301 C 4.344143 -5.005109 0.959834 C 3.403154 -3.992957 0.694736 C 7.257401 -3.779360 -1.238390 C 7.126788 -2.313461 -1.699227 C 5.590429 -2.104289 -1.940983 C 5.279007 -0.615869 -2.057288 C 5.441919 -0.206108 -3.390577 C 5.616314 -1.406097 -4.297382 C 5.214743 -2.584593 -3.380677 C 5.411089 1.143754 -3.723463 C 5.223956 2.087067 -2.713802 C 4.982895 1.712636 -1.380055 C 4.964847 0.332726 -1.088026 O 4.567088 -0.096529 0.190743 P 3.015311 -0.569136 0.362229 O 2.083095 0.420851 -0.391406 O 2.901669 -1.929118 -0.511548 O 2.730097 -0.763867 1.824576 N -0.637487 0.409337 1.108970 C -1.338776 0.078165 2.326826 O -1.787684 1.178426 2.930016 C -2.633584 1.089556 4.149924 C 0.239806 1.621138 1.085870 C 0.925522 1.844733 2.313053 O 1.178975 3.082687 2.676390 C 2.080961 3.310060 3.785820 O -1.487968 -1.070358 2.669065 O 1.367754 0.907101 3.107838 O -3.451716 1.668371 0.026668 C -4.521832 1.933546 -0.585792 O -5.020304 1.363216 -1.592571 Rh -4.018462 -0.293941 -2.331732 O -2.919109 -1.933764 -2.951811 C -1.866712 -2.216526 -2.320243 O -1.355094 -1.629781 -1.324757 Rh -2.320819 0.059303 -0.603834 O -1.280767 1.150981 -2.028708 C -1.796372 1.310843 -3.166707 O -2.908693 0.896965 -3.595384 O -3.498164 -1.138351 0.628652 C -4.556863 -1.631350 0.154264 O -5.049294 -1.491863 -0.997731 H 4.061269 -5.799305 1.643565 H 6.323293 -5.792340 0.632619	**(C(7'-10))‡** E_0 = -5293.0493094 G_{298} = -5292.194631 NImag = 1 (-954.7892 cm^{-1}) C -5.399195 0.448108 0.003563 C -6.264976 -0.519578 -0.499092 C -7.598646 -0.547437 -0.063863 C -8.082539 0.438992 0.788616 C -7.232070 1.473666 1.175628 C -5.877762 1.509793 0.797251 C -8.321200 -1.745985 -0.640904 C -7.162106 -2.603670 -1.197596 C -6.054844 -1.567892 -1.583230 C -4.714925 -2.237563 -1.846860 C -4.582572 -2.542517 -3.210033 C -5.741048 -1.970426 -3.996253 C -6.355016 -0.964744 -2.998906 C -3.483301 -3.257537 -3.673138 C -2.524924 -3.689549 -2.757735 C -2.613791 -3.381240 -1.389264 C -3.705979 -2.603689 -0.960354 O -3.776077 -2.157103 0.366839 P -3.179682 -0.668793 0.699368 O -1.726054 -0.598810 0.166425 O -4.021784 0.335454 -0.266562 O -3.379367 -0.398377 2.164466 N 1.453970 -0.709247 1.464944 C 2.515705 -0.979711 2.411022 O 3.327685 -1.902619 1.893772 C 4.438886 -2.483040 2.692398 C 0.144277 -0.304920 2.060994 C -0.355648 -1.263255 2.994257 O 0.333762 -2.365925 3.221789 C -0.232800 -3.369636 4.098391 O 2.606079 -0.434079 3.484729 O -1.490950 -1.169451 3.616073 O 2.436101 -1.324118 -1.397899 C 2.870046 -1.317212 -2.585328 O 3.263209 -0.345473 -3.280796 Rh 3.190915 1.552697 -2.431031 O 3.067250 3.367106 -1.457984 C 2.721419 3.353755 -0.243062 O 2.399447 2.370500 0.477318 Rh 2.365680 0.491962 -0.384053 O 0.471713 0.787509 -1.149571 C 0.336757 1.339754 -2.276096 O 1.230199 1.763379 -3.056007 O 4.373911 0.275409 0.172765 C 5.253662 0.727237 -0.611083 O 5.108546 1.303061 -1.721510 H -7.618607 2.287014 1.782383 H -9.114085 0.423315 1.131258

H 5.543176 1.466863 -4.752876	H -3.372782 -3.487671 -4.729654
H 5.255908 3.144590 -2.958112	H -1.682363 -4.284349 -3.098724
H 4.995088 -1.341149 -5.197908	H -5.424464 -1.497839 -4.932895
H 6.656667 -1.500318 -4.638847	H -6.460994 -2.756243 -4.265950
H 4.131637 -2.743361 -3.429903	H -5.841468 -0.000587 -3.085426
H 5.703855 -3.527235 -3.645665	H -7.423452 -0.789009 -3.158169
H 7.365058 -4.459510 -2.095486	H -9.015475 -1.445534 -1.438413
H 8.127485 -3.944801 -0.592933	H -8.917019 -2.278614 0.109258
H 7.450169 -1.644509 -0.893516	H -6.773291 -3.257780 -0.408858
H 7.723751 -2.078716 -2.585829	H -7.454790 -3.235693 -2.042318
H 1.361203 1.025455 0.270904	H -0.905879 -0.478584 0.971095
H -0.126954 -0.435965 0.846343	H 1.325729 -1.549293 0.896392
H 3.021697 2.781431 3.630576	H -1.238167 -3.632593 3.772926
H 2.247003 4.385469 3.792372	H 0.435278 -4.223742 4.013731
H 1.614756 2.979610 4.716328	H -0.256676 -2.986984 5.121013
H 1.805509 0.108803 2.603541	H -2.238250 -0.668278 3.086405
C -1.105325 -3.477183 -2.790967	C -0.014166 1.142963 2.489387
C -5.306777 3.145253 -0.031601	C -0.498259 2.120157 1.609055
C -5.393467 -2.515680 1.108384	C 0.325730 1.532998 3.797320
C -0.980214 2.149497 -4.178507	C -0.592986 3.454488 2.008214
F -1.096151 1.635613 -5.410832	H -0.797488 1.843291 0.606110
F 0.317893 2.185034 -3.854634	C 0.209487 2.860820 4.202586
F -1.452568 3.408879 -4.196277	H 0.711549 0.794860 4.490562
F -4.882130 4.269926 -0.634144	C -0.238678 3.829417 3.303408
F -6.618444 3.011792 -0.251570	H -0.946784 4.200046 1.305190
F -5.107772 3.274829 1.291583	H 0.483291 3.138113 5.217363
F -5.693228 -3.679141 0.515585	H -0.319197 4.869110 3.609112
F -6.538090 -1.880885 1.414279	C 6.713863 0.520372 -0.145551
F -4.737921 -2.775746 2.248744	C -1.130451 1.507017 -2.740201
F -1.522286 -3.886081 -3.990697	C 2.872586 -2.700745 -3.275256
F -1.309402 -4.468386 -1.902363	C 2.642515 4.743066 0.432327
F 0.213381 -3.231164 -2.854410	F 3.654307 -2.715230 -4.355244
C -0.239416 2.862956 0.366628	F 3.295896 -3.651891 -2.425062
C 0.429228 3.299897 -0.784818	F 1.612775 -3.004753 -3.651917
C -1.299845 3.639867 0.857661	F 7.584135 1.117992 -0.959307
C 0.045393 4.474481 -1.434707	F 6.878936 1.009960 1.095075
H 1.242966 2.707405 -1.187722	F 6.991990 -0.799696 -0.117618
C -1.688037 4.811827 0.208834	F 3.623092 5.539956 -0.015825
H -1.822822 3.315469 1.748238	F 1.460759 5.310786 0.123424
C -1.014999 5.234348 -0.939862	F 2.740292 4.648777 1.759736
H 0.565613 4.784783 -2.336814	F -1.200273 2.141864 -3.914918
H -2.520060 5.392039 0.598468	F -1.713934 0.308886 -2.864172
H -1.318204 6.147072 -1.446538	F -1.812557 2.229240 -1.829084
C 4.790991 2.765407 -0.348323	C -1.591110 -3.949254 -0.470413
C 5.388765 2.679704 0.899285	C -1.960417 -4.758986 0.589069
C 4.045822 3.940629 -0.662055	C -0.205081 -3.789329 -0.761512
C 5.288527 3.730479 1.847687	C -0.995665 -5.465774 1.354665
H 5.966317 1.799485 1.163314	H -3.013262 -4.900608 0.818129
C 3.925121 4.973921 0.236197	C 0.756804 -4.442699 -0.025207
H 3.549164 4.006845 -1.624952	H 0.088003 -3.148390 -1.585964
C 4.546527 4.909801 1.511433	C 0.394444 -5.311269 1.040309
H 3.338153 5.852139 -0.020678	H 1.806696 -4.315339 -0.275733
C -2.861239 2.561782 4.498854	C -5.060364 2.695089 1.162477
H -3.392458 3.074188 3.690393	C -5.174112 3.276568 2.458792
H -3.464770 2.637100 5.409345	C -4.283189 3.337112 0.213078
H -1.908786 3.073555 4.672046	C -4.553699 4.465307 2.760822
C -1.870375 0.368970 5.264900	H -5.751750 2.758317 3.218592
H -0.892184 0.836239 5.422202	C -3.635018 4.567099 0.491320
H -2.440120 0.445822 6.197709	H -4.177122 2.910360 -0.779174
H -1.720856 -0.685891 5.031375	C -3.779456 5.154781 1.789772
C -3.954607 0.405047 3.792069	H -4.647072 4.891897 3.756795
H -4.447109 0.943958 2.975789	C 5.151474 -3.364022 1.664835
H -3.799531 -0.631946 3.491988	H 5.572592 -2.751500 0.862897
H -4.618005 0.422192 4.664194	H 5.966691 -3.913437 2.147213
C 2.090376 -4.029111 1.390070	H 4.457649 -4.088069 1.224853
C 0.871771 -3.804167 0.685602	C 3.829321 -3.318296 3.822097
C 2.031051 -4.349026 2.736129	H 3.276786 -2.684184 4.519678
C -0.339750 -3.902649 1.327459	H 3.154096 -4.080865 3.420014
H 0.906559 -3.568893 -0.371370	H 4.628215 -3.824157 4.375676
C 0.796340 -4.462160 3.424809	C 5.381176 -1.401063 3.226758
H 2.950744 -4.500433 3.295751	H 4.904364 -0.798662 3.999939
C -0.420291 -4.230951 2.707223	H 6.264909 -1.889022 3.654198
H -1.258535 -3.730169 0.775472	H 5.712312 -0.741784 2.423033
C 5.914631 3.656299 3.123839	C -2.851287 5.242006 -0.485829
H 6.480943 2.762935 3.376460	H -2.732313 4.784910 -1.464860
C 4.459202 5.963997 2.460547	C -3.137206 6.393011 2.058898
H 3.899004 6.858624 2.198167	H -3.248444 6.836721 3.045768
C 5.811202 4.694893 4.022886	C -2.239727 6.441106 -0.193370
C 5.077258 5.861233 3.688194	C -2.385279 7.023267 1.091447
H 5.009037 6.676767 4.403209	H -1.639540 6.944788 -0.946207
H 6.297380 4.626188 4.992303	H -1.898677 7.970031 1.309880

C 0.727000 -4.792949 4.806128 H 1.652876 -4.966719 5.350062 C -1.657449 -4.333306 3.396159 H -2.576411 -4.130809 2.853335 C -1.691940 -4.658873 4.734081 C -0.488317 -4.893188 5.445381 H -0.529034 -5.149880 6.500847 H -2.644653 -4.734076 5.251747	C -1.367031 -6.353502 2.402961 H -2.422850 -6.477035 2.633079 C 1.353906 -6.045562 1.788937 H 2.406703 -5.935896 1.538969 C -0.413163 -7.053748 3.108362 C 0.962022 -6.897925 2.799474 H -0.711850 -7.733961 3.901421 H 1.705434 -7.461873 3.356402
(C(7'-10'))‡ E_0 = -5293.0525221 G_{298} = -5292.202112 NImag = 1 (-1029.2056 cm^{-1}) C 5.778467 1.669280 -0.145996 C 6.974507 0.960798 -0.078455 C 8.052948 1.330441 -0.895536 C 7.962381 2.446075 -1.720613 C 6.791766 3.202651 -1.703192 C 5.679241 2.840104 -0.923168 C 9.200852 0.358251 -0.730442 C 8.531766 -0.828250 -0.001478 C 7.379660 -0.179928 0.838925 C 6.402735 -1.234139 1.340130 C 6.813671 -1.700702 2.599050 C 7.963928 -0.871759 3.127404 C 7.944819 0.358697 2.195809 C 6.175597 -2.780465 3.198148 C 5.142808 -3.415039 2.511521 C 4.680593 -2.954510 1.265672 C 5.292594 -1.806880 0.721073 O 4.774007 -1.216300 -0.444317 P 3.765316 0.059040 -0.265816 O 2.634229 -0.320472 0.725138 O 4.661120 1.169844 0.542963 O 3.319331 0.547773 -1.614328 N -0.773924 -0.509372 0.514003 C -0.458898 -0.378355 1.920645 O -0.840480 -1.494501 2.542680 C -0.720274 -1.628404 4.019209 C 0.254676 0.014294 -0.421996 C 0.314695 1.438042 -0.537242 O -0.510940 2.174589 0.142005 C -0.387584 3.615627 0.143342 O 0.067204 0.600141 2.390052 O 1.216900 2.045538 -1.254661 O -2.597681 1.308690 -1.483589 C -3.561333 1.855774 -2.087726 O -4.797867 1.710040 -1.905286 Rh -5.383442 0.397157 -0.417679 O -5.850387 -0.927742 1.103540 C -4.899330 -1.432832 1.753001 O -3.655336 -1.258669 1.614127 Rh -3.013562 0.012136 0.102000 O -3.070661 -1.584588 -1.211407 C -4.148146 -1.799936 -1.835955 O -5.246767 -1.189607 -1.752644 O -3.141458 1.624311 1.406895 C -4.254800 2.208340 1.521228 O -5.348465 1.958753 0.948415 H 6.725636 4.105091 -2.303999 H 8.791731 2.736741 -2.360380 H 6.488015 -3.142530 4.174335 H 4.680417 -4.301425 2.935940 H 7.840913 -0.605267 4.183408 H 8.914223 -1.418696 3.048610 H 7.252596 1.110959 2.590586 H 8.923916 0.834135 2.079463 H 10.006792 0.796186 -0.124559 H 9.648987 0.067648 -1.687427 H 8.090032 -1.510973 -0.736114 H 9.224845 -1.406748 0.617607 H 1.577654 -0.179371 0.239236 H -0.902121 -1.500238 0.306355 H -0.495217 3.995618 -0.873006 H -1.208085 3.951297 0.773933 H 0.574608 3.907915 0.561358 H 1.997637 1.434763 -1.533188 C -5.287472 -2.381843 2.910035 C -3.136564 2.868354 -3.176404 C -4.236591 3.415746 2.486894 C -4.078952 -2.941474 -2.876996	**(D(7-10))‡** E_0 = -5293.0639203 G_{298} = -5292.214607 NImag = 1 (-1018.2903 cm^{-1}) C -5.826284 1.911753 0.631340 C -7.028648 1.328186 1.024168 C -7.702140 1.833808 2.147108 C -7.215136 2.945824 2.826664 C -6.041990 3.553518 2.379773 C -5.320303 3.051781 1.284173 C -8.911857 0.982663 2.466649 C -8.636892 -0.300744 1.653137 C -7.825192 0.185657 0.404562 C -7.174264 -0.985928 -0.322649 C -8.045405 -1.485315 -1.303545 C -9.255358 -0.586750 -1.444519 C -8.808937 0.692698 -0.702327 C -7.725620 -2.635903 -2.017078 C -6.523833 -3.290192 -1.746685 C -5.604671 -2.791394 -0.808709 C -5.943791 -1.607288 -0.125824 O -5.000469 -1.004906 0.720102 P -4.045270 0.138642 0.052618 O -3.479805 -0.378090 -1.296285 O -5.085717 1.312169 -0.399037 O -3.042635 0.567233 1.085831 N -0.838628 -1.315647 0.204431 C 0.085375 -1.103073 1.177308 O -0.286419 -1.722861 2.299171 C 0.484748 -1.689203 3.562751 C -0.857602 -0.715650 -1.105656 C -0.597586 0.687246 -1.108973 O -0.043312 1.220441 -2.168307 C 0.059696 2.661797 -2.264448 O 1.091182 -0.389502 1.051128 O -0.973651 1.508351 -0.169813 H -5.658767 4.432272 2.890782 H -7.734358 3.335846 3.698426 H -8.398797 -3.023865 -2.777374 H -6.274965 -4.204112 -2.278536 H -9.518542 -0.397768 -2.491464 H -10.141369 -1.034731 -0.972554 H -8.259643 1.345916 -1.389813 H -9.642038 1.269120 -0.287586 H -9.840036 1.471788 2.138483 H -9.019946 0.788690 3.539764 H -8.008156 -0.980664 2.239217 H -9.545362 -0.843627 1.373729 H -2.314674 -0.541267 -1.291678 H -1.617840 -1.902837 0.479377 H 0.710150 3.041040 -1.476093 H 0.503779 2.833469 -3.242965 H -0.925771 3.122230 -2.191808 H -1.686845 1.111182 0.448489 C -0.339751 -1.565560 -2.233896 C -0.903422 -1.464143 -3.514086 C 0.684588 -2.499826 -2.025533 C -0.445043 -2.263908 -4.561262 H -1.711307 -0.758080 -3.687704 C 1.144186 -3.301097 -3.071228 H 1.132595 -2.596716 -1.042167 C 0.580784 -3.186907 -4.344501 H -0.895453 -2.170403 -5.546176 H 1.953935 -4.002753 -2.888194 H 0.937710 -3.810480 -5.160038 C -4.327849 -3.518633 -0.576948 C -3.927102 -3.888491 0.696379 C -3.525549 -3.910553 -1.687865 C -2.759577 -4.668532 0.910572 H -4.527106 -3.602840 1.555860 C -2.378898 -4.649232 -1.512476 H -3.817589 -3.590447 -2.683288

F -5.291302 -3.455705 -3.112964	C -1.964381 -5.058507 -0.216720
F -3.271774 -3.923390 -2.455863	H -1.765985 -4.915565 -2.369402
F -3.590547 -2.449946 -4.030490	C -4.060961 3.728268 0.868066
F -2.248665 2.307800 -4.016658	C -3.013904 3.912348 1.816964
F -4.177088 3.305338 -3.885240	C -3.903037 4.235842 -0.408258
F -2.543589 3.928159 -2.587589	C -1.856420 4.570842 1.476353
F -5.459081 3.909499 2.691318	H -3.132951 3.495260 2.812396
F -3.466564 4.392457 1.958954	C -2.728609 4.938828 -0.786411
F -3.711118 3.059687 3.668075	H -4.695555 4.110619 -1.141429
F -6.581961 -2.698274 2.879652	C -1.675041 5.102897 0.171580
F -5.020214 -1.780001 4.087105	H -1.057714 4.685993 2.205095
F -4.566304 -3.515674 2.846935	C -0.465284 -2.402509 4.528927
C 0.294658 -0.783755 -1.702783	H -0.700390 -3.406236 4.162940
C 0.633237 -2.145224 -1.660688	H 0.003322 -2.487149 5.515000
C -0.091361 -0.228475 -2.934362	H -1.400570 -1.843235 4.633982
C 0.558750 -2.933902 -2.809699	C 0.724586 -0.245796 4.015484
H 0.964574 -2.594350 -0.727381	H 1.447267 0.267879 3.382443
C -0.134988 -1.010681 -4.086808	H -0.217709 0.312804 4.011732
H -0.385702 0.812466 -2.994256	H 1.108735 -0.256470 5.041827
C 0.178713 -2.368920 -4.027234	C 1.776952 -2.487639 3.380219
H 0.807860 -3.987267 -2.753995	H 2.439263 -2.018982 2.652310
H -0.438939 -0.558710 -5.027280	H 2.312391 -2.543802 4.334770
H 0.127549 -2.983600 -4.921751	H 1.548409 -3.507221 3.052021
C 3.652565 -3.764921 0.561767	C -2.562108 5.489530 -2.087682
C 3.857488 -4.199230 -0.736552	H -3.366864 5.375726 -2.810472
C 2.513299 -4.247029 1.270613	C -0.487823 5.779259 -0.217477
C 2.990446 -5.138211 -1.352394	H 0.323187 5.868675 0.500754
H 4.721388 -3.847294 -1.292966	C -1.404731 6.154480 -2.430460
C 1.643338 -5.144405 0.695979	C -0.353366 6.292855 -1.489258
H 2.337833 -3.892237 2.282254	H -1.291697 6.571919 -3.427524
C 1.859817 -5.630410 -0.621895	H 0.561980 6.803809 -1.775061
H 0.778941 -5.501181 1.251640	C -2.363360 -5.095159 2.208686
C -1.221448 -3.053363 4.259876	H -2.974179 -4.808640 3.061444
H -0.584191 -3.779437 3.743773	C -0.795707 -5.837434 0.000749
H -1.200177 -3.276615 5.331741	H -0.190107 -6.119518 -0.857013
H -2.246051 -3.173126 3.898821	C -1.234379 -5.863954 2.384495
C -1.628861 -0.598860 4.695320	C -0.438219 -6.233243 1.270500
H -2.665573 -0.735799 4.376233	H -0.949651 -6.193435 3.380314
H -1.583974 -0.736315 5.781552	H 0.453551 -6.835047 1.423202
H -1.313493 0.420564 4.463759	O 2.836201 2.108855 0.429645
C 0.746350 -1.483341 4.435763	C 3.805128 2.884107 0.198957
H 1.378463 -2.172275 3.865126	O 4.991982 2.598783 -0.116072
H 1.110269 -0.467712 4.277255	Rh 5.454310 0.592998 -0.374097
H 0.842929 -1.733392 5.498285	O 5.767316 -1.441003 -0.609139
C 4.500377 3.744788 -0.909134	C 4.811795 -2.217733 -0.340976
C 3.967938 4.240549 -2.134835	O 3.652248 -1.934094 0.072495
C 3.985887 4.223833 0.282774	Rh 3.170908 0.068475 0.282431
C 2.977490 5.193629 -2.144855	O 3.843832 0.032317 2.248789
H 4.350627 3.842243 -3.069920	C 5.075894 0.213338 2.455597
C 2.972902 5.217017 0.307426	O 5.988908 0.451978 1.620994
H 4.383017 3.861743 1.226951	O 2.686043 0.163877 -1.729283
C 2.458023 5.720593 -0.932155	C 3.588634 0.479569 -2.550369
H 2.578782 5.557542 -3.088951	O 4.809685 0.712937 -2.330016
C 3.219837 -5.624641 -2.669189	C 5.059696 -3.724668 -0.582759
H 4.077767 -5.249765 -3.221931	C 3.452600 4.388276 0.277730
C 1.001083 -6.580080 -1.237803	C 3.129625 0.666173 -4.015205
H 0.141221 -6.946745 -0.682018	C 5.495101 0.110780 3.940068
C 2.372394 -6.549957 -3.236821	F 5.249929 -1.134286 4.387021
C 1.250922 -7.031556 -2.515199	F 4.777960 0.974530 4.676801
H 0.588464 -7.759863 -2.974888	F 6.791928 0.377365 4.107728
H 2.559501 -6.914139 -4.243350	F 2.733319 4.649086 1.380384
C 2.461940 5.743920 1.526659	F 4.544309 5.154333 0.285633
H 2.856617 5.363781 2.465929	F 2.705051 4.717718 -0.797702
C 1.449205 6.720668 -0.902385	F 4.132132 0.423935 -4.866751
H 1.060600 7.099838 -1.844914	F 2.739630 1.952283 -4.177297
C 0.971832 7.207566 0.295331	F 2.103404 -0.128414 -4.314240
C 1.485046 6.715248 1.521877	F 4.554551 -4.451220 0.423832
H 1.103764 7.108827 2.460188	F 6.361338 -3.996166 -0.698830
H 0.202311 7.974730 0.304093	F 4.442123 -4.092581 -1.723694

(D(7-10'))‡	**(D(7'-10))‡**
E_0 = -5293.0564507	E_0 = -5293.0574959
G_{298} = -5292.207404	G_{298} = -5292.212190
NImag = 1 (-902.6305 cm^{-1})	NImag = 1 (-927.1457 cm^{-1})
N 0.770371 1.316434 0.398799	C 6.348897 1.235621 -0.350641
C -0.334368 1.889567 -0.157426	C 7.468306 0.432520 -0.559954
O -0.133801 3.195534 -0.351290	C 8.383872 0.776538 -1.566603
C -1.156796 4.102654 -0.925360	C 8.221922 1.945958 -2.301695
C 0.861929 -0.090327 0.707372	C 7.144567 2.782061 -2.013441
C 0.623930 -0.884028 -0.457443	C 6.184649 2.452231 -1.040409
O 0.005663 -2.030301 -0.363288	C 9.452996 -0.285982 -1.699906

C -0.201995 -2.814656 -1.562982	C 8.844312 -1.470270 -0.918427
O -1.352974 1.259947 -0.470788	C 7.957065 -0.803134 0.186228
O 1.057432 -0.552742 -1.645971	C 7.018596 -1.815857 0.827221
H 2.330204 -0.334377 0.834374	C 7.633883 -2.406763 1.941617
H 1.552802 1.935048 0.574416	C 8.946021 -1.717869 2.248531
H -0.891794 -2.287328 -2.223434	C 8.842625 -0.418468 1.419239
H -0.638153 -3.744623 -1.205566	C 7.019522 -3.457132 2.615450
H 0.748368 -2.996671 -2.064540	C 5.783132 -3.919107 2.165061
H 1.855070 0.081931 -1.597511	C 5.117331 -3.320666 1.081847
C 0.342671 -0.530301 2.047135	C 5.747603 -2.233668 0.443949
C 0.769611 -1.749786 2.596982	O 5.074367 -1.524961 -0.560007
C -0.512407 0.278431 2.809308	P 4.225391 -0.203766 -0.095182
C 0.334560 -2.157260 3.856302	O 3.332362 -0.591543 1.109877
H 1.448956 -2.381816 2.033141	O 5.349002 0.791675 0.533237
C -0.945740 -0.128075 4.072326	O 3.530795 0.354418 -1.303921
H -0.850784 1.230715 2.415854	N 0.226487 -1.408746 1.575336
C -0.526389 -1.349167 4.601993	C -1.068673 -1.557873 1.944678
H 0.675390 -3.107745 4.259260	O -1.176607 -2.576203 2.816457
H -1.623535 0.508841 4.633487	C -2.456118 -2.985372 3.435467
H -0.861390 -1.664896 5.586547	C 0.739364 -0.424550 0.652773
C -0.393178 5.424007 -1.031581	C 0.533163 -0.776760 -0.718189
H -0.025334 5.736329 -0.049984	O -0.247837 -1.798181 -0.985912
H -1.057256 6.202186 -1.422481	C -0.350304 -2.271462 -2.350178
H 0.463021 5.322557 -1.705259	O -2.009100 -0.842456 1.586143
C -1.581968 3.621466 -2.315730	O 1.108982 -0.206168 -1.734263
H -2.148358 2.692832 -2.275031	H 7.030994 3.719432 -2.550088
H -0.700289 3.477556 -2.950077	H 8.927206 2.213823 -3.084358
H -2.212096 4.388322 -2.780161	H 7.492773 -3.917898 3.478759
C -2.319158 4.233642 0.061642	H 5.310606 -4.762231 2.661010
H -2.812337 3.278554 0.237538	H 9.080797 -1.526774 3.319206
H -3.065795 4.927208 -0.340376	H 9.800246 -2.330628 1.927302
H -1.960095 4.630097 1.017760	H 8.321770 0.350376 2.001057
O -3.172785 -0.696423 -2.118912	H 9.814755 -0.011801 1.123227
C -4.147745 -1.358619 -2.572870	H 10.400277 0.044883 -1.250786
O -5.267585 -1.584170 -2.039765	H 9.670669 -0.536302 -2.744458
Rh -5.616202 -0.782444 -0.163277	H 8.198453 -2.056881 -1.581652
O -5.838338 0.082694 1.703245	H 9.594285 -2.147695 -0.497737
C -4.893179 0.798712 2.131870	H 2.203935 -0.547560 0.842063
O -3.788702 1.064372 1.580055	H 0.851870 -2.144139 1.882248
Rh -3.401896 0.215267 -0.266710	H 0.600090 -2.706745 -2.663353
O -4.300180 1.842583 -1.194940	H -1.129318 -3.030002 -2.317092
C -5.552553 1.831867 -1.350469	H -0.631573 -1.452712 -3.010406
O -6.377419 0.931368 -1.039689	H 2.046798 0.181106 -1.519121
O -2.697096 -1.512326 0.635762	C 0.627233 1.008834 1.116226
C -3.514721 -2.443797 0.858948	C 0.763527 1.273747 2.489581
O -4.766822 -2.454085 0.688955	C 0.393975 2.088598 0.251932
C -5.085627 1.434870 3.528353	C 0.628140 2.568031 2.986615
C -3.923902 -1.942303 -3.986964	H 0.964955 0.454748 3.173139
C -2.906647 -3.786113 1.328962	C 0.265095 3.384304 0.753888
C -6.120499 3.109848 -2.009027	H 0.283575 1.925156 -0.812436
F -5.829436 4.176528 -1.241968	C 0.371440 3.632941 2.121904
F -5.553266 3.287951 -3.213412	H 0.727651 2.742521 4.055041
F -7.444018 3.042532 -2.163057	H 0.071481 4.204007 0.068254
F -3.891645 -0.940174 -4.880757	H 0.269373 4.643428 2.504475
F -4.892727 -2.793339 -4.329686	C 3.804522 -3.864696 0.646241
F -2.746562 -2.592616 -4.036737	C 3.564468 -4.196827 -0.675488
F -3.752503 -4.442735 2.131485	C 2.791509 -4.138159 1.613135
F -2.685612 -4.550691 0.232521	C 2.354924 -4.820531 -1.079716
F -1.749192 -3.615479 1.962450	H 4.324949 -4.002860 -1.426338
F -4.787659 2.742429 3.483112	C 1.599819 -4.724352 1.251105
F -6.339971 1.295526 3.962869	H 2.973375 -3.868325 2.649938
F -4.258863 0.840212 4.408526	C 1.345708 -5.090946 -0.098999
C 6.165130 1.726664 -0.655017	H 0.834248 -4.914244 1.999929
C 7.266739 1.061385 -1.183840	C 5.091972 3.421314 -0.759237
C 7.982117 1.640099 -2.242606	C 4.360226 3.997084 -1.838068
C 7.667605 2.921284 -2.682855	C 4.853032 3.877074 0.525264
C 6.647305 3.625486 -2.045082	C 3.453064 5.006718 -1.620995
C 5.861710 3.053804 -1.026175	H 4.522186 3.616587 -2.842347
C 9.046976 0.689288 -2.746563	C 3.935271 4.928498 0.781216
C 8.663737 -0.642836 -2.061072	H 5.402843 3.452633 1.360703
C 7.964122 -0.213569 -0.728945	C 3.224088 5.516343 -0.314843
C 7.251975 -1.380236 -0.055528	H 2.901362 5.433750 -2.455421
C 8.120320 -2.017489 0.845794	C -2.010455 -4.111273 4.373577
C 9.411786 -1.242196 0.980701	H -1.291083 -3.740363 5.110756
C 9.046751 0.119863 0.355409	H -2.876436 -4.515863 4.907423
C 7.742359 -3.190681 1.489042	H -1.541956 -4.925734 3.810643
C 6.493403 -3.741873 1.208699	C -3.404605 -3.521180 2.360185
C 5.582703 -3.114494 0.341316	H -3.717200 -2.737491 1.670852
C 5.972038 -1.895201 -0.248246	H -2.921246 -4.322799 1.790529
O 5.057672 -1.178490 -1.031359	H -4.299620 -3.934703 2.838521
P 4.209376 0.044023 -0.354353	C -3.057559 -1.825739 4.235307

O 3.479659 -0.468778 0.915028 O 5.343302 1.045731 0.254266 O 3.346274 0.661928 -1.414851 H 6.451205 4.651999 -2.337494 H 8.221848 3.383689 -3.495670 H 8.413097 -3.683534 2.188147 H 6.205168 -4.686344 1.660505 H 9.745462 -1.155263 2.020951 H 10.225970 -1.731732 0.427498 H 8.593640 0.764910 1.116731 H 9.905375 0.653183 -0.064036 H 10.051106 1.020585 -2.446599 H 9.056223 0.612459 -3.839915 H 7.940653 -1.185021 -2.680908 H 9.518769 -1.304269 -1.888957 C 4.298586 -3.801357 0.039734 C 3.510937 -4.310795 1.057465 C 3.928946 -4.070913 -1.311184 C 2.361957 -5.101571 0.790296 H 3.770593 -4.101481 2.092295 C 2.838495 -4.857032 -1.601999 H 4.540117 -3.670732 -2.113835 C 2.025450 -5.400341 -0.569624 H 2.590012 -5.080453 -2.637408 C 4.826851 3.880183 -0.350902 C 4.130967 4.888896 -1.082978 C 4.593053 3.785062 1.013224 C 3.287288 5.774709 -0.457114 H 4.267277 4.949396 -2.158322 C 3.711617 4.671188 1.685554 H 5.110982 3.035215 1.601357 C 3.055924 5.705200 0.942766 H 2.779223 6.542838 -1.035241 C 3.478390 4.580085 3.086211 H 3.975187 3.792925 3.648354 C 2.203867 6.611862 1.628139 H 1.718263 7.403708 1.062287 C 2.640146 5.469119 3.720942 C 1.998474 6.497010 2.985791 H 2.469109 5.387131 4.790831 H 1.344906 7.196895 3.499427 C 1.537088 -5.614126 1.829021 H 1.794599 -5.386994 2.860902 C 0.887861 -6.209591 -0.834838 H 0.641830 -6.445188 -1.868075 C 0.430593 -6.380567 1.539312 C 0.103763 -6.684284 0.194150 H -0.195495 -6.758931 2.342482 H -0.769031 -7.294109 -0.021940	H -3.390665 -1.018083 3.584144 H -3.920721 -2.190452 4.803367 H -2.322717 -1.433922 4.947282 C 3.726034 5.444776 2.089223 H 4.267040 4.997269 2.919551 C 2.330042 6.590429 -0.058750 H 1.792435 7.034344 -0.893731 C 2.860902 6.494238 2.304246 C 2.154057 7.072283 1.219911 H 2.715879 6.883767 3.308447 H 1.474265 7.900545 1.401571 C 2.121756 -5.210099 -2.428289 H 2.892925 -5.013737 -3.169487 C 0.141417 -5.724828 -0.506039 H -0.623540 -5.924310 0.240796 C 0.947679 -5.834068 -2.789523 C -0.054256 -6.090914 -1.820124 H 0.785354 -6.133250 -3.821516 H -0.976747 -6.581990 -2.117426 O -3.751597 -1.720998 -0.874559 C -4.668813 -1.772897 -1.740886 O -5.440698 -0.858566 -2.134516 Rh -5.223021 1.021301 -1.276751 O -4.885103 2.836402 -0.351811 C -3.964431 2.890597 0.512302 O -3.214271 1.966355 0.925579 Rh -3.420228 0.096519 0.076481 O -4.860303 -0.368035 1.491885 C -6.061596 -0.068859 1.246953 O -6.542125 0.487930 0.223663 O -2.129212 0.642734 -1.481424 C -2.628464 1.216079 -2.489247 O -3.832073 1.515582 -2.712582 C -3.684527 4.292280 1.102335 C -4.856682 -3.166965 -2.382493 C -1.641202 1.556146 -3.632316 C -7.061464 -0.392890 2.380701 F -8.300977 -0.546151 1.905264 F -7.061923 0.620329 3.265836 F -6.705113 -1.515900 3.021265 F -5.267857 -4.039946 -1.446823 F -5.752268 -3.143791 -3.370569 F -3.683185 -3.604596 -2.879767 F -0.484165 2.028851 -3.152729 F -2.157598 2.458680 -4.468561 F -1.382449 0.429500 -4.333072 F -3.158317 4.208415 2.326868 F -4.808505 5.017323 1.164541 F -2.809953 4.930901 0.300036
(D(7'-10'))‡ E_0 = -5293.0538562 G_{298} = -5292.203194 NImag = 1 (-1016.7153 cm^{-1}) N -0.311998 -1.702256 -1.184658 C 0.933950 -1.822318 -1.705014 O 0.889007 -2.607761 -2.792258 C 2.099894 -3.081041 -3.496917 C -0.777495 -0.881535 -0.090348 C -0.593889 0.521902 -0.290108 O 0.056491 0.930471 -1.349617 C 0.040211 2.339523 -1.694131 O 1.974709 -1.315301 -1.273984 O -1.113570 1.446904 0.467361 H -2.224019 -0.813768 -0.469442 H -1.008447 -2.270879 -1.651496 H -0.965128 2.625891 -2.003352 H 0.748651 2.428079 -2.514644 H 0.355117 2.941593 -0.842626 H -2.001254 1.177974 0.894117 C -0.586551 -1.461075 1.302993 C -1.309463 -1.029051 2.427704 C 0.378685 -2.464216 1.497233 C -1.055225 -1.560463 3.693968 H -2.096736 -0.293662 2.333013 C 0.633472 -2.991314 2.763309 H 0.956765 -2.832998 0.660274 C -0.080007 -2.540632 3.874608 H -1.633969 -1.201448 4.541267 H 1.411191 -3.741314 2.876954 H 0.122386 -2.945457 4.862666	**(E(7-10))‡** E_0 = -5293.0565261 G_{298} = -5292.210354 NImag = 1 (-869.6852 cm^{-1}) C -6.707776 1.425013 -0.457306 C -7.827381 0.659542 -0.771145 C -9.042712 0.919461 -0.118395 C -9.155654 1.985048 0.768172 C -8.043480 2.791797 1.004148 C -6.794296 2.529561 0.414277 C -10.084571 -0.106775 -0.506771 C -9.232258 -1.210664 -1.170216 C -8.017802 -0.448410 -1.800771 C -6.916056 -1.414951 -2.223219 C -7.132805 -1.833924 -3.545389 C -8.257742 -1.043817 -4.177244 C -8.428354 0.135195 -3.194856 C -6.349659 -2.836513 -4.107274 C -5.340954 -3.417943 -3.341699 C -5.045553 -2.978635 -2.038343 C -5.843749 -1.942891 -1.508364 O -5.544832 -1.413330 -0.246168 P -4.625450 -0.069897 -0.152318 O -3.342356 -0.248078 -1.007840 O -5.463998 1.050990 -0.988360 O -4.441182 0.243064 1.302968 N -1.689345 -1.364032 1.465693 C -1.202982 -1.457081 2.749781 O -1.707682 -2.555263 3.353683 C -1.400769 -2.840419 4.766764 C -1.206054 -0.366112 0.551549

C 1.498809 -3.982669 -4.579318	C -1.240294 0.948651 1.137409
H 0.916533 -4.790947 -4.125250	O -0.266952 1.785042 0.886687
H 2.297613 -4.423340 -5.184544	C -0.348817 3.138975 1.393886
H 0.839141 -3.409454 -5.238888	O -0.442385 -0.639561 3.243412
C 2.843594 -1.898092 -4.123553	O -2.219779 1.394565 1.860368
H 3.303962 -1.264703 -3.364788	H -8.132708 3.646815 1.667634
H 2.156701 -1.294009 -4.726599	H -10.096384 2.192621 1.271710
H 3.632353 -2.276257 -4.783871	H -6.523229 -3.173044 -5.126200
C 2.977962 -3.893795 -2.540236	H -4.756933 -4.233541 -3.756579
H 3.432652 -3.261354 -1.776325	H -8.019649 -0.715215 -5.195295
H 3.780752 -4.376961 -3.108313	H -9.176080 -1.643887 -4.246355
H 2.384872 -4.676388 -2.054094	H -7.732815 0.940064 -3.458428
O 3.240013 1.537184 -1.422516	H -9.438825 0.555632 -3.189470
C 4.000517 2.528642 -1.248919	H -10.814542 0.313968 -1.212744
O 4.873213 2.712609 -0.357585	H -10.654931 -0.473161 0.354312
Rh 5.070760 1.256241 1.104976	H -8.856924 -1.898506 -0.404022
O 5.153493 -0.265089 2.503871	H -9.782772 -1.801807 -1.908735
C 4.403400 -1.264005 2.324706	H -2.373487 -0.260691 -0.383467
O 3.583094 -1.480369 1.391624	H -2.307133 -2.099175 1.142100
Rh 3.349994 -0.021025 -0.053105	H -0.288104 3.118590 2.483341
O 4.875574 -0.901853 -1.150376	H 0.515523 3.643449 0.966501
C 6.063881 -0.559162 -0.895551	H -1.277350 3.611247 1.074535
O 6.480906 0.274465 -0.048093	H -3.081487 0.841035 1.759595
O 1.961750 0.976615 1.126392	C -0.031702 -0.724151 -0.294404
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(E(7-10'))‡ E_0 = -5293.0534497 G_{298} = -5292.204832 NImag = 1 (-822.2838 cm^{-1}) C -6.828273 0.432008 -0.756393 C -7.755267 -0.604479 -0.807500 C -9.030222 -0.416084 -0.252663 C -9.402087 0.827168 0.248223 C -8.498112 1.886289 0.175819 C -7.190276 1.722589 -0.317317 C -9.826671 -1.702313 -0.302871 C -8.747807 -2.753804 -0.648830 C -7.682968 -1.968066 -1.484617 C -6.397001 -2.768574 -1.653710 C -6.463382 -3.545179 -2.821348 C -7.699903 -3.198029 -3.621117 C -8.149399 -1.868719 -2.977930 C -5.462514 -4.463870 -3.119067 C -4.395544 -4.613763 -2.234344 C -4.271644 -3.823925 -1.078135 C -5.277223 -2.867260 -0.832702 O -5.143419 -1.976711 0.240939 P -4.507175 -0.502269 -0.044982 O -3.182817 -0.652862 -0.842350 O -5.506431 0.171203 -1.141529 O -4.419890 0.234849 1.258927 N -1.762171 1.916057 0.664681 C -1.267125 2.679793 1.700843 O -1.867585 3.883116 1.730643 C -1.536737 4.853315 2.794471 C -1.222112 0.606131 0.414298 C -1.174284 -0.152847 1.639575 O -0.130675 -0.882049 1.918791 C -0.088160 -1.614457 3.167950 O -0.406868 2.275101 2.469379 O -2.163244 -0.191419 2.482821 H -8.808983 2.873184 0.504010 H -10.390582 0.983829 0.672478 H -5.511217 -5.066586 -4.022339 H -3.633646 -5.361506 -2.434165 H -7.494295 -3.100570 -4.693170 H -8.470902 -3.974666 -3.517139 H -7.625434 -1.032512 -3.454616 H -9.224181 -1.682363 -3.067254 H -10.605382 -1.657455 -1.077233 H -10.337051 -1.917258 0.642949 H -8.275907 -3.117243 0.271084 H -9.141490 -3.621237 -1.187849 H -2.308331 -0.131205 -0.312617 H -0.969746 -2.246017 3.274215 H 0.815599 -2.215978 3.101031	**(E(7'-10))‡** E_0 = -5293.0505057 G_{298} = -5292.198597 NImag = 1 (-1066.1251 cm^{-1}) N 1.248477 2.692939 -1.220558 C 0.200308 3.589236 -1.258933 O 0.657252 4.774834 -1.738712 C -0.252211 5.918454 -1.901514 C 1.150569 1.433450 -0.528550 C 1.179846 1.554588 0.901050 O 1.199369 2.761595 1.416509 C 1.440324 2.910320 2.836260 O -0.945906 3.332039 -0.941556 O 1.283298 0.569373 1.742509 O -2.881897 -1.693437 1.494389 C -3.829451 -1.782484 2.322860 O -4.916233 -1.144361 2.354158 Rh -5.277243 0.234688 0.840905 O -5.479449 1.579349 -0.714440 C -4.527868 1.664123 -1.542657 O -3.455397 1.005888 -1.586896 Rh -3.098050 -0.361571 -0.079352 O -4.097314 -1.825775 -1.173548 C -5.343233 -1.948107 -1.022434 O -6.121781 -1.272593 -0.297618 O -2.303657 1.149159 1.119938 C -3.102381 1.828401 1.818657 O -4.353229 1.712514 1.934470 H 2.427514 0.749889 -0.826196 H 2.171868 3.096616 -1.318887 H 0.596820 2.510946 3.398202 H 1.536756 3.983907 2.984563 H 2.362004 2.400043 3.116969 C -4.707498 2.748714 -2.629521 C -3.659901 -2.857244 3.422005 C -2.452229 2.924011 2.694028 C -5.981412 -3.121787 -1.801035 F -7.288958 -2.929569 -1.991809 F -5.390505 -3.282253 -2.992607 F -5.815351 -4.257728 -1.090725 F -4.298344 -3.981764 3.035194 F -4.190996 -2.447633 4.578845 F -2.369847 -3.153895 3.622543 F -3.360477 3.778094 3.170356 F -1.836120 2.331351 3.743902 F -1.533133 3.611426 2.005197 F -4.591047 3.964816 -2.063702 F -3.789433 2.639749 -3.593385 F -5.925720 2.654885 -3.184302 C 0.266404 0.413068 -1.193393 C 0.076084 0.494748 -2.578143

H -0.023263 -0.899455 3.990209	C -0.343250 -0.663597 -0.514811
H -3.041857 0.128046 2.065137	C -0.703723 -0.439491 -3.270716
C -0.075201 0.507733 -0.528305	H 0.541536 1.308645 -3.122549
C 0.370138 -0.753076 -0.973023	C -1.116854 -1.609186 -1.211661
C 0.532059 1.662680 -1.065732	H -0.191389 -0.807121 0.547447
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H -0.111230 -1.653939 -0.606787	H -0.829498 -0.329958 -4.344573
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O 3.536868 -1.891555 -0.009282	H 0.829167 -4.801898 -3.279936
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Rh 6.088204 -0.147097 0.482082	C 5.597125 2.687522 1.218546
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O 6.950675 -1.049649 -1.175330	H 6.108036 2.004896 1.892127
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C 3.139102 1.676506 3.089588	H -1.578257 -5.310277 -2.869546
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F 3.956033 1.837761 4.136235	H -3.466121 -5.555406 -1.286591
F 5.199463 4.496954 -1.571537	H -3.075681 -5.355197 1.166665

F 6.487672 3.450209 -2.984721 F 7.279769 4.107985 -1.065908 F 6.144774 -2.798677 -3.970435 F 7.136928 -0.894003 -4.346267 F 8.100057 -2.401720 -3.104001 F 3.112859 -4.447906 0.578048 F 4.899945 -4.505010 1.816098 F 3.122584 -3.464227 2.523586 H -2.540268 2.281087 0.130801	C 4.959165 4.100774 3.162681 H 5.474935 3.411599 3.827331 C 3.641146 5.881769 1.438536 H 3.132707 6.570543 0.768009 C 3.673031 6.123122 2.795209 C 4.341904 5.225132 3.665011 H 4.366914 5.429407 4.732018 H 3.190498 7.007284 3.202882 H 1.855994 -0.236823 1.389608
(E(7'-10'))‡ E_0 = -5293.040671 G_{298} = -5292.191482 NImag = 1 (-1253.7096 cm^{-1})	**(8-10)‡** E_0 = -5293.0557275 G_{298} = -5292.205737 NImag = 1 (-606.7250 cm^{-1})
C -6.440006 0.170097 0.306737 C -7.352311 -0.880205 0.368578 C -8.387070 -0.836799 1.316313 C -8.571373 0.289889 2.110751 C -7.719403 1.380298 1.946973 C -6.627961 1.349076 1.059737 C -9.175598 -2.128140 1.303954 C -8.269256 -3.065526 0.476334 C -7.512612 -2.114703 -0.511948 C -6.361177 -2.840323 -1.198926 C -6.819685 -3.450548 -2.377054 C -8.234488 -3.013713 -2.688183 C -8.425053 -1.804546 -1.747192 C -5.997688 -4.317719 -3.088440 C -4.716692 -4.584111 -2.608083 C -4.199765 -3.950949 -1.462893 C -5.041864 -3.034594 -0.799188 O -4.549547 -2.291590 0.281240 P -4.011981 -0.775493 0.031419 O -3.037886 -0.726633 -1.158728 O -5.316936 0.041641 -0.517568 O -3.526043 -0.267696 1.369582 N -0.939596 1.745627 -1.862632 C -0.028091 2.783466 -1.932875 O -0.606511 3.814565 -2.592669 C 0.105245 5.086036 -2.797324 C -0.773222 0.634539 -0.963440 C -1.013486 0.941773 0.412664 O -1.444800 2.145734 0.696697 C -1.855161 2.449160 2.056682 O 1.105040 2.743164 -1.491004 O -1.022492 0.016884 1.340593 O 3.357456 -1.496685 1.849711 C 4.260350 -1.225455 2.690964 O 5.198467 -0.388362 2.603570 Rh 5.351652 0.710728 0.847472 O 5.369027 1.732212 -0.945456 C 4.477662 1.443865 -1.794184 O 3.552210 0.594460 -1.712146 Rh 3.378964 -0.477286 0.044443 O 4.692610 -1.902087 -0.722298 C 5.931413 -1.724583 -0.560470 O 6.523567 -0.780127 0.026842 O 2.251192 1.037321 0.932659 C 2.865934 1.973520 1.510122 O 4.108295 2.148780 1.634108 H -7.897293 2.287443 2.516046 H -9.379623 0.333530 2.836289 H -6.349580 -4.798190 -3.997867 H -4.092381 -5.305265 -3.126417 H -8.371972 -2.753140 -3.743873 H -8.955758 -3.812504 -2.464589 H -8.058961 -0.893919 -2.234941 H -9.467895 -1.633570 -1.462468 H -10.155562 -1.991378 0.825322 H -9.369780 -2.510141 2.312754 H -7.535243 -3.546218 1.132913 H -8.819167 -3.855700 -0.044147 H -1.981044 -0.084005 -1.051013 H -1.890598 2.005418 -2.091510 H -1.088929 2.115269 2.755429 H -1.954797 3.531646 2.074416 H -2.813010 1.969295 2.258028 H -2.027568 -0.178309 1.561916 C 4.573562 2.234924 -3.117730 C 4.191509 -2.061355 3.989840 C 1.970022 3.021392 2.209517	C 4.012537 -3.322482 -0.517709 C 5.275462 -3.610281 -1.025433 C 5.980286 -4.719804 -0.534794 C 5.397987 -5.570988 0.398701 C 4.105862 -5.302037 0.847657 C 3.388708 -4.170831 0.419080 C 7.365814 -4.776200 -1.139087 C 7.528238 -3.356539 -1.723875 C 6.075643 -2.916459 -2.118729 C 6.020055 -1.414273 -2.379414 C 6.320399 -1.159042 -3.727383 C 6.368687 -2.450606 -4.515541 C 5.726149 -3.463681 -3.541720 C 6.512858 0.143128 -4.176389 C 6.424856 1.194029 -3.264294 C 6.063554 0.984756 -1.921976 C 5.809410 -0.341149 -1.516141 O 5.295442 -0.576531 -0.230417 P 3.682880 -0.781173 -0.086842 O 2.950366 0.308332 -0.921709 O 3.379740 -2.146358 -0.934667 O 3.311131 -0.868617 1.360113 N 0.722721 0.178105 1.502813 C 0.145596 0.617811 2.824438 O 0.968021 0.205981 3.761519 C 0.769727 0.567933 5.205357 C 0.926690 1.296011 0.502258 C -0.089129 1.243670 -0.516247 O -0.042104 2.275043 -1.358673 C -0.678294 2.180165 -2.646426 O -0.875707 1.242686 2.875333 O -0.828204 0.233617 -0.684637 O -3.188580 2.229331 -0.525385 C -4.331936 2.764729 -0.460729 O -5.463683 2.219430 -0.535747 Rh -5.528606 0.164452 -0.821317 O -5.426815 -1.881888 -1.101840 C -4.287319 -2.419232 -1.137320 O -3.150086 -1.875075 -1.061638 Rh -3.084291 0.183490 -0.800337 O -3.184000 0.436064 -2.861229 C -4.322003 0.512446 -3.404325 O -5.459226 0.446604 -2.868446 O -3.189144 -0.134823 1.248016 C -4.333823 -0.222425 1.769179 O -5.465607 -0.119498 1.221237 H 3.629124 -5.977103 1.551987 H 5.937316 -6.436407 0.775339 H 6.749688 0.343222 -5.218337 H 6.638307 2.208242 -3.588122 H 5.829816 -2.380536 -5.467384 H 7.403291 -2.730122 -4.759673 H 4.637215 -3.456912 -3.664445 H 6.073501 -4.491138 -3.690527 H 7.424779 -5.541725 -1.925971 H 8.138918 -5.021680 -0.402108 H 7.902158 -2.679200 -0.947607 H 8.222351 -3.309789 -2.568722 H 2.091242 0.769859 -0.347991 H 0.053843 -0.472685 1.052396 H -1.704228 2.540444 -2.575214 H -0.094183 2.827132 -3.302543 H -0.671168 1.151745 -3.007999 C 1.408816 2.571054 1.121708 C 0.630238 3.742183 1.128236 C 2.657678 2.593737 1.766955 C 1.100154 4.904022 1.738335

C 6.836055 -2.794946 -1.213571	H -0.347063 3.743644 0.658242
F 6.991089 -2.500085 -2.517864	C 3.113806 3.752628 2.396825
F 6.276925 -4.009751 -1.117660	H 3.274589 1.699751 1.781816
F 8.041184 -2.831461 -0.637888	C 2.342368 4.915341 2.376304
F 4.400436 -3.357288 3.695721	H 0.485052 5.800067 1.725592
F 5.110003 -1.672225 4.877358	H 4.086688 3.750879 2.878343
F 2.976565 -1.942650 4.547571	H 2.709012 5.822732 2.848011
F 2.678099 4.060041 2.655565	C 6.029237 2.139749 -0.986817
F 1.361062 2.435929 3.265544	C 6.669358 2.054053 0.286038
F 1.018156 3.474247 1.380831	C 5.485751 3.353140 -1.372557
F 5.733096 1.938538 -3.731295	C 6.779524 3.156439 1.099100
F 4.555177 3.555057 -2.864712	H 7.093316 1.106144 0.599595
F 3.568076 1.945245 -3.946940	C 5.575113 4.508098 -0.552548
C 0.217200 -0.412027 -1.391610	H 4.970589 3.432917 -2.326470
C 0.495054 -0.545525 -2.754074	C 6.249880 4.415958 0.707640
C 0.852248 -1.308562 -0.497165	H 7.291619 3.077150 2.055624
C 1.379404 -1.523696 -3.228825	C 2.027076 -3.921573 0.959006
H 0.017741 0.129319 -3.455821	C 1.771784 -4.086381 2.309881
C 1.731784 -2.293779 -0.978800	C 0.943644 -3.577084 0.097562
H 0.602848 -1.295672 0.555590	C 0.468197 -3.939835 2.849243
C 2.001362 -2.401884 -2.353633	H 2.589542 -4.320020 2.986755
H 1.571980 -1.587990 -4.296404	C -0.334508 -3.430389 0.586445
H 2.135196 -3.022816 -0.283398	H 1.131632 -3.448269 -0.962950
H 2.687915 -3.160661 -2.715415	C -0.615423 -3.613683 1.969915
C -2.838676 -4.310599 -0.986118	H -1.150539 -3.197237 -0.091767
C -2.563887 -4.503044 0.358594	C -4.307643 4.303869 -0.322738
C -1.803483 -4.571585 -1.932436	C -4.282680 -3.962691 -1.217670
C -1.297547 -4.963248 0.802905	C -4.390713 -0.534839 3.281723
H -3.333085 -4.317201 1.101224	C -4.281185 0.714090 -4.936405
C -0.571986 -5.033447 -1.534823	C 0.836272 2.089264 5.339226
H -1.993585 -4.386126 -2.985289	H -0.007928 2.571248 4.841577
C -0.279296 -5.251737 -0.162074	H 0.808674 2.354696 6.401827
H 0.202260 -5.223523 -2.273914	H 1.764669 2.477044 4.909039
C 0.440168 5.720457 -1.442493	C 1.967223 -0.114261 5.864587
H 1.147047 5.107186 -0.882024	H 1.930053 -1.196249 5.704921
H 0.880933 6.711437 -1.599512	H 2.907017 0.265341 5.452553
H -0.469073 5.841722 -0.842692	H 1.953000 0.080767 6.941849
C -0.931949 5.927029 -3.547572	C -0.552058 -0.016741 5.699662
H -1.201773 5.453003 -4.496960	H -1.408165 0.468829 5.230260
H -1.842596 6.042688 -2.949827	H -0.599752 -1.091832 5.499262
H -0.528222 6.922615 -3.759318	H -0.619509 0.133351 6.783094
C 1.348388 4.865849 -3.664508	F -4.922161 -1.763189 3.452940
H 1.783478 5.835267 -3.933355	F -5.169253 0.354733 3.912198
H 2.103166 4.279419 -3.141872	F -3.178669 -0.520451 3.842255
H 1.077681 4.347182 -4.590895	F -5.311472 -4.412911 -1.941579
C -5.762836 2.550289 0.924674	F -4.390858 -4.453056 0.034890
C -5.298234 2.983068 -0.355042	F -3.143928 -4.418045 -1.752260
C -5.460326 3.330229 2.029836	F -3.540789 1.799115 -5.226642
C -4.570877 4.141186 -0.492414	F -3.712201 -0.355338 -5.517027
H -5.537503 2.390586 -1.230600	F -5.502453 0.881068 -5.446822
C -4.719000 4.535601 1.920806	F -5.478173 4.778112 0.108950
H -5.783518 3.013183 3.018132	F -3.345042 4.685326 0.529210
C -4.258397 4.954339 0.630654	F -4.043207 4.840867 -1.530052
H -4.230908 4.456258 -1.476448	C 5.028952 5.759842 -0.947016
C -1.009919 -5.160945 2.181981	H 4.511239 5.826756 -1.900987
H -1.783763 -4.940226 2.913397	C 6.363121 5.579180 1.514772
C 0.981046 -5.729319 0.287303	H 6.884839 5.507186 2.466742
H 1.749408 -5.954604 -0.449182	C 5.827185 6.779368 1.101588
C 0.224134 -5.617498 2.587543	C 5.151052 6.869356 -0.140650
C 1.229944 -5.906280 1.631017	H 5.923181 7.663378 1.726547
H 2.198614 -6.269738 1.963019	H 4.730020 7.820418 -0.455408
H 0.432619 -5.759181 3.644415	C -1.925098 -3.492405 2.507320
C -4.403110 5.335436 3.053957	H -2.746669 -3.269269 1.832831
H -4.753056 5.017056 4.033349	C 0.197710 -4.118330 4.234330
C -3.507198 6.155076 0.523738	H 1.020777 -4.371454 4.899077
H -3.165742 6.473066 -0.458733	C -2.155939 -3.675360 3.853100
C -3.215993 6.907659 1.640946	C -1.083460 -3.989753 4.725078
C -3.668530 6.492903 2.918490	H -3.161411 -3.572384 4.248597
H -3.434420 7.094573 3.792465	H -1.278859 -4.139558 5.783767
H -2.639042 7.823416 1.546470	H 1.633393 -0.326535 1.652873
(8-10')‡	**(8'-10)‡**
E_0 = -5293.0563183	E_0 = -5293.0544765
G_{298} = -5292.199585	G_{298} = -5292.202633
NImag = 1 (-404.8694 cm^{-1})	NImag = 1 (-668.8801 cm^{-1})
C 5.782281 1.168640 0.639482	C -3.943382 -1.463537 -2.487268
C 6.048571 2.311055 1.388250	C -4.240361 -2.818414 -2.612078
C 6.705823 2.191628 2.621970	C -5.445717 -3.204877 -3.218711
C 7.213006 0.962429 3.030348	C -6.309349 -2.253969 -3.752273
C 7.091929 -0.134472 2.178202	C -5.970320 -0.905401 -3.663182
C 6.370814 -0.070396 0.971063	C -4.797525 -0.474435 -3.017521

C 6.751054 3.530113 3.329656	C -5.615535 -4.705919 -3.154287
C 5.792333 4.399886 2.481289	C -4.582080 -5.106963 -2.081475
C 5.873266 3.784257 1.046934	C -3.431829 -4.048451 -2.214236
C 4.797656 4.320480 0.111534	C -2.518203 -4.105178 -0.993054
C 5.284317 5.431885 -0.594549	C -1.514237 -5.063447 -1.202701
C 6.753577 5.645911 -0.312690	C -1.515490 -5.529544 -2.642876
C 7.164881 4.301985 0.319233	C -2.432269 -4.492440 -3.332149
C 4.445205 6.170154 -1.420660	C -0.667014 -5.437381 -0.164675
C 3.107734 5.799114 -1.525477	C -0.831314 -4.852854 1.090911
C 2.587128 4.669143 -0.866806	C -1.775756 -3.836529 1.320729
C 3.476627 3.915992 -0.072141	C -2.580188 -3.445890 0.231549
O 3.035658 2.754827 0.574114	O -3.420133 -2.327241 0.367284
P 3.295527 1.265738 -0.030545	P -2.864486 -0.901130 -0.176481
O 2.582956 1.132498 -1.413034	O -1.369914 -0.738728 0.216831
O 4.882577 1.251267 -0.436597	O -2.783921 -1.096207 -1.801838
O 2.913634 0.263603 1.010630	O -3.795260 0.194643 0.244139
C 0.714873 -0.832464 -1.300212	N -2.162763 2.392935 0.205231
C -0.492773 -0.117180 -1.622120	C -2.479187 3.758302 0.739766
O -0.749623 -0.030449 -2.925000	O -3.531059 3.653159 1.515761
C -1.799046 0.860938 -3.358449	C -4.048152 4.821775 2.305812
O -1.170632 0.498842 -0.751976	C -0.850048 1.819248 0.732902
O -3.041381 -1.897907 -0.853026	C 0.256711 2.135435 -0.140749
C -3.860300 -2.798318 -0.520985	O -0.129103 2.465840 -1.395855
O -4.807371 -2.736145 0.309512	C 0.893940 2.733081 -2.371973
Rh -5.090097 -0.944726 1.317268	O -1.796397 4.701136 0.442689
O -5.235167 0.889421 2.264824	O 1.455967 2.050934 0.180671
C -4.367810 1.760825 1.986274	O 2.689727 -0.417052 1.502609
O -3.390281 1.684528 1.190954	C 3.423160 -1.395036 1.805599
Rh -3.135327 -0.088212 0.137773	O 4.366540 -1.916917 1.148133
O -1.981797 -0.788070 1.715094	Rh 4.876980 -1.044775 -0.647200
C -2.569687 -1.392661 2.654701	O 5.311305 -0.070327 -2.425994
O -3.799547 -1.616125 2.799402	C 4.649066 0.966163 -2.692215
O -4.423952 0.593387 -1.329911	O 3.723635 1.509489 -2.025181
C -5.659777 0.385120 -1.173649	Rh 3.119451 0.598313 -0.258083
O -6.249771 -0.212938 -0.234575	O 1.847486 -0.614413 -1.358221
H 7.571948 -1.071026 2.444291	C 2.305844 -1.710217 -1.784691
H 7.732306 0.860128 3.979840	O 3.461508 -2.192594 -1.641947
H 4.817362 7.035538 -1.963101	O 4.515684 1.717907 0.787320
H 2.429231 6.401589 -2.120931	C 5.696561 1.277104 0.848047
H 7.328022 5.883862 -1.215290	O 6.169121 0.207803 0.373594
H 6.904349 6.480586 0.386858	H -6.624179 -0.156681 -4.100194
H 7.430333 3.589883 -0.470397	H -7.237811 -2.552864 -4.232039
H 8.020898 4.380265 0.996370	H 0.110290 -6.180704 -0.321699
H 7.769070 3.943855 3.335906	H -0.205470 -5.175684 1.917423
H 6.436476 3.457815 4.377197	H -0.506628 -5.544944 -3.068992
H 4.766663 4.297347 2.853019	H -1.917503 -6.548056 -2.736170
H 6.048202 5.464117 2.493146	H -1.839156 -3.624165 -3.637265
H 1.789790 0.357369 -1.410767	H -2.943159 -4.882449 -4.218471
H -1.772529 1.791362 -2.793219	H -5.387246 -5.171502 -4.123570
H -1.596630 1.043218 -4.413950	H -6.637049 -5.004933 -2.893352
H -2.771971 0.381621 -3.235621	H -5.031221 -5.015787 -1.085912
N 0.730904 -1.140899 0.196357	H -4.216410 -6.132627 -2.188672
H -0.040318 -0.577190 0.597141	H -1.067312 0.332855 0.440216
C 0.471169 -2.569624 0.555715	H -2.059797 2.481862 -0.817561
O -0.622233 -3.053918 0.432128	H 1.315465 1.796881 -2.738989
O 1.594619 -3.097451 0.979777	H 0.392459 3.268053 -3.179281
C 1.665092 -4.544876 1.382266	H 1.685881 3.343908 -1.937428
C 1.207216 -1.958565 -2.161773	C -0.742467 1.934119 2.223370
C 2.582931 -2.163749 -2.352335	C 0.293957 2.639355 2.858926
C 0.307036 -2.858217 -2.763404	C -1.734465 1.337719 3.024231
C 3.046429 -3.236015 -3.116811	C 0.334217 2.741361 4.249805
H 3.298759 -1.477167 -1.911289	H 1.076232 3.095748 2.264983
C 0.769749 -3.918140 -3.541550	C -1.699317 1.454276 4.413507
H -0.759213 -2.728413 -2.614898	H -2.542709 0.779242 2.560347
C 2.141739 -4.112889 -3.718086	C -0.662262 2.156041 5.032955
H 4.114891 -3.379830 -3.242930	H 1.148084 3.287556 4.719665
H 0.055950 -4.597390 -4.000271	H -2.469746 0.975671 5.010988
H 2.503279 -4.942170 -4.320760	H -0.626766 2.236658 6.116275
C 6.356108 -1.247788 0.064216	C -1.894391 -3.228286 2.671498
C 6.495245 -1.069044 -1.346661	C -0.717265 -2.965147 3.430236
C 6.353635 -2.540666 0.562932	C -3.125552 -2.960413 3.248056
C 6.655990 -2.143825 -2.187818	C -0.787881 -2.466546 4.708568
H 6.496277 -0.064483 -1.753548	H 0.250548 -3.144974 2.977451
C 6.525756 -3.671513 -0.277759	C -3.233451 -2.444754 4.565317
H 6.224963 -2.707358 1.629240	H -4.038435 -3.154159 2.693716
C 6.688287 -3.473734 -1.687193	C -2.040779 -2.197754 5.320062
H 6.781386 -1.981960 -3.256046	H 0.125930 -2.256193 5.257496
C 1.133250 4.388781 -0.999861	C -4.521886 0.983135 -2.919390
C 0.331733 4.100519 0.144633	C -5.543277 1.862543 -2.599859
C 0.506642 4.542610 -2.225529	C -3.234473 1.521241 -3.218542
C -1.036263 4.009986 0.046015	C -5.351296 3.268076 -2.581595

H 0.813309 3.974450 1.108447 C -0.902397 4.455848 -2.362255 H 1.101275 4.739779 -3.114039 C -1.696908 4.193346 -1.199622 H -1.634229 3.802578 0.928009 C -6.558611 0.995253 -2.273823 C -4.541692 3.137023 2.668736 C -1.670194 -1.915827 3.796783 C -3.649431 -4.173760 -1.195737 H 1.630857 -0.794576 0.620893 F -1.942618 -1.255303 4.931351 F -0.367996 -1.745434 3.509877 F -1.891159 -3.223497 3.998076 F -3.349963 3.649655 3.012808 F -5.304293 3.054195 3.760285 F -5.129032 3.982164 1.796442 F -5.990031 0.853852 -3.479453 F -6.715017 2.312297 -2.029580 F -7.763950 0.421699 -2.296652 F -3.018357 -4.043384 -2.372546 F -4.822106 -4.782854 -1.409437 F -2.902019 -4.953058 -0.395247 C 3.135318 -4.691978 1.765113 H 3.326665 -5.720090 2.089612 H 3.783647 -4.469904 0.913708 H 3.390457 -4.014103 2.585970 C 1.304728 -5.418572 0.180136 H 1.922804 -5.162036 -0.685618 H 1.494401 -6.466290 0.438792 H 0.252520 -5.316031 -0.092151 C 0.749164 -4.777408 2.583699 H 0.985158 -4.080056 3.392832 H -0.303715 -4.668119 2.319710 H 0.906551 -5.796505 2.953639 C 6.564517 -4.998203 0.234488 H 6.452710 -5.148087 1.305904 C 6.882001 -4.604282 -2.525020 H 7.012471 -4.447526 -3.593517 C -1.554269 4.632157 -3.614531 H -0.948907 4.834662 -4.495367 C -3.109627 4.121753 -1.334003 H -3.708455 3.929645 -0.449244 C -2.925833 4.549493 -3.713385 C -3.711664 4.290358 -2.562207 H -3.411723 4.685574 -4.676079 H -4.791537 4.213550 -2.651878 C 6.752541 -6.074980 -0.603759 C 6.912293 -5.876873 -1.997576 H 7.063528 -6.733616 -2.648577 H 6.784726 -7.082329 -0.197448	H -6.523870 1.472252 -2.340880 C -3.015427 2.881174 -3.209630 H -2.425717 0.844784 -3.473197 C -4.058473 3.797551 -2.897924 H -2.036453 3.275387 -3.470449 C 3.155743 -2.072067 3.169352 C 6.704622 2.204717 1.565296 C -2.947854 5.309017 3.249194 H -2.111177 5.744075 2.698960 H -3.363791 6.078340 3.909060 H -2.576513 4.487503 3.869296 C -5.209423 4.192428 3.073145 H -5.959464 3.791071 2.384676 H -4.853863 3.379330 3.713022 H -5.685524 4.950269 3.703805 C -4.527231 5.900748 1.335771 H -3.696025 6.327146 0.770576 H -5.260832 5.494367 0.632539 H -5.006469 6.703821 1.906614 F 7.102301 3.162052 0.706170 F 7.781477 1.528048 1.976742 F 6.136954 2.794283 2.625615 F 2.697781 -3.324634 2.966912 F 4.294552 -2.150586 3.873100 F 2.252370 -1.402236 3.890941 C -4.493424 -2.169425 5.166064 H -5.397435 -2.357426 4.591461 C -2.154958 -1.685569 6.640374 H -1.246402 -1.499509 7.208574 C -3.390362 -1.427869 7.193424 C -4.571541 -1.671900 6.447676 H -3.464507 -1.038965 8.205616 H -5.540821 -1.466124 6.894150 C -3.868859 5.205579 -2.895749 H -2.885699 5.603387 -3.135437 C -6.404436 4.172168 -2.270803 H -7.385825 3.769225 -2.031946 C -4.912336 6.055415 -2.600822 C -6.192226 5.533289 -2.285004 H -4.757806 7.130823 -2.609654 H -7.008343 6.213922 -2.057698 H -2.948047 1.709131 0.367097 C 1.344996 -2.552767 -2.655958 F 0.070253 -2.198963 -2.474171 F 1.659291 -2.360636 -3.953097 F 1.475286 -3.859533 -2.380993 C 5.005451 1.705707 -4.001869 F 3.883433 1.972406 -4.694514 F 5.820681 0.983202 -4.772595 F 5.607850 2.870984 -3.708557
(8'-10')‡ E_0 = -5293.0525004 G_{298} = -5292.199182 NImag = 1 (-567.7817 cm^{-1}) C 6.351006 -0.193629 0.487371 C 7.231240 -1.252431 0.286812 C 8.491377 -1.004651 -0.277390 C 8.900048 0.298268 -0.545394 C 8.034706 1.353699 -0.261126 C 6.735813 1.140230 0.235664 C 9.222164 -2.305233 -0.531130 C 8.093974 -3.352694 -0.396259 C 7.093256 -2.729666 0.635467 C 5.761938 -3.476291 0.645666 C 5.809272 -4.521312 1.583162 C 7.079227 -4.443732 2.402386 C 7.588892 -3.019591 2.092382 C 4.763943 -5.433209 1.685522 C 3.665896 -5.306637 0.834821 C 3.558229 -4.245892 -0.079494 C 4.612769 -3.313368 -0.124080 O 4.475188 -2.169919 -0.928725 P 3.927115 -0.812590 -0.222973 O 2.680117 -1.147006 0.644484 O 5.055438 -0.479831 0.919359 O 3.771008 0.268219 -1.245002 C 0.933772 0.859043 0.484317 C -0.060535 0.218607 -0.339357 O 0.180690 0.373378 -1.658738 C -0.616229 -0.391203 -2.587663	

O -0.967501 -0.518739 0.092089 O -3.454698 -1.970395 1.160537 C -4.632994 -2.289568 1.477086 O -5.699584 -1.629709 1.343291 Rh -5.568015 0.241097 0.461338 O -5.270627 2.085916 -0.455648 C -4.102219 2.368556 -0.832216 O -3.044653 1.688318 -0.721506 Rh -3.170644 -0.146252 0.225472 O -2.941375 0.768226 2.068458 C -3.977223 1.163591 2.668904 O -5.181992 1.096260 2.299535 O -3.610879 -1.031003 -1.613945 C -4.816141 -1.070139 -1.981980 O -5.841846 -0.638562 -1.389571 H 8.363766 2.374338 -0.431198 H 9.881792 0.498190 -0.967058 H 4.801213 -6.241145 2.411872 H 2.862657 -6.036463 0.873296 H 6.900067 -4.604365 3.471545 H 7.805121 -5.206321 2.086310 H 7.117348 -2.302384 2.773751 H 8.673654 -2.912296 2.192632 H 10.012541 -2.469604 0.214957 H 9.707127 -2.330104 -1.513605 H 7.581359 -3.469627 -1.357789 H 8.451742 -4.339549 -0.086613 H 1.904812 -0.331642 0.587531 H -1.582232 0.094172 -2.732754 H -0.043967 -0.399152 -3.515816 H -0.765857 -1.404731 -2.217310 N 1.754778 1.854555 -0.286135 H 2.439068 1.342268 -0.907649 C 0.996924 2.892810 -1.093187 O -0.077328 3.289316 -0.740586 O 1.749413 3.213061 -2.118111 C 1.255940 4.159923 -3.178409 C 0.641033 1.223129 1.902252 C 0.432823 0.192851 2.836072 C 0.609841 2.550516 2.361185 C 0.194806 0.482132 4.177328 H 0.460590 -0.839424 2.503530 C 0.392292 2.836560 3.711090 H 0.712727 3.374719 1.661766 C 0.183041 1.805020 4.625422 H 0.029638 -0.331896 4.877896 H 0.362894 3.872376 4.039921 H 0.002978 2.028220 5.673247 C 5.835259 2.300016 0.467320 C 4.980459 2.363618 1.610199 C 5.844258 3.379482 -0.401639 C 4.189020 3.465316 1.850098 H 4.963980 1.532621 2.305559 C 5.056926 4.537945 -0.175870 H 6.459722 3.343642 -1.296365 C 4.206191 4.589284 0.976014 H 3.555913 3.494181 2.733572 C 2.376579 -4.160196 -0.977930 C 2.557689 -4.016485 -2.385317 C 1.092029 -4.298919 -0.482388 C 1.483978 -4.044900 -3.241895 H 3.562685 -3.901046 -2.778171 C -0.040763 -4.315001 -1.338919 H 0.934102 -4.381276 0.590000 C 0.158235 -4.201609 -2.754027 H 1.640205 -3.953762 -4.314568 C -5.080934 -1.788727 -3.325092 C -3.899743 3.730610 -1.535516 C -3.717902 1.826609 4.042134 C -4.756959 -3.687950 2.124229 H 2.358210 2.355289 0.385559 F -2.995834 2.947073 3.874632 F -3.031851 0.988148 4.835308 F -4.862555 2.147332 4.654659 F -3.056136 4.494999 -0.825615 F -5.051262 4.388250 -1.688998 F -3.359928 3.529503 -2.756377 F -5.293982 -3.100355 -3.086454 F -4.031945 -1.675917 -4.151228 F -6.161019 -1.291550 -3.936380 F -4.164485 -4.608619 1.338423	

F -6.031321 -4.042006 2.303453 F -4.137004 -3.690607 3.315904 C 0.899334 5.506529 -2.548553 H 0.685496 6.222088 -3.350314 H 0.017623 5.430899 -1.909869 H 1.738246 5.893788 -1.962022 C 0.070758 3.506010 -3.888090 H -0.793672 3.407424 -3.228105 H -0.221731 4.129467 -4.740177 H 0.347705 2.517695 -4.268677 C 2.476147 4.269905 -4.090314 H 3.327597 4.687763 -3.544670 H 2.759457 3.287715 -4.480785 H 2.245419 4.927622 -4.934642 C 5.093476 5.659514 -1.049987 H 5.746314 5.623603 -1.919161 C 3.428259 5.755184 1.209321 H 2.789555 5.791962 2.088768 C -1.367227 -4.438589 -0.840849 H -1.526878 -4.501502 0.232130 C -0.971935 -4.238897 -3.613706 H -0.815571 -4.160594 -4.687454 C -2.442619 -4.461606 -1.700782 C -2.243789 -4.367579 -3.100747 H -3.449354 -4.547470 -1.303340 H -3.101696 -4.383761 -3.765112 C 4.333461 6.780025 -0.792923 C 3.492366 6.828908 0.347652 H 2.901544 7.719693 0.542250 H 4.381916 7.635729 -1.460980	

Table S7(b): The Total Electronic Energies (E_0 in a.u), Gibbs Free Energies (G_{298} in a.u) and Cartesian coordinates of stereodetermining transition states geometry given in main text obtained using different DFT Functionals. The Number of Imaginary Frequencies, along with their values (in cm^{-1}) is provided

Optimized Cartesian Coordinates for the stereodetermining transition states at the M06 level of theory in gas phase

(7-10)‡	**(7-10')‡**
E_0 = -5290.5672462 G_{298} = -5289.688271 NImag = 1 (-1118.4808 cm^{-1}) C -5.316807 1.955719 0.477038 C -6.390058 1.409668 1.162416 C -6.836669 2.010647 2.342038 C -6.249366 3.180367 2.800780 C -5.195159 3.732976 2.081561 C -4.693286 3.132369 0.920665 C -7.919815 1.177951 2.969764 C -7.746956 -0.167603 2.255460 C -7.240481 0.203952 0.837142 C -6.708850 -1.011945 0.108913 C -7.742227 -1.618865 -0.611635 C -8.981377 -0.768823 -0.564630 C -8.435314 0.577250 -0.075844 C -7.533937 -2.817821 -1.276354 C -6.275424 -3.405475 -1.226553 C -5.206045 -2.802089 -0.554954 C -5.443950 -1.583182 0.097553 O -4.383549 -0.900242 0.685179 P -3.638984 0.199842 -0.248333 O -3.247988 -0.415652 -1.593834 O -4.809582 1.257739 -0.615740 O -2.559419 0.807884 0.594715 N -0.787824 -1.347013 -0.260329 C -0.321160 -0.831036 0.895594 O -0.982650 -1.316033 1.927612 C -0.791920 -0.846867 3.308431 C -0.676100 -0.802304 -1.588770 C -0.331741 0.583295 -1.726806 O 0.315385 0.917112 -2.808074 C 0.629231 2.301214 -3.013194 O 0.562082 0.034677 0.975333 O -0.700177 1.548344 -0.962472 H -4.721929 4.649584 2.429389 H -6.593066 3.651014 3.720098 H -8.339416 -3.289065 -1.836556 H -6.096377 -4.353851 -1.730162 H -9.482768 -0.701479 -1.537361	E_0 = -5290.5538598 G_{298} = -5289.678568 NImag = 1 (-849.8146 cm^{-1}) N -0.873037 -1.470271 0.214694 C 0.256818 -1.916488 -0.387622 O 0.191652 -3.202798 -0.694989 C 1.354505 -3.920938 -1.242581 C -0.990260 -0.075570 0.560891 C -0.805595 0.714988 -0.624022 O -0.160143 1.835622 -0.575230 C 0.172524 2.499297 -1.801060 O 1.194344 -1.156625 -0.653781 O -1.311455 0.376664 -1.765929 H -2.356403 0.231721 0.771738 H -1.641984 -2.122920 0.336937 H 0.803859 1.843477 -2.408078 H 0.721506 3.393499 -1.496214 H -0.733351 2.771388 -2.347822 H -2.056266 -0.308065 -1.653578 C -0.312443 0.357751 1.817699 C -0.549902 1.637451 2.329742 C 0.535755 -0.497271 2.524505 C 0.097713 2.073715 3.477719 H -1.228382 2.311347 1.802726 C 1.168676 -0.066711 3.684969 H 0.708729 -1.510652 2.164316 C 0.969084 1.226755 4.158478 H -0.075757 3.088786 3.832956 H 1.831902 -0.747926 4.214217 H 1.478045 1.565243 5.058452 C 0.803581 -5.307596 -1.521465 H 0.459468 -5.782670 -0.596618 H 1.592341 -5.931310 -1.956665 H -0.034095 -5.258690 -2.226276 C 1.810298 -3.295227 -2.552078 H 2.168569 -2.272713 -2.436764 H 0.983416 -3.304562 -3.272077 H 2.629956 -3.897130 -2.962954 C 2.423344 -3.994356 -0.165092 H 2.707328 -3.008043 0.206061

H -9.718590 -1.181411 0.140780	H 3.326822 -4.469370 -0.565747
H -8.049560 1.152959 -0.928585	H 2.058813 -4.588841 0.681498
H -9.177881 1.198181 0.439660	O 3.002923 0.732903 -2.171156
H -8.914111 1.608168 2.775785	C 3.978528 1.405282 -2.597339
H -7.818546 1.102687 4.058844	O 5.074763 1.652804 -2.043454
H -6.964336 -0.753496 2.757309	Rh 5.373460 0.923315 -0.128554
H -8.657199 -0.778891 2.229303	O 5.522211 0.125935 1.769182
H -2.040351 -0.594939 -1.772437	C 4.610616 -0.653565 2.141563
H -1.549042 -2.009108 -0.128671	O 3.583957 -1.030533 1.523563
H -0.283701 2.893823 -3.125129	Rh 3.217431 -0.178291 -0.324077
H 1.208475 2.682521 -2.165596	O 4.220445 -1.745445 -1.227531
H 1.221107 2.321747 -3.928442	C 5.474736 -1.698603 -1.281164
H -1.367510 1.289434 -0.229020	O 6.249116 -0.782871 -0.917393
C -0.103651 -1.752588 -2.592660	O 2.388387 1.493969 0.551101
C -0.602391 -1.774174 -3.896478	C 3.134945 2.481334 0.744379
C 0.921339 -2.634246 -2.245028	O 4.383689 2.571565 0.617484
C -0.059874 -2.628993 -4.848731	C 4.767021 -1.180895 3.578378
H -1.423354 -1.107223 -4.160321	C 3.755155 2.001280 -3.998072
C 1.462495 -3.492788 -3.195789	C 2.445888 3.796237 1.155486
H 1.289080 -2.653920 -1.219232	C 6.107734 -2.986424 -1.836535
C 0.978921 -3.489116 -4.501631	F 5.976002 -3.949204 -0.921213
H -0.454676 -2.630427 -5.862346	F 5.471227 -3.372025 -2.938193
H 2.262494 -4.172354 -2.906197	F 7.389763 -2.831187 -2.112040
H 1.404469 -4.160381 -5.244340	F 3.485415 1.027603 -4.860613
C -3.876249 -3.446435 -0.581530	F 4.808059 2.673987 -4.423013
C -3.139560 -3.654624 0.567778	F 2.707275 2.827466 -3.954949
C -3.354440 -3.901008 -1.822247	F 2.793483 4.746388 0.282662
C -1.881721 -4.305725 0.529109	F 1.131033 3.689620 1.143411
H -3.516175 -3.299842 1.526961	F 2.845342 4.165612 2.366557
C -2.146363 -4.544299 -1.888181	F 3.981880 -2.226365 3.801305
H -3.918578 -3.695078 -2.730089	F 6.022871 -1.532703 3.813762
C -1.375591 -4.764752 -0.721488	F 4.429938 -0.208606 4.424682
H -1.742789 -4.863998 -2.848268	C -6.070975 -2.018139 -0.243085
C -3.509670 3.712528 0.250774	C -7.218254 -1.591093 -0.886313
C -2.385033 4.078422 1.040628	C -7.849516 -2.431201 -1.804759
C -3.462870 3.918217 -1.110836	C -7.396905 -3.731653 -1.977461
C -1.270732 4.634225 0.471873	C -6.294279 -4.171179 -1.251135
H -2.413375 3.877103 2.110022	C -5.577433 -3.325208 -0.392525
C -2.332372 4.506676 -1.726140	C -8.956855 -1.688859 -2.503117
H -4.312325 3.640062 -1.733327	C -8.670345 -0.226321 -2.123087
C -1.216466 4.879780 -0.921766	C -8.011719 -0.314455 -0.724162
H -0.402930 4.888352 1.079907	C -7.402691 0.993673 -0.254467
C -2.073168 -1.328948 3.966912	C -8.332926 1.704360 0.512851
H -2.167042 -2.419401 3.899153	C -9.586852 0.898261 0.695964
H -2.082077 -1.047939 5.025768	C -9.104996 -0.514188 0.361959
H -2.935893 -0.873477 3.464245	C -8.025480 2.950429 1.037159
C -0.709023 0.668992 3.404532	C -6.767211 3.490459 0.801821
H 0.258784 1.053992 3.078525	C -5.799871 2.798713 0.064755
H -1.501266 1.131620 2.805293	C -6.142251 1.542066 -0.454588
H -0.859696 0.947123 4.454875	O -5.179851 0.814690 -1.140851
C 0.437888 -1.531237 3.873046	P -4.267916 -0.216126 -0.286083
H 1.340137 -1.229614 3.330082	O -3.517115 0.514661 0.833027
H 0.565529 -1.248041 4.925020	O -5.368976 -1.091778 0.511369
H 0.334813 -2.621612 3.817203	O -3.439645 -1.002221 -1.251411
C -2.280916 4.757076 -3.120510	H -5.960847 -5.199938 -1.368192
H -3.138581 4.477792 -3.731234	H -7.889527 -4.403867 -2.677571
C -0.091983 5.478558 -1.536949	H -8.754494 3.493192 1.636009
H 0.756570 5.752564 -0.913127	H -6.509480 4.472354 1.194011
C -1.178715 5.346912 -3.689878	H -10.004663 0.985734 1.705772
C -0.070208 5.708595 -2.890619	H -10.372932 1.228172 -0.000395
H -1.155551 5.538151 -4.760427	H -8.630601 -0.959380 1.247437
H 0.800160 6.171801 -3.350609	H -9.900278 -1.193618 0.032980
C -1.081472 -4.462603 1.688932	H -9.945320 -2.010824 -2.142994
H -1.469866 -4.098995 2.639389	H -8.952394 -1.855536 -3.586842
C -0.099424 -5.376671 -0.765613	H -7.942598 0.205839 -2.823735
H 0.276969 -5.724727 -1.726481	H -9.561968 0.412504 -2.128489
C 0.164276 -5.029824 1.609846	C -4.471843 3.415182 -0.144121
C 0.657178 -5.499997 0.371132	C -3.774539 3.939513 0.923048
H 0.778385 -5.127954 2.502525	C -3.936181 3.562203 -1.451111
H 1.644089 -5.952285 0.324730	C -2.570646 4.659511 0.741948
O 2.608923 2.181395 0.164794	H -4.154416 3.797272 1.935057
C 3.704728 2.793399 0.078140	C -2.783864 4.274995 -1.659735
O 4.874913 2.347781 0.138532	H -4.476012 3.133899 -2.292496
Rh 5.112225 0.293856 0.279935	C -2.075437 4.857240 -0.579339
O 5.137957 -1.780930 0.395407	H -2.411918 4.429782 -2.673037
C 4.052050 -2.373945 0.590128	C -4.338053 -3.780067 0.275065
O 2.897685 -1.898100 0.758512	C -3.538798 -4.787199 -0.334004
Rh 2.692975 0.138982 0.490202	C -3.906640 -3.259439 1.482813
O 2.932569 0.454685 2.516603	C -2.383244 -5.235655 0.248401
C 4.106988 0.478692 2.967202	H -3.838782 -5.191430 -1.297857
O 5.195500 0.417201 2.350243	C -2.686249 -3.656437 2.075701

O 2.641913 -0.123971 -1.560405	H -4.490041 -2.501288 1.996588
C 3.713294 0.008380 -2.200365	C -1.906163 -4.675043 1.457556
O 4.880161 0.169577 -1.764399	H -1.794351 -6.011077 -0.239035
C 4.095734 -3.911314 0.581720	C -2.193582 -3.026516 3.247520
C 3.550566 4.303793 -0.177746	H -2.786668 -2.233870 3.701923
C 3.598035 0.058891 -3.735486	C -0.672476 -5.043881 2.045295
C 4.169683 0.595253 4.499196	H -0.089538 -5.840926 1.583237
F 5.413771 0.600035 4.944821	C -0.979771 -3.384295 3.775865
F 3.521649 -0.434575 5.040945	C -0.213348 -4.408179 3.172080
F 3.569325 1.718457 4.882504	H -0.596218 -2.871166 4.654791
F 2.692920 4.834873 0.690026	H 0.743977 -4.690327 3.605312
F 4.702346 4.941493 -0.085077	C -1.861334 5.226188 1.831028
F 3.060643 4.481547 -1.408238	H -2.238028 5.058801 2.839971
F 4.582558 -0.624192 -4.301721	C -0.909291 5.639107 -0.765528
F 3.708239 1.343064 -4.100710	H -0.545788 5.800393 -1.780847
F 2.442754 -0.400898 -4.174746	C -0.736939 5.982788 1.618870
F 3.439750 -4.400798 1.629208	C -0.259219 6.198022 0.306063
F 5.333524 -4.371509 0.599381	H -0.204185 6.417105 2.461984
F 3.494736 -4.343513 -0.530974	H 0.632176 6.800876 0.149844

Optimized Cartesian Coordinates for the stereodetermining transition states optimized at the M06 level of theory in the condensed phase

(7-10)‡	**(7-10')‡**
E_0 = -5290.6177984	E_0 = -5290.6068097
G_{298} = -5289.740306	G_{298} = -5289.736173
NImag = 1 (-1101.6327 cm^{-1})	NImag = 1 (-774.5829 cm^{-1})
C -5.267607 2.039873 0.511280	N -0.857037 -1.510461 0.180497
C -6.335134 1.511303 1.220054	C 0.272128 -1.978237 -0.412943
C -6.746554 2.123363 2.407718	O 0.183748 -3.263038 -0.719483
C -6.134266 3.288727 2.846529	C 1.335330 -4.004704 -1.270439
C -5.091796 3.827342 2.099510	C -0.961024 -0.113900 0.516046
C -4.621841 3.214132 0.930715	C -0.769084 0.672152 -0.666945
C -7.827491 1.310740 3.063285	O -0.123184 1.791095 -0.625068
C -7.701740 -0.037982 2.345328	C 0.207966 2.453436 -1.855145
C -7.218036 0.322002 0.916053	O 1.228271 -1.241809 -0.671467
C -6.729542 -0.904050 0.172675	O -1.270470 0.326334 -1.812392
C -7.791813 -1.484668 -0.528929	H -2.340816 0.206926 0.723737
C -9.010297 -0.608208 -0.451443	H -1.633146 -2.153013 0.310305
C -8.425648 0.723308 0.030957	H 0.816032 1.788188 -2.474691
C -7.621887 -2.683375 -1.206236	H 0.779556 3.335807 -1.558840
C -6.374501 -3.297461 -1.190191	H -0.695940 2.746846 -2.394435
C -5.276702 -2.722576 -0.536893	H -2.013825 -0.349694 -1.696269
C -5.478677 -1.505309 0.131258	C -0.308170 0.326657 1.782206
O -4.394876 -0.850143 0.709943	C -0.562629 1.607335 2.287628
P -3.633137 0.241964 -0.214296	C 0.525874 -0.524701 2.511373
O -3.257142 -0.370315 -1.568418	C 0.053502 2.046416 3.452295
O -4.783186 1.321548 -0.581859	H -1.234970 2.277690 1.746885
O -2.540108 0.824238 0.627797	C 1.129560 -0.089680 3.686770
N -0.786011 -1.343462 -0.196736	H 0.706669 -1.541144 2.162942
C -0.299460 -0.835055 0.954440	C 0.912822 1.203399 4.154708
O -0.903469 -1.381598 1.993663	H -0.136683 3.058438 3.806592
C -0.690847 -0.943820 3.383355	H 1.782876 -0.767741 4.232930
C -0.689361 -0.813138 -1.531279	H 1.396681 1.545062 5.067651
C -0.326923 0.561565 -1.703626	C 0.755718 -5.376138 -1.559165
O 0.297928 0.861923 -2.806044	H 0.394888 -5.852299 -0.640842
C 0.615964 2.236872 -3.065308	H 1.533857 -6.014984 -1.992020
O 0.555118 0.060872 1.023871	H -0.073107 -5.308130 -2.273363
O -0.667740 1.550063 -0.951530	C 1.813872 -3.380436 -2.571238
H -4.602193 4.740702 2.433428	H 2.227957 -2.380165 -2.440775
H -6.450737 3.768174 3.771100	H 0.985989 -3.334371 -3.289437
H -8.448635 -3.134617 -1.751993	H 2.597268 -4.020069 -2.997132
H -6.228535 -4.243875 -1.708177	C 2.401849 -4.104702 -0.195215
H -9.529965 -0.525980 -1.413269	H 2.736509 -3.125047 0.152976
H -9.739329 -1.008874 0.268681	H 3.274805 -4.635636 -0.594216
H -8.049909 1.296058 -0.828567	H 2.019102 -4.668171 0.664773
H -9.143541 1.354228 0.568330	O 3.012197 0.695144 -2.169378
H -8.816582 1.762915 2.896373	C 3.982252 1.364961 -2.607920
H -7.696548 1.233555 4.148945	O 5.075792 1.631992 -2.058003
H -6.925067 -0.644324 2.832267	Rh 5.385338 0.948834 -0.120982
H -8.628361 -0.624094 2.335849	O 5.518738 0.175442 1.796994
H -2.056225 -0.584246 -1.717778	C 4.612282 -0.608782 2.171782
H -1.521188 -2.034482 -0.060902	O 3.592974 -1.001261 1.554410
H -0.295907 2.838488 -3.117475	Rh 3.231285 -0.177382 -0.304623
H 1.276644 2.622489 -2.280834	O 4.238220 -1.753649 -1.179279
H 1.126106 2.234514 -4.029212	C 5.490857 -1.697101 -1.241823
H -1.322178 1.307884 -0.208907	O 6.262516 -0.776492 -0.883979
C -0.158212 -1.793025 -2.530702	O 2.391461 1.501435 0.557035
C -0.704568 -1.853011 -3.815091	C 3.125861 2.499687 0.728695
C 0.866541 -2.677410 -2.188709	O 4.371896 2.606737 0.586396
C -0.212311 -2.754763 -4.752878	C 4.762969 -1.119844 3.613710

H -1.523722 -1.182556 -4.076951	C 3.756973 1.935063 -4.018487
C 1.360098 -3.580094 -3.124712	C 2.430544 3.803763 1.159075
H 1.271071 -2.660552 -1.176667	C 6.132933 -2.979114 -1.797172
C 0.826091 -3.619091 -4.410887	F 6.084779 -3.921479 -0.853818
H -0.645718 -2.788817 -5.750271	F 5.455241 -3.415226 -2.854317
H 2.158409 -4.263137 -2.839187	F 7.394903 -2.790824 -2.145104
H 1.212168 -4.326245 -5.142195	F 3.442400 0.953711 -4.857549
C -3.962918 -3.401678 -0.601527	F 4.827450 2.562499 -4.474422
C -3.208402 -3.661045 0.526828	F 2.739330 2.797591 -3.983198
C -3.485990 -3.853244 -1.862472	F 2.813168 4.791784 0.346778
C -1.983212 -4.371308 0.446480	F 1.116262 3.706445 1.103497
H -3.548078 -3.319825 1.505099	F 2.794753 4.119484 2.399703
C -2.310664 -4.550660 -1.968092	F 4.006966 -2.186241 3.835918
H -4.060640 -3.611236 -2.755161	F 6.026050 -1.431530 3.873202
C -1.529169 -4.836392 -0.822265	F 4.386224 -0.151594 4.449466
H -1.942659 -4.867965 -2.943708	C -6.088191 -1.999147 -0.241598
C -3.445754 3.777920 0.232051	C -7.232303 -1.553930 -0.878101
C -2.308589 4.154772 0.999979	C -7.883476 -2.387306 -1.790508
C -3.414982 3.956887 -1.134733	C -7.451146 -3.695570 -1.963059
C -1.198991 4.694503 0.405910	C -6.352554 -4.152717 -1.240098
H -2.322515 3.980223 2.074362	C -5.619774 -3.316750 -0.384119
C -2.288449 4.526791 -1.776247	C -8.987730 -1.631232 -2.478204
H -4.274382 3.677419 -1.743130	C -8.682519 -0.172434 -2.100433
C -1.159856 4.909871 -0.993564	C -8.010749 -0.268910 -0.708006
H -0.323599 4.958501 0.999212	C -7.384697 1.033438 -0.241889
C -1.873054 -1.580008 4.091302	C -8.305126 1.751951 0.531991
H -1.851557 -2.671639 3.991599	C -9.562454 0.955436 0.726939
H -1.847123 -1.334681 5.158924	C -9.095755 -0.460462 0.388832
H -2.813865 -1.207654 3.666150	C -7.984534 2.997280 1.051547
C -0.761954 0.567874 3.517365	C -6.724654 3.528999 0.805456
H 0.140547 1.062594 3.150293	C -5.764835 2.829792 0.063230
H -1.628059 0.957294 2.969901	C -6.121438 1.573435 -0.449897
H -0.884030 0.813149 4.579357	O -5.169093 0.835803 -1.144604
C 0.626828 -1.511989 3.867994	P -4.263972 -0.216383 -0.313731
H 1.469691 -1.052674 3.342677	O -3.485460 0.495179 0.803290
H 0.741322 -1.307334 4.939867	O -5.359098 -1.079804 0.500710
H 0.659214 -2.598431 3.718390	O -3.459809 -0.998966 -1.301606
C -2.251919 4.744432 -3.177285	H -6.035836 -5.186810 -1.359421
H -3.118430 4.457562 -3.772125	H -7.957743 -4.361628 -2.659296
C -0.037592 5.486645 -1.635017	H -8.705311 3.546741 1.654431
H 0.820584 5.767652 -1.026890	H -6.461323 4.510831 1.193942
C -1.150623 5.311126 -3.772240	H -9.968640 1.047206 1.740890
C -0.029774 5.683054 -2.994429	H -10.351488 1.291434 0.037497
H -1.136995 5.475294 -4.847653	H -8.619298 -0.910191 1.271404
H 0.839026 6.127365 -3.476189	H -9.900869 -1.130385 0.065103
C -1.171753 -4.603365 1.586674	H -9.975096 -1.943650 -2.107763
H -1.521634 -4.247088 2.554326	H -8.994381 -1.798216 -3.561716
C -0.293892 -5.525922 -0.904555	H -7.959307 0.253424 -2.809989
H 0.038330 -5.880192 -1.879579	H -9.568211 0.474079 -2.093627
C 0.033281 -5.249587 1.471917	C -4.435220 3.443076 -0.153544
C 0.476879 -5.719922 0.213766	C -3.753745 4.006749 0.905422
H 0.651746 -5.408860 2.352967	C -3.884059 3.555897 -1.459003
H 1.434233 -6.231749 0.136764	C -2.550695 4.727626 0.716414
O 2.645736 2.194844 0.135527	H -4.145437 3.902981 1.917527
C 3.749020 2.785989 0.014745	C -2.733530 4.270178 -1.675713
O 4.912504 2.321673 0.061914	H -4.411596 3.107800 -2.298034
Rh 5.129444 0.255263 0.230769	C -2.040686 4.889119 -0.604822
O 5.093081 -1.826168 0.394993	H -2.349474 4.393686 -2.688468
C 3.996068 -2.383446 0.629335	C -4.387483 -3.789974 0.285728
O 2.860807 -1.868794 0.800526	C -3.594955 -4.800252 -0.328424
Rh 2.706545 0.159908 0.494392	C -3.955580 -3.278110 1.497437
O 3.009259 0.512107 2.510684	C -2.439447 -5.255108 0.250433
C 4.193278 0.516036 2.933361	H -3.901157 -5.203855 -1.290746
O 5.266585 0.410214 2.295267	C -2.739757 -3.688366 2.091244
O 2.617291 -0.141358 -1.552393	H -4.536376 -2.522262 2.018251
C 3.675779 -0.041951 -2.216623	C -1.962158 -4.704414 1.464729
O 4.855764 0.105122 -1.810967	H -1.854927 -6.032098 -0.239736
C 3.991160 -3.920596 0.663228	C -2.251069 -3.078050 3.275597
C 3.611753 4.291884 -0.270354	H -2.843644 -2.289671 3.738338
C 3.535313 -0.018644 -3.749039	C -0.732001 -5.087329 2.051978
C 4.297803 0.665418 4.459312	H -0.150657 -5.879298 1.579964
F 5.555816 0.711149 4.866694	C -1.044841 -3.455687 3.809408
F 3.695151 -0.368989 5.043563	C -0.278786 -4.473671 3.194033
F 3.681048 1.779716 4.843017	H -0.669535 -2.969413 4.707369
F 2.767840 4.851285 0.592086	H 0.673038 -4.769658 3.630654
F 4.774066 4.917407 -0.196954	C -1.856043 5.327378 1.797967
F 3.117514 4.453380 -1.500346	H -2.247741 5.194136 2.806196
F 4.525053 -0.694185 -4.320237	C -0.875181 5.670564 -0.801507
F 3.619416 1.259491 -4.139356	H -0.500924 5.803570 -1.816776
F 2.384570 -0.507974 -4.168397	C -0.728288 6.078036 1.576373
F 3.232247 -4.369012 1.656352	C -0.237216 6.258614 0.262880

F 5.210920 -4.414037 0.799796	H -0.206962 6.539371 2.412557
F 3.478516 -4.364287 -0.487435	H 0.654426 6.860219 0.100308

Optimized Cartesian Coordinates for the stereodetermining transition states at the B3LYP-D level of theory in gas phase

(7-10)‡

E_0 = -5293.42957
G_{298} = -5292.568516
NImag = 1 (-1045.4793 cm^{-1})

C	-5.335076	1.879597	0.616004
C	-6.407734	1.253187	1.234872
C	-6.875427	1.739560	2.463166
C	-6.294743	2.862810	3.044866
C	-5.229919	3.492103	2.395325
C	-4.719243	3.013122	1.177928
C	-7.974985	0.845075	2.991915
C	-7.771954	-0.444174	2.164174
C	-7.230636	0.059555	0.787830
C	-6.647623	-1.080431	-0.029870
C	-7.639094	-1.645813	-0.844570
C	-8.918116	-0.843192	-0.744134
C	-8.426463	0.482603	-0.120775
C	-7.364077	-2.763244	-1.627376
C	-6.084756	-3.323286	-1.588172
C	-5.063786	-2.765180	-0.803940
C	-5.366600	-1.619477	-0.047965
O	-4.333352	-0.955422	0.627265
P	-3.602668	0.230708	-0.219523
O	-3.190567	-0.272690	-1.621907
O	-4.796480	1.290086	-0.537204
O	-2.530953	0.796007	0.674311
N	-0.750315	-1.307882	-0.326773
C	-0.300569	-0.916612	0.880795
O	-0.949259	-1.525356	1.862898
C	-0.674923	-1.237153	3.288752
C	-0.599577	-0.645139	-1.600372
C	-0.303846	0.751145	-1.632426
O	0.278234	1.215112	-2.715504
C	0.455454	2.650094	-2.818164
O	0.571964	-0.044245	1.061501
O	-0.663189	1.634175	-0.758146
H	-4.761202	4.365092	2.839790
H	-6.649264	3.238093	4.001008
H	-8.130227	-3.193820	-2.266317
H	-5.854725	-4.203482	-2.181252
H	-9.408726	-0.704562	-1.713447
H	-9.639723	-1.341539	-0.081927
H	-8.049802	1.144432	-0.907954
H	-9.197307	1.017651	0.442246
H	-8.963762	1.282817	2.795637
H	-7.903059	0.676128	4.071630
H	-7.003605	-1.066945	2.634941
H	-8.680133	-1.044032	2.051137
H	-2.029552	-0.420903	-1.782097
H	-1.489505	-2.000851	-0.293492
H	1.109095	2.997771	-2.017049
H	0.922298	2.797298	-3.790079
H	-0.506814	3.156902	-2.755972
H	-1.344727	1.295399	-0.059455
C	-0.020693	-1.524455	-2.665306
C	-0.529041	-1.483150	-3.967851
C	1.007265	-2.425525	-2.361662
C	-0.011612	-2.319313	-4.958116
H	-1.336663	-0.793873	-4.198175
C	1.528387	-3.259008	-3.350237
H	1.387285	-2.479889	-1.348658
C	1.020171	-3.211237	-4.651859
H	-0.417083	-2.279580	-5.965306
H	2.331030	-3.946235	-3.099479
H	1.424023	-3.863739	-5.420941
C	-3.711682	-3.378607	-0.790586
C	-3.128005	-3.782877	0.398212
C	-3.011288	-3.588394	-2.013071
C	-1.857910	-4.416041	0.417713
H	-3.642784	-3.609464	1.338231
C	-1.767268	-4.177726	-2.024450
H	-3.458157	-3.232169	-2.935556
C	-1.155843	-4.609263	-0.816296

(7-10')‡

E_0 = -5293.4140197
G_{298} = -5292.553282
NImag = 1 (-850.5987 cm^{-1})

N	-0.753302	-1.168775	0.023094
C	0.245958	-1.676345	-0.737200
O	0.055270	-2.957244	-1.032320
C	1.081068	-3.780570	-1.727587
C	-0.838042	0.242030	0.322686
C	-0.664686	1.014208	-0.870463
O	0.001809	2.133817	-0.843705
C	0.327211	2.790601	-2.090388
O	1.184562	-0.979408	-1.176268
O	-1.200022	0.664174	-2.008502
H	-2.260235	0.535816	0.540708
H	-1.518691	-1.793793	0.246358
H	0.976152	2.135436	-2.675108
H	0.858395	3.690035	-1.788227
H	-0.585299	3.032953	-2.636250
H	-1.948028	-0.016007	-1.867042
C	-0.244968	0.703703	1.611024
C	-0.505979	2.007609	2.059312
C	0.530331	-0.144542	2.410554
C	0.054296	2.473367	3.244573
H	-1.124083	2.667881	1.461347
C	1.086005	0.322399	3.603342
H	0.715837	-1.160252	2.090712
C	0.863240	1.636659	4.020138
H	-0.127718	3.499191	3.550787
H	1.702660	-0.342068	4.200324
H	1.307875	2.003827	4.940617
C	0.330460	-5.076479	-2.017829
H	0.034028	-5.558332	-1.086362
H	0.991816	-5.750203	-2.571954
H	-0.563653	-4.880707	-2.617587
C	1.529096	-3.138813	-3.042555
H	2.145114	-2.258132	-2.883099
H	0.652919	-2.871266	-3.643132
H	2.113607	-3.881482	-3.596745
C	2.224391	-4.033395	-0.749751
H	2.681437	-3.100695	-0.436128
H	2.992912	-4.643327	-1.235504
H	1.848330	-4.556804	0.133332
O	3.289273	1.208814	-1.964818
C	4.276612	1.993159	-1.888929
O	5.299366	1.913419	-1.157131
Rh	5.292208	0.519145	0.393149
O	5.063866	-0.885490	1.912542
C	3.985937	-1.534009	1.936400
O	2.982102	-1.430520	1.179162
Rh	3.080868	-0.137260	-0.414680
O	4.029139	-1.601379	-1.519925
C	5.283218	-1.709028	-1.433373
O	6.092732	-0.993734	-0.787070
O	2.368643	1.530806	0.591008
C	3.192775	2.264421	1.192956
O	4.398051	2.016839	1.490062
C	3.839157	-2.652608	2.992033
C	4.128525	3.285709	-2.717815
C	2.735111	3.705142	1.517815
C	5.855946	-2.930909	-2.183818
F	7.177578	-2.843531	-2.349570
F	5.583006	-4.036941	-1.458953
F	5.275175	-3.063273	-3.385494
F	5.305928	3.829968	-3.027638
F	3.432906	4.162974	-1.954342
F	3.434026	3.073892	-3.844409
F	3.604688	4.558245	0.938204
F	1.520312	3.965031	1.026132
F	2.735959	3.934653	2.839060
F	2.702533	-2.480532	3.698453
F	3.753399	-3.840739	2.360955
F	4.866320	-2.687674	3.840124

H -1.218323 -4.282520 -2.955305	C -5.853151 -2.029774 -0.231340
C -3.537198 3.657428 0.554825	C -7.078925 -1.629695 -0.747516
C -2.387082 3.928557 1.352999	C -7.800777 -2.496912 -1.576411
C -3.522920 4.001647 -0.783615	C -7.354811 -3.799806 -1.770940
C -1.273859 4.526021 0.812038	C -6.176961 -4.217137 -1.150785
H -2.393086 3.618354 2.393164	C -5.366114 -3.346169 -0.393136
C -2.399214 4.642582 -1.366802	C -9.022981 -1.799045 -2.133256
H -4.386397 3.787345 -1.406065	C -8.750387 -0.315364 -1.784413
C -1.249422 4.912586 -0.555281	C -7.907691 -0.385734 -0.475324
H -0.388036 4.699654 1.417074	C -7.324485 0.957146 -0.068283
C -1.844860 -1.933891 3.980258	C -8.205012 1.620925 0.800672
H -1.834791 -3.005046 3.764795	C -9.390560 0.741673 1.123152
H -1.762395 -1.791601 5.062330	C -8.863220 -0.653577 0.735672
H -2.791878 -1.508379 3.633101	C -7.908428 2.889723 1.286033
C -0.721393 0.267674 3.575219	C -6.707791 3.493391 0.912753
H 0.192078 0.766839 3.252239	C -5.785605 2.845187 0.074498
H -1.577472 0.713726 3.059708	C -6.124670 1.569064 -0.411690
H -0.841901 0.405658 4.655657	O -5.207092 0.869113 -1.204286
C 0.661840 -1.875355 3.654787	P -4.144472 -0.090023 -0.431203
H 1.475865 -1.397989 3.109817	O -3.396821 0.706159 0.664200
H 0.845511 -1.746703 4.727072	O -5.093466 -1.077102 0.447377
H 0.641177 -2.944914 3.420433	O -3.289416 -0.774797 -1.459197
C -2.381678 5.036525 -2.732968	H -5.874057 -5.251140 -1.265670
H -3.256929 4.832735 -3.344717	H -7.917241 -4.495198 -2.387991
C -0.125698 5.552267 -1.140335	H -8.592376 3.398963 1.959379
H 0.746451 5.737531 -0.523345	H -6.456513 4.483556 1.279984
C -1.279392 5.666521 -3.271209	H -9.696320 0.810308 2.172483
C -0.138759 5.923435 -2.468235	H -10.260675 1.015626 0.510137
H -1.279270 5.964049 -4.316058	H -8.270850 -1.064832 1.560053
H 0.728184 6.411901 -2.903940	H -9.648866 -1.372071 0.485199
C -1.246691 -4.838923 1.629192	H -9.938453 -2.155954 -1.642399
H -1.795562 -4.714498 2.557194	H -9.147355 -1.967665 -3.208482
C 0.143848 -5.182765 -0.785610	H -8.143856 0.149105 -2.569172
H 0.681157 -5.296291 -1.721043	H -9.660735 0.277351 -1.653552
C 0.013387 -5.392454 1.626433	C -4.492139 3.501885 -0.228584
C 0.719730 -5.558224 0.407129	C -3.765727 4.084863 0.794599
H 0.474869 -5.702380 2.559778	C -3.997459 3.586788 -1.561388
H 1.722600 -5.969241 0.420705	C -2.557418 4.780679 0.545212
O 2.520643 2.189273 0.343882	H -4.114652 3.991781 1.819031
C 3.601830 2.833750 0.249511	C -2.839789 4.277830 -1.837733
O 4.785903 2.403715 0.227550	H -4.557447 3.112737 -2.359913
Rh 5.067218 0.343394 0.192724	C -2.090140 4.900661 -0.803470
O 5.123113 -1.741933 0.129472	H -2.489600 4.366606 -2.863316
C 4.047209 -2.365906 0.319464	C -4.076313 -3.821209 0.178432
O 2.896197 -1.908595 0.574519	C -3.437394 -4.969882 -0.384523
Rh 2.652790 0.135498 0.490248	C -3.459425 -3.220722 1.271210
O 2.979740 0.292253 2.522509	C -2.268218 -5.473869 0.129389
C 4.173716 0.279336 2.933946	H -3.868319 -5.450289 -1.255138
O 5.239007 0.289072 2.262650	C -2.215197 -3.678481 1.779586
O 2.529955 0.032117 -1.571960	H -3.914052 -2.368897 1.758570
C 3.571800 0.237185 -2.251114	C -1.596926 -4.831923 1.201641
O 4.757129 0.387516 -1.845456	H -1.821136 -6.356920 -0.317153
C 4.092840 -3.906148 0.204920	C -1.538724 -2.987359 2.822892
C 3.404160 4.356873 0.082829	H -1.998852 -2.099293 3.247788
C 3.367333 0.410983 -3.773379	C -0.328653 -5.250769 1.681440
C 4.298900 0.234495 4.472679	H 0.137334 -6.125020 1.233906
F 3.709425 1.317485 5.006794	C -0.297166 -3.402660 3.250431
F 5.572723 0.198043 4.870959	C 0.317660 -4.542523 2.672507
F 3.670951 -0.863290 4.935177	H 0.226088 -2.844000 4.018585
F 2.491650 4.816077 0.958676	H 1.308643 -4.838644 3.001942
F 4.538523 5.036862 0.251125	C -1.793321 5.363239 1.594206
F 2.940983 4.593357 -1.165149	H -2.146310 5.254204 2.616509
F 4.460099 0.041093 -4.452108	C -0.897279 5.630797 -1.053237
F 3.149910 1.728126 -4.005594	H -0.556341 5.737078 -2.079823
F 2.322914 -0.276769 -4.228580	C -0.628314 6.043060 1.321074
F 3.580873 -4.468720 1.312468	C -0.179944 6.185752 -0.017127
F 5.333404 -4.361604 0.025741	H -0.043791 6.471352 2.129784
F 3.339114 -4.291273 -0.849156	H 0.740466 6.725609 -0.218441

Optimized Cartesian Coordinates for the stereodetermining transition states optimized at the B3LYP-D level of theory in the condensed phase

(7-10)‡	**(7-10')‡**
E_0 = -5293.4785682	E_0 = -5293.4652229
G_{298} = -5292.618314	G_{298} = -5292.605419
NImag = 1 (-1054.6174 cm^{-1})	NImag = 1 (-830.5182 cm^{-1})
C -5.508626 1.911999 0.688193	N -0.736899 -1.171564 0.034096
C -6.658747 1.307318 1.180142	C 0.254025 -1.685512 -0.734336
C -7.226870 1.779275 2.372669	O 0.061253 -2.970117 -1.009541
C -6.669284 2.865256 3.042566	C 1.074709 -3.806212 -1.713729
C -5.527602 3.475629 2.517035	C -0.814677 0.238289 0.334024

C -4.920238 3.012342 1.338324	C -0.637013 1.014347 -0.853899
C -8.404308 0.915810 2.766591	O 0.027786 2.133449 -0.825068
C -8.170384 -0.358388 1.926225	C 0.367878 2.789773 -2.071523
C -7.479689 0.157800 0.623261	O 1.183412 -0.990769 -1.195529
C -6.861801 -0.985616 -0.163436	O -1.166229 0.663775 -1.997892
C -7.792926 -1.498294 -1.079860	H -2.255748 0.533238 0.538520
C -9.044718 -0.648788 -1.081522	H -1.481491 -1.801674 0.308597
C -8.566259 0.645090 -0.385597	H 0.993252 2.121291 -2.666213
C -7.483007 -2.609557 -1.859276	H 0.926527 3.672403 -1.769254
C -6.230449 -3.213122 -1.718184	H -0.536010 3.064105 -2.616131
C -5.265844 -2.706641 -0.832085	H -1.910187 -0.014575 -1.861608
C -5.603620 -1.568119 -0.077130	C -0.231759 0.692426 1.629463
O -4.616086 -0.946667 0.704213	C -0.495896 1.992832 2.088576
P -3.763366 0.211095 -0.061190	C 0.535370 -0.164301 2.429906
O -3.303266 -0.286913 -1.452519	C 0.043283 2.442973 3.290620
O -4.875327 1.343104 -0.428940	H -1.102957 2.661342 1.487343
O -2.700649 0.689253 0.891212	C 1.074181 0.288255 3.636483
N -0.746367 -1.264423 -0.057726	H 0.725995 -1.176758 2.101402
C -0.124126 -0.862803 1.068146	C 0.840147 1.596086 4.069064
O -0.594129 -1.496885 2.136213	H -0.146949 3.463363 3.610694
C 0.014898 -1.355162 3.482261	H 1.684997 -0.383062 4.232500
C -0.705061 -0.651630 -1.361777	H 1.266913 1.951137 5.003130
C -0.454485 0.749368 -1.430055	C 0.316265 -5.100842 -1.981878
O 0.080918 1.223035 -2.528593	H 0.031048 -5.576410 -1.043194
C 0.240451 2.660087 -2.644947	H 0.969669 -5.781526 -2.537494
O 0.733139 0.043251 1.111531	H -0.582926 -4.910685 -2.576525
O -0.828052 1.622769 -0.544951	C 1.507579 -3.177533 -3.038776
H -5.077389 4.320363 3.030205	H 2.139395 -2.304562 -2.895640
H -7.102912 3.225947 3.971565	H 0.625612 -2.899663 -3.626813
H -8.199893 -3.000435 -2.576385	H 2.068980 -3.932228 -3.600830
H -5.976502 -4.085925 -2.312808	C 2.228794 -4.054910 -0.748921
H -9.434447 -0.473963 -2.089906	H 2.717967 -3.125398 -0.475903
H -9.842331 -1.131538 -0.500637	H 2.967368 -4.706014 -1.228374
H -8.093096 1.305994 -1.120141	H 1.855908 -4.541130 0.157178
H -9.367785 1.197042 0.114260	O 3.317262 1.228948 -1.966318
H -9.350503 1.398871 2.486998	C 4.303291 2.010862 -1.873501
H -8.442517 0.717766 3.842896	O 5.327136 1.915857 -1.143468
H -7.476246 -1.023085 2.451954	Rh 5.311435 0.500183 0.390564
H -9.086374 -0.915243 1.707763	O 5.058977 -0.927372 1.895454
H -2.139831 -0.458545 -1.536890	C 3.972883 -1.563732 1.906860
H -1.450404 -1.982233 0.072784	O 2.974629 -1.439559 1.146904
H 0.966887 3.006336 -1.908815	Rh 3.091286 -0.131580 -0.428958
H 0.610776 2.815984 -3.657133	O 4.019458 -1.590912 -1.552305
H -0.715797 3.159989 -2.496945	C 5.271142 -1.713314 -1.466608
H -1.485235 1.251193 0.149689	O 6.089402 -1.010692 -0.817920
C -0.182838 -1.539797 -2.448933	O 2.389584 1.532070 0.598001
C -0.766710 -1.502502 -3.721136	C 3.214731 2.251282 1.212330
C 0.854259 -2.447281 -2.201028	O 4.418346 1.993688 1.511869
C -0.312886 -2.346782 -4.735536	C 3.806613 -2.691660 2.947857
H -1.584161 -0.811749 -3.909606	C 4.156368 3.327708 -2.659970
C 1.310825 -3.291092 -3.213939	C 2.760276 3.683033 1.575703
H 1.292281 -2.498879 -1.211772	C 5.830577 -2.934717 -2.225145
C 0.729016 -3.245564 -4.485075	F 7.154792 -2.859827 -2.390586
H -0.776988 -2.309204 -5.717474	F 5.549575 -4.045169 -1.511180
H 2.119090 -3.986644 -3.006721	F 5.250294 -3.052882 -3.428802
H 1.082187 -3.905982 -5.272534	F 5.337032 3.850038 -3.003661
C -3.929885 -3.344888 -0.732218	F 3.522358 4.199728 -1.839829
C -3.389239 -3.690570 0.495161	F 3.409809 3.173716 -3.761230
C -3.189595 -3.625039 -1.917114	F 3.636079 4.553682 1.030105
C -2.121665 -4.324030 0.589837	F 1.548390 3.965618 1.093221
H -3.935526 -3.477650 1.409109	F 2.761539 3.870249 2.905696
C -1.947601 -4.214540 -1.856169	F 2.652183 -2.536281 3.625215
H -3.603397 -3.323352 -2.874103	F 3.750535 -3.875311 2.305545
C -1.375341 -4.579167 -0.607626	F 4.813486 -2.724645 3.823713
H -1.371093 -4.373025 -2.762485	C -5.868194 -2.014381 -0.243923
C -3.672939 3.646594 0.842300	C -7.089089 -1.599301 -0.759939
C -2.564224 3.792323 1.726793	C -7.818927 -2.459703 -1.591145
C -3.565257 4.107327 -0.456391	C -7.385956 -3.767403 -1.786987
C -1.388990 4.363379 1.299123	C -6.214261 -4.199567 -1.164188
H -2.653130 3.411160 2.739398	C -5.397528 -3.337816 -0.401520
C -2.376696 4.731208 -0.919762	C -9.034192 -1.750536 -2.147193
H -4.402692 4.002214 -1.140302	C -8.750499 -0.269978 -1.797258
C -1.257473 4.847700 -0.031066	C -7.909160 -0.349004 -0.487207
H -0.538336 4.444274 1.971026	C -7.316423 0.989248 -0.076154
C -0.967806 -2.116193 4.367448	C -8.197231 1.658271 0.790172
H -1.027394 -3.164051 4.063418	C -9.388225 0.786062 1.108436
H -0.622609 -2.069908 5.405358	C -8.869913 -0.612082 0.721125
H -1.965907 -1.668870 4.307879	C -7.897443 2.928197 1.272290
C 0.084921 0.112221 3.910183	C -6.694543 3.528506 0.899423
H 0.894633 0.642369 3.409411	C -5.771053 2.875526 0.065099
H -0.864810 0.613076 3.692417	C -6.112976 1.596947 -0.415253

H 0.254510 0.146344 4.992432	O -5.194292 0.890890 -1.205632
C 1.380306 -2.035408 3.468958	P -4.142277 -0.084891 -0.443409
H 2.066099 -1.518498 2.801262	O -3.384280 0.696665 0.659475
H 1.800890 -2.013418 4.480314	O -5.092087 -1.068857 0.432727
H 1.278893 -3.077159 3.147694	O -3.294771 -0.759972 -1.484375
C -2.259588 5.245133 -2.240949	H -5.920967 -5.236235 -1.282172
H -3.113588 5.164458 -2.909009	H -7.954337 -4.455427 -2.407068
C -0.054875 5.431917 -0.507591	H -8.581836 3.441978 1.941903
H 0.798771 5.483929 0.160689	H -6.444411 4.519972 1.263964
C -1.083603 5.826105 -2.669266	H -9.695047 0.856310 2.157277
C 0.033266 5.909293 -1.798430	H -10.253223 1.067150 0.492110
H -1.005117 6.211790 -3.682058	H -8.284219 -1.029259 1.547604
H 0.964370 6.341961 -2.152847	H -9.661044 -1.321993 0.464552
C -1.556246 -4.685278 1.843503	H -9.950812 -2.101111 -1.654810
H -2.135471 -4.502361 2.743596	H -9.158471 -1.918317 -3.222443
C -0.075153 -5.143825 -0.500977	H -8.141995 0.191220 -2.582690
H 0.497771 -5.302461 -1.408901	H -9.657267 0.326878 -1.663405
C -0.297408 -5.239566 1.913576	C -4.476601 3.531043 -0.241681
C 0.456303 -5.459113 0.730685	C -3.757632 4.136026 0.775329
H 0.128629 -5.503106 2.877633	C -3.972539 3.590408 -1.573457
H 1.459986 -5.865160 0.801395	C -2.545970 4.825892 0.519301
O 2.742006 2.230566 0.181315	H -4.113637 4.069966 1.799578
C 3.830804 2.812109 -0.083229	C -2.811654 4.273706 -1.856283
O 4.979387 2.318191 -0.233973	H -4.528101 3.105209 -2.368678
Rh 5.179656 0.241009 -0.167215	C -2.068351 4.916462 -0.828716
O 5.124582 -1.853039 -0.100438	H -2.451857 4.337108 -2.880244
C 4.036387 -2.405062 0.204043	C -4.117125 -3.829439 0.178325
O 2.932674 -1.869710 0.504320	C -3.479749 -4.976634 -0.391381
Rh 2.792163 0.176910 0.378660	C -3.508516 -3.242106 1.282776
O 3.336853 0.379552 2.366847	C -2.314167 -5.488529 0.124767
C 4.564102 0.319003 2.652332	H -3.908187 -5.449398 -1.267723
O 5.555485 0.276895 1.876456	C -2.270138 -3.709717 1.796709
O 2.445309 0.045670 -1.646972	H -3.962443 -2.393651 1.776639
C 3.419676 0.165142 -2.435612	C -1.650276 -4.858522 1.209952
O 4.652232 0.206294 -2.166894	H -1.864778 -6.367150 -0.328121
C 3.987616 -3.948351 0.207451	C -1.601397 -3.032423 2.854933
C 3.691548 4.338919 -0.270790	H -2.066576 -2.151183 3.289085
C 3.057156 0.387743 -3.919267	C -0.386278 -5.286812 1.694828
C 4.849184 0.225806 4.165697	H 0.081417 -6.155053 1.238037
F 6.144120 0.404284 4.446387	C -0.365359 -3.458753 3.290105
F 4.483399 -1.000677 4.592795	C 0.251249 -4.593948 2.703070
F 4.132285 1.137026 4.840663	H 0.151123 -2.915239 4.074411
F 3.105006 4.887547 0.808747	H 1.236698 -4.900769 3.040686
F 4.871230 4.934006 -0.463496	C -1.788113 5.428982 1.562082
F 2.909316 4.581754 -1.343148	H -2.149991 5.345245 2.583737
F 4.060109 0.018700 -4.727855	C -0.869203 5.634695 -1.086312
F 2.845172 1.714910 -4.089334	H -0.518356 5.712646 -2.111782
F 1.953484 -0.264163 -4.278764	C -0.618407 6.100115 1.281800
F 3.545882 -4.391200 1.397750	C -0.158407 6.210749 -0.056129
F 5.182636 -4.491671 -0.036531	H -0.040380 6.547462 2.085320
F 3.123845 -4.368488 -0.741277	H 0.764870 6.744761 -0.262271

Optimized Cartesian Coordinates of the intermediates and transition states at the B3LYP$_{(Chloroform)}$/Lanl2DZ (Rh), 6-31g (C, H, N, O, F, P) level of theory in the condensed phase**

1

E_0 = -607.6904095
G_{298} = -607.569107
NImag = 0

C	-2.6683619679	0.0076695079	-2.2763176866
C	-1.7614742609	-1.0701836884	-2.6997860477
O	-0.7186149781	-0.9108519132	-3.3110361399
O	-2.2292205961	-2.2813874513	-2.3242780177
N	-3.7410797504	-0.397080007	-1.6274422132
C	-2.5007480041	1.4602139519	-2.4977538086
C	-1.3850537278	1.9666821071	-3.1900330704
C	-3.4621709597	2.370396317	-2.0157537684
C	-1.2454211533	3.3406167531	-3.3883077634
H	-0.6364333545	1.2831513527	-3.5669531741
C	-3.3117180012	3.7396718206	-2.2201040608
H	-4.335707628	2.0149846454	-1.4769902651
C	-2.2019639821	4.2358147254	-2.907970739
H	-0.3757629997	3.7090184476	-3.9257219863
H	-4.0677196227	4.4201238611	-1.8381792195
H	-2.0859839264	5.3039793094	-3.0664743954
N	-4.673671289	-0.7257072045	-1.0654989481
C	-1.4127309258	-3.409060715	-2.6928451184
H	-1.9410993769	-4.2839967806	-2.3137167737
H	-0.4236182566	-3.3370875912	-2.2336336205

2

E_0 = -402.4098925
G_{298} = -402.280622
NImag = 0

N	-2.9728210763	0.0789847412	0.8873289154
C	-4.25437786	0.4083302642	0.5472190781
O	-4.7398632467	1.5189554198	0.7123025629
O	-4.8642705582	-0.6582475858	-0.0190830947
C	-6.2356892824	-0.5668171729	-0.5514074856
H	-2.7059769563	-0.894067461	0.921008486
H	-2.4910720651	0.719076849	1.5006957884
C	-7.2171775474	-0.2412976792	0.5783845803
H	-7.0430140743	0.75847979	0.9780372519
H	-8.2440528265	-0.2936155311	0.2015374932
H	-7.1185099393	-0.9679492476	1.3918264602
C	-6.476473832	-1.9797928092	-1.0870060325
H	-6.3922157782	-2.7187583124	-0.2841417089
H	-7.478834205	-2.0540083152	-1.5193270336
H	-5.7468929481	-2.2301619097	-1.8633105904
C	-6.2894225635	0.4593615913	-1.6868476977
H	-6.1019007857	1.4685722535	-1.3177902195
H	-5.5443105608	0.220685904	-2.4530546528
H	-7.2779102742	0.437540461	-2.1575679407

H -1.3080074989 -3.4724654682 -3.7788404432

(R)-SPA

E_0 = -2068.6291355
G_{298} = -2068.145884
NImag = 0

C	5.5852651031	2.2255550952	-0.1026209121
C	6.8792968387	1.7144898052	-0.077706365
C	7.8739629683	2.3398787307	-0.8481833224
C	7.5931755449	3.5011707935	-1.5619500591
C	6.3044170438	4.0335391442	-1.5185587395
C	5.2684459275	3.4066691186	-0.8044079485
C	9.1650815397	1.5556212591	-0.7832493216
C	8.7027348174	0.1998457527	-0.2079138503
C	7.4809801745	0.5530209056	0.7079368148
C	6.6968148379	-0.698631721	1.0932977966
C	7.2186330484	-1.241821383	2.2791945391
C	8.2439717442	-0.3084347654	2.8833474258
C	7.9919021015	1.0079848452	2.1166648449
C	6.7590499547	-2.4639851718	2.7608726457
C	5.7670104365	-3.1456939664	2.0558663707
C	5.178448754	-2.6087548583	0.8972588214
C	5.6495548862	-1.3566575436	0.4536171847
O	5.0095792415	-0.7203049052	-0.6272200463
P	3.8169625321	0.3029519439	-0.2257526128
O	2.6968038222	-0.2023173573	0.5928107068
O	4.5624184245	1.5222466592	0.5512348949
O	3.4969689146	0.8014598052	-1.7139688228
H	6.0836485295	4.9496974129	-2.057883121
H	8.3635266646	3.9889103325	-2.1530796476
H	7.164018544	-2.8872580255	3.6761167645
H	5.4237639425	-4.1124698803	2.4113292251
H	8.121143047	-0.1978012065	3.9656070053
H	9.2637183737	-0.6797767796	2.7162176066
H	7.1998524518	1.5787165329	2.6134674772
H	8.8751180629	1.6490073723	2.0501847555
H	9.890587574	2.045220371	-0.1201297652
H	9.6457869701	1.4586826832	-1.762096494
H	8.3592563917	-0.4478280553	-1.0217973911
H	9.487449547	-0.3333030056	0.3354417005
H	2.6501249012	1.2764151791	-1.7615705064
C	3.8944437541	3.9784203518	-0.8336004934
C	3.1341584319	4.1215713227	0.3166571973
C	3.3469595548	4.429142912	-2.0730392467
C	1.8408926471	4.706602199	0.2860727625
H	3.5288732384	3.794236692	1.2732624151
C	2.0958469974	4.997669835	-2.1350229929
H	3.9279727316	4.3037561647	-2.9818096087
C	1.3052785787	5.1574673137	-0.9648886242
C	4.1015988511	-3.3607093855	0.1973820225
C	4.1149905068	-3.5406792377	-1.1760609489
C	3.0507134155	-3.9575416095	0.9552600479
C	3.1175613434	-4.3061439247	-1.8348793652
H	4.9086107236	-3.1031928666	-1.7740726999
C	2.0677538102	-4.7007714778	0.3456403122
H	3.0216110469	-3.8012879522	2.0292816631
C	2.067848197	-4.9012375164	-1.0611480461
H	1.2691943335	-5.1398550668	0.9383847569
C	3.1296335863	-4.5067147421	-3.243595416
H	3.9262433502	-4.0543265579	-3.8290059691
C	1.0724111347	-5.6690302218	-1.7241390236
H	0.2773073173	-6.1172969662	-1.133432472
C	1.112133564	-5.8437267106	-3.0902245623
C	2.1513069524	-5.2576968543	-3.8566504883
H	0.3464402692	-6.4335682223	-3.5864854578
H	2.1713055637	-5.4032653573	-4.9331696812
H	1.6941806206	5.328901134	-3.0894360587
C	1.0582243539	4.8630879222	1.464153288
H	1.4649889471	4.5185849666	2.4114765788
C	0.0113948593	5.7450571052	-0.9902686271
H	-0.3910525142	6.0854022698	-1.941142227
C	-0.7208667903	5.8823162888	0.1686170965
C	-0.1921381313	5.4373579022	1.4068931219
H	-1.7085545403	6.3338666311	0.1385020068
H	-0.7807195207	5.5507154716	2.3129624651

$[Rh_2(TFA)_4]$

E_0 = -2323.9273177
G_{298} = -2323.873585
NImag = 0

C	2.031302494	1.6683044141	0.015191174
O	1.6133164313	1.3125552188	-1.1209399858
Rh	0.0126172068	-0.0001205671	-1.1985468543
O	-1.2990637906	1.6017856039	-1.1207251981
C	-1.6510431661	2.0225263763	0.0159433075
O	-1.3007477788	1.6035721722	1.1521689286
Rh	0.012874101	0.0026461823	1.2313219353
O	1.3262264757	-1.5983171588	1.1570092646
C	1.676368863	-2.0200393099	0.0217758636
O	1.324533408	-1.6021605613	-1.1159377262
O	-1.5881586622	-1.3127867741	-1.1176766576
C	-2.0071557668	-1.6641841314	0.0195459682
O	-1.5871506368	-1.312497853	1.155162454
O	1.6145379018	1.3158587251	1.1518985402
C	3.1806619254	2.7006999769	-0.006500476
C	-2.64668473	3.2038772001	-0.0147298742
C	-3.2111532359	-2.6327844128	-0.0038805076
C	2.6718667944	-3.2016063634	-0.0054696899
F	2.9771944613	-3.6159377609	1.2267465433
F	3.8014975383	-2.8218931195	-0.6251424673
F	2.1386512464	-4.227973731	-0.6869907881
F	-3.4401301802	-3.1593374077	1.2023531034
F	-2.9850405583	-3.6277966735	-0.8736054829
F	-4.3095467192	-1.9649805266	-0.3977297777
F	4.0881873407	2.36998623	-0.934962899
F	3.7878778774	2.7812506081	1.1809046256
F	2.6766499909	3.9094265274	-0.31439754
F	-2.9529441691	3.6209458761	1.2163322664
F	-3.7757375763	2.8226170945	-0.6344048974
F	-2.113059086	4.228677145	-0.6982331527

N_2

E_0 = -109.5155669
G_{298} = -109.528408
NImag = 0

N	-3.7201667278	-0.4030282991	-1.6510593136
N	-4.6131522822	-0.7481201709	-1.0994656564

3

E_0 = -2931.6358654
G_{298} = -2931.441078
NImag = 0

Rh	-2.0555914272	0.2770518658	1.3706313192
Rh	-0.4034376278	-0.1250401508	-0.3800206365

	O -1.9545365599 -0.7318694772 -1.6115126405 C -3.118808759 -0.7208306732 -1.1266312238 O -3.493001421 -0.3736306904 0.0262448942 C -4.2343624734 -1.256076922 -2.0514106871 O 1.043026429 0.5034242749 0.9660134865 C 0.6677869055 0.8869391374 2.109069202 O -0.4951217946 0.9132239126 2.5914628465 C 1.7883097129 1.4509901226 3.0107712365 O -0.6826532265 1.8303313626 -0.9915319757 C -1.5124106153 2.5365586365 -0.3536578349 O -2.2348574325 2.215605243 0.627083061 C -1.6701110691 3.9771584459 -0.8889813551 O -1.7373797163 -1.6860000028 1.9831264903 C -0.9118856965 -2.3838592265 1.3365707368 O -0.2135383382 -2.059784163 0.3363938347 C -0.6836498537 -3.8168261435 1.8670712877 F -0.4677292238 4.5135406178 -1.1457760381 F -2.310532762 4.7593084655 -0.0142334293 F -2.3753891761 3.9497362088 -2.0348328305 F -5.4005737218 -0.6490218328 -1.799561612 F -4.3859917913 -2.5762458043 -1.8298421583 F -3.9263527384 -1.0762981398 -3.340811044 F -0.3254416237 -4.6460834964 0.8777833165 F -1.7877823083 -4.2967886103 2.4505640977 F 0.3058005318 -3.7930427546 2.7800394515 F 2.9636550526 0.8605087912 2.7461569588 F 1.9163437779 2.7698342957 2.7727070904 F 1.5048772546 1.2780375005 4.305688541 C 3.2807195672 0.2015159645 -1.5446069178 C 2.3031204902 -0.7916930882 -1.9364501757 N 2.7661887283 1.3991681163 -1.3152710977 N 2.3463211852 2.4332620234 -1.1213696069 O 1.0785810743 -0.5761463932 -2.0282500032 O 2.8391074014 -1.9734484402 -2.2213977233 C 1.9260064663 -3.0365640725 -2.589787652 H 2.5642186121 -3.895935841 -2.7919611342 H 1.2437427938 -3.2511255083 -1.7652068269 H 1.3615150569 -2.759493903 -3.4823825703 C 4.7415361581 0.0295832945 -1.3341666439 C 5.5285108786 -0.6540620302 -2.275085971 C 5.3508097931 0.5703362724 -0.1901726057 C 6.8988187467 -0.8010879979 -2.0639528345 H 5.0677798745 -1.0697707919 -3.1641231461 C 6.7248903212 0.4339177906 0.0052348987 H 4.7460301963 1.0786981078 0.555706198 C 7.5022540492 -0.2541991112 -0.9286617399 H 7.4976405215 -1.3359881624 -2.7955835338 H 7.1843593509 0.8557623261 0.8943597673 H 8.5711284261 -0.3662993491 -0.7717550664
(3-4)‡ E_0 = -2931.6205654 G_{298} = -2931.420767 NImag = 1 (-43.9052 cm^{-1}) C -2.1540183076 -2.2622912521 -0.3318530251 O -1.3053533247 -1.9358335455 0.5425683874 Rh -0.3807457216 -0.0997609929 0.3382673375 O -1.9078751665 0.8072281314 1.3969993577 C -2.9128464634 1.2124113856 0.7503913998 O -3.12870444 1.1457194688 -0.4910431705 Rh -1.6798045116 0.2533296081 -1.6736843961 O -0.1469971712 -0.6567126943 -2.7381212469 C 0.85611246 -1.0559641473 -2.0849590412 O 1.0669035322 -0.9868197517 -0.8418356189 O 0.4844126197 1.7497383404 0.0079880244 C 0.1088903005 2.4097732429 -0.999998197 O -0.7394685486 2.0913110913 -1.8781655588 O -2.5372106726 -1.6062150939 -1.338516288 C 2.4540044346 -0.016998969 2.4401371088 C 1.6101472098 -1.1848130379 2.7361293927 O 0.5192195146 -1.099702201 3.2925931761 O 2.1579053837 -2.3391055205 2.3296853771 N 1.8698942653 1.112817214 2.796921929 C -2.8365342324 -3.6299999021 -0.1076893265 C -4.0089474851 1.8743946816 1.6152127412 C 0.7490994552 3.8091913448 -1.135679264 C 1.9933288646 -1.7231952347 -2.890371366 F 1.7070725192 -1.7799382975 -4.1941173589 F 2.1928004518 -2.9719757925 -2.4381254071 F 3.128758885 -1.0258865506 -2.7283386233 F 0.6206478276 4.2875432285 -2.3763411505 F 2.0537710447 3.7629742192 -0.8256443149	**4** E_0 = -2931.6236631 G_{298} = -2931.426942 NImag = 0 C -1.5732853895 -2.1559083074 -0.8769742983 O -0.8602682214 -1.8942173545 0.1314064945 Rh -0.0281847574 -0.0035974351 0.2958179812 O -1.7390319299 0.6820263846 1.2367278071 C -2.6838501449 1.1039943656 0.510089442 O -2.7472467678 1.1711834916 -0.7441636866 Rh -1.1103961338 0.514784032 -1.8497167235 O 0.6069393528 -0.1787081168 -2.7899809628 C 1.5492959543 -0.5857438172 -2.0602578019 O 1.6123173058 -0.64657922 -0.800990839 O 0.6865741786 1.9430750201 0.3076452628 C 0.4052269882 2.6842975141 -0.6760633437 O -0.267406993 2.4117777944 -1.7035724987 O -1.88000222 -1.4143247251 -1.8461955559 C 1.0795859244 -0.4752142034 2.429157278 C 0.2804701729 -1.6844006476 2.8508368696 O -0.7170205449 -1.6002939553 3.5409333105 O 0.7711320333 -2.8130694622 2.3421991424 N 0.564538328 0.6059976449 3.0845169162 C -2.1185032531 -3.6011071848 -0.8941890682 C -3.9063999115 1.6245803935 1.2983792774 C 0.9199294911 4.1373340742 -0.5682532115 C 2.8182590723 -1.092734571 -2.7815098849 F 3.8920864265 -0.4118948134 -2.3484309458 F 2.726488324 -0.9464045011 -4.1068944214 F 3.0044537265 -2.3956460001 -2.5068419822 F 1.1119832296 4.6742441369 -1.7777215271 F 2.073078937 4.189834368 0.1135366231

F 0.1404596284 4.6521240782 -0.2831248387 F -1.9570482781 -4.5208505096 0.3722153555 F -3.3533531994 -4.1061767636 -1.2448697798 F -3.8291068204 -3.4853440566 0.7875111703 F -5.0425824141 2.2807636927 0.8726754716 F -3.4968370763 2.9357795768 2.2586667814 F -4.4532998489 0.997224434 2.5291157768 C 3.8041794582 0.0692168119 1.8365087687 C 4.7552476381 -0.9466015405 2.03742116 C 4.166999067 1.1989084959 1.0805031907 C 6.0302679426 -0.8336774104 1.4846711426 H 4.4954123842 -1.8199565637 2.622813002 C 5.4494011115 1.3104063542 0.5458702028 H 3.4415074463 1.9860515529 0.8959715509 C 6.3870609421 0.2943870241 0.7425817382 H 6.7517819262 -1.6294591062 1.6470675181 H 5.7106589557 2.1912290133 -0.0337260798 H 7.3840869028 0.3797087493 0.3205483576 N 1.372430988 2.0859907437 3.105243612 C 1.3680016597 -3.5270497633 2.5612268908 H 1.9905852152 -4.3545153704 2.2213577166 H 0.4413666579 -3.487306482 1.9845382938 H 1.1365543602 -3.6342644239 3.6232208998	F 0.0066259793 4.8774047973 0.0884140223 F -1.0906470701 -4.4683213964 -0.9127517378 F -2.8923918651 -3.8312075321 -1.9570372639 F -2.8382399961 -3.8301371694 0.2199519781 F -4.9335393714 1.900139004 0.4893382529 F -3.5664194759 2.7475780965 1.9565297235 F -4.3002044736 0.7103308915 2.1981340464 C 2.5687389913 -0.3849561968 2.2323791814 C 3.3912277015 -1.5218420794 2.2851303632 C 3.1599964582 0.8710816267 2.0013683607 C 4.7693224318 -1.3975653048 2.1041737268 H 2.9628495788 -2.498436932 2.4614754382 C 4.5376920615 0.9842799477 1.832329144 H 2.5480135192 1.7635066546 1.9297626684 C 5.3509862856 -0.1497689359 1.880302732 H 5.3886036102 -2.2888873831 2.1463162094 H 4.9724741852 1.9637954445 1.656034591 H 6.424669311 -0.0607073215 1.744319184 N 0.1182671804 1.5222964774 3.5529852672 C 0.0013903143 -4.0096336562 2.6104940313 H 0.5300224478 -4.809273729 2.0931271393 H -1.0107026037 -3.9019353505 2.2191735859 H -0.0307013781 -4.2052998582 3.6845187023
(4-5)‡ E_0 = -2931.6099342 G_{298} = -2931.414928 NImag = 1 (-389.4004 cm^{-1}) C 2.4677569662 1.3510708098 -0.8511238245 O 1.550911741 0.693840874 -1.4226234346 Rh -0.0068043557 -0.0357133019 -0.2604367381 O 1.0948785801 -1.7517621734 0.139130049 C 1.9098810523 -1.7436017984 1.1055860398 O 2.1751363523 -0.8232918582 1.9176362721 Rh 1.1466579091 0.9761604424 1.7021143705 O 0.0223934543 2.6969340279 1.3440871184 C -0.749363566 2.7033525723 0.3551431204 O -0.9678216057 1.793245336 -0.4994284235 O -1.4727676066 -0.6765339816 1.0643917633 C -1.3283361503 -0.4118568255 2.2919909101 O -0.4035754388 0.2128308837 2.8701041519 O 2.5987455969 1.6412851589 0.3641969381 C -1.0160365225 -0.9962795278 -1.9463413173 C -0.168882979 -2.1699496145 -2.3773835923 O 0.7410429738 -2.1240810501 -3.1810673371 O -0.5237940884 -3.2451112512 -1.6691064368 C 0.3416414154 -4.3990438917 -1.7872058938 H -0.0480715643 -5.1234379322 -1.0731470234 H 0.296568854 -4.8018010206 -2.8017903821 H 1.3686167676 -4.1289437845 -1.5395841694 N -0.5500612751 0.1269597433 -3.2300292732 N -0.3696097422 1.0917827773 -3.7434522915 C -2.4844339246 -1.0925317339 -2.0630694238 C -3.3194632369 -0.1466990299 -1.4325368234 C -3.0807566625 -2.1272454156 -2.8196286354 C -4.7034759537 -0.2460382943 -1.5409823718 H -2.881840503 0.6683586187 -0.8712432214 C -4.4639505136 -2.2276649313 -2.9134890791 H -2.4609197464 -2.8575634257 -3.3282831236 C -5.2779462013 -1.2875975606 -2.2740250648 H -5.3351471513 0.4877952867 -1.0499502692 H -4.9081755631 -3.0334360186 -3.4896959274 H -6.3586047604 -1.3655068545 -2.3510162415 C 3.6069455158 1.8183349954 -1.7852432536 C -2.4919263718 -0.8840765342 3.1931288768 C 2.6611539437 -3.0814383214 1.2901595684 C -1.5646937252 3.9919631475 0.1055804344 F -3.0178081217 -2.0316272665 2.7445528381 F -3.4587128382 0.0554634317 3.1853432086 F -2.0886438042 -1.0638340617 4.4562469137 F 1.777750741 -4.0663803396 1.5353350262 F 3.5336820098 -3.029204549 2.2993465701 F 3.328739527 -3.3917135577 0.162768446 F 3.1497129186 2.056583267 -3.0221423657 F 4.5421156244 0.8523788123 -1.8561467067 F 4.1847565296 2.9332832451 -1.321363552 F -1.195582934 4.5424984704 -1.0647579836 F -2.875135537 3.694878077 0.0348005704 F -1.3834210295 4.8910389286 1.0758529945	
(5-6)‡ E_0 = -3224.536274	**6** E_0 = -3224.5639674

G_{298} = -3224.194646
NImag = 1 (-76.1423 cm^{-1})

C	-1.2220838638	0.3819642938	-1.2207326816
C	-1.5831618239	-0.8550108703	-1.9896844658
O	-2.1553380106	-1.8285032324	-1.5431841043
Rh	0.4800603862	0.0319952737	-0.0844836251
O	1.4949545495	1.583284329	-1.0184004775
C	2.7088381543	1.7785177068	-0.7136477713
O	3.4342719287	1.1672589668	0.1067556751
Rh	2.5975020454	-0.4097951508	1.1876230704
O	1.5828408507	-1.9550648305	2.1573473395
C	0.3881632298	-2.1633306502	1.8327485486
O	-0.3310692777	-1.5627908461	0.9814718518
O	1.2027811455	-1.2937744347	-1.5037219893
C	2.3113646101	-1.8688592744	-1.2979185188
O	3.1136618274	-1.7392893817	-0.342807576
O	-0.0700763923	1.282053299	1.4892932639
C	0.7545023789	1.4535869042	2.439461195
O	1.889461069	0.951884155	2.6069849848
O	-1.0703502338	-0.7695160988	-3.2285480212
C	-1.0583946633	-1.9952525554	-3.9974010099
H	-0.5162414934	-1.7557527525	-4.9115807692
H	-2.0788259374	-2.3080679276	-4.2306713235
H	-0.5451871405	-2.7836624791	-3.4443179784
N	-2.8224446916	-0.069890535	0.712386108
C	-4.1196660836	0.3163232677	0.4483602513
O	-4.521442592	1.4568904592	0.6246381713
O	-4.8140192834	-0.7174111508	-0.0568004494
C	-6.2352281182	-0.5860330313	-0.4419826948
H	-2.5986292453	-1.0571607915	0.7324044493
H	-2.3121808524	0.5277145918	1.3505495939
C	-0.3155163393	-3.3502290589	2.5298569337
C	0.2473297895	2.4369385129	3.5171980702
C	3.3521273637	2.9621790648	-1.4711395551
C	2.6807873815	-2.8858059527	-2.4013870015
C	-1.7683561187	1.6454438317	-1.5993747863
C	-2.7252251924	1.7496981333	-2.6515354621
C	-1.3567142529	2.8415742936	-0.9469115795
C	-3.2105278701	2.985535949	-3.0481192717
H	-3.0637319417	0.8556204407	-3.1621692177
C	-1.8564559987	4.071782799	-1.3445172529
H	-0.6573613471	2.7843674226	-0.1242477665
C	-2.775956654	4.1472782232	-2.3974362767
H	-3.9288477201	3.0517566763	-3.8589741838
H	-1.5336903082	4.9760799313	-0.8386825767
H	-3.160125454	5.1143141437	-2.7090748267
C	-7.0714540619	-0.1988602838	0.7801299296
H	-6.8225436393	0.8041432747	1.1290637841
H	-8.1341191099	-0.2233614086	0.5180855364
H	-6.9074933176	-0.9083970217	1.5976510684
C	-6.578828161	-1.9994997144	-0.9147969998
H	-6.4455337369	-2.7239720705	-0.1056336137
H	-7.6204824121	-2.0409117719	-1.247155769
H	-5.9367300715	-2.2958376848	-1.7498345561
C	-6.3753235881	0.4199618813	-1.5868166532
H	-6.0965952424	1.4253594813	-1.2685889337
H	-5.7456975295	0.1264120222	-2.4330307998
H	-7.4144254359	0.438359501	-1.9314361533
F	-1.6214439625	-3.0942675924	2.7062753949
F	-0.2003630699	-4.4488904076	1.7607384189
F	0.2316014278	-3.6087478528	3.7229575712
F	1.1059283911	2.5481909194	4.5332348627
F	-0.9359332371	2.0154197455	3.9980057936
F	0.0696510523	3.6535052565	2.9691473737
F	1.7993417042	-3.9054189519	-2.3817653267
F	3.9083636871	-3.3830868349	-2.2314508129
F	2.6147931018	-2.3035234327	-3.6110507299
F	2.7326515827	4.1070267111	-1.1270080475
F	3.215293715	2.7924271804	-2.7968509628
F	4.6526285639	3.0835770104	-1.1894735681

G_{298} = -3224.218753
NImag = 0

C	3.1766398054	-0.1132146242	-1.1792579781
O	1.9820555204	0.0994584913	-1.5297580342
Rh	0.5049694663	0.0187693089	-0.0763372204
O	0.3270290703	-2.0352883592	-0.3471937005
C	1.101199447	-2.7920968201	0.3099953478
O	1.9919031839	-2.4919863328	1.1413513437
Rh	2.323164877	-0.4723296907	1.568596529
O	2.487632174	1.5860383158	1.8491544701
C	1.7270213375	2.3334235465	1.1823168676
O	0.8351427273	2.0315320046	0.3397810563
O	-0.8369585731	-0.1685140585	1.5132791886
C	-0.3698442416	-0.3981127416	2.6724349561
O	0.8203640108	-0.5490552093	3.0273673744
O	3.6491600816	-0.3538539414	-0.038350064
C	-1.2411213994	0.3958491501	-1.4404271008
C	-0.7627680343	-0.1593743438	-2.7447052449
O	-0.9370127065	-1.3406584431	-3.0398296488
O	-0.0650830927	0.6875880901	-3.4993066295
N	-2.2274664017	-0.6430955919	-0.9406430576
H	-2.1989379045	-0.7409250078	0.0821035147
C	-3.6579837092	-0.4917277147	-1.4070096911
O	-3.8952085612	-0.1845737436	-2.5415090679
O	-4.4311477496	-0.7801164158	-0.3920190978
C	-5.9434326994	-0.7971464067	-0.5244977767
C	4.2084199024	-0.1259354808	-2.3299438149
C	0.9340595595	-4.2953613693	-0.0049973749
C	-1.4555005127	-0.525046613	3.763005958
C	1.8729697666	3.8542533753	1.4156528234
F	0.7381905037	4.3436745182	1.9491790455
F	2.8839239529	4.1357288235	2.2455598632
F	2.0933949683	4.4830978314	0.2485076931
F	-2.3140546167	0.5073383419	3.6885768728
F	-2.1528083099	-1.6618997	3.5652396894
F	-0.9303299103	-0.5563754711	4.9892533381
F	3.7377280971	0.485361217	-3.4260029095
F	5.3457220231	0.4797320289	-1.9602381802
F	4.4953553473	-1.4027162971	-2.6514194492
F	1.4584228558	-5.0615838325	0.9576812721
F	-0.3652966939	-4.6113691669	-0.139409061
F	1.5576552363	-4.5796235959	-1.1635054046
C	-1.7586278499	1.7905680629	-1.2653029933
C	-1.5562969312	2.8125977187	-2.2118866261
C	-2.4643193539	2.1210100317	-0.0879142243
C	-2.0489662268	4.098930131	-1.9931312673
H	-1.0156950901	2.6036376383	-3.1239488723
C	-2.962318468	3.4061046352	0.1201990436
H	-2.6033716302	1.3871541646	0.6984369349
C	-2.7600105565	4.4055997137	-0.8325849498
H	-1.8793281044	4.8636596125	-2.7460345902
H	-3.5009685152	3.6250834826	1.0379700807
H	-3.1449908066	5.4080796628	-0.6701966582
H	-1.8732889104	-1.5213919501	-1.3759583707
C	-6.3225287584	-1.8898939582	-1.5193454442
H	-7.4120431444	-1.9912308216	-1.532478379
H	-5.9914874418	-1.6507545018	-2.5318214075
H	-5.8978437542	-2.8529381632	-1.2201319957
C	-6.4151873773	0.5922169804	-0.9414436658
H	-7.508789807	0.614545954	-0.9069241396
H	-6.0374690373	1.3536363619	-0.2531460581
H	-6.0996538264	0.8417952369	-1.9556588564
C	-6.3789578714	-1.1424892744	0.8950493742
H	-5.9799282623	-2.1129413601	1.2041827224
H	-6.0431099017	-0.3814346747	1.6053503499
H	-7.4708114356	-1.1914144839	0.934757187
C	0.5547963137	0.1278761182	-4.6780113669
H	-0.201988251	-0.2944932794	-5.3426460635
H	1.0602650427	0.9637658635	-5.1601585005
H	1.2740661576	-0.643063973	-4.3977409605

(6-7)‡

E_0 = -3224.5558096
G_{298} = -3224.213937
NImag = 1 (-1193.2574 cm^{-1})

C	-1.2864583922	0.4705532978	-1.4773797917
C	-0.7617577564	-0.0998441938	-2.7324213454
O	-1.1411124961	-1.2750808703	-3.0146521251
Rh	0.4624208103	-0.0113526058	-0.0548980421
O	1.7431783046	1.4121213459	-0.8536041759
C	2.8943339377	1.5287645097	-0.3473158566
O	3.4125749131	0.9128097619	0.6197217514

(7-8)‡

E_0 = -3224.5297461
G_{298} = -3224.184623
NImag = 1 (-134.6220 cm^{-1})

C	3.603990165	-0.4375036924	-0.9790502399
O	2.4860465797	-0.1521511016	-1.4887264169
Rh	0.8424297622	-0.1127821502	-0.2333583106
O	0.5453153809	-2.1419302585	-0.5391287288
C	1.1644990307	-2.9521195304	0.2048397992
O	1.9610468902	-2.7043901513	1.1510205174
Rh	2.3277866033	-0.7108759897	1.5922985889

Rh 2.281354143 -0.5618161947 1.5646331692	O 2.6224002394 1.3103052385 1.9207019749
O 0.9741848207 -1.9907742562 2.3735627908	C 2.0239886686 2.1210771544 1.1575160761
C -0.1644261516 -2.1115848368 1.8649921506	O 1.2437872613 1.8725443664 0.1992558809
O -0.6707011649 -1.4861689675 0.8850959984	O -0.7191009727 -0.1410049345 1.1369588429
O 1.3090200338 -1.4350565433 -1.3180350644	C -0.4553802643 -0.4210157393 2.3409779889
C 2.3306462601 -2.063190588 -0.9156238552	O 0.6639471805 -0.6786039392 2.8545168713
O 2.9602890054 -1.9557058549 0.1657901288	O 3.8732283981 -0.7119117887 0.2220628738
O -0.217024921 1.3441389299 1.3722027229	C -2.1306496046 1.3071252269 -1.603106355
C 0.4299905189 1.4687179512 2.4498493851	C -1.1036568999 1.1008361435 -2.5503405254
O 1.466979811 0.8709133879 2.8350916965	O -0.7094822481 -0.0646995624 -2.8640848496
O 0.0987739833 0.5536109353 -3.4631799875	O -0.5497121266 2.1978712407 -3.1127912124
C 0.6746067901 -0.1377860964 -4.6062549848	N -2.6048376183 -0.0151415434 -1.1623848556
H 1.3424861618 0.5898551955 -5.0640666902	H -2.4559764692 -0.2060086663 -0.1610700703
H -0.1135615674 -0.4300793079 -5.3019143375	C -4.0027616689 -0.4245482806 -1.5462594081
H 1.2303151551 -1.0104869407 -4.2627960677	O -4.4929217139 -0.0621439299 -2.5787114273
N -2.3432842858 -0.5277870405 -1.1164727058	O -4.4498670002 -1.2103135064 -0.5924216649
C -3.7296669326 -0.2475481088 -1.454902893	C -5.8008429257 -1.879974498 -0.6820806048
O -4.0353558937 0.2756780076 -2.498925299	C 4.780332744 -0.4596529141 -1.979811867
O -4.4923423822 -0.7135979049 -0.4798811895	C 0.8759663953 -4.4408855823 -0.0920837907
C -5.9905708068 -0.726408618 -0.5775712253	C -1.6617750022 -0.410774931 3.3062318488
H -1.9145769194 -1.310157889 -2.0265054543	C 2.3211059169 3.6099984452 1.445238321
H -2.2504167323 -0.9241771889 -0.1786187434	F 2.1000694771 3.8790629975 2.7412069854
C 2.8352804181 -3.1322871383 -1.9109938937	F 3.6138437911 3.8644932634 1.1745437431
C -0.1595907173 2.5252028164 3.4109905879	F 1.5615475778 4.4166084015 0.7016690475
C 3.8082184433 2.5433496815 -1.0708679076	F -1.732030211 0.7815811454 3.9189294913
C -1.0702157845 -3.204779987 2.474343744	F -2.8077555987 -0.6151895871 2.6371346957
C -6.3911937514 -1.3571428225 0.7540080491	F -1.5335381068 -1.3639411349 4.2358968252
H -5.9769924337 -2.3651053952 0.8512730957	F 4.5777699727 -1.429905063 -2.8861916546
H -7.4811293853 -1.4258148421 0.8145487963	F 4.8495963096 0.7160347921 -2.624147489
H -6.037311416 -0.7527460162 1.5945127789	F 5.9457571287 -0.6817550883 -1.3660451866
C -6.500385435 0.7086442363 -0.6944167175	F 1.6420999557 -5.2484599891 0.6456063982
H -6.1930072347 1.1703894374 -1.6337646131	F -0.4150726509 -4.7054144622 0.1815704117
H -6.1367529037 1.3191312645 0.1377450435	F 1.0946478093 -4.7021785039 -1.3890147889
H -7.5941978847 0.7008908356 -0.6552519665	C -2.718013858 2.4871052951 -1.0084192073
C -6.3993911656 -1.6029776589 -1.7596630311	C -2.3824339239 3.8014054104 -1.4259278628
H -7.4886548555 -1.7087584894 -1.7661600394	C -3.6676132951 2.3769099313 0.0394483946
H -5.9631239543 -2.602751114 -1.6693351204	C -2.9628708423 4.9166174048 -0.8312246822
H -6.0930602469 -1.165176857 -2.7114786896	H -1.6632126946 3.9342859971 -2.223199224
F -0.8266876482 -4.3760425379 1.8560793565	C -4.2444607815 3.5031751534 0.6255221026
F -2.3673377341 -2.9042476163 2.3080725809	H -3.9603891979 1.4029037567 0.4212847114
F -0.8320583016 -3.3578116654 3.7817094994	C -3.9014433798 4.7859887362 0.1983418056
F 1.9247616791 -4.1179911735 -2.0109027715	H -2.6776699715 5.905785974 -1.1814745367
F 3.9972483358 -3.6651643984 -1.523653179	H -4.9674004362 3.3691703177 1.4264816408
F 3.0022622849 -2.592569758 -3.1339887453	H -4.3513422153 5.6626000459 0.6549911377
F 4.8068184418 2.9570977801 -0.2825728694	H -1.9383057638 -0.6265914439 -1.7170584872
F 4.3445235518 1.9507695476 -2.1580653251	C -5.8094489311 -2.7996583712 -1.900244576
F 3.1142878398 3.6149852507 -1.4792847042	H -6.7418512561 -3.3725986539 -1.9045141779
F -0.0686271886 3.7467434327 2.8565589038	H -5.7522255801 -2.2365114764 -2.8335950548
F -1.4594639623 2.2639186211 3.6406187897	H -4.9772493801 -3.5092101003 -1.8579849565
F 0.4808111307 2.5432826008 4.5849436537	C -6.8815867008 -0.8033241735 -0.7346477391
C -1.6282038103 1.9104364987 -1.3057876931	H -7.8626364116 -1.2855560579 -0.6834747257
C -1.0479198441 2.9259709829 -2.0903693362	H -6.7947794875 -0.1220051421 0.1170672191
C -2.5330125636 2.2951122893 -0.2962667689	H -6.8329148606 -0.2249560471 -1.6588180619
C -1.3765690906 4.2645393335 -1.8788520592	C -5.8482577383 -2.6681974757 0.6227297442
H -0.3394629398 2.6749504063 -2.8679273362	H -5.0460158221 -3.411158032 0.6602679577
C -2.8623252428 3.6334163089 -0.0941647801	H -5.7505915665 -2.0027738412 1.4854604429
H -2.9749552059 1.5464857721 0.3531151527	H -6.8053943178 -3.1921325853 0.6969911185
C -2.2867977187 4.6291125077 -0.8854759401	C 0.5116463523 1.964647617 -4.0537465277
H -0.9173893224 5.0261401463 -2.5030762582	H 0.1517149205 1.4022919517 -4.9194075443
H -3.5652832961 3.8964241881 0.6913092777	H 0.8417356929 2.9563365481 -4.3666336886
H -2.5413723339 5.6731382152 -0.727827524	H 1.340582291 1.4244853637 -3.5897579581

Optimized Cartesian Coordinates of the intermediates and transition states at the B3LYP $_{(Chloroform)}$/DGDZVP (Rh), 6-31g (C, H, N, O, F, P) level of theory in the condensed phase**

[$Rh_2(TFA)_4$]	**3**
E_0 = -11480.2213993	E_0 = -12087.9296903
G_{298} = -11480.168189	G_{298} = -12087.736329
NImag = 0	NImag = 0
C 2.0397514439 1.6760908681 0.0145688767	Rh -2.0681970561 0.2713741477 1.3651643678
O 1.622652607 1.3202326058 -1.1213424525	Rh -0.4257884947 -0.1567554865 -0.3942831796
Rh 0.0134415926 -0.0009897725 -1.2018090217	O -1.9992636509 -0.7597223158 -1.6203933462
O -1.3065010022 1.6098508568 -1.1213823169	C -3.1613478602 -0.7319201387 -1.1314036227
C -1.6579627671 2.0304573219 0.0149799557	O -3.5283064095 -0.372995555 0.0196758838
O -1.3079848756 1.6118347819 1.1509487692	C -4.2819521544 -1.2627346878 -2.0531735171
Rh 0.0132929189 0.0021052487 1.2327845414	O 1.0445270329 0.4721785343 0.9447862462
O 1.3344808194 -1.6078369447 1.1562661761	C 0.6792890659 0.8647269524 2.0874823476
C 1.6846387527 -2.0293618354 0.021457036	O -0.4790502803 0.8952508735 2.5791712985
O 1.3336437369 -1.6118424757 -1.1161377615	C 1.8044168098 1.439660159 2.9765580176
O -1.5960556263 -1.322049167 -1.1181848844	O -0.6844566494 1.8099924762 -1.0150002322
C -2.0153477042 -1.672262628 0.0187783126	C -1.4810438429 2.5379701484 -0.3592921729

O -1.5958795788 -1.3205398315 1.1540999356 O 1.6234259129 1.3235885004 1.1509330157 C 3.1880584818 2.7099972811 -0.0061705167 C -2.6531806684 3.2125065265 -0.0147486056 C -3.2209629613 -2.6392920012 -0.0036970478 C 2.6796338511 -3.2117013364 -0.0045457954 F 2.9833385765 -3.6256680646 1.228337263 F 3.8101317403 -2.8334060235 -0.6234452427 F 2.1466180415 -4.2380114341 -0.6863667578 F -3.4484374846 -3.1664649584 1.2027062765 F -2.9982698175 -3.6337418976 -0.8749604198 F -4.3192111146 -1.9697929914 -0.3949983808 F 4.094447856 2.3830039154 -0.9371614103 F 3.7969481615 2.7874428815 1.1807564737 F 2.6829014196 3.9192253996 -0.3097444948 F -2.9571791428 3.6300321515 1.2168659988 F -3.7834174801 2.8320868217 -0.6327476704 F -2.120267689 4.2368192013 -0.6995598516	O -2.2107919213 2.2304836488 0.619210963 C -1.5298338855 4.0043818623 -0.8424461341 O -1.7684081167 -1.7090824587 1.973689095 C -0.9463839892 -2.4153651254 1.332520504 O -0.245370499 -2.1017406507 0.3316861945 C -0.7269186503 -3.8446493636 1.8772490335 F -0.3056697341 4.5504121481 -0.7307402816 F -2.3902428588 4.7345755266 -0.1266911524 F -1.8960230354 4.0505945062 -2.1336355181 F -5.4566442845 -0.6890510217 -1.7659364949 F -4.4024496885 -2.5918280256 -1.870057933 F -3.9970687367 -1.0375925518 -3.3413212842 F -0.3082827844 -4.6721894165 0.9107442557 F -1.853864657 -4.3359654683 2.4062677277 F 0.21359796 -3.8066819348 2.8400417285 F 2.9875431782 0.8778106158 2.6848476736 F 1.9009086088 2.7636314483 2.7540529512 F 1.5463772233 1.2440471212 4.2738800815 C 3.2556683565 0.2058417761 -1.5721155679 C 2.294661934 -0.8133121757 -1.9359548554 N 2.7228704197 1.3974298371 -1.3504895379 N 2.2878119486 2.4260698377 -1.1619884171 O 1.0646569351 -0.6267716556 -2.0212337305 O 2.8530439521 -1.9885411706 -2.204499493 C 1.9585104198 -3.0842020912 -2.5201081326 H 2.6134369766 -3.9345912355 -2.7065815281 H 1.2966396876 -3.287278212 -1.6759075015 H 1.3709719285 -2.8504202138 -3.4101042355 C 4.7192341799 0.0578089859 -1.3599976292 C 5.5188432338 -0.6114272979 -2.300373576 C 5.316809445 0.6051179026 -0.21309269 C 6.8908546665 -0.7373769062 -2.0861725562 H 5.0667773428 -1.0326020963 -3.1913948517 C 6.6923999171 0.4903166729 -0.0146316576 H 4.7009822231 1.0989129488 0.5333303962 C 7.4827572433 -0.1831727066 -0.9483262006 H 7.4999220502 -1.26141724 -2.8171941163 H 7.1429106687 0.9168439594 0.8768539842 H 8.5528758318 -0.2787648867 -0.7889816039
(3-4)‡ E_0 = -12087.9130263 G_{298} = -12087.713449 NImag = 1 (-41.0096 cm^{-1}) C -2.1655108528 -2.2737413801 -0.326749478 O -1.3189981785 -1.9475239435 0.5495599449 Rh -0.3883087708 -0.1019768631 0.3465614688 O -1.9284542034 0.8153291611 1.4072504521 C -2.9281793884 1.224015087 0.7558726032 O -3.1392786647 1.1584363046 -0.4861956537 Rh -1.6824866951 0.2541181259 -1.6712785715 O -0.1418542307 -0.6647112211 -2.7389111278 C 0.8584976299 -1.0667671006 -2.0835035128 O 1.0674653723 -0.9995941839 -0.840490457 O 0.4903618082 1.7561853098 0.0146444912 C 0.1180128544 2.415682695 -0.9943905487 O -0.7300429417 2.0993651858 -1.8731962983 O -2.5496463118 -1.6166366495 -1.3318395524 C 2.4595533415 -0.0193106319 2.438179456 C 1.6177743904 -1.1883673896 2.73510076 O 0.5305518306 -1.1043741089 3.2985101397 O 2.1621068563 -2.3407817623 2.3192366995 N 1.8744350118 1.1091416747 2.7977329483 C -2.8436108992 -3.6446192826 -0.106698875 C -4.0276270702 1.8906417033 1.6135932004 C 0.7616004029 3.8136998418 -1.1313702157 C 1.9950407847 -1.7360235886 -2.88901406 F 1.7098975243 -1.7879642677 -4.1933977677 F 2.1900596212 -2.9865978793 -2.4402217473 F 3.1327736761 -1.0434127697 -2.7237323873 F 0.6418858529 4.287035004 -2.3749603414 F 2.0645860306 3.7667438161 -0.8127887285 F 0.1495743707 4.661367041 -0.286445733 F -1.9624721213 -4.53163576 0.3781872315 F -3.3514034167 -4.122491165 -1.247422121 F -3.8420792629 -3.5060036748 0.7824573431 F -5.0547217829 2.3004059736 0.8634705708 F -3.5164534352 2.9503968344 2.260320462 F -4.4816086068 1.0158986509 2.5250845695 C 3.8085727251 0.0704192312 1.8330305889 C 4.7609708116 -0.9450028536 2.0294788341 C 4.1698492183 1.2040143939 1.0822639109	**4** E_0 = -12087.9164815 G_{298} = -12087.720529 NImag = 0 C -1.5918027926 -2.1721044564 -0.8767547645 O -0.8792292145 -1.9089085752 0.131145954 Rh -0.0332897252 -0.0112669962 0.2866141784 O -1.7475720094 0.6934386413 1.2379491874 C -2.6943274476 1.1133551991 0.5133983922 O -2.7632185805 1.1736138467 -0.7406559329 Rh -1.1217261497 0.5098473996 -1.8583492616 O 0.6040843857 -0.1892158759 -2.8069150227 C 1.546605992 -0.6006296272 -2.0802127606 O 1.6098937334 -0.6701369334 -0.8219783335 O 0.7008730123 1.9400953578 0.2966846799 C 0.4132036758 2.685823096 -0.6813796154 O -0.2685424939 2.419620061 -1.7041838795 O -1.8964567747 -1.4331760515 -1.8483015738 C 1.0911154051 -0.4773881905 2.4437157529 C 0.290518996 -1.6879465561 2.8566702771 O -0.7120375094 -1.6059966851 3.5394901465 O 0.7854591635 -2.8158042375 2.3487680687 N 0.5629478945 0.604479213 3.0824424687 C -2.1381311153 -3.617246741 -0.892098128 C -3.9133849406 1.6408367211 1.303286487 C 0.9297636608 4.1382947734 -0.5731559062 C 2.8162100979 -1.0998597838 -2.8066667482 F 3.888969718 -0.4196109128 -2.3702113606 F 2.7216714733 -0.9438263689 -4.1309615922 F 3.0069298755 -2.4040601165 -2.542141594 F 1.155158598 4.6618948154 -1.783289364 F 2.0645558544 4.1954027959 0.1383154134 F 0.0012961748 4.8877311646 0.0503321786 F -1.1110435426 -4.4851635787 -0.9231419996 F -2.922923574 -3.8439143506 -1.9478740572 F -2.8462095309 -3.8497779765 0.2286544927 F -4.9362221368 1.9312187225 0.493576424 F -3.5645662243 2.7558859984 1.9697706504 F -4.3175810227 0.724377635 2.1961662417 C 2.5777466142 -0.3797627709 2.2453862095 C 3.4020048022 -1.5164547697 2.2781470658 C 3.1679269821 0.8809804025 2.0361123531

C 6.0363743714 -0.8271530981 1.4787209847 H 4.5019138537 -1.8218785179 2.6099454228 C 5.4523869618 1.3200998474 0.5491999438 H 3.4425719716 1.9899019888 0.8996950153 C 6.3919148825 0.3051115395 0.7424581467 H 6.7590961361 -1.6224757309 1.6380093721 H 5.7124640725 2.2037908079 -0.0265559603 H 7.3893317282 0.3944000155 0.3221660848 N 1.377624609 2.0824247527 3.1066228003 C 1.3722684148 -3.529096242 2.5494599402 H 2.0033439666 -4.3579166816 2.228788878 H 0.4557577283 -3.4985429735 1.9559458005 H 1.1223553925 -3.6262177561 3.6080338535	C 4.7804966132 -1.3870542832 2.1048630977 H 2.9738409883 -2.4964943781 2.4342045764 C 4.545890724 0.9986260399 1.8733857574 H 2.5554158457 1.774219002 1.978464931 C 5.3611236363 -0.134589672 1.9061341135 H 5.4006631066 -2.27836302 2.1318414524 H 4.9798440778 1.9814151248 1.7142765433 H 6.4351650332 -0.0414817489 1.7757468426 N 0.1035099743 1.5191239128 3.5425412911 C 0.0107812652 -4.0119298692 2.6050018089 H 0.5389759382 -4.8093126845 2.0836326766 H -0.9991289929 -3.8977374326 2.2101327542 H -0.026452535 -4.2153402803 3.6773784274
(4-5)‡ E_0 = -12087.9012472 G_{298} = -12087.707067 NImag = 1 (-383.2010 cm^{-1}) C 2.4762714093 1.3603760237 -0.853706061 O 1.5627077184 0.6979243253 -1.4232166419 Rh -0.0014821135 -0.0375177082 -0.2517490231 O 1.1115938125 -1.7629330517 0.1387489298 C 1.9338505193 -1.7521269274 1.0985410755 O 2.1956409965 -0.8344778054 1.9140737865 Rh 1.1523330118 0.9779769759 1.7141811636 O 0.0036799684 2.7031374305 1.3551518121 C -0.7649265181 2.7062862458 0.3642548659 O -0.9729625343 1.7976314632 -0.493641488 O -1.4779432177 -0.6829832543 1.0777016036 C -1.3330821958 -0.4232231132 2.3060093764 O -0.4069214519 0.1961270979 2.8869939344 O 2.606690247 1.6530188973 0.3607185994 C -1.0246348129 -1.009353186 -1.9536222316 C -0.1860934514 -2.1910301668 -2.3756434383 O 0.7200619661 -2.1613974221 -3.184271425 O -0.5429629927 -3.2545564037 -1.6499851798 C 0.3236085108 -4.4091100482 -1.7495500708 H -0.0575603951 -5.1181856844 -1.0156963821 H 0.2700758804 -4.8352126137 -2.7541601005 H 1.3521106737 -4.130768203 -1.5182595716 N -0.533958411 0.1144294251 -3.2446070095 N -0.3217777923 1.0784633337 -3.7471744808 C -2.4911860076 -1.0925313056 -2.0748659992 C -3.3208840106 -0.1346821233 -1.4545217474 C -3.0937996599 -2.1287376455 -2.8251849416 C -4.7050042083 -0.2235315525 -1.567794655 H -2.8799276953 0.6820829104 -0.8981739823 C -4.477263014 -2.2179351694 -2.9241051575 H -2.4780444183 -2.8684635139 -3.3253158767 C -5.2854841301 -1.2657285544 -2.2951540582 H -5.3326303077 0.5192919233 -1.0852724829 H -4.9264081807 -3.0243213477 -3.4956116761 H -6.3664715946 -1.3347892269 -2.3759321218 C 3.6135982494 1.8313205989 -1.7887113274 C -2.4990798903 -0.8920671559 3.2063189739 C 2.7043038742 -3.0815349876 1.2679004138 C -1.5845599704 3.9917672132 0.1121984542 F -3.0426162961 -2.0268719447 2.7468005124 F -3.4535181674 0.0598082225 3.2155858795 F -2.0915082036 -1.0922534827 4.4653863981 F 1.8369940324 -4.0816908271 1.5092700775 F 3.5819800118 -3.025731375 2.27264346 F 3.3696475468 -3.3729659158 0.1341135813 F 3.1557369283 2.0637058256 -3.0266690789 F 4.5547526923 0.8712329422 -1.856868101 F 4.185045762 2.9507080784 -1.3270459665 F -1.1803165601 4.5680374935 -1.0339395869 F -2.8891507997 3.6857705215 -0.0102107514 F -1.4451998099 4.8736877682 1.1052697168	**5** E_0 = -11978.412963 G_{298} = -11978.224696 NImag = 0 C -0.6617457073 -1.6538063135 -1.5500258718 C 0.4887852584 -2.3057735393 -2.2305566503 O 0.9850717173 -1.8330467851 -3.2358892866 Rh -0.0535714922 -0.1581828934 -0.2460286502 O -1.1081248577 -1.0104067398 1.3458327055 C -1.0244354612 -0.4615322093 2.4846166176 O -0.3810626187 0.555497979 2.8351407129 Rh 0.7416493136 1.5853144715 1.3837393133 O 1.7780543902 2.4532079543 -0.2213046727 C 1.6976656713 1.8989147286 -1.34507668 O 1.0623299059 0.8607889338 -1.6895821402 O 1.6449661335 -1.2552500512 0.2731171187 C 2.4524306017 -0.7612875654 1.1127951297 O 2.386501838 0.3203120705 1.7430138841 O -1.664608621 1.1128325809 -0.645566979 C -1.7505001454 2.2003403835 -0.0007854144 O -0.9768849573 2.681228161 0.8597510047 O 0.9074010506 -3.3941282136 -1.584211991 C 2.1603744801 -3.9656199788 -2.0349217091 H 2.3036932335 -4.8585372552 -1.4277369895 H 2.1051373251 -4.2274063151 -3.0933974645 H 2.972844811 -3.2561821081 -1.8661306501 C 2.4986639133 2.5467176503 -2.4985867897 C -3.0173628716 3.0165534553 -0.3431680987 C -1.8705240054 -1.1616869955 3.5726763165 C 3.6763943259 -1.6631193654 1.3930481547 C -1.9693229785 -2.1049541015 -1.8432474899 C -2.1848951279 -3.1489140153 -2.7992953803 C -3.1055294536 -1.5560793332 -1.1743050228 C -3.4602978558 -3.6093964925 -3.0662589484 H -1.3396363818 -3.5765928661 -3.3278777895 C -4.3765217543 -2.0358470578 -1.4416598716 H -2.965856972 -0.7648262866 -0.4514630862 C -4.5552345971 -3.0557387294 -2.3852628665 H -3.61483404 -4.3971925857 -3.7961343087 H -5.2343678461 -1.620102188 -0.9236825239 H -5.5559382824 -3.4236978708 -2.59319423 F 1.6959894746 2.7787963668 -3.5501604048 F 3.4779721251 1.7128063656 -2.8919647387 F 3.0533651099 3.7045182415 -2.1234427538 F -3.0586431206 4.1745599125 0.3216672384 F -3.0600495985 3.2759085012 -1.660415458 F -4.1113538041 2.2990812834 -0.0210421798 F 4.251187101 -2.0392666086 0.2357748321 F 4.5929698899 -1.0376110618 2.1373147983 F 3.2815091886 -2.7727309763 2.043441684 F -3.177585286 -1.040929825 3.2707859812 F -1.5728831921 -2.4703416227 3.6260945823 F -1.6633758299 -0.6273340896 4.7797020165
(5-6)‡ E_0 = -12380.8270067 G_{298} = -12380.485845 NImag = 1 (-76.8627 cm^{-1}) C -1.2273362711 0.4055820789 -1.2374945482 C -1.6001447703 -0.8211750526 -2.0138564841 O -2.202974948 -1.7820061719 -1.5808162435 Rh 0.4920140316 0.0307544998 -0.0934150823 O 1.5198206106 1.5891371835 -1.0250109806 C 2.7347050415 1.7756615873 -0.7200062435 O 3.4570463647 1.1546698932 0.0951877224 Rh 2.6042128161 -0.4290515437 1.1873365439	**6** E_0 = -12380.8559389 G_{298} = -12380.510669 NImag = 0 C 3.1955858984 -0.1170558698 -1.1962318444 O 2.0025289893 0.1044730456 -1.5451143244 Rh 0.5212031595 0.0320541148 -0.0786471506 O 0.3177712336 -2.032970915 -0.3544098536 C 1.0796908134 -2.8009501278 0.3046744722 O 1.9781876896 -2.5150612079 1.131268474 Rh 2.3374124507 -0.4844149893 1.5709267506 O 2.5170233717 1.5865230079 1.863188659

O 1.5528388769 -1.969569516 2.1606289387	C 1.765067021 2.3427391867 1.1965216307
C 0.359327002 -2.1689886204 1.8282751736	O 0.8741680468 2.0531280865 0.3491906072
O -0.3456492949 -1.5696036056 0.9649544831	O -0.8344047666 -0.1472800185 1.5148578328
O 1.2086892572 -1.304460865 -1.5233145807	C -0.374735014 -0.3869357683 2.6748999069
C 2.3091742118 -1.8925662439 -1.3136890241	O 0.8118276332 -0.5520008432 3.0344221139
O 3.1095406877 -1.7729988367 -0.3557409896	O 3.6672037986 -0.3658275688 -0.0573826189
O -0.0666708089 1.2856245502 1.485457422	C -1.2480111787 0.4168985596 -1.4471188803
C 0.753626942 1.4559864101 2.4388961065	C -0.7669089995 -0.1414521492 -2.7474345868
O 1.8863181035 0.9521681488 2.6114884872	O -0.9369315016 -1.3242803315 -3.0384556547
O -1.0636308454 -0.742690997 -3.2432122577	O -0.0725639052 0.7051818729 -3.5065188471
C -1.0564130674 -1.9686474255 -4.0114817379	N -2.2217269376 -0.6240790705 -0.935014147
H -0.4972354576 -1.7367989778 -4.9174400654	H -2.1920763903 -0.7121999079 0.0889050288
H -2.0771100102 -2.2685693344 -4.2600209328	C -3.6541694213 -0.489779263 -1.4044765774
H -0.5616145941 -2.7630712004 -3.4501879805	O -3.8921822813 -0.1834842069 -2.5389244497
N -2.8235793732 -0.0333870393 0.7230097188	O -4.4254494061 -0.7893777788 -0.391697214
C -4.1256571784 0.3286631208 0.4478274759	C -5.937135565 -0.8250365795 -0.5281547704
O -4.5414018484 1.4689390656 0.5901954188	C 4.2278865605 -0.1270397607 -2.3468426136
O -4.8070403379 -0.7278829865 -0.0268168904	C 0.8526129886 -4.3014574102 0.0119054613
C -6.2256541776 -0.6223225909 -0.4272855974	C -1.4664925058 -0.512182542 3.7601957136
H -2.5893730485 -1.0170301957 0.7770009672	C 1.9230773097 3.8612938036 1.4387765407
H -2.3237191507 0.5870129343 1.3479295653	F 0.7917049773 4.3571450796 1.9736152957
C -0.3626716685 -3.339288179 2.5352865608	F 2.9353668212 4.1296164267 2.2717078889
C 0.2401726981 2.4396197951 3.5134257875	F 2.1498833806 4.49556509 0.2758651277
C 3.3845076615 2.9606916526 -1.470257052	F -2.3432943933 0.5026730498 3.6618446967
C 2.6710611401 -2.9142036295 -2.4155964927	F -2.1422735789 -1.6645313837 3.5790624374
C -1.7664037809 1.6746937109 -1.6035567088	F -0.9484509763 -0.5118227857 4.9902329649
C -2.730630429 1.789344089 -2.6482156029	F 3.7470778132 0.461213228 -3.4515023366
C -1.342804822 2.8648288115 -0.9474005452	F 5.3533943529 0.5049834528 -1.9837454929
C -3.2138980538 3.0293508361 -3.0334924377	F 4.5400590277 -1.4016695725 -2.6513758879
H -3.0766749529 0.8993199817 -3.161216567	F 1.5492936405 -5.0803523608 0.845308495
C -1.8393945748 4.099178272 -1.3351044396	F -0.4531643115 -4.6042848864 0.1366384144
H -0.6366829264 2.801289868 -0.1308822332	F 1.2275164174 -4.5810844639 -1.2488118843
C -2.7677638765 4.184939136 -2.3796365214	C -1.7631050668 1.8093049255 -1.2683163912
H -3.9384099327 3.1038438059 -3.8380644979	C -1.5510671093 2.8346323674 -2.209816799
H -1.5078941704 4.9995195409 -0.8279695213	C -2.4802486556 2.1363258251 -0.0964330503
H -3.1495516194 5.1557146006 -2.6824727104	C -2.0506756348 4.1185101144 -1.9945430619
C -7.0765822793 -0.2131209774 0.7774604649	H -0.9983902339 2.6285375495 -3.1151941794
H -6.8425592241 0.8018918406 1.1012735892	C -2.9839063492 3.4196515973 0.1082096145
H -8.1369257782 -0.2578484883 0.5087017275	H -2.6251363464 1.4010187632 0.6876964529
H -6.9100810555 -0.898334857 1.615035435	C -2.7764200366 4.4206255412 -0.8417821563
C -6.5489500418 -2.051247868 -0.8671651323	H -1.8741962376 4.8854357103 -2.743584093
H -6.4189471875 -2.752922618 -0.0376607378	H -3.5315301645 3.6360665263 1.0211962972
H -7.5854843798 -2.1123553034 -1.2122659507	H -3.1667733124 5.4214794345 -0.6823138764
H -5.8918887746 -2.3615410615 -1.6852538129	H -1.8608152622 -1.5041186412 -1.3608322129
C -6.3677266883 0.3516927994 -1.5994074275	C -6.299317335 -1.9253398763 -1.5209716171
H -6.1052125128 1.3687063972 -1.3053227706	H -7.3875157899 -2.0392659445 -1.5387626048
H -5.7263145631 0.044127284 -2.431701452	H -5.9663273127 -1.6855506575 -2.5326911372
H -7.4036016708 0.3474906456 -1.9541044322	H -5.8647069174 -2.8823382925 -1.2167489051
F -1.6715732483 -3.0762217092 2.6788733878	C -6.4251621742 0.5570900918 -0.9504497727
F -0.2347807807 -4.4559598129 1.7955200297	H -7.5190002279 0.5661202159 -0.9175129101
F 0.159335418 -3.5713663337 3.7453236731	H -6.0577811864 1.3252792486 -0.2640381167
F 1.096124449 2.5574055976 4.5310822565	H -6.1110743724 0.8072391571 -1.9649325751
F -0.9426052354 2.0138050615 3.9922997672	C -6.3724168854 -1.1715454688 0.89115041
F 0.0572213721 3.6540737832 2.9622080719	H -5.9612125617 -2.1353876205 1.2049036935
F 1.7815109029 -3.9268733291 -2.3953168068	H -6.0491773964 -0.4036812492 1.5999485844
F 3.894719257 -3.4210211743 -2.243937082	H -7.4636367537 -1.2351882131 0.9274700298
F 2.6102139003 -2.3342525927 -3.6266877262	C 0.5590190831 0.1385608978 -4.6757906549
F 2.7661471964 4.1058411215 -1.1254221354	H -0.1894043381 -0.3033113164 -5.3370350131
F 3.2538726166 2.7965870289 -2.7972896907	H 1.0548335052 0.9750111632 -5.166998401
F 4.6841033125 3.0776736252 -1.1814655486	H 1.2878878099 -0.6179590918 -4.3818199318
(6-7)‡	**(7-8)‡**
E_0 = -12380.8480954	E_0 = -12380.8221753
G_{298} = -12380.506139	G_{298} = -12380.478784
NImag = 1 (-1191.1257 cm^{-1})	NImag = 1 (-201.9003 cm^{-1})
C -1.299113885 0.4797813012 -1.4794284164	C 3.6340906522 -0.4474344206 -0.9754558256
C -0.7699079662 -0.0961645292 -2.7276938319	O 2.5231795961 -0.1587376537 -1.4974566786
O -1.1445570896 -1.2744931715 -3.0038508725	Rh 0.8578623841 -0.118994173 -0.2528223106
Rh 0.4738137488 -0.0109547373 -0.0534967713	O 0.5541642836 -2.1604222646 -0.5646860757
O 1.765343403 1.4196202337 -0.8598023234	C 1.1613052302 -2.9721866924 0.1863690581
C 2.9170681909 1.5333568658 -0.3549587841	O 1.9492883914 -2.7282435577 1.1404306609
O 3.4353673162 0.9158411794 0.610662755	Rh 2.3213554832 -0.7269293687 1.5929899947
Rh 2.296275228 -0.5669921818 1.5680888586	O 2.6214177997 1.3043032991 1.9288307544
O 0.9677752516 -2.0011365805 2.3805952367	C 2.0359857756 2.118253547 1.1593643028
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O 1.318937762 -1.4440911943 -1.3280296225	C -0.4806173696 -0.4256777065 2.3154156706
C 2.3394728652 -2.0746469887 -0.9278850798	O 0.6301127589 -0.6934309783 2.8404764461
O 2.9695814184 -1.9716274361 0.1532862132	O 3.8886006208 -0.7256067853 0.2274393812
O -0.2101087877 1.3539173663 1.3807241164	C -2.1400660405 1.3162813863 -1.6126212412
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H -2.5445386061 5.6821380135 -0.7299885196	H 1.3900336545 1.5768676512 -3.5434501666
(7-10')‡	**(7-10)‡**
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G_{298} = -14448.635406	G_{298} = -14448.640206
NImag = 1 (-926.0358 cm^{-1})	NImag = 1 (-1060.0143 cm^{-1})
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C 0.5218474604 -1.7696349505 -0.2325331054	C -6.7592111153 1.558034851 0.7378086483
O 0.3970166957 -3.0923325482 -0.3544045524	C -7.3597770714 2.1894248398 1.839255254
C 1.4385340894 -3.9727008657 -0.949262551	C -6.8285882689 3.3664536639 2.3575124795
C -0.7405525803 0.1756897621 0.5995117414	C -5.6905599568 3.9152450611 1.7667293579
C -0.5928921079 0.9057070541 -0.6251972245	C -5.0350911449 3.2869119354 0.6934987049
O -0.0101810452 2.0724531957 -0.6370320156	C -8.5549977767 1.3958674402 2.3182156911
C 0.1308934977 2.7819242918 -1.8942413071	C -8.3622577042 0.0382446871 1.6089657787
O 1.4728718951 -1.0867958364 -0.6427284286	C -7.6208874307 0.3896992948 0.2745402013
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H -2.2229566915 0.3498407186 0.769301685	C -7.9999648671 -1.3964056454 -1.2807308877
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H 0.8109244926 2.2329779469 -2.546784251	C -8.6593720075 0.843389582 -0.8067154315
H 0.5573997331 3.7435641341 -1.6187864583	C -7.766157635 -2.6125162601 -1.9146049855
H -0.8398038318 2.9079507643 -2.373147439	C -6.5793432563 -3.295556832 -1.6531432572
H -1.840590822 -0.1860731291 -1.6328064199	C -5.5871158502 -2.7675437787 -0.8073765629
C -0.1724065137 0.7077738627 1.8831834332	C -5.8368271825 -1.5133388713 -0.2143904142
C -0.4621909999 2.0169366825 2.3082285677	O -4.8300146276 -0.8876835721 0.5438452913
C 0.5953959137 -0.1066153474 2.73052589	P -3.8700367922 0.192016988 -0.2106146299
C 0.0256961294 2.5007768715 3.5204116673	O -3.2838025398 -0.4314112499 -1.5027878085
H -1.0736273724 2.6606759886 1.6850435788	O -4.8881530399 1.3380765782 -0.7654767495
C 1.0825071349 0.3792264669 3.9463083942	O -2.87521924 0.70055188 0.7983925941
H 0.8165976681 -1.1287798881 2.4436287312	N -0.7115630512 -1.3309197542 0.1550463689
C 0.8038751056 1.6858925397 4.3478693875	C 0.163227781 -1.0392787652 1.1528040385
H -0.2070838597 3.5191431248 3.819778745	O -0.224142501 -1.632242077 2.2848033541
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H	1.407374506	-6.0804828456	-1.4078871592
H	-0.1545501304	-5.2717405525	-1.6502560862
C	1.7997600771	-3.5081941265	-2.3616456526
H	2.3376792991	-2.5629872814	-2.3628385152
H	0.8944178364	-3.4065890391	-2.9688771058
H	2.4361165498	-4.2661756513	-2.8300527452
C	2.6287483828	-4.0320335946	0.0079608558
H	3.0788361068	-3.051786866	0.15651233
H	3.3976711318	-4.6961951765	-0.3990324388
H	2.3126927859	-4.4274017518	0.9786245068
O	3.2636179813	0.8783714777	-2.3539232329
C	4.2200864189	1.5584917699	-2.8179928027
O	5.3440897199	1.80127331	-2.304331692
Rh	5.7103042408	1.0688788634	-0.375287962
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O	3.8647751808	-0.7431166281	1.4326838964
Rh	3.5000832566	0.0324248121	-0.4636157675
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H	-1.3243944069	5.9698975252	-4.766906431
H	0.5341312004	6.6618200421	-3.2589808039
C	-2.3709653188	-5.0218484901	2.2766083485
H	-2.8749121177	-4.55889769	3.1209601051
C	-1.0796489589	-6.2216017808	0.0885247819
H	-0.5827130467	-6.6828294348	-0.7611446777
C	-1.3288339258	-5.9000105241	2.4786508986
C	-0.6744003225	-6.5031979224	1.3746108295
H	-1.0060678106	-6.1384636961	3.4882504714
H	0.1478049687	-7.1915383763	1.5489359939

H	-4.0975343436	4.1801017152	1.8759852101
C	-3.0974357432	4.586138447	-1.8574515439
H	-4.6890408472	3.2273008805	-2.2774411906
C	-2.3662412479	5.305384867	-0.8719839442
H	-2.829591564	4.710307012	-2.9039218339
C	-4.4334145352	-4.1264483229	0.0552444671
C	-3.6589122534	-5.1388345384	-0.5886213931
C	-4.2219456816	-3.900472953	1.4080438806
C	-2.7509045959	-5.8976379822	0.1104194796
H	-3.7881366345	-5.3071016992	-1.6530663296
C	-3.2766895076	-4.653162773	2.153357501
H	-4.8041474732	-3.1507199188	1.9328594569
C	-2.5311714602	-5.6867584094	1.4986639054
H	-2.1819576561	-6.6706173119	-0.399044033
C	-3.0621803653	-4.4267224483	3.5421027758
H	-3.6287330005	-3.6424129879	4.0375882531
C	-1.6039561513	-6.4539992623	2.2545675995
H	-1.0464245475	-7.2427147908	1.755501443
C	-2.1527938684	-5.1842638423	4.2465180744
C	-1.4172290156	-6.2080009484	3.5976560989
H	-1.9960010354	-5.000506116	5.305690778
H	-0.7057667128	-6.800208081	4.166365309
C	-1.9968057464	5.8435784185	1.4990928188
H	-2.2780931924	5.7202404168	2.5420013891
C	-1.2847460451	6.1680676941	-1.1989518017
H	-1.0154475104	6.2975951723	-2.2443840462
C	-0.9457121326	6.663091712	1.1508989384
C	-0.587632661	6.8292492223	-0.2107014791
H	-0.3885914509	7.1905153076	1.9199998372
H	0.2398017926	7.4830562928	-0.4717367675
O	2.8089403983	2.2659870751	0.3063630387
C	3.7534883102	3.0705875293	0.0805899499
O	4.9761259445	2.827924135	-0.1063392559
Rh	5.5831702182	0.8264119501	-0.0677712648
O	6.0326362618	-1.2169032813	0.0064666928
C	5.0912080717	-2.0143430452	0.259879424
O	3.8796114638	-1.759972039	0.5047565289
Rh	3.2695023949	0.2312507022	0.4269002939
O	3.7330824459	0.4693089513	2.4470229908
C	4.9172751473	0.771477006	2.7541464564
O	5.9026054091	0.9808607134	1.9963849924
O	2.9726414908	0.0415867447	-1.6225272126
C	3.9375407407	0.2966252347	-2.3906995705
O	5.1170820774	0.6343462687	-2.0968602701
C	5.4349351447	-3.5205116189	0.2363300082
C	3.3312886636	4.5539226616	-0.0252117467
C	3.6068139587	0.2379848097	-3.898646108
C	5.1796972423	0.9511930624	4.2661531929
F	6.4324134693	0.5991333972	4.5820950219
F	4.3300405206	0.2131425867	4.993457401
F	5.0053721507	2.2450900316	4.5938872844
F	2.4190557677	4.8621831772	0.9076163063
F	4.3775160819	5.3741723016	0.1092911585
F	2.7779886526	4.7669581364	-1.2381959483
F	4.7046501188	0.0034445046	-4.6280199773
F	3.0982636202	1.4312394067	-4.2765601935
F	2.702714466	-0.7093775789	-4.1614303518
F	4.9078997146	-4.1381757551	1.3043582788
F	6.755949705	-3.7252186165	0.2308752449
F	4.9109657987	-4.0750746414	-0.8728205248

Optimized Cartesian Coordinates Stereodetermining transition states at the B3LYP-D$_{(Chloroform)}$/DGDZVP (for all atoms Rh, C, H, N, O, F, P) level of theory in the condensed phase

(7-10')‡

E_0 = -14450.4370583
G_{298} = -14449.583637
NImag = 1 (-958.1255 cm^{-1})

N	-0.809975531	-1.2670045198	0.1817286242
C	0.2635628496	-1.8333760914	-0.4264014553
O	0.0802453394	-3.1293473863	-0.6778713499
C	1.1754963414	-3.9709668634	-1.2460818934
C	-0.845213954	0.1498053365	0.4534599793
C	-0.6339250399	0.9027155651	-0.7411017151
O	-0.01536114	2.0499127815	-0.7075154114
C	0.2454230817	2.7425944064	-1.9592951311
O	1.2685840127	-1.1808285025	-0.7626973096
O	-1.0885010976	0.5088633608	-1.9106226489
H	-2.296181729	0.4732540875	0.6174982869
H	-1.6020109655	-1.8643891544	0.4025133539
H	0.8737609299	2.1115119048	-2.590135598
H	0.7690174799	3.6501783959	-1.6647587394
H	-0.6930110078	2.979886173	-2.4616344582
H	-1.8365321988	-0.1637881774	-1.7949669094
C	-0.2460250247	0.6007497465	1.7479390463
C	-0.493760448	1.9003534154	2.2248577582
C	0.5286441435	-0.270599713	2.5293375433
C	0.0462546423	2.3259283703	3.4390059288
H	-1.09848713	2.5850752706	1.636774297
C	1.064856583	0.1551337135	3.7492966015
H	0.7231974881	-1.2820232116	2.1893851534
C	0.8321575033	1.45643782	4.2089795361
H	-0.1404704319	3.3408025843	3.7820253207
H	1.6680162364	-0.5324647563	4.336885853
H	1.2537593358	1.789495692	5.1548152944
C	0.5014011407	-5.3240760675	-1.4546437123
H	0.1635028211	-5.7387830587	-0.5036584775
H	1.2280837704	-6.012619077	-1.8995522871
H	-0.3546559917	-5.2301676398	-2.1309395905
C	1.639614126	-3.4218559981	-2.5974361111
H	2.1824087392	-2.4841389432	-2.504506792
H	0.7733505708	-3.2792339165	-3.2541306068
H	2.299443716	-4.1654951199	-3.0582844012
C	2.2820160055	-4.0840580942	-0.1987563664
H	2.6908805184	-3.1096426762	0.0631650725
H	3.093379257	-4.7032477445	-0.5966481097
H	1.8856044298	-4.5593547112	0.7053144988
O	3.0873067681	0.8774815574	-2.1228598771
C	4.1088547483	1.5229408576	-2.4913625963
O	5.2175844729	1.6600819	-1.9081922323
Rh	5.4343858218	0.8200166867	0.0012510666
O	5.4415981101	-0.0719854018	1.8914331808

(7-10)‡

E_0 = -14450.446091
G_{298} = -14449.593783
NImag = 1 (-1056.6591 cm^{-1})

C	-5.8084055946	1.7383116247	0.7366051626
C	-6.9216028845	1.0875177115	1.2554527611
C	-7.5032740242	1.5615927167	2.4413586816
C	-7.0057823712	2.7048843527	3.0658394679
C	-5.9134900486	3.372724058	2.4988639347
C	-5.286547798	2.9029687867	1.3308489939
C	-8.6249788001	0.6420679358	2.8756700743
C	-8.3453693034	-0.6338606042	2.0488858895
C	-7.6992621811	-0.1055377235	0.7293179473
C	-7.0498267572	-1.22571391	-0.0665883102
C	-7.9722351956	-1.7692776918	-0.9746515415
C	-9.2592156195	-0.9732939571	-0.9536454757
C	-8.8241914653	0.3367648229	-0.2600867591
C	-7.6292406184	-2.8654957597	-1.7645693361
C	-6.3494386583	-3.4196209309	-1.6448426748
C	-5.3912396049	-2.880181963	-0.7679747782
C	-5.7686968713	-1.762593386	0.0009624163
O	-4.8008003646	-1.1141527925	0.7907778552
P	-3.9824311444	0.0875743183	0.0686075782
O	-3.4342908822	-0.3887460187	-1.3015024968
O	-5.132543113	1.1540455062	-0.3530013487
O	-2.9833227558	0.6112655243	1.0583465287
N	-0.8400642928	-1.2645821286	0.1720579115
C	-0.0335435187	-0.9740931594	1.2168564618
O	-0.4302503432	-1.5954586325	2.3275799061
C	0.392370954	-1.6033642944	3.5705611357
C	-0.8059793447	-0.6408372639	-1.1251373505
C	-0.5589118293	0.7605658978	-1.1301387843
O	0.0047014329	1.2971555179	-2.183878654
C	0.115443632	2.7486357775	-2.2345213947
O	0.9149742055	-0.1662859614	1.1662163537
O	-0.9373603211	1.5864171527	-0.1885526776
H	-5.5220647033	4.2692712101	2.972896849
H	-7.4492642677	3.0722600858	3.9889936586
H	-8.3403155739	-3.2828554913	-2.4743105193
H	-6.0743256535	-4.2813204837	-2.2478178877
H	-9.669550148	-0.8107560782	-1.9558539291
H	-10.0236659689	-1.4938829567	-0.3619241112
H	-8.3953730527	1.0203876024	-1.0012874862
H	-9.6409463575	0.8499947028	0.2563576721
H	-9.6000208708	1.0722846899	2.612386046
H	-8.6238923189	0.4592140014	3.9552945959
H	-7.6166936676	-1.2606911754	2.5746079713
H	-9.2410402027	-1.2307051594	1.8516294946

C	4.4581936822	-0.8017226616	2.2005684604	H	-2.2670028996	-0.4866690558	-1.337307659
O	3.4242874478	-1.0689952917	1.5316691815	H	-1.5692468603	-1.9511611058	0.3458645323
Rh	3.1904454871	-0.1241442631	-0.3020053558	H	0.6958764278	3.1010671717	-1.3824904318
O	4.1154688838	-1.7351863397	-1.2412044329	H	0.6302612743	2.9537971379	-3.1736174333
C	5.3747600123	-1.7899464634	-1.2474760783	H	-0.8798380612	3.1920899001	-2.2321788001
O	6.2059199461	-0.9422931341	-0.8247711074	H	-1.6369862013	1.1792728715	0.4312230632
O	2.4593947431	1.6014124097	0.6083864877	C	-0.2688357827	-1.4919138862	-2.2354042041
C	3.2755445085	2.5186927736	0.8828728503	C	-0.8115968833	-1.3969030934	-3.5249877285
O	4.5378603696	2.5166280282	0.7932408415	C	0.7539511867	-2.4192809024	-1.992062209
C	4.5462149679	-1.4413560957	3.6119920137	C	-0.3277028611	-2.2015841713	-4.5608199735
C	3.9334940116	2.2659299501	-3.8432158248	H	-1.618316946	-0.6927046473	-3.7155700047
C	2.671002205	3.8488854366	1.4110681799	C	1.2433380995	-3.2208912233	-3.0261089917
C	5.9551726823	-3.1155132083	-1.8066368697	H	1.1671681816	-2.5146403303	-0.9933885706
F	5.8684937764	-4.0674044871	-0.8470298131	C	0.7059963058	-3.1156574194	-4.3159639766
F	5.2563546328	-3.538088665	-2.8762359776	H	-0.7574162751	-2.1178811189	-5.5566614909
F	7.2432559421	-2.9932633001	-2.1613273315	H	2.0443760395	-3.9283440476	-2.8233773001
F	5.0814786313	2.8022953396	-4.2798071489	H	1.0862924209	-3.7409035408	-5.1207965527
F	3.0318194883	3.2649705484	-3.6870823866	C	-4.0345564664	-3.4787639492	-0.6906022219
F	3.4660932031	1.4283225671	-4.7888732616	C	-3.4403203227	-3.7714801043	0.5276237421
F	3.3745190743	4.9040270673	0.9432244456	C	-3.3341811072	-3.7918168709	-1.8941911996
F	1.3982836171	4.0027338937	1.0354884967	C	-2.1658674919	-4.4005323643	0.5944296866
F	2.7352314228	3.8765931515	2.7605778496	H	-3.9545659187	-3.5339119598	1.4550509706
F	3.537132912	-2.2969423475	3.8423030513	C	-2.0878360009	-4.3781836745	-1.8604995611
F	5.7080302552	-2.1112424917	3.7511243591	H	-3.7832234697	-3.5259318149	-2.8473264176
F	4.5041156662	-0.473848651	4.5531943187	C	-1.4707126333	-4.706994518	-0.6217912209
C	-5.9246433685	-2.0387241768	-0.3216240369	H	-1.5487909292	-4.5714404062	-2.7846183484
C	-7.1136559635	-1.6083399404	-0.8976831583	C	-4.1038186696	3.6111939379	0.7792118258
C	-7.7917739663	-2.4442697626	-1.7956063064	C	-3.0354840629	3.9841416467	1.6496771063
C	-7.3418861196	-3.7462541161	-2.004802732	C	-4.021135073	3.9367172807	-0.564486671
C	-6.2076782771	-4.1974645704	-1.3218503433	C	-1.9321248834	4.656471535	1.1715220817
C	-5.4422883486	-3.3574886657	-0.4823790269	H	-3.0907918805	3.7020168373	2.697805527
C	-8.9749721418	-1.7175197098	-2.4007792965	C	-2.9076660237	4.6514265254	-1.0836375614
C	-8.7175440155	-0.2476529456	-1.9873461621	H	-4.8246153459	3.6580366137	-1.2414976999
C	-7.9462258618	-0.3645646061	-0.6375837861	C	-1.8362204719	5.0157849972	-0.2022370387
C	-7.3699924299	0.9601377376	-0.1650712489	H	-1.1132955	4.9135163841	1.8403358188
C	-8.2869389122	1.6093495864	0.6789295206	C	-0.475494836	-2.4126246443	4.5317826297
C	-9.4942272857	0.7323341621	0.9214785832	H	-0.6302234039	-3.426344148	4.1517606592
C	-8.9669026055	-0.6571711351	0.5129468469	H	0.0282377264	-2.4738808166	5.5022311547
C	-8.0060181321	2.8688727916	1.2038012529	H	-1.4493408128	-1.9303431442	4.6714793796
C	-6.7891390942	3.4811004051	0.8885049015	C	0.590489116	-0.1825554475	4.1004498422
C	-5.8330949454	2.8476288861	0.0733025472	H	1.2669925069	0.3948896872	3.4707910286
C	-6.1527061792	1.5753598538	-0.4393354746	H	-0.3746695108	0.3326809345	4.1691385812
O	-5.1959573512	0.8788458675	-1.2001800459	H	1.0180314226	-0.2493146168	5.1077394234
P	-4.1899503494	-0.1270117709	-0.4232354821	C	1.7097135267	-2.3236021026	3.2912727979
O	-3.4396855953	0.6357394706	0.6999517615	H	2.3346669952	-1.7559034737	2.6043185221
O	-5.179569721	-1.1010810885	0.4116578163	H	2.2537717216	-2.4433342716	4.2352651185
O	-3.3319381839	-0.8151686141	-1.4429974378	H	1.5144025032	-3.3144812967	2.86828698
H	-5.9067056883	-5.2311953881	-1.4543868023	C	-2.8228395445	5.0161755883	-2.4587967506
H	-7.8676886727	-4.4168230804	-2.68121958	H	-3.6363191942	4.7382819661	-3.1260193651
H	-8.7164319366	3.3687678903	1.8586804467	C	-0.7134035574	5.7138176893	-0.7278826401
H	-6.5610078059	4.4688239347	1.2800384879	H	0.104822317	5.9696154006	-0.0583422666
H	-9.84083066	0.7711022893	1.9594047135	C	-1.7255261284	5.7056949412	-2.9385298131
H	-10.3297615399	1.0395746633	0.2787063092	C	-0.6572909148	6.053588591	-2.0662265788
H	-8.4279999249	-1.1061802243	1.3545726328	H	-1.6695791224	5.9767791371	-3.9903486321
H	-9.7506150347	-1.3495875764	0.1928813434	H	0.2070146259	6.5841727486	-2.4589318359
H	-9.9168121378	-2.0866524053	-1.9751748863	C	-1.548562872	-4.7148236842	1.8391743086
H	-9.0309994257	-1.8494361263	-3.4866616537	H	-2.0745517028	-4.4711717323	2.7588108008
H	-8.0731607093	0.2412677745	-2.7263614882	C	-0.1811070984	-5.3039813489	-0.5507076644
H	-9.6344823546	0.3396471672	-1.8815116054	H	0.3480353337	-5.5165211902	-1.4757657221
C	-4.5448825356	3.5293993348	-0.2058126735	C	-0.2989374951	-5.2987941763	1.8773697424
C	-3.8482472448	4.1453886302	0.8213336552	C	0.3943241233	-5.5933111342	0.6706626981
C	-4.0366890201	3.619105486	-1.5367058842	H	0.1670108442	-5.5275296801	2.832889852
C	-2.6576493737	4.8792346924	0.5750906693	H	1.3837973329	-6.0424312742	0.715119848
H	-4.2063134326	4.0613055762	1.8447315636	O	2.6654820666	2.1924465202	0.1484157432
C	-2.8952386515	4.3423340967	-1.8092999559	C	3.6720053697	2.8778904464	-0.1834962899
H	-4.5754675951	3.129791314	-2.3426272563	O	4.8509341206	2.4992954622	-0.4242409009
C	-2.1776610033	5.00008225	-0.7702074479	Rh	5.2610505973	0.4446379254	-0.364315183
H	-2.5357477974	4.4265155578	-2.832965065	O	5.4645896667	-1.6413140807	-0.2712622087
C	-4.2144454628	-3.8741322511	0.1856378549	C	4.4397830859	-2.3128191812	0.0225206695
C	-3.544824346	-5.0199783815	-0.3540172487	O	3.2758042805	-1.9099359497	0.3020886397
C	-3.6942687231	-3.3178789989	1.3512601553	Rh	2.9114826927	0.1292071268	0.2651235477
C	-2.4513651998	-5.5791115252	0.2661834403	O	3.5189502657	0.3101388844	2.2522075883
H	-3.8893583838	-5.4576105584	-1.2851509118	C	4.7470250148	0.4698359121	2.491018836
C	-2.5327329048	-3.8403589559	1.9827760103	O	5.7083574417	0.5595695333	1.6804147782
H	-4.1718410544	-2.4653313206	1.8171527273	O	2.4892697177	0.031284524	-1.7658015754
C	-1.9021674371	-5.0079326174	1.4465302486	C	3.4372840059	0.1612746343	-2.5832763474
H	-1.9751771634	-6.4543429102	-0.1678321549	O	4.6727256739	0.3079426347	-2.3552015811
C	-1.9643550719	-3.2134193985	3.1298335688	C	4.5799511995	-3.8582943313	0.0432512144
H	-2.4333032194	-2.3146592486	3.5251951505	C	3.3939075631	4.3931341955	-0.3787147043
C	-0.7392024193	-5.5231185428	2.0815983438	C	3.0700416052	0.1345720365	-4.0909797737
H	-0.2658762798	-6.4133773922	1.6729965938	C	5.0864141131	0.5987275637	3.9999434342

C	-0.8224126562	-3.7236547021	3.7155681533	F	4.7012569154	1.8172258302	4.4421025807
C	-0.2068990876	-4.8935072952	3.1906189306	F	6.4003609966	0.4614204359	4.2354551848
H	-0.3861970548	-3.2282020224	4.5796990661	F	4.426707224	-0.3332596001	4.7162795173
H	0.6904687042	-5.2867444945	3.6630494028	F	2.4572992651	4.8376561473	0.4767468558
C	-1.9299481233	5.5062309607	1.6276472633	F	4.5027699111	5.1310206694	-0.216786558
H	-2.2897074463	5.4010116758	2.6493528114	F	2.9362469443	4.5897033427	-1.640042347
C	-1.0002978804	5.7602079043	-1.0185542927	F	3.5463937697	-0.9989029965	-4.6530898978
H	-0.6420470417	5.853318284	-2.0417418598	F	3.6438295843	1.1839726663	-4.7225973305
C	-0.7881546505	6.2330344676	1.3569646993	F	1.7526634564	0.1934531839	-4.2948512202
C	-0.3219010103	6.3666567417	0.0200804905	F	4.1864297398	-4.3447892752	1.2391307105
H	-0.2357783723	6.703817335	2.166818882	F	5.8387841797	-4.2582560729	-0.1832955213
H	0.5814688146	6.9390191638	-0.1775021035	F	3.7839652124	-4.3972149177	-0.9080608438