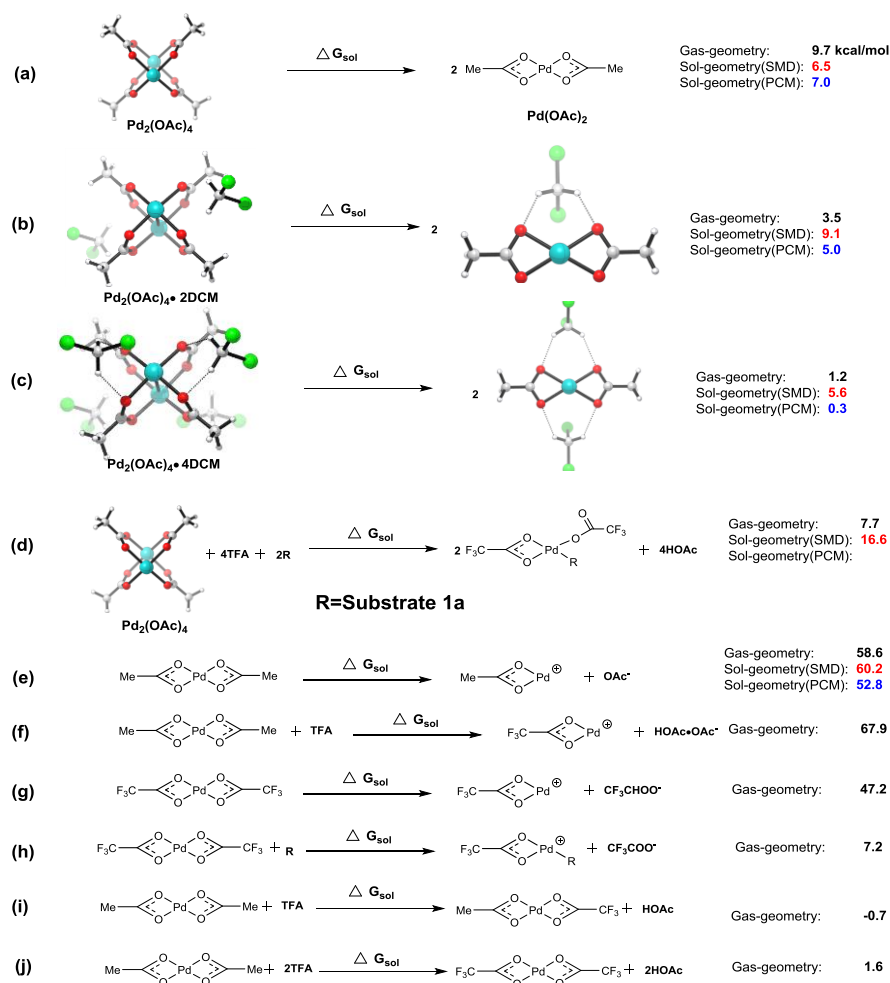


Exploring the necessity of acidic additive for Pd(II)-catalyzed exclusive C4-fluoroalkylation of 3-acetylindole? a detailed DFT study on the mechanism and regioselectivity

Supporting Information

Part 1

1. The free energy files and the partial geometries in Pd(OAc)₂-catalyzed C-H activation process, as well as the corresponding thermodynamic process of the generation of various Palladium catalysts



Scheme S1. Generation Pathways of Monomeric Pd(OAc)₂, Pd(OAc)(TFA), Pd(TFA)₂ and Pd(TFA)₂·R from

Preliminary Palladium Acetate Catalysts $[\text{Pd}_2(\text{OAc})_4]$, as well as the formation of $\text{Pd}(\text{OAc})^+$, $\text{Pd}(\text{CF}_3\text{COO})^+$ along with the Calculated Free Energy Changes (kcal/mol).

In modern organometallic chemistry, palladium acetate has been the most widely used palladium catalyst, but its structural determination both in the solid state and in solution remains issue. The experiments suggested that polymeric form $[\text{Pd}(\text{OAc})_2]_n$ ($n=2,3$) exist in the solid state, but both polymeric $[\text{Pd}(\text{OAc})_2]_n$ ($n=2,3$) and monomeric form $\text{Pd}(\text{OAc})_2$ coexist in solution and their relative contents should depend on the solvent, concentration, and temperature.¹ Our calculation results confirm that monomer could be generated from dimer in solution with free energy change of 1.2 kcal/mol (Scheme S1(c)) in this work. In addition, when adding additive TFA, electrophilic species, e.g., $\text{Pd}(\text{CF}_3\text{COO})^+$ $\text{Pd}(\text{OAc})^+$ electrophilic species were also acted as efficient catalyst in previous report,²⁻³ whereas the generation of these electrophilic species from monomer $\text{Pd}(\text{OAc})_2$ and $\text{Pd}(\text{TFA})_2$ is difficult with quite high free energy change of 58.6, 47.2 kcal/mol (Scheme S1(e) (g)) in this work. The pathway of $[\text{R-Pd}(\text{CF}_3\text{COO})^+]$ -catalyzed C-H activation is difficult (37.3 kcal/mol, Figure S11(c)) though the generation of this species is feasible (7.2 kcal/mol, Scheme S1(h)). Therefore, only the monomeric form of the catalyst $\text{Pd}(\text{OAc})_2$ will be used to discuss the reaction mechanism afterward.

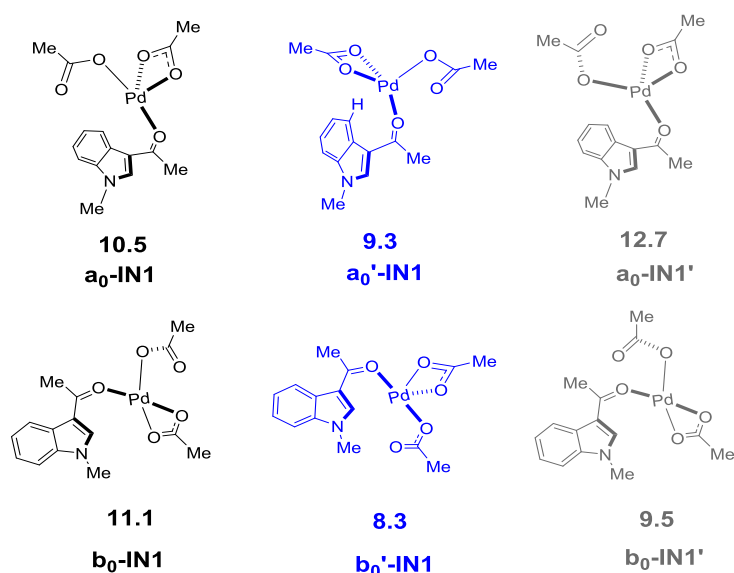


Figure S1. IN1 species represents the whole group of isomers sharing the same coordination mode around the Pd center. The relative energies of these isomers are calculated to be quite close to each other, less than 3 kcal/mol.

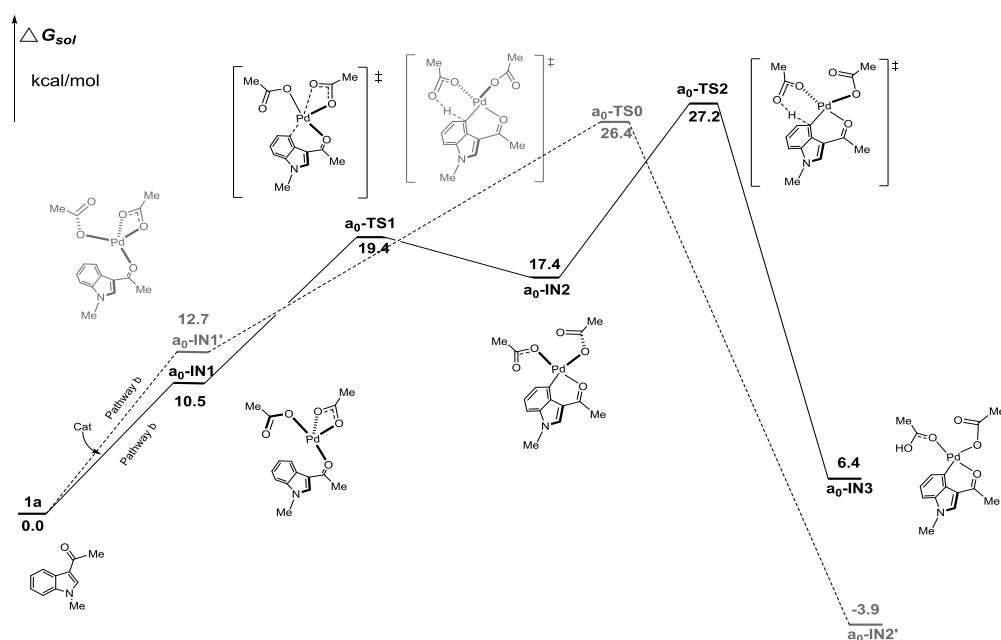


Figure S2. The comparison of the concerted and the stepwise in pathway **b** in C4-H activation in indole with Pd(OAc)₂ as efficient catalyst.

In the text, pathway **b** (in Figure 2) is also a directed one. Besides leading directly to the final product **INT3** in a concerted pattern via **TS0**, there is another possibility for pathway **b** to proceed in a directed stepwise process. The latter consists of two steps: first the formation of Pd... π interaction, leading to **IN2**, occurs via **TS1** and then the proton at C4/C2 position of **IN2** transfers via **TS2**, leading to **IN3** eventually. Being different from pathway **a**, the proton transfer here is completed by the ligand L₁ which is formally in η^2 coordination mode to the Pd center, i.e., η^2 -L₁. As will be demonstrated below, the preference to either concerted process or stepwise process in pathway **b** depends on two factors: 1) the closest distance between C4/C2 proton and O atom of η^2 -L₁ ligands, 2) the capability of abstracting proton of η^2 -L₁. It is not hard for us to understand that shorter H...O distance and η^2 -L₁ from weaker acid will result in higher degree of preference to the concerted process.

In the situation of Pd(OAc)₂-catalyzed C4-H activation, besides the stepwise version (Figure 1), the corresponding concerted one of pathway **b** is also found (Figure S2). This version, starting from a similar intermediate **a₀-IN1'**, needs a barrier of 26.4 kcal/mol which should be impossible at room temperature too (see ESI, Figure S2). What is the reason for the coexistence of two different mechanisms, stepwise and concerted, even starting from intermediates of similar energies (**a₀-IN1** and **a₀-IN1'**)? Although being similar to each other in the aspects of energy and coordination mode around the Pd center, the two intermediates, **a₀-IN1** and **a₀-IN1'**, show clear difference in the closest distance

between the transferred H and O_L. Such closest distance in **a₀-IN1** is 3.45 Å (H₁...O₁), a large value which precludes the direct transfer of H from this intermediate. However, in the case of **a₀-IN1'**, this closest distance is reduced to be only 2.29 Å (H₁...O₁, see ESI, Figure S3) and thus the transfer of H, starting from **a₀-IN1'**, changes to be possible in concerted pattern. It should be emphasized that the concerted process is also facilitated by the strong capability to bind proton H of the OAc⁻ ligand due to the weak acidity of acetic acid.

In the aspect of the highest TS of these two versions of pathway **b**, i.e., **a₀-TS2**, **a₀-TS0** (ESI, Figure S3), they have quite similar lengths for a given bond. For example, the distances of Pd-C4 are 2.18/2.16 Å and those of Pd-O_{DG} are 2.09/2.10 Å for **a₀-TS2**/**a₀-TS0** respectively. Thus this similarity in the geometries of the TS leads to the small difference of only 0.8 kcal/mol in the free energy barrier (see ESI, Figure S2).

For the corresponding C2-H activation, we have also explored all the three pathways **a**, **b** and **c** as shown in Figure S4. The highest TS are calculated to be **b₀'-TS1**, **b₀-TS0** and **b₀''-TS2** for the pathways **a**, **b** and **c** respectively. Therefore, the energy barriers for C2-H activation, in relative to initial material **1a**, are predicted to be 37.0, 28.2 and 25.5 kcal/mol respectively. Clearly, the obtained free energy data suggests that C2-H activation, catalyzed by Pd(OAc)₂ alone, is also difficult at the experimental condition, e.g., room temperature, because of the high barrier energies along all the three paths. The pathway **b** here is of concerted version because of the small value, 2.20 Å, of the closest distance between the transferred H and O_L in **b₀-IN1** (in Figure S3). Actually we have located another concerted pathway **b** of which the TS **b₀-TS0'** is energetically higher than **b₀-TS0** by 1.9 kcal/mol (see ESI, Figure S4). Clearly, the existence of **b₀-TS0'** does not change the above theoretical prediction on the feasibility of C2-H activation, catalyzed by Pd(OAc)₂ alone.

However, when Pd(TFA)₂ works as the catalyst, the concerted pattern is not adopted by pathway **b** as shown in Figure S8 ~ S9. As a ligand from strong acid, the capability of abstracting proton H should be obviously poor for CF₃COO⁻. This could be the reason for the nonexistence of concerted pathway **b** even though there are indeed close H₂...O₁ distances (2.17 ~ 2.19 Å, Figure S10) in some of the starting intermediates.

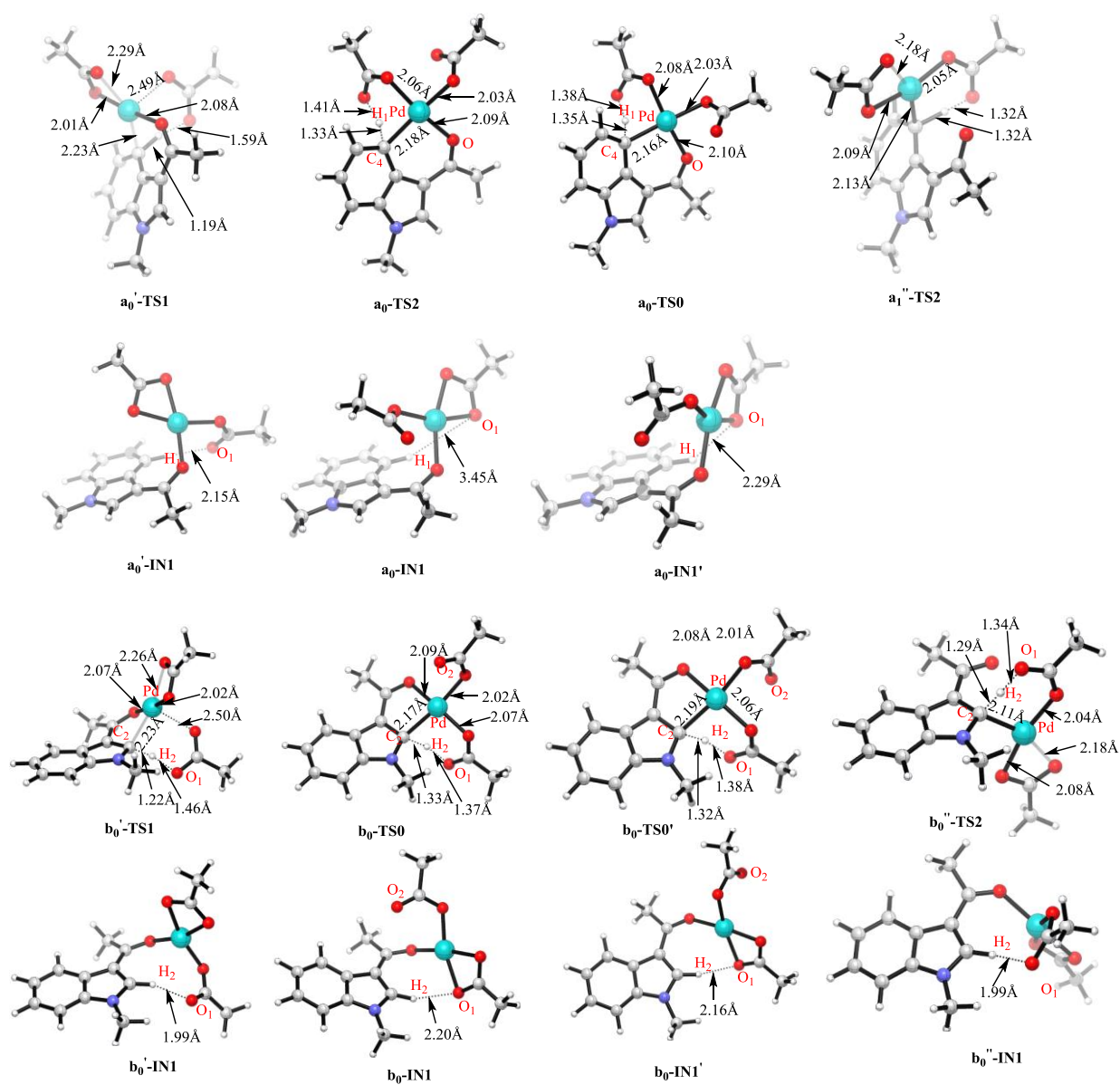


Figure S3. The partial bond length and geometry of local minimal and transition state in the $\text{Pd}(\text{OAc})_2$ -catalyzed C4 & C2-H activation.

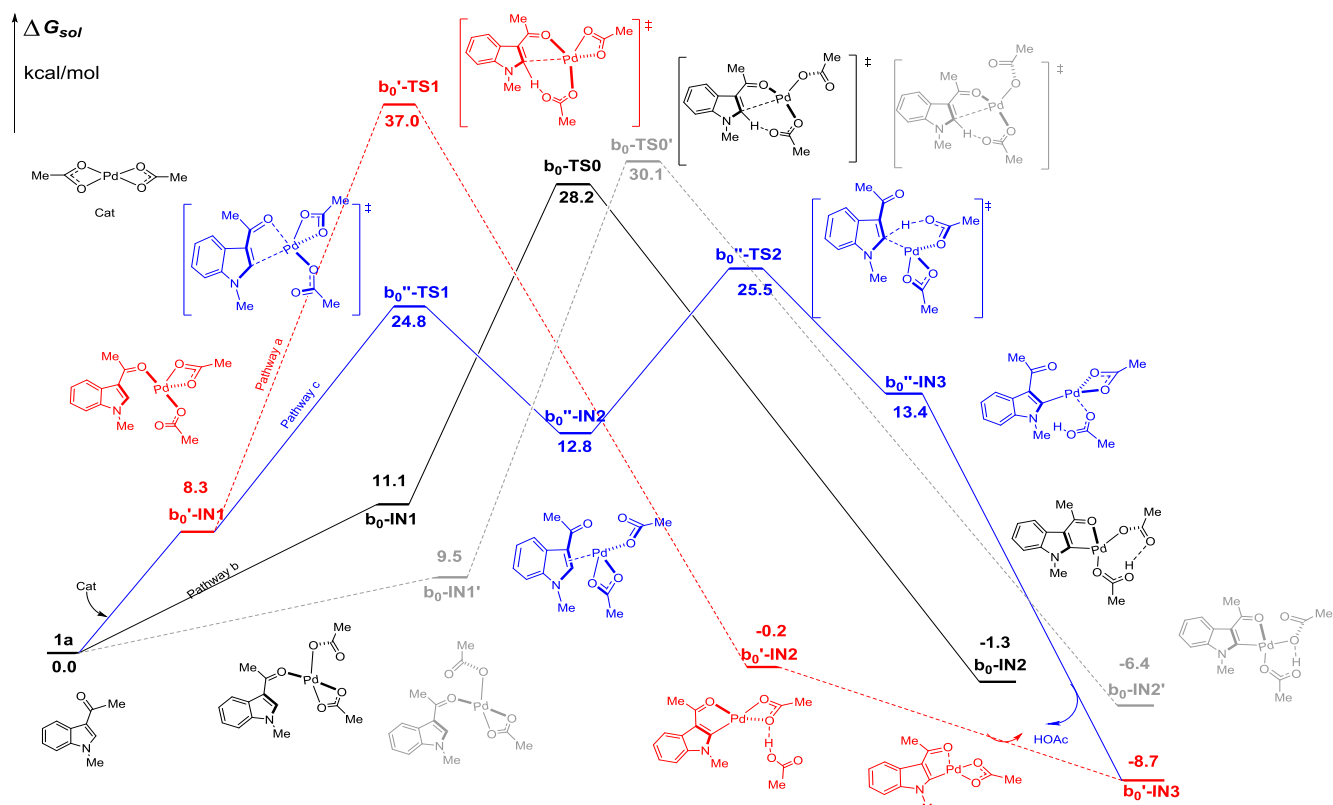


Figure S4. Three possible pathways of C2-H activation in indole with $\text{Pd}(\text{OAc})_2$ as efficient catalyst.

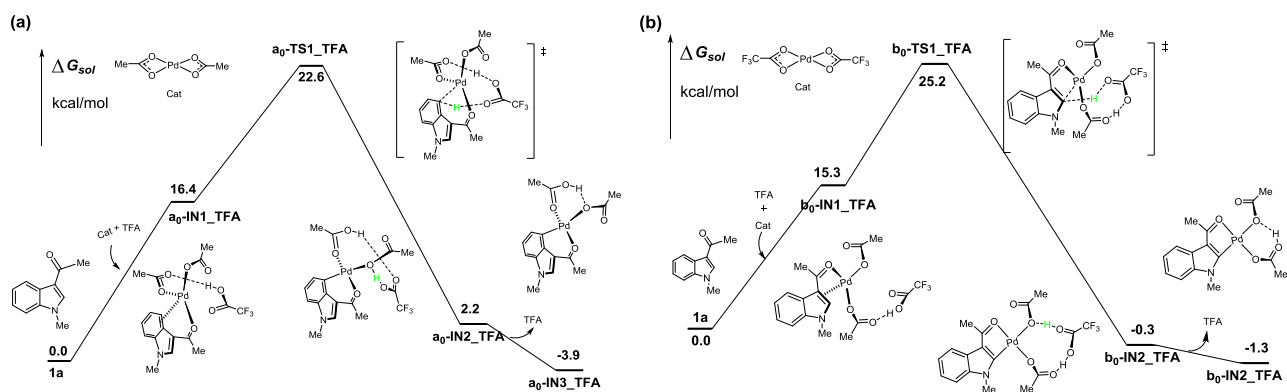


Figure S5. The pathway of C-H bond activation of the $\text{Pd}(\text{OAc})_2$ -catalyzed with the participation of additive TFA. **(a)** C4-H activation. **(b)** C2-H activation.

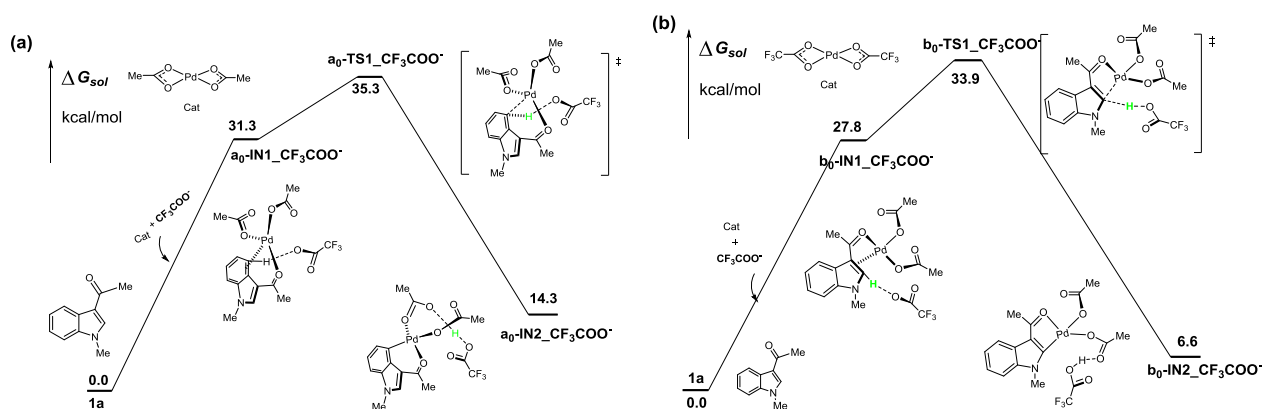


Figure S6. The pathway of C-H bond activation of the $\text{Pd}(\text{OAc})_2$ -catalyzed with the participation of CF_3COO^- anion. **(a)** C4-H activation. **(b)** C2-H activation.

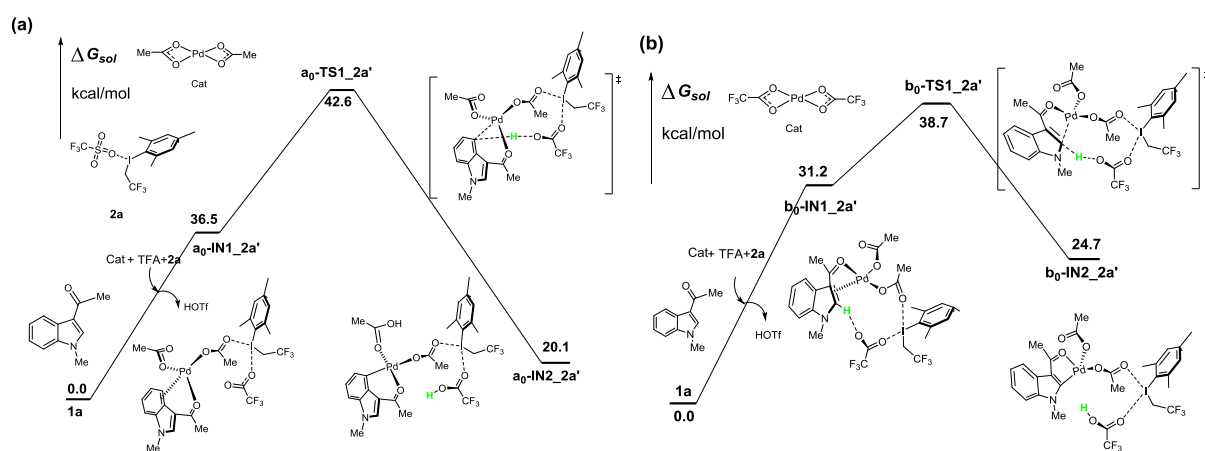
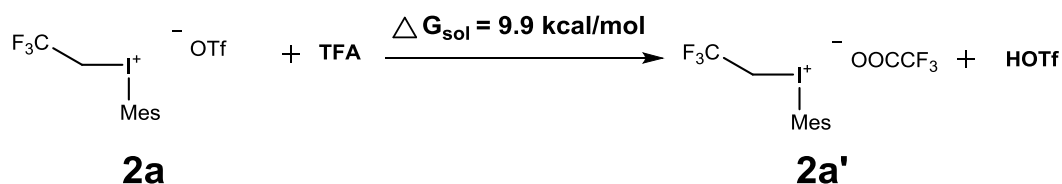


Figure S7. The pathway of C-H bond activation of the $\text{Pd}(\text{OAc})_2$ -catalyzed with the participation of additive TFA and substrate **2a**. **(a)** C4-H activation. **(b)** C2-H activation.



Scheme S2. Generation Pathways of **2a'** from substrate **2a** with additive TFA, along with the Calculated Free Energy Changes (kcal/mol).

2. The C-H activation catalyzed by $\text{Pd}(\text{TFA})_2$ and $\text{Pd}(\text{OAc})(\text{TFA})$, the oxidative addition and the reductive elimination catalyzed by $\text{Pd}(\text{TFA})_2$, as well as the underlying basis of the improvement of the performance of $\text{Pd}(\text{TFA})_2$ as the catalyst

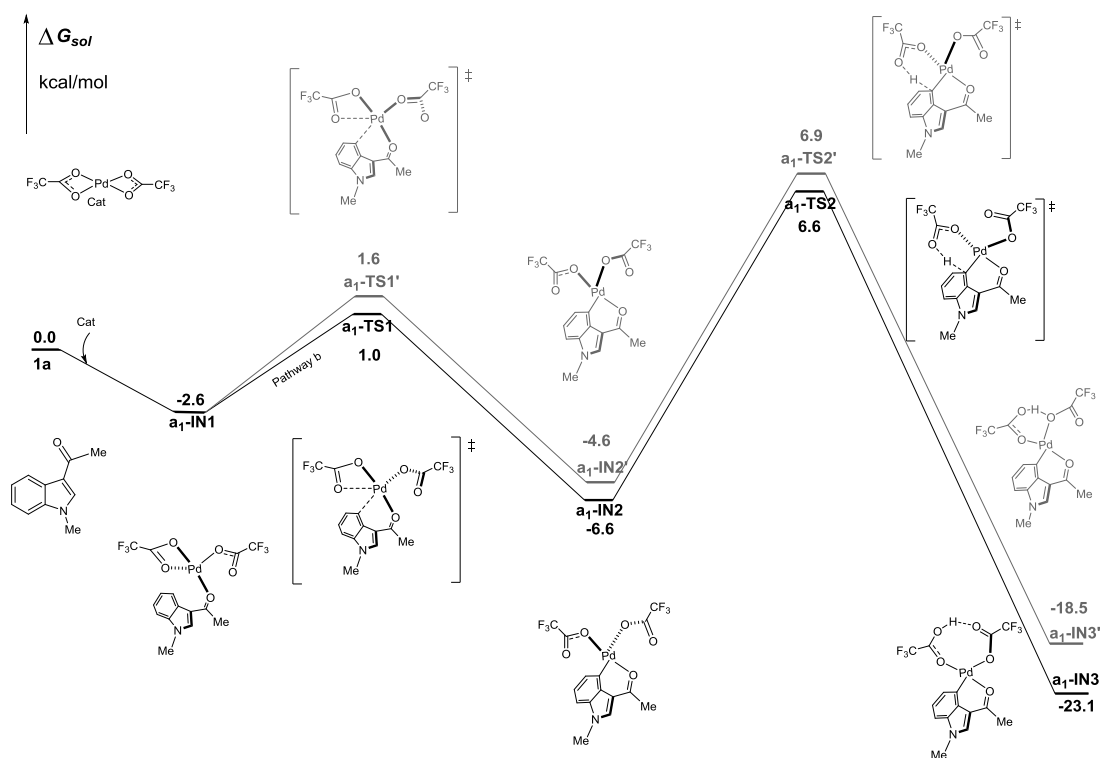


Figure S8. The other possible isomers in pathway **b** in C4-H activation in indole with $\text{Pd}(\text{TFA})_2$ as efficient catalyst.

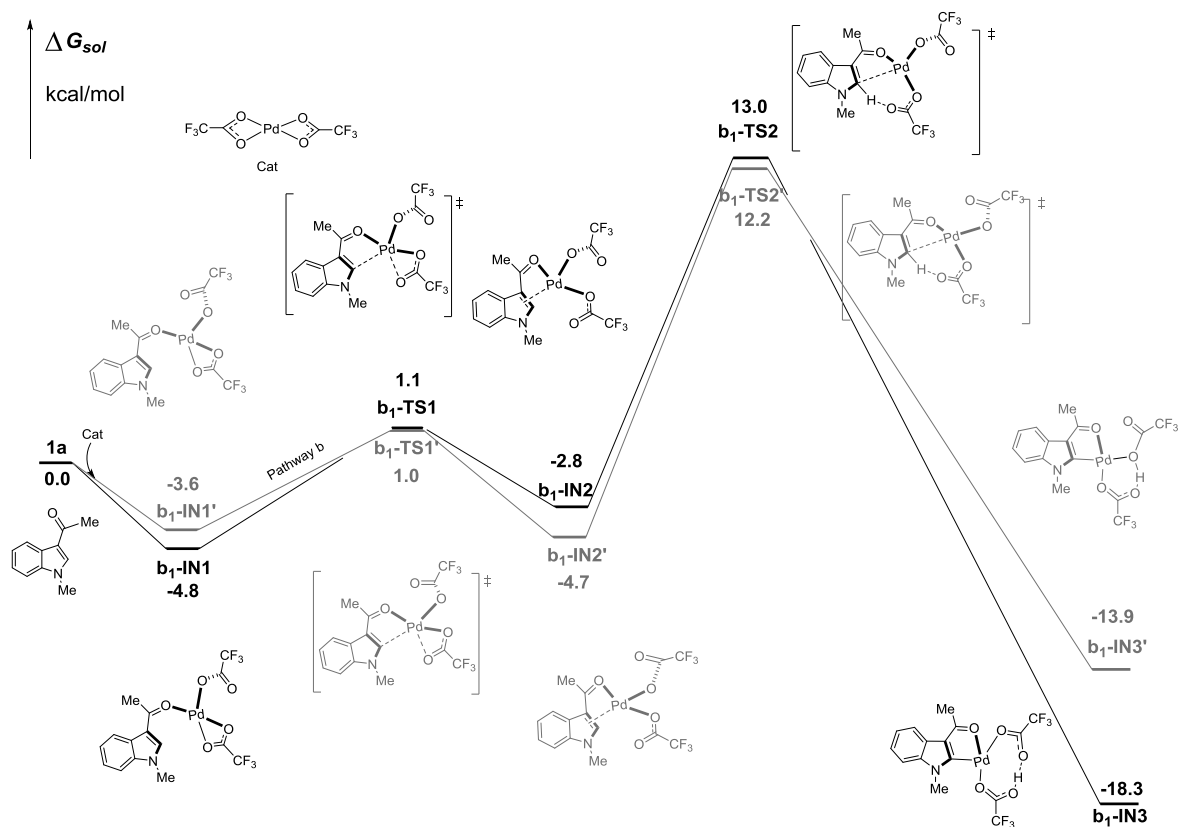


Figure S9. Three possible pathways of C2-H activation in indole with $\text{Pd}(\text{TFA})_2$ as efficient catalyst.

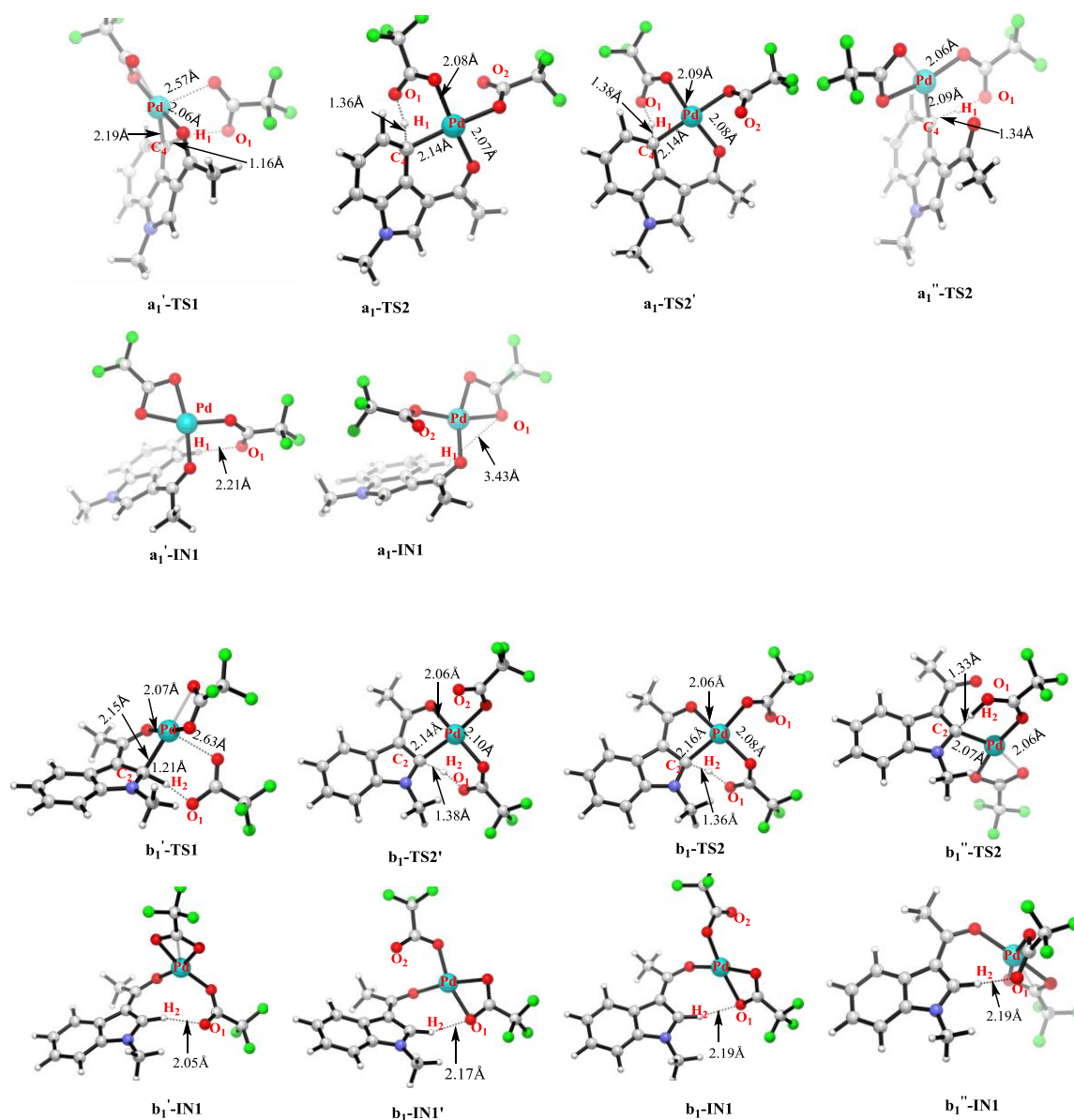
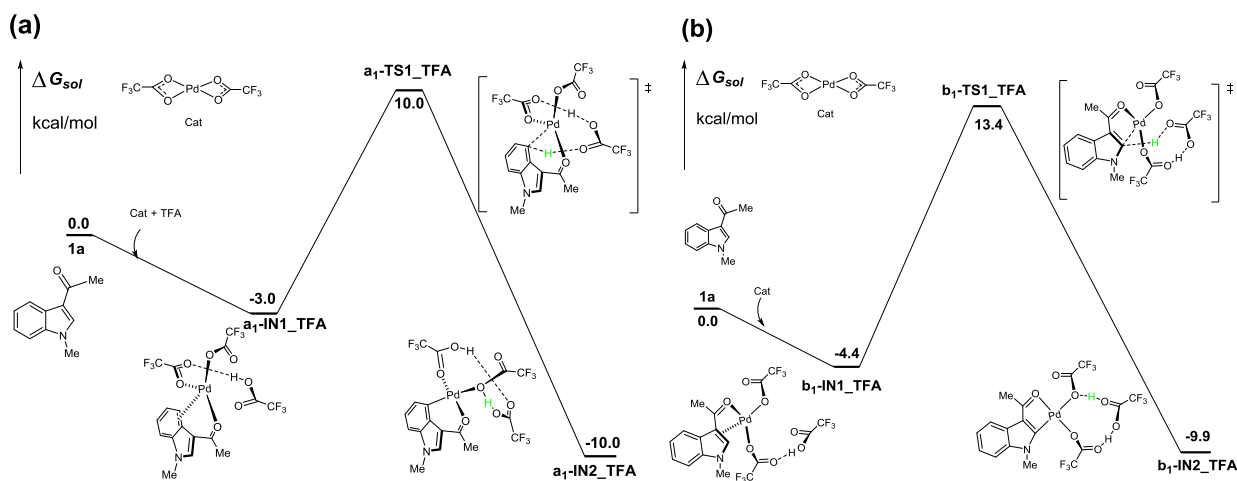


Figure S10. The partial bond length and geometry of local minimal and transition state in the Pd(TFA)₂-catalyzed C4 & C2-H activation.



(c)

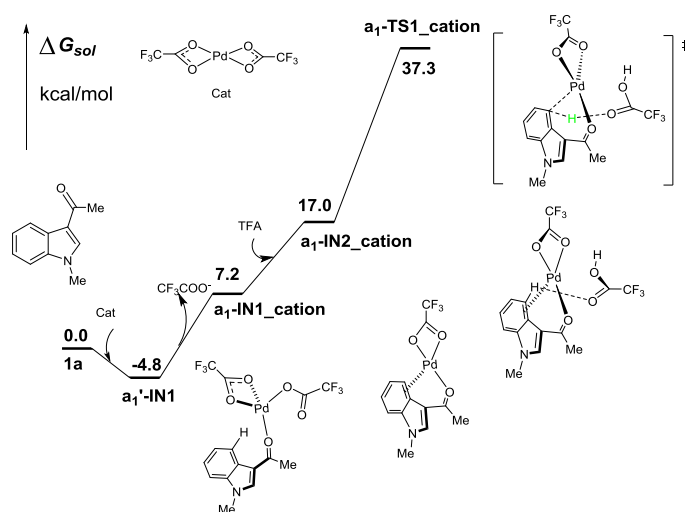


Figure S11. (a) The pathway of C4-H bond activation of the $Pd(TFA)_2$ -catalyzed with the participation of additive TFA acid. C-H activation. (b) The pathway of C2-H bond activation of the $Pd(TFA)_2$ -catalyzed with the participation of additive TFA acid. (c) The pathway of C4-H bond activation catalyzed by $[R-Pd(CF_3COO)]^+$ species (R =substrate **1a**) with the participation of additive TFA acid.

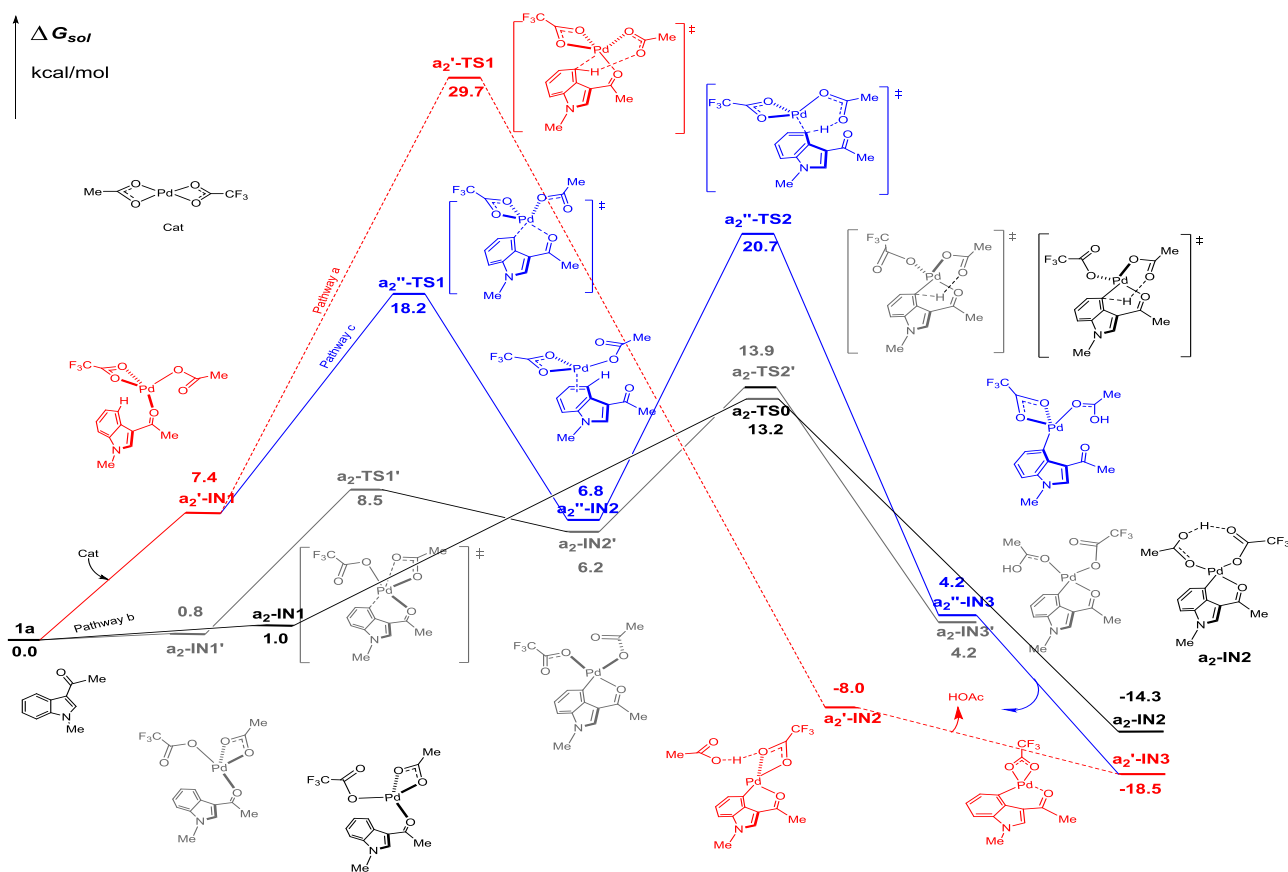


Figure S12. Three possible pathways of C4-H activation in indole with $Pd(OAc)(TFA)$ as efficient catalyst.

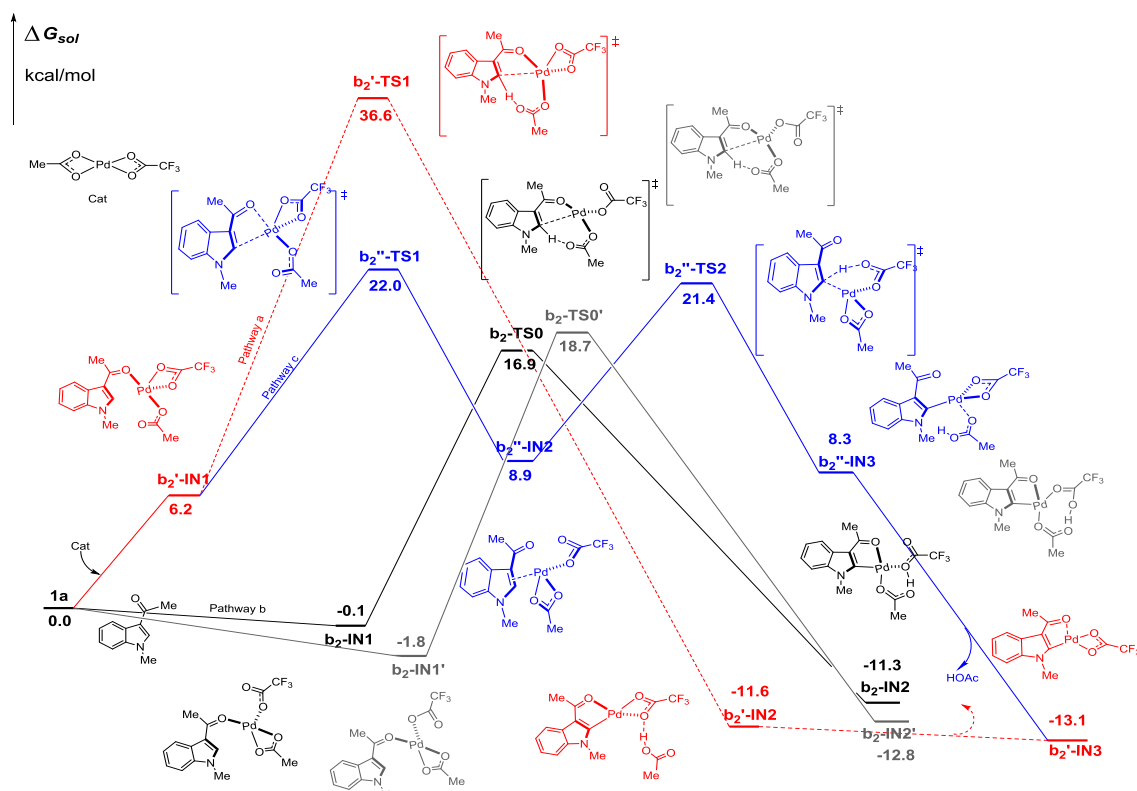


Figure S13. Three possible pathways of C2-H activation in indole with Pd(OAc)(TFA) as efficient catalyst.

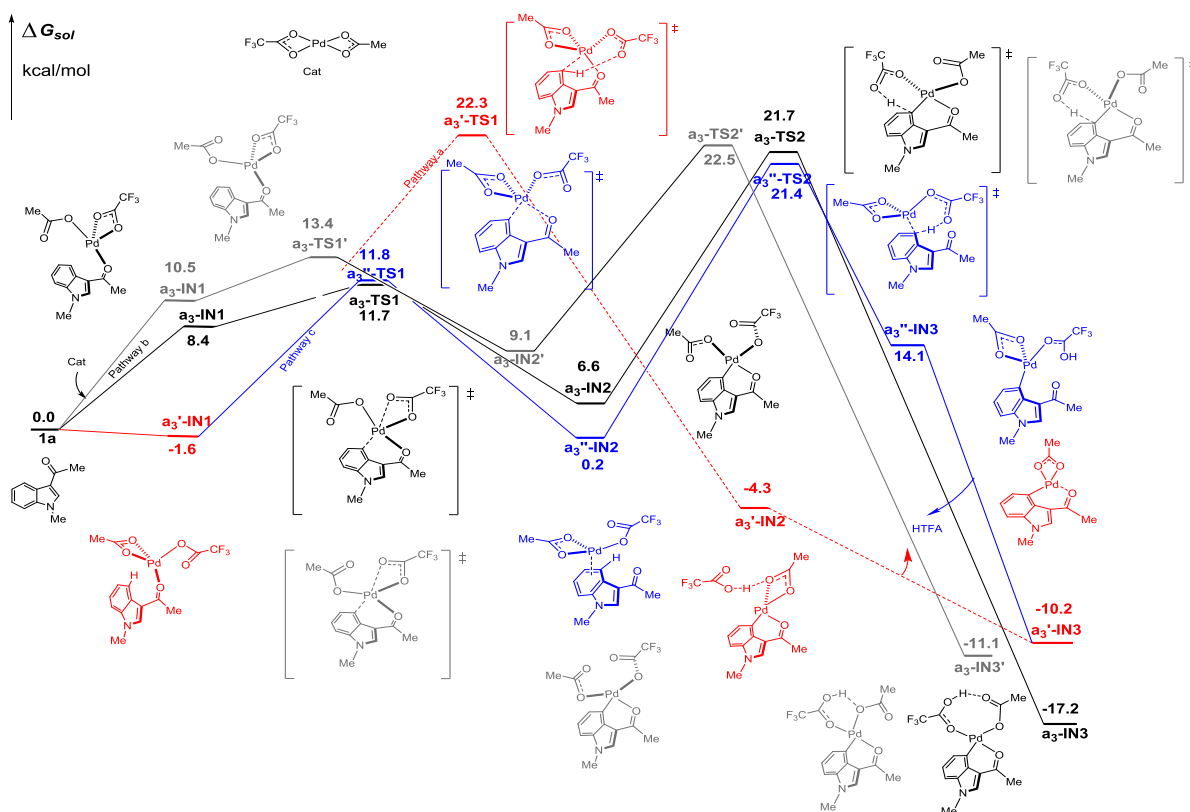


Figure S14. Three possible pathways of C4-H activation in indole with Pd(TFA)(OAc) as efficient catalyst.

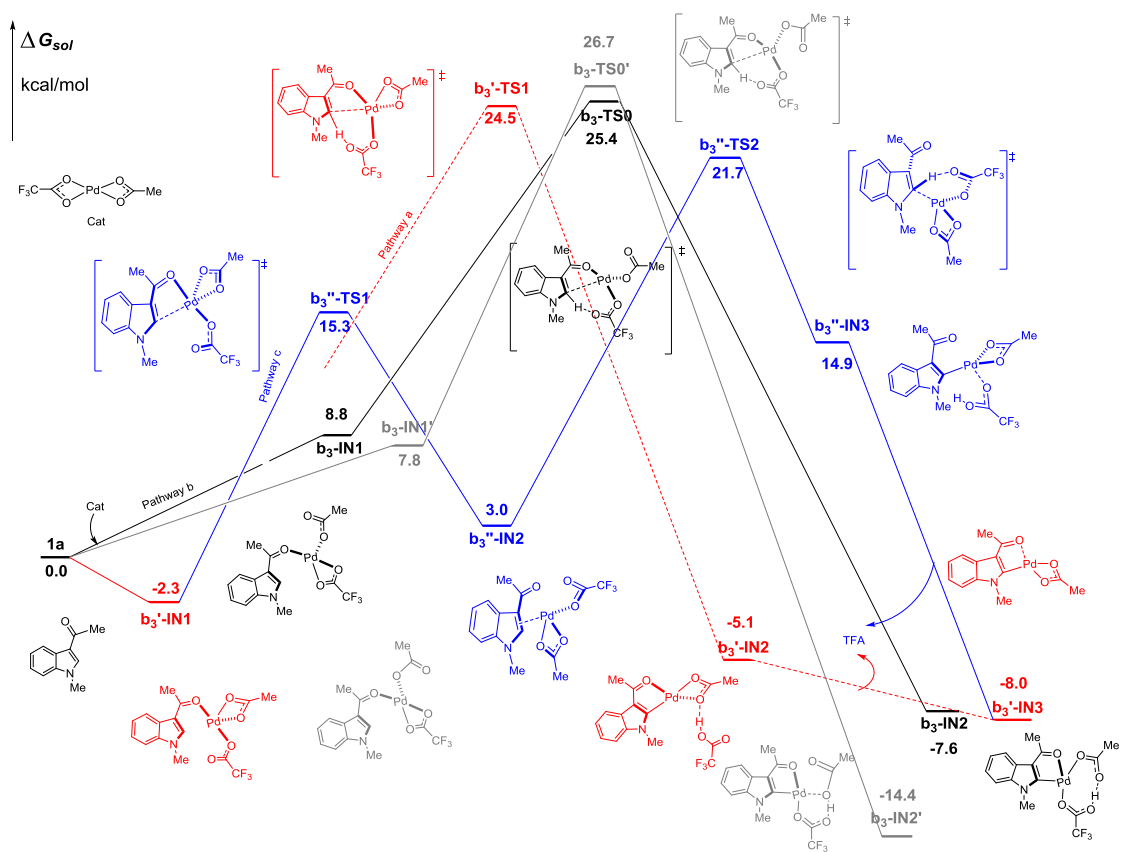


Figure S15. Three possible pathways of C2-H activation in indole with Pd(TFA)(OAc) as efficient catalyst.

Table S1. Comparison of overall free energies of TS including single-point energies at different theoretical levels in the C2 & C4-H activation under various Pd-catalysts (kcal/mol).

C-H activation	Pathway a			Pathway b			Pathway c		
The free energies	C2-H	C4-H	Δ	C2-H	C4-H	Δ	C2-H	C4-H	Δ
Pd(OAc) ₂	37.0/36.6 ^a	35.8/36.3 ^a	1.3/0.3 ^a	30.1/30.4	27.2/28.3	2.9/2.0	25.5/24.8	25.8/25.1	-0.4/-0.3
	34.0/34.0 ^b	31.6/32.7 ^b	2.4/1.3 ^b	25.1/24.9	21.1/22.4	4.0/2.5	20.7/20.1	19.8/19.5	0.9/0.7
Pd(TFA)(OAc)	24.5/25.2	22.3/23.7	2.2/1.4	25.4/25.9	21.7/23.4	3.7/2.4	21.7/21.6	21.4/21.2	0.4/0.4
	22.0/23.0	15.6/17.8	6.3/5.3	20.2/20.8	15.3/17.3	4.9/3.5	16.1/15.9	14.8/14.9	1.3/1.0
Pd(OAc)(TFA)	36.6/37.1	29.7/31.0	6.9/6.1	16.9/18.6	13.2/16.1	3.6/2.4	21.4/21.1	20.7/20.6	0.7/0.6
	28.5/29.4	25.9/27.8	2.6/1.7	12.6/14.2	7.9/10.7	4.7/3.5	16.6/16.3	14.7/14.8	1.9/1.5
Pd(TFA) ₂	18.8/18.8	15.9/	2.9/	13.0/15.0	6.6/10.0	6.4/5.0	15.4/15.8	14.0/14.7	1.4/1.1
	16.3/17.7	10.5/13.3	5.8/4.4	7.4/9.5	0.6/4.1	6.8/5.4	9.4/9.8	7.3/8.2	2.2/1.7
Pd(OAc)(OTf)	35.2/35.6	29.5/30.6	5.6/5.0	14.0/16.0	9.1/11.9	4.9/4.0	20.1/19.6	18.2/18.0	1.9/1.6
	27.1/28.1	25.9/27.8	1.2/0.3	10.5/12.6	3.9/6.9	6.6/5.7	14.3/14.2	11.6/11.9	2.7/2.3
Pd(OTf)(OAc)	16.6/18.5	11.0/14.1	5.6/4.4	29.3/30.4	25.7/28.1	3.6/2.4	13/28.3	26.5/28.0	-13.5/0.3
	15.2/17.4	7.8/11.2	7.4/6.2	23.6/25.1	18.9/21.6	4.7/3.5	19.5/21.4	18.2/20.3	1.3/1.1
Pd(TFA)(OTf)	18.6/19.2	15.0/16.8	3.6/2.4	9.3/11.4	2.4/5.8	6.8/5.5	13.8/14.1	11.8/11.7	2.0/2.4
	15.5/17.0	/11.8	/5.2	4.8/7.1	-3.5/0.0	8.3/7.1	/7.3	/4.7	3.6/2.6
Pd(OTf)(TFA)	10.9/13.2	4.8/8.1	6.1/5.0	16.3/19.1	10.3/14.6	6/4.5	20.0/22.0	18.2/20.5	1.8/1.5
	9.2/11.9	1.0/4.9	8.2/7.1	10.4/13.4	3.7/8.1	6.8/5.3	12.0/14.4	9.2/12.1	2.8/2.3
Pd(OTf) ₂	9.3/11.6	3.3/6.5	6.0/5.1	12.5/15.7	5.1/9.1	7.4/6.6	19.1/21.2	16.6/18.6	2.5/2.6
	6.3/9.6	-1.7/2.4	8.0/7.2	6.7/10.3	-2.3/2.1	9/8.3	10.1/12.8	6.3/9.1	3.9/3.8
The energy barriers	C2-H	C4-H	Δ	C2-H	C4-H	Δ	C2-H	C4-H	Δ
Pd(OAc) ₂	37.0/36.6	35.8/36.3	1.3/0.3	30.1/30.4	27.2/28.3	2.9/2.0	25.5/24.8	25.8/25.1	-0.4/-0.3
	34.0/34.0	31.6/32.7	2.4/1.3	25.1/24.9	21.1/22.4	4.0/2.5	20.7/20.2	19.8/19.5	0.9/0.7
Pd(TFA)(OAc)	26.8/27.3	23.9/24.8	2.9/2.5	16.6/18.0	15.1/15.8	1.5/2.2	24.0/23.7	22.9/22.3	1.1/1.4
	30.0/31.0	24.1/25.6	5.9/5.4	19.6/20.8	16.8/17.7	2.9/3.1	24.2/23.9	23.4/22.8	0.8/1.1
Pd(OAc)(TFA)	36.6/37.1	29.7/31.0	6.9/6.1	16.9/18.4	13.2/16.1	3.7/2.3	21.4/21.1	20.7/20.6	0.7/0.6
	28.5/29.4	25.9/28.0	2.6/1.5	20.4/21.6	15.5/17.2	4.9/4.4	17.4/16.8	15.0/14.9	2.5/2.0

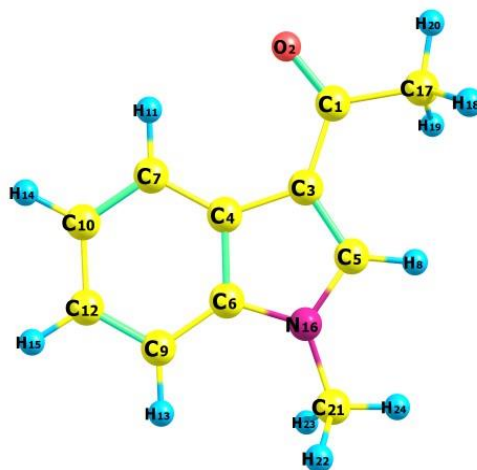
Pd(TFA) ₂	25.1/25.4	20.7/	4.5/	17.8/18.9	13.2/14.1	4.6/4.8	18.3/17.8	19.0/18.3	-0.8/-0.4
	28.3/29.2	22.6/24.2	5.7/5.0	18.1/19.5	15.3/16.3	2.8/3.2	22.6/21.7	19.3/18.8	3.3/2.9
Pd(OAc)(OTf)	35.2/35.6	29.5/30.6	5.6/5.0	17.0/18.0	11/.012.3	6.0/5.7	20.1/19.6	18.2/18.0	1.9/1.6
	28.9/30.4	25.9/29.7	2.9/0.8	21.4/21.9	14.6/15.2	6.8/6.7	17.7/17.4	14.3/14.3	3.5/3.1
Pd(OTf)(OAc)	20.6/21.7	13.6/15.8	7.0/5.9	29.3/30.4	25.7/28.1	3.6/2.4	20.8/28.3	26.9/28.0	-6/0.3
	25.2/26.5	18.0/20.1	7.2/6.4	23.6/25.1	18.9/22.1	4.7/3.0	28.2/28.0	25.3/25.8	2.9/2.2
Pd(TFA)(OTf)	25.9/25.8	20.7/21.5	5.2/4.4	16.6/16.2	10.1/10.9	6.5/5.2	18.2/18.3	17.7/17.1	0.5/1.1
	28.8/29.8	/24.2	28.8/5.6	21.5/20.6	14.9/15.3	6.7/5.3	0.3/22.0	-0.6/17.4	0.9/4.7
Pd(OTf)(TFA)	18.7/18.4	10.3/12.4	8.4/6.0	22.9/23.2	15.6/17.2	7.3/6.0	24.1/26.7	23.6/24.0	0.5/2.6
	25.4/24.6	14.5/16.5	10.8/8.1	26.2/26.3	19.1/20.4	7.1/5.8	22.9/23.1	21.4/22.1	1.5/1.0
Pd(OTf) ₂	18.0/18.5	10.3/11.6	7.7/6.9	22.1/21.7	14.5/15.5	7.6/6.3	23.9/25.1	24.1/24.2	-0.1/0.9
	21.1/22.4	13.5/15.2	7.6/7.3	26.0/25.3	17.9/18.4	8.2/6.9	21.9/23.2	21.2/21.5	0.6/1.7

^a the left of “/” is from the B3LYP/BS2 level, the right of “/” is from the B3LYP/BS1 level ($\Delta G_{sol}/\Delta G_{sol\ B3LYP}$);

^b the left of “/” is from the M06-2X/BS2 level, the right of “/” is from the M06-2X /BS1 level ($\Delta G_{sol\ M06-2X_Larg}/\Delta G_{sol\ M06-2X}$);

The analysis on the reaction mechanism was mainly based on the free energies, i.e., ΔG_{sol} , including free energy of solvation in DCM at 298K from M06-2X/BS1 level (BS1, denoting 6-31G(d)+LANL2DZ after), electronic energies from B3LYP/BS2 level (BS2, denoting 6-311+G(d,p)+SDD after) and the zero-point vibration energy (ZPVE) as well as thermal corrections from B3LYP/BS1 level based on gas-phase structures. In addition, we have pointed here $\Delta G_{sol\ B3LYP}$ representing relative Gibbs free energies with electronic energies from B3LYP/BS1; $\Delta G_{sol\ M06-2X}$ representing relative Gibbs free energies with electronic energies from M06-2X/BS1 level; $\Delta G_{sol\ M06-2X_Larg}$ representing relative Gibbs free energies with electronic energies from M06-2X/BS2 level; $\Delta G_{sol\ B3LYP+sol}$ representing relative Gibbs free energies based on solvent-phase structures; $\Delta G_{sol\ D_1}$ represented the results from the optimized geometry with B3LYP-D3(BJ)/BS1 level, and the electronic energy from B3LYP/BS2 level; $\Delta G_{sol\ D_2}$ represented the results from the optimized geometry with B3LYP-D3(BJ)/BS1 level, and the electronic energy from B3LYP-D3(BJ)/BS2 level; $\Delta G_{sol\ D_3}$ represented the results from the optimized geometry with B3LYP-D3(BJ)/BS1 level, and the electronic energy from M06-2X/BS2 level; $\Delta G_{sol\ M06-2X_opt}$ represented the results from the optimized geometry with M06-2X/BS1 level, and the electronic energy from M06-2X/BS2 level.

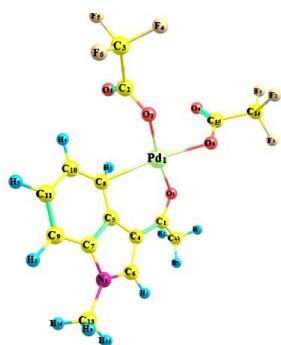
The results of M06-2X ($\Delta G_{sol\ M06-2X}$) is consistent with that of B3LYP (ΔG_{sol}), as shown in Table.S1. For example, in pathway **b**, the differences between of free energies of the highest points of C4-H and C2-H activation are 1.5, 2.8 and 5.4 kcal/mol for Pd(OAc)₂, Pd(OAc)(TFA) and Pd(TFA)₂ respectively. They are consistent with B3LYP results (1.0, 3.0 and 6.4 kcal/mol). In addition, the influence of basis set on relative energies is also small, as shown in Figure S16 ~ S17. For example, in situation of small basis set (BS1, 6-31G(d)+LANL2DZ), this difference between C4-H and C2-H activation in pathway **b** catalyzed by Pd(TFA)₂ is 5.0 kcal/mol (**b1-TS2**→**a1-TS2**, $\Delta G_{sol\ B3LYP}$), which is also consistent with larger basis set (BS2, 6-311+G(d,p)+SDD) results (6.4 kcal/mol). Besides the consideration of both functional and basis set, for Pd(TFA)₂, we have re-optimized all the stationary points in pathway **b** for both C2-H and C4-H activation in DCM solvent. The difference between gas-phase geometry and that in solvent are actually small (seen in Table. S2 ~ S6). Thus, these results completely support the regioselectivity of C4 over C2 could be achieved by Pd(TFA)₂.



1a

Table. S2 The comparison of bond distances of **1a** at both gas and solvent phase with the theoretical level of B3LYP/BS1.

	Distances _{-gas}	Distances _{-sol}	Error (Dis _{-sol} - Dis _{-gas})
C1-O2	1.227	1.234	0.007
C1-C17	1.525	1.521	-0.004
C1-C3	1.465	1.460	-0.005
C3-C5	1.384	1.389	0.005
C3-C4	1.448	1.449	0.001
C6-C4	1.418	1.420	0.002
C6-N16	1.392	1.391	-0.001
C5-H8	1.369	1.363	-0.006
N16-C21	1.450	1.455	0.005
C7-C4	1.404	1.405	0.001
C6-C9	1.399	1.399	0.000
C9-H13	1.084	1.084	0.000
Average			0.000

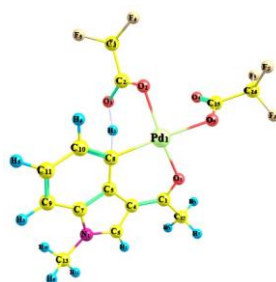


a₁-IN2

Table. S3 The comparison of bond distances of **a₁-IN2** at both gas and solvent phase with the theoretical level of B3LYP/BS1.

	Distance _{-gas}	Distance _{-sol}	Error (Dis _{-sol} - Dis _{-gas})
Pd1-O1	2.097	2.091	-0.006
Pd1-O2	2.002	2.020	0.018

Pd1-O5	2.011	2.058	0.047
Pd1-C8	2.454	2.315	-0.139
O2-C2	1.294	1.290	-0.004
O3-C2	1.224	1.223	-0.001
C2-C3	1.551	1.552	0.001
C3-F4	1.241	1.348	0.107
C3-F5	1.339	1.342	0.003
C3-F6	1.355	1.352	-0.003
O4-C15	1.216	1.222	0.006
O5-C15	1.301	1.288	-0.013
C15-C14	1.555	1.553	-0.002
C14-F1	1.338	1.342	0.004
C14-F2	1.345	1.350	0.005
C14-F3	1.351	1.352	0.001
C1-O1	1.251	1.262	0.011
C1-C12	1.508	1.500	-0.008
C12-H6	1.098	1.099	0.001
C12-H7	1.092	1.092	0.000
C12-H8	1.094	1.094	0.000
C1-C4	1.442	1.435	-0.007
C4-C5	1.446	1.437	-0.009
C4-C6	1.393	1.399	0.006
C6-N1	1.357	1.351	-0.006
N1-C7	1.396	1.397	0.001
C5-C7	1.415	1.415	0.000
C5-C8	1.410	1.418	0.008
C8-C10	1.399	1.412	0.013
C10-C11	1.404	1.398	-0.006
C9-C11	1.394	1.401	0.007
C7-C9	1.396	1.393	-0.003
C9-H3	1.086	1.086	0.000
C11-H5	1.085	1.085	0.000
C10-H4	1.084	1.084	0.000
C8-H2	1.107	1.100	-0.007
C6-H1	1.081	1.082	0.001
N1-C13	1.455	1.460	0.005
Average			0.001



a₁-TS2

Table. S4 The comparison of bond distances of **a₁-TS2** at both gas and solvent phase with the theoretical level of B3LYP/BS1.

	Distance _{-gas}	Distance _{-sol}	Error (Dis _{-sol} - Dis _{-gas})
Pd1-O1	2.074	2.060	-0.014
Pd1-O2	2.080	2.101	0.021
Pd1-O5	2.044	2.099	0.055
Pd1-C8	2.144	2.101	-0.043
O2-C2	1.261	1.257	-0.004
O3-C2	1.261	1.264	0.003
C2-C3	1.544	1.543	-0.001
C3-F4	1.334	1.337	0.003
C3-F5	1.337	1.341	0.004
C3-F6	1.352	1.348	-0.004
O4-C15	1.222	1.227	0.005
O5-C15	1.293	1.282	-0.011
C15-C14	1.552	1.553	0.001
C14-F1	1.340	1.344	0.004
C14-F2	1.348	1.352	0.004
C14-F3	1.352	1.353	0.001
C1-O1	1.253	1.265	0.012
C1-C12	1.510	1.505	-0.005
C12-H6	1.097	1.091	-0.006
C12-H7	1.092	1.097	0.005
C12-H8	1.092	1.095	0.003
C1-C4	1.437	1.426	-0.011
C4-C5	1.444	1.439	-0.005
C4-C6	1.396	1.405	0.009
C6-N1	1.355	1.346	-0.009
N1-C7	1.398	1.399	0.001
C5-C7	1.414	1.414	0.000
C5-C8	1.414	1.414	0.000
C8-C10	1.410	1.417	0.007
C10-C11	1.404	1.402	-0.002
C9-C11	1.394	1.397	0.003
C7-C9	1.396	1.394	-0.002
C9-H3	1.086	1.086	0.000
C11-H5	1.086	1.086	0.000
C10-H4	1.086	1.087	0.001
C8-H2	1.358	1.373	0.015
C6-H1	1.081	1.081	0.000
N1-C13	1.455	1.459	0.004
Average			0.001

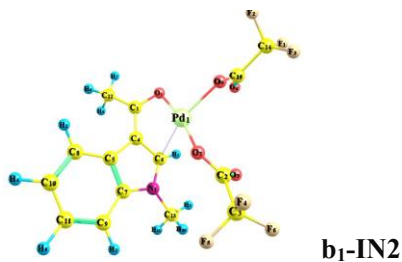
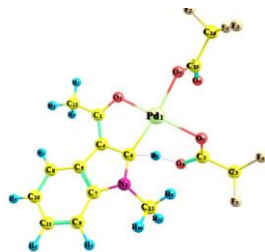


Table. S5 The comparison of bond distances of **b₁-IN2** at both gas and solvent phase with the theoretical level of B3LYP/BS1.

	Distance _{-gas}	Distance _{-sol}	Error (Dis _{-sol} - Dis _{-gas})
Pd1-O1	2.074	2.109	0.035
Pd1-O2	2.009	2.025	0.016
Pd1-O5	2.014	2.066	0.052
Pd1-C6	2.544	2.437	-0.107
O2-C2	1.289	1.291	0.002
O3-C2	1.230	1.232	0.002
C2-C3	1.549	1.551	0.002
C3-F4	1.338	1.344	0.006
C3-F5	1.355	1.358	0.003
C3-F6	1.339	1.341	0.002
O4-C15	1.216	1.223	0.007
O5-C15	1.302	1.289	-0.013
C15-C14	1.555	1.552	-0.003
C14-F1	1.338	1.342	0.004
C14-F2	1.349	1.352	0.003
C14-F3	1.346	1.350	0.004
C1-O1	1.258	1.257	-0.001
C1-C12	1.502	1.486	-0.016
C12-H6	1.093	1.098	0.005
C12-H7	1.092	1.092	0.000
C12-H8	1.098	1.096	-0.002
C1-C4	1.446	1.475	0.029
C4-C5	1.442	1.453	0.011
C4-C6	1.413	1.432	0.019
C6-N1	1.361	1.347	-0.014
N1-C7	1.387	1.399	0.012
C5-C7	1.421	1.415	-0.006
C5-C8	1.408	1.402	-0.006
C8-C10	1.387	1.391	0.004
C10-C11	1.412	1.408	-0.004
C9-C11	1.388	1.393	0.005
C7-C9	1.400	1.396	-0.004
C9-H3	1.085	1.085	0.000
C11-H5	1.086	1.086	0.000

C10-H4	1.086	1.086	0.000
C8-H2	1.085	1.085	0.000
C6-H1	1.092	1.082	-0.010
N1-C13	1.462	1.461	-0.001
Average			0.001



b₁-TS2

Table. S6 The comparison of bond distances of **b₁-TS2** at both gas and solvent phase with the theoretical level of B3LYP/BS1.

	Distance _{-gas}	Distance _{-sol}	Error (Dis _{-sol} - Dis _{-gas})
Pd1-O1	2.064	2.055	-0.009
Pd1-O2	2.082	2.096	0.014
Pd1-O5	2.021	2.061	0.040
Pd1-C6	2.157	2.119	-0.038
O2-C2	1.259	1.257	-0.002
O3-C2	1.266	1.267	0.001
C2-C3	1.544	1.543	-0.001
C3-F4	1.332	1.339	0.007
C3-F5	1.354	1.348	-0.006
C3-F6	1.335	1.339	0.004
O4-C15	1.220	1.224	0.004
O5-C15	1.299	1.288	-0.011
C15-C14	1.552	1.552	0.000
C14-F1	1.339	1.342	0.003
C14-F2	1.349	1.351	0.002
C14-F3	1.348	1.351	0.003
C1-O1	1.266	1.273	0.007
C1-C12	1.502	1.495	-0.007
C12-H6	1.097	1.097	0.000
C12-H7	1.091	1.092	0.001
C12-H8	1.095	1.096	0.001
C1-C4	1.433	1.431	-0.002
C4-C5	1.439	1.436	-0.003
C4-C6	1.419	1.423	0.004
C6-N1	1.374	1.375	0.001
N1-C7	1.390	1.387	-0.003
C5-C7	1.422	1.424	0.002
C5-C8	1.407	1.409	0.002
C8-C10	1.388	1.387	-0.001

C10-C11	1.411	1.414	0.003
C9-C11	1.388	1.387	-0.001
C7-C9	1.401	1.403	0.002
C9-H3	1.085	1.085	0.000
C11-H5	1.086	1.086	0.000
C10-H4	1.086	1.086	0.000
C8-H2	1.085	1.085	0.000
C6-H1	1.364	1.380	0.016
N1-C13	1.460	1.462	0.002
Average			0.001

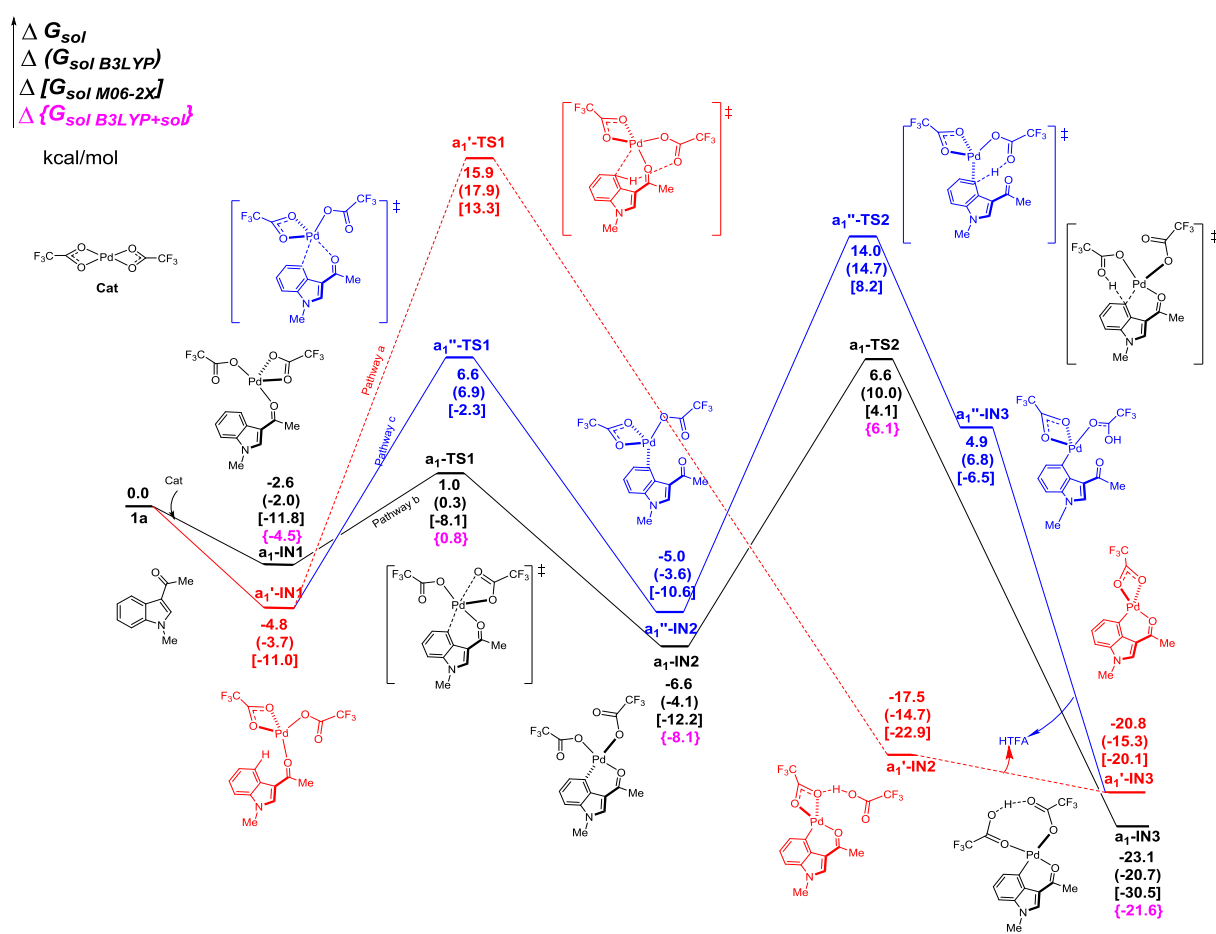


Figure S16. The comparison of three possible pathways of C4-H activation in indole with Pd(TFA)₂ as efficient catalyst at various functionals, as well as the comparison between gas- and solvent-phase geometry.

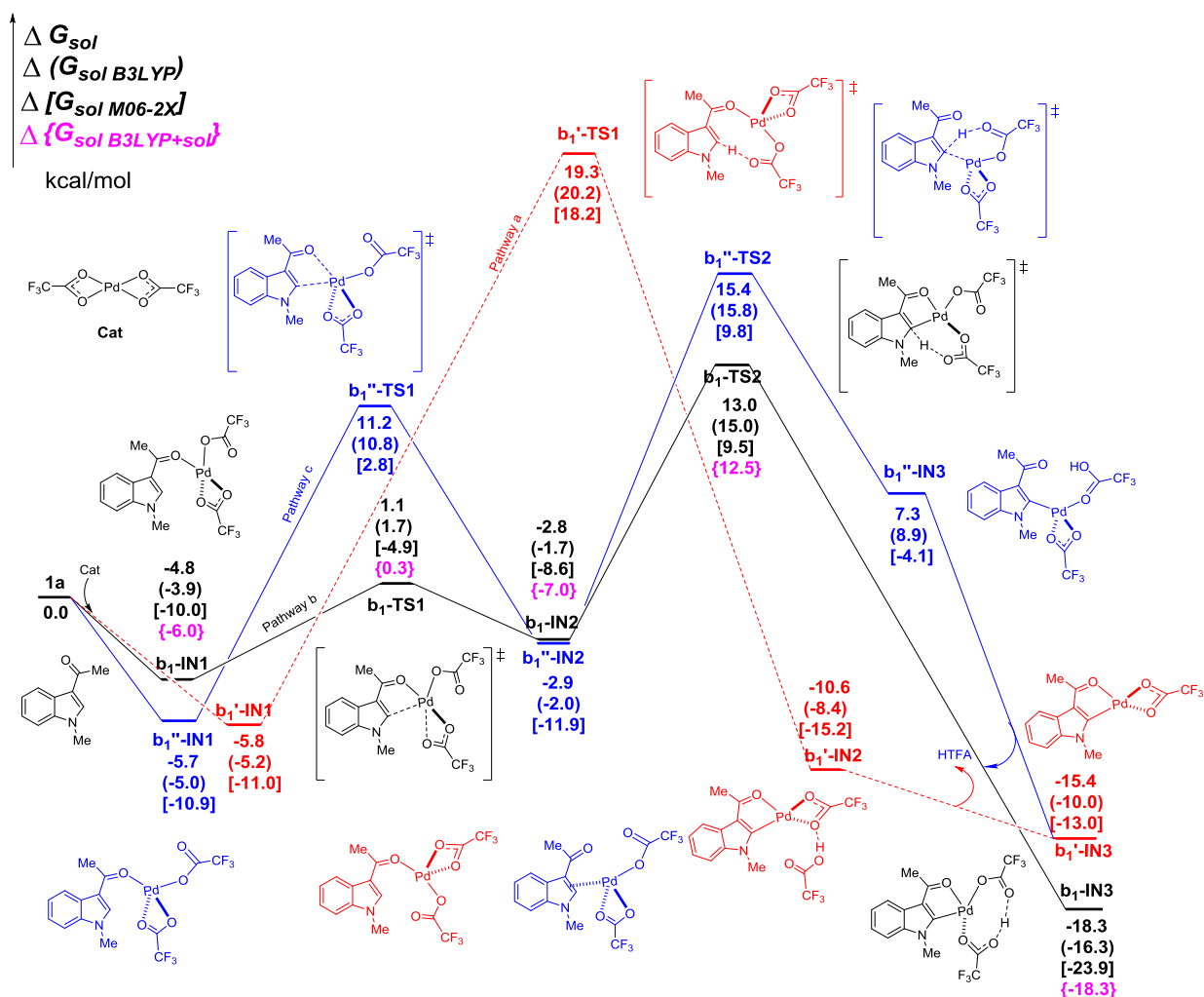


Figure S17. Three possible pathways of C2-H activation in indole with $\text{Pd}(\text{TFA})_2$ as efficient catalyst.

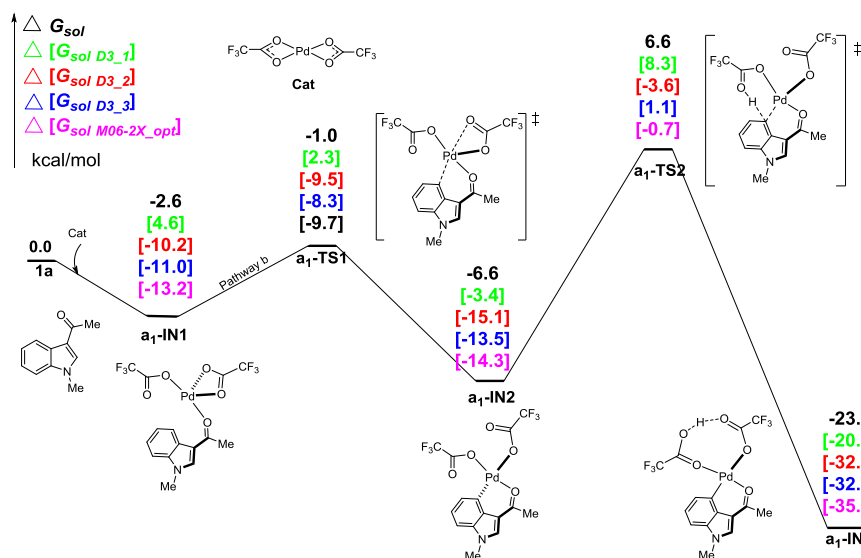


Figure S18. The comparison of the free energies(kcal/mol) from different optimized-geometries with three B3LYP, B3LYP-D3(BJ) and M06-2X methods along pathway **b** of C4-H activation catalyzed by $\text{Pd}(\text{TFA})_2$.

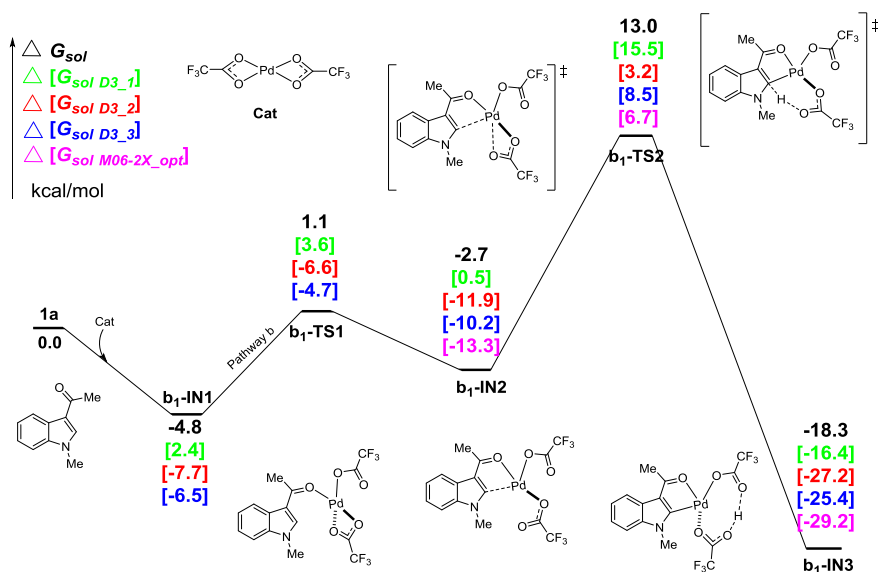


Figure S19. The comparison of the free energies(kcal/mol) from different optimized-geometries with three B3LYP, B3LYP-D3(BJ) and M06-2X methods along pathway **b** of C2-H activation catalyzed by Pd(TFA)₂.

Table S7. The comparison of the energy barriers among three methods B3LYP and B3LYP-D3(BJ) and M06-2X and the corresponding difference along pathway **b** of C4/C2-H activation catalyzed by Pd(TFA)₂ (kcal/mol).

	(kcal/mol)	ΔG_{sol}	$\Delta G_{sol D_1}$	$\Delta G_{sol D_2}$	$\Delta G_{sol D_3}$	$\Delta G_{sol M06-2X_opt}$
Barrier	C4	13.2	11.7	11.5	14.6	13.6
	C2	17.8	15.5	15.1	18.7	20.0
Difference	C4	0.0	-1.5	-1.8	1.4	0.4
	C2	0.0	-2.3	-2.7	1.0	2.2

For some important pathways in C4/C2-H bond activation process catalyzed by Pd(TFA)₂, we have reoptimized local minimal geometries and transition states with both B3LYP-D3(BJ) and M06-2X methods. The results suggest that the differences of geometry and the energy barrier among different methods are small (Figure S18 ~ S19 and Table S7 ~ S21).

In the aspect of energy barrier, the results obtained from B3LYP, B3LYP-D3(BJ) and M06-2X methods are close to each other as shown in Figure S18 ~ S19 and Table S7. The corresponding differences are small (in Table S7). For example, in pathway **b** of C4-H activation, the energy barriers from B3LYP, B3LYP-D3(BJ), and M06-2X (ΔG_{sol} , $\Delta G_{sol D_2}$, and $\Delta G_{sol M06-2X_opt}$) levels are 13.2, 11.5, and 13.6 kcal/mol respectively. The corresponding differences are 0.4 ~ 1.8 kcal/mol which are permissible. Similar results exist in C2-H activation too (in Table S7). Thus, the results from B3LYP method should be reliable.

In the aspect of optimized geometries, the differences from various methods are small too (Table S8 ~ S21). As shown Table S8, the average differences of inter-atomic distances (denotes as Ave Δ (Δ =

Δ_1 or Δ_2)) lie within the range of 0.000 ~ 0.009 Å. The corresponding average deviations (denotes as Ave Δ_D) are of the range of 0.000 ~ 0.020 Å. For some important inter-atomic distances, as shown Table S9, the corresponding Ave Δ and Ave Δ_D values lie within the range of 0.000 ~ 0.021 Å and 0.000 ~ 0.045 Å respectively. The calculated details of three methods (B3LYP, B3LYP-D3(BJ) M06-2X) are provided in Table S10 ~ S21.

Therefore, in this system, the differences of the energy barriers and the optimized geometries from B3LYP method are small compared to both B3LYP-D3(BJ) and M06-2X, and thus the following discussion are mainly based on the optimized-geometry at B3LYP level.

Table S8. The difference (denotes as Δ_1) of the optimized-geometries between B3LYP and B3LYP-D3(BJ) methods and the corresponding difference (denotes as Δ_2) between B3LYP and M06-2X methods, including maximum difference (denotes as Max Δ_1 or Δ_2) and average difference (denotes as Ave Δ_1 or Δ_2) and Average Deviation (denotes as Ave Δ_D) (Å).

Distances(Å)	$\Delta_1(\text{Å})$			$\Delta_2(\text{Å})$		
	Max Δ_1	Ave Δ_1	Ave Δ_D	Max Δ_2	Ave Δ_2	Ave Δ_D
1a	0.003	0.000	0.001	0.009	0.003	0.004
Pd(TFA)₂	0.002	0.000	0.001	0.015	0.007	0.009
a₁-IN1	0.016	0.002	0.004	0.021	0.006	0.008
a₁-TS1	0.091	0.004	0.016	0.069	0.009	0.018
a₁-IN2	0.020	0.002	0.004	0.019	0.007	0.009
a₁-TS2	0.011	0.002	0.003	0.043	0.008	0.012
a₁-IN3	0.009	0.001	0.002	0.041	0.008	0.012
b₁-IN1	0.025	0.003	0.005			
b₁-TS1	0.005	0.001	0.020			
b₁-IN2	0.079	0.006	0.016	0.076	0.009	0.016
b₁-TS2	0.024	0.002	0.004	0.069	0.008	0.013
b₁-IN3	0.009	0.002	0.003	0.032	0.007	0.009

$\Delta_1 = D_{\text{B3LYP}} - D_{\text{B3LYP-D3(BJ)}}$ denoted as the difference of optimized geometry based on between B3LYP and B3LYP-D3(BJ) theoretical levels.

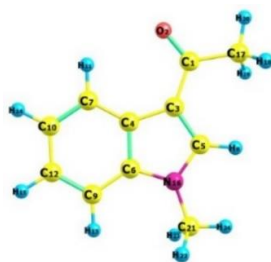
$\Delta_2 = D_{\text{B3LYP}} - D_{\text{M06-2X}}$ denoted as the difference of optimized geometry based on between B3LYP and M06-2X theoretical levels.

Table S9. The difference (denotes as Δ_1) of some important inter-atomic distances for the optimized-geometries between B3LYP and B3LYP-D3(BJ) methods and the corresponding difference (denotes as Δ_2) between B3LYP and M06-2X methods, including Average Difference (denotes as Ave Δ ($\Delta = \Delta_1$ or Δ_2)) and Average Deviation (denotes as Ave Δ_D) (Å).

Pd(TFA)₂	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O1-Pd5	2.089	2.089	2.087	0.000	0.002
O3-Pd5	2.089	2.089	2.087	0.000	0.002

Pd5-O8	2.089	2.089	2.087	0.000	0.002
Pd5-O9	2.089	2.089	2.087	0.000	0.002
Ave Δ				0.000	0.002
Ave Δ_D				0.000	0.002
a₁-IN1	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.067	2.066	2.088	0.000	-0.021
O3-Pd29	2.113	2.116	2.118	-0.004	-0.005
Pd29-O38	2.008	2.009	2.005	-0.001	0.003
Ave Δ				0.002	0.010
Ave Δ_D				0.002	0.013
a₁-TS1	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.090	2.084	2.108	0.006	-0.018
O3-Pd29	2.005	2.005	2.003	-0.001	0.002
O5-Pd29	2.723	2.681	2.640	0.042	0.083
C11-H15	1.093	1.092	1.093	0.001	0.000
C11-Pd29	2.743	2.652	2.674	0.091	0.069
Pd29-O38	2.015	2.018	2.006	-0.003	0.009
Ave Δ				0.024	0.030
Ave Δ_D				0.041	0.045
a₁-IN2	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.098	2.097	2.124	0.000	-0.027
O3-Pd29	2.002	1.998	1.992	0.004	0.010
C11-H15	1.107	1.104	1.100	0.003	0.007
C11-Pd29	2.454	2.434	2.473	0.020	-0.019
Pd29-O38	2.011	2.007	1.994	0.004	0.017
Ave Δ				0.006	0.016
Ave Δ_D				0.009	0.017
a₁-TS2	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.074	2.068	2.100	0.006	-0.025
O3-Pd29	2.080	2.071	2.069	0.009	0.011
O5-H15	1.364	1.376	1.388	-0.011	-0.023
C11-H15	1.358	1.355	1.325	0.003	0.033
C11-Pd29	2.144	2.134	2.187	0.011	-0.043
Pd29-O38	2.044	2.042	2.027	0.002	0.017
Ave Δ				0.007	0.025
Ave Δ_D				0.008	0.027
a₁-IN3	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.076	2.071	2.117	0.005	-0.041
O3-Pd29	2.065	2.057	2.080	0.009	-0.015
C11-Pd29	1.977	1.970	1.946	0.007	0.032
Pd29-O38	2.277	2.271	2.291	0.006	-0.014
Ave Δ				0.007	0.026
Ave Δ_D				0.007	0.028
b₁-IN1	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2

O2-Pd29	2.058	2.050		0.007	
O3-Pd29	2.120	2.145		-0.025	
Pd29-O38	1.993	1.991		0.001	
Ave Δ				0.011	
Ave Δ_D				0.015	
b₁-TS1	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.065	2.065		0.000	
O3-Pd29	2.012	2.017		-0.005	
C9-H12	1.089	1.086		0.003	
C9-Pd29	2.748	2.748		0.001	
Pd29-O38	2.010	2.009		0.001	
Ave Δ				0.002	
Ave Δ_D				0.003	
b₁-IN2	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.0736	2.1321	2.1497	-0.059	-0.076
O3-Pd29	2.0085	2.0035	1.9958	0.005	0.013
C9-H12	1.0922	1.0825	1.0835	0.010	0.009
C9-Pd29	2.5437	2.4651	2.5054	0.079	0.038
Pd29-O38	2.0135	2.0143	1.9968	-0.001	0.017
Ave Δ				0.031	0.031
Ave Δ_D				0.044	0.039
b₁-TS2	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.0641	2.0664	2.0786	-0.002	-0.015
O3-Pd29	2.0819	2.0765	2.0764	0.005	0.006
O5-H12	1.3293	1.327	1.3315	0.002	-0.002
C9-H12	1.3644	1.3653	1.341	-0.001	0.023
C9-Pd29	2.1566	2.1329	2.2258	0.024	-0.069
Pd29-O38	2.0213	2.0212	2.0019	0.000	0.019
Ave Δ				0.006	0.022
Ave Δ_D				0.010	0.031
b₁-IN3	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
O2-Pd29	2.0649	2.0693	2.0974	-0.004	-0.032
C9-Pd29	1.9677	1.9591	1.949	0.009	0.019
Pd29-O38	2.21	2.2031	2.2172	0.007	-0.007
Ave Δ				0.007	0.019
Ave Δ_D				0.007	0.022



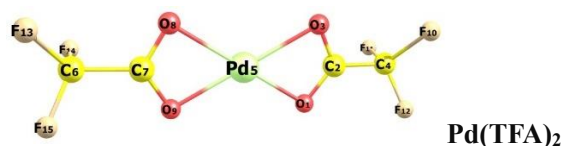
1a

Table. S10 The comparison of bond distances of **1a** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

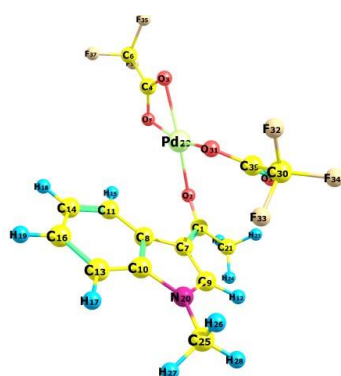
Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.227	1.227	1.218	0.000	0.009
C1-C3	1.465	1.462	1.466	0.003	-0.001
C1-C17	1.526	1.524	1.518	0.002	0.007
C3-C4	1.448	1.448	1.443	0.000	0.005
C3-C5	1.384	1.385	1.377	-0.001	0.007
C6-C4	1.418	1.418	1.411	0.000	0.007
C7-C4	1.404	1.403	1.402	0.001	0.002
C5-H8	1.082	1.081	1.083	0.001	-0.001
C6-N16	1.369	1.370	1.364	-0.001	0.005
C6-C9	1.399	1.397	1.397	0.002	0.001
C6-N16	1.392	1.392	1.384	0.000	0.008
C7-C10	1.391	1.391	1.385	0.000	0.006
C7-H11	1.084	1.083	1.084	0.000	0.000
C9-C12	1.392	1.392	1.385	0.000	0.006
C9-H13	1.086	1.086	1.086	0.000	0.000
C10-C12	1.409	1.409	1.408	0.000	0.001
C10-H14	1.087	1.086	1.085	0.000	0.001
C12-H15	1.087	1.086	1.085	0.000	0.001
N16-C21	1.450	1.448	1.445	0.002	0.005
C17-H18	1.097	1.097	1.095	0.000	0.002
C17-H19	1.097	1.097	1.095	0.000	0.002
C17-H20	1.092	1.091	1.090	0.000	0.002
C21-H22	1.096	1.096	1.094	0.000	0.002
C21-H23	1.096	1.096	1.094	0.000	0.002
C21-H24	1.092	1.092	1.091	0.000	0.001
Average Value (Ave Δ)				0.001	0.003
Average Deviation (Ave Δ_D)				0.001	0.004

$\Delta_1 = D_{B3LYP} - D_{B3LYP-D3(BJ)}$ denoted as the difference of optimized geometry based on between B3LYP and B3LYP-D3(BJ) theoretical levels.

$\Delta_2 = D_{B3LYP} - D_{M06-2X}$ denoted as the difference of optimized geometry based on between B3LYP and M06-2X theoretical levels.



C2-O3	1.269	1.269	1.261	0.000	0.008
C2-C4	1.535	1.534	1.532	0.002	0.003
C2-Pd5	2.425	2.424	2.410	0.001	0.015
O3-Pd5	2.089	2.089	2.087	0.000	0.002
C4-F10	1.336	1.336	1.326	0.000	0.010
C4-F11	1.343	1.343	1.333	0.000	0.010
C4-F12	1.336	1.336	1.326	0.000	0.010
Pd5-C7	2.425	2.424	2.410	0.001	0.015
Pd5-O8	2.089	2.089	2.087	0.000	0.002
Pd5-O9	2.089	2.089	2.087	0.000	0.002
C6-C7	1.535	1.534	1.532	0.002	0.003
C6-F13	1.336	1.336	1.326	0.000	0.010
C6-F14	1.343	1.343	1.333	0.000	0.010
C6-F15	1.336	1.336	1.326	0.000	0.010
C7-O8	1.269	1.269	1.261	0.000	0.008
C7-O9	1.269	1.269	1.261	0.000	0.008
Ave Δ				0.000	0.007
Ave Δ_D				0.001	0.009

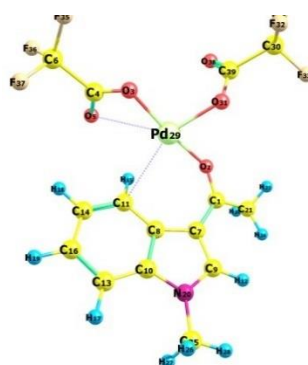


a₁-IN1

Table. S12 The comparison of bond distances of **a₁-IN1** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.262	1.262	1.251	0.000	0.012
C1-C7	1.432	1.428	1.434	0.003	-0.002
C1-C21	1.508	1.504	1.501	0.005	0.008
O2-Pd29	2.067	2.066	2.088	0.000	-0.021
O3-C4	1.268	1.267	1.259	0.000	0.009
O3-Pd29	2.113	2.116	2.118	-0.004	-0.005
C4-O5	1.267	1.267	1.261	-0.001	0.006
C4-C6	1.536	1.534	1.533	0.002	0.003
C6-F35	1.337	1.337	1.326	0.000	0.011
C6-F36	1.339	1.338	1.331	0.000	0.008
C6-F37	1.347	1.347	1.335	0.000	0.012
C7-C8	1.454	1.452	1.445	0.002	0.008

C7-C9	1.396	1.397	1.388	0.000	0.008
C8-C10	1.415	1.415	1.408	0.001	0.007
C8-C11	1.403	1.401	1.401	0.002	0.001
C9-H12	1.081	1.080	1.082	0.001	-0.001
C9-N20	1.351	1.353	1.348	-0.002	0.003
C10-C13	1.396	1.394	1.394	0.002	0.002
C10-N20	1.399	1.399	1.391	-0.001	0.007
C11-C14	1.392	1.392	1.387	0.000	0.006
C11-H15	1.085	1.085	1.086	0.000	-0.002
C13-C16	1.392	1.392	1.386	0.000	0.006
C13-H17	1.086	1.085	1.085	0.000	0.000
C14-C16	1.407	1.407	1.406	0.000	0.000
C14-H18	1.086	1.086	1.085	0.000	0.001
C16-H19	1.086	1.086	1.085	0.000	0.001
N20-C25	1.454	1.453	1.450	0.001	0.004
C21-H22	1.094	1.092	1.091	0.002	0.002
C21-H23	1.097	1.093	1.097	0.004	0.000
C21-H24	1.092	1.097	1.091	-0.005	0.001
C25-H26	1.095	1.093	1.093	0.002	0.002
C25-H27	1.094	1.094	1.093	0.000	0.001
C25-H28	1.091	1.091	1.090	0.001	0.001
Pd29-O31	2.008	2.009	2.005	-0.001	0.003
C30-F32	1.340	1.342	1.333	-0.002	0.007
C30-F33	1.363	1.348	1.337	0.015	0.026
C30-F34	1.339	1.355	1.344	-0.016	-0.006
C30-C39	1.555	1.554	1.549	0.001	0.007
O31-C39	1.293	1.289	1.282	0.004	0.011
O38-C39	1.220	1.221	1.216	-0.001	0.004
Ave Δ				0.002	0.006
Ave Δ_D				0.004	0.008

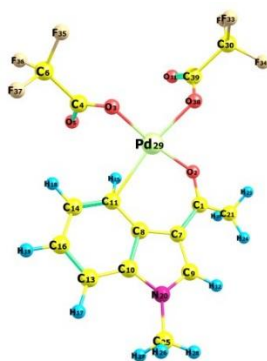


a₁-TS1

Table. S13 The comparison of bond distances of **a₁-TS1** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.254	1.255	1.243	0.000	0.012

C1-C7	1.439	1.437	1.444	0.002	-0.005
C1-C21	1.509	1.506	1.502	0.004	0.007
O2-Pd29	2.090	2.084	2.108	0.006	-0.018
O3-C4	1.290	1.288	1.281	0.001	0.009
O3-Pd29	2.005	2.005	2.003	-0.001	0.002
C4-O5	1.232	1.233	1.228	-0.001	0.005
C4-C6	1.545	1.541	1.537	0.004	0.008
O5-Pd29	2.723	2.681	2.640	0.042	0.083
C6-F35	1.339	1.338	1.328	0.001	0.011
C6-F36	1.340	1.340	1.331	0.000	0.009
C6-F37	1.353	1.356	1.343	-0.003	0.010
C7-C8	1.449	1.450	1.445	-0.001	0.004
C7-C9	1.394	1.394	1.386	0.000	0.008
C8-C10	1.414	1.414	1.408	0.000	0.006
C8-C11	1.405	1.405	1.405	0.000	0.000
C9-H12	1.081	1.081	1.082	0.000	-0.001
C9-N20	1.357	1.358	1.353	-0.002	0.004
C10-C13	1.397	1.396	1.396	0.001	0.001
C10-N20	1.397	1.398	1.389	0.000	0.008
C11-C14	1.394	1.395	1.389	-0.001	0.006
C11-H15	1.093	1.092	1.093	0.001	0.000
C11-Pd29	2.743	2.652	2.674	0.091	0.069
C13-C16	1.393	1.394	1.387	0.000	0.006
C13-H17	1.086	1.085	1.085	0.000	0.000
C14-C16	1.406	1.406	1.406	0.001	0.000
C14-H18	1.085	1.084	1.085	0.001	0.000
C16-H19	1.086	1.085	1.085	0.000	0.001
N20-C25	1.455	1.453	1.450	0.002	0.004
C21-H22	1.098	1.093	1.095	0.005	0.002
C21-H23	1.092	1.097	1.090	-0.005	0.002
C21-H24	1.093	1.092	1.092	0.001	0.000
C25-H26	1.095	1.095	1.093	0.000	0.002
C25-H27	1.095	1.095	1.093	0.000	0.002
C25-H28	1.091	1.091	1.090	0.000	0.001
Pd29-O31	2.015	2.018	2.006	-0.003	0.009
C30-F32	1.345	1.345	1.335	0.000	0.010
C30-F33	1.352	1.352	1.341	-0.001	0.011
C30-F34	1.337	1.337	1.328	0.000	0.009
C30-C39	1.555	1.552	1.544	0.003	0.011
O31-C39	1.302	1.301	1.295	0.002	0.007
O38-C39	1.215	1.215	1.210	0.000	0.005
Ave Δ				0.004	0.009
Ave Δ_D				0.016	0.018

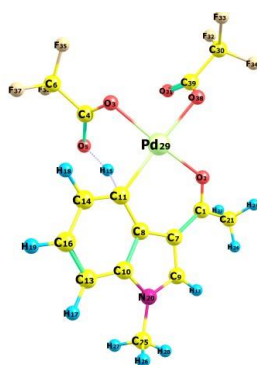


a₁-IN2

Table. S14 The comparison of bond distances of **a₁-IN2** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.251	1.251	1.240	0.001	0.011
C1-C7	1.442	1.441	1.447	0.001	-0.006
C1-C21	1.509	1.506	1.502	0.003	0.006
O2-Pd29	2.098	2.097	2.124	0.000	-0.027
O3-C4	1.294	1.294	1.287	0.001	0.007
O3-Pd29	2.002	1.998	1.992	0.004	0.010
C4-O5	1.224	1.224	1.219	0.000	0.005
C4-C6	1.551	1.546	1.540	0.005	0.011
C6-F35	1.341	1.339	1.329	0.002	0.012
C6-F36	1.339	1.338	1.329	0.001	0.010
C6-F37	1.355	1.358	1.347	-0.004	0.008
C7-C8	1.446	1.447	1.444	-0.001	0.002
C7-C9	1.393	1.393	1.385	0.000	0.008
C8-C10	1.415	1.416	1.409	-0.001	0.005
C8-C11	1.410	1.409	1.409	0.001	0.001
C9-H12	1.081	1.081	1.082	0.000	-0.001
C9-N20	1.357	1.359	1.353	-0.002	0.004
C10-C13	1.396	1.395	1.395	0.002	0.002
C10-N20	1.396	1.396	1.388	0.000	0.008
C11-C14	1.399	1.399	1.393	0.000	0.006
C11-H15	1.107	1.104	1.100	0.003	0.007
C11-Pd29	2.454	2.434	2.473	0.020	-0.019
C13-C16	1.394	1.394	1.388	-0.001	0.006
C13-H17	1.086	1.085	1.086	0.001	0.000
C14-C16	1.404	1.403	1.404	0.001	0.001
C14-H18	1.084	1.083	1.084	0.001	-0.001
C16-H19	1.085	1.085	1.084	0.000	0.001
N20-C25	1.455	1.453	1.450	0.002	0.005
C21-H22	1.098	1.097	1.095	0.000	0.002
C21-H23	1.092	1.091	1.090	0.000	0.002
C21-H24	1.094	1.094	1.093	0.000	0.001
C25-H26	1.095	1.095	1.093	0.000	0.002

C25-H27	1.095	1.094	1.093	0.000	0.002
C25-H28	1.091	1.091	1.090	0.000	0.001
Pd29-O38	2.011	2.007	1.994	0.004	0.017
C30-F32	1.338	1.338	1.329	0.000	0.010
C30-F33	1.346	1.347	1.337	-0.001	0.009
C30-F34	1.351	1.350	1.340	0.001	0.012
C30-C39	1.555	1.552	1.544	0.002	0.010
O31-C39	1.216	1.215	1.209	0.001	0.006
O38-C39	1.301	1.301	1.296	0.000	0.005
Ave Δ				0.002	0.007
Ave Δ_D				0.004	0.009



a₁-TS2

Table. S15 The comparison of bond distances of **a₁-TS2** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.253	1.253	1.240	0.000	0.013
C1-C7	1.437	1.435	1.441	0.002	-0.004
C1-C21	1.510	1.508	1.507	0.002	0.003
O2-Pd29	2.074	2.068	2.100	0.006	-0.025
O3-C4	1.261	1.262	1.258	-0.001	0.004
O3-Pd29	2.080	2.071	2.069	0.009	0.011
C4-O5	1.261	1.260	1.252	0.002	0.010
C4-C6	1.544	1.541	1.536	0.003	0.008
O5-H15	1.364	1.376	1.388	-0.011	-0.023
C6-F35	1.334	1.334	1.325	0.000	0.009
C6-F36	1.337	1.336	1.326	0.001	0.011
C6-F37	1.352	1.353	1.342	-0.001	0.009
C7-C8	1.444	1.444	1.440	0.000	0.004
C7-C9	1.396	1.397	1.388	-0.001	0.008
C8-C10	1.414	1.414	1.409	0.000	0.005
C8-C11	1.414	1.411	1.410	0.003	0.004
C9-H12	1.081	1.081	1.083	0.000	-0.001
C9-N20	1.356	1.357	1.350	-0.001	0.005
C10-C13	1.396	1.395	1.395	0.001	0.001
C10-N20	1.398	1.398	1.390	0.000	0.008

C11-C14	1.410	1.409	1.400	0.001	0.010
C11-H15	1.358	1.355	1.325	0.003	0.033
C11-Pd29	2.144	2.134	2.187	0.011	-0.043
C13-C16	1.394	1.394	1.387	-0.001	0.007
C13-H17	1.086	1.086	1.086	0.000	0.000
C14-C16	1.404	1.403	1.404	0.001	0.000
C14-H18	1.086	1.086	1.087	0.001	-0.001
C16-H19	1.086	1.085	1.085	0.000	0.001
N20-C25	1.455	1.453	1.450	0.002	0.005
C21-H22	1.097	1.097	1.092	0.000	0.005
C21-H23	1.092	1.092	1.090	0.001	0.003
C21-H24	1.093	1.093	1.096	0.000	-0.003
C25-H26	1.095	1.095	1.093	0.000	0.002
C25-H27	1.095	1.094	1.093	0.000	0.002
C25-H28	1.091	1.091	1.090	0.000	0.001
Pd29-O38	2.044	2.042	2.027	0.002	0.017
C30-F32	1.341	1.340	1.330	0.000	0.010
C30-F33	1.348	1.348	1.337	0.000	0.011
C30-F34	1.352	1.351	1.341	0.000	0.011
C30-C39	1.552	1.550	1.543	0.003	0.009
O31-C39	1.222	1.223	1.217	-0.001	0.005
O38-C39	1.293	1.293	1.287	0.001	0.006
Ave Δ				0.002	0.008
Ave Δ_D				0.003	0.012

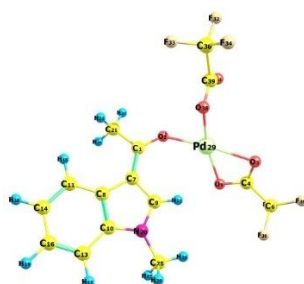


a₁-IN3

Table. S16 The comparison of bond distances of **a₁-IN3** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.258	1.258	1.244	0.000	0.015
C1-C7	1.424	1.422	1.431	0.002	-0.007
C1-C21	1.510	1.508	1.505	0.002	0.005
O2-Pd29	2.076	2.071	2.117	0.005	-0.041
O3-C4	1.270	1.269	1.260	0.000	0.010
O3-Pd29	2.065	2.057	2.080	0.009	-0.015
C4-O5	1.241	1.241	1.237	0.000	0.004

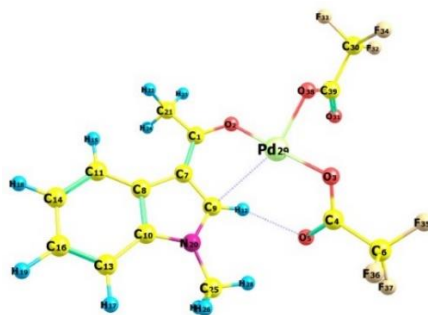
C4-C6	1.551	1.548	1.543	0.003	0.009
O5-H15	1.523	1.519	1.495	0.004	0.028
C6-F35	1.346	1.345	1.336	0.001	0.010
C6-F36	1.337	1.337	1.328	0.000	0.009
C6-F37	1.352	1.353	1.340	-0.001	0.012
C7-C8	1.445	1.445	1.441	-0.001	0.004
C7-C9	1.396	1.397	1.387	-0.001	0.008
C8-C10	1.413	1.413	1.407	0.000	0.006
C8-C11	1.401	1.399	1.400	0.002	0.001
C9-H12	1.081	1.081	1.082	0.000	-0.001
C9-N20	1.356	1.357	1.351	-0.001	0.004
C10-C13	1.395	1.394	1.395	0.001	0.000
C10-N20	1.402	1.402	1.393	0.000	0.009
C11-C14	1.396	1.396	1.388	0.000	0.008
C11-Pd29	1.977	1.970	1.946	0.007	0.032
C13-C16	1.393	1.394	1.387	0.000	0.006
C13-H17	1.086	1.085	1.085	0.000	0.001
C14-C16	1.410	1.410	1.410	0.001	0.001
C14-H18	1.083	1.083	1.084	0.001	-0.001
C16-H19	1.087	1.086	1.085	0.000	0.001
N20-C25	1.454	1.452	1.449	0.002	0.005
C21-H22	1.096	1.096	1.092	0.000	0.004
C21-H23	1.095	1.094	1.091	0.001	0.004
C21-H24	1.092	1.092	1.095	0.000	-0.003
C25-H26	1.095	1.095	1.093	0.000	0.002
C25-H27	1.095	1.095	1.093	0.000	0.002
C25-H28	1.092	1.091	1.090	0.000	0.001
Pd29-O38	2.277	2.271	2.291	0.006	-0.014
C30-F32	1.343	1.341	1.330	0.001	0.013
C30-F33	1.335	1.335	1.326	0.000	0.009
C30-F34	1.346	1.347	1.340	-0.001	0.006
C30-C39	1.545	1.543	1.537	0.002	0.008
O31-C39	1.297	1.296	1.290	0.000	0.007
O38-C39	1.226	1.226	1.221	0.000	0.005
Ave Δ				0.001	0.008
Ave Δ_D				0.002	0.012



b₁-IN1

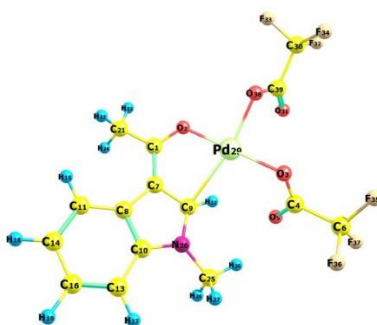
Table. S17 The comparison of bond distances of **b₁-IN1** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.261	1.265		-0.005	
C1-C7	1.437	1.432		0.005	
C1-C21	1.510	1.502		0.008	
O2-Pd29	2.058	2.050		0.007	
O3-C4	1.262	1.262		0.001	
O3-Pd29	2.120	2.145		-0.025	
C4-O5	1.271	1.271		0.000	
C4-C6	1.536	1.533		0.003	
C6-F35	1.333	1.333		0.001	
C6-F36	1.350	1.357		-0.007	
C6-F37	1.340	1.338		0.003	
C7-C8	1.458	1.455		0.003	
C7-C9	1.398	1.400		-0.002	
C8-C10	1.418	1.419		-0.001	
C8-C11	1.405	1.403		0.002	
C9-H12	1.081	1.081		0.000	
C9-N20	1.350	1.350		0.000	
C10-C13	1.396	1.394		0.002	
C10-N20	1.396	1.398		-0.002	
C11-C14	1.392	1.392		0.000	
C11-H15	1.084	1.084		0.000	
C13-C16	1.391	1.392		0.000	
C13-H17	1.086	1.085		0.001	
C14-C16	1.406	1.406		0.000	
C14-H18	1.086	1.086		0.001	
C16-H19	1.086	1.085		0.000	
N20-C25	1.456	1.455		0.001	
C21-H22	1.098	1.098		0.000	
C21-H23	1.091	1.092		-0.001	
C21-H24	1.093	1.092		0.002	
C25-H26	1.095	1.094		0.001	
C25-H27	1.095	1.095		0.000	
C25-H28	1.091	1.092		0.000	
Pd29-O38	1.993	1.991		0.001	
C30-F32	1.338	1.336		0.002	
C30-F33	1.351	1.362		-0.011	
C30-F34	1.346	1.342		0.004	
C30-C39	1.553	1.549		0.003	
O31-C39	1.216	1.214		0.002	
O38-C39	1.304	1.304		0.001	
Ave Δ				0.003	

**b₁-TS1****Table. S18** The comparison of bond distances of **b₁-TS1** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.260	1.262		-0.001	
C1-C7	1.440	1.436		0.004	
C1-C21	1.504	1.501		0.003	
O2-Pd29	2.065	2.065		0.000	
O3-C4	1.286	1.282		0.004	
O3-Pd29	2.012	2.017		-0.005	
C4-O5	1.234	1.239		-0.005	
C4-C6	1.547	1.542		0.006	
C6-F35	1.339	1.336		0.003	
C6-F36	1.352	1.353		-0.002	
C6-F37	1.340	1.341		-0.002	
C7-C8	1.448	1.448		0.000	
C7-C9	1.406	1.406		0.000	
C8-C10	1.420	1.421		-0.001	
C8-C11	1.406	1.404		0.002	
C9-H12	1.089	1.086		0.003	
C9-N20	1.354	1.354		0.001	
C9-Pd29	2.748	2.748		0.001	
C10-C13	1.398	1.396		0.002	
C10-N20	1.392	1.394		-0.002	
C11-C14	1.389	1.390		0.000	
C11-H15	1.085	1.084		0.000	
C13-C16	1.390	1.390		-0.001	
C13-H17	1.085	1.085		0.000	
C14-C16	1.409	1.408		0.001	
C14-H18	1.086	1.086		0.000	
C16-H19	1.086	1.085		0.000	
N20-C25	1.461	1.459		0.002	
C21-H22	1.098	1.098		0.000	
C21-H23	1.092	1.092		0.000	
C21-H24	1.094	1.093		0.000	

C25-H26	1.094	1.093	0.001
C25-H27	1.095	1.095	0.000
C25-H28	1.090	1.090	0.000
Pd29-O38	2.010	2.009	0.001
C30-F32	1.337	1.337	0.000
C30-F33	1.349	1.349	0.000
C30-F34	1.345	1.345	0.000
C30-C39	1.556	1.553	0.003
O31-C39	1.215	1.215	0.000
O38-C39	1.303	1.302	0.001
Ave Δ			0.005
Ave Δ_D			0.020



b₁-IN2

Table. S19 The comparison of bond distances of **b₁-IN2** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.2577	1.2539	1.2417	0.004	0.016
C1-C7	1.4458	1.4574	1.4667	-0.012	-0.021
C1-C21	1.5021	1.498	1.4965	0.004	0.006
O2-Pd29	2.0736	2.1321	2.1497	-0.059	-0.076
O3-C4	1.2891	1.2933	1.2867	-0.004	0.002
O3-Pd29	2.0085	2.0035	1.9958	0.005	0.013
C4-O5	1.23	1.2235	1.2184	0.006	0.012
C4-C6	1.5495	1.5471	1.541	0.002	0.009
C6-F35	1.3381	1.3369	1.327	0.001	0.011
C6-F36	1.3551	1.3645	1.3523	-0.009	0.003
C6-F37	1.3391	1.3367	1.3277	0.002	0.011
C7-C8	1.442	1.4418	1.445	0.000	-0.003
C7-C9	1.4128	1.4234	1.4127	-0.011	0.000
C8-C10	1.4207	1.4197	1.4089	0.001	0.012
C8-C11	1.4078	1.405	1.4025	0.003	0.005
C9-H12	1.0922	1.0825	1.0835	0.010	0.009
C9-N20	1.361	1.3622	1.3493	-0.001	0.012
C9-Pd29	2.5437	2.4651	2.5054	0.079	0.038
C10-C13	1.4001	1.398	1.3971	0.002	0.003
C10-N20	1.3871	1.3866	1.385	0.000	0.002

C11-C14	1.3872	1.3873	1.3833	0.000	0.004
C11-H15	1.0847	1.0846	1.0852	0.000	0.000
C13-C16	1.3878	1.3887	1.3838	-0.001	0.004
C13-H17	1.085	1.0844	1.0846	0.001	0.000
C14-C16	1.4115	1.4109	1.4085	0.001	0.003
C14-H18	1.0858	1.0853	1.0845	0.001	0.001
C16-H19	1.0858	1.0854	1.0847	0.000	0.001
N20-C25	1.4619	1.4597	1.4569	0.002	0.005
C21-H22	1.0983	1.0982	1.0967	0.000	0.002
C21-H23	1.0921	1.0924	1.0914	0.000	0.001
C21-H24	1.0934	1.0926	1.0912	0.001	0.002
C25-H26	1.09	1.0873	1.0923	0.003	-0.002
C25-H27	1.094	1.0928	1.0927	0.001	0.001
C25-H28	1.0947	1.0938	1.0877	0.001	0.007
Pd29-O38	2.0135	2.0143	1.9968	-0.001	0.017
C30-F32	1.3376	1.3379	1.3287	0.000	0.009
C30-F33	1.3487	1.3486	1.3388	0.000	0.010
C30-F34	1.3456	1.3472	1.3369	-0.002	0.009
C30-C39	1.5555	1.5531	1.5448	0.002	0.011
O31-C39	1.2157	1.2149	1.2095	0.001	0.006
O38-C39	1.3019	1.3014	1.2956	0.001	0.006
Ave Δ				0.006	0.009
Ave Δ_D				0.016	0.016

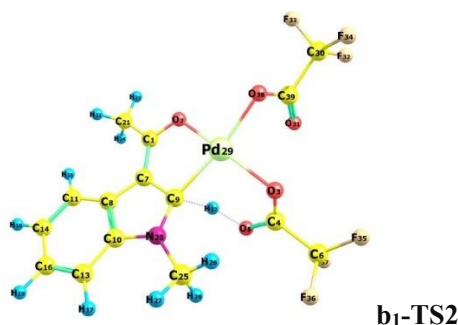


Table. S20 The comparison of bond distances of **b₁-TS2** at various functionals (B3LYP, B3LYP-D3(BJ) and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.2656	1.2656	1.2516	0.000	0.014
C1-C7	1.4334	1.431	1.4407	0.002	-0.007
C1-C21	1.5016	1.4991	1.4977	0.002	0.004
O2-Pd29	2.0641	2.0664	2.0786	-0.002	-0.015
O3-C4	1.2586	1.2581	1.2524	0.000	0.006
O3-Pd29	2.0819	2.0765	2.0764	0.005	0.006
C4-O5	1.2661	1.2657	1.2583	0.000	0.008
C4-C6	1.5439	1.5408	1.5363	0.003	0.008
O5-H12	1.3293	1.327	1.3315	0.002	-0.002

C6-F35	1.3318	1.3314	1.3225	0.000	0.009
C6-F36	1.3535	1.3548	1.3441	-0.001	0.009
C6-F37	1.3353	1.3346	1.3254	0.001	0.010
C7-C8	1.4393	1.4379	1.4373	0.001	0.002
C7-C9	1.4193	1.418	1.4074	0.001	0.012
C8-C10	1.4218	1.4237	1.4148	-0.002	0.007
C8-C11	1.4074	1.4059	1.407	0.002	0.000
C9-H12	1.3644	1.3653	1.341	-0.001	0.023
C9-N20	1.3744	1.3731	1.3629	0.001	0.012
C9-Pd29	2.1566	2.1329	2.2258	0.024	-0.069
C10-C13	1.4014	1.3998	1.4009	0.002	0.000
C10-N20	1.3896	1.389	1.3829	0.001	0.007
C11-C14	1.3876	1.3874	1.3811	0.000	0.006
C11-H15	1.0848	1.0843	1.0842	0.000	0.001
C13-C16	1.3879	1.388	1.3811	0.000	0.007
C13-H17	1.085	1.0846	1.0844	0.000	0.001
C14-C16	1.4109	1.4107	1.4102	0.000	0.001
C14-H18	1.086	1.0856	1.0848	0.000	0.001
C16-H19	1.0859	1.0855	1.0847	0.000	0.001
N20-C25	1.4602	1.4582	1.457	0.002	0.003
C21-H22	1.0974	1.0972	1.0962	0.000	0.001
C21-H23	1.0914	1.091	1.0899	0.000	0.001
C21-H24	1.0952	1.095	1.0933	0.000	0.002
C25-H26	1.09	1.0898	1.0912	0.000	-0.001
C25-H27	1.0914	1.0908	1.0898	0.001	0.002
C25-H28	1.0943	1.0935	1.0925	0.001	0.002
Pd29-O38	2.0213	2.0212	2.0019	0.000	0.019
C30-F32	1.3389	1.3389	1.329	0.000	0.010
C30-F33	1.3489	1.3484	1.3376	0.000	0.011
C30-F34	1.3479	1.3481	1.3372	0.000	0.011
C30-C39	1.5524	1.5497	1.5429	0.003	0.010
O31-C39	1.2196	1.2204	1.2139	-0.001	0.006
O38-C39	1.2986	1.2976	1.293	0.001	0.006
Ave Δ				0.002	0.008
Ave Δ_D				0.004	0.013

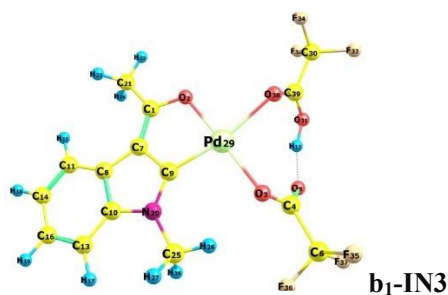


Table. S21 The comparison of bond distances of **b₁-IN3** at various functionals (B3LYP, B3LYP-D3(BJ))

and M06-2X) with the BS1 basis set.

Distances(Å)	B3LYP	B3LYP-D3(BJ)	M06-2X	Δ_1	Δ_2
C1-O2	1.2815	1.2817	1.2645	0.000	0.017
C1-C7	1.4071	1.4053	1.4142	0.002	-0.007
C1-C21	1.502	1.4997	1.4981	0.002	0.004
O2-Pd29	2.0649	2.0693	2.0974	-0.004	-0.032
O3-C4	1.2741	1.2735	1.265	0.001	0.009
O3-Pd29	2.0642	2.0579	2.0728	0.006	-0.009
C4-O5	1.2386	1.2386	1.2337	0.000	0.005
C4-C6	1.5516	1.5487	1.5431	0.003	0.009
O5-H12	1.5369	1.5329	1.5229	0.004	0.014
C6-F35	1.3449	1.3438	1.3344	0.001	0.011
C6-F36	1.3524	1.3531	1.342	-0.001	0.010
C6-F37	1.3352	1.3347	1.3256	0.000	0.010
C7-C8	1.4466	1.446	1.4423	0.001	0.004
C7-C9	1.4183	1.4184	1.4068	0.000	0.011
C8-C10	1.4175	1.4191	1.4119	-0.002	0.006
C8-C11	1.4006	1.3991	1.399	0.002	0.002
C9-N20	1.3501	1.3497	1.3441	0.000	0.006
C9-Pd29	1.9677	1.9591	1.949	0.009	0.019
C10-C13	1.3936	1.3917	1.3923	0.002	0.001
C10-N20	1.4106	1.4109	1.4022	0.000	0.008
C11-C14	1.3943	1.3944	1.3883	0.000	0.006
C11-H15	1.086	1.0856	1.0855	0.000	0.001
C13-C16	1.3952	1.3955	1.3888	0.000	0.006
C13-H17	1.0855	1.0851	1.0852	0.000	0.000
C14-C16	1.4042	1.4038	1.4031	0.000	0.001
C14-H18	1.0863	1.0859	1.0851	0.000	0.001
C16-H19	1.086	1.0856	1.0848	0.000	0.001
N20-C25	1.4576	1.4556	1.4537	0.002	0.004
C21-H22	1.0965	1.0963	1.095	0.000	0.002
C21-H23	1.0915	1.0912	1.0898	0.000	0.002
C21-H24	1.0965	1.0963	1.0949	0.000	0.002
C25-H26	1.0864	1.0858	1.0865	0.001	0.000
C25-H27	1.0949	1.0943	1.0931	0.001	0.002
C25-H28	1.0953	1.095	1.094	0.000	0.001
Pd29-O38	2.21	2.2031	2.2172	0.007	-0.007
C30-F32	1.343	1.3422	1.3324	0.001	0.011
C30-F33	1.3424	1.3333	1.3242	0.009	0.018
C30-F34	1.3335	1.3429	1.3323	-0.009	0.001
C30-C39	1.5449	1.5427	1.538	0.002	0.007
O31-C39	1.2953	1.2947	1.2888	0.001	0.006
O38-C39	1.229	1.2292	1.2218	0.000	0.007
Ave Δ				0.002	0.007

Based on the discussion above, Pd(TFA)₂ is thought to be the most efficient catalyst in the reported experimental condition. Therefore, we have calculated the oxidative addition and reductive elimination steps catalyzed by Pd(TFA)₂.

Firstly, the formed intermediates **a₁-IN3**, **b₁-IN3** after C4-H and C2-H activation are stable Pd(II)-species, which could be oxidized to Pd(IV) intermediate by the substrate **2a**. Due to the co-existence of OAc⁻, CF₃COO⁻ and OTf⁻ anions as well as **2a** cation in the reaction, the oxidative addition process may be achieved by one of them alone or via a concerted manner. Our results suggest that the combination of **2a** cation with OAc⁻ anion provides the most feasible access for oxidative addition and the reductive elimination steps (Figure S20). The oxidant cation of **2a** exhibits a strong oxidizing ability due to the existence of high valent iodonium salt, in which the C-I bond can cleave to form the Pd-C bond and further lead to stable intermediates (**a₁/b₁-IN4**) after the release of IMes moiety. From **a₁/b₁-IN3** to **a₁/b₁-IN4**, the overall oxidative addition process is completed and the oxidation state of palladium changes from +2 to +4, the coordination number of palladium changes from 4 to 6. The thermodynamic data suggests this process is irreversible with the 22.8, 20.0 kcal/mol exergonic for C4 and C2 sites (Figure S20 ~ S21), respectively. However, for C4 site, the oxidative addition TS is not found which is consistent with the results of the scan of the PES along the reaction coordinate as shown in Figure S20.

Subsequently, from **a₁/b₁-IN4**, the reductive elimination process proceeds via a three-center TS **a₁-TS3/b₁-TS4** to generate species **a₁/b₁-IN5**. This step could recover the oxidation state of palladium from +4 to +2, concomitant with the change of the coordination number of palladium from 6 to 4 (Figure S20 ~ S21). Then the products **3aa/3ba** are obtained with the release of Pd(II)-catalyst. The thermodynamic data suggests this process is irreversible with the 34.4, 40.5 kcal/mol exergonic for C4 and C2 sites, respectively. For C4 site, the reductive elimination **a₁-TS3** has a free energy barrier of 18.0 kcal/mol, which is surmountable barrier at the experimental condition. For the C2 site, the free energy of **b₁-TS4** is higher than **a₁-TS3** by 6.9 kcal/mol, thus it is unfavorable in this work.

For the other two pathways, the kinetics and thermodynamics are poor in oxidative addition and the reductive elimination steps as shown in ESI (e and f, Figure S20 ~ S21). In Pd(TFA)₂, due to the

exergonic and irreversible character in the oxidative addition and reductive elimination steps, the regioselectivity of C4 and C2 site should arise from the step of C-H activation.

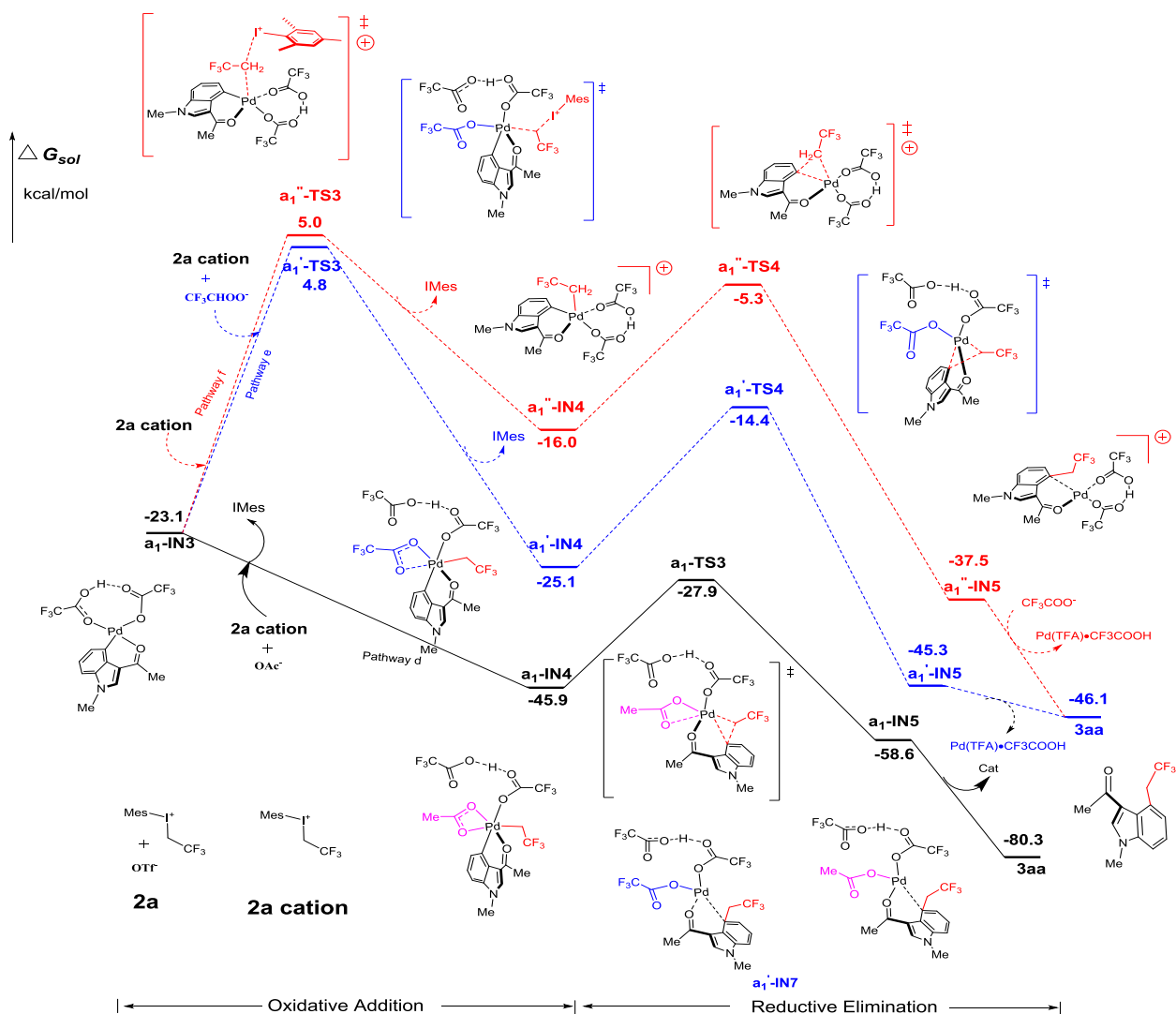


Figure S20. The Oxidative Addition and Reductive Elimination steps of C4-fluoroalkylation with Pd(TFA)₂ catalyst.

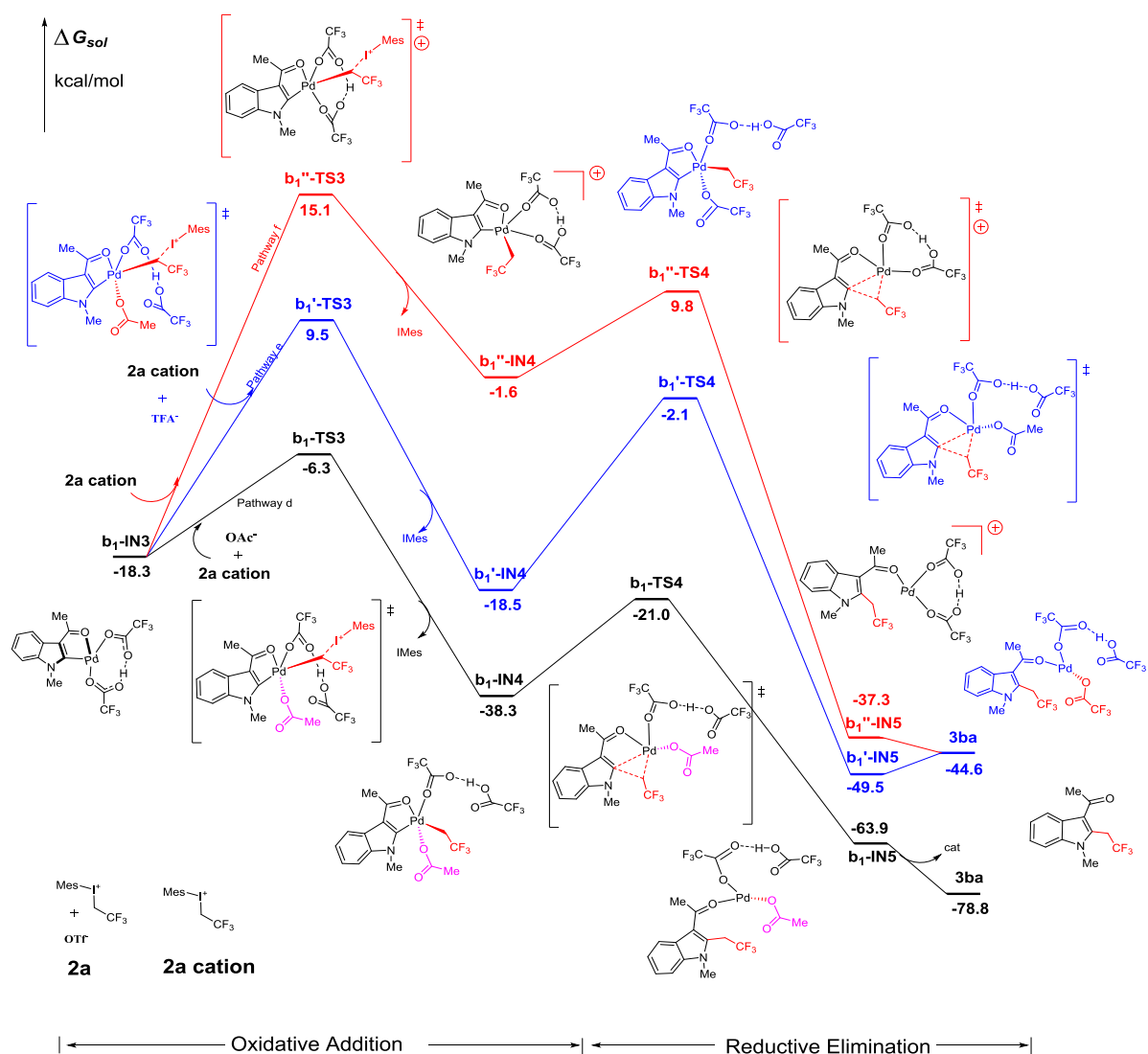


Figure S21. The Oxidative Addition and Reductive Elimination steps of C2-fluoroalkylation with $\text{Pd}(\text{TFA})_2$ catalyst.

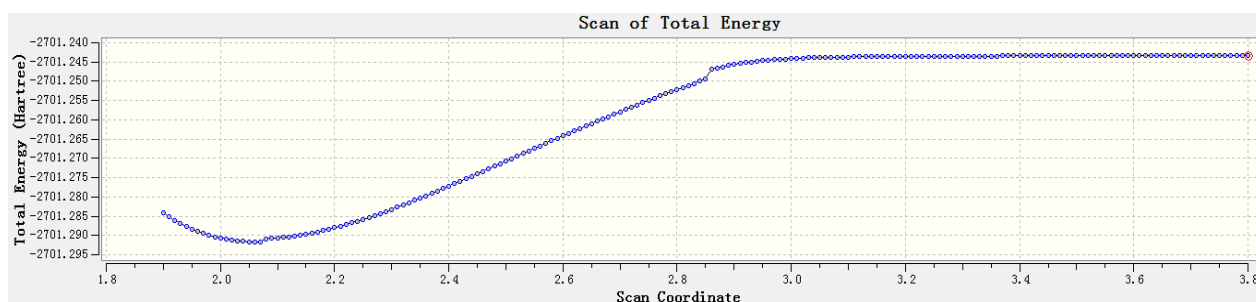


Figure S22. The scan profile of the oxidative addition step ($\text{a}_1\text{-IN3} \rightarrow \text{a}_1\text{-IN4}$) in C4-functionalization catalyzed by $\text{Pd}(\text{TFA})_2$.

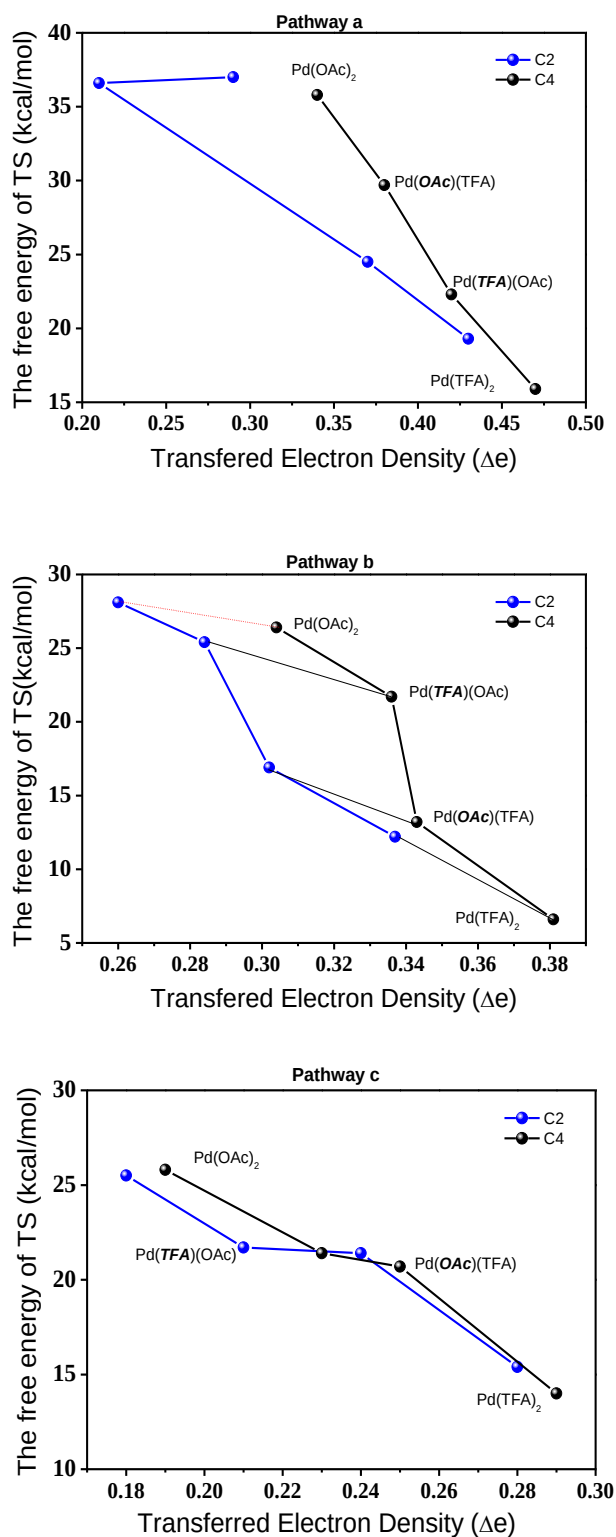


Figure S23. The correlation between the free energy of the TS and the amount of the transferred electron density in various pathways under various Pd-catalysts.

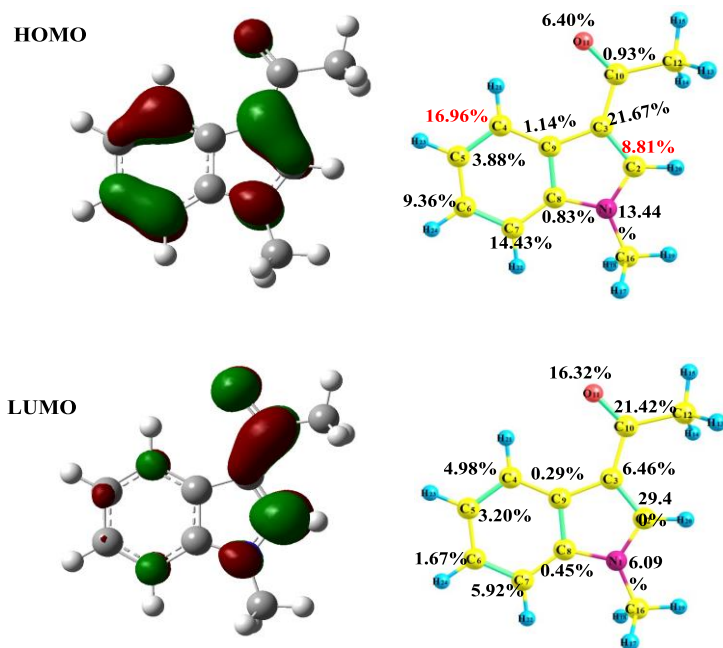


Figure S24. The HOMO and LUMO and the corresponding distributions of substrate **1a**.

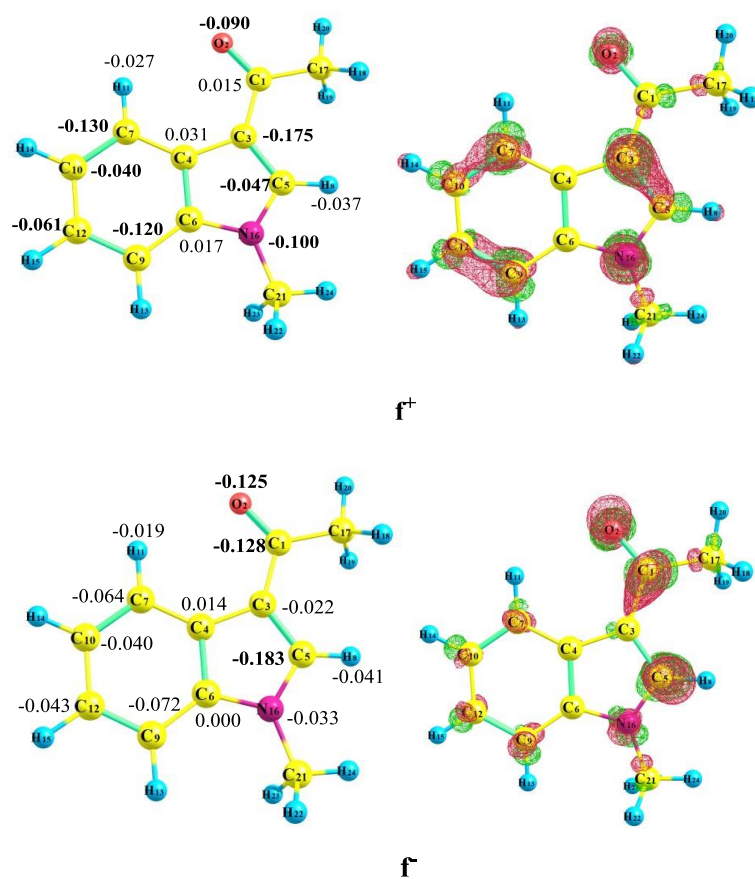


Figure S25. The $f^+ f^-$ function of substrate **1a**.

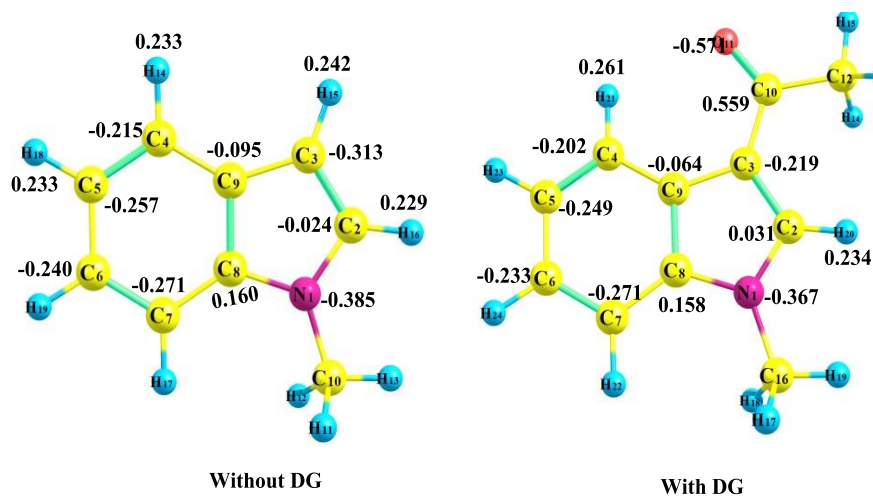


Figure S26. The natural charges of substrate **1a**.

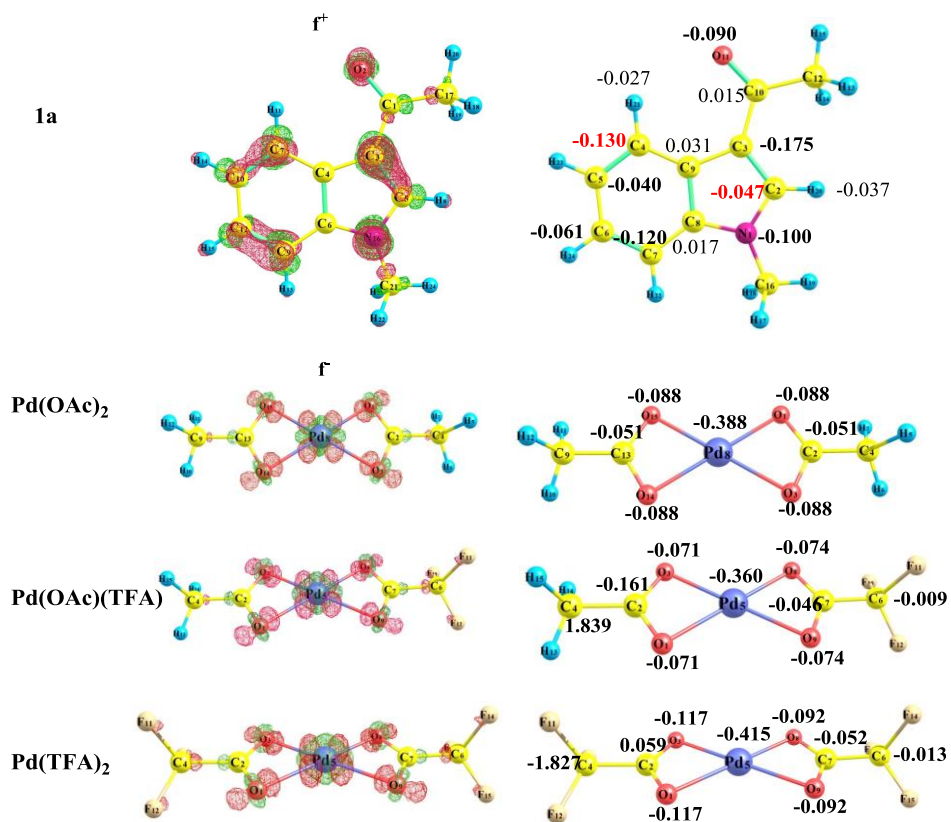


Figure S27. The f^+ of substrate **1a** and f^- of Pd-catalysts as well as the corresponding distributions.

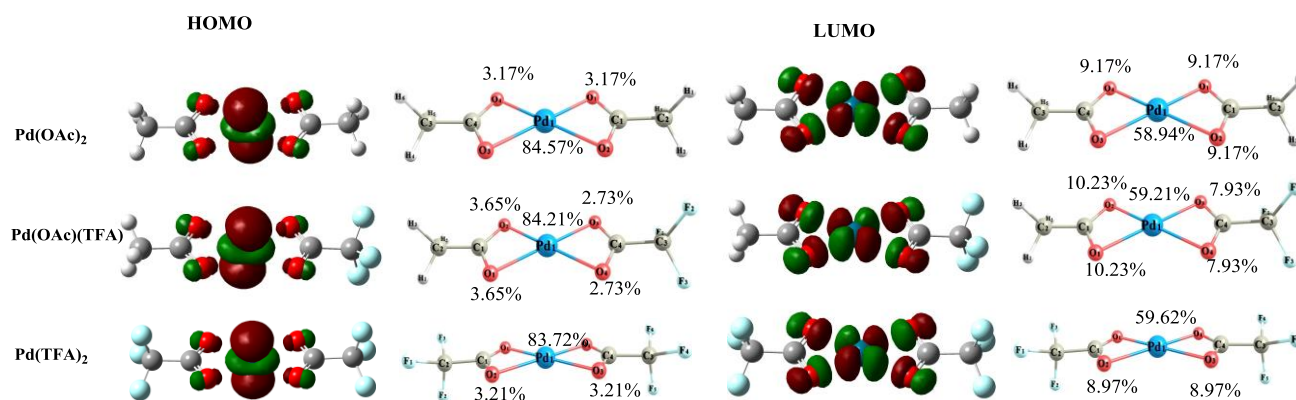


Figure S28. The HOMO and LUMO and the corresponding distributions of Pd(II)-catalysts.

Table S22. The energy differences between the LUMO of one reactant and the HOMO of the other one for different Pd-catalysts (in a.u.)

Molecule	HOMO	LUMO	LUMO _{indole} -HOMO _{Pd}	LUMO _{Pd} -HOMO _{indole}
Indole	-0.2087	-0.0325		
Pd(OAc) ₂	-0.2646	-0.1181	0.2321	0.0906
Pd(OAc)(TFA)	-0.2854	-0.1425	0.2529	0.0662
Pd(TFA) ₂	-0.3064	-0.1670	0.2719	0.0417

Table S23. The natural charges of Pd atom both in the isolated catalyst and the transferred electron density (Δe) from the substrate to Pd(II)-catalysts in proton transfer transition states (TS) among three pathways (a, b, and c) (|e|).

Δe	Pd center	Pathway a		Pathway b		Pathway c	
		C2	C4	C2	C4	C2	C4
Pd(OAc) ₂	0.729	0.29	0.34	0.26	0.30	0.18	0.19
Pd(TFA)(OAc)	0.754	0.37	0.42	0.28	0.34	0.21	0.23
Pd(OAc)(TFA)	0.754	0.21	0.38	0.30	0.34	0.24	0.25
Pd(TFA) ₂	0.781	0.43	0.47	0.34	0.38	0.28	0.29

Now that Pd-catalyst could provide LUMO, Pd center should accept extra electron. As shown in Table S23, along the order of Pd(OAc)₂, Pd(TFA)(OAc) and Pd(TFA)₂, the positive natural charge of Pd center is 0.729, 0.754, 0.781. When nucleophilic **1a** attack Pd center of catalyst, the transferred electrons density (Δe) from indole moiety to Pd-catalyst should increase along the order above. In order to confirm this prediction, we have chosen the proton-transfer TS among three pathways to analyze the Δe values as shown in Table S23. Generally, the larger Δe values in reaction process, the smaller the barrier energies. Luckily, the Δe values are directly corrected to the barrier energies as shown in Figure S23.

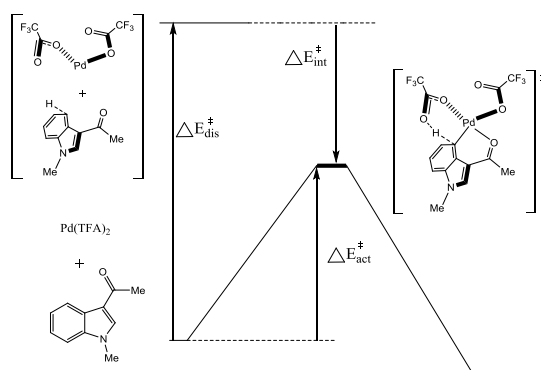


Figure S29. Relationship between the activation energy and the distortion and interaction energies of reactants.

Activation strain model (ASM)⁴⁻⁵ to analyze the distortion of substrate or catalyst and the interaction between them in the C-H activation process. ASM is a fragment approach to understand organic reactions, in which the height of the energetic barrier is described in terms of the original reactants. As depicted in Figure S29, the activation energy of the TSs of the nucleophilic attack ($\Delta E_{\text{act}}^{\ddagger}$) is decomposed into two parts: the energies that are required for the distorting the separate reactants (indole and Pd-catalyst) from ground state to the TS geometries [$\Delta E_{\text{dis}}^{\ddagger}(\text{indole})$, $\Delta E_{\text{dis}}^{\ddagger}(\text{Pd})$], and the interaction energy between these deformed reactants ($\Delta E_{\text{int}}^{\ddagger}(\text{indole-Pd})$), namely, $\Delta E_{\text{act}}^{\ddagger} = \Delta E_{\text{dis}}^{\ddagger}(\text{indole}) + \Delta E_{\text{dis}}^{\ddagger}(\text{Pd}) + \Delta E_{\text{int}}^{\ddagger}(\text{indole-Pd})$.

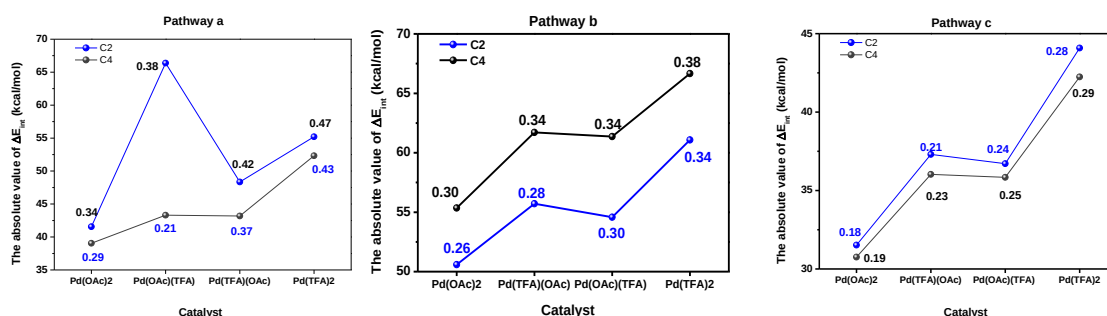


Figure S30. The calculated absolute values of $\Delta E_{\text{int}}^{\ddagger}(\text{indole-Pd})$ for Pd(OAc)₂, Pd(TFA)(OAc), Pd(OAc)(TFA) and Pd(TFA)₂ in pathways **a**, **b**, and **c**.

Table S24. Comparison of overall free energies about C2 & C4-H activation under various Pd(II)-catalysts (kcal/mol).

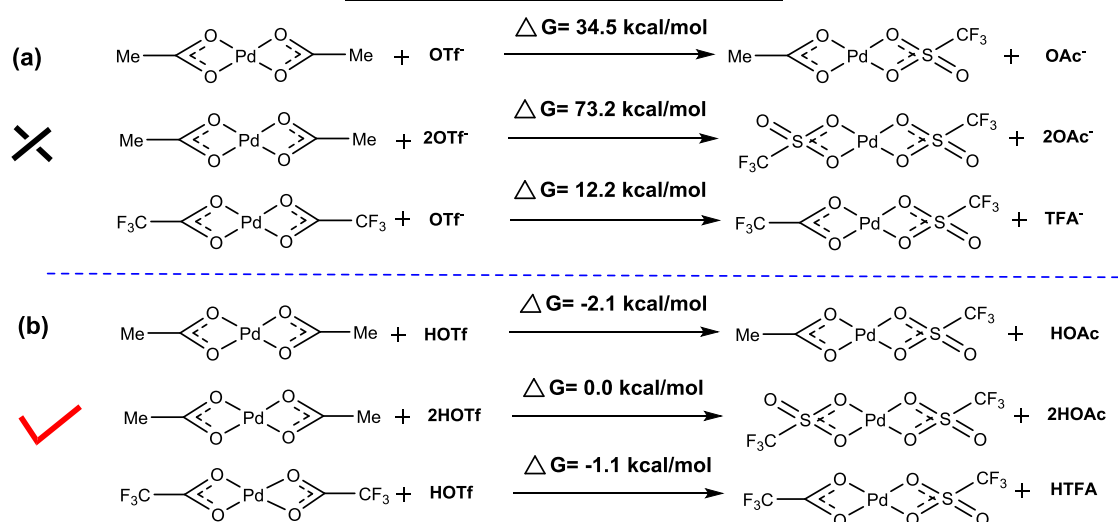
		Pathway a		Pathway b		Pathway c	
		C2-H	C4-H	C2-H	C4-H	C2-H	C4-H
Pd(OAc) ₂	$\Delta G_{\text{sol}}^{\ddagger}$	37.0	35.8	28.2	27.2	25.5	25.8
	$\Delta E_{\text{act}}^{\ddagger}$	26.4	24.9	16.7	15.4	14.9	16.0
	$\Delta E_{\text{dis}}^{\ddagger}(\text{indole})$	19.7	16.3	35.1	38.7	28.3	28.9
	$\Delta E_{\text{dis}}^{\ddagger}(\text{Pd})$	48.3	47.7	32.2	32.1	18.0	17.9
	$\Delta E_{\text{int}}^{\ddagger}(\text{indole-Pd})$	-41.6	-39.0	-50.6	-55.3	-31.5	-30.8

Pd(TFA)(OAc)	$\Delta G_{\text{sol}}^{\ddagger}$	24.5	22.3	25.4	21.7	21.7	21.4
	$\Delta E_{\text{act}}^{\ddagger}$	11.7	8.8	13.8	10.8	11.1	11.6
	$\Delta E_{\text{dis}}^{\ddagger}(\text{indole})$	20.5	13.8	42.7	45.7	37.9	37.0
	$\Delta E_{\text{dis}}^{\ddagger}(\text{Pd})$	39.5	38.2	26.8	26.8	10.5	10.6
	$\Delta E_{\text{int}}^{\ddagger}(\text{indole-Pd})$	-48.3	-43.2	-55.7	-61.7	-37.3	-36.0
Pd(OAc)(TFA)	$\Delta G_{\text{sol}}^{\ddagger}$	36.6	29.7	16.9	13.2	21.4	20.7
	$\Delta E_{\text{act}}^{\ddagger}$	25.3	20.1	5.2	1.9	11.1	10.9
	$\Delta E_{\text{dis}}^{\ddagger}(\text{indole})$	59.3	21.3	34.3	37.8	29.4	28.4
	$\Delta E_{\text{dis}}^{\ddagger}(\text{Pd})$	32.4	42.1	25.5	25.4	18.6	18.3
	$\Delta E_{\text{int}}^{\ddagger}(\text{indole-Pd})$	-66.4	-43.3	-54.6	-61.4	-36.7	-35.8
Pd(TFA) ₂	$\Delta G_{\text{sol}}^{\ddagger}$	19.3	15.9	13.0	6.6	15.4	14.0
	$\Delta E_{\text{act}}^{\ddagger}$	7.2	3.4	0.4	-4.1	5.5	4.6
	$\Delta E_{\text{dis}}^{\ddagger}(\text{indole})$	21.7	17.7	42.0	44.9	38.9	36.3
	$\Delta E_{\text{dis}}^{\ddagger}(\text{Pd})$	40.7	38.0	19.6	19.4	10.7	10.5
	$\Delta E_{\text{int}}^{\ddagger}(\text{indole-Pd})$	-55.2	-52.3	-61.1	-68.4	-44.1	-42.2

3. The prediction of the role of super-acid HOTf in C-H activation process

Table S25. The natural charge of Pd center in various catalysts.

Catalyst	Pd center
Pd(OAc) ₂	0.729
Pd(TFA)(OAc)	0.754
Pd(TFA) ₂	0.781
Pd(OAc)(OTf)	0.749
Pd(TFA)(OTf)	0.773
Pd(OTf) ₂	0.762



Scheme S3. Calculated free energy changes along interconversions among possible Pd-catalysts after the addition of HOTf.

Based on the discussions above, other acidic additive, which is capable of introducing strong

electron-withdrawing ligand into Pd-catalyst, would also realize the exclusive C4-fluoroalkylation under mild reaction condition. It should be indicated that OTf anion, which arises from stronger acid HOTf, exists in the system of Shi's reaction and the OTf ligand has been verified to be capable of accelerating some C-H activation under Pd-catalyst. However, as shown in Scheme S3(a), OTf anion alone is not capable of resulting into Pd-catalyst containing stronger electron withdrawing ligand of OTf, i.e., Pd(OTf)L (L=OAc⁻, TFA⁻ and OTf⁻), in the aspect of thermodynamics. Thus it is highly probable for the nonexistence of Pd(OTf)L in Shi's reaction. What if the reaction condition was modified by adding HOTf? As shown in Scheme S3(b), the creation of Pd(OTf)L should be thermodynamically available. Therefore, we explore here both the C4-H and C2-H activation, catalyzed by these Pd(OTf)L (L=OAc⁻, TFA⁻ and OTf⁻) catalysts generated by HOTf acid. (Scheme S3(b)), Similar as above sections, all the three pathways were investigated.

Similar to Pd(OAc)(TFA), there are two different ligands (OTf⁻ and L) responsible for abstracting proton H on target carbon center in each Pd(OTf)L (L=OAc⁻, TFA⁻), i.e., Pd(**OTf**)L and Pd**L**(OTf) are denoted as the cases where OTf⁻ and L anion abstract proton H on target sites respectively. For all these potential catalysts, the calculated free energy profiles of C4-H and C2-H activation along three pathways are shown in Figure S31 ~ S40, and the corresponding free energies, as well as energy barriers, are summarized in Table S26.

The free energies of the rate-determining TS in C4-H activation, catalyzed by Pd(**TFA**)(OTf) and Pd(OTf)₂, are 2.4 kcal/mol and 3.3 kcal/mol respectively. These values are apparently lower than that of Pd(TFA)₂ by 4.2 and 3.3 kcal/mol respectively. The corresponding free energy barriers in both catalysts are also lower (10.1, 10.2 kcal/mol) when comparing to Pd(TFA)₂ (13.2 kcal/mol). Due to the markedly decreased free energy of TS, the step of C4-H activation should become easier when adding HOTf acid. Moreover, the regioselectivity of C4 over C2 site should also be improved due to the increased difference of free energy of rate-determining TS between C4-H and C2-H activation when introducing HOTf (Table S26). For example, these differences are 6.9 and 8.4 kcal/mol in that catalyzed by Pd(**TFA**)(OTf) and Pd(OTf)₂ respectively, which are higher than that of Pd(TFA)₂ (6.4 kcal/mol).

The significant improvement due to the addition of HOTf is also related to the stronger electron-accepting ability of these potential Pd-catalysts arising from the strong electron-withdrawing ligand of

OTf. This increased ability is indicated in the larger amount of positive charge of Pd center and the lower LUMO energy of Pd(OTf)L. These results are consistent with correlation between the increased amount of transferred electron density (Δe) and reduced free energy barrier as shown in Table. S26 ~ S27 and Figure S44. Once again, the regioselectivity of C4 over C2 site is echoed in the Δe value of C4-H activation which is larger than that of C2-H activation.

Among these Pd(OTf)L (L=OAc⁻, TFA⁻ and OTf⁻) catalysts, the most efficient ones are Pd(TFA)(OTf) and Pd(OTf)₂ in the C-H activation step. In order to provide a thorough and reliable prediction, we also show here other steps, i.e., oxidative addition and reductive elimination, of C4-functionalization with Pd(TFA)(OTf) as the catalyst. Similar as Pd(TFA)₂, Pd(TFA)(OTf) could also support feasible C4-functionalization due to the low free energy barriers which are 10.1, 9.4 and 19.9 kcal/mol for C-H activation, oxidative addition and reductive elimination respectively. Moreover, the thermodynamic is also feasible with 78.7 kcal/mol exergonic. Therefore, the formed Pd(TFA)(OTf) after adding HOTf should be a promising catalyst for this reaction.

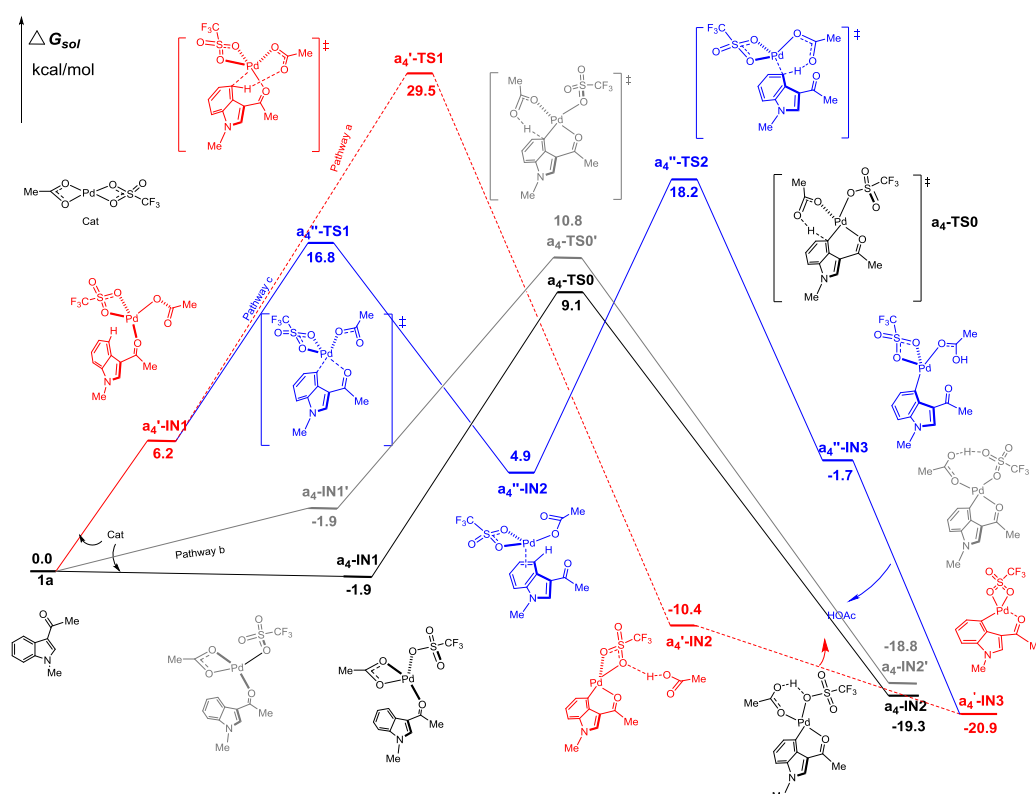


Figure S31. Three possible pathways of C4-H activation in indole with Pd(OAc)(OTf) as efficient catalyst.

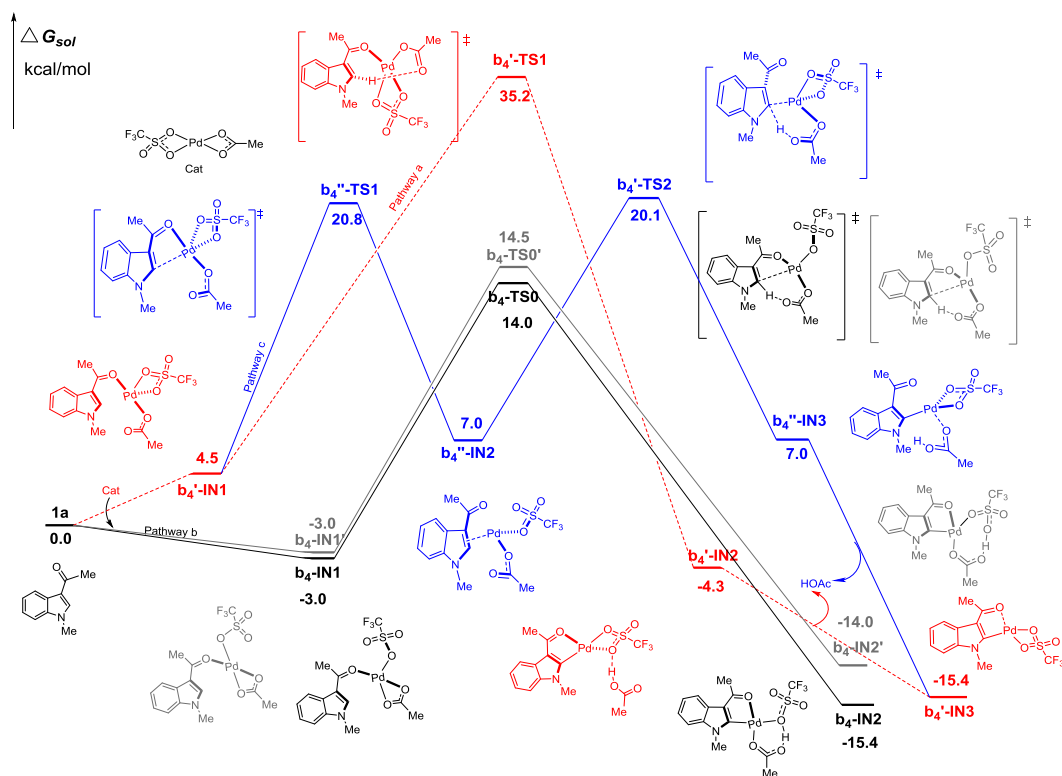


Figure S32. Three possible pathways of C2-H activation in indole with $\text{Pd}(\text{OAc})(\text{OTf})$ as efficient catalyst.

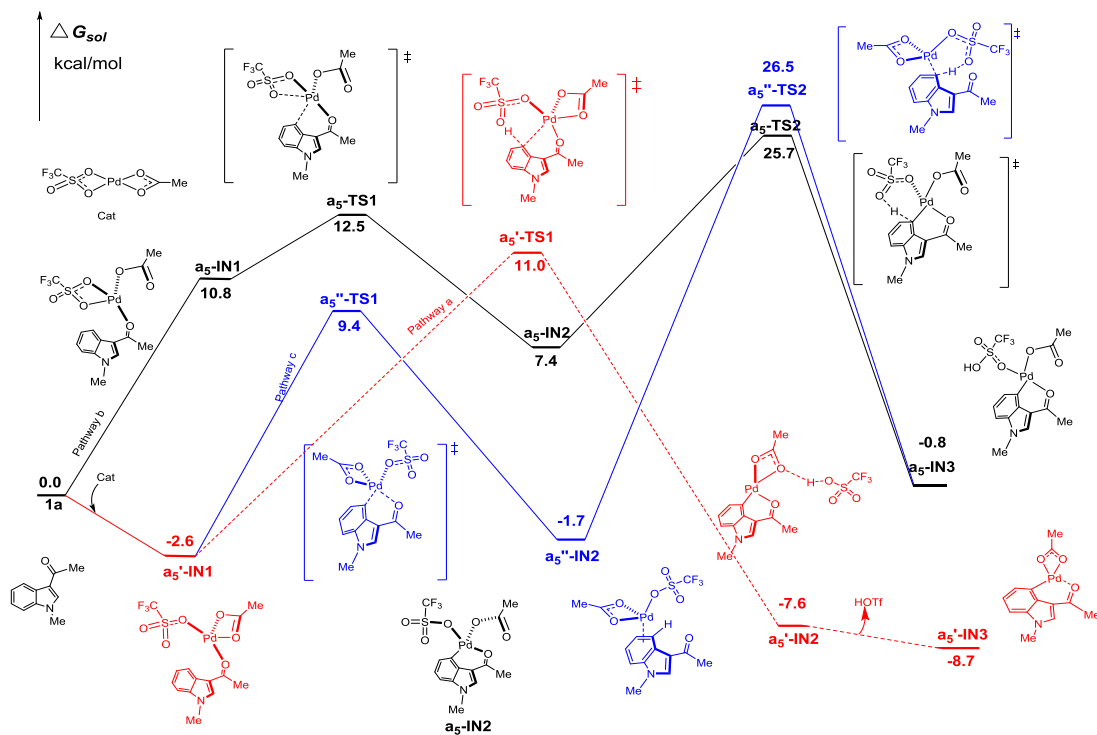


Figure S33. Three possible pathways of C4-H activation in indole with $\text{Pd}(\text{OTf})(\text{OAc})$ as efficient catalyst.

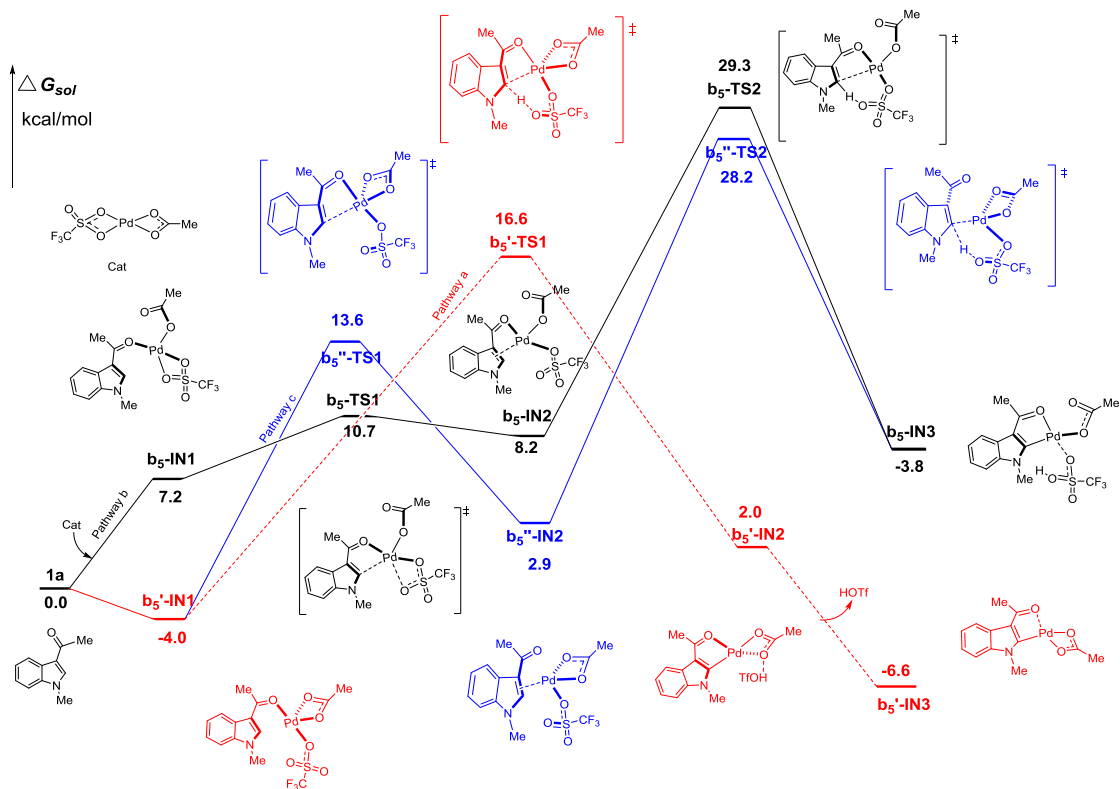


Figure S34. Three possible pathways of C2-H activation in indole with Pd(OTf)(OAc) as efficient catalyst.

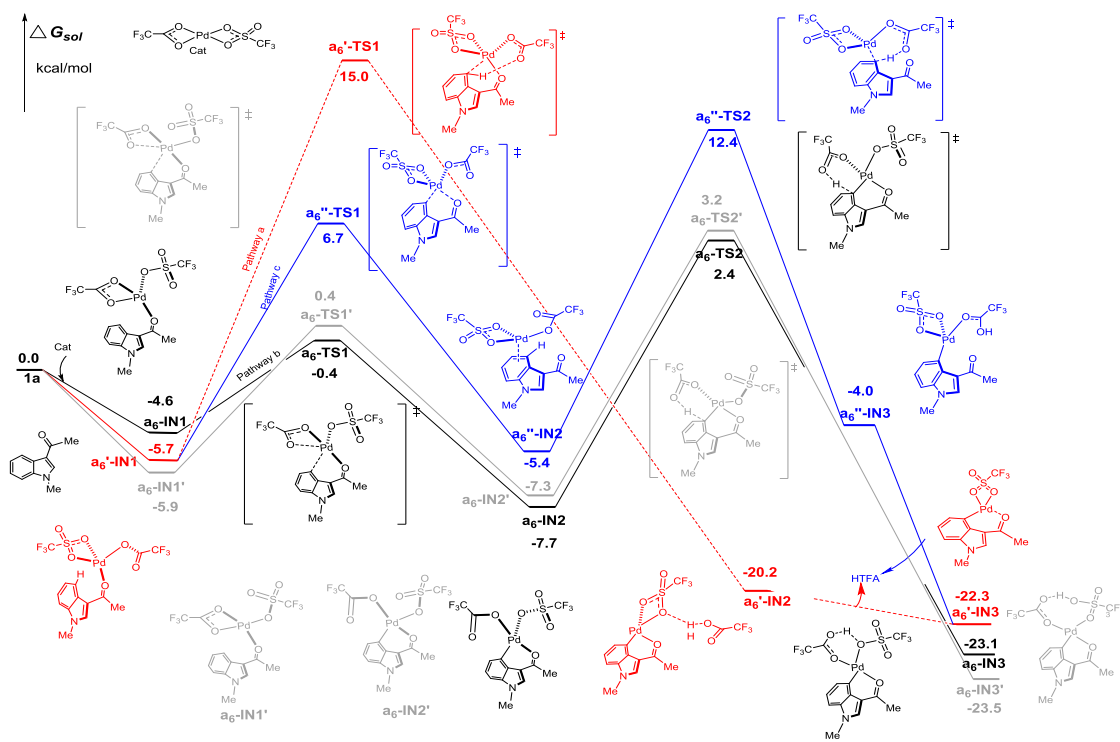


Figure S35. Three possible pathways of C4-H activation in indole with Pd(TFA)(OTf) as efficient catalyst.

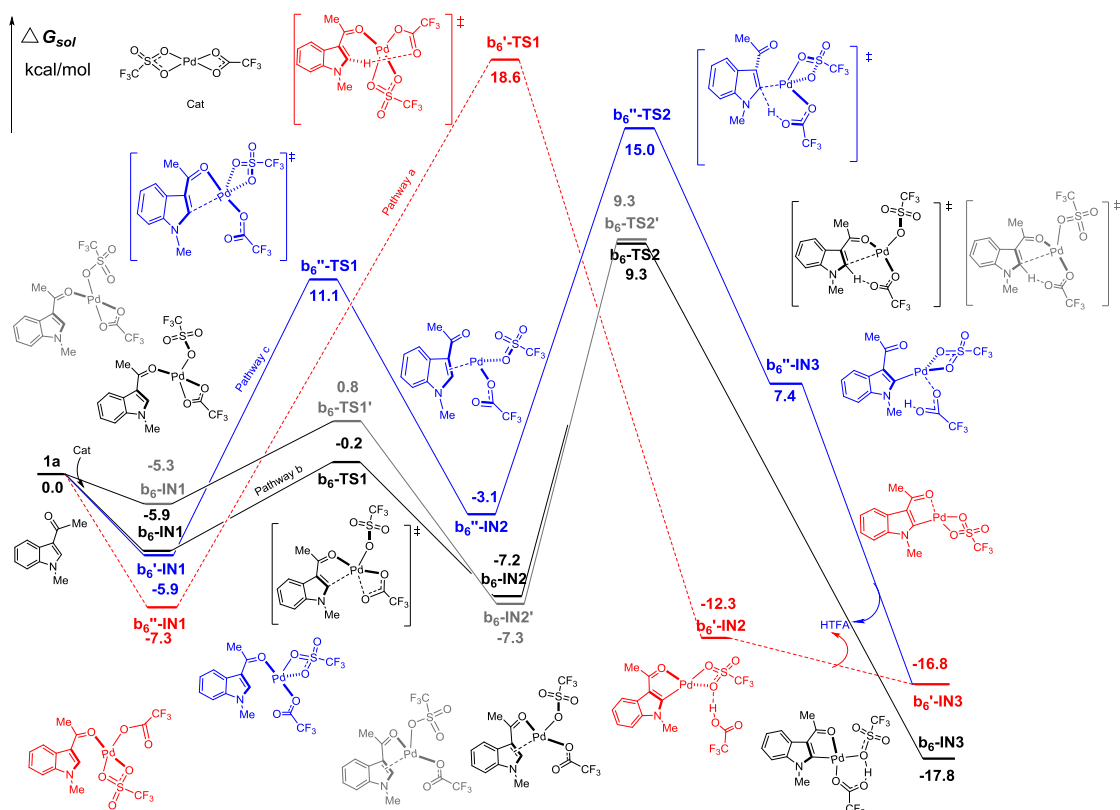


Figure S36. Three possible pathways of C2-H activation in indole with Pd(TFA)(OTf) as efficient catalyst.

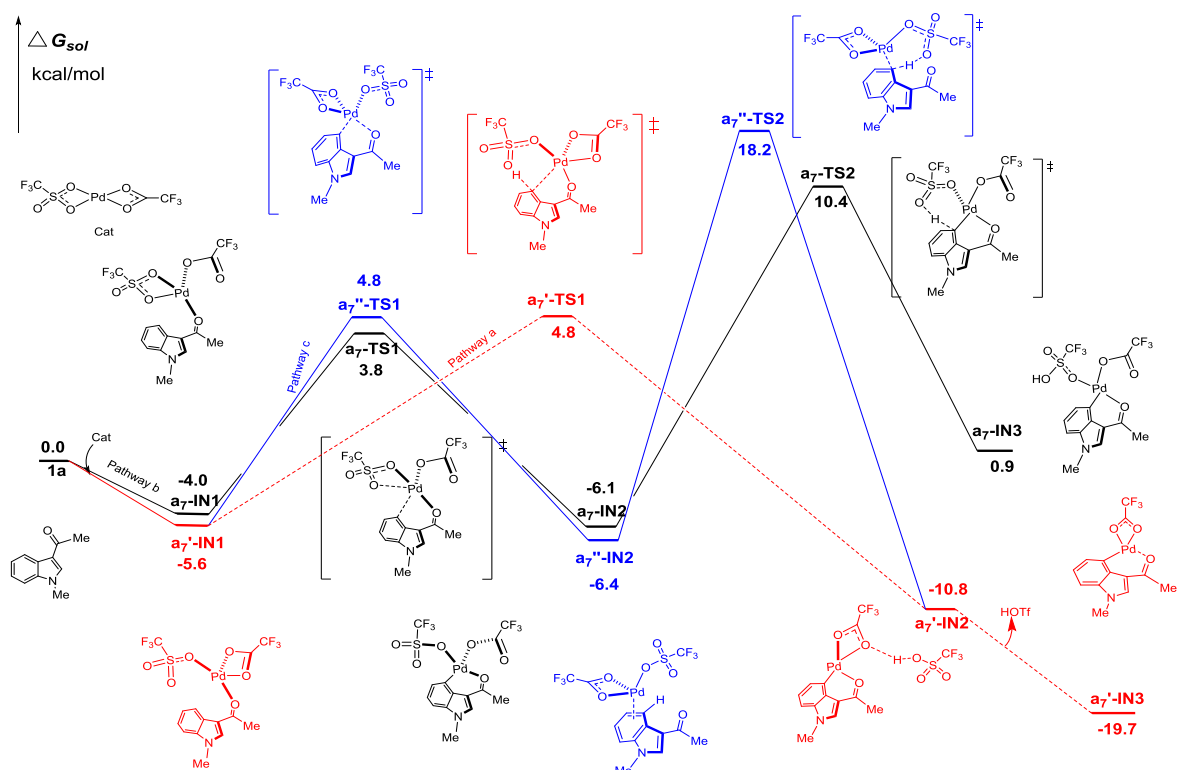


Figure S37. Three possible pathways of C4-H activation in indole with Pd(OTf)(TFA) as efficient catalyst.

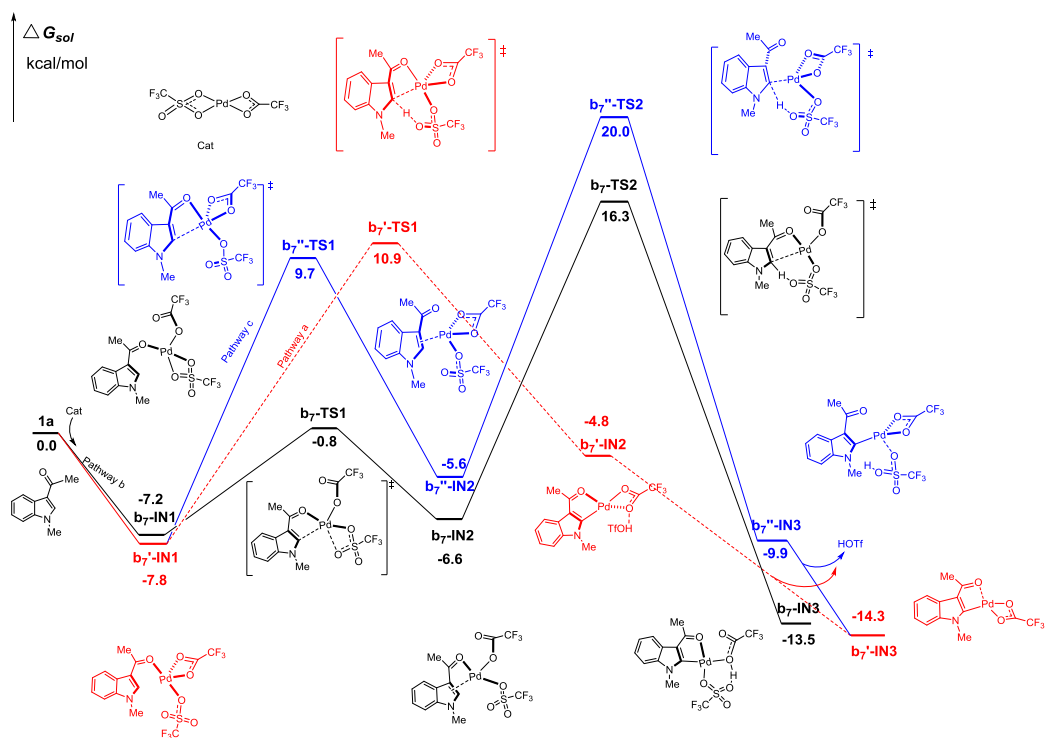


Figure S38. Three possible pathways of C2-H activation in indole with $\text{Pd}(\text{OTf})(\text{TFA})$ as efficient catalyst.

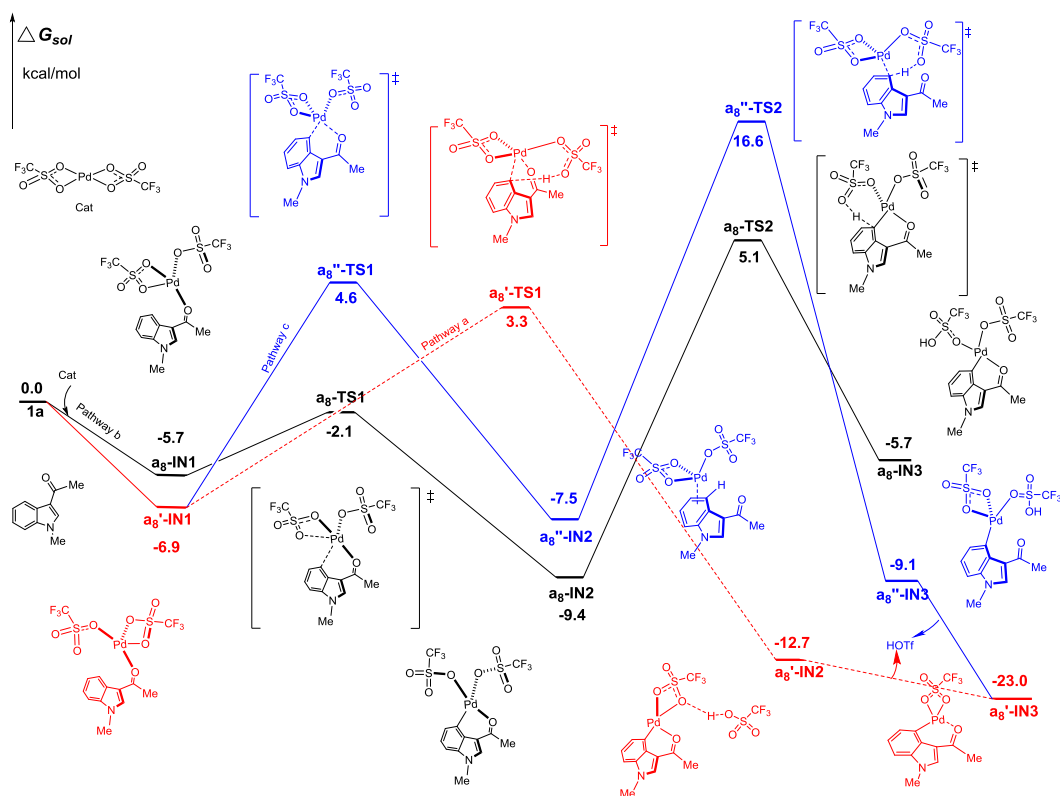


Figure S39. Three possible pathways of C4-H activation in indole with $\text{Pd}(\text{OTf})_2$ as efficient catalyst.

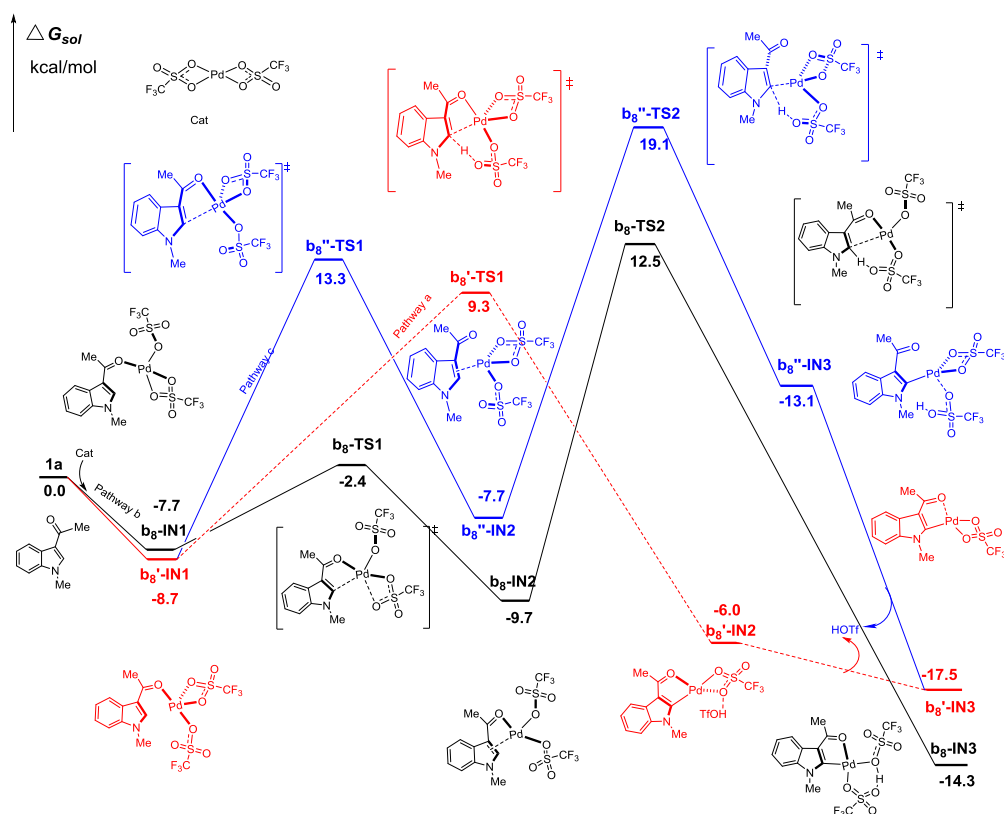


Figure S40. Three possible pathways of C2-H activation in indole with Pd(OTf)₂ as efficient catalyst.

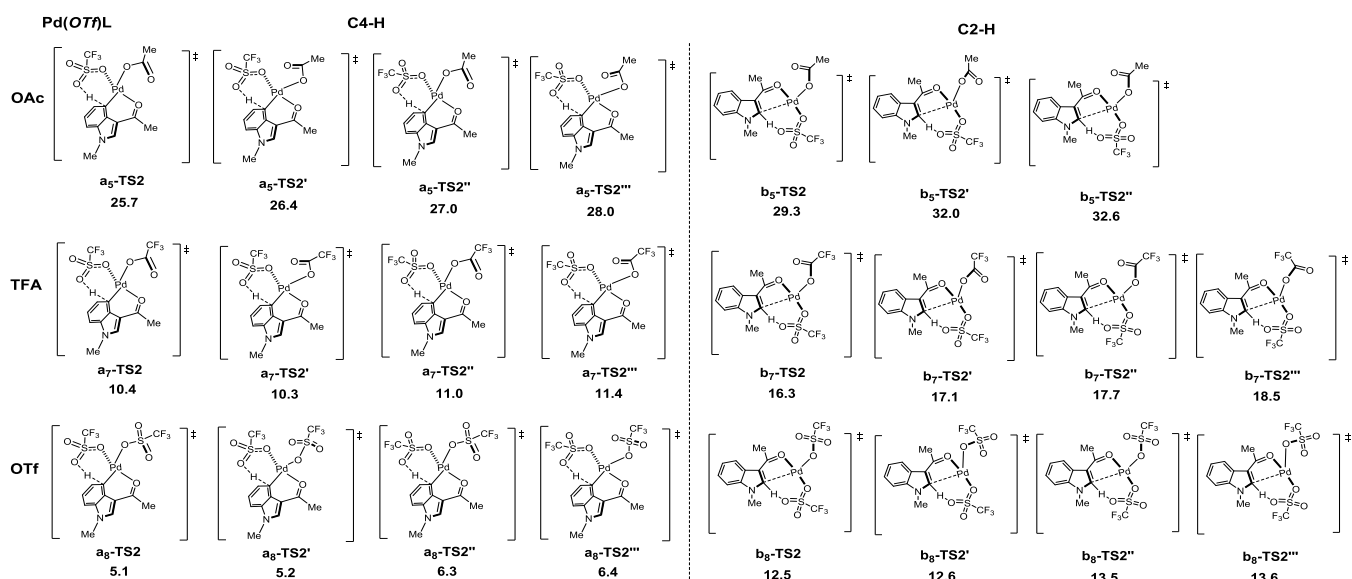
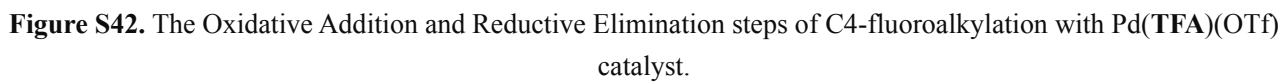


Figure S41. The other possible isomers of proton transfer TS in pathway b catalyzed Pd(OTf)L (L=OAc⁻, TFA⁻, OTf⁻).



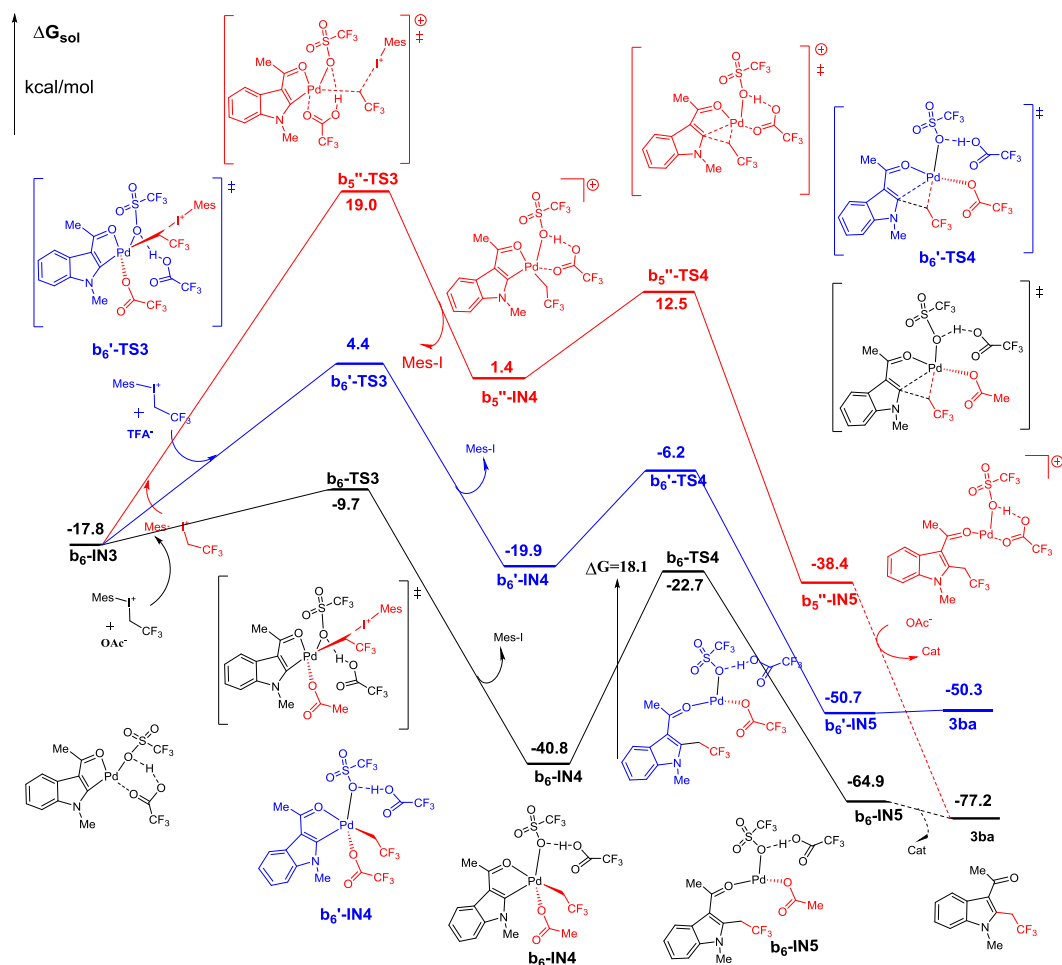


Figure S43. The Oxidative Addition and Reductive Elimination steps of C2-fluoroalkylation with Pd(TFA)(OTf) catalyst.

Table S26. Comparison of overall free energies of TS in the C2 & 4-H activation under various Pd-catalysts including OTf⁻ anion (kcal/mol).

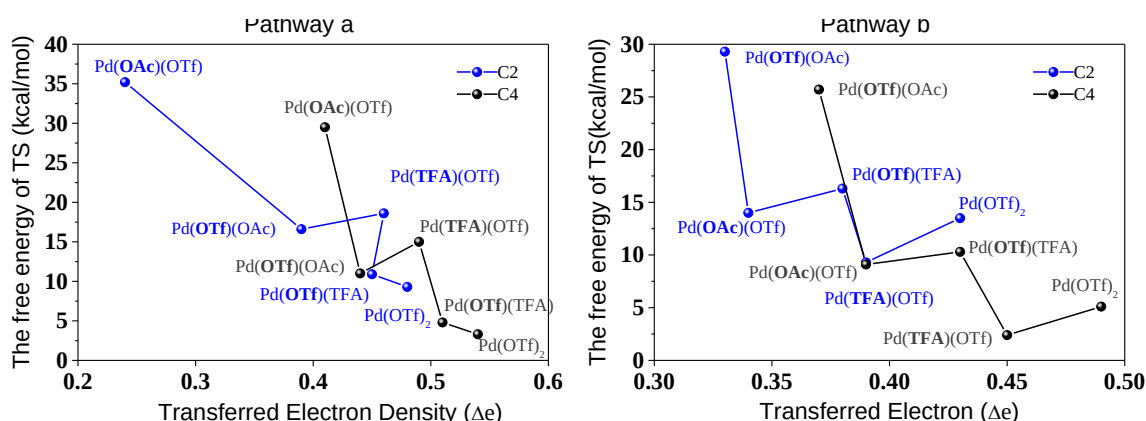
C-H activation	Pathway a			Pathway b			Pathway c		
The free energies	C2-H	C4-H	$\Delta(\text{C2-C4})$	C2-H	C4-H	$\Delta(\text{C2-C4})$	C2-H	C4-H	$\Delta(\text{C2-C4})$
Pd(OAc)(OTf)	35.2	29.5	5.7	14.0	9.1	4.9	20.1	18.2	1.9
Pd(OTf)(OAc)	16.6	11.0	5.6	29.3	25.7	3.6	28.2	26.5	1.7
Pd(TFA)(OTf)	18.6	15.0	3.6	9.3	2.4	6.9	15.0	12.4	2.6
Pd(OTf)(TFA)	10.9	4.8	6.1	16.3	10.3	6.0	20.0	18.2	1.8
Pd(OTf) ₂	9.3	3.3	6.0	12.5	5.1	7.4	19.1	16.6	2.5
The energy barrier	C2-H	C4-H	$\Delta(\text{C2-C4})$	C2-H	C4-H	$\Delta(\text{C2-C4})$	C2-H	C4-H	$\Delta(\text{C2-C4})$
Pd(OAc)(OTf)	35.2	29.5	5.7	17.0	11.0	6.0	20.1	18.2	1.9
Pd(OTf)(OAc)	20.6	13.6	7.0	29.3	25.7	3.6	32.2	29.1	3.1
Pd(TFA)(OTf)	25.9	20.7	5.2	16.5	10.1	6.4	20.9	18.1	2.8
Pd(OTf)(TFA)	18.7	10.4	8.3	23.6	16.5	7.1	27.8	24.6	3.2
Pd(OTf) ₂	18.0	10.2	7.8	22.2	14.5	7.7	27.8	24.1	3.7

Table S27. The gap of LUMO in indole and HOMO in Pd-catalyst and the gap of LUMO in Pd-catalyst and HOMO in indole.

Molecule	Pd center	HOMO(a.u.)	LUMO(a.u.)	LUMO _{indole} -HOMO _{Pd} (a.u.)	LUMO _{Pd} -HOMO _{indole} (a.u.)
Indole	-	-0.2087	-0.0325		
Pd(OAc) ₂	0.729	-0.2646	-0.1181	0.2321	0.0906
Pd(OAc)(TFA)	0.754	-0.2854	-0.1425	0.2529	0.0662
Pd(TFA) ₂	0.781	-0.3064	-0.1670	0.2719	0.0417
Pd(OAc)(OTf)	0.749	-0.2910	-0.1497	0.2585	0.0589
Pd(TFA)(OTf)	0.773	-0.3109	-0.1725	0.2784	0.0361
Pd(OTf) ₂	0.762	-0.3154	-0.1773	0.2829	0.0314

Table S28. The natural charge of Pd atom both in the isolated catalyst and the transferred electron density (Δe) from the substrate to Pd(II)-catalysts in proton transfer transition states (TS) among three pathways (**a**, **b**, and **c**) (|e|).

Δe	Pd center	Pathway a		Pathway b		Pathway c	
		C2	C4	C2	C4	C2	C4
Pd(OAc) ₂	0.729	0.29	0.34	0.26	0.30	0.18	0.19
Pd(OAc)(TFA)	0.754	0.21	0.38	0.30	0.34	0.24	0.25
Pd(OAc)(OTf)	0.749	0.24	0.41	0.34	0.39	0.27	0.27
Pd(TFA)(OAc)	0.754	0.37	0.42	0.28	0.34	0.21	0.23
Pd(TFA) ₂	0.781	0.43	0.47	0.34	0.38	0.28	0.29
Pd(TFA)(OTf)	0.773	0.46	0.49	0.39	0.45	0.30	0.32
Pd(OTf)(OAc)	0.749	0.39	0.44	0.33	0.37	0.27	0.29
Pd(OTf)(TFA)	0.773	0.45	0.51	0.38	0.43	0.34	0.36
Pd(OTf) ₂	0.762	0.48	0.54	0.43	0.49	0.36	0.39



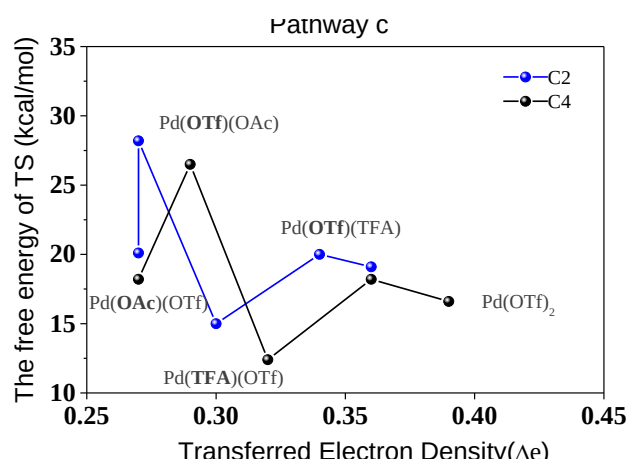


Figure S44. The relation of the free energy of highest-point with the transferred electron density (Δe) in C-H activation catalyzed by Pd(OTf)L formed after adding HOTf acid along pathways **a**, **b** and **c**.

Part II

4. The energies for the overall catalytic cycle with various Pd-catalysts

Sum of electronic energies (E, in Hartree), sum of electronic and thermal enthalpies (H, in Hartree), sum of electronic and thermal free energies (G, in Hartree), thermal correction to Gibbs free energy (TCGFE, in Hartree), electronic energy in solution (E_{sol}, in Hartree), electronic energy in gas (E_{gas}, in Hartree) and total free energy in DCM solution (G_{sol}, which equals to $\Delta E_{\text{sol}} + E_{\text{gas_lar}} + \text{TCGFE}$, in Hartree). Relative energies (ΔG_{sol} and $\Delta G_{\text{sol M06-2X}}$) are reported in kcal/mol.

Table S29. Potential energy surface for the functionalization catalyzed by Pd(OAc)₂

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol}	ΔG_{sol}	$\Delta G_{\text{sol M06-2X}}$
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(OAc)₂	-583.729	-583.614	-583.665	0.064	-583.426	-583.412	-0.013	-585.061	-585.010		
a₀-IN1	-1139.504	-1139.178	-1139.262	0.242	-1138.999	-1138.964	-0.035	-1140.991	-1140.785	10.5	1.7
a₀-TS1	-1139.483	-1139.159	-1139.240	0.243	-1138.987	-1138.943	-0.044	-1140.970	-1140.771	19.4	10.4
a₀-IN2	-1139.483	-1139.158	-1139.242	0.241	-1138.987	-1138.943	-0.044	-1140.971	-1140.774	17.4	8.8
a₀-TS2	-1139.468	-1139.147	-1139.227	0.241	-1138.965	-1138.924	-0.042	-1140.958	-1140.758	27.2	22.4
a₀-IN3	-1139.505	-1139.178	-1139.260	0.245	-1139.006	-1138.968	-0.038	-1140.998	-1140.791	6.4	-0.6
a₀'-IN1	-1139.505	-1139.179	-1139.264	0.242	-1138.999	-1138.963	-0.037	-1140.992	-1140.787	9.1	1.5
a₀'-TS1	-1139.451	-1139.130	-1139.212	0.240	-1138.948	-1138.904	-0.044	-1140.940	-1140.745	35.8	32.7
a₀'-IN2	-1139.526	-1139.199	-1139.283	0.243	-1139.017	-1138.983	-0.034	-1141.017	-1140.808	-4.3	-8.8
a₀'-IN3	-910.430	-910.173	-910.241	0.189	-910.013	-909.982	-0.031	-911.839	-911.681	-10.9	-10.8
a₀''-TS1	-1139.487	-1139.162	-1139.247	0.240	-1138.982	-1138.947	-0.035	-1140.972	-1140.767	21.8	11.3
a₀''-IN2	-1139.503	-1139.178	-1139.262	0.242	-1138.997	-1138.961	-0.036	-1140.991	-1140.785	10.4	3.3
a₀''-TS2	-1139.478	-1139.158	-1139.240	0.238	-1138.967	-1138.933	-0.034	-1140.965	-1140.761	25.8	19.5
a₀''-IN3	-1139.508	-1139.182	-1139.264	0.244	-1139.005	-1138.972	-0.033	-1140.998	-1140.787	9.1	-0.8

a₀-IN1'	-1139.505	-1139.179	-1139.262	0.243	-1138.997	-1138.964	-0.032	-1140.992	-1140.781	12.7	3.9
a₀-TS0	-1139.467	-1139.147	-1139.228	0.240	-1138.965	-1138.923	-0.042	-1140.957	-1140.760	26.4	22.0
a₀-IN2'	-1139.523	-1139.199	-1139.282	0.241	-1139.021	-1138.987	-0.034	-1141.015	-1140.808	-3.9	-12.4
b₀-IN1	-1139.510	-1139.184	-1139.266	0.244	-1139.001	-1138.969	-0.032	-1140.996	-1140.784	11.1	2.1
b₀-TS0	-1139.474	-1139.153	-1139.233	0.240	-1138.963	-1138.928	-0.035	-1140.962	-1140.757	28.2	23.9
b₀-IN2	-1139.528	-1139.203	-1139.284	0.244	-1139.017	-1138.988	-0.029	-1141.019	-1140.804	-1.3	-7.7
b₀'-IN1	-1139.517	-1139.190	-1139.272	0.244	-1139.003	-1138.973	-0.030	-1141.003	-1140.788	8.3	1.2
b₀'-TS1	-1139.461	-1139.141	-1139.222	0.239	-1138.945	-1138.912	-0.033	-1140.948	-1140.743	37.0	34.0
b₀'-IN2	-1139.529	-1139.202	-1139.285	0.244	-1139.010	-1138.984	-0.026	-1141.021	-1140.802	-0.2	-3.3
b₀'-IN3	-910.435	-910.178	-910.245	0.190	-910.008	-909.985	-0.023	-911.844	-911.678	-8.7	-6.8
b₀''-TS1	-1139.490	-1139.166	-1139.248	0.242	-1138.979	-1138.950	-0.029	-1140.975	-1140.762	24.8	14.6
b₀''-IN2	-1139.505	-1139.180	-1139.261	0.244	-1138.999	-1138.966	-0.032	-1140.993	-1140.781	12.8	3.5
b₀''-TS2	-1139.483	-1139.163	-1139.244	0.239	-1138.967	-1138.938	-0.030	-1140.971	-1140.761	25.5	20.1
b₀''-IN3	-1139.505	-1139.179	-1139.261	0.244	-1139.000	-1138.971	-0.029	-1140.995	-1140.780	13.4	2.7
b₀-IN1'	-1139.506	-1139.180	-1139.264	0.243	-1138.999	-1138.963	-0.036	-1140.993	-1140.787	9.5	2.4
b₀-TS0	-1139.473	-1139.153	-1139.231	0.242	-1138.963	-1138.929	-0.034	-1140.962	-1140.754	30.1	24.9
b₀-IN2'	-1139.541	-1139.215	-1139.296	0.246	-1139.026	-1139.000	-0.026	-1141.032	-1140.812	-6.3	-12.5
HOAc	-229.078	-229.010	-229.043	0.035	-228.988	-228.980	-0.008	-229.165	-229.138		

Table S30. Potential energy surface for the functionalization catalyzed by Pd(TFA)₂

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE _{sol}	E _{gas_lar}	G _{sol}	ΔG _{sol}	ΔG _{sol} M06-2X
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(TFA)₂	-1179.117	-1179.044	-1179.106	0.010	-1178.653	-1178.646	-0.007	-1180.654	-1180.651		
a₁-IN1	-1734.913	-1734.629	-1734.723	0.190	-1734.250	-1734.221	-0.029	-1736.608	-1736.446	-2.6	-11.8
a₁-TS1	-1734.896	-1734.614	-1734.709	0.188	-1734.242	-1734.202	-0.039	-1736.592	-1736.444	-1.0	-8.1
a₁-IN2	-1734.899	-1734.615	-1734.711	0.187	-1734.248	-1734.204	-0.044	-1736.596	-1736.452	-6.6	-12.2

a₁-TS2	-1734.879	-1734.601	-1734.693	0.186	-1734.221	-1734.181	-0.039	-1736.578	-1736.431	6.6	4.1
a₁-IN3	-1734.944	-1734.661	-1734.754	0.190	-1734.280	-1734.253	-0.027	-1736.642	-1736.479	-23.1	-30.5
a₁'-IN1	-1734.912	-1734.628	-1734.723	0.188	-1734.247	-1734.216	-0.031	-1736.607	-1736.450	-4.8	-11.0
a₁'-TS1	-1734.866	-1734.586	-1734.678	0.188	-1734.208	-1734.166	-0.042	-1736.563	-1736.417	15.9	13.3
a₁'-IN2	-1734.929	-1734.645	-1734.742	0.187	-1734.265	-1734.235	-0.030	-1736.627	-1736.470	-17.5	-22.9
a₁'-IN3	-1208.134	-1207.898	-1207.973	0.161	-1207.640	-1207.611	-0.029	-1209.648	-1209.516	-20.8	-20.1
a₁''-TS1	-1734.894	-1734.612	-1734.707	0.187	-1734.232	-1734.201	-0.030	-1736.588	-1736.431	6.6	-2.3
a₁''-IN2	-1734.909	-1734.626	-1734.723	0.187	-1734.245	-1734.213	-0.032	-1736.605	-1736.450	-5.0	-10.6
a₁''-TS2	-1734.880	-1734.603	-1734.697	0.183	-1734.211	-1734.183	-0.028	-1736.575	-1736.420	14.0	8.2
a₁''-IN3	-1734.896	-1734.612	-1734.710	0.186	-1734.238	-1734.210	-0.028	-1736.592	-1736.434	4.9	-6.5
a₁-IN1'	-1734.901	-1734.619	-1734.711	0.190	-1734.244	-1734.211	-0.033	-1736.596	-1736.439	1.6	-8.2
a₁-TS1'	-1734.903	-1734.619	-1734.714	0.188	-1734.250	-1734.211	-0.038	-1736.599	-1736.449	-4.6	-12.7
a₁-IN2'	-1734.903	-1734.619	-1734.714	0.188	-1734.250	-1734.211	-0.038	-1736.599	-1736.449	-4.6	-12.7
a₁-TS2'	-1734.879	-1734.601	-1734.693	0.186	-1734.220	-1734.181	-0.039	-1736.578	-1736.431	6.9	4.4
a₁-IN3'	-1734.933	-1734.651	-1734.744	0.189	-1734.271	-1734.243	-0.028	-1736.632	-1736.471	-18.5	-26.1
b₁-IN1	-1734.913	-1734.629	-1734.724	0.189	-1734.246	-1734.215	-0.030	-1736.608	-1736.450	-4.8	-10.0
b₁-TS1	-1734.901	-1734.618	-1734.711	0.190	-1734.238	-1734.204	-0.035	-1736.595	-1736.440	1.1	-4.9
b₁-IN2	-1734.901	-1734.618	-1734.714	0.187	-1734.242	-1734.205	-0.037	-1736.596	-1736.446	-2.8	-8.6
b₁-TS2	-1734.881	-1734.603	-1734.693	0.188	-1734.214	-1734.183	-0.031	-1736.578	-1736.421	13.0	9.5
b₁-IN3	-1734.947	-1734.663	-1734.755	0.192	-1734.271	-1734.251	-0.020	-1736.643	-1736.471	-18.3	-23.9
b₁'-IN1	-1734.921	-1734.637	-1734.731	0.190	-1734.248	-1734.223	-0.025	-1736.615	-1736.451	-5.8	-11.0
b₁'-TS1	-1734.871	-1734.592	-1734.683	0.187	-1734.200	-1734.166	-0.033	-1736.565	-1736.411	19.3	18.2
b₁'-IN2	-1734.928	-1734.644	-1734.739	0.189	-1734.254	-1734.232	-0.022	-1736.625	-1736.459	-10.6	-15.2
b₁'-IN3	-1208.136	-1207.900	-1207.973	0.163	-1207.631	-1207.610	-0.021	-1209.649	-1209.507	-15.4	-13.0
b₁''-IN1	-1734.921	-1734.637	-1734.731	0.190	-1734.248	-1734.223	-0.025	-1736.615	-1736.451	-5.7	-10.9
b₁''-TS1	-1734.894	-1734.612	-1734.706	0.188	-1734.225	-1734.199	-0.025	-1736.587	-1736.424	11.2	2.8
b₁''-IN2	-1734.911	-1734.628	-1734.721	0.190	-1734.250	-1734.219	-0.030	-1736.606	-1736.446	-2.9	-11.9
b₁''-TS2	-1734.883	-1734.605	-1734.699	0.184	-1734.209	-1734.185	-0.024	-1736.577	-1736.417	15.4	9.8
b₁''-IN3	-1734.900	-1734.617	-1734.712	0.188	-1734.236	-1734.213	-0.023	-1736.596	-1736.430	7.3	-4.1

b₁-IN1'	-1734.916	-1734.632	-1734.726	0.190	-1734.248	-1734.221	-0.027	-1736.610	-1736.448	-3.6	-10.8
b₁-TS1'	-1734.903	-1734.620	-1734.713	0.190	-1734.241	-1734.208	-0.033	-1736.597	-1736.440	1.0	-6.3
b₁-IN2'	-1734.904	-1734.621	-1734.715	0.189	-1734.249	-1734.211	-0.038	-1736.601	-1736.449	-4.7	-11.5
b₁-TS2'	-1734.881	-1734.603	-1734.694	0.187	-1734.214	-1734.182	-0.031	-1736.578	-1736.422	12.2	9.1
b₁-IN3'	-1734.934	-1734.652	-1734.744	0.190	-1734.263	-1734.240	-0.022	-1736.632	-1736.464	-13.9	-19.6
HTFA	-526.771	-526.725	-526.764	0.007	-526.602	-526.595	-0.007	-526.960	-526.959		
2a cation	-737.605	-737.370	-737.437	0.168	-737.357	-737.267	-0.090	-737.855	-737.777		
OAc-	-228.493	-228.439	-228.473	0.021	-228.489	-228.401	-0.088	-228.602	-228.669		
IMes	-360.973	-360.787	-360.838	0.135	-360.772	-360.761	-0.011	-361.100	-360.975		
a₁-IN4	-2340.313	-2339.922	-2340.041	0.272	-2339.427	-2339.390	-0.038	-2342.221	-2341.986	-45.9	-58.7
a₁-TS3	-2340.283	-2339.895	-2340.013	0.271	-2339.412	-2339.372	-0.040	-2342.188	-2341.958	-27.9	-49.8
a₁-IN5	-2340.347	-2339.955	-2340.073	0.274	-2339.486	-2339.453	-0.033	-2342.248	-2342.007	-58.6	-94.6
3aa	-932.120	-931.873	-931.935	0.185	-931.792	-931.769	-0.023	-932.404	-932.242	-80.3	-101.6
Pd_cat	-1408.232	-1408.091	-1408.168	0.063	-1407.680	-1407.669	-0.011	-1409.852	-1409.799		
TFA-	-526.230	-526.197	-526.236	-0.006	-526.141	-526.063	-0.077	-526.445	-526.528		
a₁-TS3	-2998.955	-2998.400	-2998.552	0.403	-2997.821	-2997.767	-0.054	-3001.088	-3000.740	4.8	-26.4
a₁'-IN4	-2638.011	-2637.642	-2637.767	0.243	-2637.050	-2637.012	-0.038	-2640.021	-2639.815	-27.3	-41.5
a₁'-TS4	-2637.989	-2637.621	-2637.745	0.244	-2637.040	-2637.000	-0.041	-2639.998	-2639.795	-14.4	-35.6
a₁'-IN5	-2638.052	-2637.682	-2637.807	0.245	-2637.115	-2637.083	-0.032	-2640.057	-2639.844	-45.3	-81.4
Pd_cat'	-1705.905	-1705.784	-1705.870	0.036	-1705.279	-1705.268	-0.011	-1707.628	-1707.603		
a₁''-TS3	-2472.573	-2472.053	-2472.188	0.385	-2471.625	-2471.540	-0.084	-2474.512	-2474.211	5.0	-6.2
a₁''-IN4	-2111.605	-2111.271	-2111.376	0.228	-2110.852	-2110.772	-0.081	-2113.417	-2113.269	-16.0	-19.1
a₁''-TS4	-2111.584	-2111.252	-2111.355	0.229	-2110.842	-2110.758	-0.084	-2113.398	-2113.252	-5.3	-12.2
a₁''-IN5	-2111.634	-2111.300	-2111.404	0.229	-2110.906	-2110.818	-0.088	-2113.445	-2113.304	-37.5	-52.3
b₁-TS3	-2701.251	-2700.676	-2700.822	0.429	-2700.184	-2700.136	-0.048	-2703.280	-2702.899	-6.3	-35.5
b₁-IN4	-2340.313	-2339.923	-2340.039	0.273	-2339.414	-2339.385	-0.029	-2342.219	-2341.974	-38.3	-49.5
b₁-TS4	-2340.283	-2339.895	-2340.012	0.271	-2339.394	-2339.364	-0.030	-2342.187	-2341.947	-21.0	-38.7
b₁-IN5	-2340.350	-2339.959	-2340.079	0.271	-2339.482	-2339.448	-0.034	-2342.252	-2342.015	-63.9	-93.7
3ba	-932.122	-931.875	-931.937	0.185	-931.793	-931.772	-0.021	-932.404	-932.240	-78.8	-101.5

b1'-TS3	-2998.960	-2998.405	-2998.556	0.403	-2997.810	-2997.766	-0.044	-3001.091	-3000.732	9.5	-19.2
b1'-IN4	-2638.010	-2637.641	-2637.763	0.246	-2637.034	-2637.008	-0.027	-2640.017	-2639.797	-16.0	-30.0
b1'-TS4	-2637.985	-2637.618	-2637.741	0.244	-2637.033	-2637.006	-0.027	-2639.992	-2639.775	-2.1	-31.1
b1'-IN5	-2638.057	-2637.687	-2637.812	0.245	-2637.113	-2637.080	-0.033	-2640.062	-2639.851	-49.5	-80.4
b1''-TS3	-2472.559	-2472.040	-2472.174	0.385	-2471.604	-2471.521	-0.083	-2474.497	-2474.195	15.1	6.5
b1''-IN4	-2111.584	-2111.251	-2111.357	0.227	-2110.823	-2110.746	-0.078	-2113.396	-2113.246	-1.6	-1.9
b1''-TS4	-2111.564	-2111.232	-2111.336	0.228	-2110.813	-2110.730	-0.083	-2113.373	-2113.228	9.8	5.2
b1''-IN5	-2111.638	-2111.304	-2111.409	0.229	-2110.912	-2110.824	-0.088	-2113.446	-2113.304	-37.7	-56.0

Table S31. Potential energy surface for the functionalization catalyzed by Pd(TFA)₂ based on solvent-phase geometry.

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD		
	E _{sol}	H _{sol}	G _{sol}	TCGFE _{sol}	E _{sol}	E _{gas}	ΔE _{sol}	E _{gas_lar}	G _{sol B3LYP+sol}	ΔG _{sol B3LYP+sol}
1a	-555.793	-555.585	-555.635	0.158	-555.558	-555.536	-0.023	-555.929	-555.793	
Pd(TFA)₂	-1179.122	-1179.050	-1179.110	0.012	-1178.653	-1178.646	-0.007	-1180.654	-1180.650	
a1-IN1	-1734.942	-1734.659	-1734.753	0.189	-1734.247	-1734.214	-0.033	-1736.606	-1736.450	-4.5
a1-TS1	-1734.934	-1734.652	-1734.743	0.191	-1734.241	-1734.200	-0.041	-1736.592	-1736.442	0.8
a1-IN2	-1734.943	-1734.661	-1734.755	0.189	-1734.249	-1734.198	-0.051	-1736.594	-1736.456	-8.1
a1-TS2	-1734.918	-1734.641	-1734.731	0.187	-1734.222	-1734.179	-0.043	-1736.577	-1736.433	6.1
a1-IN3	-1734.971	-1734.687	-1734.779	0.192	-1734.280	-1734.252	-0.028	-1736.641	-1736.477	-21.6
b1-IN1	-1734.944	-1734.661	-1734.754	0.191	-1734.247	-1734.213	-0.034	-1736.609	-1736.452	-6.0
b1-TS1	-1734.934	-1734.652	-1734.744	0.190	-1734.238	-1734.200	-0.038	-1736.594	-1736.442	0.3
b1-IN2	-1734.943	-1734.660	-1734.752	0.191	-1734.248	-1734.201	-0.047	-1736.597	-1736.454	-7.0
b1-TS2	-1734.912	-1734.634	-1734.723	0.189	-1734.214	-1734.180	-0.034	-1736.578	-1736.423	12.5
b1-IN3	-1734.965	-1734.682	-1734.774	0.191	-1734.271	-1734.251	-0.020	-1736.643	-1736.472	-18.3

Table S32. Potential energy surface for the functionalization catalyzed by Pd(OAc)(TFA)

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lac}	G _{sol}	ΔG_{sol}	ΔG_{sol} M06-2X
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(OAc)(TFA)	-881.424	-881.330	-881.387	0.037	-881.041	-881.031	-0.010	-882.860	-882.833		
a2-IN1	-1437.214	-1436.909	-1436.999	0.215	-1436.628	-1436.597	-0.031	-1438.807	-1438.623	1.0	-6.4
a2-TS0	-1437.178	-1436.879	-1436.965	0.213	-1436.599	-1436.557	-0.042	-1438.774	-1438.603	13.2	10.7
a2-IN2	-1437.234	-1436.930	-1437.018	0.217	-1436.654	-1436.621	-0.033	-1438.831	-1438.647	-14.4	-21.6
a2'-IN1	-1437.159	-1436.900	-1436.990	0.215	-1436.618	-1436.586	-0.032	-1438.795	-1438.612	7.4	-0.2
a2'-TS1	-1437.153	-1436.854	-1436.942	0.210	-1436.569	-1436.528	-0.041	-1438.746	-1438.577	29.7	27.8
a2'-IN2	-1437.223	-1436.918	-1437.009	0.214	-1436.636	-1436.604	-0.032	-1438.819	-1438.637	-8.0	-12.2
a2'-IN3	-1208.134	-1207.898	-1207.973	0.161	-1207.640	-1207.611	-0.029	-1209.648	-1209.516	-18.5	-18.4
a2''-TS1	-1437.188	-1436.885	-1436.974	0.214	-1436.604	-1436.572	-0.031	-1438.778	-1438.595	18.2	8.1
a2''-IN2	-1437.204	-1436.899	-1436.990	0.214	-1436.617	-1436.585	-0.032	-1438.795	-1438.613	6.8	-0.1
a2''-TS2	-1437.180	-1436.881	-1436.969	0.211	-1436.590	-1436.559	-0.031	-1438.771	-1438.591	20.7	14.8
a2''-IN3	-1437.214	-1436.910	-1436.996	0.219	-1436.634	-1436.604	-0.030	-1438.807	-1438.618	4.2	-7.8
a2-IN1'	-1437.216	-1436.911	-1436.999	0.217	-1436.634	-1436.601	-0.032	-1438.808	-1438.623	0.8	-8.7
a2-TS1'	-1437.192	-1436.889	-1436.976	0.216	-1436.618	-1436.576	-0.042	-1438.784	-1438.611	8.5	0.6
a2-IN2'	-1437.193	-1436.888	-1436.978	0.215	-1436.620	-1436.576	-0.044	-1438.786	-1438.614	6.2	-1.2
a2-TS2'	-1437.179	-1436.880	-1436.965	0.214	-1436.600	-1436.560	-0.041	-1438.775	-1438.602	13.9	10.4
a2-IN3'	-1437.237	-1436.933	-1437.021	0.216	-1436.621	-1436.583	-0.038	-1438.795	-1438.618	4.2	-1.7
PdOAcTFA	-881.424	-881.330	-881.387	0.037	-881.041	-881.031	-0.010	-882.860	-882.833		
b2-IN1	-1437.219	-1436.913	-1437.001	0.217	-1436.632	-1436.600	-0.032	-1438.810	-1438.624	-0.1	-7.4
b2-TS0	-1437.182	-1436.883	-1436.969	0.214	-1436.594	-1436.559	-0.034	-1438.776	-1438.597	16.9	14.2

b2-IN2	-1437.237	-1436.932	-1437.019	0.218	-1436.647	-1436.620	-0.027	-1438.833	-1438.642	-11.3	-16.6
b2'-IN1	-1437.215	-1436.910	-1436.998	0.217	-1436.621	-1436.594	-0.026	-1438.805	-1438.614	6.2	-0.5
b2'-TS1	-1437.162	-1436.862	-1436.949	0.213	-1436.569	-1436.544	-0.025	-1438.754	-1438.566	36.6	29.4
b2'-IN2	-1437.244	-1436.938	-1437.024	0.220	-1436.654	-1436.628	-0.025	-1438.837	-1438.643	-11.6	-19.4
b2'-IN3	-1208.136	-1207.900	-1207.973	0.163	-1207.631	-1207.610	-0.021	-1209.649	-1209.507	-13.1	-11.3
b2''-TS1	-1437.189	-1436.886	-1436.975	0.214	-1436.597	-1436.572	-0.026	-1438.778	-1438.589	22.0	12.4
b2''-IN2	-1437.206	-1436.901	-1436.989	0.217	-1436.620	-1436.591	-0.030	-1438.797	-1438.610	8.9	-0.5
b2''-TS2	-1437.184	-1436.885	-1436.972	0.211	-1436.588	-1436.561	-0.027	-1438.774	-1438.590	21.4	16.3
b2''-IN3	-1437.207	-1436.902	-1436.990	0.216	-1436.624	-1436.597	-0.027	-1438.801	-1438.611	8.3	-2.8
b2-IN1'	-1437.216	-1436.911	-1437.000	0.216	-1436.630	-1436.595	-0.035	-1438.808	-1438.627	-1.8	-7.1
b2-TS0'	-1437.183	-1436.883	-1436.967	0.216	-1436.594	-1436.561	-0.033	-1438.776	-1438.594	18.7	15.1
b2-IN2'	-1437.240	-1436.936	-1437.023	0.217	-1436.648	-1436.622	-0.026	-1438.835	-1438.645	-12.8	-17.8

Table S33. Potential energy surface for the functionalization catalyzed by Pd(OAc)(TFA)

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol}	ΔG_{sol}	ΔG_{sol} M06-2X
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(OAc)(TFA)	-881.424	-881.330	-881.387	0.037	-881.041	-881.031	-0.010	-882.860	-882.833		
a3-IN1	-1437.203	-1436.898	-1436.988	0.215	-1436.618	-1436.586	-0.032	-1438.794	-1438.611	8.4	-0.2
a3-TS1	-1437.189	-1436.886	-1436.974	0.215	-1436.612	-1436.572	-0.041	-1438.780	-1438.605	11.7	3.5
a3-IN2	-1437.191	-1436.887	-1436.977	0.214	-1436.618	-1436.574	-0.044	-1438.784	-1438.614	6.6	-0.4
a3-TS2	-1437.169	-1436.870	-1436.956	0.212	-1436.588	-1436.548	-0.039	-1438.763	-1438.590	21.7	17.3
a3-IN3	-1437.244	-1436.939	-1437.026	0.218	-1436.661	-1436.630	-0.031	-1438.839	-1438.652	-17.2	-25.2
a3'-IN1	-1437.214	-1436.909	-1436.999	0.215	-1436.630	-1436.595	-0.035	-1438.806	-1438.627	-1.6	-7.9
a3'-TS1	-1437.168	-1436.866	-1436.951	0.217	-1436.591	-1436.547	-0.044	-1438.761	-1438.589	22.3	17.8
a3'-IN2	-1437.220	-1436.915	-1437.006	0.214	-1436.629	-1436.599	-0.030	-1438.816	-1438.631	-4.3	-7.4
a3'-IN3	-910.430	-910.173	-910.241	0.189	-910.013	-909.982	-0.031	-911.839	-911.681	-10.2	-9.8

a3''-TS1	-1437.195	-1436.891	-1436.981	0.213	-1436.613	-1436.578	-0.034	-1438.785	-1438.605	11.8	2.3
a3''-IN2	-1437.211	-1436.906	-1436.996	0.214	-1436.627	-1436.591	-0.035	-1438.803	-1438.624	0.2	-5.8
a3''-TS2	-1437.179	-1436.880	-1436.968	0.210	-1436.589	-1436.559	-0.031	-1438.770	-1438.590	21.4	14.9
a3''-IN3	-1437.192	-1436.888	-1436.980	0.212	-1436.611	-1436.581	-0.030	-1438.785	-1438.602	14.1	2.9
a3-IN1'	-1437.204	-1436.899	-1436.989	0.215	-1436.615	-1436.587	-0.028	-1438.794	-1438.607	10.5	1.9
a3-TS1'	-1437.195	-1436.891	-1436.978	0.217	-1436.616	-1436.581	-0.035	-1438.785	-1438.603	13.4	2.5
a3-IN2'	-1437.195	-1436.891	-1436.980	0.216	-1436.619	-1436.581	-0.038	-1438.787	-1438.610	9.1	-0.5
a3-TS2'	-1437.168	-1436.870	-1436.956	0.212	-1436.587	-1436.548	-0.038	-1438.762	-1438.588	22.5	18.0
a3-IN3'	-1437.233	-1436.928	-1437.016	0.218	-1436.651	-1436.620	-0.031	-1438.829	-1438.642	-11.1	-19.0
b3-IN1	-1437.209	-1436.904	-1436.993	0.217	-1436.619	-1436.592	-0.028	-1438.799	-1438.610	8.8	0.0
b3-TS0	-1437.174	-1436.875	-1436.960	0.213	-1436.583	-1436.552	-0.031	-1438.766	-1438.584	25.4	20.8
b3-IN2	-1437.235	-1436.930	-1437.017	0.218	-1436.642	-1436.618	-0.024	-1438.830	-1438.636	-7.6	-13.2
b3'-IN1	-1437.224	-1436.919	-1437.007	0.217	-1436.633	-1436.604	-0.029	-1438.816	-1438.628	-2.3	-8.0
b3'-TS1	-1437.174	-1436.874	-1436.958	0.215	-1436.582	-1436.547	-0.035	-1438.766	-1438.585	24.5	23.0
b3'-IN2	-1437.231	-1436.925	-1437.014	0.217	-1436.632	-1436.609	-0.023	-1438.826	-1438.632	-5.1	-7.6
b3''-TS1	-1437.197	-1436.893	-1436.982	0.215	-1436.608	-1436.580	-0.029	-1438.786	-1438.600	15.3	6.0
b3''-IN2	-1437.212	-1436.908	-1436.995	0.217	-1436.629	-1436.597	-0.033	-1438.804	-1438.619	3.0	-6.0
b3''-TS2	-1437.184	-1436.885	-1436.972	0.212	-1436.589	-1436.563	-0.027	-1438.775	-1438.590	21.7	15.9
b3''-IN3	-1437.200	-1436.895	-1436.983	0.216	-1436.613	-1436.589	-0.024	-1438.792	-1438.600	14.9	3.8
b3-IN1'	-1437.206	-1436.901	-1436.991	0.215	-1436.617	-1436.586	-0.031	-1438.796	-1438.612	7.8	0.5
b3-TS0'	-1437.173	-1436.874	-1436.958	0.215	-1436.584	-1436.552	-0.031	-1438.765	-1438.582	26.7	21.4
b3-IN2'	-1437.249	-1436.944	-1437.030	0.220	-1436.655	-1436.631	-0.023	-1438.843	-1438.647	-14.4	-20.3

Table S34. Potential energy surface for the functionalization catalyzed by Pd(OAc)(OTf)

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol}	ΔG_{sol}	ΔG_{sol} M06-2X
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		

Pd(OAc)(OTf)	-1316.648	-1316.552	-1316.612	0.037	-1316.220	-1316.209	-0.011	-1318.120	-1318.094		
a4-IN1	-1872.439	-1872.132	-1872.223	0.215	-1871.811	-1871.776	-0.035	-1874.069	-1873.889	-1.9	-8.4
a4-TS0	-1872.405	-1872.104	-1872.193	0.212	-1871.784	-1871.738	-0.046	-1874.038	-1873.871	9.1	6.9
a4-IN2	-1872.462	-1872.155	-1872.246	0.217	-1871.840	-1871.804	-0.036	-1874.097	-1873.916	-19.3	-25.8
a4'-IN1	-1872.430	-1872.123	-1872.215	0.214	-1871.800	-1871.767	-0.033	-1874.016	-1873.834	32.2	-1.9
a4'-TS1	-1872.377	-1872.076	-1872.166	0.211	-1871.749	-1871.706	-0.043	-1874.007	-1873.838	29.5	27.8
a4'-IN2	-1872.450	-1872.143	-1872.236	0.214	-1871.821	-1871.787	-0.034	-1874.082	-1873.902	-10.4	-15.5
a4'-IN3	-1643.361	-1643.124	-1643.200	0.162	-1642.825	-1642.793	-0.032	-1644.911	-1644.781	-20.9	-21.4
a4''-TS1	-1872.414	-1872.109	-1872.200	0.214	-1871.787	-1871.754	-0.033	-1874.041	-1873.859	16.8	6.2
a4''-IN2	-1872.430	-1872.124	-1872.216	0.214	-1871.800	-1871.766	-0.033	-1874.058	-1873.878	4.9	-2.3
a4''-TS2	-1872.407	-1872.106	-1872.196	0.211	-1871.774	-1871.741	-0.033	-1874.034	-1873.857	18.2	11.9
a4''-IN3	-1872.442	-1872.135	-1872.226	0.216	-1871.819	-1871.787	-0.032	-1874.072	-1873.888	-1.7	-12.9
a4-IN1'	-1872.416	-1872.110	-1872.201	0.215	-1871.802	-1871.754	-0.048	-1874.046	-1873.879	4.3	-2.6
a4-TS0'	-1872.406	-1872.105	-1872.192	0.215	-1871.784	-1871.739	-0.045	-1874.038	-1873.868	10.8	7.9
a4-IN2'	-1872.464	-1872.157	-1872.247	0.217	-1871.841	-1871.806	-0.035	-1874.098	-1873.916	-18.8	-26.2
b4-IN1	-1872.441	-1872.135	-1872.225	0.216	-1871.813	-1871.778	-0.036	-1874.071	-1873.890	-3.0	-9.3
b4-TS0	-1872.406	-1872.105	-1872.193	0.213	-1871.775	-1871.736	-0.039	-1874.037	-1873.863	14.0	12.6
b4-IN2	-1872.464	-1872.157	-1872.246	0.217	-1871.830	-1871.801	-0.030	-1874.098	-1873.910	-15.4	-19.3
b4'-IN1	-1872.441	-1872.134	-1872.224	0.217	-1871.803	-1871.775	-0.028	-1874.067	-1873.878	4.5	-2.4
b4'-TS1	-1872.387	-1872.086	-1872.175	0.212	-1871.750	-1871.724	-0.026	-1874.016	-1873.829	35.2	28.1
b4'-IN2	-1872.449	-1872.142	-1872.235	0.215	-1871.808	-1871.784	-0.025	-1874.082	-1873.892	-4.3	-7.3
b4'-IN3	-1643.363	-1643.125	-1643.200	0.163	-1642.814	-1642.791	-0.023	-1644.912	-1644.772	-15.4	-13.6
b4''-TS1	-1872.415	-1872.110	-1872.200	0.215	-1871.781	-1871.753	-0.027	-1874.040	-1873.852	20.8	10.5
b4''-IN2	-1872.432	-1872.126	-1872.216	0.217	-1871.804	-1871.773	-0.031	-1874.059	-1873.874	7.3	-3.1
b4''-TS2	-1872.410	-1872.109	-1872.198	0.212	-1871.772	-1871.743	-0.028	-1874.037	-1873.854	20.1	14.2
b4''-IN3	-1872.433	-1872.127	-1872.216	0.217	-1871.807	-1871.779	-0.028	-1874.063	-1873.874	7.0	-5.2
b4-IN1'	-1872.443	-1872.136	-1872.226	0.217	-1871.814	-1871.779	-0.035	-1874.072	-1873.890	-3.0	-9.3
b4-TS0'	-1872.407	-1872.106	-1872.193	0.214	-1871.776	-1871.738	-0.038	-1874.038	-1873.862	14.5	12.6
b4-IN2'	-1872.461	-1872.154	-1872.243	0.218	-1871.830	-1871.799	-0.031	-1874.094	-1873.908	-14.0	-19.3

Table S35. Potential energy surface for the functionalization catalyzed by Pd(OTf)(OAc)

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol}	ΔG_{sol}	ΔG_{sol} M06-2X
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(OAc)(OTf)	-1316.648	-1316.552	-1316.612	0.037	-1316.220	-1316.209	-0.011	-1318.120	-1318.094		
a5-IN1	-1872.429	-1872.122	-1872.213	0.216	-1871.797	-1871.767	-0.030	-1874.055	-1873.868	10.8	0.8
a5-TS1	-1872.417	-1872.111	-1872.200	0.217	-1871.796	-1871.758	-0.038	-1874.045	-1873.866	12.5	2.1
a5-IN2	-1872.417	-1872.111	-1872.202	0.215	-1871.799	-1871.758	-0.042	-1874.047	-1873.874	7.4	-1.1
a5-TS2	-1872.384	-1872.084	-1872.173	0.210	-1871.758	-1871.719	-0.039	-1874.015	-1873.845	25.7	21.6
a5-IN3	-1872.436	-1872.130	-1872.223	0.213	-1871.798	-1871.768	-0.031	-1874.069	-1873.887	-0.8	-1.9
a5'-IN1	-1872.437	-1872.131	-1872.222	0.216	-1871.812	-1871.773	-0.039	-1874.067	-1873.890	-2.6	-8.9
a5'-TS1	-1872.401	-1872.101	-1872.190	0.211	-1871.775	-1871.731	-0.045	-1874.034	-1873.868	11.0	11.2
a5'-IN2	-1872.448	-1872.142	-1872.233	0.214	-1871.815	-1871.783	-0.032	-1874.080	-1873.898	-7.6	-11.7
a5'-IN3	-910.430	-910.173	-910.241	0.189	-910.013	-909.982	-0.031	-911.839	-911.681	-8.7	-5.4
a5''-TS1	-1872.420	-1872.115	-1872.207	0.213	-1871.795	-1871.759	-0.037	-1874.047	-1873.871	9.4	0.0
a5''-IN2	-1872.435	-1872.128	-1872.221	0.214	-1871.808	-1871.769	-0.038	-1874.064	-1873.888	-1.7	-7.2
a5''-TS2	-1872.390	-1872.091	-1872.181	0.209	-1871.759	-1871.727	-0.032	-1874.021	-1873.843	26.5	20.3
a5''-IN3	-1872.436	-1872.130	-1872.223	0.213	-1871.798	-1871.768	-0.031	-1874.069	-1873.887	-0.8	-1.9
a5-TS2'	-1872.382	-1872.082	-1872.171	0.211	-1871.757	-1871.717	-0.040	-1874.014	-1873.843	27.0	22.8
a5-TS2'	-1872.385	-1872.085	-1872.174	0.211	-1871.759	-1871.721	-0.039	-1874.016	-1873.843	26.4	21.3
a5-TS2'	-1872.383	-1872.083	-1872.171	0.212	-1871.757	-1871.719	-0.038	-1874.014	-1873.841	28.0	23.1
b5-IN1	-1872.435	-1872.129	-1872.219	0.216	-1871.801	-1871.772	-0.028	-1874.062	-1873.874	7.2	-1.4
b5-TS1	-1872.422	-1872.117	-1872.205	0.217	-1871.794	-1871.759	-0.035	-1874.050	-1873.868	10.7	3.1
b5-IN2	-1872.422	-1872.116	-1872.208	0.214	-1871.795	-1871.759	-0.036	-1874.050	-1873.872	8.2	0.8
b5-TS2	-1872.422	-1872.116	-1872.208	0.214	-1871.795	-1871.759	-0.036	-1874.050	-1873.872	8.2	0.9

b5-IN3	-1872.390	-1872.090	-1872.178	0.211	-1871.754	-1871.723	-0.031	-1874.019	-1873.839	29.3	25.1
b5'-IN1	-1872.448	-1872.141	-1872.231	0.217	-1871.813	-1871.782	-0.031	-1874.077	-1873.892	-4.0	-9.1
b5'-TS1	-1872.405	-1872.104	-1872.193	0.212	-1871.766	-1871.731	-0.035	-1874.036	-1873.859	16.6	17.4
b5'-IN2	-1872.436	-1872.130	-1872.223	0.213	-1871.789	-1871.763	-0.026	-1874.069	-1873.882	2.0	4.1
b5'-IN3	-910.435	-910.178	-910.245	0.190	-910.008	-909.985	-0.023	-911.844	-911.678	-6.6	-1.5
b5''-TS1	-1872.116	-1872.207	-1871.792	0.214	-1874.048	-1873.864	-0.184	-1874.048	-1873.864	13.6	3.1
b5''-IN2	-1872.130	-1872.221	-1871.811	0.216	-1874.066	-1873.881	-0.185	-1874.066	-1873.881	2.6	-8.4
b5''-TS2	-1872.096	-1872.185	-1871.758	0.211	-1874.025	-1873.841	-0.184	-1874.025	-1873.841	28.2	22.1
b5''-IN3	-1872.137	-1872.227	-1871.811	0.217	-1874.077	-1873.892	-3.807	-1874.077	-1873.892	-3.8	-7.7
b5-TS2'	-1872.387	-1872.087	-1872.174	0.213	-1871.752	-1871.721	-0.030	-1874.017	-1873.834	32.0	27.4
b5-TS2'	-1872.384	-1872.083	-1872.171	0.213	-1871.750	-1871.718	-0.032	-1874.014	-1873.834	32.6	28.2

Table S36. Potential energy surface for the functionalization catalyzed by Pd(TFA)(OTf)

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol}	ΔG_{sol}	$\Delta G_{sol} M06-2X$
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(TFA)(OTf)	-1614.340	-1614.265	-1614.330	0.010	-1613.831	-1613.824	-0.007	-1615.914	-1615.911		
a6-IN1	-2170.123	-2169.838	-2169.940	0.184	-2169.402	-2169.379	-0.024	-2171.851	-2171.691	7.4	0.6
a6-TS1	-2170.125	-2169.840	-2169.935	0.190	-2169.425	-2169.389	-0.036	-2171.857	-2171.703	-0.4	-9.7
a6-IN2	-2170.126	-2169.841	-2169.939	0.187	-2169.431	-2169.390	-0.042	-2171.861	-2171.715	-7.7	-15.3
a6-TS2	-2170.105	-2169.825	-2169.920	0.185	-2169.405	-2169.361	-0.043	-2171.840	-2171.699	2.4	0.0
a6-IN3	-2170.160	-2169.875	-2169.971	0.189	-2169.455	-2169.424	-0.031	-2171.897	-2171.739	-23.1	-29.6
a6'-IN1	-2170.136	-2169.851	-2169.948	0.188	-2169.427	-2169.396	-0.032	-2171.868	-2171.712	-5.7	-12.3
a6'-TS1	-2170.091	-2169.809	-2169.903	0.188	-2169.389	-2169.346	-0.043	-2171.824	-2171.679	15.0	11.8
a6'-IN2	-2170.155	-2169.869	-2169.969	0.186	-2169.445	-2169.415	-0.030	-2171.891	-2171.735	-20.2	-24.7
a6'-IN3	-1643.361	-1643.124	-1643.200	0.162	-1642.825	-1642.793	-0.032	-1644.911	-1644.781	-23.6	-23.6
a6''-TS1	-2170.120	-2169.836	-2169.932	0.187	-2169.414	-2169.382	-0.031	-2171.850	-2171.694	6.7	-3.0
a6''-IN2	-2170.135	-2169.850	-2169.948	0.187	-2169.426	-2169.394	-0.033	-2171.867	-2171.713	-5.4	-11.6

a6''-TS2	-2170.107	-2169.828	-2169.924	0.183	-2169.395	-2169.365	-0.030	-2171.838	-2171.685	12.4	5.7
a6''-IN3	-2170.138	-2169.853	-2169.949	0.188	-2169.434	-2169.405	-0.028	-2171.871	-2171.711	-4.0	-15.2
a6-TS1'	-2170.123	-2169.839	-2169.933	0.190	-2169.425	-2169.388	-0.037	-2171.856	-2171.702	0.4	-9.3
a6-IN2'	-2170.125	-2169.840	-2169.938	0.187	-2169.432	-2169.389	-0.043	-2171.859	-2171.714	-7.3	-15.5
a6-TS2'	-2170.106	-2169.826	-2169.919	0.186	-2169.406	-2169.363	-0.043	-2171.841	-2171.698	3.2	0.1
a6-IN3'	-2170.163	-2169.878	-2169.974	0.189	-2169.457	-2169.428	-0.030	-2171.899	-2171.740	-23.5	-30.7
b6-IN1	-2170.139	-2169.853	-2169.950	0.189	-2169.428	-2169.398	-0.030	-2171.871	-2171.712	-5.9	-11.8
b6-TS1	-2170.125	-2169.841	-2169.936	0.189	-2169.422	-2169.387	-0.035	-2171.857	-2171.703	-0.2	-8.2
b6-IN2	-2170.128	-2169.843	-2169.939	0.189	-2169.430	-2169.389	-0.041	-2171.862	-2171.714	-7.2	-13.5
b6-TS2	-2170.105	-2169.826	-2169.919	0.187	-2169.395	-2169.360	-0.035	-2171.839	-2171.688	9.3	6.7
b6-IN3	-2170.160	-2169.875	-2169.970	0.190	-2169.444	-2169.419	-0.025	-2171.896	-2171.731	-17.8	-21.9
b6'-IN1	-2170.146	-2169.860	-2169.957	0.189	-2169.429	-2169.403	-0.026	-2171.877	-2171.714	-7.3	-12.7
b6'-TS1	-2170.095	-2169.815	-2169.908	0.188	-2169.380	-2169.346	-0.034	-2171.827	-2171.673	18.6	17.0
b6'-IN2	-2170.147	-2169.861	-2169.962	0.185	-2169.427	-2169.402	-0.024	-2171.883	-2171.722	-12.3	-14.0
b6'-IN3	-1643.363	-1643.125	-1643.200	0.163	-1642.814	-1642.791	-0.023	-1644.912	-1644.772	-18.1	-15.9
b6''-TS1	-2170.119	-2169.835	-2169.931	0.188	-2169.406	-2169.380	-0.026	-2171.849	-2171.687	11.1	1.7
b6''-IN2	-2170.137	-2169.852	-2169.947	0.190	-2169.433	-2169.401	-0.032	-2171.868	-2171.710	-3.1	-13.7
b6''-TS2	-2170.109	-2169.829	-2169.924	0.184	-2169.392	-2169.367	-0.026	-2171.839	-2171.681	15.0	8.3
b6''-IN3	-2170.126	-2169.841	-2169.937	0.189	-2169.419	-2169.395	-0.024	-2171.858	-2171.693	7.5	-5.3
b6-TS1'	-2170.124	-2169.840	-2169.934	0.190	-2169.422	-2169.386	-0.036	-2171.856	-2171.701	0.8	-7.7
b6-IN2'	-2170.127	-2169.842	-2169.938	0.189	-2169.430	-2169.388	-0.042	-2171.861	-2171.714	-7.3	-13.5
b6-TS2'	-2170.105	-2169.825	-2169.918	0.186	-2169.395	-2169.359	-0.036	-2171.838	-2171.688	9.3	7.1
b6-IN3'	-2170.160	-2169.875	-2169.970	0.190	-2169.444	-2169.419	-0.025	-2171.896	-2171.731	-17.8	-21.9
2a cation	-737.605	-737.370	-737.437	0.168	-737.357	-737.267	-0.090	-737.855	-737.777		
OAc-	-228.493	-228.439	-228.473	0.021	-228.489	-228.401	-0.088	-228.602	-228.669		
IMes	-360.973	-360.787	-360.838	0.135	-360.772	-360.761	-0.011	-361.100	-360.975		
a6-TS3	-3136.475	-3135.898	-3136.048	0.427	-3135.376	-3135.321	-0.055	-3138.543	-3138.171	-13.7	-45.2
a6-IN4	-2775.540	-2775.147	-2775.266	0.274	-2774.613	-2774.573	-0.040	-2777.485	-2777.251	-48.2	-62.1
a6-TS4	-2775.505	-2775.115	-2775.233	0.272	-2774.596	-2774.552	-0.044	-2777.447	-2777.219	-28.4	-52.7

a6-IN5	-2775.567	-2775.174	-2775.298	0.269	-2774.664	-2774.629	-0.035	-2777.509	-2777.275	-63.4	-96.6
3aa	-932.120	-931.873	-931.935	0.185	-931.792	-931.769	-0.023	-932.404	-932.242	-78.7	-98.9
TFA-	-526.230	-526.197	-526.236	-0.006	-526.141	-526.063	-0.077	-526.445	-526.528		
a6-TS3	-3434.191	-3433.633	-3433.791	0.400	-3433.026	-3432.967	-0.059	-3436.365	-3436.024	-10.0	-44.5
a6'-IN4	-3073.237	-3072.866	-3072.991	0.245	-3072.234	-3072.194	-0.039	-3075.284	-3075.078	-28.8	-43.8
a6'-TS4	-3073.208	-3072.838	-3072.963	0.244	-3072.223	-3072.178	-0.045	-3075.253	-3075.053	-13.0	-37.6
a6'-IN5	-3073.273	-3072.902	-3073.031	0.242	-3072.292	-3072.258	-0.034	-3075.320	-3075.111	-49.4	-82.2
a6''-TS3	-2907.786	-2907.266	-2907.402	0.384	-2906.792	-2906.709	-0.084	-2909.766	-2909.466	8.7	0.2
a6''-IN4	-2546.807	-2546.473	-2546.580	0.227	-2546.016	-2545.927	-0.089	-2548.663	-2548.524	-12.3	-10.4
a6''-TS4	-2546.793	-2546.460	-2546.566	0.228	-2546.009	-2545.922	-0.086	-2548.646	-2548.505	-0.1	-5.6
a6''-IN5	-2546.845	-2546.509	-2546.617	0.228	-2546.075	-2545.983	-0.091	-2548.695	-2548.559	-34.1	-47.0
b6-IN3	-2170.160	-2169.875	-2169.970	0.190	-2169.444	-2169.419	-0.025	-2171.896	-2171.731	-17.8	-21.9
b6-TS3	-3136.473	-3135.895	-3136.045	0.427	-3135.362	-3135.310	-0.053	-3138.539	-3138.165	-9.7	-36.3
b6-IN4	-2775.535	-2775.143	-2775.262	0.273	-2774.595	-2774.562	-0.033	-2777.479	-2777.239	-40.8	-51.4
b6-TS4	-2775.501	-2775.110	-2775.229	0.271	-2774.576	-2774.538	-0.038	-2777.443	-2777.210	-22.7	-40.5
b6-IN5	-2775.569	-2775.176	-2775.299	0.270	-2774.666	-2774.627	-0.039	-2777.509	-2777.277	-64.9	-97.3
3ba	-932.122	-931.875	-931.937	0.185	-931.793	-931.772	-0.021	-932.404	-932.240	-77.2	-98.9
b6'-TS3	-3434.181	-3433.624	-3433.779	0.401	-3432.993	-3432.942	-0.052	-3436.351	-3436.001	4.4	-22.8
b6'-IN4	-3073.231	-3072.860	-3072.987	0.245	-3072.214	-3072.182	-0.031	-3075.278	-3075.064	-19.9	-31.6
b6'-TS4	-3073.203	-3072.834	-3072.959	0.244	-3072.201	-3072.165	-0.037	-3075.249	-3075.042	-6.2	-24.6
b6'-IN5	-3073.276	-3072.904	-3073.032	0.244	-3072.294	-3072.257	-0.037	-3075.320	-3075.113	-50.7	-82.8
b6''-TS3	-2907.769	-2907.250	-2907.386	0.383	-2906.767	-2906.684	-0.083	-2909.750	-2909.450	19.0	15.4
b6''-IN4	-2546.785	-2546.452	-2546.559	0.226	-2545.987	-2545.899	-0.088	-2548.641	-2548.503	1.3	7.0
b6''-TS4	-2546.775	-2546.442	-2546.547	0.228	-2545.981	-2545.895	-0.086	-2548.627	-2548.485	12.5	11.9
b6''-IN5	-2546.853	-2546.518	-2546.627	0.226	-2546.081	-2545.993	-0.089	-2548.703	-2548.566	-38.4	-52.1

Table S37. Potential energy surface for the functionalization catalyzed by Pd(OTf)(TFA)

B3LYP/6-31G(d)+LANL2DZ	M06-2X/6-31G(d)+LANL2DZ	B3LYP/6-
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311+G(d,p)+SDD											
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol}	ΔG_{sol}	$\Delta G_{sol} M06-2X$
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(TFA)(OTf)	-1614.340	-1614.265	-1614.330	0.010	-1613.831	-1613.824	-0.007	-1615.914	-1615.911		
a7-IN1	-2170.138	-2169.853	-2169.949	0.189	-2169.431	-2169.401	-0.029	-2171.869	-2171.709	-4.0	-13.6
a7-TS1	-2170.126	-2169.842	-2169.936	0.190	-2169.431	-2169.401	-0.029	-2171.857	-2171.697	3.8	-13.3
a7-IN2	-2170.127	-2169.842	-2169.939	0.188	-2169.430	-2169.390	-0.040	-2171.860	-2171.712	-6.1	-14.1
a7-TS2	-2170.094	-2169.815	-2169.910	0.184	-2169.392	-2169.353	-0.039	-2171.831	-2171.686	10.4	7.2
a7-IN3	-2170.113	-2169.828	-2169.925	0.188	-2169.415	-2169.377	-0.038	-2171.851	-2171.701	0.9	-5.2
a7'-IN1	-2170.134	-2169.848	-2169.945	0.188	-2169.427	-2169.393	-0.034	-2171.866	-2171.712	-5.6	-11.7
a7'-TS1	-2170.100	-2169.820	-2169.915	0.185	-2169.397	-2169.352	-0.045	-2171.835	-2171.695	4.8	4.9
a7'-IN2	-2170.139	-2169.854	-2169.954	0.185	-2169.424	-2169.395	-0.029	-2171.876	-2171.720	-10.8	-12.2
a7'-IN3	-1208.134	-1207.898	-1207.973	0.161	-1207.640	-1207.611	-0.029	-1209.648	-1209.516	-19.7	-16.2
a7''-TS1	-2170.114	-2169.830	-2169.928	0.186	-2169.410	-2169.376	-0.034	-2171.847	-2171.695	4.8	-3.0
a7''-IN2	-2170.131	-2169.845	-2169.944	0.186	-2169.424	-2169.388	-0.036	-2171.863	-2171.713	-6.4	-11.2
a7''-TS2	-2170.091	-2169.813	-2169.910	0.181	-2169.382	-2169.352	-0.030	-2171.825	-2171.674	18.2	12.1
a7''-IN3	-2170.139	-2169.854	-2169.954	0.185	-2169.424	-2169.395	-0.029	-2171.876	-2171.720	-10.8	-12.3
a7-TS2'	-2170.093	-2169.814	-2169.909	0.184	-2169.391	-2169.351	-0.040	-2171.830	-2171.686	10.3	8.1
a7-TS2''	-2170.092	-2169.813	-2169.907	0.185	-2169.391	-2169.350	-0.040	-2171.830	-2171.685	11.0	8.8
a7-TS2'''	-2170.094	-2169.815	-2169.909	0.185	-2169.392	-2169.353	-0.039	-2171.830	-2171.685	11.4	8.1
b7-IN1	-2170.142	-2169.856	-2169.952	0.189	-2169.427	-2169.396	-0.030	-2171.873	-2171.714	-7.2	-11.1
b7-TS1	-2170.128	-2169.843	-2169.938	0.190	-2169.422	-2169.387	-0.034	-2171.859	-2171.704	-0.8	-7.7
b7-IN2	-2170.128	-2169.843	-2169.940	0.188	-2169.428	-2169.390	-0.038	-2171.863	-2171.713	-6.6	-12.9
b7-TS2	-2170.097	-2169.818	-2169.912	0.185	-2169.383	-2169.353	-0.030	-2171.832	-2171.677	16.3	13.4
b7-IN3	-2170.154	-2169.869	-2169.965	0.189	-2169.438	-2169.415	-0.023	-2171.890	-2171.724	-13.5	-18.3
b7'-IN1	-2170.125	-2169.840	-2169.937	0.188	-2169.428	-2169.384	-0.044	-2171.859	-2171.715	-7.8	-12.6
b7'-TS1	-2170.102	-2169.822	-2169.917	0.185	-2169.385	-2169.351	-0.034	-2171.835	-2171.685	10.9	11.9
b7'-IN2	-2170.136	-2169.851	-2169.951	0.185	-2169.411	-2169.388	-0.023	-2171.872	-2171.710	-4.8	-4.1
b7'-IN3	-1208.136	-1207.900	-1207.973	0.163	-1207.631	-1207.610	-0.021	-1209.649	-1209.507	-14.3	-9.2

b7''-TS1	-2170.117	-2169.833	-2169.931	0.186	-2169.406	-2169.380	-0.027	-2171.847	-2171.687	9.7	-0.4
b7''-IN2	-2170.132	-2169.848	-2169.945	0.188	-2169.427	-2169.394	-0.034	-2171.866	-2171.712	-5.6	-12.4
b7''-TS2	-2170.094	-2169.815	-2169.912	0.182	-2169.378	-2169.353	-0.025	-2171.827	-2171.671	20.0	14.4
b7''-IN3	-2170.137	-2169.852	-2169.950	0.187	-2169.424	-2169.395	-0.029	-2171.876	-2171.718	-9.9	-11.3
b7-TS2'	-2170.095	-2169.816	-2169.909	0.186	-2169.383	-2169.352	-0.031	-2171.830	-2171.674	17.7	14.7
b7-TS2''	-2170.094	-2169.815	-2169.909	0.185	-2169.381	-2169.349	-0.032	-2171.829	-2171.675	17.1	15.2
b7-TS2'''	-2170.091	-2169.812	-2169.905	0.186	-2169.380	-2169.347	-0.033	-2171.827	-2171.673	18.5	16.2

Table S38. Potential energy surface for the functionalization catalyzed by **Pd(OTf)₂**

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD			
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas, Inr}	G _{sol}	ΔG_{sol}	ΔG_{sol} M06-2X
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791		
Pd(OTf)₂	-2049.563	-2049.487	-2049.554	0.009	-2049.008	-2049.001	-0.007	-2051.173	-2051.171		
a8-IN1	-2605.359	-2605.072	-2605.170	0.188	-2604.604	-2604.574	-0.031	-2607.129	-2606.972	-5.7	-11.6
a8-TS1	-2605.348	-2605.063	-2605.159	0.189	-2604.604	-2604.567	-0.037	-2607.118	-2606.966	-2.1	-10.4
a8-IN2	-2605.350	-2605.064	-2605.163	0.187	-2604.611	-2604.568	-0.043	-2607.122	-2606.978	-9.4	-16.3
a8-TS2	-2605.321	-2605.040	-2605.138	0.183	-2604.578	-2604.534	-0.044	-2607.094	-2606.954	5.1	2.1
a8-IN3	-2605.343	-2605.056	-2605.155	0.188	-2604.606	-2604.564	-0.042	-2607.117	-2606.972	-5.7	-12.6
a8'-IN1	-2605.358	-2605.071	-2605.170	0.188	-2604.606	-2604.572	-0.035	-2607.127	-2606.974	-6.9	-12.8
a8'-TS1	-2605.325	-2605.043	-2605.138	0.187	-2604.581	-2604.533	-0.047	-2607.096	-2606.957	3.3	2.4
a8'-IN2	-2605.366	-2605.079	-2605.178	0.187	-2604.610	-2604.578	-0.032	-2607.138	-2606.983	-12.7	-15.7
a8'-IN3	-1643.361	-1643.124	-1643.200	0.162	-1642.825	-1642.793	-0.032	-1644.911	-1644.781	-23.0	-20.1
a8''-TS1	-2605.341	-2605.055	-2605.153	0.187	-2604.592	-2604.558	-0.034	-2607.109	-2606.955	4.6	-4.2
a8''-IN2	-2605.356	-2605.069	-2605.169	0.186	-2604.604	-2604.568	-0.036	-2607.125	-2606.975	-7.5	-12.4
a8''-TS2	-2605.318	-2605.038	-2605.135	0.182	-2604.566	-2604.535	-0.031	-2607.087	-2606.936	16.6	9.1
a8''-IN3	-2605.355	-2605.068	-2605.166	0.189	-2604.614	-2604.577	-0.037	-2607.129	-2606.977	-9.1	-16.9
a8-TS2'	-2605.319	-2605.039	-2605.136	0.184	-2604.576	-2604.531	-0.045	-2607.093	-2606.954	5.2	3.2

a8-TS2''	-2605.318	-2605.037	-2605.133	0.185	-2604.576	-2604.531	-0.045	-2607.093	-2606.953	6.3	4.4
a8-TS2'''	-2605.320	-2605.039	-2605.134	0.186	-2604.579	-2604.534	-0.045	-2607.094	-2606.952	6.4	3.3
b8-IN1	-2605.364	-2605.077	-2605.175	0.189	-2604.608	-2604.577	-0.030	-2607.134	-2606.975	-7.7	-13.0
b8-TS1	-2605.350	-2605.064	-2605.161	0.189	-2604.601	-2604.564	-0.036	-2607.119	-2606.966	-2.4	-8.7
b8-IN2	-2605.352	-2605.065	-2605.165	0.187	-2604.609	-2604.567	-0.041	-2607.124	-2606.978	-9.7	-15.0
b8-TS2	-2605.321	-2605.040	-2605.136	0.184	-2604.566	-2604.531	-0.035	-2607.092	-2606.943	12.5	10.3
b8-IN3	-2605.373	-2605.087	-2605.186	0.187	-2604.610	-2604.586	-0.024	-2607.148	-2606.985	-14.3	-15.6
b8'-IN1	-2605.367	-2605.080	-2605.179	0.189	-2604.607	-2604.579	-0.028	-2607.137	-2606.976	-8.7	-12.9
b8'-TS1	-2605.327	-2605.046	-2605.141	0.186	-2604.568	-2604.532	-0.036	-2607.097	-2606.948	9.3	9.6
b8'-IN2	-2605.363	-2605.077	-2605.176	0.188	-2604.598	-2604.573	-0.024	-2607.135	-2606.972	-6.0	-7.7
b8'-IN3	-1643.363	-1643.125	-1643.200	0.163	-1642.814	-1642.791	-0.023	-1644.912	-1644.772	-17.5	-1343.6
b8''-TS1	-2605.341	-2605.056	-2605.155	0.186	-2604.610	-2604.610	0.000	-2607.128	-2606.941	13.3	-16.3
b8''-IN2	-2605.358	-2605.071	-2605.170	0.188	-2604.610	-2604.575	-0.035	-2607.128	-2606.975	-7.7	-15.2
b8''-TS2	-2605.319	-2605.039	-2605.136	0.183	-2604.560	-2604.534	-0.026	-2607.089	-2606.932	19.1	12.8
b8''-IN3	-2605.369	-2605.082	-2605.180	0.189	-2604.615	-2604.585	-0.030	-2607.143	-2606.983	-13.1	-17.5
b8-TS2'	-2605.317	-2605.037	-2605.133	0.185	-2604.562	-2604.526	-0.036	-2607.089	-2606.941	13.5	12.6
b8-TS2''	-2605.317	-2605.037	-2605.133	0.185	-2604.565	-2604.530	-0.035	-2607.092	-2606.943	12.6	10.9
b8-TS2'''	-2605.317	-2605.037	-2605.133	0.185	-2604.563	-2604.527	-0.036	-2607.090	-2606.941	13.6	12.4
HOTf	-961.989	-961.942	-961.984	0.005	-961.772	-961.765	-0.007	-962.216	-962.218		

Table S39. Potential energy surface for the functionalization catalyzed by Pd(TFA)₂ with the geometry-optimization of B3LYP/BS1 level

	B3LYP/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD		
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol}	ΔG_{sol}
1a	-555.772	-555.563	-555.614	0.158	-555.557	-555.535	-0.021	-555.928	-555.791	
Pd(TFA) ₂	-1179.117	-1179.044	-1179.106	0.010	-1178.653	-1178.646	-0.007	-1180.654	-1180.651	
a1-IN1	-1734.913	-1734.629	-1734.723	0.190	-1734.250	-1734.221	-0.029	-1736.608	-1736.446	-2.607
a1-TS1	-1734.896	-1734.614	-1734.709	0.188	-1734.242	-1734.202	-0.039	-1736.592	-1736.444	-1.013
a1-IN2	-1734.899	-1734.615	-1734.711	0.187	-1734.248	-1734.204	-0.044	-1736.596	-1736.452	-6.643

a₁-TS2	-1734.879	-1734.601	-1734.693	0.186	-1734.221	-1734.181	-0.039	-1736.578	-1736.431	6.591
a₁-IN3	-1734.944	-1734.661	-1734.754	0.190	-1734.280	-1734.253	-0.027	-1736.642	-1736.479	-23.071
b₁-IN1	-1734.913	-1734.629	-1734.724	0.189	-1734.246	-1734.215	-0.030	-1736.608	-1736.450	-4.785
b₁-TS1	-1734.901	-1734.618	-1734.711	0.190	-1734.238	-1734.204	-0.035	-1736.595	-1736.440	1.087
b₁-IN2	-1734.901	-1734.618	-1734.714	0.187	-1734.242	-1734.205	-0.037	-1736.596	-1736.446	-2.738
b₁-TS2	-1734.881	-1734.603	-1734.693	0.188	-1734.214	-1734.183	-0.031	-1736.578	-1736.421	13.007
b₁-IN3	-1734.947	-1734.663	-1734.755	0.192	-1734.271	-1734.251	-0.020	-1736.643	-1736.471	-18.327

Table S40. Potential energy surface for the functionalization catalyzed by Pd(TFA)₂ with the geometry-optimization of B3LYP-D3(BJ)/BS1 level

	B3LYP-D3(BJ)/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP/6-311+G(d,p)+SDD		
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE _{sol}	E _{gas_lar}	G _{sol} D3_1	ΔG _{sol} D3_1
1a	-555.819	-555.610	-555.660	0.158	-555.558	-555.536	-0.022	-555.929	-555.793	
Pd(TFA)₂	-1179.140	-1179.067	-1179.130	0.010	-1178.653	-1178.646	-0.007	-1180.654	-1180.651	
a₁-IN1	-1735.005	-1734.721	-1734.812	0.193	-1734.252	-1734.225	-0.026	-1736.603	-1736.436	4.643
a₁-TS1	-1734.985	-1734.702	-1734.795	0.189	-1734.242	-1734.203	-0.039	-1736.590	-1736.440	2.335
a₁-IN2	-1734.987	-1734.704	-1734.798	0.189	-1734.249	-1734.206	-0.044	-1736.595	-1736.449	-3.409
a₁-TS2	-1734.968	-1734.690	-1734.782	0.187	-1734.221	-1734.182	-0.039	-1736.578	-1736.430	8.316
a₁-IN3	-1735.032	-1734.748	-1734.841	0.191	-1734.280	-1734.253	-0.027	-1736.641	-1736.477	-20.941
b₁-IN1	-1734.997	-1734.713	-1734.805	0.193	-1734.245	-1734.216	-0.029	-1736.603	-1736.440	2.394
b₁-TS1	-1734.987	-1734.704	-1734.797	0.190	-1734.238	-1734.205	-0.034	-1736.594	-1736.438	3.593
b₁-IN2	-1734.991	-1734.707	-1734.799	0.191	-1734.247	-1734.208	-0.039	-1736.595	-1736.443	0.505
b₁-TS2	-1734.971	-1734.693	-1734.782	0.189	-1734.214	-1734.183	-0.031	-1736.577	-1736.419	15.468
b₁-IN3	-1735.034	-1734.750	-1734.842	0.192	-1734.271	-1734.252	-0.020	-1736.642	-1736.470	-16.360

Table S41. Potential energy surface for the functionalization catalyzed by Pd(TFA)₂ with the geometry-optimization of B3LYP-D3(BJ)/BS1 level

	B3LYP-D3(BJ)/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			B3LYP-D3(BJ)/6-311+G(d,p)+SDD		
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	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol} D3_2	ΔG_{sol} D3_2
1a	-555.819	-555.610	-555.660	0.158	-555.558	-555.536	-0.022	-555.976	-555.840	
Pd(TFA)₂	-1179.140	-1179.067	-1179.130	0.010	-1178.653	-1178.646	-0.007	-1180.678	-1180.674	
a₁-IN1	-1735.005	-1734.721	-1734.812	0.193	-1734.252	-1734.225	-0.026	-1736.697	-1736.530	-10.171
a₁-TS1	-1734.985	-1734.702	-1734.795	0.189	-1734.242	-1734.203	-0.039	-1736.680	-1736.529	-9.508
a₁-IN2	-1734.987	-1734.704	-1734.798	0.189	-1734.249	-1734.206	-0.044	-1736.684	-1736.538	-15.110
a₁-TS2	-1734.968	-1734.690	-1734.782	0.187	-1734.221	-1734.182	-0.039	-1736.667	-1736.520	-3.631
a₁-IN3	-1735.032	-1734.748	-1734.841	0.191	-1734.280	-1734.253	-0.027	-1736.729	-1736.565	-32.159
b₁-IN1	-1734.997	-1734.713	-1734.805	0.193	-1734.245	-1734.216	-0.029	-1736.690	-1736.526	-7.687
b₁-TS1	-1734.987	-1734.704	-1734.797	0.190	-1734.238	-1734.205	-0.034	-1736.681	-1736.525	-6.615
b₁-IN2	-1734.991	-1734.707	-1734.799	0.191	-1734.247	-1734.208	-0.039	-1736.685	-1736.533	-11.921
b₁-TS2	-1734.971	-1734.693	-1734.782	0.189	-1734.214	-1734.183	-0.031	-1736.667	-1736.509	3.176
b₁-IN3	-1735.034	-1734.750	-1734.842	0.192	-1734.271	-1734.252	-0.020	-1736.730	-1736.557	-27.197

Table S42. Potential energy surface for the functionalization catalyzed by Pd(TFA)₂ with the geometry-optimization of B3LYP-D3(BJ)/BS1 level.

	B3LYP-D3(BJ)/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			M06-2X/6-311+G(d,p)+SDD		
	E	H	G	TCGFE	E _{sol}	E _{gas}	ΔE_{sol}	E _{gas_lar}	G _{sol} D3_3	ΔG_{sol} D3_3
1a	-555.819	-555.610	-555.660	0.158	-555.558	-555.536	-0.022	-555.691	-555.554	
Pd(TFA)₂	-1179.140	-1179.067	-1179.130	0.010	-1178.653	-1178.646	-0.007	-1180.163	-1180.160	
a₁-IN1	-1735.005	-1734.721	-1734.812	0.193	-1734.252	-1734.225	-0.026	-1735.898	-1735.732	-10.962
a₁-TS1	-1734.985	-1734.702	-1734.795	0.189	-1734.242	-1734.203	-0.039	-1735.878	-1735.727	-8.321
a₁-IN2	-1734.987	-1734.704	-1734.798	0.189	-1734.249	-1734.206	-0.044	-1735.881	-1735.736	-13.498
a₁-TS2	-1734.968	-1734.690	-1734.782	0.187	-1734.221	-1734.182	-0.039	-1735.860	-1735.712	1.140
a₁-IN3	-1735.032	-1734.748	-1734.841	0.191	-1734.280	-1734.253	-0.027	-1735.929	-1735.766	-32.309
b₁-IN1	-1734.997	-1734.713	-1734.805	0.193	-1734.245	-1734.216	-0.029	-1735.888	-1735.725	-6.499
b₁-TS1	-1734.987	-1734.704	-1734.797	0.190	-1734.238	-1734.205	-0.034	-1735.878	-1735.722	-4.687
b₁-IN2	-1734.991	-1734.707	-1734.799	0.191	-1734.247	-1734.208	-0.039	-1735.883	-1735.730	-10.196
b₁-TS2	-1734.971	-1734.693	-1734.782	0.189	-1734.214	-1734.183	-0.031	-1735.859	-1735.701	8.547

b₁-IN3	-1735.034	-1734.750	-1734.842	0.192	-1734.271	-1734.252	-0.020	-1735.927	-1735.755	-25.420
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Table S43. Potential energy surface for the functionalization catalyzed by Pd(TFA)₂ with the geometry-optimization of M06-2X/BS1 level.

	M06-2X/6-31G(d)+LANL2DZ				M06-2X/6-31G(d)+LANL2DZ			M06-2X/6-311+G(d,p)+SDD		
	E _{gas}	H	G	TCGFE	E _{sol}	E _{gas}	ΔE _{sol}	E _{gas_lar}	G _{sol M06-2X_opt}	ΔG _{sol M06-2X_opt}
1a	-555.537	-555.326	-555.376	0.161	-555.559	-555.537	-0.022	-555.691	-555.553	
Pd(TFA)₂	-1178.647	-1178.574	-1178.629	0.018	-1178.654	-1178.647	-0.007	-1180.165	-1180.154	
a₁-IN1	-1734.227	-1733.940	-1734.029	0.198	-1734.253	-1734.227	-0.025	-1735.900	-1735.727	-13.244
a₁-TS1	-1734.205	-1733.919	-1734.010	0.195	-1734.243	-1734.205	-0.037	-1735.880	-1735.722	-9.718
a₁-IN2	-1734.208	-1733.920	-1734.012	0.196	-1734.250	-1734.208	-0.042	-1735.883	-1735.729	-14.300
a₁-TS2	-1734.184	-1733.902	-1733.992	0.192	-1734.222	-1734.184	-0.038	-1735.861	-1735.708	-0.702
a₁-IN3	-1734.255	-1733.968	-1734.060	0.196	-1734.282	-1734.255	-0.027	-1735.932	-1735.763	-35.822
b₁-IN1										
b₁-TS1										
b₁-IN2	-1734.211	-1733.923	-1734.015	0.196	-1734.249	-1734.211	-0.038	-1735.886	-1735.728	-13.252
b₁-TS2	-1734.186	-1733.904	-1733.991	0.195	-1734.216	-1734.186	-0.030	-1735.861	-1735.696	6.736
b₁-IN3	-1734.254	-1733.966	-1734.057	0.197	-1734.273	-1734.254	-0.019	-1735.930	-1735.753	-29.236

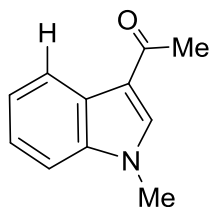
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5. Coordinates of All Stationary Points

as well as the Imaginary Frequency

for TS



1a

C	-2.40493000	-0.52698200	0.00008700
O	-2.53071900	-1.74790100	0.00039800
C	-1.08389100	0.10665400	0.00008100
C	0.19820100	-0.56633700	-0.00006200
C	-0.80616800	1.46259200	0.00015500
C	1.19202900	0.44475200	-0.00006700
C	0.59359500	-1.91337900	-0.00006600
H	-1.48411500	2.30564100	0.00023500
C	2.56038700	0.15557800	-0.00000500
C	1.95295100	-2.20757800	-0.00010200
H	-0.16028200	-2.69173500	-0.00002500
C	2.92518900	-1.18730300	-0.00007200
H	3.31082500	0.94100800	0.00008000
H	2.27533300	-3.24529400	-0.00011700
H	3.97889700	-1.45256600	-0.00008100
N	0.54611400	1.67783500	0.00004700
C	-3.63516100	0.37505100	-0.00039000
H	-3.64852300	1.02372000	0.88413600
H	-3.64847000	1.02296500	-0.88544800
H	-4.52990600	-0.25036000	-0.00010500
C	1.20818600	2.96761100	0.00006800
H	1.83529900	3.08294600	0.89156000
H	1.83811500	3.08127500	-0.88962300
H	0.45344400	3.75681600	-0.00188900

Pd(OAc)₂-catalyst

Pd(OAc)₂

O	1.77253300	1.08859500	-0.00962200
C	2.44439100	0.00002500	-0.00473800
O	1.77250500	-1.08854800	-0.00962700
C	3.94034400	-0.00007600	0.03538000

H	4.27076300	-0.00653700	1.08086400
H	4.32865300	-0.89640300	-0.45398700
H	4.32864300	0.90185100	-0.44349400
Pd	-0.00000100	0.00003500	-0.00926200
C	-3.94034000	-0.00007000	0.03541600
H	-4.32869700	-0.89497800	-0.45652300
H	-4.32866500	0.90325900	-0.44075600
H	-4.27067600	-0.00977200	1.08090700
C	-2.44439000	0.00006900	-0.00478300
O	-1.77251200	-1.08851600	-0.00967600
O	-1.77252500	1.08862800	-0.00965300

ao-IN1

C	-0.71488500	-1.16144900	-1.63747400
O	0.47469900	-0.76562800	-1.61910600
O	3.35246400	0.50466900	1.06943900
C	3.92988600	0.90650400	-0.00044300
O	3.30505900	0.76047900	-1.10357100
C	5.30812400	1.49751100	0.04708900
C	-1.79336800	-0.45154900	-0.99847000
C	-1.83031700	0.91122100	-0.49554000
C	-3.04816500	-0.99351300	-0.73465900
C	-3.12085700	1.10072900	0.05671200
C	-0.93842800	1.99445500	-0.50948000
H	-3.41474400	-1.99207600	-0.92842900
C	-3.53717800	2.30987600	0.61841200
C	-1.34348800	3.20281000	0.04940700
H	0.04691300	1.89406700	-0.95021300
C	-2.62381400	3.35973700	0.61193700
H	-4.53133000	2.43247500	1.03788100
H	-0.65646200	4.04411000	0.05097900
H	-2.90710400	4.31625900	1.04158200
N	-3.83437300	-0.09014600	-0.09583900
C	-0.97891600	-2.44026500	-2.39544700
H	-0.28679900	-2.49868800	-3.23940800
H	-0.74376900	-3.26444300	-1.71156400
H	-2.00723600	-2.53199500	-2.75279900
C	-5.19175200	-0.31311200	0.36938200
H	-5.25011000	-0.18795200	1.45583000
H	-5.88118700	0.39247700	-0.10665900
H	-5.49438600	-1.33027500	0.11378200
Pd	1.71422700	-0.15302900	-0.04428100
C	-0.56543300	-2.31688500	2.84037200
O	0.54122500	-0.77868000	1.45168300

O	0.13789400	-2.83712500	0.59056100	H	4.79023700	-1.80870400	1.99353900
C	0.07915000	-2.00343700	1.49120100	H	3.81994100	-3.24877100	1.66760700
H	0.21929100	-2.43375700	3.59629200	H	5.15722400	-2.80326500	0.55818100
H	-1.21061700	-1.49498000	3.16465700	H	2.96127900	4.41894600	-0.34635200
H	-1.13531400	-3.24612000	2.77059000	H	3.03279000	3.76760200	1.32606200
H	5.45836800	2.17083500	-0.80006600	H	4.18151800	3.20353300	0.10667900
H	5.45989800	2.02534500	0.99185500				
H	6.04668100	0.68957100	-0.01657500				
a₀-TS1				a₀-IN2			
Imaginary Frequency: -32.2122				C	-1.12633800	-2.20170500	-0.63170400
C	-1.08547600	-2.16956000	-0.70083900	O	0.07961600	-1.88122600	-0.62058200
O	0.11194000	-1.81826400	-0.72750300	O	2.08414200	1.44341000	0.71959400
O	2.11968500	1.45379100	0.73207100	C	2.22785300	2.38812100	-0.17499800
C	2.20746500	2.41486600	-0.14988800	O	1.65151000	2.41656800	-1.26546600
O	1.60091100	2.42036800	-1.22669500	C	3.20571100	3.46922700	0.25817900
C	3.14803100	3.53272400	0.26404200	C	-2.18430500	-1.26341700	-0.33705800
C	-2.15820500	-1.26618100	-0.35570400	C	-2.09335300	0.18143000	-0.30998500
C	-2.11275900	0.18115400	-0.32136500	C	-3.46040300	-1.58025400	0.11838600
C	-3.40883500	-1.62604300	0.13686800	C	-3.32580100	0.65501300	0.20118400
C	-3.34343700	0.61243600	0.22953500	C	-1.11898900	1.11742800	-0.70050900
C	-1.18218800	1.14834400	-0.73760800	H	-3.91691100	-2.54891400	0.26784500
H	-3.82955000	-2.60946000	0.29478600	C	-3.59280100	2.01367300	0.38597300
C	-3.64832200	1.96121100	0.42853100	C	-1.37062600	2.47552400	-0.50378400
C	-1.46901300	2.49617200	-0.52557500	H	-0.24334500	0.85990600	-1.31939500
H	-0.30424500	0.91084300	-1.35317900	C	-2.58992800	2.91603100	0.03967100
C	-2.68517100	2.89590600	0.05620600	H	-4.54440200	2.35822000	0.77975600
H	-4.59764500	2.27395800	0.85306600	H	-0.60613700	3.18288100	-0.80358200
H	-0.73433800	3.22998300	-0.83676000	H	-2.76121200	3.97974500	0.17445300
H	-2.88522800	3.95311200	0.20260900	N	-4.13981400	-0.45119400	0.45012600
N	-4.11319100	-0.52098000	0.49690100	C	-1.45450700	-3.63222900	-0.99336100
C	-1.38853200	-3.60164900	-1.07887200	H	-1.76404300	-3.67816600	-2.04505800
H	-1.72256800	-3.63732100	-2.12346900	H	-0.56536900	-4.25137500	-0.86229200
H	-0.48203400	-4.20138400	-0.98029900	H	-2.27522700	-4.03230900	-0.39003900
H	-2.18472600	-4.03144400	-0.46334800	C	-5.48123000	-0.39016800	1.00619500
C	-5.43743700	-0.50610600	1.09526700	H	-5.46339400	0.07211200	1.99869700
H	-5.40289600	-0.04989400	2.09016800	H	-6.14006100	0.19205900	0.35346600
H	-6.13449700	0.05940500	0.46799800	H	-5.87750400	-1.40333200	1.09467500
H	-5.79888500	-1.53180900	1.18850700	Pd	1.02917100	-0.10858800	0.04739400
Pd	1.06720300	-0.07567900	0.00718700	C	4.42969300	-2.36198300	1.09633300
C	4.35691600	-2.42120300	1.19507400	O	2.33886100	-1.28930200	0.99894800
O	2.29822200	-1.29895500	1.01172500	O	3.65062900	-1.14280400	-0.84093000
O	3.69505000	-1.17161400	-0.76624700	C	3.42763100	-1.52940900	0.29718800
C	3.41165400	-1.56037800	0.35741300	H	4.87692000	-1.73721600	1.87743300
				H	3.93505300	-3.20381000	1.58958600
				H	5.21435600	-2.72246100	0.42815200

H	3.07483700	4.35687600	-0.36451800
H	3.07205200	3.71890000	1.31462800
H	4.22751600	3.09341000	0.13238700

a₀-TS2

Imaginary Frequency: -1151.0605

C	1.05952600	-2.23362500	0.36305000
O	-0.07618200	-1.97629300	-0.09209700
O	-2.09033200	1.60820000	-0.40081700
C	-1.96927300	2.17617400	0.73938100
O	-0.99703500	1.98679900	1.52837700
C	-3.08489400	3.10766300	1.14901400
C	2.11303600	-1.25272200	0.40771500
C	1.98891800	0.14728100	0.06848000
C	3.47925700	-1.52049600	0.48300100
C	3.30616600	0.63236200	-0.11094700
C	0.87612900	0.99856500	-0.11853400
H	3.99092000	-2.44936500	0.69357100
C	3.57410600	1.92756600	-0.55743200
C	1.16498700	2.28088600	-0.62242100
H	-0.07253200	1.23648900	0.77789400
C	2.47570900	2.73696700	-0.83875100
H	4.58902100	2.29082200	-0.68941500
H	0.34085400	2.96684200	-0.79276000
H	2.63709600	3.74619700	-1.20636600
N	4.19343700	-0.40694200	0.17954600
C	1.28698700	-3.64552600	0.85308900
H	1.06860400	-3.68484500	1.92791100
H	0.59710900	-4.31990700	0.34179900
H	2.31517200	-3.98665400	0.70576000
C	5.64223700	-0.30822600	0.11980600
H	5.96466600	-0.02970400	-0.88896800
H	6.00515500	0.44223500	0.82978900
H	6.07714600	-1.27616400	0.37565200
Pd	-0.96621000	-0.11409300	-0.44652300
C	-4.80188100	-1.93211100	-0.61243000
O	-3.51633600	-0.69831300	1.01662800
O	-2.60639600	-1.16562900	-1.00212900
C	-3.56212300	-1.19533900	-0.10663000
H	-5.52663100	-2.03568600	0.19789000
H	-5.25366200	-1.36994900	-1.43745300
H	-4.52983900	-2.91862300	-1.00122000
H	-2.75292500	3.79152100	1.93190500
H	-3.46373200	3.65686100	0.28382400

H	-3.89790300	2.48214500	1.53538600
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a₀-IN3

C	-1.43824100	2.24827800	0.16170200
O	-0.21795800	2.02366600	-0.03246100
O	1.98576900	-1.46564400	-0.58290700
C	2.53212100	-1.97423600	0.41012800
O	2.11008300	-1.80086500	1.64875700
C	3.69869800	-2.89959400	0.27618500
C	-2.40998200	1.20242400	0.16898200
C	-2.10722300	-0.19080800	-0.06703500
C	-3.79046700	1.28739400	0.34363500
C	-3.33758400	-0.88402200	-0.03048200
C	-0.89499000	-0.85317500	-0.31150200
H	-4.41660300	2.14773700	0.53675400
C	-3.42061700	-2.26180400	-0.24113900
C	-0.98579600	-2.23199800	-0.53633100
H	1.45705500	-1.06434200	1.64278300
C	-2.21834600	-2.91704700	-0.49958400
H	-4.36405800	-2.79861500	-0.21314400
H	-0.08875900	-2.80204300	-0.75685700
H	-2.23004300	-3.98908100	-0.68001600
N	-4.34594100	0.05332400	0.22842700
C	-1.82494600	3.69744000	0.34969100
H	-1.08124500	4.18723800	0.98398700
H	-1.80740500	4.20120400	-0.62432400
H	-2.81785300	3.81995900	0.78883000
C	-5.75889300	-0.26202200	0.34638700
H	-6.12850400	-0.71031700	-0.58195600
H	-5.92629600	-0.96463600	1.16966000
H	-6.31683400	0.65534700	0.54397800
Pd	0.79133700	0.23422200	-0.32744100
C	4.71341700	2.24821200	-0.27739100
O	3.94254200	0.19087100	0.69836000
O	2.48432100	1.48740900	-0.45217600
C	3.64485200	1.19737200	0.03496500
H	5.65374700	1.99593200	0.21801000
H	4.87337500	2.30176900	-1.36047700
H	4.37515800	3.23803600	0.04706800
H	3.67895400	-3.67359000	1.04663100
H	3.72071300	-3.33741000	-0.72268500
H	4.58860900	-2.27662900	0.41919600

a₀-IN1'

C	0.80304300	-1.26176100	1.50048200	O	2.21953700	1.76288600	0.11191900
O	-0.39145800	-0.88754600	1.59667400	C	1.87287200	2.59177000	-0.79220600
O	-3.16862200	0.96061100	-0.86624700	O	0.81283900	2.49141800	-1.48490500
C	-3.00392800	1.97381700	-0.10429200	C	2.80354100	3.75573400	-1.05352600
O	-2.13717000	1.88017300	0.82975500	C	-2.00305100	-1.11827200	-0.66470200
C	-3.82787500	3.21452300	-0.28521800	C	-1.85671900	0.18846400	-0.06429700
C	1.84415600	-0.54124300	0.81143700	C	-3.35413300	-1.44652200	-0.57818900
C	1.90698300	0.83277000	0.34143300	C	-3.13851400	0.54952200	0.41556100
C	3.03492600	-1.13783500	0.41074500	C	-0.74675200	1.04175900	0.13099000
C	3.14843900	0.96979700	-0.33092000	H	-3.86643800	-2.34549500	-0.89279200
C	1.08701300	1.96435600	0.47051600	C	-3.36197500	1.70728600	1.16281800
H	3.35392500	-2.16384600	0.52836700	C	-0.98224100	2.17386600	0.93367700
C	3.57875400	2.17071900	-0.89899200	H	0.06388200	1.53016500	-0.83239200
C	1.50750500	3.16478400	-0.09607600	C	-2.25179200	2.50166500	1.43751900
H	0.14363200	1.91822800	0.99891600	H	-4.34981200	1.97495400	1.52589800
C	2.73356400	3.26959100	-0.77752500	H	-0.15862500	2.85331600	1.12966300
H	4.53404500	2.24958500	-1.40952100	H	-2.37340900	3.40119300	2.03400600
H	0.87262000	4.04167000	-0.00572700	N	-4.03559300	-0.46019100	0.05870800
H	3.03002800	4.22187200	-1.20803900	C	-1.23540100	-3.36934000	-1.62833600
N	3.80538900	-0.25968300	-0.27971400	H	-0.36200300	-3.69784500	-2.19554200
C	1.14157000	-2.55462900	2.21156600	H	-1.41620300	-4.10594900	-0.83551200
H	0.41200300	-2.72114600	3.00724900	H	-2.11098700	-3.33942800	-2.28278700
H	1.03782000	-3.36293000	1.47822300	C	-5.45428700	-0.46398700	0.37325700
H	2.15313300	-2.56415600	2.62494700	H	-5.60537400	-0.42405600	1.45716800
C	5.08887800	-0.54563000	-0.89459800	H	-5.95178600	0.39574000	-0.08764100
H	5.03752400	-0.39312400	-1.97793900	H	-5.90326900	-1.38090400	-0.01300700
H	5.86702800	0.10503400	-0.48081600	Pd	1.13926400	-0.00423700	-0.03214500
H	5.35528300	-1.58554700	-0.69685000	C	4.23754600	-2.65859100	1.05239100
Pd	-1.73134100	-0.11223000	0.19932800	O	2.88907500	-1.03149500	-0.00677600
C	-1.58882500	-3.88837100	-1.85315300	O	2.05642600	-1.99331000	1.85378700
O	-1.97069700	-1.86060000	-0.74375300	C	2.93972600	-1.85731600	1.00798700
O	0.16628400	-2.63259200	-0.77492800	H	3.48711300	3.47550100	-1.86347700
C	-1.02865900	-2.71093600	-1.05488300	H	2.23580800	4.63198700	-1.37381200
H	-4.74395000	3.12650100	0.31086200	H	3.39802700	3.97803800	-0.16549600
H	-3.27349700	4.08908800	0.06358700	H	5.09157100	-1.98032100	1.15481400
H	-4.11080300	3.32964000	-1.33425800	H	4.21557200	-3.35174200	1.89598600
H	-2.04317600	-3.52638200	-2.78120700	H	4.37259300	-3.21297900	0.11758400
H	-0.78678700	-4.59264700	-2.08341200				
H	-2.37483500	-4.39154800	-1.28061800				
ao-TS0				ao-IN2'			
Imaginary Frequency: -1236.5073				C	-1.33724100	-2.13688400	-0.38716200
C	-0.93721200	-2.02386000	-1.00229200	O	-0.13029300	-1.80436200	-0.46364700
O	0.25796100	-1.78187500	-0.73513300	O	1.82021800	1.86365800	0.02161000
				C	3.04403300	2.05359600	-0.18125700
				O	3.90971900	1.14253800	-0.47268100

C	3.58986100	3.45805100	-0.09160100
C	-2.36720100	-1.17423900	-0.15919800
C	-2.12460200	0.24163300	-0.01088500
C	-3.74599100	-1.35454000	-0.07344000
C	-3.38648100	0.85491500	0.15501700
C	-0.94314100	0.99512300	-0.00463200
H	-4.33563900	-2.25898100	-0.13429900
C	-3.52615500	2.23362000	0.32495200
C	-1.08160000	2.37557900	0.16199100
H	3.46216400	0.13967600	-0.45552100
C	-2.34731700	2.97699900	0.32256800
H	-4.49454700	2.70793800	0.45275500
H	-0.19720000	3.00260100	0.17604200
H	-2.40381300	4.05503100	0.45185700
N	-4.35651000	-0.15482200	0.11322300
C	-1.63265200	-3.60881200	-0.55563200
H	-1.22672500	-3.94932900	-1.51389900
H	-1.11126400	-4.16294200	0.23228700
H	-2.69891400	-3.84182500	-0.51439000
C	-5.78481400	0.06348200	0.25789700
H	-6.00668200	0.51132100	1.23251900
H	-6.15092000	0.73097900	-0.52950100
H	-6.30439500	-0.89366200	0.18111000
Pd	0.78642100	0.03125200	-0.16637400
C	4.48353500	-2.37146200	0.46308900
O	2.71844000	-0.97255800	-0.33219700
O	2.27430500	-2.31215000	1.42453500
C	3.04382600	-1.88513100	0.58064500
H	4.39200100	3.49067900	0.65264200
H	4.02779500	3.73765700	-1.05560000
H	2.80143700	4.16176500	0.17659000
H	5.17871800	-1.52843800	0.55532600
H	4.69667900	-3.10663500	1.24129600
H	4.64804400	-2.81829000	-0.52366000

ao'-IN1

C	0.55170500	-1.86237600	-1.22413300
O	-0.64070500	-1.53229100	-1.03440400
O	-3.12811700	-0.67108600	0.06582300
C	-3.06215800	-1.30869900	1.20913100
O	-2.08080300	-1.37352000	1.94541000
C	-4.38223900	-1.98883200	1.55791200
C	1.69210100	-1.22042000	-0.61528400
C	1.78850300	-0.45250200	0.61785700

C	2.96597100	-1.20352600	-1.17996200
C	3.12770400	0.00061100	0.70170100
C	0.90986000	-0.18166800	1.67993400
H	3.31164300	-1.63083800	-2.11093000
C	3.60929000	0.75516900	1.77432100
C	1.38450800	0.57281400	2.74985700
H	-0.10713700	-0.56638800	1.69151100
C	2.70991600	1.04412600	2.79596100
H	4.64041300	1.09327700	1.81811200
H	0.71267000	0.79299000	3.57448400
H	3.04255800	1.62874900	3.64920000
N	3.81480900	-0.46624800	-0.42035100
C	0.76366900	-3.06543200	-2.12049200
H	-0.08904600	-3.17402600	-2.79365300
H	1.68971500	-3.00467800	-2.69863700
H	0.82824600	-3.96384400	-1.49351200
C	5.20677800	-0.18411700	-0.72038800
H	5.36477500	0.89426300	-0.82860600
H	5.85457800	-0.55848500	0.07963000
H	5.47916300	-0.67753000	-1.65539000
Pd	-1.49895900	0.31271300	-0.53653600
C	-0.77173800	4.16492800	-1.08158100
O	-0.16089900	1.82016700	-1.21343700
O	-2.11838700	2.29342500	-0.35550300
C	-1.01903400	2.69953800	-0.87014000
H	-1.14926500	4.73423900	-0.22788500
H	0.29472600	4.35097000	-1.22513000
H	-1.31460700	4.49757300	-1.97400900
H	-4.27759400	-2.53341900	2.49833200
H	-5.17467500	-1.23862700	1.65029900
H	-4.67545700	-2.67656000	0.75804400

ao'-TS1

Imaginary Frequency: -221.4093

C	-1.14320800	1.60544700	-1.46919300
O	0.07688700	1.32409400	-1.47300500
O	2.44708800	1.49708100	0.68823800
C	1.84752600	2.11610200	1.60627400
O	0.64426400	1.91512700	1.97507000
C	2.62156100	3.18761000	2.37637200
C	-2.10118500	0.82877800	-0.72498700
C	-1.77095200	-0.12131000	0.30532800
C	-3.46229300	0.67379400	-0.97995500
C	-2.94905000	-0.84281400	0.59245600

C	-0.57413100	-0.36067600	1.01800000
H	-4.09519100	1.17946400	-1.69646200
C	-2.96610800	-1.87988900	1.52670000
C	-0.59750000	-1.43563600	1.92951500
H	0.08905700	0.57768000	1.31763700
C	-1.76241800	-2.17703000	2.17403000
H	-3.87084200	-2.43847800	1.74819800
H	0.30616500	-1.66352400	2.48693400
H	-1.74086500	-2.98390100	2.90089700
N	-3.97163100	-0.32383300	-0.20842100
C	-1.57062800	2.80254700	-2.28092300
H	-0.86520900	2.96487600	-3.09843000
H	-2.58491300	2.69715400	-2.67643600
H	-1.55448300	3.68703900	-1.63146500
C	-5.34407700	-0.80163400	-0.22291900
H	-5.37835400	-1.85783500	-0.51020900
H	-5.79982400	-0.68627700	0.76607900
H	-5.91816200	-0.21940400	-0.94607900
Pd	1.07171800	-0.21631900	-0.48630600
C	4.13640300	-2.73520400	-0.89272000
O	2.65110200	-1.09802700	-1.88998000
O	2.21845600	-1.73634100	0.16690000
C	2.94815800	-1.81585500	-0.90183900
H	3.93598900	-3.61479700	-0.27513000
H	4.38701800	-3.03153700	-1.91396200
H	4.99288300	-2.20320000	-0.46225700
H	1.98196000	4.05523400	2.56783600
H	2.92547400	2.78409000	3.35020400
H	3.51675800	3.49008100	1.82704700

ao'-IN2

C	2.77022500	-1.80183400	0.28899900
O	1.58587700	-2.21939800	0.21952800
O	-5.10721500	0.77500400	0.99951400
C	-4.63741900	1.73752100	0.42190900
O	-3.55609000	1.68498200	-0.36925800
C	-5.20399900	3.13835000	0.50179600
C	3.07853000	-0.41502400	0.16315600
C	2.08463400	0.61133400	-0.04293400
C	4.31298800	0.23278600	0.21741700
C	2.77270800	1.84265700	-0.10183600
C	0.69247300	0.55596600	-0.17304600
H	5.30615200	-0.17098400	0.35903200
C	2.10729000	3.05592000	-0.28857800

C	0.01873500	1.76503400	-0.35520900
H	-3.17245000	0.76434300	-0.35966000
C	0.72041500	2.98830200	-0.41148700
H	2.63262300	4.00503700	-0.33460700
H	-1.06157300	1.78450100	-0.45074500
H	0.15736600	3.90660600	-0.55548600
N	4.13805000	1.56981500	0.06017100
C	3.83624800	-2.84620000	0.52172600
H	3.75253200	-3.62149300	-0.24679800
H	4.84843700	-2.43632600	0.50945000
H	3.65891200	-3.32909500	1.48915300
C	5.18748100	2.57469000	0.06054100
H	5.19682900	3.11577800	-0.89142100
H	5.02922400	3.29087700	0.87371400
H	6.15347400	2.08581100	0.20062700
Pd	-0.19571900	-1.19929300	-0.08961900
C	-4.12376800	-2.11191500	-0.45613900
O	-1.82988400	-2.81262300	-0.10310400
O	-2.19681300	-0.66157500	-0.39433100
C	-2.64510200	-1.88347300	-0.30202500
H	-4.41060900	-1.93089500	-1.49923200
H	-4.37155100	-3.14123200	-0.19065300
H	-4.67562300	-1.40126800	0.16734000
H	-4.45738200	3.81991200	0.92354800
H	-5.44611000	3.50283800	-0.50217700
H	-6.09916200	3.13858700	1.12465600

ao'-IN3

C	1.05658800	2.19499800	-0.00410100
O	-0.19111900	2.04497300	-0.00431700
C	1.94456000	1.07574000	-0.00529800
C	1.50364100	-0.29864800	-0.00090200
C	3.33889900	1.04270500	-0.00704800
C	2.66211100	-1.10487200	0.00011100
C	0.22767400	-0.87052400	0.00198000
H	4.05547800	1.85269500	-0.00952700
C	2.59308200	-2.50002300	0.00402600
C	0.14862500	-2.26403200	0.00584000
C	1.31463300	-3.05833400	0.00691400
H	3.48119700	-3.12477500	0.00493500
H	-0.82580200	-2.74305900	0.00787600
H	1.21308500	-4.14062000	0.01004900
N	3.76989200	-0.24608700	-0.00362000
C	1.56343300	3.61850400	0.01439300

H	1.30079300	4.07943200	0.97365100
H	2.64399800	3.69116300	-0.12769500
H	1.05654000	4.19010600	-0.76919500
C	5.15507000	-0.68314700	-0.00473400
H	5.36698100	-1.28203000	0.88738100
H	5.36388300	-1.28722600	-0.89407300
H	5.80849700	0.19147600	-0.00842500
Pd	-1.34492300	0.30431100	-0.00119300
C	-5.18580200	-0.92377200	-0.00057300
H	-5.92931400	-0.12462000	-0.00109000
H	-5.32207000	-1.55754300	0.88222700
H	-5.32200600	-1.55838100	-0.88280300
C	-3.79278300	-0.34125700	-0.00091500
O	-2.79603600	-1.16611300	0.00164600
O	-3.58690100	0.89784500	-0.00373500

ao''-TS1

Imaginary Frequency: -87.2211

C	-0.84303100	-0.65063800	2.32412800
O	0.36873600	-0.63437500	2.08389200
O	3.01771500	-0.33452000	-0.16505300
C	3.23105200	-1.62496200	-0.07409300
O	2.37554900	-2.50475800	-0.03103100
C	4.72167600	-1.94394200	-0.01423700
C	-1.81625200	-0.74359400	1.24242300
C	-1.50257600	-0.97546900	-0.14401600
C	-3.16582500	-0.42400400	1.28530300
C	-2.68823900	-0.74397000	-0.88022500
C	-0.32523500	-1.35776000	-0.81967900
H	-3.78586800	-0.16264000	2.13247800
C	-2.73263400	-0.83771500	-2.27314000
C	-0.36863400	-1.43189400	-2.21943300
H	0.54224000	-1.77244200	-0.29303900
C	-1.54871800	-1.16708800	-2.93435900
H	-3.65000700	-0.66231200	-2.82794200
H	0.52646800	-1.74011900	-2.75154000
H	-1.54925900	-1.24315800	-4.01781100
N	-3.69633500	-0.42216700	0.02731700
C	-1.33373000	-0.53481800	3.75710100
H	-0.47600700	-0.56280700	4.43153900
H	-1.86787200	0.41258100	3.90354100
H	-2.02492900	-1.34847400	4.00510000
C	-5.06920800	-0.10785400	-0.32330200
H	-5.10756500	0.76342100	-0.98625400

H	-5.54518600	-0.95711000	-0.82586400
H	-5.62715100	0.11863100	0.58740100
Pd	1.23218200	0.53048200	-0.09088400
C	0.14097400	4.35985800	-0.35934400
C	0.59675900	2.93285100	-0.24188700
O	-0.25624200	1.99074000	-0.05717700
O	1.82273100	2.62240400	-0.34787700
H	4.86789900	-3.02174600	-0.10837000
H	5.12803900	-1.60261100	0.94425300
H	5.26096500	-1.41599000	-0.80623200
H	0.88377500	5.02772000	0.08442900
H	0.04226800	4.61968800	-1.41994500
H	-0.82999500	4.49044500	0.12424300

ao''-IN2

C	2.61597900	-2.28361000	-1.14878300
O	1.63483700	-3.01730100	-1.15665400
O	-2.44063300	-1.32873500	-0.28522600
C	-3.45537000	-1.35164500	0.55297100
O	-3.62015600	-0.57455900	1.48895800
C	-4.43954800	-2.46869500	0.22839100
C	2.66783400	-1.10038900	-0.27698100
C	1.62339000	-0.63983200	0.60118100
C	3.71647500	-0.20926200	-0.12161000
C	2.10819700	0.51292500	1.25532400
C	0.31309000	-1.09967800	0.89395000
H	4.68654300	-0.19314100	-0.59922400
C	1.35912800	1.22078100	2.21720500
C	-0.44655300	-0.38949000	1.86154700
H	-0.02908600	-2.04558000	0.49220900
C	0.09391900	0.76012400	2.51455900
H	1.76369400	2.09915600	2.71119200
H	-1.39211200	-0.78738800	2.21306100
H	-0.51273900	1.27009700	3.25575200
N	3.38982900	0.75704600	0.79370400
C	3.81499800	-2.57215900	-2.04165500
H	3.62375400	-3.48773300	-2.60419200
H	3.98676400	-1.74659700	-2.74321300
H	4.72858100	-2.69709000	-1.44739300
C	4.23214400	1.86984000	1.19831000
H	3.75364700	2.82357700	0.95215000
H	4.42785300	1.83580200	2.27538400
H	5.18368800	1.80551000	0.66729700
Pd	-1.24034900	0.26875400	-0.20611200

C	-0.94907500	3.68646300	-2.23861600
C	-1.06116500	2.38100400	-1.50342800
O	-0.20685900	2.06084300	-0.60162300
O	-2.01636800	1.57590300	-1.74069100
H	-5.13187300	-2.59980900	1.06243000
H	-3.91289300	-3.40412800	0.01844100
H	-5.00470800	-2.20035400	-0.67132300
H	-1.18109300	3.53874900	-3.29693000
H	-1.68203600	4.39225600	-1.83085400
H	0.05203700	4.10717300	-2.12186100

ao''-TS2

Imaginary Frequency: -1106.3399

C	-0.94283100	-0.59865000	2.33744100
O	0.24419600	-0.86320500	2.17597100
O	2.66997500	-1.21078500	-0.23025600
C	2.25190900	-2.40863600	-0.16861900
O	1.04598900	-2.76700100	-0.31446100
C	3.28350900	-3.47770300	0.12437000
C	-1.85045100	-0.38094000	1.20469600
C	-1.53924200	-0.41223400	-0.20591800
C	-3.20804900	-0.11144900	1.29724800
C	-2.75816300	-0.15822800	-0.88949600
C	-0.35203900	-0.64035200	-0.95764500
H	-3.82801100	-0.00599700	2.17726000
C	-2.85137200	-0.11485900	-2.28162700
C	-0.47524200	-0.60641900	-2.36409300
H	0.36671500	-1.67129200	-0.56018900
C	-1.69000500	-0.35013400	-3.01584000
H	-3.79549800	0.08652700	-2.78026000
H	0.40757700	-0.80405200	-2.96674900
H	-1.73003900	-0.33457800	-4.10126300
N	-3.76078400	0.02407300	0.05749800
H	3.00652900	-4.41503200	-0.36270800
H	4.27504700	-3.15117700	-0.19400600
H	3.30362400	-3.64603300	1.20738900
C	-1.51593300	-0.48608800	3.74627800
H	-1.89977000	0.52450800	3.93268300
H	-2.34394900	-1.18938100	3.89679800
H	-0.72377900	-0.70547300	4.46438900
C	-5.15415500	0.30335100	-0.23573200
H	-5.25242000	1.24163900	-0.79286300
H	-5.59702700	-0.50693700	-0.82557800
H	-5.70385200	0.39412700	0.70325100

Pd	1.38945800	0.38556600	-0.28707400
C	1.73510000	4.30686700	0.33868300
H	2.51058300	4.53688200	1.07334600
H	0.77024100	4.70752500	0.65900300
H	2.00912500	4.78405900	-0.60980300
C	1.64366600	2.81911600	0.13356600
O	0.52385700	2.28626800	-0.19929800
O	2.66287300	2.07325900	0.25583800

ao''-IN3

C	0.73470800	-1.27949700	1.92786100
O	-0.27937800	-0.60659300	2.17155400
O	-1.73185300	2.13918800	0.10682800
C	-1.34254800	2.63132200	1.17789700
O	-0.68153600	1.99546800	2.10974700
C	-1.62089400	4.07433900	1.50296200
C	1.72677100	-0.88319000	0.94112900
C	1.58169700	0.00217900	-0.20598700
C	3.07510900	-1.20128700	1.02200900
C	2.89137500	0.18685200	-0.72804300
C	0.49181000	0.58031700	-0.88858800
H	3.59719300	-1.80961700	1.74752400
C	3.16706700	0.97856400	-1.84600000
C	0.76746500	1.39033000	-1.99139300
H	-0.53456300	1.01221100	1.91863800
C	2.08168300	1.59297300	-2.45902400
H	4.17725200	1.10328000	-2.22434500
H	-0.05186500	1.85982100	-2.52886600
H	2.24384200	2.22307000	-3.32984000
N	3.77718800	-0.55816100	0.04784100
H	-0.67678400	4.59573600	1.69110100
H	-2.15377400	4.54817200	0.67867700
H	-2.21722700	4.13425000	2.41930300
C	0.92028400	-2.58644800	2.67425900
H	0.57859500	-3.40595700	2.02910000
H	1.96493400	-2.78803400	2.92995400
H	0.31154800	-2.57789700	3.58080900
C	5.21162500	-0.62148900	-0.15724700
H	5.44203900	-1.02085500	-1.15124600
H	5.65986100	0.37413000	-0.06523400
H	5.65229300	-1.27765000	0.59620100
Pd	-1.39780400	0.14564600	-0.49288900
C	-3.22404500	-3.38696600	-1.11348700
H	-4.18833400	-3.48618800	-0.61074300

H	-2.54284600	-4.18104100	-0.79470600
H	-3.37569900	-3.49281300	-2.19416100
C	-2.62334800	-2.03137700	-0.82671200
O	-1.36415400	-1.86407800	-1.05025200
O	-3.32562600	-1.07435300	-0.40437800

b₀-IN1

C	0.80628700	-1.41790900	-0.88576800
O	-0.43100800	-1.22275000	-0.91763900
O	-2.99697000	1.69933700	0.57868100
C	-2.39202200	2.52470200	-0.18117900
O	-1.38810700	2.09987100	-0.85410400
C	-2.87190600	3.94128000	-0.31042600
C	1.78230200	-0.47052400	-0.40246100
C	3.19852800	-0.66079100	-0.11388000
C	1.52225000	0.88256600	-0.18236000
C	3.69857900	0.60888100	0.27636400
C	4.08928900	-1.74775400	-0.11169300
H	0.60442000	1.43535700	-0.33227000
C	5.02602300	0.82739100	0.64908800
C	5.41587400	-1.53972200	0.25526800
H	3.76201300	-2.74366400	-0.38657500
C	5.88354700	-0.26799500	0.63055000
H	5.37804200	1.81125400	0.94434900
H	6.10414600	-2.38009200	0.25424300
H	6.92423300	-0.13923500	0.91290800
N	2.64754100	1.52311200	0.21224500
C	1.26282300	-2.75797500	-1.41800200
H	1.54940300	-3.40567000	-0.57948100
H	0.43447100	-3.22882400	-1.94999000
H	2.12996700	-2.65770900	-2.07770000
C	2.75386600	2.94307500	0.50478200
H	1.77903200	3.40777700	0.34867200
H	3.06109500	3.09727800	1.54451400
H	3.48619700	3.41620800	-0.15774300
Pd	-1.75410800	0.14151900	-0.04827500
C	-3.91609800	-3.14765800	1.42070900
O	-3.92551300	-1.75525400	-0.55755500
O	-2.38579700	-1.39048500	1.05394900
C	-3.41225600	-2.02457200	0.52052800
H	-2.03786700	4.60455100	-0.55269800
H	-3.60141700	3.99557800	-1.12712700
H	-3.36459600	4.25956200	0.61123300
H	-3.09196700	-3.80424100	1.71691000

H	-4.34260000	-2.72322400	2.33626300
H	-4.68178900	-3.72029500	0.89363400

b₀-TS0

Imaginary Frequency: -1199.7971			
C	-0.90441500	-2.08591300	0.50154500
O	0.32242500	-2.12690800	0.20591600
O	1.97683200	1.57871300	-0.51020700
C	1.74902900	2.25953700	0.54648700
O	0.81508500	2.00979000	1.37107200
C	2.67575600	3.41955200	0.81808500
C	-1.61485400	-0.84249300	0.40413900
C	-3.01707400	-0.57989800	0.19479700
C	-0.90077000	0.35671800	0.15604200
C	-3.09743500	0.77944100	-0.21213700
C	-4.20300600	-1.33265500	0.27576400
H	0.04425500	1.00002200	0.82220500
C	-4.31627200	1.40429000	-0.50474400
C	-5.41241200	-0.71759900	-0.01968100
H	-4.18485900	-2.37394300	0.57932300
C	-5.46979600	0.63737700	-0.40476500
H	-4.36565100	2.44804700	-0.79769000
H	-6.33360700	-1.28862500	0.05154400
H	-6.43221700	1.08995800	-0.62468600
N	-1.81038200	1.30166700	-0.24847700
C	-1.57015600	-3.37828400	0.88691400
H	-2.23846200	-3.70583500	0.08036500
H	-0.81119700	-4.14621500	1.04711400
H	-2.17555200	-3.25391800	1.79086500
C	-1.49659600	2.68735700	-0.57756400
H	-0.49194900	2.73291700	-0.99743300
H	-2.20442400	3.04098100	-1.33027000
H	-1.55364100	3.32724400	0.30868400
Pd	1.12987400	-0.29026100	-0.35875100
C	5.13448900	-1.60933800	-0.61050000
O	3.78000000	-0.38235700	0.97162700
O	2.84853900	-1.14497300	-0.94413600
C	3.84384100	-0.97372000	-0.10091500
H	2.21741500	4.13070700	1.50722400
H	3.58269000	3.00834200	1.27653000
H	2.96374100	3.90718700	-0.11617300
H	4.97881800	-2.67454000	-0.80974300
H	5.43443100	-1.14085100	-1.55394400
H	5.92367900	-1.48147800	0.13300300

C	-1.58722900	2.65171000	-0.62550500
O	-0.55943500	2.46438300	-1.35348700
C	-2.31005400	3.97592400	-0.72821500
C	1.49885100	-0.72831800	-0.64878500
C	2.86075000	-0.62182300	-0.18855200
C	0.81023500	0.45171200	-0.26627400
C	2.93832400	0.61911700	0.49915400
C	4.00783700	-1.43363100	-0.25160300
H	0.01973400	1.29913000	-0.93521500
C	4.12341000	1.07694500	1.08821900
C	5.18288200	-0.98554700	0.33748600
H	3.98841100	-2.38990500	-0.76344700
C	5.24147800	0.25750700	0.99950100
H	4.17483200	2.03461700	1.59602100
H	6.07594800	-1.60147300	0.28445000
H	6.17685700	0.58125900	1.44641000
N	1.68724300	1.22329200	0.45549200
C	1.38970300	-3.13118600	-1.58648200
H	1.90039700	-3.64376400	-0.76136100
H	0.62314900	-3.79542200	-1.98977600
H	2.13739600	-2.90919200	-2.35517100
C	1.38956200	2.52743900	1.03513600
H	0.33755400	2.55841400	1.31854900
H	1.99245700	2.65900100	1.93601900
H	1.60596100	3.33478100	0.32825400
Pd	-1.28518100	-0.10250900	-0.15291100
C	-4.65375100	-2.22304800	1.17418300
O	-2.39990100	-1.72465800	1.89860000
O	-3.14361700	-0.87740500	-0.04996900
C	-3.27698600	-1.58227300	1.04895800
H	-1.60225300	4.78091900	-0.93786100
H	-3.01603700	3.91784700	-1.56496500
H	-2.87421400	4.17740900	0.18406000
H	-5.43115700	-1.45242300	1.14806000
H	-4.83188800	-2.89619400	0.32894100
H	-4.71515200	-2.78065700	2.11074000

b₀-IN2'

C	1.11588100	-2.08919300	-0.35540400
O	-0.16004200	-2.03730600	-0.41016300
O	-1.63453400	1.85074600	0.00781400
C	-2.80015800	2.24919300	-0.22652600
O	-3.79495000	1.49339100	-0.56042500
C	-3.12090700	3.71760900	-0.11896100

C	1.82513400	-0.88665200	-0.16329500
C	3.20936200	-0.48703800	-0.03601600
C	1.01650600	0.27083000	-0.04452100
C	3.17285400	0.91790700	0.15779400
C	4.45252300	-1.13207100	-0.06072700
H	-3.51962500	0.46364400	-0.54052000
C	4.32569500	1.68304800	0.32234100
C	5.61150800	-0.37383100	0.10393500
H	4.52016100	-2.20646000	-0.20485600
C	5.55139100	1.01602200	0.29291400
H	4.27887900	2.75790900	0.46916300
H	6.57908900	-0.86777200	0.08600000
H	6.47009200	1.58171400	0.41877300
N	1.82836000	1.33760000	0.14750000
C	1.76045800	-3.43946600	-0.49910200
H	2.32679600	-3.68400600	0.40760000
H	0.99803400	-4.20268700	-0.66512700
H	2.46750000	-3.43735000	-1.33707000
C	1.42865400	2.72445400	0.32845900
H	0.34247200	2.77992100	0.29640800
H	1.78771200	3.09548200	1.29494200
H	1.85380600	3.34637500	-0.46759200
Pd	-0.92361000	-0.13648500	-0.16276900
C	-4.77280700	-2.12776100	0.37479000
O	-2.70957600	-1.85595300	1.59554700
O	-2.93151100	-0.81128100	-0.38710000
C	-3.36888800	-1.59078100	0.60537400
H	-3.59928000	4.05596000	-1.04317700
H	-3.83808300	3.86973600	0.69483500
H	-2.21840500	4.29818900	0.07324900
H	-5.48216600	-1.30100300	0.25133800
H	-4.79866200	-2.71576600	-0.54890500
H	-5.07910500	-2.74917900	1.21809500

b₀'-IN1

C	0.86586400	-0.83639100	-1.64955100
O	-0.38896800	-0.77389500	-1.74078200
O	-2.27966500	1.39116500	-1.20510400
C	-1.96307800	2.46285600	-0.53091300
O	-1.28682300	2.49073900	0.50284700
C	-2.53589800	3.73337500	-1.14591400
C	1.64650800	-0.25649100	-0.59386500
C	3.06607600	-0.40106900	-0.28896400
C	1.14742200	0.67913200	0.31824100

C	3.32472800	0.46514400	0.80612000
C	4.13179500	-1.16817400	-0.78712300
H	0.15708200	1.11957700	0.40206800
C	4.58125900	0.59404600	1.39826900
C	5.39120200	-1.04423800	-0.20481400
H	3.99158900	-1.85699300	-1.61236500
C	5.61804700	-0.17323500	0.87432800
H	4.74580400	1.26359800	2.23713100
H	6.21515400	-1.63672000	-0.59245700
H	6.61121300	-0.10042500	1.30772000
N	2.13121400	1.11067100	1.13414300
C	1.55227300	-1.57808000	-2.77492500
H	1.90636100	-2.55122700	-2.41130100
H	0.83592300	-1.74827900	-3.58043800
H	2.41850000	-1.02517700	-3.15074600
C	1.96414500	2.12618300	2.16468000
H	0.95266800	2.52905100	2.08884100
H	2.11467700	1.69291200	3.15929900
H	2.68724600	2.93421000	2.01428800
Pd	-1.88170100	-0.38379600	-0.34850400
C	-3.67435400	-2.52694700	2.44550900
O	-1.95228400	-2.17216900	0.77449900
O	-3.37350400	-0.54064000	1.09671400
C	-2.96470700	-1.71359000	1.40402500
H	-2.05815600	4.60907000	-0.70190800
H	-2.39972500	3.73370100	-2.23112800
H	-3.61332000	3.77349900	-0.94942400
H	-2.99573100	-3.27052600	2.86948300
H	-4.06915100	-1.87359400	3.22762100
H	-4.51811500	-3.04948700	1.97950400

b₀'-TS1

Imaginary Frequency: -426.3036

C	-0.97279600	-0.36708800	2.13521800
O	0.28335300	-0.52006600	2.20791500
O	2.60466800	1.38184200	0.75321900
C	2.17140000	2.49837400	0.38700500
O	0.96231900	2.74092500	0.02285300
C	3.12086600	3.69128600	0.35457400
C	-1.53096100	0.07350700	0.89240100
C	-2.82805200	-0.08263200	0.29307600
C	-0.65653000	0.63568000	-0.08460000
C	-2.68351300	0.36295500	-1.05284300
C	-4.07722300	-0.57120700	0.71787700

H	0.19082200	1.50319600	0.07170600
C	-3.74905800	0.35227400	-1.96064900
C	-5.13421300	-0.58298800	-0.18211700
H	-4.22175400	-0.92519800	1.73374600
C	-4.97236500	-0.12518900	-1.50679700
H	-3.62440300	0.69325300	-2.98345200
H	-6.10534500	-0.94967600	0.13730800
H	-5.81966200	-0.15084600	-2.18582700
N	-1.37550000	0.78376100	-1.23938700
C	-1.79612400	-0.69120700	3.34846100
H	-2.30599200	-1.65208800	3.19830800
H	-1.14672800	-0.77678000	4.22195300
H	-2.56294100	0.07091100	3.51961300
C	-0.85039400	1.41285400	-2.44599400
H	0.06161700	1.94736900	-2.17691700
H	-0.62701200	0.65680700	-3.20585200
H	-1.58164200	2.12368200	-2.84160600
Pd	1.14880100	-0.60797200	0.33433800
C	3.74010500	-2.50158600	-2.02591200
O	2.57435000	-2.34119800	0.09414600
O	2.00482400	-0.91889900	-1.47426200
C	2.72864200	-1.91821200	-1.08279100
H	2.71587500	4.50526600	0.96561000
H	4.10938000	3.40715700	0.72206700
H	3.20435900	4.06795900	-0.67141900
H	3.94256000	-3.54184200	-1.76093200
H	3.38669700	-2.42878800	-3.05779800
H	4.67301700	-1.93175400	-1.94276400

b₀'-IN2

C	-2.07844100	-2.00809100	0.76635600
O	-0.93396400	-2.57513600	0.67337000
O	4.71188800	1.52071200	0.85454000
C	3.79851900	2.32225000	0.90514200
O	2.59794400	2.12189800	0.33598500
C	3.86886300	3.65720700	1.61031300
C	-2.19976200	-0.68722800	0.29022600
C	-3.22982500	0.32003600	0.15362600
C	-1.00499300	-0.15560100	-0.24669700
C	-2.59203600	1.42344200	-0.47376700
C	-4.58848900	0.42082000	0.47771400
H	2.58798500	1.22973900	-0.09845100
C	-3.26518700	2.60550400	-0.77497000
C	-5.26956100	1.60012200	0.17711300

H	-5.10893100	-0.40283700	0.95788100
C	-4.61813700	2.67950900	-0.44062000
H	-2.76070800	3.44258400	-1.24779200
H	-6.32341800	1.68600100	0.42674900
H	-5.17265900	3.58715500	-0.66049900
N	-1.24238100	1.08987400	-0.70847400
C	-3.20265800	-2.79945600	1.37224100
H	-4.03424100	-2.88109500	0.66215600
H	-2.85643000	-3.79830300	1.64394600
H	-3.58470200	-2.29048400	2.26537200
C	-0.27929100	1.97209400	-1.35420000
H	0.59640400	1.38793500	-1.63401400
H	-0.72757800	2.40424200	-2.25398800
H	0.03018300	2.77442600	-0.67743300
Pd	0.53601900	-1.35867700	-0.14596000
C	4.44733100	-1.21304800	-1.04928500
O	2.50349500	-2.41297100	-0.23174900
O	2.20405400	-0.33256200	-0.87449100
C	2.99827500	-1.35812700	-0.69734900
H	3.11200400	3.70195100	2.40073500
H	4.86163900	3.79387700	2.03994100
H	3.65172800	4.46663800	0.90530300
H	4.97144900	-2.15484100	-0.87849400
H	4.54374900	-0.91507800	-2.09906000
H	4.87834100	-0.41399600	-0.43518400

b₀'-IN3

C	0.76248400	2.15345700	0.00005100
O	-0.51299600	2.25014900	-0.00001100
C	1.32827600	0.86085200	0.00005900
C	2.64433300	0.25825100	0.00007800
C	0.37751700	-0.18425500	-0.00002900
C	2.41322500	-1.14385200	0.00000100
C	3.96549400	0.72286300	0.00015400
C	3.44956500	-2.07473700	-0.00000500
C	5.00862100	-0.20316300	0.00014000
H	4.18109200	1.78750100	0.00022000
C	4.75634300	-1.58419000	0.00006200
H	3.25354400	-3.14274800	-0.00006200
H	6.03586100	0.15070400	0.00019300
H	5.58830000	-2.28248200	0.00005400
N	1.02244300	-1.37049900	-0.00006000
C	1.56185100	3.42631000	0.00011200
H	2.21053600	3.46632200	0.88343700

H	2.21072700	3.46629300	-0.88307200
H	0.89409800	4.28978000	0.00002900
C	0.40525100	-2.68937200	-0.00018900
H	0.71131900	-3.24797700	-0.89145800
H	0.71123500	-3.24811600	0.89102200
H	-0.67790300	-2.56829500	-0.00022700
Pd	-1.48612500	0.40349900	-0.00011100
C	-5.05240600	-1.41572100	0.00062200
H	-5.89728700	-0.72495100	-0.00513900
H	-5.10207600	-2.05691300	0.88710700
H	-5.09758500	-2.06708100	-0.87858600
C	-3.75599300	-0.65071100	-0.00014500
O	-2.64530000	-1.31431900	-0.00020200
O	-3.71727500	0.60868700	-0.00022200

b₀'-TS1

Imaginary Frequency: -91.1098

C	-0.73304200	-0.73681800	2.32595600
O	0.46036700	-0.51573000	2.53211100
O	2.91773200	-0.60129000	0.26627100
C	3.09025400	-1.70038400	-0.41467600
O	2.24113100	-2.26306000	-1.11272800
C	4.50135400	-2.25514300	-0.26535400
C	-1.24261700	-0.83368800	0.95003400
C	-2.52262600	-0.50783700	0.38701900
C	-0.43716900	-1.28325100	-0.10672300
C	-2.42218200	-0.76695800	-1.01204100
C	-3.73234700	0.00855500	0.89409400
H	0.50103400	-1.83356200	-0.09556900
C	-3.48704300	-0.54141100	-1.89468700
C	-4.78886000	0.22402100	0.02303600
H	-3.84351600	0.23011200	1.95055300
C	-4.66775000	-0.04806200	-1.35824200
H	-3.39297500	-0.74432600	-2.95695000
H	-5.72819500	0.61245900	0.40588600
H	-5.51518000	0.13595500	-2.01248600
N	-1.15640400	-1.24571300	-1.27639200
C	-1.69107700	-0.91295700	3.48779100
H	-2.22357300	0.03205200	3.65922300
H	-2.43994800	-1.68686300	3.29350800
H	-1.12118800	-1.14882900	4.38902000
C	-0.66437600	-1.69500000	-2.57247200
H	-1.25430100	-2.54566900	-2.93116800
H	-0.73315600	-0.88020400	-3.30102900

H	0.37947200	-1.98898900	-2.45544100
Pd	1.27755800	0.52908000	0.12714400
C	0.66872700	4.38406900	-0.62183100
C	0.92793600	2.92534400	-0.38629200
O	-0.02604700	2.13676800	-0.04586100
O	2.09718000	2.43448900	-0.48847100
H	4.56178300	-3.23889800	-0.73454700
H	5.21360700	-1.57490100	-0.74496400
H	4.77384700	-2.32173700	0.79210800
H	0.85964800	4.93629400	0.30594200
H	1.34481200	4.76619700	-1.39076400
H	-0.37300600	4.54092300	-0.91143400

b₀''-IN2

C	-0.83150100	-2.32994500	-0.54044900
O	-1.61700800	-2.89599100	0.19877600
O	-2.48511600	-0.07813800	-0.57791700
C	-3.21896200	-0.19239400	0.50858200
O	-2.84310900	0.08342500	1.64656500
C	-4.59928100	-0.76085300	0.22073700
C	0.16840900	-1.35586000	0.02838100
C	1.60352500	-1.28481600	-0.28173000
C	0.05417300	-0.88361200	1.37010500
C	2.23920000	-0.74879700	0.86345000
C	2.38680300	-1.61951700	-1.39395400
H	-0.83981000	-0.86482900	1.98127800
C	3.61241700	-0.51782200	0.92485800
C	3.76238500	-1.40707600	-1.33815700
H	1.93591200	-2.02502700	-2.29307000
C	4.36786800	-0.86053600	-0.19440100
H	4.07937200	-0.08962100	1.80611900
H	4.37706100	-1.66300900	-2.19615000
H	5.44202600	-0.70039900	-0.18157300
N	1.26709200	-0.52462600	1.84739500
C	-0.79587400	-2.60794600	-2.02929500
H	-0.63403900	-1.69394800	-2.60866000
H	0.02062000	-3.30632700	-2.25494000
H	-1.73821600	-3.07489700	-2.32214500
C	1.49616100	0.20421000	3.08545000
H	2.32281700	-0.25034900	3.63925100
H	1.73247800	1.25127600	2.86802800
H	0.59105400	0.15853600	3.69303700
Pd	-0.65961000	0.70594000	-0.30524200
C	1.02112900	4.29932400	-0.77752700

C	0.35512500	2.96544400	-0.58830500
O	1.03947200	1.94581800	-0.20968500
O	-0.88306800	2.81033900	-0.82051400
H	-5.26894000	-0.53974500	1.05440800
H	-5.00585900	-0.36333700	-0.71294100
H	-4.50643000	-1.84806400	0.11521300
H	1.22305700	4.45067500	-1.84441600
H	0.35518800	5.10013700	-0.44532300
H	1.96729400	4.33562800	-0.23299300

b₀''-TS2

Imaginary Frequency: -861.8391

C	-0.82914500	-1.57985200	1.80751400
O	0.34828800	-1.90913700	1.90504100
O	2.59176900	-1.25669000	-0.36769800
C	2.14730800	-2.32733500	-0.88798200
O	0.96076300	-2.50794400	-1.29304900
C	3.12316800	-3.47966900	-1.00458800
C	-1.30109500	-0.78991300	0.64805200
C	-2.60796900	-0.30224000	0.32556100
C	-0.43912300	-0.46668200	-0.43013500
C	-2.49507300	0.32749000	-0.95384100
C	-3.87564900	-0.31205700	0.95447000
H	0.25936900	-1.44651700	-0.88651200
C	-3.58966600	0.93143500	-1.59721300
C	-4.95071400	0.28530100	0.32101400
H	-4.01319900	-0.77441600	1.92471400
C	-4.80991500	0.90306200	-0.94494900
H	-3.48123400	1.41129400	-2.56471100
H	-5.92396000	0.28451000	0.80338400
H	-5.67578400	1.36649800	-1.40937400
N	-1.20108500	0.20693600	-1.38366200
H	3.00785800	-4.11329900	-0.11759000
H	2.89348500	-4.08075000	-1.88697000
H	4.14999600	-3.11198500	-1.03916700
C	-1.82407700	-1.99462900	2.87781300
H	-2.25694400	-1.11308800	3.36637400
H	-2.64980600	-2.57434500	2.44892500
H	-1.30339200	-2.59850300	3.62342200
C	-0.68936200	0.72790700	-2.63995100
H	-1.37972200	0.48894000	-3.45509700
H	-0.55296000	1.81371000	-2.58442200
H	0.27591300	0.26153800	-2.84293600
Pd	1.44520600	0.39538900	-0.01712400

C	2.14003600	4.13678700	1.14357200
H	3.13434000	4.48773100	0.85754500
H	2.06808900	4.15957700	2.23745600
H	1.36694300	4.79281300	0.73597400
C	1.93405900	2.72651900	0.66812700
O	0.74651300	2.30296000	0.41002200
O	2.90422200	1.91994800	0.53787700

b₀''-IN3

C	0.89191300	1.13120000	1.89116300
O	-0.27137400	1.53787600	1.96214100
O	-1.69844000	1.82014500	-0.94812800
C	-0.94467400	2.78896000	-1.08729400
O	0.35383000	2.77035200	-0.86817600
C	-1.46613500	4.12573000	-1.53308800
C	1.34615200	0.30540600	0.76830900
C	2.67425100	-0.18464600	0.42593300
C	0.44882700	-0.26156400	-0.16071800
C	2.50657300	-1.02265200	-0.70675000
C	3.97481600	-0.00617200	0.92814500
H	0.62802000	1.89448700	-0.49233200
C	3.56974200	-1.67224100	-1.33754600
C	5.04093800	-0.65387500	0.30866600
H	4.16117700	0.62612200	1.78902700
C	4.84459200	-1.47896400	-0.81193500
H	3.41176100	-2.30646300	-2.20474700
H	6.04533300	-0.51734000	0.70017000
H	5.69551800	-1.97092900	-1.27450800
N	1.15078100	-1.04655900	-1.03335000
H	-1.49187100	4.79712300	-0.66693400
H	-0.79651900	4.56642400	-2.27654900
H	-2.47405800	4.01758400	-1.93385900
C	1.88177000	1.49884800	2.98415300
H	2.38416300	0.61009500	3.38232000
H	2.65845300	2.16733100	2.59167400
H	1.34575300	2.01103500	3.78569500
C	0.59976900	-1.83721400	-2.12176200
H	1.00007700	-1.49968600	-3.08481300
H	0.84773500	-2.89518400	-1.98393000
H	-0.48459200	-1.72402900	-2.12022700
Pd	-1.52217100	-0.13586300	-0.14222100
C	-4.03463000	-2.99369000	1.07632100
H	-5.06702400	-2.84930100	0.75103500
H	-4.00633200	-2.99000800	2.17227900

H	-3.65514200	-3.96045900	0.73452200
C	-3.16925000	-1.87666300	0.55820500
O	-1.88952400	-2.05811600	0.50866400
O	-3.64773700	-0.76724900	0.19749500

Pd(TFA)₂-catalyst

Pd(TFA)₂

O	1.78018800	1.09343800	-0.03940700
C	2.42431400	0.00011900	-0.03269300
O	1.78019900	-1.09317500	-0.03944000
C	3.95835300	-0.00002200	0.02827400
Pd	-0.00002800	0.00015100	-0.03931800
C	-3.95832700	0.00002200	0.02835900
C	-2.42432000	0.00024100	-0.03318300
O	-1.78024100	-1.09308400	-0.04001300
O	-1.78014400	1.09353100	-0.03996600
F	4.44551800	-1.08742000	-0.57610500
F	4.34466500	-0.00685300	1.31454100
F	4.44550800	1.09355200	-0.56464800
F	-4.44569800	-1.08568100	-0.57893200
F	-4.34418300	-0.01048500	1.31473800
F	-4.44568000	1.09524400	-0.56129400

a₁-IN1

C	1.14862900	0.01099200	2.28724400
O	-0.10300300	-0.02653000	2.12951400
O	-2.81928600	-0.54796600	-0.93960700
C	-3.57260700	0.02393900	-0.09533100
O	-3.10980500	0.41762700	1.01617700
C	-5.04548700	0.28516000	-0.44321900
C	2.03404100	0.69479500	1.39412700
C	1.74189500	1.71374500	0.39960700
C	3.39006000	0.39367000	1.25214100
C	2.95102400	1.94925600	-0.29684100
C	0.61539700	2.48565900	0.07924100
H	3.98076300	-0.34752200	1.77246100
C	3.06342600	2.88924600	-1.32266100
C	0.71719800	3.42498000	-0.94317100
H	-0.31530100	2.36390300	0.62278800
C	1.92248600	3.61983600	-1.64191200
H	3.99841800	3.05015700	-1.85039600
H	-0.15147700	4.02154500	-1.20583300
H	1.96707400	4.35785400	-2.43728200
N	3.93368800	1.11745300	0.24927700

C	1.67197700	-0.73090600	3.49158700
H	0.97529600	-0.59113700	4.32291300
H	1.67772700	-1.79839400	3.24012900
H	2.67209000	-0.41233200	3.79271200
C	5.27494600	0.95266300	-0.28708300
H	5.23180100	0.47524000	-1.27126700
H	5.76796000	1.92533600	-0.37473600
H	5.85464100	0.32266000	0.38988200
Pd	-1.20898700	-0.32522200	0.40951700
C	2.13617300	-2.35889200	-1.33781800
O	0.29394900	-1.05428000	-0.70488900
F	1.65735800	-2.36518100	-2.58912000
F	3.13223000	-1.43032000	-1.28286900
F	2.68867300	-3.55296300	-1.09060100
F	-5.49865000	-0.62652200	-1.31034900
F	-5.80286300	0.25358000	0.65993300
F	-5.15804100	1.50422600	-1.00412100
O	1.06652600	-2.58248400	0.80038000
C	1.05471000	-2.00841000	-0.27633800

a₁-TS1

Imaginary Frequency: -57.4986

C	-1.62456900	-2.20828100	-1.14410000
O	-0.49448100	-1.70195300	-1.34414000
O	1.39167000	1.44991900	0.45649900
C	1.25938600	2.46832200	-0.32342100
O	0.61539400	2.48734200	-1.37403200
C	1.92661400	3.76003800	0.19804400
C	-2.69254600	-1.49374400	-0.49687300
C	-2.80106000	-0.06036700	-0.31148400
C	-3.76225000	-2.05545800	0.19756500
C	-3.92233400	0.15727000	0.52242300
C	-2.09555400	1.04954900	-0.80555100
H	-4.02353400	-3.09579900	0.33359100
C	-4.32226100	1.43338900	0.92625100
C	-2.47277300	2.32603100	-0.39018300
H	-1.33862700	0.95855100	-1.58897100
C	-3.56905000	2.51305600	0.47071900
H	-5.18415900	1.58439300	1.56902800
H	-1.90950500	3.17936900	-0.75165900
H	-3.84356800	3.51878000	0.77367000
N	-4.48571800	-1.08772300	0.81443200
C	-1.82857400	-3.61173700	-1.65981000
H	-2.07152000	-3.55727900	-2.72875600

H	-0.90065600	-4.17845100	-1.55437500
H	-2.64783100	-4.13292200	-1.15890500
C	-5.63938400	-1.29750600	1.67507500
H	-5.43380200	-0.92682700	2.68443900
H	-6.51411100	-0.77591800	1.27336700
H	-5.85687100	-2.36570300	1.72671300
Pd	0.38666100	-0.05036200	-0.41385900
C	3.46143900	-2.69558500	0.77629300
O	1.53642200	-1.37779000	0.57425200
F	3.68129300	-2.27291600	2.03429800
F	2.78040600	-3.86130100	0.84262300
F	4.64498400	-2.94080700	0.20385300
F	2.98605100	3.50927300	0.97751700
F	2.31964300	4.53375600	-0.82263200
F	1.02312600	4.45545300	0.92592500
O	3.07630400	-1.22133300	-1.09564600
C	2.65222100	-1.64799100	-0.04017800

a₁-IN2

C	-1.86976800	-2.39363100	-0.70782300
O	-0.66884700	-2.04490700	-0.74386000
O	1.21649200	1.37954000	0.47074200
C	1.32528700	2.31805300	-0.41381900
O	0.82186500	2.37969400	-1.52794500
C	2.14666000	3.51760700	0.12675300
C	-2.92261100	-1.47854400	-0.34322200
C	-2.83328900	-0.03638800	-0.29252300
C	-4.16218600	-1.81023200	0.19893600
C	-4.02189000	0.42184900	0.32307400
C	-1.88638300	0.90982100	-0.73416000
H	-4.60278100	-2.78399100	0.36236400
C	-4.26874300	1.77502400	0.56400700
C	-2.12274700	2.26538600	-0.48183600
H	-1.10319600	0.67343500	-1.48031700
C	-3.29343800	2.68835800	0.16803200
H	-5.18583600	2.10988100	1.03928000
H	-1.39370700	2.98818900	-0.82875300
H	-3.45181700	3.74741300	0.34503500
N	-4.81447500	-0.69218900	0.60640000
C	-2.17700900	-3.82191100	-1.08363500
H	-2.41755300	-3.86284200	-2.15371000
H	-1.29771300	-4.44341800	-0.90400400
H	-3.03499000	-4.22162600	-0.53590200
C	-6.11066400	-0.64764200	1.26616900

H	-6.01507200	-0.20869300	2.26442500
H	-6.81729900	-0.05279400	0.67866100
H	-6.49714000	-1.66375600	1.36120100
Pd	0.20197200	-0.23407400	-0.14217400
C	3.74160400	-2.44720000	0.52754100
O	1.67582300	-1.34955900	0.65096100
F	4.16446100	-1.89921600	1.68134100
F	3.22748500	-3.66451700	0.80970000
F	4.80458300	-2.62230700	-0.26626600
F	3.18990500	3.13181400	0.87517600
F	2.60401000	4.27589900	-0.87759200
F	1.34164100	4.28881100	0.89632100
O	2.82338100	-1.17561300	-1.30655300
C	2.67005000	-1.55666500	-0.16215500

a₁-TS2

Imaginary Frequency: -1271.5280

C	1.70138600	-2.40402000	0.58321600
O	0.58479300	-2.13572600	0.08194200
O	-1.24219900	1.49457700	-0.62626200
C	-0.99484700	2.22248000	0.37371000
O	-0.04857000	2.08312100	1.19581200
C	-1.88257900	3.47380100	0.54504100
C	2.80372200	-1.48338400	0.53392000
C	2.75172400	-0.13789400	0.01357100
C	4.15601700	-1.79693400	0.68085000
C	4.09172300	0.26450900	-0.19161500
C	1.67974600	0.72261600	-0.31606400
H	4.61985100	-2.71066700	1.02556100
C	4.42299400	1.47527800	-0.80165500
C	2.03319300	1.91132700	-0.98740300
H	0.77873700	1.18362300	0.58946000
C	3.36712300	2.28164300	-1.22233400
H	5.45461900	1.77759300	-0.95490000
H	1.24810900	2.60318800	-1.27797300
H	3.57969800	3.22381900	-1.71837000
N	4.92483200	-0.76446700	0.25627100
C	1.83330500	-3.76366200	1.22585500
H	1.46123600	-3.69722600	2.25611900
H	1.20466900	-4.47917000	0.69096900
H	2.86358400	-4.12559100	1.25837400
C	6.37915700	-0.73362400	0.22750300
H	6.73649600	-0.60331100	-0.79904800
H	6.75595000	0.08783700	0.84514800

H	6.76372700	-1.67669500	0.61963900
Pd	-0.19852700	-0.29872000	-0.47936000
C	-4.04979800	-2.10155100	-0.23317400
O	-2.68189600	-0.72520500	1.19339100
F	-4.97618900	-1.99340100	0.72964800
F	-4.60155500	-1.68136300	-1.38898000
F	-3.75072200	-3.41247200	-0.37278900
F	-3.08073500	3.31192100	-0.01848800
F	-2.04668700	3.77340800	1.83742500
F	-1.26246900	4.51256200	-0.05781300
O	-1.91934300	-1.33479500	-0.85744900
C	-2.77374900	-1.28769300	0.11211000

a₁-IN3

C	1.81807700	-2.49358600	-0.07949500
O	0.65149300	-2.05584100	-0.25499700
O	-0.84156500	1.79082800	-0.58130400
C	-1.68342200	2.25390500	0.24882500
O	-2.29877700	1.69185500	1.16833900
C	-1.93872200	3.76872700	0.03187300
C	2.93126400	-1.61404400	0.04697900
C	2.83501800	-0.17367800	-0.00776300
C	4.28078200	-1.91693300	0.23429600
C	4.14707900	0.32671600	0.14964500
C	1.75189400	0.69775100	-0.17827000
H	4.77213600	-2.87572200	0.32686800
C	4.42984700	1.69312000	0.14209800
C	2.02704800	2.06675700	-0.19148200
H	-2.70954900	0.22617900	1.20934100
C	3.34331900	2.54749000	-0.03216100
H	5.43784700	2.07762400	0.26377300
H	1.22191100	2.77915400	-0.32377700
H	3.51155000	3.62095100	-0.04681000
N	5.00459600	-0.77239300	0.29604000
C	1.96264400	-3.99484600	-0.00392000
H	1.40860800	-4.36422600	0.86636600
H	1.50642300	-4.44355700	-0.89219200
H	3.00117000	-4.32354300	0.07163100
C	6.44300000	-0.67903000	0.48265400
H	6.90462500	-0.16953700	-0.36949700
H	6.67274100	-0.12157900	1.39663200
H	6.86055800	-1.68426000	0.56474800
Pd	-0.04236000	-0.10433300	-0.39397900
C	-3.79321400	-2.65314300	0.05391000

O	-3.20688800	-0.68124000	1.20625300
F	-5.08925900	-2.30606400	0.00893400
F	-3.49784300	-3.34937900	-1.04665000
F	-3.60162200	-3.44411700	1.12576500
F	-2.47708200	3.98261700	-1.18338200
F	-2.76581600	4.27514100	0.95245400
F	-0.77454200	4.45300000	0.09569800
O	-2.02258100	-1.19604200	-0.66263800
C	-2.89954900	-1.39798700	0.16999300

a₁-TS1'

Imaginary Frequency: -52.3032

C	2.27403600	0.63061800	1.52591200
O	1.34552800	-0.15387800	1.85431800
O	-1.99863500	-0.94673500	-0.35863800
C	-2.98579300	-0.42911500	0.28872600
O	-2.89427100	0.20249600	1.34397600
C	-4.35991500	-0.58483600	-0.39845900
C	2.04923700	1.78904800	0.71016100
C	0.77510800	2.38925700	0.37480900
C	3.00367400	2.44871100	-0.05857600
C	1.03541400	3.36761700	-0.61294500
C	-0.54237900	2.21625800	0.83343300
H	4.06770000	2.26943600	-0.12907200
C	0.02392000	4.13816500	-1.18984500
C	-1.56282300	2.96417800	0.24364800
H	-0.77537000	1.60655600	1.70951300
C	-1.28144700	3.90925200	-0.75791800
H	0.23805700	4.88456600	-1.94874900
H	-2.58349400	2.81073400	0.57678900
H	-2.09410200	4.48131600	-1.19490700
N	2.41244600	3.37668100	-0.85205200
C	3.65280600	0.27224700	2.01463800
H	3.57521900	-0.21287900	2.99084600
H	4.06608400	-0.46032400	1.30972500
H	4.32089900	1.13397700	2.07776200
C	3.08074800	4.21446900	-1.83507700
H	2.70072100	3.99974900	-2.83904600
H	2.91750800	5.27315700	-1.60850500
H	4.15196100	4.00768200	-1.81023300
Pd	-0.36001100	-0.48516100	0.70804500
C	2.10542500	-3.60606700	-0.84816000
O	0.46009200	-2.23273500	0.09232600
F	2.41021800	-4.28227500	0.27899600

F	1.16879000	-4.30054300	-1.51370900
F	3.20792100	-3.55432000	-1.60934100
F	-4.40873000	-1.64757900	-1.21143200
F	-5.33301800	-0.70118300	0.51603200
F	-4.60820900	0.52154700	-1.13479900
O	2.32017300	-1.20837900	-0.74249700
C	1.61405000	-2.17318600	-0.48825000

a₁-IN2'

C	2.27883000	1.31673100	-1.26943400
O	1.07345500	1.29557900	-1.61556800
O	-1.83117800	-0.86202900	0.30793900
C	-2.33690200	-1.81824700	-0.40120400
O	-2.00205900	-2.18837200	-1.52043900
C	-3.44101800	-2.59040800	0.36539700
C	2.87507200	0.21707500	-0.55858500
C	2.29400000	-1.09470000	-0.37793000
C	4.02068300	0.24722600	0.23034200
C	3.11464800	-1.77722100	0.54959700
C	1.16745700	-1.75576300	-0.91308400
H	4.71753400	1.05762200	0.39489300
C	2.82955100	-3.07148400	0.98884500
C	0.86815800	-3.04610600	-0.45868300
H	0.64781000	-1.39888200	-1.81637100
C	1.68612900	-3.68947300	0.48282500
H	3.46759400	-3.58255300	1.70355700
H	-0.00674000	-3.54567900	-0.85887100
H	1.43188800	-4.69114600	0.81446800
N	4.16663100	-0.92622700	0.89696900
C	3.05465800	2.56450500	-1.59516900
H	2.74306700	2.93750500	-2.57441000
H	2.77762300	3.32269300	-0.85141300
H	4.13640800	2.41508500	-1.58135900
C	5.21002200	-1.24100100	1.86087700
H	4.77275400	-1.43299700	2.84592500
H	5.77326600	-2.12292800	1.53921800
H	5.89264200	-0.39296300	1.93577100
Pd	-0.36953000	0.12156400	-0.64573200
C	-1.47793900	3.98151600	0.72982900
O	-1.35534400	1.83377400	-0.20109000
F	-1.61114900	4.64738000	-0.43677200
F	-2.70690600	3.72823200	1.20917000
F	-0.85005600	4.78984700	1.59603800
F	-4.17646300	-1.79444300	1.15433000

F	-4.26316900	-3.21793800	-0.48608700
F	-2.85628700	-3.52953000	1.14673100
O	0.46508100	2.57317600	0.95362300
C	-0.66755900	2.67350400	0.50422100

a₁-TS2'

Imaginary Frequency: -1318.0044

C	1.31679000	-2.28346100	1.16702400
O	0.17324000	-1.87226500	0.86718200
O	-1.18333300	1.84720700	-0.32723100
C	-0.63992600	2.68394400	0.44024300
O	0.39662200	2.50730000	1.14256200
C	-1.24623600	4.10371700	0.45726100
C	2.51060600	-1.60557400	0.74693200
C	2.56161400	-0.37021700	0.00198800
C	3.79740200	-2.14333500	0.71191600
C	3.87847000	-0.26371500	-0.50297400
C	1.58913100	0.60968000	-0.30161000
H	4.16995500	-3.06701700	1.13312400
C	4.26374200	0.75226000	-1.37899200
C	1.98034500	1.59011100	-1.23634700
H	0.94090300	1.38576900	0.63297800
C	3.28195000	1.66474000	-1.75826700
H	5.27682200	0.82634300	-1.76264300
H	1.26895800	2.35831200	-1.52418700
H	3.53151700	2.45949600	-2.45468100
N	4.61463500	-1.35103900	-0.02421700
C	1.38059800	-3.58871100	1.92604000
H	0.52217900	-3.64954300	2.59906000
H	1.30216700	-4.42086800	1.21554400
H	2.30520800	-3.69833200	2.49816300
C	6.01707400	-1.60300700	-0.31772300
H	6.16698700	-1.70683400	-1.39720800
H	6.63842200	-0.78152700	0.05294700
H	6.32346700	-2.52825800	0.17327100
Pd	-0.41175300	-0.06764300	0.01773200
C	-4.00182000	-2.29393100	-0.43951000
O	-2.32311100	-0.77508600	0.19980600
F	-4.04631900	-2.97042100	0.73057100
F	-4.94097000	-1.32927200	-0.39158100
F	-4.33586400	-3.14751300	-1.41833200
F	-2.52337300	4.10126300	0.07202400
F	-1.16374500	4.64384000	1.67912200
F	-0.54026900	4.87298100	-0.39817900

O	-1.87353700	-2.13860400	-1.55632900
C	-2.58516500	-1.70166900	-0.66315700

a₁-IN3'

C	-2.18568900	-2.25412800	-0.34711400
O	-0.97613200	-1.91815200	-0.40918000
O	0.97500200	1.74757600	0.05071500
C	2.18693700	1.93273800	-0.14199000
O	3.10144800	1.07218900	-0.39457200
C	2.70924000	3.38387800	-0.05409300
C	-3.21658000	-1.29179300	-0.13634300
C	-2.97254200	0.12381900	0.00207200
C	-4.59810100	-1.46654700	-0.06477900
C	-4.23331300	0.74344100	0.14721800
C	-1.79389600	0.87742500	0.01420000
H	-5.18903800	-2.37013200	-0.12559700
C	-4.36796800	2.12441500	0.30059500
C	-1.92040700	2.26030300	0.16309200
H	2.70886800	0.06366500	-0.37192200
C	-3.18752100	2.86496500	0.30289000
H	-5.33546600	2.60422700	0.41209300
H	-1.03663700	2.88818700	0.17756400
H	-3.24150400	3.94418300	0.41880100
N	-5.20582100	-0.26442300	0.10342700
C	-2.47383100	-3.72379600	-0.53296700
H	-2.22905700	-4.01033600	-1.56221300
H	-1.81788500	-4.29740900	0.12886800
H	-3.51517300	-3.98385100	-0.33090100
C	-6.63636300	-0.03968600	0.22749500
H	-6.86749600	0.42012000	1.19402000
H	-6.98891500	0.61932400	-0.57274200
H	-7.15763300	-0.99606700	0.15551500
Pd	-0.07106600	-0.08881000	-0.12507700
C	3.67404700	-2.59077500	0.16429500
O	1.90953100	-1.06163200	-0.26672500
F	3.77167500	-3.13411200	-1.06705600
F	4.53430700	-1.54619500	0.21873800
F	4.07530100	-3.50300600	1.05582700
F	1.69483400	4.25477500	-0.00210300
F	3.45356900	3.52524700	1.05512300
F	3.46896200	3.67172000	-1.11985700
O	1.51109800	-2.75086900	1.19125500
C	2.22004300	-2.12333500	0.43343900

a₁'-IN1

C	0.28845100	-2.09293000	-1.59297400
O	-0.69597700	-1.32679400	-1.42515400
O	-2.70765600	0.33457900	-0.35231500
C	-3.11120100	-0.51527200	0.54018800
O	-2.45890600	-1.20945200	1.30206900
C	-4.66287100	-0.59124900	0.54814500
C	1.47236500	-2.09485500	-0.77929600
C	1.67132700	-1.64548000	0.59186000
C	2.72909000	-2.49362800	-1.24014900
C	3.05494000	-1.78056200	0.85795500
C	0.81598600	-1.23703900	1.62833400
H	3.01855500	-2.85628500	-2.21664200
C	3.62504500	-1.46978500	2.09429200
C	1.37928200	-0.92098800	2.86225600
H	-0.26103100	-1.19620400	1.49229400
C	2.76366900	-1.02397600	3.09215600
H	4.68982300	-1.57882700	2.27667600
H	0.72883900	-0.59805800	3.66979400
H	3.16565600	-0.76890000	4.06838200
N	3.67013800	-2.28881200	-0.28959400
C	0.13065200	-3.09525100	-2.71449600
H	-0.40698500	-2.63713700	-3.54811200
H	1.08107700	-3.51005700	-3.05690800
H	-0.47796800	-3.92863100	-2.34067000
C	5.09622100	-2.53096000	-0.42974800
H	5.65512300	-1.59823700	-0.30202200
H	5.43470900	-3.25476500	0.31891700
H	5.29548100	-2.93142500	-1.42538700
Pd	-0.74048800	0.57019300	-0.60752500
C	1.70199800	3.68018400	-0.15972000
O	1.21272000	1.40695300	-0.85455200
F	2.67258000	3.68336000	-1.08418800
F	1.03273200	4.83580800	-0.22833700
F	2.27290500	3.58590700	1.05548900
F	-5.20758900	0.62515300	0.73502500
F	-5.11380400	-1.07454400	-0.62759000
F	-5.09906200	-1.39846000	1.52352000
O	-0.45713000	2.58043200	-0.03018400
C	0.75903700	2.48688900	-0.37333600

a₁'-TS1

Imaginary Frequency: -91.6314

C	-2.01718000	0.46770900	-1.56251300
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O	-0.77940800	0.67260500	-1.54834800
O	0.78938400	2.21557200	0.53877200
C	-0.35262400	2.49415200	0.95618900
O	-1.20556200	1.74648000	1.50988600
C	-0.85978900	3.94192300	0.69835300
C	-2.60136900	-0.62535600	-0.82666900
C	-1.94226600	-1.32198400	0.23661200
C	-3.74986700	-1.36072100	-1.12139600
C	-2.69514800	-2.48198500	0.50897800
C	-0.80522000	-0.98517400	1.01004900
H	-4.50684900	-1.18744000	-1.87425200
C	-2.29117800	-3.39714600	1.48119800
C	-0.38678800	-1.94243300	1.96434500
H	-0.72374800	0.14043600	1.28032200
C	-1.11141400	-3.11911300	2.18592400
H	-2.86094800	-4.29730000	1.69269600
H	0.49452400	-1.73336100	2.56261400
H	-0.77284000	-3.82206100	2.94077300
N	-3.80541300	-2.47299200	-0.34177800
C	-2.85028100	1.41654800	-2.37744000
H	-2.33898400	1.65582100	-3.31344600
H	-3.85587000	1.03868900	-2.57596200
H	-2.92980000	2.34401900	-1.79624700
C	-4.83482300	-3.50089100	-0.38711900
H	-4.39452400	-4.47011400	-0.64227400
H	-5.33867300	-3.57840300	0.58158600
H	-5.57082800	-3.23492700	-1.14765600
Pd	0.69071700	-0.18117000	-0.37648700
C	4.62691600	-1.03489900	-0.19257300
O	2.76700600	-0.17135300	-1.49587900
F	5.41758100	-0.41062300	-1.07005800
F	5.01592800	-0.71368900	1.04967900
F	4.78005700	-2.36611300	-0.35118300
F	0.12416600	4.79492200	0.38149000
F	-1.73689500	3.93293700	-0.35239500
F	-1.52304100	4.44691700	1.75535300
O	2.33849200	-0.92473600	0.54146300
C	3.15169500	-0.66368400	-0.42067100

a₁'-IN2

C	3.49814000	-1.57913800	1.01664600
O	2.33832500	-2.05965200	0.91366700
O	-3.06798900	0.71214600	1.48296600
C	-3.09778300	1.52627900	0.59201800

H	0.94069600	-1.45988700	-2.89891600
H	-1.19945200	-1.75052100	-4.11213500
N	-3.32005300	-2.41556800	-0.02201000
C	-0.99911600	-1.76545700	3.68514900
H	-0.12756700	-1.64672700	4.33194600
H	-1.74101400	-1.00796600	3.96985600
H	-1.44483400	-2.75358600	3.83837200
C	-4.71270000	-2.67531000	-0.34751500
H	-5.13844300	-1.83341200	-0.90325800
H	-4.80427400	-3.58529300	-0.94982100
H	-5.27581600	-2.80745600	0.57807800
Pd	0.55025500	0.56159900	-0.01590300
C	-2.48673400	3.23554600	-0.01450700
C	-1.24141300	2.33303100	-0.01877900
O	-1.44210100	1.07571000	0.13120300
O	-0.10032100	2.80777300	-0.18084900
F	-2.15067600	4.52695300	0.02371600
F	-3.21340900	3.01259200	-1.12714000
F	-3.26065600	2.95836300	1.05078100
F	5.63062400	-1.03172500	-0.01862000
F	5.08191300	0.69062800	-1.22823000
F	5.04977100	0.82795500	0.94788800

a₁''-IN2

C	1.87568500	-3.08682300	-1.80878100
O	0.67989900	-3.27167400	-1.99760900
O	-2.37640200	-0.35920800	-0.39709600
C	-3.35709200	-0.16194400	0.43571100
O	-3.32002700	0.31621700	1.55628300
C	-4.69523800	-0.66410600	-0.17208200
C	2.34134000	-2.37676600	-0.60519000
C	1.50664200	-1.81329900	0.42253400
C	3.64483200	-2.10999600	-0.22317700
C	2.36317300	-1.23697600	1.38691800
C	0.10405800	-1.73806100	0.61352200
H	4.57421000	-2.35818300	-0.71699800
C	1.88836400	-0.60834200	2.55732700
C	-0.38036000	-1.09683500	1.79178700
H	-0.56132700	-2.28199700	-0.04658900
C	0.52485600	-0.54907400	2.75221000
H	2.57334800	-0.18455300	3.28533100
H	-1.43038900	-1.16422500	2.05331800
H	0.11865400	-0.08365600	3.64397700
N	3.66456800	-1.43040100	0.96792200

C	2.91536300	-3.57793700	-2.80369800
H	2.40740900	-4.09586000	-3.61905200
H	3.49065700	-2.73817900	-3.21252700
H	3.62515400	-4.26409100	-2.32543200
C	4.85318200	-0.95321900	1.65843800
H	4.84164100	0.13909300	1.73026500
H	4.91143000	-1.38021000	2.66483800
H	5.73606500	-1.26071100	1.09551500
Pd	-0.59916300	0.42129900	0.08992500
C	1.54736000	3.71335500	-0.74812500
C	0.68578800	2.46790700	-0.48578800
O	1.18307600	1.53430600	0.22678000
O	-0.48320500	2.39152100	-0.93805300
F	1.06602400	4.42855400	-1.76759100
F	1.56457600	4.48742000	0.35287600
F	2.81201300	3.35438200	-1.02874800
F	-5.71711300	-0.41884900	0.65588700
F	-4.94813200	-0.06044100	-1.34680500
F	-4.63867800	-1.99450700	-0.38747700

a₁''-TS2

Imaginary Frequency: -1190.9525

C	0.13694300	1.37776900	2.34152100
O	-0.65325200	0.46404500	2.12276100
O	-2.20981900	-1.23888000	-0.24585700
C	-3.01403200	-0.28215900	-0.14450400
O	-2.77030800	0.94905500	-0.27199000
C	-4.49478000	-0.65399700	0.10304700
C	0.71996000	2.16499300	1.24735900
C	0.51439000	1.99483100	-0.16904400
C	1.57424000	3.25069800	1.38723700
C	1.26687900	3.01585300	-0.81011100
C	-0.24482200	1.08770800	-0.96519700
H	1.97178500	3.69700200	2.28867200
C	1.30600200	3.16860400	-2.19585900
C	-0.19028000	1.26517400	-2.36843200
H	-1.52628900	1.02698600	-0.56818000
C	0.55674100	2.28357100	-2.97245500
H	1.89534800	3.95334900	-2.66177600
H	-0.76808700	0.59632200	-3.00085700
H	0.55915700	2.38496100	-4.05353400
N	1.90702200	3.76595300	0.17059400
C	0.53700700	1.72195300	3.76923300
H	1.61293300	1.56894300	3.91865300

H	0.31366900	2.76969100	4.00383900
H	-0.01436000	1.07523600	4.45386200
C	2.77466700	4.90567900	-0.07234300
H	3.64109300	4.60971700	-0.67335800
H	2.23190000	5.70043000	-0.59529800
H	3.12758900	5.29297200	0.88523200
Pd	-0.17519100	-0.92281500	-0.38977100
C	3.24472700	-2.98417000	0.07748400
C	1.89000100	-2.28237400	-0.11843000
O	1.91461300	-1.04574100	-0.43295700
O	0.81808900	-2.90656500	0.05718000
F	3.80085600	-2.57794200	1.23653900
F	4.08791600	-2.67282800	-0.92152800
F	3.10236100	-4.31276500	0.11894100
F	-4.61173400	-1.86853000	0.64541900
F	-5.14513600	-0.64651900	-1.07697800
F	-5.07821300	0.23771000	0.91404500

a₁''-IN3

C	-0.88735300	0.90725100	2.29618100
O	-0.53262100	-0.23778000	2.01264200
O	-0.71283200	-2.18581400	-0.42278400
C	-1.91733200	-2.14765400	-0.21947500
O	-2.68605700	-1.08854400	-0.17359300
C	-2.71898900	-3.44895300	-0.00906400
C	-1.25535900	1.87199000	1.25971200
C	-1.09762800	1.74377400	-0.18169600
C	-1.94846100	3.05196000	1.47033300
C	-1.74955600	2.87670400	-0.75352400
C	-0.45135700	0.83300500	-1.04968600
H	-2.27126800	3.49994100	2.40005600
C	-1.81916300	3.10563700	-2.12895700
C	-0.53380800	1.05486500	-2.42668500
H	-2.13513700	-0.27900900	-0.32159400
C	-1.21224500	2.16863000	-2.95788400
H	-2.31952700	3.97837600	-2.53715500
H	-0.03464500	0.37406200	-3.11012100
H	-1.24284600	2.30550200	-4.03519800
N	-2.25158100	3.65390200	0.28400000
C	-0.96110000	1.33955400	3.75261500
H	-0.24536300	2.14679700	3.94918900
H	-1.95958100	1.71056500	4.01242700
H	-0.72143200	0.48410700	4.38651500
C	-2.97682100	4.90078900	0.11561600

H	-2.35311500	5.64395700	-0.39288900
H	-3.88793600	4.74102300	-0.47111900
H	-3.25392300	5.28685400	1.09842000
Pd	0.75418900	-0.59537600	-0.41121800
C	4.72627600	-0.00049900	0.15094000
C	3.24038200	-0.35518900	-0.04778600
O	2.48550200	0.60119700	-0.43439400
O	2.82860400	-1.51179700	0.17405200
F	4.85696700	0.90610400	1.14001900
F	5.23715100	0.53478600	-0.97379000
F	5.44997400	-1.07937600	0.47115000
F	-1.90585400	-4.50179700	0.00651900
F	-3.60509200	-3.59307400	-1.00874400
F	-3.38787400	-3.39013900	1.15131800

2a cation

C	-1.88736900	-0.25353700	1.09190800
H	-2.35846400	-1.15324800	1.48609000
C	-2.92621500	0.81091800	0.76035700
C	2.86164900	1.48052400	-0.34841100
C	3.74364100	0.67809600	0.38435500
C	3.30830900	-0.58572800	0.80055200
C	2.02649600	-1.07524200	0.51774300
C	1.20617500	-0.19703000	-0.20425400
C	1.56149600	1.07355900	-0.67718900
H	3.18719100	2.46029600	-0.68695600
H	3.98406200	-1.22477800	1.36227000
I	-0.79958400	-0.91918500	-0.72161400
F	-2.35233700	1.94511300	0.32578500
F	-3.77641700	0.37729100	-0.18159300
F	-3.60619400	1.07470400	1.88050600
H	-1.10962200	0.12433300	1.75551400
C	0.67029100	1.98435600	-1.48604200
H	0.44071400	1.55708800	-2.46940900
H	-0.27864000	2.18657300	-0.98002600
H	1.16626900	2.94241600	-1.65468700
C	1.62953000	-2.45391500	0.98806500
H	0.76887000	-2.42767900	1.66709800
H	1.37463400	-3.11504700	0.15211500
H	2.45550000	-2.91754600	1.53132600
C	5.12488600	1.17080300	0.73292300
H	5.50878600	1.85808400	-0.02649700
H	5.10835100	1.71285000	1.68737800
H	5.83149900	0.34268500	0.83899500

				H	-7.94419900	0.92499800	-2.13140700
OAc⁻ anion				H	-6.99520100	0.41546900	-3.54950500
C	1.35426400	0.05381100	-0.00014900	H	-7.86112400	-0.79704200	-2.57519500
C	-0.22053700	-0.00178200	-0.00049100	Pd	-1.90316000	0.31702000	1.21311600
O	-0.80711500	1.10953000	0.00012100	C	0.97876700	-2.57338700	3.00154000
O	-0.69747900	-1.16559800	0.00010400	O	-0.55215100	-0.81240400	2.61842700
H	1.73373900	1.08364600	-0.01339600	O	1.56960900	-0.62869900	1.80112400
H	1.74926500	-0.46127300	0.88809600	F	2.24650600	-2.65525300	3.45548800
H	1.75138800	-0.48600000	-0.87266000	F	0.16428600	-2.98973500	3.97180700
				F	0.87563000	-3.46806300	1.96524000
CF₃COO⁻ anion				F	0.36691000	4.26192500	-0.37622400
C	-0.51293600	0.01361000	0.00009500	F	2.38336100	4.27942000	0.44527500
C	1.06610900	0.01019400	-0.00052300	F	2.06145800	3.75465200	-1.64129500
O	1.59101700	1.14071300	-0.00048800	C	0.49676200	-1.64202600	-0.88440600
O	1.53174300	-1.14794700	-0.00023100	H	0.21921500	-2.18895100	0.01202500
F	-1.08157100	1.24978800	-0.00150700	C	-0.33586700	-2.04628400	-2.08336500
F	-1.03254800	-0.63130100	-1.08777400	C	4.41009400	1.63773100	-1.87279700
F	-1.03044800	-0.62792500	1.09020500	C	5.15746300	1.87338400	-0.71520300
				C	5.23751000	0.86163900	0.24461300
a₁-IN4				C	4.54824000	-0.35302600	0.12299300
C	-3.86057400	-1.91242800	0.46017400	C	3.78314100	-0.48605200	-1.04221500
O	-2.78315500	-1.59415500	1.01840200	C	3.69221000	0.45259700	-2.07713700
O	0.90653700	1.38985600	-0.87759600	H	4.34431500	2.40937700	-2.63431900
C	1.39366600	2.13729000	-0.04486800	H	5.83283900	1.01923400	1.13981100
O	1.87451000	1.84360700	1.12896200	I	2.61656700	-2.32876900	-1.23897500
C	1.55213400	3.63541900	-0.39494800	F	0.02438300	-1.40011200	-3.20641800
C	-4.21977200	0.39690200	-0.54406200	F	-0.23171800	-3.37459200	-2.33136100
C	-5.79263500	-1.17931900	-1.02624800	F	-1.62212700	-1.77203200	-1.83268800
C	-5.17838500	0.94925500	-1.42336300	H	0.57995400	-0.55809500	-0.73749100
C	-3.13631600	1.15827100	-0.08059700	C	2.85434300	0.29932100	-3.31982400
H	-6.40792900	-2.06402600	-1.11772100	H	2.98536100	-0.67837500	-3.79472700
C	-5.09124900	2.26103300	-1.89283400	H	1.79329800	0.42892800	-3.08391700
C	-3.03645400	2.46577100	-0.56539700	H	3.12522300	1.06651200	-4.04933200
H	1.64230200	0.87747100	1.39057400	C	4.65903600	-1.38785300	1.21356900
C	-3.99432000	2.99964500	-1.45126100	H	3.69537100	-1.51956200	1.71586200
H	-5.82873500	2.68713000	-2.56664700	H	4.99099000	-2.35887600	0.82780500
H	-2.20139000	3.08080600	-0.25046700	H	5.38915900	-1.06496700	1.95998800
H	-3.87638400	4.02430000	-1.79559400	C	5.81282400	3.21295100	-0.48984300
N	-6.13145300	-0.04315400	-1.68977900	H	6.61099600	3.15397800	0.25594400
C	-4.29294000	-3.35636300	0.59337000	H	6.23229900	3.61909100	-1.41626800
H	-3.70293000	-3.97542500	-0.09406500	H	5.06482700	3.92843800	-0.12505100
H	-4.08337200	-3.69967500	1.61003400	C	-4.61787600	-0.97284500	-0.30491100
H	-5.35230600	-3.50596800	0.37074100	C	-1.30688400	2.69267800	2.61918500
C	-7.29782600	0.13751600	-2.53403800	C	-0.54512100	3.99678300	2.85185500

O	-2.14150700	2.27743300	3.41573600
O	-0.97130600	2.10953400	1.48944400
C	0.62531900	-1.16607600	2.44544500
H	-0.76893200	4.38315600	3.84821400
H	-0.83858900	4.73797300	2.09996300
H	0.53222700	3.83559700	2.74454500

a₁-IN5

C	-4.11295500	-2.07292900	-0.12197100
O	-2.94806800	-1.96312500	0.34809300
O	1.31893900	2.02987900	-0.47173400
C	1.75701700	2.46308500	0.57156100
O	1.97837600	1.83122000	1.70124200
C	2.07887400	3.96558600	0.72892600
C	-4.41137100	0.42108400	-0.47595400
C	-6.17155100	-0.89900000	-1.04858400
C	-5.43978100	1.22642200	-1.01366200
C	-3.21528400	1.00287600	-0.06117300
H	-6.86762300	-1.70282100	-1.24460800
C	-5.30317600	2.60739900	-1.15708000
C	-3.05238400	2.37530200	-0.21018900
H	1.67080400	0.87338200	1.65653000
C	-4.09053100	3.16127100	-0.75094200
H	-6.09328200	3.22642400	-1.57035100
H	-2.12317200	2.84957000	0.08341800
H	-3.93543900	4.23134600	-0.85454300
N	-6.50597300	0.37907000	-1.34555200
C	-4.61678900	-3.48445200	-0.28757300
H	-4.14520300	-3.92310800	-1.17534700
H	-4.31085800	-4.07935800	0.57684900
H	-5.70151900	-3.53521500	-0.40434100
C	-7.76668000	0.82283100	-1.92023200
H	-8.26891000	1.51889500	-1.24085600
H	-7.59041200	1.32232100	-2.87814400
H	-8.41064000	-0.04307900	-2.08326200
Pd	-1.89691900	-0.23044100	0.81867300
C	1.07218400	-2.90356200	2.85149000
O	-0.64760200	-1.66510300	1.85237500
O	1.42948600	-0.72744600	1.92702600
F	2.39003500	-2.88015600	3.10607500
F	0.42869700	-3.05417200	4.02783000
F	0.81559000	-3.99133900	2.09762900
F	1.07119400	4.57053900	1.40506600
F	3.21580600	4.17559000	1.41699100

F	2.19255800	4.56069300	-0.46248700
C	-0.69259100	-0.47911900	-0.84372400
H	-0.31940800	-1.48506400	-0.65883500
C	-1.28972700	-0.39576900	-2.22322800
C	4.49599900	1.59840100	-2.18428200
C	5.18387100	1.97028500	-1.02865900
C	5.28877500	1.03263900	0.00234600
C	4.73248300	-0.25114300	-0.08688100
C	4.05321900	-0.56959100	-1.27308200
C	3.91299400	0.33191000	-2.33708700
H	4.39835000	2.31195700	-2.99942000
H	5.82034200	1.29930900	0.91335800
I	3.18705100	-2.54899500	-1.47091400
F	-1.66606500	0.84315000	-2.58172000
F	-0.35050600	-0.80043300	-3.11600300
F	-2.36069300	-1.21023100	-2.39773300
H	0.06574300	0.29150500	-0.69188800
C	3.17351500	0.01075000	-3.61255500
H	3.59587800	-0.86720800	-4.11492700
H	2.11744100	-0.20751100	-3.41948500
H	3.22252200	0.85654000	-4.30500700
C	4.88223400	-1.20413200	1.07313600
H	3.91060600	-1.45043100	1.51436400
H	5.35016200	-2.14545100	0.76323800
H	5.50424100	-0.75605400	1.85409200
C	5.77659600	3.35316700	-0.88144800
H	6.76998100	3.31607000	-0.41969000
H	5.87248300	3.85211200	-1.85131100
H	5.14616200	3.98498300	-0.24440400
C	-4.88557900	-0.94172600	-0.50609700
C	-1.50729500	1.45663600	2.70734500
C	-0.95111000	2.45633700	3.68462300
O	-2.47206800	0.70599900	2.95077700
O	-0.90228400	1.37187300	1.55102700
C	0.58916100	-1.61109800	2.13404200
H	-1.76020600	2.86676600	4.29359900
H	-0.40813500	3.24889200	3.16604000
H	-0.24800000	1.93882000	4.34757300

a₁-IN6

C	-2.92490700	2.02790000	-0.05560500
O	-1.66701600	2.09107800	0.01588800
O	2.40582100	-1.83257000	1.67312300
C	3.18524400	-2.00254500	0.76034900

O	3.80399700	-1.10119900	0.03185800
C	3.51368200	-3.43045200	0.27154200
C	-2.97229100	-0.47761100	-0.45219000
C	-4.98527600	0.57767500	-0.40994300
C	-3.99990700	-1.43312300	-0.61166600
C	-1.64039800	-0.88381600	-0.43132300
H	-5.81050600	1.27414600	-0.35513400
C	-3.73168700	-2.79586700	-0.74373900
C	-1.35029700	-2.23875000	-0.54547600
H	3.44636000	-0.17938000	0.22685100
C	-2.39162700	-3.17666000	-0.70140300
H	-4.52091500	-3.53097700	-0.86619900
H	-0.32341100	-2.58464900	-0.51150200
H	-2.13689500	-4.22889700	-0.78919800
N	-5.22038700	-0.74370800	-0.58837300
C	-3.65520100	3.32296200	0.19615900
H	-3.66075400	3.51865600	1.27534200
H	-3.11335800	4.14105300	-0.28536900
H	-4.68656100	3.30321000	-0.16261400
C	-6.52586500	-1.36925900	-0.73355300
H	-6.59973000	-1.87173000	-1.70327000
H	-6.68356700	-2.10353000	0.06274800
H	-7.29987500	-0.60253000	-0.66950800
Pd	-0.27604000	0.58752700	-0.34622900
C	2.90732100	3.73647600	-0.19226700
O	1.09081500	2.26735000	-0.38161400
O	3.07533500	1.41452800	0.35307200
F	2.74796600	4.20118300	-1.44796600
F	2.26960300	4.58320500	0.64525200
F	4.21446400	3.77563400	0.09948400
F	4.76395000	-3.54605800	-0.19728600
F	3.33998700	-4.32280500	1.25168300
F	2.66051000	-3.75142600	-0.73688200
C	0.08799800	0.42674300	1.68144200
H	0.32539500	1.46445900	1.91067800
C	-0.99314500	-0.06634300	2.60661400
F	-0.57366100	0.12413100	3.88081600
F	-2.16213100	0.61200700	2.47803700
F	-1.27227100	-1.37345000	2.47166200
H	0.96180300	-0.22659400	1.71039200
C	-3.61108300	0.80968400	-0.31774500
C	1.05763200	-0.49718300	-2.23664200
C	2.08246800	-1.17112700	-3.10582600
O	0.17139600	0.26852100	-2.66499400

O	1.14126300	-0.72242400	-0.95104500
C	2.31935400	2.30267900	-0.05771500
H	2.99523800	-0.56416800	-3.10405200
H	1.70902800	-1.24752100	-4.12903700
H	2.33757000	-2.15421300	-2.70456400

a1-TS3

Imaginary Frequency: -298.3763

C	-2.83861700	2.12949300	0.10356700
O	-1.58510100	2.18484800	0.09151600
O	2.20136100	-1.98150400	1.65086300
C	3.16270100	-1.76613300	0.94528500
O	3.72598100	-0.61457200	0.65387300
C	3.89618800	-2.95142800	0.27678600
C	-2.93068900	-0.37382100	-0.37462600
C	-4.90141400	0.74806600	-0.46549000
C	-3.96047600	-1.26842900	-0.74297800
C	-1.60941300	-0.84154700	-0.24207100
H	-5.70301800	1.47361400	-0.45698900
C	-3.71847900	-2.61509400	-1.01331800
C	-1.36176900	-2.19224600	-0.52900400
H	3.16303800	0.15364600	0.96938400
C	-2.39809300	-3.05573800	-0.91163000
H	-4.51530600	-3.29677800	-1.29391500
H	-0.35028600	-2.57376100	-0.44419100
H	-2.16656100	-4.09504500	-1.12362500
N	-5.15597600	-0.54453900	-0.78515700
C	-3.56981100	3.38525600	0.50409300
H	-3.70522500	3.37959800	1.59309500
H	-2.96842900	4.25740100	0.23951500
H	-4.55656600	3.45992200	0.03935100
C	-6.45028800	-1.09712900	-1.15553800
H	-6.41912700	-1.48698500	-2.17799200
H	-6.72753000	-1.90503600	-0.47118900
H	-7.20374000	-0.30978700	-1.09809700
Pd	-0.23525900	0.66295800	-0.44654600
C	3.05346000	3.47688900	-0.05831500
O	1.14510100	2.25877300	-0.76621500
O	2.22607900	1.55167600	1.09522800
F	3.14898100	3.89155600	-1.33049100
F	2.63720600	4.52156700	0.69073900
F	4.28249700	3.13100000	0.36023000
F	4.78135000	-2.57091300	-0.65574400
F	4.54508800	-3.67424400	1.20639400

F	2.98810400	-3.75570500	-0.31559200
C	-0.52360200	-0.45117000	1.49253200
H	0.08403900	0.39869400	1.82010000
C	-1.63867400	-0.60676800	2.50035900
F	-1.07068900	-0.73067400	3.71981900
F	-2.44952300	0.47924300	2.55029600
F	-2.42290100	-1.68557200	2.32080300
H	0.11098700	-1.33042300	1.44620400
C	-3.54073000	0.92174400	-0.21630900
C	1.20893200	-0.63493600	-2.34722700
C	2.34816600	-1.46731800	-2.90200700
O	0.40687800	-0.01567400	-3.03835500
O	1.16545200	-0.64211700	-1.02386900
C	2.06021200	2.29651800	0.11178100
H	3.30481700	-1.06459200	-2.55392100
H	2.31217700	-1.45330500	-3.99270500
H	2.28181500	-2.49645200	-2.53557000

a₁-IN7

C	-1.67304100	2.77025800	0.52314100
O	-0.61934100	2.38298400	1.08705900
O	0.67774500	-2.20498800	1.72831500
C	1.39374800	-2.82309700	0.96898700
O	2.55876400	-2.47249900	0.48035200
C	0.97095400	-4.20152900	0.41076400
C	-2.03933800	0.45427500	-0.53534200
C	-2.57511900	2.29671400	-1.78216100
C	-2.31932100	0.07334400	-1.88827100
C	-1.92476100	-0.57157800	0.46242700
H	-2.69828600	3.29383400	-2.18261000
C	-2.33638200	-1.25213300	-2.31041500
C	-1.93269000	-1.89325500	0.00769600
H	2.75647800	-1.51181300	0.70768600
C	-2.10678100	-2.22606300	-1.34300900
H	-2.52425900	-1.51785200	-3.34503900
H	-1.79122600	-2.68809400	0.73019900
H	-2.08599700	-3.27230900	-1.63116800
N	-2.62034400	1.21659600	-2.60880600
C	-2.30707200	4.06543300	0.92725800
H	-3.11102900	3.83922000	1.63991200
H	-1.57501700	4.71763500	1.40743600
H	-2.76667200	4.56957300	0.07086800
C	-2.67992900	1.26889300	-4.06425500
H	-1.69325600	1.01829000	-4.46605400

H	-3.43124300	0.56605000	-4.43599600
H	-2.96057800	2.27768500	-4.37194800
Pd	0.29802700	0.84409900	-0.12010400
C	4.32296800	2.16491200	0.75119800
O	2.10307800	1.74791400	0.15746000
O	3.31661100	0.00615500	1.00820500
F	4.68605800	2.58987600	-0.47549500
F	3.97370100	3.24259000	1.47946900
F	5.38865100	1.59894600	1.32860500
F	0.67477700	-4.09615100	-0.90616400
F	1.93907100	-5.11831400	0.54703000
F	-0.12933400	-4.65020500	1.03797900
C	-1.91882600	-0.32197600	1.95835300
H	-1.27233300	0.50749200	2.25145600
C	-3.29903600	-0.01438900	2.50895800
F	-3.26307300	0.11305300	3.84938300
F	-3.78708300	1.15812500	2.01190800
F	-4.19978200	-0.97036200	2.21004100
H	-1.54391500	-1.21266100	2.46708400
C	-2.23110400	1.91198900	-0.49907700
C	1.01269100	-0.35756100	-2.56227500
C	1.75450700	-1.43077200	-3.34400900
O	0.40970600	0.57185900	-3.09568100
O	1.10891600	-0.55061700	-1.26453400
C	3.13637600	1.16386100	0.64073000
H	2.82104100	-1.17942300	-3.36858700
H	1.37807000	-1.46730400	-4.36878500
H	1.65360300	-2.40349600	-2.85640000

3aa

C	0.15877200	2.37726600	0.43221200
O	-0.91243500	2.37899200	1.03053800
C	0.64278400	-0.25542200	0.33725300
C	2.27997000	1.22400800	-0.21126500
C	1.84820000	-0.95228800	0.03502100
C	-0.50215000	-1.02735200	0.65694300
H	2.88894600	2.09115600	-0.42511100
C	1.97543900	-2.34279800	0.06906100
C	-0.36528300	-2.41662500	0.68961200
C	0.84492300	-3.07105800	0.41136500
H	2.91610100	-2.83303900	-0.16305700
H	-1.23991400	-3.01440500	0.93115300
H	0.89087100	-4.15536700	0.45420700
N	2.82508700	-0.02128600	-0.29374300

C	0.72824900	3.70610000	-0.06273700
H	0.92329600	3.68176800	-1.14089900
H	0.00308800	4.49130600	0.15770000
H	1.67152100	3.94759400	0.44248400
C	4.19245500	-0.33722900	-0.65974300
H	4.70048700	-0.86516400	0.15505900
H	4.21861300	-0.96520000	-1.55732300
H	4.72925600	0.59109400	-0.86516500
C	-1.87116700	-0.43504700	0.90274200
H	-1.79841100	0.55140900	1.36177700
C	-2.66626700	-0.26138200	-0.37776900
F	-3.87763000	0.28178100	-0.12318000
F	-2.03937400	0.54443700	-1.26305500
F	-2.88644700	-1.44265200	-1.00483300
H	-2.46117200	-1.09309500	1.54877200
C	0.95278200	1.16464500	0.18262100

IMes

C	-2.25735200	-1.19658200	-0.00950300
C	-2.97676300	0.00015300	-0.00868100
C	-2.25731200	1.19673900	-0.00947400
C	-0.85573200	1.23113900	-0.00418400
C	-0.18325700	0.00005300	-0.00049700
C	-0.85588400	-1.23108000	-0.00422500
H	-2.79584600	-2.14192700	-0.01577100
H	-2.79573300	2.14210900	-0.01568600
I	1.98268400	-0.00004200	0.00327500
C	-0.15041600	-2.56511300	-0.00660700
H	0.49477500	-2.67801000	-0.88553100
H	0.49107100	-2.68255600	0.87442800
H	-0.87680000	-3.38318800	-0.01016100
C	-0.15025100	2.56516300	-0.00662200
H	0.49203800	2.68226600	0.87386500
H	0.49414000	2.67841200	-0.88610300
H	-0.87662100	3.38325500	-0.00920700
C	-4.48766500	-0.00004500	0.01789400
H	-4.89744700	-0.88074400	-0.48806700
H	-4.86674200	-0.01152100	1.04864700
H	-4.89728500	0.89155400	-0.46859600

a₁'-IN4

C	-3.92437100	-2.07804700	0.82020900
O	-2.82085500	-1.66011100	1.25468500
O	1.13179100	0.94528500	-1.53927100

C	1.63771100	1.85979900	-0.90962800
O	1.99057100	1.88596400	0.34429800
C	2.00698700	3.16702700	-1.64802200
C	-4.29522100	-0.05694900	-0.67488500
C	-5.90862100	-1.66581000	-0.71864200
C	-5.28160200	0.29744600	-1.62193300
C	-3.18206300	0.76394800	-0.44565000
H	-6.53995800	-2.53242500	-0.57777300
C	-5.19474200	1.46026500	-2.38891300
C	-3.08174700	1.91910300	-1.22685900
H	1.67485900	1.05988800	0.84076200
C	-4.06975800	2.25475600	-2.17512800
H	-5.95347100	1.73525500	-3.11544500
H	-2.23194200	2.58003800	-1.10038800
H	-3.95102600	3.16796600	-2.75259500
N	-6.25898200	-0.70771900	-1.61303900
C	-4.36031000	-3.44252400	1.30430400
H	-3.71402100	-4.20649100	0.85535000
H	-4.22551500	-3.49582400	2.38867800
H	-5.39876500	-3.67449300	1.05766800
C	-7.45781700	-0.70058500	-2.43234200
H	-8.07237300	0.17618300	-2.20199300
H	-7.19310100	-0.67703200	-3.49483500
H	-8.03740300	-1.60359300	-2.23045600
Pd	-1.91722700	0.21517500	0.97567600
C	1.27621400	-1.01694500	3.97970500
O	-0.59525700	-0.45786500	2.62569500
O	1.49542000	-0.26451100	1.74935200
F	2.21872600	-0.16556300	4.42837700
F	0.38228900	-1.20502500	4.95468200
F	1.89225600	-2.21115900	3.74978700
F	2.28629700	4.17915100	-0.82600300
F	3.11157800	2.93711000	-2.41098600
F	1.01689500	3.53020500	-2.47079700
C	0.29806500	-1.85698900	-0.57587400
H	-0.08267700	-1.90886300	0.44016500
C	-0.55607000	-2.62607200	-1.56366100
C	4.66192700	0.20081800	-2.48335100
C	5.48255100	0.72949400	-1.48241800
C	5.42276000	0.16675700	-0.20605100
C	4.54058300	-0.87334400	0.12282400
C	3.72742800	-1.31503100	-0.92703500
C	3.75390000	-0.83685100	-2.24355900
H	4.69879600	0.62297100	-3.48388500

H	6.06655900	0.55218700	0.57977300
I	2.30009800	-2.90636700	-0.44757700
F	-0.04169400	-2.61672700	-2.80876700
F	-0.68638200	-3.92287200	-1.19257800
F	-1.77870300	-2.08544200	-1.61603700
H	0.55162900	-0.83565000	-0.88206000
C	2.86443300	-1.31345100	-3.36250500
H	2.80038000	-2.40492900	-3.41202500
H	1.85099000	-0.91618300	-3.24511400
H	3.24795800	-0.95545100	-4.32123900
C	4.52308400	-1.42583200	1.52498800
H	3.54597500	-1.26512700	1.98963100
H	4.74874700	-2.49894400	1.54470100
H	5.27659200	-0.92121800	2.13465100
C	6.37926000	1.90568500	-1.77739200
H	7.09506600	2.08212400	-0.96956500
H	6.93852900	1.76121200	-2.70852900
H	5.77241000	2.81145900	-1.89706500
C	-4.70081500	-1.32469400	-0.10856900
C	-1.34903900	2.94775700	1.55826300
C	-0.56862700	4.25987400	1.27450800
O	-2.21786200	2.93618600	2.41294000
O	-0.92987000	1.99568400	0.78587000
F	0.68344100	4.19620800	1.77287900
F	-0.46323700	4.48691800	-0.06008600
F	-1.17398300	5.32550400	1.81689000
C	0.65140200	-0.50618000	2.65237700

a₁'-TS3

Imaginary Frequency: -118.7182

C	-4.15786100	-1.94779000	0.74506000
O	-2.98912900	-1.69242000	1.13623900
O	1.31111300	1.03573000	-1.43099500
C	1.86972200	1.89472500	-0.77253200
O	2.17412100	1.87718100	0.49720500
C	2.36186700	3.18421900	-1.47023300
C	-4.30552700	0.11715800	-0.72798900
C	-6.12558400	-1.25097400	-0.71116700
C	-5.26772400	0.61175100	-1.63543000
C	-3.08406300	0.77616400	-0.54751900
H	-6.86462600	-2.02303900	-0.54672700
C	-5.04592100	1.75423900	-2.40589300
C	-2.84575400	1.90789000	-1.32923900
H	1.78489800	1.07068000	0.96154300

C	-3.81334500	2.38266500	-2.23886900
H	-5.78543500	2.13636100	-3.10298600
H	-1.90883700	2.44457500	-1.23118300
H	-3.59044500	3.27244300	-2.82154400
N	-6.37413200	-0.24813200	-1.58890800
C	-4.75944500	-3.23893100	1.24864400
H	-4.22583300	-4.08394900	0.79777000
H	-4.61279900	-3.30055900	2.33112500
H	-5.82348600	-3.33391500	1.02201100
C	-7.59207700	-0.06957700	-2.36094100
H	-8.07020000	0.88130800	-2.10353400
H	-7.36683100	-0.07473200	-3.43250400
H	-8.28169000	-0.88611000	-2.13859200
Pd	-1.87366000	0.06140200	0.85479100
C	1.09924700	-1.06652200	4.07741600
O	-0.66439500	-0.73495600	2.51623000
O	1.46524900	-0.24674900	1.88784800
F	1.79759800	-0.07563400	4.66161100
F	0.12535400	-1.44224200	4.91539100
F	1.93983200	-2.12423100	3.92741600
F	2.68553600	4.15734000	-0.61557800
F	3.46578400	2.89649200	-2.20734700
F	1.42136500	3.63812100	-2.30932300
C	-0.02518900	-1.61947900	-0.53329500
H	-0.24714700	-1.91419700	0.48290400
C	-0.81386800	-2.30192300	-1.63505100
C	4.82793700	0.10217000	-2.39256400
C	5.65864200	0.49686500	-1.33897400
C	5.50298600	-0.12773100	-0.10054100
C	4.52321700	-1.10353800	0.13662500
C	3.70850900	-1.42311400	-0.95741100
C	3.82647100	-0.86141500	-2.23811000
H	4.93701400	0.57553200	-3.36466800
H	6.14915900	0.15588800	0.72595800
I	2.15453600	-2.90943900	-0.64782100
F	-0.26495200	-2.09119600	-2.84620200
F	-0.85834600	-3.64219700	-1.43134100
F	-2.08315000	-1.87209600	-1.69286800
H	0.39136400	-0.63103600	-0.72811100
C	2.93982100	-1.20490100	-3.40773400
H	2.91629000	-2.28256100	-3.60398900
H	1.91260000	-0.87161300	-3.23162500
H	3.30026500	-0.70572300	-4.31088300
C	4.40842500	-1.72628100	1.50471800

H	3.44687400	-1.48347000	1.96686700
H	4.50446300	-2.81761000	1.46474700
H	5.20076300	-1.34791300	2.15594100
C	6.66791900	1.60025300	-1.53835200
H	7.36001700	1.67302200	-0.69439800
H	7.25436400	1.44867400	-2.45175400
H	6.15254600	2.56360000	-1.63743300
C	-4.85892900	-1.08572900	-0.14775100
C	-1.24218100	2.69469100	1.53594900
C	-0.42079300	4.00579000	1.42867600
O	-2.19485400	2.63599900	2.29590800
O	-0.76847200	1.77586500	0.75252200
F	0.71777700	3.91386800	2.14197700
F	-0.08245000	4.26945400	0.14224000
F	-1.11533600	5.05560600	1.88699500
C	0.57573800	-0.61863300	2.68436600

ai'-IN5

C	-4.16447000	-2.14862500	0.51917900
O	-3.00941100	-1.86144900	0.94439600
O	1.06828400	1.61194300	-1.54345800
C	1.66724600	2.31372000	-0.75697100
O	2.01654900	2.04932000	0.48198000
C	2.08538200	3.73925700	-1.18189700
C	-4.40208700	-0.01444000	-0.82003300
C	-6.17116300	-1.44012800	-0.88079800
C	-5.39164100	0.51223400	-1.67764800
C	-3.20500100	0.67158800	-0.62989500
H	-6.87899100	-2.24875700	-0.76179100
C	-5.21213200	1.71174700	-2.36769100
C	-2.99569700	1.85846700	-1.32505300
H	1.69020300	1.15067100	0.77329100
C	-3.99641900	2.36686500	-2.17983400
H	-5.97202400	2.11818200	-3.02761500
H	-2.06433900	2.40367100	-1.21610100
H	-3.80918400	3.29882400	-2.70503100
N	-6.46641400	-0.38872700	-1.67951200
C	-4.68237000	-3.49977300	0.93787500
H	-4.08587900	-4.26959100	0.43448600
H	-4.53206800	-3.62389400	2.01424300
H	-5.73646100	-3.64689400	0.69481200
C	-7.69897600	-0.20423000	-2.43174800
H	-8.20674300	0.70958300	-2.10767900
H	-7.48047600	-0.13302900	-3.50179500

H	-8.35574500	-1.05822900	-2.25805600
Pd	-1.92985300	-0.11593900	0.70996000
C	1.09471500	-1.60370100	3.61845000
O	-0.70847600	-0.95686500	2.26533200
O	1.37543500	-0.31618100	1.61220400
F	0.49586100	-1.14459800	4.73398300
F	0.84441200	-2.92490300	3.52483300
F	2.41970600	-1.44352300	3.76860100
F	2.89592000	4.34534500	-0.30090100
F	2.71728300	3.69475000	-2.36908700
F	0.98202500	4.49942400	-1.32862900
C	-0.71513200	-0.79390100	-0.82111600
H	0.22162500	-0.88905100	-0.27331100
C	-1.12240300	-2.08752600	-1.47450800
C	4.56336300	0.88438400	-2.26713700
C	5.32245000	1.41444200	-1.22164800
C	5.46997900	0.64711700	-0.06413700
C	4.88577500	-0.61870400	0.08011500
C	4.14450000	-1.10708400	-1.00635800
C	3.95818000	-0.37894500	-2.18984500
H	4.42434700	1.46763300	-3.17421900
H	6.05124700	1.04232600	0.76611500
I	3.25169700	-3.07741600	-0.85003900
F	-0.26129000	-2.32915900	-2.49039500
F	-1.07987900	-3.14260500	-0.64416400
F	-2.36549200	-2.04774900	-2.01305000
H	-0.68481200	0.03160300	-1.52585200
C	3.14655100	-0.88116700	-3.35853100
H	3.56118800	-1.81026300	-3.76731700
H	2.11211500	-1.09393600	-3.06716900
H	3.12622900	-0.13457700	-4.15779500
C	5.06064300	-1.36967400	1.37623100
H	4.10182300	-1.48280400	1.89346300
H	5.46746600	-2.37384000	1.21362800
H	5.74077600	-0.82877600	2.04121500
C	5.93421400	2.79280000	-1.32240500
H	6.87492600	2.85409700	-0.76453300
H	6.13757200	3.06544000	-2.36341800
H	5.25857700	3.55235700	-0.91118700
C	-4.90334700	-1.26973300	-0.31738100
C	-1.52340900	2.22984300	1.75562700
C	-0.88658600	3.57491300	2.16519000
O	-2.50118900	1.76715200	2.34158600
O	-0.91641200	1.64029200	0.77345000

F	0.16254400	3.34911900	2.97159300
F	-0.45729000	4.24886800	1.08351300
F	-1.77318400	4.33571000	2.81681100
C	0.55667500	-0.86361500	2.36200400

a₁'-IN6

C	-3.36155700	1.54486100	-0.54729100
O	-2.12807000	1.79871300	-0.44222300
O	2.10225800	-1.15609900	2.41730500
C	3.01801200	-1.34641300	1.64684600
O	3.64517300	-0.46563600	0.89544600
C	3.56394000	-2.77838000	1.45546600
C	-3.05572200	-0.95751700	-0.31717600
C	-5.18920600	-0.22820100	-0.60248000
C	-3.93214300	-2.06349400	-0.27753500
C	-1.68574700	-1.14622100	-0.15421000
H	-6.10148200	0.33363500	-0.74790000
C	-3.47408800	-3.36425100	-0.06476200
C	-1.20791400	-2.43240100	0.07988600
H	3.17069700	0.41415300	0.93089000
C	-2.10167200	-3.52352600	0.11888600
H	-4.14629900	-4.21589400	-0.03386400
H	-0.14892600	-2.61091000	0.23472700
H	-1.70214900	-4.51748800	0.29722600
N	-5.23263100	-1.57359700	-0.46483000
C	-4.25483200	2.75153600	-0.67036400
H	-4.26556700	3.27304600	0.29398400
H	-3.83071200	3.43865100	-1.40802600
H	-5.27868500	2.49690000	-0.95113200
C	-6.43041100	-2.40020200	-0.50215200
H	-6.36742300	-3.12023600	-1.32401300
H	-6.54408000	-2.94224900	0.44180800
H	-7.30193600	-1.76119300	-0.65356500
Pd	-0.53287200	0.49168600	-0.32659300
C	2.29648600	3.93154400	-0.55032100
O	0.63916600	2.26928100	-0.65092900
O	2.39199100	1.92289300	0.75779600
F	2.34307000	4.00911800	-1.89387000
F	1.49084600	4.91926100	-0.10504100
F	3.52944300	4.15782400	-0.07805200
F	4.55756800	-2.86009900	0.56438900
F	4.00687200	-3.25823500	2.63122100
F	2.55521900	-3.57496000	1.03829800
C	-0.32654900	0.54799100	1.73137000

H	0.67290700	0.97787900	1.78793000
C	-1.34847200	1.37722800	2.46174200
F	-1.06917100	1.31677800	3.78293400
F	-1.34113200	2.67116200	2.10260900
F	-2.61582400	0.91781800	2.30459100
H	-0.34370600	-0.48888700	2.05368500
C	-3.86705600	0.21742100	-0.51975400
C	1.14241400	-0.78085600	-1.82700800
C	2.38049700	-1.51701000	-2.38016900
O	0.28547100	-0.30075800	-2.57006400
O	1.10576200	-0.69405000	-0.53393800
F	3.44637600	-0.70364200	-2.33630000
F	2.64546900	-2.61307000	-1.64812000
F	2.17623000	-1.89085200	-3.64782300
C	1.74554800	2.55214400	-0.09186400

a₁'-TS4

Imaginary Frequency: -271.9514

C	-3.25758900	1.99957300	0.09639900
O	-2.00992400	2.14924000	0.07297100
O	2.19882900	-1.25442700	2.01921800
C	3.26266800	-0.95928600	1.51992500
O	3.68665200	0.23433900	1.15772600
C	4.33358900	-2.04796200	1.28323600
C	-3.15981800	-0.51639300	-0.29246500
C	-5.21226100	0.44705600	-0.40462500
C	-4.11929700	-1.49811900	-0.62757600
C	-1.80850000	-0.87994700	-0.15530500
H	-6.06695700	1.10919400	-0.41374700
C	-3.77559200	-2.82942500	-0.86067600
C	-1.45578500	-2.21302400	-0.40416200
H	2.95677700	0.91003700	1.25120300
C	-2.42513300	-3.16370300	-0.75765100
H	-4.51863100	-3.57837700	-1.11592300
H	-0.41833700	-2.51833000	-0.32540100
H	-2.11326900	-4.18629500	-0.94557300
N	-5.36736300	-0.86930800	-0.68258600
C	-4.07395800	3.21577000	0.44892200
H	-4.17115000	3.26614500	1.54085000
H	-3.55308100	4.11484200	0.11282800
H	-5.07807500	3.18527800	0.01833900
C	-6.61758100	-1.53169400	-1.02651200
H	-6.56048700	-1.94935900	-2.03661100
H	-6.82732700	-2.33652300	-0.31529300

H	-7.42915900	-0.80331000	-0.98774600
Pd	-0.54852900	0.72515000	-0.36662500
C	2.44055300	3.83173100	-0.42526300
O	0.63754400	2.37967200	-0.92890600
O	1.71537200	2.06887300	1.03478000
F	2.66119200	3.91430000	-1.74560100
F	1.84579300	4.97738500	-0.02714200
F	3.62695200	3.74197200	0.19406200
F	5.31563900	-1.65452400	0.46405800
F	4.88391500	-2.39121000	2.46641200
F	3.75469500	-3.14142700	0.76114900
C	-0.72968800	-0.35253600	1.58736000
H	-0.16505100	0.53737900	1.88425200
C	-1.84018800	-0.54043200	2.59537900
F	-1.26880600	-0.58682300	3.81711100
F	-2.71333200	0.49625700	2.60242000
F	-2.55567700	-1.66985800	2.44998800
H	-0.05122400	-1.19784900	1.54849700
C	-3.86684800	0.73284900	-0.16995700
C	1.09225300	-0.78806600	-2.04786300
C	2.26369400	-1.78229200	-2.26148100
O	0.38516300	-0.43107700	-2.96946300
O	0.98748200	-0.49671900	-0.78024500
F	3.39284300	-1.35549500	-1.66797200
F	1.93377500	-2.97772000	-1.71727400
F	2.51182000	-1.96928200	-3.55990600
C	1.53142200	2.62990300	-0.05721700

a₁'-IN7

C	-2.25103500	2.63271800	-0.02703700
O	-1.27281000	2.49076200	0.75193600
O	0.47383000	-1.39945100	2.38333100
C	1.36307400	-2.11726600	1.97264700
O	2.56129800	-1.77296200	1.56995600
C	1.15649300	-3.64190700	1.82237600
C	-2.09453800	0.17483300	-0.74103300
C	-2.65620500	1.71178600	-2.34032100
C	-2.05778200	-0.42843600	-2.04159800
C	-2.02663400	-0.67147400	0.41800800
H	-2.85030700	2.60893500	-2.91246800
C	-1.78810800	-1.77831800	-2.23722000
C	-1.74270200	-2.02204200	0.19010300
H	2.64078200	-0.77114600	1.54256700
C	-1.59504600	-2.55553000	-1.09706300

H	-1.72733300	-2.21128900	-3.22965400
H	-1.63240800	-2.67663900	1.04645200
H	-1.34858900	-3.60673400	-1.20347400
N	-2.38752400	0.53915600	-2.97682600
C	-3.10563400	3.85780500	0.06593300
H	-3.98651700	3.60858200	0.67209200
H	-2.55887100	4.67231700	0.54482700
H	-3.46834800	4.16636100	-0.91994300
C	-2.21735800	0.37476300	-4.41573900
H	-1.15533700	0.22743000	-4.63446300
H	-2.79762200	-0.48321700	-4.76745700
H	-2.57654800	1.27321000	-4.92026500
Pd	0.03035600	0.96986200	-0.00920400
C	3.61412100	3.11570200	1.08395800
O	1.59561000	2.21193300	0.33552500
O	2.98826700	0.84467800	1.52850500
F	3.98711900	3.50998300	-0.14837300
F	3.00204100	4.15274800	1.68786800
F	4.71527300	2.81660100	1.78005500
F	1.04269100	-3.95960800	0.51515300
F	2.17322200	-4.34295900	2.34050300
F	0.02135600	-4.02449500	2.43565100
C	-2.36667900	-0.22912400	1.82830000
H	-1.91539200	0.72743400	2.09886500
C	-3.86060000	-0.08781400	2.05581800
F	-4.12253700	0.20596600	3.34335900
F	-4.38912800	0.91975100	1.30335800
F	-4.53908100	-1.20777100	1.74103700
H	-1.98523600	-0.96851600	2.53509800
C	-2.50053900	1.56917200	-0.97322300
C	1.30017000	-0.43130300	-2.09670800
C	2.16185600	-1.62789400	-2.58189700
O	0.77991600	0.32536100	-2.90322500
O	1.20592300	-0.43667000	-0.80361100
F	3.33665200	-1.69002900	-1.94007800
F	1.49480400	-2.78303700	-2.35621300
F	2.40075700	-1.54224800	-3.89778600
C	2.65268600	1.89470000	0.99283000

a₁''-IN4

C	3.87535300	-2.13683600	-0.85748600
O	2.66037900	-1.87573300	-0.62374500
O	0.75149900	1.40620700	1.02184300
C	0.05772500	1.30360900	2.08170500

O	-0.23876000	0.31087800	2.76090300
C	-0.51148900	2.67725900	2.52105800
C	4.90151100	-1.20161000	-0.55954200
C	4.66568800	0.09962100	0.01870800
C	6.28370200	-1.30409600	-0.75115300
C	5.92584800	0.72525200	0.14618600
C	3.50584000	0.76229600	0.42752800
H	6.86883500	-2.11675600	-1.15923000
C	6.06971700	2.00932600	0.67221700
C	3.63233800	2.04781300	0.95320400
H	-0.21182900	-1.17138500	2.32838800
C	4.90062000	2.65435000	1.06991700
H	7.03790700	2.48959000	0.77097800
H	2.75605000	2.59421300	1.28123200
H	4.96368800	3.65590000	1.48552200
N	6.89142200	-0.17002600	-0.33661500
C	4.15782400	-3.48170800	-1.47786100
H	3.67880400	-4.26270000	-0.87876300
H	3.70898400	-3.51757400	-2.47714300
H	5.22429300	-3.69823100	-1.56213800
C	8.32331100	0.09758200	-0.37349600
H	8.52675400	0.97582600	-0.99370500
H	8.69948300	0.27732600	0.63822600
H	8.83822300	-0.76588100	-0.79757200
Pd	1.79934700	-0.20264800	0.21805500
C	-0.91240400	-3.69049200	0.32909400
O	-0.43283200	-2.14444000	2.05954900
F	0.15963200	-4.49361400	0.32720000
F	-1.83638900	-4.20918900	1.15276200
F	-1.42405100	-3.65234500	-0.91063100
F	-1.32216700	3.15535600	1.52090400
F	-1.24921800	2.60046900	3.62600100
F	0.46520900	3.57352300	2.70487800
O	-0.19824800	-1.43057000	-0.07821100
C	-1.26822300	1.46029900	-1.32917600
H	-0.96626400	2.26061800	-0.65823900
C	-0.59937200	1.55172800	-2.68927600
C	-4.28295200	-2.31964100	0.08130500
C	-4.66486200	-2.09423800	1.41027900
C	-4.73425200	-0.77646100	1.87030400
C	-4.41952000	0.32605800	1.06139700
C	-4.02622100	0.00698000	-0.24325100
C	-3.95686100	-1.27935000	-0.79753700
H	-4.22946500	-3.33752700	-0.29354100

H	-5.03795200	-0.58377400	2.89532200
I	-3.47072900	1.67656000	-1.54841300
F	-0.92844600	0.51370700	-3.47739700
F	-0.94610100	2.68495800	-3.32826500
F	0.72660700	1.54683500	-2.50654000
H	-1.13787900	0.47754500	-0.87548900
C	-3.56430400	-1.59052400	-2.22141900
H	-4.25715200	-1.13426200	-2.93775300
H	-2.55585900	-1.23842300	-2.46240500
H	-3.57831100	-2.66925600	-2.38635000
C	-4.52018900	1.72234300	1.62629200
H	-3.55422300	2.23703800	1.62573900
H	-5.23042500	2.33955400	1.06414700
H	-4.86914200	1.68287600	2.66039000
C	-4.97677500	-3.25568600	2.31932500
H	-5.71333600	-3.92740100	1.86462700
H	-4.07073200	-3.84419300	2.50470700
H	-5.36781200	-2.92097300	3.28350000
C	-0.48303400	-2.27318100	0.77306300

a₁''-TS3

Imaginary Frequency: -176.2527

C	-3.25796300	-2.35350200	-0.34989200
O	-2.06071600	-1.98710000	-0.54847500
O	-0.32024000	1.73439200	-0.85890600
C	0.04348900	2.09620200	-2.03381800
O	0.08582900	1.43094700	-3.07236600
C	0.46720400	3.58748100	-2.07960100
C	-4.29492400	-1.40783700	-0.15141900
C	-4.09636800	0.02013800	-0.12908400
C	-5.66386300	-1.61856200	0.06241900
C	-5.36156200	0.60627600	0.09904900
C	-2.97127800	0.83278400	-0.27947700
H	-6.22107300	-2.54375500	0.11514200
C	-5.53775700	1.98678000	0.18692200
C	-3.12472500	2.21552000	-0.19072900
H	0.52107900	-0.07615300	-3.24561700
C	-4.39869600	2.77551700	0.03743400
H	-6.51012500	2.43538600	0.36242600
H	-2.27553300	2.87624100	-0.31390000
H	-4.48972200	3.85600000	0.09410900
N	-6.29477100	-0.43539300	0.20895900
C	-3.49548900	-3.84048000	-0.33454200
H	-3.09452700	-4.27967800	-1.25371700

H	-2.94417900	-4.28165200	0.50358600
H	-4.55052300	-4.10338000	-0.24210300
C	-7.72395200	-0.24705700	0.43592800
H	-7.88728100	0.27935000	1.38080200
H	-8.16033900	0.33352700	-0.38209100
H	-8.20992300	-1.22264800	0.48133000
Pd	-1.26140400	-0.09281200	-0.66437700
C	2.02061000	-2.85764200	-2.37089900
O	1.00690200	-0.96718600	-3.36246000
F	1.38367200	-3.75535800	-3.13261800
F	3.19714400	-2.55915700	-2.94238600
F	2.25146300	-3.39547800	-1.16773200
F	1.55391000	3.77353800	-1.29893700
F	0.76149400	3.97849300	-3.31565700
F	-0.52465700	4.36417600	-1.60245500
O	0.66270300	-1.29072200	-1.14550100
C	-0.03124800	0.06248400	1.58209600
H	-0.24177300	1.11520800	1.46504500
C	-0.83204800	-0.74460800	2.58964300
C	4.59652300	-1.30048400	-0.10248900
C	5.09664100	-0.23592600	-0.86242300
C	4.76826600	1.06641300	-0.47643900
C	3.95208000	1.34220700	0.63009400
C	3.47722400	0.22792900	1.33700100
C	3.78218600	-1.10670200	1.01924600
H	4.84510300	-2.31960700	-0.38552600
H	5.15507200	1.90519100	-1.04889300
I	2.16455100	0.58396800	3.02301100
F	-0.31729900	-1.97799500	2.72492600
F	-0.83151000	-0.14601800	3.79728500
F	-2.12073800	-0.87345700	2.22385100
H	0.63117200	-0.45576600	0.90513700
C	3.29945300	-2.30282200	1.80448700
H	3.68486800	-2.28769500	2.83058000
H	2.20700100	-2.34921200	1.86977600
H	3.64006100	-3.22671700	1.33224500
C	3.63950900	2.77547400	0.98502800
H	2.57044800	2.99326700	0.89119400
H	3.94083500	3.01502000	2.01062100
H	4.17027600	3.45498400	0.31419800
C	5.96905800	-0.50054100	-2.06444700
H	6.89986100	-1.00116900	-1.77210500
H	5.45798200	-1.15794300	-2.77666700
H	6.23339600	0.42505500	-2.58286600

C	1.14721300	-1.58878000	-2.23549500
a₁^{''}-IN5			
C	-3.47649300	1.66043500	-1.28634500
O	-2.25129500	1.66037200	-0.94015900
O	-0.13628400	-0.64492100	1.68308500
C	0.03079000	0.08363500	2.73150900
O	-0.31476600	1.26444700	2.85108700
C	0.65575300	-0.68997900	3.91948500
C	-4.39192900	0.72816000	-0.74777800
C	-4.03185200	-0.31104800	0.18072600
C	-5.77202400	0.59591700	-0.96836500
C	-5.21558100	-1.02179800	0.48469500
C	-2.83557000	-0.70352100	0.77517800
H	-6.42779200	1.18093900	-1.59853800
C	-5.22789700	-2.10629600	1.35956000
C	-2.81228500	-1.78945600	1.64573200
H	0.42178100	2.55480300	2.05767900
C	-4.01079600	-2.47262200	1.93365600
H	-6.13762200	-2.65085000	1.59006400
H	-1.89326800	-2.10916800	2.12104800
H	-3.97753700	-3.31013700	2.62326600
N	-6.25862800	-0.42855800	-0.24365100
C	-3.85756300	2.70090200	-2.30132200
H	-3.46186600	3.67379900	-1.99476500
H	-3.38447400	2.44254400	-3.25635100
H	-4.93640400	2.77574800	-2.44679600
C	-7.65276300	-0.86631400	-0.20163600
H	-7.72759600	-1.90380300	-0.53905600
H	-8.03848100	-0.78495300	0.81842300
H	-8.24508700	-0.23106500	-0.86121700
Pd	-1.24279700	0.41282700	0.33086700
C	1.65020400	3.88866700	-0.65168800
O	0.89882100	3.22955300	1.49337000
F	0.80924600	4.91865400	-0.83531100
F	2.77140000	4.34104000	-0.07855000
F	1.94636400	3.35385300	-1.83648600
F	1.78781700	-1.30134500	3.54452500
F	0.91547000	0.12939600	4.93348700
F	-0.22377300	-1.62765900	4.32337900
O	0.46256500	1.83410300	-0.24483000
C	-0.55047200	-1.00473400	-1.02983900
H	-0.87656600	-1.96274200	-0.63359400
C	-1.01622700	-0.77421200	-2.45019200

C	4.12149800	1.20358100	-0.35600600
C	4.39001300	1.01662500	1.00433500
C	4.21115700	-0.26152100	1.53853200
C	3.78853400	-1.34996200	0.76027900
C	3.52227900	-1.10194600	-0.59542100
C	3.68477600	0.16187200	-1.18711800
H	4.27323700	2.18503400	-0.79765600
H	4.42027500	-0.43255700	2.59163200
I	2.86273100	-2.75120100	-1.83726100
F	-0.58404000	0.39441100	-2.94676100
F	-0.52860800	-1.76570100	-3.21466400
F	-2.36430100	-0.80092100	-2.55719100
H	0.51675200	-0.82717500	-0.90172500
C	3.41915300	0.44348200	-2.64671200
H	4.01840300	-0.20406900	-3.29566100
H	2.36782300	0.27531000	-2.91086100
H	3.65946400	1.48230000	-2.88584200
C	3.65641200	-2.70972000	1.40121800
H	2.62950200	-3.08828300	1.34325700
H	4.29752600	-3.44673200	0.90520600
H	3.94058600	-2.66662700	2.45562500
C	4.89092100	2.15928100	1.85727800
H	5.95134800	2.36067100	1.65934100
H	4.34342900	3.08452600	1.64880600
H	4.79408400	1.93681700	2.92443300
C	0.94467400	2.84810000	0.24882600

a₁''-IN6

C	-1.62654500	-2.06797600	-1.05748200
O	-0.47285400	-1.68910400	-0.66978500
O	0.92434700	1.84492300	0.79661200
C	1.48917700	2.37257500	-0.23411500
O	1.55453600	1.83807200	-1.34993600
C	2.05076200	3.79141600	0.02526500
C	-2.73914900	-1.19927700	-1.00807700
C	-2.69309200	0.14052600	-0.48419200
C	-4.06352200	-1.41057700	-1.42547000
C	-3.99248500	0.68129800	-0.61416400
C	-1.69056000	0.92236000	0.08064600
H	-4.51219500	-2.28587100	-1.87492100
C	-4.30517200	1.97269800	-0.19424700
C	-1.97044400	2.21231500	0.52078400
H	2.63943000	0.55123700	-1.71827000
C	-3.27473900	2.72480500	0.36989100

H	-5.30356900	2.38555200	-0.29411600
H	-1.20274500	2.83718200	0.96091000
H	-3.47640800	3.73658200	0.70704800
N	-4.79977900	-0.30748500	-1.19906500
C	-1.70271700	-3.48588500	-1.54780400
H	-0.90622400	-3.66473800	-2.27662100
H	-1.52280400	-4.15553000	-0.69827600
H	-2.66754900	-3.72796600	-1.99607600
C	-6.21842400	-0.14108700	-1.51218500
H	-6.77862100	0.07162500	-0.59749100
H	-6.34924200	0.68118800	-2.22109200
H	-6.59484400	-1.06270900	-1.95746700
Pd	0.12139700	0.08840100	0.14040400
C	4.08924700	-2.17379600	-0.65236700
O	3.28659600	-0.20822100	-1.72060000
F	3.65909600	-3.13034100	-1.49162900
F	5.30447600	-1.77521600	-1.02534100
F	4.14008700	-2.66719500	0.58408000
F	2.90603500	3.76417000	1.05448400
F	2.67125600	4.25624100	-1.05437300
F	1.02506500	4.60632700	0.33325600
O	2.18080100	-0.93021400	0.12590000
C	-0.09349100	-0.38052300	2.14248700
H	-0.63797400	0.45581500	2.57441100
C	-0.75912200	-1.70659200	2.43588000
F	-0.09458200	-2.74789600	1.91624700
F	-0.79197100	-1.84979400	3.77329400
F	-2.02950200	-1.75433000	1.98156900
H	0.96249700	-0.38893600	2.41423400
C	3.07817500	-1.00375200	-0.70971500

a₁''-TS4

Imaginary Frequency: -267.4634

C	-1.36532800	-2.53877100	-0.24367400
O	-0.25927500	-2.06770700	0.15425500
O	1.11898000	1.74968500	0.50575400
C	1.83631800	2.23768700	-0.44892300
O	2.26502300	1.66470800	-1.44866100
C	2.10726900	3.75233900	-0.23847900
C	-2.38893900	-1.68492400	-0.74011300
C	-2.35299100	-0.25152000	-0.67737200
C	-3.57559900	-2.01994600	-1.40912000
C	-3.50714300	0.21704100	-1.34646100
C	-1.45549300	0.67636400	-0.11789100

H	-3.97044700	-2.99437400	-1.66224000	C	-1.96201600	-0.48194000	-0.69445600
C	-3.77383800	1.57375600	-1.51226100	C	-2.28432100	-2.00858500	-2.33979500
C	-1.70585400	2.04828400	-0.29953100	C	-2.46594500	0.16366600	-1.84958100
H	2.97681900	0.22945200	-1.51783700	C	-1.74692000	0.25631800	0.53268000
C	-2.84390300	2.47906700	-0.99188000	H	-2.32005700	-2.89287100	-2.96214600
H	-4.66162500	1.92614900	-2.02735300	C	-2.65646400	1.53985300	-1.89979500
H	-1.01924000	2.78593400	0.09764400	C	-1.92356000	1.67987200	0.41455100
H	-3.01086600	3.54412200	-1.11477000	H	2.79814700	0.56216000	-1.18651000
N	-4.23168400	-0.90215600	-1.77498500	C	-2.32521200	2.29645400	-0.76163200
C	-1.52930300	-4.02863700	-0.13605000	H	-3.03175800	2.03111000	-2.79257500
H	-0.56906300	-4.52117300	-0.30486300	H	-1.76867100	2.28671100	1.30014500
H	-1.85644900	-4.26998700	0.88364200	H	-2.43334400	3.37475500	-0.79049800
H	-2.27360100	-4.41751900	-0.83448700	N	-2.66993200	-0.81059500	-2.83122300
C	-5.48648700	-0.84735500	-2.52467500	C	-1.10712000	-4.25181600	-0.34426800
H	-6.24642900	-0.32062600	-1.94110900	H	-0.19191500	-4.74070200	-0.00640300
H	-5.33133800	-0.33169400	-3.47645300	H	-1.93403100	-4.55332700	0.31280900
H	-5.82724500	-1.86477700	-2.71967400	H	-1.36299600	-4.58562700	-1.35500600
Pd	0.36818400	-0.11519900	0.27895400	C	-3.17810400	-0.55450700	-4.17923100
C	4.20460200	-2.49670800	-0.16045200	H	-4.18223100	-0.12482600	-4.12625400
O	3.56380900	-0.59270200	-1.43488200	H	-2.51055500	0.13112600	-4.70862600
F	3.72438900	-3.52505500	-0.88137000	H	-3.22415000	-1.49831100	-4.72367800
F	5.44491000	-2.22303900	-0.55841800	Pd	0.41696800	-0.22065000	0.54623100
F	4.21170000	-2.83405700	1.12848500	C	4.52445700	-1.91247000	0.16347400
F	2.70341200	3.95594400	0.94259300	O	3.51568900	-0.16545300	-1.09378800
F	2.87004800	4.24065400	-1.20920500	F	4.28721700	-2.97938400	-0.61958300
F	0.92521700	4.40913700	-0.23992100	F	5.69099000	-1.36879200	-0.17659400
O	2.32417000	-1.11542000	0.39320800	F	4.56482300	-2.30336400	1.43478200
C	-0.98224900	0.50480500	1.97855500	F	1.94196500	4.21679500	1.17979300
H	-0.83496900	1.57205100	2.10592200	F	2.09161000	4.51073000	-0.97150200
C	-2.33513000	0.03453900	2.47803000	F	0.13357200	4.29003800	-0.04008200
F	-2.52632600	-1.28093100	2.24214800	O	2.41263500	-0.94228000	0.73870600
F	-2.33533300	0.21833300	3.81131300	C	-2.11452800	-0.34843700	1.89742100
F	-3.37755400	0.70705300	1.97231000	H	-1.71305200	0.26973800	2.70566800
H	-0.22420300	-0.05911400	2.53139100	C	-3.62905200	-0.41773400	2.08905800
C	3.26542900	-1.28686500	-0.38563900	F	-4.20267300	-1.19715900	1.14320500
a₁''-IN7				F	-3.91798600	-0.93897500	3.28910800
C	-0.95817800	-2.76177900	-0.28199800	F	-4.19567100	0.80171800	2.00718600
O	-0.06349100	-2.27767800	0.45929900	H	-1.73095300	-1.36034700	2.03612400
O	0.90141800	1.72329200	0.76587500	C	3.36457300	-0.90811500	-0.05232400
C	1.46207600	2.34576500	-0.20698200	b₁-IN1			
O	1.96187300	1.87316600	-1.23230700	C	-1.35427400	-1.34490700	1.27433500
C	1.42486900	3.88472100	-0.00745400	O	-0.13019000	-1.06536500	1.38531500
C	-1.80039500	-1.86265700	-1.03470000	O	2.28791800	1.71544800	-0.55109000

C	1.62088900	2.57292800	0.09200900
O	0.68421400	2.21785700	0.87383600
C	1.89890900	4.07252900	-0.08917500
C	-2.32360300	-0.55483100	0.56614500
C	-3.68300200	-0.89729600	0.16406800
C	-2.13824000	0.78058600	0.19528900
C	-4.22375400	0.26673900	-0.43936400
C	-4.48452300	-2.04986800	0.21207000
H	-1.29060200	1.42828800	0.37039400
C	-5.51257200	0.32435000	-0.97193100
C	-5.77288200	-2.00198900	-0.31293600
H	-4.11750300	-2.97352900	0.64421900
C	-6.28528700	-0.83015800	-0.89695100
H	-5.89859900	1.23019400	-1.42923000
H	-6.39453200	-2.89169700	-0.27369000
H	-7.29393800	-0.82677600	-1.29897100
N	-3.25268500	1.26891900	-0.38999000
C	-1.77688500	-2.61254600	1.97766100
H	-1.88046300	-3.41651100	1.23715600
H	-0.99984900	-2.90277600	2.68700000
H	-2.73620800	-2.49411200	2.48882800
C	-3.42727600	2.63131000	-0.87154700
H	-3.64419000	2.62894600	-1.94449200
H	-4.25010300	3.12048700	-0.34047300
H	-2.50584900	3.18904500	-0.69585400
Pd	1.11138300	0.18017100	0.31739500
C	3.09999900	-3.37410700	-0.77142400
O	3.28864300	-1.77182600	1.02550400
F	4.15883100	-3.96986000	-0.21204900
F	2.07155900	-4.25028900	-0.75901800
F	3.39769600	-3.10448400	-2.05624200
F	2.96908300	4.28209700	-0.85633900
F	0.82672000	4.64659100	-0.67468100
F	2.08977100	4.65713200	1.10181600
O	1.73491400	-1.47203500	-0.60603600
C	2.71418100	-2.08360100	0.00062300

b₁-TS1

Imaginary Frequency: -33.2198

C	1.44406800	-2.29709700	-0.60432300
O	0.20237000	-2.09282400	-0.67154700
O	-1.34177600	1.47720300	0.54758600
C	-0.88968800	2.44154100	-0.17304800
O	-0.06422100	2.35531700	-1.08604200

C	-1.43193600	3.82834500	0.24689400
C	2.37288100	-1.20504000	-0.47239300
C	3.71754300	-1.17305200	0.06362400
C	2.05798600	0.11806600	-0.82846300
C	4.12754200	0.18550100	0.01887500
C	4.59837400	-2.12592400	0.60494500
H	1.22318300	0.51674400	-1.40288000
C	5.38050700	0.61217800	0.46892300
C	5.84555100	-1.70811300	1.05226200
H	4.32125900	-3.17231700	0.67263100
C	6.23423900	-0.35529900	0.98470300
H	5.67577100	1.65538100	0.42181800
H	6.53578700	-2.43828200	1.46410200
H	7.21609100	-0.06338800	1.34486600
N	3.09403300	0.93852200	-0.53199100
C	1.90439300	-3.72802500	-0.65214300
H	2.08317900	-4.08273200	0.37179500
H	1.11663000	-4.34507300	-1.08913600
H	2.83438300	-3.83646200	-1.21700000
C	3.15870100	2.36908800	-0.82069500
H	3.46220000	2.90675600	0.08225400
H	3.88572800	2.56242700	-1.61617700
H	2.16786600	2.71044300	-1.12192300
Pd	-0.55212600	-0.27027800	-0.06069000
C	-4.36716600	-2.01797600	0.34075300
O	-3.14294400	-0.87768100	-1.40328200
F	-5.36608300	-2.06962000	-0.54679100
F	-4.03812200	-3.28189400	0.67687900
F	-4.81498900	-1.39476900	1.44512400
F	-2.72153800	3.77818900	0.60235100
F	-0.71835700	4.27737600	1.30351300
F	-1.29698400	4.71282400	-0.75022600
O	-2.18916600	-1.20446000	0.63660700
C	-3.13498800	-1.27915700	-0.25639700

b₁-IN2

C	1.53740500	-2.40924200	-0.63438300
O	0.28482400	-2.29778500	-0.65431600
O	-1.08993800	1.33686800	0.59549300
C	-0.89164400	2.28266200	-0.25774200
O	-0.29332800	2.22293800	-1.33076300
C	-1.42324800	3.65208800	0.23512800
C	2.36186000	-1.22734800	-0.51795700
C	3.67238900	-1.06120900	0.06024700

C	1.92131200	0.06036100	-0.89709900
C	3.95082900	0.33115300	0.01212500
C	4.61953900	-1.92382200	0.64390700
H	1.10223700	0.36366600	-1.55285000
C	5.14445700	0.87747300	0.49911400
C	5.80446600	-1.38632800	1.12483800
H	4.43854200	-2.99096200	0.71421400
C	6.06530000	-0.00098300	1.05272600
H	5.34125400	1.94342700	0.45176400
H	6.54738000	-2.04271600	1.56778600
H	7.00271500	0.38467200	1.44194700
N	2.87475200	0.97763100	-0.57789600
C	2.12171200	-3.79111300	-0.70737100
H	2.33593900	-4.14529200	0.30996600
H	1.38851000	-4.46873300	-1.15009800
H	3.05425000	-3.80811700	-1.27799000
C	2.83861600	2.40264100	-0.90223600
H	3.01892600	2.98537100	0.00589000
H	3.61063900	2.63779100	-1.64190400
H	1.85097600	2.64958400	-1.29178300
Pd	-0.41140100	-0.45061100	-0.01990300
C	-4.39982700	-1.79240600	0.35580500
O	-3.10518500	-0.63759800	-1.32516200
F	-5.41841600	-1.67038800	-0.50257100
F	-4.20719500	-3.10592600	0.59355100
F	-4.75246400	-1.20610200	1.51445700
F	-2.51271900	3.53852900	1.00368100
F	-0.45268800	4.25235400	0.96585200
F	-1.71226000	4.45118600	-0.79983000
O	-2.13179000	-1.26903900	0.63172900
C	-3.10736500	-1.14792000	-0.22180800

b₁-TS2

Imaginary Frequency: -1297.2609

C	-1.55495200	-2.33368200	0.68549100
O	-0.31839500	-2.32466900	0.41618700
O	1.14055600	1.39794400	-0.58743600
C	0.76607800	2.15684100	0.34421600
O	-0.13247500	1.92224000	1.20475100
C	1.37986000	3.57313800	0.37383600
C	-2.32493700	-1.14529700	0.46329300
C	-3.73019500	-0.96710000	0.20812300
C	-1.65223600	0.04883800	0.09443700
C	-3.85662800	0.33451100	-0.34976000

C	-4.88548900	-1.75608100	0.36135800
H	-0.77928000	0.84064500	0.78195400
C	-5.09602500	0.87264400	-0.72167500
C	-6.11241400	-1.22829500	-0.01471900
H	-4.82917300	-2.75466800	0.78128800
C	-6.21740300	0.07321100	-0.54928100
H	-5.18476600	1.87446400	-1.12866400
H	-7.01157600	-1.82446900	0.10943700
H	-7.19380000	0.45757700	-0.82860800
N	-2.59149800	0.90351300	-0.43130100
C	-2.14930500	-3.62621900	1.16615800
H	-2.80160700	-4.04504800	0.38938800
H	-1.35205000	-4.34021200	1.37993000
H	-2.75905800	-3.46481300	2.06147000
C	-2.33530200	2.25852200	-0.91153200
H	-1.34091200	2.30223500	-1.35580000
H	-3.06574100	2.50189100	-1.68514400
H	-2.40601100	2.98777300	-0.09875900
Pd	0.38993500	-0.52229500	-0.29814200
C	4.45660100	-1.71729100	-0.28359000
O	3.02399700	-0.40927600	1.15057700
F	5.42085900	-1.43070500	0.60003000
F	4.33788200	-3.05920000	-0.35165400
F	4.85303000	-1.27454600	-1.49345900
F	2.54646000	3.62162600	-0.26678600
F	0.51244600	4.40672500	-0.24648600
F	1.54894300	3.99735600	1.62862800
O	2.18354300	-1.34142700	-0.74262300
C	3.10785500	-1.06776900	0.12748900

b₁-IN3

C	-1.60335400	-2.47629600	-0.02940000
O	-0.34451000	-2.30231700	-0.19459800
O	0.64311200	1.69001900	-0.55376800
C	1.41574400	2.26899500	0.27753900
O	2.07001400	1.79745700	1.21763600
C	1.50892200	3.79688100	0.02364300
C	-2.43033700	-1.33823000	0.00078800
C	-3.84380200	-1.06181100	0.13597000
C	-1.75862400	-0.09965600	-0.16171300
C	-3.95644100	0.34815100	0.04293000
C	-5.00539000	-1.82267000	0.31919900
H	2.70447200	0.39988400	1.29723500
C	-5.17943200	1.01078300	0.12803500

C	-6.23343500	-1.16794500	0.40487100
H	-4.95774500	-2.90496500	0.39489800
C	-6.32137400	0.23033400	0.31092400
H	-5.24742000	2.09177700	0.05658000
H	-7.13939500	-1.75021300	0.54747000
H	-7.29143200	0.71345100	0.38199700
N	-2.66976600	0.89636400	-0.14060700
C	-2.09654600	-3.88766600	0.11510500
H	-2.82315300	-4.11713800	-0.67338300
H	-1.26045000	-4.58650900	0.05258100
H	-2.60714800	-4.01413500	1.07721500
C	-2.43779800	2.32770600	-0.28888200
H	-1.38210000	2.50146000	-0.47777800
H	-3.02763000	2.70947100	-1.12865500
H	-2.73968100	2.85189700	0.62426000
Pd	0.18634900	-0.31446800	-0.36852800
C	4.26242900	-2.19087900	0.02676500
O	3.33438600	-0.41512100	1.27797900
F	5.45040800	-1.58932000	-0.14778800
F	4.33132000	-2.96634100	1.12035100
F	4.00918800	-2.96014500	-1.03269100
F	2.03060000	4.03405800	-1.19309600
F	0.27649400	4.35226100	0.06336500
F	2.26814000	4.40754700	0.93654300
O	2.26132300	-1.03042600	-0.62514900
C	3.15911200	-1.12493100	0.20875700

b₁-IN1'

C	1.55564200	0.44979500	1.53105800
O	0.33898400	0.71799000	1.75016500
O	-3.02053200	-0.26089400	-0.49139500
C	-2.87563100	-1.40588400	0.01986200
O	-1.92205600	-1.64364500	0.82521300
C	-3.84197700	-2.54723100	-0.33068100
C	2.02485900	-0.65126200	0.74073700
C	3.36031400	-0.92071000	0.22340500
C	1.24356700	-1.75307800	0.38250400
C	3.28931700	-2.18055100	-0.42343800
C	4.58322200	-0.23104800	0.19691600
H	0.20885400	-1.96322500	0.61340500
C	4.37860300	-2.77484600	-1.06226900
C	5.67679700	-0.81592700	-0.43531300
H	4.68529900	0.74917700	0.64758100
C	5.58073500	-2.07424500	-1.05527700

H	4.29431400	-3.74148300	-1.54943100
H	6.62386200	-0.28463900	-0.45567200
H	6.45253900	-2.50167500	-1.54151800
N	1.98275800	-2.65737000	-0.29597400
C	2.53407100	1.37616300	2.20347300
H	2.84836000	2.11947000	1.45884400
H	2.03053500	1.90335000	3.01624400
H	3.41757600	0.85201900	2.57570000
C	1.50283300	-3.93521700	-0.79935400
H	1.65117500	-3.99379700	-1.88230400
H	2.03759800	-4.76166200	-0.31980000
H	0.43689400	-4.02275100	-0.58205300
Pd	-1.28604200	0.39362400	0.54867200
C	-0.33055100	4.32056300	-0.80766500
O	-1.21297600	2.31330400	0.00908900
F	-1.35543300	4.48704100	-1.66303000
F	-0.60343900	5.01739300	0.31391200
F	0.76877800	4.84535500	-1.36486400
F	-4.74494500	-2.16210900	-1.23325200
F	-3.14073200	-3.58331200	-0.83200500
F	-4.47802400	-2.96518400	0.77466100
O	0.96562800	2.29166100	-0.66513200
C	-0.11789900	2.81683000	-0.47235500

b₁-TS1'

Imaginary Frequency: -31.4248

C	0.69531300	-2.22675400	-1.30866100
O	-0.38315000	-1.64915900	-1.61537100
O	-0.93675500	1.90225900	0.32033300
C	-0.24088000	2.81657300	-0.25406200
O	0.49037300	2.68049700	-1.24022000
C	-0.30343600	4.20083800	0.43237900
C	1.80250200	-1.45233100	-0.80687600
C	2.90287400	-1.81897800	0.05230500
C	1.91737600	-0.06456900	-1.03386900
C	3.62016900	-0.62005300	0.30855800
C	3.33165300	-3.01083700	0.66401000
H	1.40858800	0.56948800	-1.75730800
C	4.75756300	-0.58221500	1.12178400
C	4.46101800	-2.97833700	1.47037000
H	2.79555400	-3.94169600	0.51410700
C	5.16788200	-1.77883000	1.69544100
H	5.29593500	0.34224000	1.30342700
H	4.80641200	-3.89340500	1.94187800

H	6.04583600	-1.78995400	2.33426700
N	2.99602700	0.42168500	-0.36968600
C	0.75268100	-3.71736500	-1.45943300
H	0.42961500	-4.16693400	-0.51028300
H	0.04286200	-4.03016100	-2.22878900
H	1.75831000	-4.07345300	-1.69570000
C	3.48078300	1.79896900	-0.42016000
H	3.66462300	2.15390900	0.59781200
H	4.41088700	1.85365300	-0.99529100
H	2.71276600	2.42449700	-0.87596400
Pd	-0.66898400	0.14933600	-0.64127900
C	-4.21065400	-1.72189200	0.70822700
O	-2.59930100	-0.31893500	-0.26015900
F	-4.88464600	-0.67521000	1.21508100
F	-4.78433000	-2.06454500	-0.46265500
F	-4.34137700	-2.75307100	1.55242400
F	-1.29793500	4.30337900	1.31935400
F	0.86579500	4.40982500	1.08225000
F	-0.44521200	5.17072000	-0.48376300
O	-1.83678700	-2.06633500	0.98261700
C	-2.71085100	-1.37354400	0.48942800

b₁-IN2'

C	0.19253200	-2.72388000	-0.98290200
O	-0.85513400	-2.19616900	-1.42489700
O	-0.00394800	1.40075800	0.40909000
C	0.46452200	2.31548200	-0.37366600
O	0.62952300	2.27970500	-1.58687900
C	0.96158600	3.55824000	0.40959900
C	1.30071600	-1.81420000	-0.67789800
C	2.33146100	-1.89099400	0.33572500
C	1.62981000	-0.69615700	-1.50067700
C	3.21085600	-0.80798100	0.08893500
C	2.56001800	-2.72846800	1.43889900
H	1.23437700	-0.42385400	-2.47012300
C	4.31427600	-0.54236400	0.90466800
C	3.66393600	-2.47830700	2.24405500
H	1.88962700	-3.55092100	1.66664600
C	4.52857700	-1.39737000	1.98000700
H	4.97234900	0.29902400	0.71499100
H	3.85965100	-3.11918200	3.09814400
H	5.37637300	-1.22291800	2.63565100
N	2.77242800	-0.12455000	-1.04173500
C	0.24802100	-4.19861500	-0.73260100

H	-0.10390900	-4.38868900	0.29064700
H	-0.43966200	-4.70593300	-1.41379100
H	1.26129500	-4.59532200	-0.83298800
C	3.44540500	1.03125600	-1.62897600
H	3.47956300	1.84635400	-0.90214600
H	4.46029200	0.75455100	-1.93084600
H	2.87243800	1.37268500	-2.48943200
Pd	-0.55379700	-0.28412700	-0.54388900
C	-4.61987800	-0.09399600	0.57750000
O	-2.49622200	0.28362800	-0.35834300
F	-4.73887800	1.18460900	0.98039300
F	-5.23947400	-0.21577400	-0.61420800
F	-5.26222600	-0.87062500	1.45984500
F	0.32286400	3.75058000	1.56830800
F	2.28433400	3.38095500	0.69088200
F	0.85133500	4.66896500	-0.32851100
O	-2.69696400	-1.46593100	1.07376200
C	-3.12756400	-0.50404700	0.45600300

b₁-TS2'

Imaginary Frequency: -1313.2880

C	-1.15229800	-2.18447900	1.23099700
O	0.09196800	-1.95662400	1.17347000
O	1.04638500	1.79669000	-0.25757500
C	0.35990300	2.59487800	0.42870500
O	-0.62761700	2.30997500	1.17219200
C	0.67777800	4.09896300	0.28129000
C	-2.05909200	-1.22193400	0.68240000
C	-3.39602700	-1.37072300	0.17064200
C	-1.53764800	0.01189600	0.20991900
C	-3.62665600	-0.22497400	-0.63840900
C	-4.40882200	-2.34146000	0.27974600
H	-0.96489500	1.07419100	0.87568600
C	-4.84085600	-0.01094500	-1.30413700
C	-5.60852300	-2.13613800	-0.38674800
H	-4.26824900	-3.23057000	0.88508700
C	-5.82342400	-0.98215400	-1.16920400
H	-5.01504100	0.87609300	-1.90410600
H	-6.40069900	-2.87404900	-0.30155700
H	-6.77575100	-0.85004500	-1.67392700
N	-2.48407800	0.56674200	-0.61785000
C	-1.58946600	-3.49498600	1.81897700
H	-1.98456800	-4.14079300	1.02453500
H	-0.73649000	-3.99222100	2.28409000

H	-2.38610600	-3.34621900	2.55558100
C	-2.36472100	1.84419200	-1.31454400
H	-1.32523400	2.00200000	-1.60259100
H	-2.96654800	1.80617300	-2.22411200
H	-2.70283400	2.67398300	-0.68638800
Pd	0.59556400	-0.18895900	0.23720300
C	4.40414200	-1.83891400	-0.54070500
O	2.57364800	-0.63298300	0.31818900
F	5.19302000	-0.74688900	-0.55357700
F	4.64301800	-2.51025100	0.60488900
F	4.76409900	-2.62416700	-1.56413700
F	1.90320100	4.30123000	-0.20013600
F	-0.21852700	4.62725600	-0.58131100
F	0.55889000	4.72872400	1.45467300
O	2.20057700	-1.89755500	-1.52397700
C	2.90671100	-1.44534700	-0.63571200

bi-IN3'

C	1.93482900	-2.29987900	-0.32198600
O	0.65623500	-2.23130400	-0.36733800
O	-0.78444100	1.65863700	0.04748100
C	-1.93936600	2.06052400	-0.17147700
O	-2.98207500	1.37515800	-0.46066700
C	-2.20174700	3.57903500	-0.05835400
C	2.65517400	-1.10497300	-0.13787600
C	4.04142700	-0.70740000	-0.02710000
C	1.85502000	0.05847200	-0.02454600
C	4.01017900	0.69898300	0.15017600
C	5.28130700	-1.35814800	-0.05523500
H	-2.76769300	0.32621500	-0.43845200
C	5.16648500	1.46292000	0.29659300
C	6.44333300	-0.60153000	0.09088000
H	5.34364500	-2.43426600	-0.18739200
C	6.38881000	0.79081400	0.26442800
H	5.12499100	2.53924000	0.43201400
H	7.40923100	-1.09825500	0.07057600
H	7.31027800	1.35462000	0.37628400
N	2.66598700	1.12659200	0.14568800
C	2.55548300	-3.65889600	-0.47015200
H	3.12434500	-3.91127200	0.43278100
H	1.78018600	-4.41015200	-0.63009100
H	3.25623400	-3.66685100	-1.31325600
C	2.28475500	2.52366700	0.30509100
H	1.20282000	2.61281700	0.24539800

H	2.62836200	2.89566700	1.27638900
H	2.74413200	3.12597700	-0.48603700
Pd	-0.08161300	-0.33635000	-0.12312900
C	-4.09443400	-2.19776900	0.13956900
O	-2.13864600	-0.93038200	-0.30501600
F	-4.81711900	-1.05228200	0.10094100
F	-4.20101200	-2.78922000	-1.06604900
F	-4.64040500	-3.00273700	1.05439200
F	-1.04916900	4.26049000	-0.09031900
F	-2.97955900	3.99934700	-1.06125000
F	-2.81870400	3.83313200	1.10640300
O	-2.01756900	-2.51287100	1.31246800
C	-2.61102000	-1.88919600	0.46222000

bi'-IN1

C	-1.58942300	0.09298500	1.88473400
O	-0.33918400	0.23296300	2.02196200
O	1.68254100	1.79196600	0.69703500
C	1.38615500	2.44853000	-0.37518000
O	0.74987700	2.07996700	-1.35587900
C	1.93031600	3.90090700	-0.30457200
C	-2.27917300	0.00229700	0.63459700
C	-3.66436200	-0.36705200	0.35987800
C	-1.72566600	0.37279900	-0.59835400
C	-3.84726200	-0.20097200	-1.03687600
C	-4.74771600	-0.84297100	1.11560700
H	-0.74690600	0.78176600	-0.82747600
C	-5.04964400	-0.47538700	-1.68864300
C	-5.95413400	-1.11638700	0.47540400
H	-4.66164000	-1.00550300	2.18382700
C	-6.10793100	-0.93425300	-0.90950100
H	-5.15768400	-0.34070200	-2.76048600
H	-6.79347300	-1.48171200	1.06004800
H	-7.06112400	-1.15845800	-1.37882600
N	-2.64477400	0.26335800	-1.57680600
C	-2.35745300	0.03938700	3.18447600
H	-2.64245500	-0.99946700	3.39571800
H	-1.71628400	0.39137300	3.99446400
H	-3.27125800	0.63826600	3.13703600
C	-2.42397200	0.61947800	-2.97228800
H	-1.42399900	1.04524700	-3.06844400
H	-2.50741000	-0.26678800	-3.60972100
H	-3.16298500	1.36126300	-3.29054200
Pd	1.20183700	-0.16120300	0.72998200

C	2.94265300	-3.47024200	-0.61694100
O	1.18192700	-2.28249600	0.55937000
F	3.67250600	-3.22435100	-1.71002500
F	3.75666300	-3.92660300	0.35136400
F	2.04112500	-4.42035500	-0.89862100
F	1.30130300	4.58169100	0.67527600
F	3.24864200	3.91375300	-0.04371500
F	1.72392200	4.54788800	-1.45882300
O	2.74442100	-1.05949000	-0.39054000
C	2.24095000	-2.19327700	-0.13097500

b₁'-TS1

Imaginary Frequency: -125.2703

C	-2.24032600	-0.31678500	2.17162200
O	-1.03272100	-0.50543400	2.49737200
O	1.72397500	1.34342900	1.33662000
C	1.36265100	2.30100400	0.64017900
O	0.17416200	2.65896500	0.33638100
C	2.44795200	3.16366100	-0.05562000
C	-2.49866300	0.06175500	0.80725200
C	-3.61239000	-0.10648000	-0.06879800
C	-1.38812800	0.52891400	0.03359900
C	-3.13015100	0.23419100	-1.37207300
C	-4.94928400	-0.53127300	0.08008800
H	-0.65665600	1.43592100	0.34826800
C	-3.95676600	0.18295500	-2.50519400
C	-5.75932300	-0.58332100	-1.04078900
H	-5.34271400	-0.80147000	1.05477800
C	-5.26696200	-0.22862400	-2.32005100
H	-3.58289400	0.44137800	-3.49022400
H	-6.79336900	-0.89929500	-0.94196500
H	-5.93227100	-0.28577400	-3.17642600
N	-1.80490500	0.60200000	-1.27588600
C	-3.30736800	-0.52889900	3.20187200
H	-3.85481600	-1.45366700	2.97635400
H	-2.85431900	-0.62316600	4.19051500
H	-4.02766900	0.29572400	3.19189900
C	-0.97631100	1.11855400	-2.36427000
H	-0.17377200	1.71750400	-1.93124200
H	-0.54872400	0.29128000	-2.93902600
H	-1.58243800	1.75005200	-3.01854300
Pd	0.16963100	-0.71318300	0.82759900
C	3.32747300	-2.50113500	-0.87636600
O	1.83086500	-2.26853200	1.02748800

F	3.02175000	-2.79362400	-2.15175100
F	4.31012800	-1.58716500	-0.87353400
F	3.76854100	-3.61056300	-0.27443500
F	3.68321500	2.89093200	0.38422700
F	2.41897200	2.91105700	-1.39128800
F	2.22523000	4.48133100	0.11040600
O	1.36048800	-1.10578000	-0.78906900
C	2.09364100	-1.94200800	-0.14907000

b₁'-IN2

C	-2.88096400	-1.72225300	1.35223000
O	-1.75797600	-2.33976200	1.41367700
O	2.98091100	0.88140300	1.25972300
C	2.64122100	1.80367800	0.55835800
O	2.04370900	1.72743500	-0.62731700
C	2.84841400	3.28023900	0.95740500
C	-2.98153600	-0.63964200	0.45818200
C	-3.97341800	0.32198400	0.02691600
C	-1.79737600	-0.38370900	-0.26936000
C	-3.32335300	1.11550800	-0.95449200
C	-5.30759000	0.60108300	0.34758200
H	1.90641700	0.76543100	-0.83752700
C	-3.95983800	2.16795500	-1.60923000
C	-5.95218100	1.65084300	-0.30526500
H	-5.83589800	0.01460200	1.09352100
C	-5.28855400	2.42520800	-1.27045400
H	-3.44632500	2.77229800	-2.35042200
H	-6.98659800	1.87554200	-0.06156400
H	-5.81461700	3.23936500	-1.76001600
N	-2.00098400	0.64692100	-1.11313300
C	-3.99129300	-2.20880400	2.23681300
H	-4.86139500	-2.48927400	1.63140700
H	-3.65988900	-3.06976500	2.81993100
H	-4.30910900	-1.40870900	2.91608600
C	-1.03653300	1.21508800	-2.04726100
H	-0.22128500	0.50603500	-2.18461000
H	-1.52439100	1.38819500	-3.01046900
H	-0.63413000	2.15909400	-1.66662800
Pd	-0.30244300	-1.55113100	0.18739200
C	3.61447300	-1.82103300	-0.86984300
O	1.72295200	-2.63930800	0.39892800
F	3.72238900	-2.65611300	-1.92209700
F	4.01560500	-0.60006000	-1.26450600
F	4.42001500	-2.25098400	0.10083600

F	3.45877000	3.36672900	2.14038000
F	3.59481300	3.91819900	0.03839200
F	1.65853900	3.90803400	1.04023600
O	1.37547300	-0.90010300	-0.92755100
C	2.14765800	-1.79594300	-0.40435800

b₁'-IN3

C	-1.75696800	2.16672000	0.00267900
O	-0.50378400	2.43361700	0.00002700
C	-2.13905000	0.81015600	0.00125700
C	-3.35624500	0.02676300	0.00297900
C	-1.05261100	-0.09309400	-0.00294200
C	-2.92911600	-1.32770600	-0.00043500
C	-4.72941800	0.30123400	0.00678100
C	-3.82289600	-2.39633400	-0.00012400
C	-5.63054600	-0.76303700	0.00712700
H	-5.09295100	1.32472100	0.00938800
C	-5.18534900	-2.09465500	0.00372900
H	-3.47821500	-3.42583200	-0.00275300
H	-6.69741600	-0.55831300	0.01006300
H	-5.91031500	-2.90329600	0.00409000
N	-1.51889600	-1.35802800	-0.00395600
C	-2.71679500	3.32159500	0.00697000
H	-3.36637600	3.27642900	-0.87537900
H	-3.36318300	3.27260900	0.89144800
H	-2.16985200	4.26611000	0.00798700
C	-0.72676200	-2.58140400	-0.00798400
H	-0.95303700	-3.17617400	0.88321300
H	-0.95787500	-3.17340000	-0.89978300
H	0.33017800	-2.31765800	-0.01047400
Pd	0.70410200	0.74885100	-0.00594600
C	4.48270700	-0.68244300	0.00506500
C	3.09101400	-0.02501500	-0.01136300
O	2.08608600	-0.81937500	-0.01195800
O	2.96577200	1.21602800	-0.01117100
F	4.59279500	-1.56484500	-1.00427400
F	4.65993200	-1.34609000	1.16343100
F	5.45285600	0.22815800	-0.11628900

b₁''-IN1

C	1.58367100	0.20974000	1.88960200
O	0.33062800	0.31188000	2.03509900
O	-1.76496700	1.74921000	0.68954900
C	-1.49897100	2.39067400	-0.39961500

O	-0.85235600	2.02376300	-1.37415100
C	-2.09907700	3.82206500	-0.36128600
C	2.26415200	0.10219100	0.63572200
C	3.65711100	-0.23382700	0.35787500
C	1.68796800	0.41839400	-0.60203800
C	3.82154900	-0.10533800	-1.04511700
C	4.76125500	-0.65429600	1.11637300
H	0.69538200	0.79177500	-0.83275600
C	5.02531100	-0.36402100	-1.70077000
C	5.96911700	-0.91149200	0.47219900
H	4.69013600	-0.78653800	2.18987800
C	6.10417700	-0.76738800	-0.91913700
H	5.11904600	-0.25919800	-2.77728400
H	6.82451500	-1.23385600	1.05883100
H	7.05909500	-0.97767900	-1.39138500
N	2.60059900	0.30637700	-1.58625900
C	2.36516300	0.22349200	3.18228300
H	2.68311100	-0.79870600	3.42546300
H	3.26004700	0.84730500	3.10531100
H	1.72120300	0.58332300	3.98661500
C	2.35587600	0.61231500	-2.98963600
H	3.06808400	1.36671300	-3.33795200
H	2.46126700	-0.29018400	-3.60045400
H	1.34206400	1.00325000	-3.08866600
Pd	-1.20261800	-0.18061600	0.76771500
C	-2.73313000	-3.58293400	-0.60361900
C	-2.15336300	-2.27474500	-0.04561700
O	-1.09523000	-2.30302300	0.65117600
O	-2.71360400	-1.17098900	-0.31794900
F	-2.13452600	-3.86659500	-1.77585200
F	-2.50926800	-4.59494000	0.24364000
F	-4.04861400	-3.46963700	-0.81198000
F	-1.48596800	4.55286700	0.59235800
F	-1.93093600	4.44504400	-1.53478400
F	-3.41383500	3.79123400	-0.08469100

b₁''-TS1

Imaginary Frequency: -104.6961

C	-0.54544000	-1.67484900	2.22672300
O	0.36719900	-0.88716700	2.48426600
O	2.53467200	0.28595600	0.36071300
C	3.16852800	-0.47451400	-0.46751900
O	2.72734100	-1.24979800	-1.30749600
C	4.70456300	-0.33210500	-0.27423500

C	-1.00070600	-1.84133700	0.83817000
C	-2.30540700	-2.05221500	0.28986800
C	-0.10957900	-1.74767800	-0.24825000
C	-2.14718900	-2.06199100	-1.12882900
C	-3.60127300	-2.18721400	0.83178300
H	0.96869000	-1.86197200	-0.27295100
C	-3.23286100	-2.21903200	-2.00104100
C	-4.67183800	-2.35284100	-0.03006300
H	-3.76057600	-2.16873600	1.90500400
C	-4.48922900	-2.36832300	-1.43283100
H	-3.09800400	-2.22262900	-3.07791100
H	-5.67310500	-2.46818300	0.37400000
H	-5.35365800	-2.49495300	-2.07805100
N	-0.81076500	-1.89210700	-1.42119900
C	-1.20120000	-2.47469700	3.33158200
H	-2.12866600	-1.96914700	3.63222300
H	-1.46154600	-3.48748600	3.01056100
H	-0.53678600	-2.50373900	4.19764600
C	-0.21619300	-1.92536900	-2.75254700
H	-0.38032200	-2.90239600	-3.21930800
H	-0.66414100	-1.14820000	-3.38024600
H	0.85331300	-1.73668900	-2.65423800
Pd	0.55632000	0.57528400	0.32794700
C	-2.00832500	3.62764800	-0.15634700
C	-0.95045300	2.52784600	0.02854100
O	-1.35584800	1.35130900	0.32414300
O	0.26693200	2.77211400	-0.14029600
F	-2.57113900	3.50218200	-1.37352200
F	-2.97235200	3.51407300	0.76872900
F	-1.45699000	4.84073400	-0.06343400
F	5.05887700	-0.74606400	0.95720300
F	5.36900800	-1.07035800	-1.17163200
F	5.08778200	0.94904800	-0.41451700

b₁''-IN2

C	1.71216000	2.07834000	-0.52354900
O	2.61128500	2.32523700	0.25795000
O	2.07210100	-0.64110800	-0.56444400
C	2.84091900	-0.76452000	0.47837000
O	2.53242800	-0.73819200	1.65810400
C	4.31717600	-0.95689700	0.04373500
C	0.35074900	1.69497500	0.01812100
C	-0.93254900	2.30305100	-0.36990900
C	0.19463900	1.36584300	1.40760900

C	-1.76936700	2.24927400	0.76745800
C	-1.42497000	2.87507900	-1.54873600
H	0.96019600	0.98412900	2.07139800
C	-3.07998600	2.71784000	0.76318600
C	-2.73106000	3.36147800	-1.56214700
H	-0.81092300	2.93197500	-2.44104800
C	-3.54886500	3.28036400	-0.42366100
H	-3.71503400	2.65122200	1.64055300
H	-3.12544500	3.80612100	-2.47080500
H	-4.56494100	3.66083700	-0.46633800
N	-1.04313100	1.67247900	1.82666400
C	1.89819300	2.18369000	-2.02178200
H	1.24983400	1.49582600	-2.57099000
H	1.67601600	3.20945300	-2.34457900
H	2.94388300	1.97031300	-2.25255200
C	-1.62068700	1.28696400	3.10747600
H	-2.11502400	2.14810600	3.56545100
H	-2.34662900	0.48103000	2.96027000
H	-0.82183700	0.94053400	3.76473200
Pd	0.10118800	-0.47963400	-0.20763700
C	-3.20636400	-2.78392000	-0.25110000
C	-1.89747200	-1.97699100	-0.24056200
O	-1.97657700	-0.73178000	0.03376700
O	-0.80368900	-2.52394400	-0.51170000
F	-3.92102400	-2.51905700	0.85749500
F	-3.94441100	-2.43463800	-1.32067000
F	-2.96810700	-4.09634000	-0.30492000
F	4.70375600	0.03518000	-0.78295700
F	5.13415700	-0.96355900	1.10180500
F	4.46426100	-2.12523500	-0.61163000

b₁''-TS2

Imaginary Frequency: -1106.0115

C	-0.73001200	1.69708100	2.08072100
O	-1.41601700	0.69210300	2.23342500
O	-2.03529300	-1.42390500	-0.04035300
C	-2.91224700	-0.58191600	-0.34457900
O	-2.74617900	0.61794300	-0.70217900
C	-4.37735800	-1.08231700	-0.34222300
C	-0.05495900	1.94753300	0.78449700
C	0.72512100	3.05639200	0.33892400
C	-0.20178000	1.05161000	-0.31070200
C	1.07003800	2.78361000	-1.02373500
C	1.18133200	4.26666200	0.91730100

H	-1.49885800	0.86216800	-0.56224100
C	1.84324100	3.66920600	-1.79704900
C	1.94677500	5.12958000	0.15725700
H	0.94495300	4.51745600	1.94435500
C	2.27620900	4.83315600	-1.18951000
H	2.10163000	3.44305800	-2.82635800
H	2.30725400	6.05478900	0.59696100
H	2.88467200	5.53499300	-1.75254200
N	0.51043200	1.58977800	-1.38526700
C	-0.57228600	2.69559100	3.21085200
H	0.48452200	2.82531700	3.47299100
H	-0.96627800	3.67766800	2.92303600
H	-1.11942400	2.32842200	4.08098100
C	0.65673800	0.96334200	-2.68995600
H	0.51376100	1.70545800	-3.48111600
H	1.64732900	0.50668300	-2.79014900
H	-0.10116300	0.18508200	-2.79167400
Pd	-0.02141300	-0.98896600	-0.02732700
C	3.50178100	-2.89878600	0.24029900
C	2.10603400	-2.25643900	0.16910300
O	2.05491600	-0.99234900	-0.02370600
O	1.07099300	-2.95279200	0.26937300
F	-4.74735300	-1.33406100	-1.61265200
F	-5.19208500	-0.14673700	0.16048500
F	-4.51211600	-2.20145600	0.37144100
F	4.29693600	-2.20381400	1.06927500
F	4.06106300	-2.89104000	-0.98573500
F	3.43071500	-4.16188800	0.66829800

b1''-IN3

C	1.47302200	-0.35928400	2.14878100
O	0.69331000	0.58475200	2.30881800
O	0.21483600	2.17938600	-0.36510800
C	1.40099000	2.47968000	-0.30646100
O	2.42481600	1.69463400	-0.11518300
C	1.83193400	3.94941100	-0.50859100
C	1.55985800	-1.05150200	0.85768100
C	2.42663700	-2.12983200	0.39871900
C	0.60202000	-0.84969400	-0.15882100
C	1.94480900	-2.50938600	-0.87971200
C	3.55119700	-2.79912900	0.90996200
H	2.12858700	0.75624300	0.06239400
C	2.53795800	-3.51194100	-1.64978000
C	4.14525900	-3.80506500	0.15244500

H	3.96137000	-2.54480000	1.88095000
C	3.64714700	-4.15976500	-1.11326400
H	2.15135300	-3.77997700	-2.62822200
H	5.01297200	-4.32555400	0.54780400
H	4.13324200	-4.94769000	-1.68109200
N	0.83605800	-1.71457400	-1.18472700
C	2.36286200	-0.80865100	3.29189400
H	2.26135700	-1.88472800	3.47247500
H	3.41709600	-0.61226800	3.05924900
H	2.08877800	-0.25478000	4.19171400
C	0.06196400	-1.84485900	-2.41090200
H	0.67222300	-1.57830000	-3.28097600
H	-0.29006500	-2.87533500	-2.52129900
H	-0.80103500	-1.18163000	-2.35499300
Pd	-0.91817600	0.38463100	-0.07566900
C	-4.77337300	-0.77042900	0.17420400
C	-3.34278400	-0.20800400	0.09276900
O	-2.39817100	-1.06994300	-0.01053700
O	-3.13110500	1.02113200	0.10439200
F	2.58205400	4.03959100	-1.61907000
F	2.56031800	4.35803800	0.53822700
F	0.76655100	4.73584600	-0.63724700
F	-4.85579700	-1.71170100	1.12841800
F	-5.10275700	-1.33519200	-1.00446400
F	-5.65689200	0.19440000	0.44449700

b1-TS3

Imaginary Frequency: -117.8322

C	-4.06026100	-1.82841700	-0.35267200
O	-2.91751400	-2.23044100	0.05935900
O	1.08112400	1.80475500	-0.34521800
C	1.66951600	2.14061800	0.66550700
O	2.03480600	1.40803700	1.68264700
C	2.05556200	3.62274800	0.87073800
C	-5.43429900	0.41581100	-0.71039400
C	-3.31917100	0.36874400	0.22562000
C	-4.99027500	1.73249500	-0.42144300
C	-6.70108500	0.24226700	-1.28241500
C	-5.76509800	2.86020100	-0.68358400
C	-7.48317600	1.36606000	-1.54820700
H	1.69718600	0.45787200	1.59627400
C	-7.02322900	2.65925700	-1.25329700
H	-5.41057100	3.85965700	-0.45090600
H	-8.46785500	1.23832300	-1.98938200

H	-7.65484900	3.51647900	-1.46792900	C	6.28079800	2.93192700	0.10429000
N	-3.69931600	1.66018700	0.13894100	H	6.70676500	3.55870900	-0.68652800
C	-5.01492900	-2.86294400	-0.88162600	H	5.68456400	3.58332900	0.75514300
H	-5.92418000	-2.88449700	-0.26883300	H	7.10231600	2.52502900	0.70142800
H	-5.31670600	-2.61576400	-1.90638900	C	-4.35020700	-0.44964400	-0.29805000
H	-4.54671900	-3.84895100	-0.86551800	C	-1.30926000	0.99455600	3.08730900
C	-2.93003700	2.83190000	0.53458400	C	-0.53415600	1.98708600	3.94183500
H	-2.87883900	3.53665800	-0.30186000	O	-2.27918700	0.37301000	3.51507500
H	-3.40494900	3.32589900	1.38944600	O	-0.82860600	0.85859900	1.86901000
H	-1.92696300	2.51014600	0.80945800	H	-7.07708000	-0.75000500	-1.51390900
Pd	-1.81189700	-0.67662800	0.94552900	C	0.78873300	-2.03698700	1.94543800
C	1.42400800	-3.21107400	2.74064700	H	0.37596500	1.50291400	4.31430900
O	1.59761600	-1.16622500	1.56149100	H	-0.22245800	2.85830100	3.35987500
O	-0.45013600	-2.13804400	1.75043500	H	-1.14398600	2.29285100	4.79435200
F	2.32809900	-3.85245600	1.95569100				
F	2.08267500	-2.74386700	3.81805400	b₁-IN4			
F	0.53193700	-4.11644100	3.15453700	C	2.44021400	-2.37011900	-0.06145700
F	1.05948500	4.26033700	1.52169200	O	1.17968600	-2.57853200	0.08743500
F	3.18151500	3.76601400	1.59121700	O	-1.78087100	2.18787100	1.60777400
F	2.23498100	4.22901900	-0.31174300	C	-2.53561300	2.56497100	0.73744400
C	0.04916200	-0.96898900	-1.24893300	O	-3.42974400	1.86723200	0.07210100
H	-0.10021900	-1.86150800	-0.65664500	C	-2.47075000	4.01985500	0.22391300
C	-0.74009500	-0.86809900	-2.54030500	C	4.14721200	-0.36918700	-0.45267300
C	4.55853800	2.09594200	-1.54229700	C	1.86849000	-0.07434900	-0.34248600
C	5.41000800	1.83818600	-0.46326600	C	3.81424600	1.00434200	-0.56852500
C	5.40735900	0.55705600	0.09269700	C	5.49518400	-0.74528100	-0.49517100
C	4.55588100	-0.46146500	-0.35864600	C	4.77618600	2.00091000	-0.71919200
C	3.70620900	-0.11899500	-1.41987200	C	6.46409600	0.24474200	-0.65017000
C	3.68258100	1.13152000	-2.05542100	H	-3.33111700	0.89126900	0.28152600
H	4.55463000	3.08328000	-1.99660700	C	6.11123700	1.59972500	-0.76001200
H	6.07671000	0.33215900	0.91880200	H	4.50357200	3.04810300	-0.80250100
I	2.33046200	-1.64613300	-2.13103500	H	7.51252900	-0.03666100	-0.68533300
F	-2.03326600	-0.59580600	-2.31694100	H	6.88869700	2.34846700	-0.87852400
F	-0.26121600	0.10329600	-3.34256400	N	2.41004600	1.14205600	-0.49658600
F	-0.68379800	-2.03298500	-3.22655600	C	3.34260000	-3.56267100	0.05179500
H	0.36403700	-0.04588700	-0.76497800	H	3.96342800	-3.65469700	-0.84654200
C	2.77571000	1.49141400	-3.20420800	H	4.01477100	-3.43590000	0.90925500
H	2.85755200	0.77671100	-4.03038000	H	2.75316300	-4.47125600	0.18517400
H	1.72995200	1.51941100	-2.88485700	C	1.72894500	2.43285400	-0.47322600
H	3.03238700	2.48183300	-3.58870200	H	2.09358900	3.01993200	0.37471000
C	4.60508200	-1.81724600	0.29855600	H	1.93090500	2.97473500	-1.40251400
H	3.66071700	-2.04475400	0.80119800	H	0.65833600	2.27300800	-0.36780000
H	4.80934200	-2.61368700	-0.42637900	Pd	0.05419400	-0.89192200	-0.30248500
H	5.39951700	-1.84097900	1.04907800	C	-3.82745500	-3.00415400	-0.24964800

O	-3.31051800	-0.76704500	0.44017900	H	6.54103000	3.02174300	-1.05976000
O	-1.66387600	-2.11202700	-0.38167100	N	2.24734700	1.38038300	-0.43074700
F	-5.08285700	-2.68661900	0.08948300	C	3.74543400	-3.20074600	0.03036300
F	-3.82605900	-3.38569300	-1.54164700	H	4.39080000	-3.15816800	-0.85493200
F	-3.44440200	-4.05822600	0.49814600	H	4.37565400	-3.02603300	0.91064400
F	-1.59019400	4.06988600	-0.81260100	H	3.28542600	-4.18780500	0.09911800
F	-3.65033900	4.47207500	-0.21785600	C	1.41752300	2.57973400	-0.48603500
F	-2.02315000	4.84214600	1.17741000	H	1.56704900	3.18467800	0.41450200
C	-0.28648300	-0.66648300	1.73012400	H	1.69298700	3.16669300	-1.36668700
H	-0.62750000	-1.66619000	1.99414500	H	0.37145400	2.28773900	-0.56262900
C	0.83954500	-0.23733400	2.63267000	Pd	0.17359500	-0.96249400	-0.54336900
F	1.34144600	0.97534200	2.32089300	C	-3.60924900	-3.02763400	0.05068800
F	0.35837600	-0.16083900	3.89358300	O	-2.38318100	-1.24762300	1.07123900
F	1.87127000	-1.11032900	2.65559000	O	-1.47911100	-2.29884500	-0.71721300
H	-1.07982900	0.08134900	1.72081500	F	-4.74098700	-2.35302800	0.31772100
C	2.88131300	-1.05646600	-0.29992500	F	-3.73448800	-3.58919000	-1.16002000
C	-0.86528400	0.49381700	-2.24467900	F	-3.48569000	-4.01513700	0.96120300
C	-1.63015300	1.38490700	-3.18282800	F	-2.90998800	4.56553900	0.66607900
O	-0.17618000	-0.48018400	-2.61500400	F	-3.65793500	3.40105100	-1.01430200
O	-0.96162700	0.75203800	-0.96863000	F	-4.80871600	3.51591000	0.83346200
H	5.78776500	-1.78729600	-0.40921900	C	0.53905200	0.05412300	1.47207800
C	-2.85507800	-1.80953100	-0.03524700	H	-0.26830900	-0.63378300	1.73468200
H	-2.64361700	0.98258400	-3.29660300	C	1.59208800	-0.01494800	2.55402900
H	-1.71261700	2.39337100	-2.77228300	F	2.59767500	0.87221700	2.40327400
H	-1.14782600	1.39544000	-4.16260100	F	0.97994500	0.27830100	3.72229500
br-TS4				F	2.14213400	-1.23955800	2.68618100
Imaginary Frequency: -303.9683				H	0.12306700	1.05143200	1.36418500
C	2.68542000	-2.14426300	-0.05112000	C	2.95880700	-0.75304100	-0.17328900
O	1.46730000	-2.51037300	-0.01434600	C	-1.00233000	0.35171200	-2.49903400
O	-1.68291900	2.29132000	1.28682500	C	-1.97634000	1.18519300	-3.29607300
C	-2.81030300	2.20073900	0.84943800	O	-0.22774500	-0.46766900	-3.00767200
O	-3.55781700	1.12939900	0.70873800	O	-1.03669000	0.52619200	-1.19570100
C	-3.56589600	3.44799300	0.33531400	H	5.90716000	-1.18359800	-0.39703800
C	4.12269600	0.05567700	-0.40296900	C	-2.38223500	-2.08305600	0.14716600
C	1.83107100	0.10871300	-0.19397600	H	-1.48240700	1.56695300	-4.19395000
C	3.63781600	1.38607600	-0.55194200	H	-2.80063200	0.53846800	-3.61796800
C	5.50386600	-0.18195600	-0.50584000	H	-2.38686500	2.00415500	-2.70289800
C	4.48876100	2.46997800	-0.78641700	br-IN5			
C	6.35106500	0.89288800	-0.74216100	C	1.55643100	-2.73907800	0.31649900
H	-3.06166100	0.28602900	0.93012200	O	0.40197300	-2.91000600	0.76103200
C	5.85006900	2.20372500	-0.87950700	O	-0.54689700	2.25478500	1.60135500
H	4.10743500	3.48046200	-0.88986400	C	-1.33134000	2.80787400	0.85501600
H	7.42087900	0.72347900	-0.81959600	O	-2.48696500	2.37632000	0.42676900

C	-1.04167900	4.22737600	0.31269600
C	2.63996000	-0.94926800	-1.31039400
C	1.75781700	-0.22751700	0.70859100
C	2.91545600	0.41987600	-1.11861500
C	3.05265500	-1.57957100	-2.49081900
C	3.60890100	1.18092900	-2.06232900
C	3.76094200	-0.83571900	-3.42740400
H	-2.64518400	1.41847700	0.70511300
C	4.03540600	0.52762600	-3.21491900
H	3.81413300	2.23480600	-1.90817000
H	4.09307300	-1.30926600	-4.34601000
H	4.58377200	1.08490600	-3.96845900
N	2.38331100	0.81960800	0.11205800
C	2.55788000	-3.84870900	0.28325700
H	3.04579200	-3.90580800	-0.69447600
H	3.34009700	-3.62500500	1.02023400
H	2.07896100	-4.79860100	0.52734000
C	2.49383800	2.19117500	0.60831700
H	3.50266600	2.37308500	0.98849600
H	2.27704600	2.87729400	-0.21268700
H	1.75391300	2.36975800	1.38388400
Pd	-0.40032900	-1.17354500	-0.28825200
C	-4.65483800	-1.77518600	0.22468200
O	-3.15236700	-0.08616700	1.03781900
O	-2.38554900	-1.71378100	-0.35703500
F	-5.57447600	-1.13011200	0.95280800
F	-5.07151700	-1.79471200	-1.05563600
F	-4.58944400	-3.04733600	0.66344200
F	0.25387300	4.54224300	0.49459400
F	-1.31002400	4.32264400	-1.00166500
F	-1.78849500	5.13645400	0.96100500
C	1.35071200	-0.20654600	2.15698000
H	0.65569300	-1.02135400	2.36362100
C	2.54044300	-0.39854600	3.08697900
F	3.46096200	0.58161900	2.95903500
F	2.14145000	-0.42538400	4.36727600
F	3.17374500	-1.57206500	2.82723000
H	0.83161000	0.72054600	2.40810800
C	1.85766600	-1.36944700	-0.15892600
C	-0.65383900	0.33861900	-2.59794400
C	-1.09017000	1.57139800	-3.37502500
O	-0.27191300	-0.69231100	-3.13633200
O	-0.75689900	0.50663800	-1.28905000
H	2.80734600	-2.61832600	-2.68790600

C	-3.26251900	-1.09110800	0.32973500
H	-0.47223300	1.67263700	-4.27081400
H	-2.12909800	1.42704000	-3.69370600
H	-1.04367500	2.47655300	-2.76692300

3ba

C	-0.08371900	2.31225100	0.30303500
O	-1.24101200	2.61244200	0.59435900
C	1.71371000	0.39190400	0.01429600
C	-0.43171800	-0.18688800	0.53712500
C	1.62149600	-1.01885400	0.14042800
C	2.97039900	0.94117600	-0.30495600
C	2.71500400	-1.87421900	-0.02758900
C	4.06201200	0.09760100	-0.47854900
C	3.93998400	-1.29720400	-0.34123800
H	2.61768600	-2.94963500	0.08540100
H	5.02977400	0.52551800	-0.72499200
H	4.81143600	-1.93059000	-0.47999200
N	0.30665700	-1.34340200	0.44746200
C	0.90282200	3.42056400	-0.02870100
H	1.73737600	3.43000100	0.68254400
H	1.32453900	3.28705700	-1.03175700
H	0.37711000	4.37604200	0.02005100
C	-0.14167000	-2.70667300	0.68475200
H	0.26480900	-3.36089000	-0.09189700
H	0.19613400	-3.06815300	1.66334700
H	-1.22627100	-2.75928300	0.62822400
C	-1.89223500	-0.19192900	0.87592200
H	-2.14411300	0.78922000	1.28049500
C	-2.80428600	-0.40797600	-0.32276000
F	-2.63796500	-1.64333600	-0.87082300
F	-4.09765700	-0.31673800	0.05005400
F	-2.58794900	0.48716700	-1.29861800
H	-2.13881700	-0.95983000	1.61615400
C	0.38498700	0.91537200	0.27450700
H	3.10325400	2.01022700	-0.41785900

b₁¹-IN4

C	-3.57741100	-2.05979400	1.12245300
O	-2.49994000	-1.78668600	1.75916900
O	0.51892500	0.54742300	-1.66072800
C	1.06802300	1.59460900	-1.35863700
O	1.65784100	1.90885900	-0.24055400
C	1.12650600	2.73018100	-2.40535500

C	-5.16263100	-1.04367600	-0.74717900
C	-3.29396500	0.06292900	0.06598900
C	-4.99271600	0.19835200	-1.41248800
C	-6.24415700	-1.85814700	-1.10543000
C	-5.86252000	0.64067300	-2.40664800
C	-7.11984200	-1.42254100	-2.10037400
H	1.51344100	1.19217200	0.46266200
C	-6.93339600	-0.18921500	-2.74374900
H	-5.72049900	1.59686000	-2.90084000
H	-7.96281200	-2.04831500	-2.38067800
H	-7.63220100	0.12734200	-3.51281200
N	-3.84635300	0.83463500	-0.89568600
C	-4.23802700	-3.38203100	1.40294300
H	-5.27197300	-3.22910400	1.73358800
H	-4.27314700	-3.98959300	0.49031300
H	-3.68700300	-3.92046800	2.17665500
C	-3.36790700	2.12447500	-1.37662900
H	-3.28201900	2.09837700	-2.46777500
H	-4.06783400	2.91828500	-1.09285300
H	-2.39125300	2.32506100	-0.94208100
Pd	-1.78389600	0.13282000	1.32145100
C	1.82504300	-0.28573600	3.93417000
O	1.61777000	0.03218400	1.59677100
O	-0.27624600	-0.05911200	2.85380800
F	2.48034700	-1.47513900	3.81876500
F	2.76445400	0.67400400	4.04562900
F	1.11903800	-0.31802000	5.06518900
F	-0.09580400	3.25085300	-2.58646400
F	1.96927600	3.71608500	-2.06541200
F	1.53968900	2.22307500	-3.58808900
C	0.55333600	-2.18570200	-0.24880000
H	0.27365700	-2.19470000	0.80179900
C	-0.23511100	-3.19630800	-1.05852600
C	4.10426400	0.49593000	-2.83257700
C	4.88152400	1.29256100	-1.98686000
C	5.09624100	0.86016600	-0.67585000
C	4.51519100	-0.30608200	-0.15910700
C	3.70723600	-1.01345500	-1.05745200
C	3.48697200	-0.68589700	-2.40045500
H	3.93775200	0.80846200	-3.85942200
H	5.71981200	1.45250000	-0.01201100
I	2.70676800	-2.79710300	-0.25886600
F	-1.53334500	-2.87629300	-1.00069200
F	0.13415400	-3.22219200	-2.35292800

F	-0.08167300	-4.44716600	-0.56955500
H	0.54551300	-1.17474600	-0.67143700
C	2.61823200	-1.45625400	-3.36084300
H	2.76504000	-2.53782900	-3.28584700
H	1.55990500	-1.24047200	-3.18097700
H	2.84339300	-1.15690900	-4.38744300
C	4.78865500	-0.71255800	1.26602400
H	3.86326200	-0.73805300	1.84598200
H	5.26858600	-1.69724200	1.32391300
H	5.46111000	0.00772100	1.73790600
C	5.43368900	2.60890200	-2.47321700
H	5.79642700	2.53824700	-3.50408700
H	4.64152400	3.36788500	-2.45377500
H	6.25269100	2.96344400	-1.84088800
C	-4.06601700	-1.12158200	0.19380700
C	-1.44621500	2.96414900	1.58051600
C	-0.69109000	4.26387900	1.19365600
O	-2.25119300	2.97626900	2.49370300
O	-1.07235500	1.98223400	0.81774000
H	-6.40722700	-2.81479000	-0.61738600
F	0.59993000	4.19380800	1.58249300
F	-0.70153600	4.45900100	-0.14773400
F	-1.23686200	5.34482400	1.76523600
C	0.95966600	-0.06362500	2.66449800

b₁'-TS3

Imaginary Frequency: -150.3280

C	-4.01778700	-2.01671200	0.64425000
O	-2.85861900	-2.09859300	1.18812000
O	1.00370200	1.08457200	-1.44510900
C	1.66376000	1.93995500	-0.88370200
O	2.06295700	1.97220000	0.35995600
C	2.11809400	3.18886200	-1.67437700
C	-5.44362900	-0.38586100	-0.89168200
C	-3.31875200	0.12682300	-0.13863500
C	-5.01943800	0.86381800	-1.41248500
C	-6.71375900	-0.86497100	-1.23619200
C	-5.81756600	1.63629700	-2.25342900
C	-7.51869900	-0.09854800	-2.07827300
H	1.71249800	1.18382800	0.87625600
C	-7.07835300	1.13622000	-2.58104900
H	-5.47931000	2.59347700	-2.63777300
H	-8.50628200	-0.46201200	-2.34811900
H	-7.72819700	1.71375000	-3.23198300

O	-0.40649500	-1.63917300	2.14440100
F	1.37971300	-3.53209500	3.08439800
F	2.77733700	-1.93716600	3.57122900
F	0.85548200	-2.03680300	4.58281700
F	0.18788600	4.26092700	-0.65556400
F	2.22382900	4.45576200	0.09665400
F	1.88087200	3.92005100	-1.98376800
C	-0.51418500	-1.28039200	-0.73385400
H	-0.19618000	-2.26349000	-0.39309100
C	-1.07760200	-1.34271000	-2.13035500
C	4.40526800	1.68381300	-2.14690800
C	5.09875900	2.14550000	-1.02522100
C	5.35565000	1.23945300	0.00509900
C	4.93716400	-0.09824600	-0.04550000
C	4.24681800	-0.50708500	-1.19604200
C	3.96421100	0.35775400	-2.26380700
H	4.18992100	2.37145100	-2.96142900
H	5.89367000	1.57624200	0.88835800
I	3.59297300	-2.57136400	-1.33459500
F	-1.54665300	-0.16036700	-2.57176000
F	-0.07278300	-1.71373000	-2.95620900
F	-2.06421900	-2.25363400	-2.27127100
H	0.24600400	-0.50370700	-0.65417600
C	3.21484500	-0.06319600	-3.50372800
H	3.71921300	-0.88912800	-4.01842700
H	2.20175700	-0.40364400	-3.26377200
H	3.13223000	0.77480900	-4.20201800
C	5.23133300	-1.00671900	1.12231000
H	4.30816900	-1.31294100	1.62614700
H	5.75139000	-1.91791500	0.80713600
H	5.85916600	-0.49193900	1.85581700
C	5.52521900	3.59134100	-0.91748300
H	5.82778800	3.99404400	-1.89044300
H	4.70114400	4.21386500	-0.54785700
H	6.36433200	3.71061800	-0.22431700
C	-4.29153800	-1.10908800	-0.37045300
C	-1.64694800	1.46930900	2.19937000
C	-1.25319300	2.81966100	2.83274400
O	-2.53753800	0.75701500	2.67316500
O	-0.96177900	1.14829700	1.15270200
H	-7.01370400	-1.97984100	-1.27777600
F	-0.11387600	2.67906900	3.52640600
F	-1.06043700	3.74286600	1.87314700
F	-2.21118500	3.25300900	3.65707700

C	0.83029500	-1.34735000	2.30093200
b₁'-IN6			
C	2.78056300	-2.26920500	-0.26587900
O	1.55391600	-2.60887900	-0.05697300
O	-1.59399900	1.65804100	2.13930800
C	-2.47601500	2.09844100	1.43085000
O	-3.38841000	1.43045000	0.76159500
C	-2.57728400	3.62225000	1.20266600
C	4.27224100	-0.08654400	-0.55416700
C	1.99132100	-0.02368400	-0.26142500
C	3.80977900	1.25298800	-0.50273300
C	5.64082000	-0.32545500	-0.72658300
C	4.66391800	2.34795200	-0.61534300
C	6.50218200	0.76407000	-0.84336800
H	-3.20372700	0.44989900	0.81893400
C	6.02199700	2.08289300	-0.78829000
H	4.29307200	3.36697100	-0.57406400
H	7.56561000	0.59034600	-0.97897800
H	6.71783300	2.91104600	-0.88263000
N	2.40804300	1.24748800	-0.31907700
C	3.78213000	-3.38192800	-0.34017800
H	4.34780500	-3.32035600	-1.27660700
H	4.49608500	-3.28875800	0.48739900
H	3.27980500	-4.34856100	-0.27708900
C	1.61640200	2.45955800	-0.11968800
H	2.05277600	3.04127000	0.69690200
H	1.61695200	3.06117800	-1.03401900
H	0.59543900	2.18988800	0.13913000
Pd	0.26588800	-1.01860400	-0.20454200
C	-3.45251700	-3.37900500	-0.21007100
O	-2.98478200	-1.23145500	0.75534500
O	-1.33982800	-2.36389700	-0.33749500
F	-3.01512800	-4.47929300	0.43587400
F	-4.71244200	-3.14277300	0.17268200
F	-3.45416300	-3.64090900	-1.52950500
F	-1.52321700	4.01243800	0.44893100
F	-3.69874900	3.99305900	0.57781800
F	-2.50613400	4.26781200	2.37624900
C	0.03529500	-1.02659100	1.85585900
H	-0.22918900	-2.06977300	2.01854100
C	1.19454700	-0.62401800	2.73118900
F	1.59821200	0.64536100	2.53257700
F	0.78234700	-0.72406900	4.01361400

F	2.27459400	-1.42316000	2.59554700
H	-0.79592100	-0.32809600	1.95904300
C	3.08790800	-0.90463900	-0.38988900
C	-0.89590900	0.52391000	-1.91019900
C	-1.81126900	1.52382100	-2.64578600
O	-0.19543100	-0.29264100	-2.51788300
O	-0.93956100	0.59630900	-0.62127400
H	6.03086400	-1.33772300	-0.76965600
F	-3.08226300	1.10019200	-2.58227700
F	-1.73257100	2.73626200	-2.06976800
F	-1.45498000	1.63470900	-3.92851300
C	-2.52433000	-2.17382300	0.11062500

b₁'-TS4

Imaginary Frequency: -277.6148

C	-3.03818300	-2.03853500	0.29196900
O	-1.86318200	-2.51960300	0.21389600
O	1.59660800	1.76410800	-1.87665000
C	2.74498700	1.63561100	-1.50755200
O	3.39772300	0.52663400	-1.23316800
C	3.67334400	2.85819600	-1.32456000
C	-4.25580800	0.31007000	0.47880000
C	-1.99181400	0.13318800	0.12497600
C	-3.65313000	1.59969300	0.43324500
C	-5.64070700	0.21153000	0.69918500
C	-4.39165300	2.77684000	0.58968100
C	-6.37524500	1.37879600	0.85626900
H	2.81233600	-0.27925300	-1.28159800
C	-5.75865700	2.64677200	0.80113400
H	-3.92137200	3.75351600	0.54749300
H	-7.44654000	1.31791600	1.02254800
H	-6.36487300	3.53885600	0.92578300
N	-2.28078100	1.45539800	0.22367300
C	-4.18697100	-2.99364400	0.40219300
H	-4.74870500	-2.80315000	1.32432900
H	-4.87234300	-2.84705600	-0.44124000
H	-3.82085100	-4.02147100	0.40366700
C	-1.36144700	2.58239800	0.07673700
H	-1.56261600	3.10660700	-0.86311500
H	-1.50165400	3.27110800	0.91425200
H	-0.33471400	2.22242900	0.08189200
Pd	-0.40528400	-1.05040600	0.45907000
C	3.09050900	-3.54923400	0.16546500
O	2.02446800	-1.81905200	-1.12279700

O	1.08685400	-2.47946400	0.82830300
F	4.18774900	-3.26973600	-0.55041800
F	3.43567300	-3.60999800	1.46053700
F	2.64109200	-4.76491500	-0.20907000
F	2.97664000	3.99403400	-1.44965500
F	4.25715000	2.84555800	-0.11633900
F	4.63956500	2.84640500	-2.26219900
C	-0.79162200	-0.24075300	-1.62526600
H	-0.07682200	-1.03702300	-1.84755300
C	-1.93277300	-0.32430100	-2.61450300
F	-2.83316800	0.67223700	-2.50628900
F	-1.38073400	-0.23099800	-3.84317800
F	-2.60174000	-1.49331300	-2.55985300
H	-0.27989300	0.71724000	-1.64608300
C	-3.18292200	-0.62074100	0.27405900
C	1.02782200	0.62883500	2.05908900
C	2.12193700	1.67396500	2.38705000
O	0.32819700	0.12898700	2.92410100
O	0.96766600	0.40057500	0.77729500
H	-6.13221700	-0.75504900	0.74044500
F	3.34032500	1.18347000	2.11478900
F	1.93588600	2.78202800	1.63128200
F	2.07789900	2.03220200	3.67212100
C	1.97984500	-2.49435700	-0.08249300

b₁'-IN7

C	-2.17368500	2.66887400	-0.22792100
O	-1.05991800	3.16116100	0.05269700
O	0.87032600	-1.36802600	2.41108300
C	1.80442400	-1.90142600	1.84468600
O	2.84979500	-1.33190900	1.30083100
C	1.89001400	-3.44203000	1.74221200
C	-2.83652000	0.36075000	-1.34469800
C	-1.85929400	0.32629500	0.76087000
C	-2.78697100	-0.95734600	-0.84694500
C	-3.35655800	0.60097700	-2.62285200
C	-3.24046300	-2.05155000	-1.58606100
C	-3.83461700	-0.47900800	-3.35586100
H	2.75691900	-0.33295500	1.30818900
C	-3.77359800	-1.78835800	-2.84458600
H	-3.17807900	-3.06432600	-1.20365500
H	-4.24410800	-0.31315200	-4.34733100
H	-4.13991100	-2.61314300	-3.44808100
N	-2.21395400	-0.93966000	0.42949700

C	-3.38383900	3.52030100	-0.42710000
H	-3.92124000	3.22809500	-1.33463500
H	-4.06316600	3.34336800	0.41738500
H	-3.10719900	4.57538500	-0.46662400
C	-1.96271200	-2.16899700	1.18396000
H	-2.91459600	-2.61908200	1.47843800
H	-1.39874700	-2.85462000	0.54887100
H	-1.35870000	-1.95889200	2.06135100
Pd	0.05356900	1.38680300	-0.48545700
C	4.12964400	2.73980400	-0.25673000
O	2.74817300	1.31625000	1.11040300
O	1.91048100	2.19722900	-0.80559200
F	5.10956400	2.39913600	0.58861100
F	4.53769100	2.46722100	-1.50778700
F	3.93168700	4.06971200	-0.15841900
F	0.66113500	-3.97878400	1.86211300
F	2.41428900	-3.84436700	0.58014300
F	2.65180000	-3.91966800	2.74419300
C	-1.48361100	0.72991300	2.16025700
H	-1.02065900	1.71812500	2.15448800
C	-2.70274800	0.82078600	3.06758800
F	-3.33803900	-0.36268000	3.19623500
F	-2.35241700	1.23987600	4.29194400
F	-3.60786300	1.70555300	2.57125400
H	-0.75068900	0.04223300	2.58909900
C	-2.19287500	1.19149800	-0.34062800
C	0.54238200	-0.85756300	-2.11328300
C	0.96716500	-2.34424200	-2.25346100
O	0.10879100	-0.23496300	-3.06307400
O	0.69938200	-0.46908200	-0.87911200
H	-3.36827900	1.60021400	-3.04740700
F	2.25942400	-2.51550900	-1.93853900
F	0.22922100	-3.11724500	-1.41098700
F	0.76696400	-2.79298200	-3.49557400
C	2.81296000	1.98395300	0.07519800

b₁''-IN4

C	4.14067800	1.70154300	-1.11987100
O	2.94728300	2.18223700	-1.10155200
O	0.25159400	-0.19073500	0.94925800
C	-0.33144200	0.22245500	2.01101100
O	-0.36960000	1.35342800	2.50283800
C	-1.03128500	-0.91720600	2.79618100
C	5.49048100	-0.39086600	-0.19994500

C	3.23054100	-0.07031400	0.18823300
C	4.96924100	-1.44512900	0.58825800
C	6.84865300	-0.40676400	-0.54157300
C	5.75290200	-2.50502000	1.04165100
C	7.64055300	-1.46233800	-0.09309000
H	-0.19482200	2.74648000	1.78355300
C	7.10180600	-2.49811200	0.68796900
H	5.33931500	-3.30535700	1.64697900
H	8.69510600	-1.48444600	-0.35104700
H	7.74443900	-3.30614200	1.02372000
N	3.59126000	-1.21509700	0.80374400
C	5.18932900	2.48549100	-1.85058400
H	5.65045900	1.86758300	-2.62996000
H	4.75097900	3.37626400	-2.30372400
H	5.98519800	2.78452700	-1.15786900
C	2.76457400	-2.11279400	1.59928100
H	2.75639200	-3.11031800	1.14875000
H	3.16715300	-2.18477100	2.61461900
H	1.75130800	-1.72400100	1.63747700
Pd	1.61323000	1.03264200	-0.05997300
C	-0.81134000	4.77652300	-0.71428300
O	-0.35549900	3.64451900	1.32199400
F	-2.15150700	4.62893600	-0.88690500
F	-0.59563000	5.89279800	-0.02422600
F	-0.24504700	4.87349800	-1.91483600
F	-0.13090800	-1.53265900	3.58188700
F	-2.02848300	-0.46116500	3.55678800
F	-1.54017600	-1.85128600	1.95294000
O	0.08440400	2.55511300	-0.61897600
C	-0.88443300	-2.18821100	-1.29215300
H	-0.27392700	-1.89154100	-2.14375100
C	-0.61134700	-3.63125000	-0.90242400
C	-4.59813100	-0.05875300	1.63337100
C	-4.36335100	1.31007000	1.45915200
C	-3.79106900	1.74411500	0.25812000
C	-3.41383300	0.85803800	-0.76169500
C	-3.64286700	-0.49425400	-0.47991500
C	-4.24747600	-1.01456800	0.67157600
H	-5.05839100	-0.40871800	2.55307200
H	-3.62020900	2.80464400	0.09863300
I	-2.97716500	-1.94027700	-1.98725700
F	-1.33700000	-4.01833700	0.15678500
F	-0.86999100	-4.47147900	-1.91891300
F	0.69079500	-3.72451300	-0.58739900

H	-0.76995400	-1.50618000	-0.44557800
C	-4.52402700	-2.47605400	0.92434400
H	-5.21548600	-2.89158300	0.18224500
H	-3.60710800	-3.07225400	0.90433500
H	-4.98070800	-2.60640600	1.90766600
C	-2.81379400	1.39243900	-2.03987900
H	-1.77663600	1.06548900	-2.17571800
H	-3.38756000	1.08030800	-2.91944200
H	-2.80261600	2.48296000	-2.02115100
C	-4.69212000	2.28831500	2.55737000
H	-4.81138300	3.30456100	2.17183800
H	-5.60923600	2.00730900	3.08419400
H	-3.88099500	2.30469500	3.29689600
C	4.36701500	0.48690400	-0.45128000
H	7.28452100	0.38523000	-1.14272100
C	-0.28715500	3.52938200	0.03359900

bl''-TS3

Imaginary Frequency: -165.2240

C	-3.27140100	2.22256900	-0.30914700
O	-1.98711100	2.31015800	-0.40625300
O	-0.19517600	-1.35890200	-0.88630200
C	0.29830800	-1.63314300	-2.03985000
O	0.40269800	-0.90085200	-3.02623200
C	0.74821000	-3.11038600	-2.18947400
C	-5.15963500	0.36135300	-0.15754200
C	-2.91890000	-0.13662500	-0.36271500
C	-4.95745900	-1.04103900	-0.16050900
C	-6.46376200	0.86064900	-0.04718800
C	-6.00622200	-1.95451000	-0.05766200
C	-7.51726000	-0.04416900	0.05776000
H	0.77311200	0.62845600	-3.14638500
C	-7.29315300	-1.43238200	0.05278500
H	-5.83663200	-3.02615300	-0.06351800
H	-8.53307900	0.32889400	0.14452400
H	-8.13671000	-2.11043300	0.13531300
N	-3.57396600	-1.30621400	-0.28307100
C	-4.04096000	3.50407200	-0.22746200
H	-4.62026500	3.53357500	0.70320600
H	-3.36426300	4.35933500	-0.26177200
H	-4.75314200	3.56848300	-1.05870500
C	-3.02716300	-2.66036800	-0.27953000
H	-3.31526700	-3.16499000	0.64733100
H	-3.42438000	-3.22024600	-1.13158800

H	-1.94371200	-2.60981400	-0.34909600
Pd	-1.07030800	0.49561900	-0.62971200
C	2.21817700	3.32582600	-1.98164700
O	1.22106400	1.54351000	-3.18295400
F	3.50332300	2.94717600	-2.10816200
F	1.90251200	4.14245300	-2.98575200
F	2.07348300	3.97164900	-0.82136700
F	-0.22669200	-3.79626900	-2.80800200
F	1.86673100	-3.19224100	-2.91956300
F	0.97531000	-3.68783000	-0.99659500
O	0.81579500	1.65940000	-0.95646000
C	-0.04000600	0.33272100	1.60986300
H	0.36085900	1.30558900	1.36380700
C	-1.17398700	0.24383300	2.61794100
C	3.87630100	-2.22665800	-0.32593700
C	4.52780400	-1.26519500	-1.10845700
C	4.58474100	0.04856300	-0.63333400
C	3.99972600	0.43643400	0.58078800
C	3.33646500	-0.57052700	1.29988100
C	3.26912600	-1.91598500	0.89593100
H	3.83278000	-3.25484100	-0.67414500
H	5.09988300	0.80453100	-1.21928900
I	2.29070400	-0.00817400	3.10647900
F	-1.81553900	-0.93105000	2.49506000
F	-0.74271200	0.34545000	3.88848300
F	-2.05529800	1.23914900	2.42133900
H	0.33043600	-0.57119600	1.15166800
C	2.59380600	-3.01042900	1.68725000
H	2.98058200	-3.06802000	2.71002000
H	1.50924900	-2.86225900	1.75372600
H	2.75888600	-3.97833200	1.20936000
C	4.11422400	1.87196500	1.03436300
H	3.13915700	2.37100400	1.06995400
H	4.55783400	1.94598900	2.03282700
H	4.74411400	2.43789000	0.34475900
C	5.15377900	-1.65271400	-2.42495600
H	5.53487400	-0.78097300	-2.96375500
H	5.99000800	-2.34586100	-2.27280400
H	4.42438400	-2.16152200	-3.06523600
C	-3.83813600	0.93823700	-0.28133600
H	-6.65785100	1.92848800	-0.04344800
C	1.32163400	2.06586400	-2.00568300

bl''-IN5

C	-3.09594500	-0.53812400	-2.37714300
O	-1.80422700	-0.65198600	-2.30829900
O	-0.44478200	-0.40502400	1.56177700
C	-0.46233200	-1.65266800	1.84170500
O	-0.81015300	-2.52829100	1.02030700
C	-0.09027400	-2.06843500	3.28333300
C	-5.14920800	0.08441700	-0.81462900
C	-2.98033600	0.02735900	-0.05993600
C	-5.08433400	0.42293300	0.55886900
C	-6.39451500	0.06236200	-1.45444900
C	-6.21297000	0.74348800	1.31215900
C	-7.52803200	0.37975000	-0.71020300
H	0.34786700	-3.18549900	-0.04960100
C	-7.43964000	0.71617000	0.65240500
H	-6.14908700	1.00254100	2.36352900
H	-8.50086900	0.36858100	-1.19148000
H	-8.34325700	0.95893200	1.20228100
N	-3.73330700	0.37769200	0.98630300
C	-3.72485600	-0.81926300	-3.70481300
H	-4.28487800	0.06054200	-4.04405600
H	-2.96431100	-1.07414000	-4.44437000
H	-4.43683500	-1.64815000	-3.61231700
C	-3.32602000	0.72683500	2.34834200
H	-3.64291500	1.75054800	2.56395100
H	-3.80238100	0.04102600	3.05450500
H	-2.24556600	0.65844200	2.43241200
Pd	-1.09154200	-0.44505900	-0.40906200
C	2.33603300	-2.53431700	-2.55215600
O	1.03636500	-3.35429900	-0.75237500
F	3.31887700	-3.34027400	-2.14409400
F	1.66647600	-3.13009100	-3.55108500
F	2.84857700	-1.38819400	-2.99414400
F	-1.19929900	-2.50638900	3.89422900
F	0.80902100	-3.05911200	3.24219800
F	0.41280400	-1.04573400	3.97981600
O	0.84364900	-1.14686800	-1.26467900
C	-0.48814200	1.48455500	-0.92563400
H	-0.68950400	1.51790900	-1.99468900
C	-1.11847100	2.63737700	-0.17636200
C	3.23756700	-0.70992100	1.97788100
C	3.91882100	-1.60716700	1.15081700
C	4.44566000	-1.12144400	-0.05082400
C	4.30244400	0.21552300	-0.44947700
C	3.58563700	1.06636300	0.40757000

C	3.06041400	0.64073200	1.63828200
H	2.84979300	-1.05591800	2.93230300
H	5.00160600	-1.79479200	-0.69812600
I	3.29120200	3.12560100	-0.18941200
F	-1.00450900	2.49865700	1.15926700
F	-0.47662500	3.75651900	-0.54386900
F	-2.42415100	2.79475600	-0.46463000
H	0.57012300	1.37091900	-0.68246500
C	2.34504900	1.55746300	2.60156200
H	2.98880300	2.38953600	2.90762100
H	1.44451600	1.99805600	2.15962300
H	2.04459700	1.01091800	3.49864300
C	4.92161600	0.67056600	-1.74791200
H	4.16970800	1.06098200	-2.44275400
H	5.64749200	1.47382900	-1.58004400
H	5.43906700	-0.15773200	-2.23885200
C	4.11441100	-3.05029600	1.55527200
H	4.06751000	-3.71757700	0.68791600
H	5.09476600	-3.19844200	2.02541200
H	3.35518900	-3.37049200	2.27568800
C	-3.77981000	-0.16691900	-1.21389800
H	-6.48359200	-0.19399800	-2.50506700
C	1.32476000	-2.27126000	-1.41101600

bl''-IN6

C	1.41033100	-2.44580400	-0.74989300
O	0.16409900	-2.24999300	-0.44015200
O	-0.59112200	1.68745400	0.43840500
C	-0.90246000	2.02410400	-0.75555600
O	-0.92708000	1.19641400	-1.69581900
C	-1.17610500	3.52597600	-0.99432000
C	3.72316300	-1.13994500	-0.72835300
C	1.74707700	-0.18924600	-0.04127200
C	3.92211000	0.20366100	-0.32774300
C	4.81728100	-1.88671200	-1.18170700
C	5.16974800	0.82518700	-0.36046200
C	6.06753300	-1.27402500	-1.22039700
H	-2.38188200	0.27173800	-1.97883200
C	6.24222500	0.06130000	-0.81577600
H	5.30836800	1.85546400	-0.05091600
H	6.92613900	-1.83882500	-1.56954400
H	7.23054000	0.50753100	-0.85913300
N	2.68312400	0.75400100	0.09129800
C	1.75785100	-3.78861600	-1.30980100

H	2.51081500	-4.27249100	-0.67594000
H	0.87146500	-4.42195300	-1.36913200
H	2.19299300	-3.67374900	-2.30975600
C	2.55592000	2.12899900	0.58143100
H	3.23878800	2.27059300	1.42272300
H	2.81657200	2.82403300	-0.22162000
H	1.53612100	2.30625600	0.90853200
Pd	-0.22047000	-0.32913000	0.11574800
C	-4.55867200	-1.65535900	-0.48589900
O	-3.21801700	-0.25711200	-1.86048800
F	-5.61168900	-0.93122800	-0.86134600
F	-4.49134300	-2.76791200	-1.22949900
F	-4.67421700	-1.98669300	0.79761500
F	0.00947700	4.16213100	-0.98882300
F	-1.76934400	3.70788800	-2.17052400
F	-1.94249100	4.02048200	-0.02141900
O	-2.37546800	-0.86357500	0.16107700
C	-0.02107600	-1.06614700	2.04625300
H	0.89149700	-1.65602400	2.07870500
C	-0.02360300	0.03462300	3.08505400
F	-1.13742200	0.77341100	3.04041500
F	0.05455700	-0.55357900	4.29156900
F	1.03897000	0.85460900	2.94994100
H	-0.92691300	-1.67206200	2.08141400
C	2.30868400	-1.39269600	-0.53809400
H	4.70341600	-2.91860900	-1.49741200
C	-3.25099800	-0.85486900	-0.70648900

b₁''-TS4

Imaginary Frequency: -255.7776

C	1.31190200	-2.63580700	-0.34095000
O	0.09923700	-2.39150300	-0.01294700
O	-0.53642400	1.65568300	0.24328700
C	-0.91935900	2.09517900	-0.90433700
O	-1.20026200	1.40744000	-1.89176700
C	-0.92573600	3.64262400	-1.00198500
C	3.59279800	-1.32189600	-0.66044400
C	1.70240700	-0.30147100	0.15429400
C	3.82525900	0.06854600	-0.43251500
C	4.63208600	-2.11700500	-1.17811700
C	5.05434500	0.67659900	-0.70631400
C	5.85215200	-1.51567600	-1.44455000
H	-2.45734100	0.35299400	-2.00573800
C	6.06045100	-0.13615000	-1.21206800

H	5.22066500	1.73559500	-0.54277000
H	6.66759300	-2.11239400	-1.84051000
H	7.02940600	0.29780000	-1.43735500
N	2.65844000	0.65360700	0.07593500
C	1.65836700	-4.02251100	-0.77857400
H	2.47744800	-4.41818300	-0.16620400
H	0.78800500	-4.67522700	-0.69650300
H	2.00421500	-4.00768600	-1.81984000
C	2.54503900	2.07063000	0.43776400
H	3.46699200	2.38077100	0.93372700
H	2.38491300	2.67839400	-0.45632100
H	1.70517700	2.20252800	1.11485200
Pd	-0.27544700	-0.36265700	0.17851300
C	-4.54142000	-1.71984200	-0.55960200
O	-3.27463000	-0.22505600	-1.90879700
F	-5.61906200	-1.10794600	-1.04644400
F	-4.35867400	-2.88208200	-1.20541200
F	-4.70883900	-1.95962000	0.73899900
F	0.34697100	4.04867600	-1.21541500
F	-1.68147100	4.04519600	-2.01800300
F	-1.36500700	4.19701700	0.13015100
O	-2.39059600	-0.86500300	0.08230000
C	0.89767400	-0.54498000	2.17331600
H	1.94216800	-0.35241700	2.39719100
C	0.03106800	0.33925600	3.06125300
F	-1.28211500	0.19307500	2.83729600
F	0.28888400	-0.04737400	4.32488100
F	0.34724200	1.63834300	2.94764300
H	0.64712000	-1.59783100	2.27534400
C	2.23220700	-1.55196400	-0.27483900
H	4.48876100	-3.17589900	-1.36445000
C	-3.27484300	-0.85578700	-0.77807300

b₁''-IN7

C	0.50138200	-2.21575700	-1.98623900
O	-0.68309800	-2.27552700	-1.60624000
O	0.25232100	0.93899200	0.76860000
C	0.01234900	2.18198500	0.55770200
O	-0.82314800	2.69668600	-0.18594500
C	0.92596000	3.09916300	1.41770100
C	2.12465400	-0.14582500	-1.74861900
C	1.91635700	-1.55245000	0.09998600
C	3.04666000	0.21410700	-0.75020000
C	2.08696600	0.56672000	-2.95199100

C	3.93483700	1.27713500	-0.89677600
C	2.98736100	1.61709600	-3.12187100
H	-2.22542900	2.10747800	-0.50957500
C	3.89335700	1.96940700	-2.10710200
H	4.62544300	1.56663900	-0.11293700
H	2.98182300	2.18010100	-4.04954500
H	4.57257800	2.80098300	-2.26433800
N	2.89347600	-0.66821500	0.34101200
C	1.01666100	-3.00309100	-3.13913100
H	1.84975200	-3.63767500	-2.80932800
H	0.22244100	-3.61487700	-3.57118300
H	1.42675800	-2.32629900	-3.89889600
C	3.68304200	-0.50875100	1.56694000
H	4.73921700	-0.44160600	1.29751800
H	3.36454300	0.40823400	2.06899200
H	3.52769100	-1.35182500	2.23396200
Pd	-0.53923100	-0.53070000	-0.36810400
C	-4.94141800	0.24593500	-0.22767600
O	-3.21347600	1.84292100	-0.57199700
F	-5.68628200	1.27845800	0.16170600
F	-5.28193900	-0.10041800	-1.47981900
F	-5.15024400	-0.78846000	0.58509300
F	2.19680100	2.62826700	1.42405500
F	0.94175600	4.34057000	0.94498400
F	0.47970900	3.10884000	2.68075900
O	-2.61683000	-0.26646100	0.03084600
C	1.64004100	-2.75208600	0.96545600
H	2.58883900	-3.19270500	1.28945500
C	0.79952600	-2.53681800	2.23372300
F	-0.48698300	-2.26522000	1.93729400
F	0.82759000	-3.65580700	2.96652300
F	1.27166600	-1.52189500	2.98122400
H	1.11836500	-3.51440300	0.38071600
C	1.31938200	-1.23328600	-1.18866100
H	1.37145900	0.32495300	-3.73255800
C	-3.43845400	0.62132100	-0.23575500

Pd(OAc)(TFA)_catalyst

Pd(OAc)(TFA)

O	2.57105900	1.08567500	-0.00506600
C	3.25021100	-0.00007600	0.00656400
O	2.57090500	-1.08574600	-0.00407100
C	4.74253800	-0.00019200	0.05929000
Pd	0.81602000	0.00009100	-0.02008000

C	-3.15482400	0.00004200	0.01257000
C	-1.62001100	0.00032100	-0.03545300
O	-0.98388100	-1.09597400	-0.03671600
O	-0.98373300	1.09651200	-0.03569900
F	-3.64244400	-1.08600200	-0.59673000
F	-3.55598000	-0.00872000	1.29589300
F	-3.64274700	1.09391800	-0.58206000
H	5.13405400	-0.89755900	-0.42565600
H	5.06325100	-0.00501100	1.10786300
H	5.13404500	0.90131400	-0.41784900

Pd(OAc)(TFA)

a2-IN1

C	-0.88258700	0.22722900	2.09963600
O	0.28609000	-0.22883200	2.03387600
O	2.87079800	-1.49875300	-0.90597500
C	2.77083900	-2.61169300	-0.28722500
O	1.96326600	-2.66077200	0.70672900
C	3.58888300	-3.80142500	-0.68686300
C	-1.91728000	-0.03556800	1.13179100
C	-2.05575600	-1.10396500	0.15585500
C	-3.00006700	0.81418200	0.93040300
C	-3.22586300	-0.81206200	-0.59045800
C	-1.37086900	-2.30092000	-0.11100900
H	-3.22924900	1.74868200	1.42322800
C	-3.70456000	-1.63953800	-1.60875300
C	-1.84069300	-3.12925800	-1.12635400
H	-0.49842900	-2.58953300	0.46355400
C	-2.98736500	-2.80200000	-1.87311600
H	-4.60220600	-1.39350100	-2.16805900
H	-1.31198700	-4.05308900	-1.34318200
H	-3.32496600	-3.47080100	-2.65949700
N	-3.76770000	0.37583400	-0.09858100
C	-1.18071700	1.08175000	3.30952700
H	-0.52174000	0.78049700	4.12732200
H	-0.93750900	2.11682700	3.04377600
H	-2.22410900	1.01782700	3.62672300
C	-4.94353100	1.04051500	-0.63331500
H	-4.78599100	1.31100400	-1.68261200
H	-5.81940600	0.38682200	-0.56131300
H	-5.13139100	1.94917000	-0.05862800
Pd	1.49653600	-0.63632600	0.40659700
C	1.25826300	3.45108000	-1.01148100
O	1.52607300	1.21843500	-0.39331100

F	2.57917200	3.69870500	-0.92719100
F	0.96921900	3.16947100	-2.29900100
F	0.60507200	4.57607300	-0.68107300
O	-0.02089300	2.44854100	0.75751800
C	0.84603300	2.26866600	-0.08621800
H	3.05403200	-4.72374600	-0.44730300
H	3.82389600	-3.75558500	-1.75279800
H	4.53008600	-3.79358100	-0.12442900

a₂-TS0

Imaginary Frequency: -1159.6670

C	-0.92021100	-2.03214200	-1.06317700
O	0.15521300	-1.44682100	-0.81092100
O	0.98085700	2.48324600	0.09072400
C	0.37002000	3.21135000	-0.76445400
O	-0.63787200	2.83136500	-1.43200300
C	0.91607400	4.60488500	-0.98255600
C	-2.19597100	-1.49672500	-0.67288300
C	-2.42100100	-0.22564600	-0.02503200
C	-3.38491200	-2.21610200	-0.55904100
C	-3.72992200	-0.27865100	0.50987700
C	-1.60838200	0.91450700	0.17264500
H	-3.61899700	-3.21707700	-0.89477400
C	-4.25198900	0.73389700	1.31631400
C	-2.12959200	1.89582900	1.03853700
H	-1.05119300	1.64594100	-0.79209900
C	-3.41575600	1.81239500	1.59532100
H	-5.25787400	0.68314500	1.72223800
H	-1.53575300	2.78179600	1.23886000
H	-3.77235700	2.61251100	2.23710500
N	-4.30075200	-1.49869600	0.13813600
C	-0.81176500	-3.38759600	-1.72439700
H	0.06587600	-3.39499800	-2.37465300
H	-0.65924700	-4.15338000	-0.95371300
H	-1.70230200	-3.64413100	-2.30406000
C	-5.64153000	-1.93498200	0.49371000
H	-5.75345800	-1.97381400	1.58219600
H	-6.38903500	-1.24938500	0.08163600
H	-5.81242100	-2.93222200	0.08440000
Pd	0.48283800	0.49527700	-0.11711700
C	4.36480900	-1.13684100	0.48790100
O	2.47716400	0.04994400	-0.25173300
F	4.53565400	-1.83967300	-0.65466900
F	5.14605400	-0.04018500	0.41395300

F	4.81230200	-1.89236100	1.50205900
O	2.23438900	-1.23495100	1.60467900
C	2.87078100	-0.75943700	0.67517600
H	0.12365200	5.27617000	-1.31896800
H	1.38557900	4.97843500	-0.07041500
H	1.68423600	4.55438700	-1.76299100

a₂-IN2

C	-1.39991600	-2.19204400	-0.36702600
O	-0.29595700	-1.59820100	-0.43748300
O	0.80044200	2.40954100	0.03256200
C	1.93434300	2.89571300	-0.16042200
O	3.00992600	2.22461200	-0.44470400
C	2.13662700	4.38562200	-0.06752400
C	-2.61741400	-1.48104900	-0.14733700
C	-2.69382300	-0.04642400	-0.00327300
C	-3.92335000	-1.96075100	-0.06591300
C	-4.06050900	0.27387200	0.15592200
C	-1.70990700	0.95054700	0.00500300
H	-4.29808700	-2.97331700	-0.12634100
C	-4.50144900	1.58810500	0.32103900
C	-2.14832800	2.26684100	0.16730400
H	2.84140300	1.20394700	-0.43861400
C	-3.51648700	2.57379300	0.32125700
H	-5.55111200	1.83728000	0.44352800
H	-1.42535100	3.07442600	0.18308800
H	-3.81015200	3.61283900	0.44714100
N	-4.78364300	-0.92525800	0.11382000
C	-1.35853000	-3.69063300	-0.54558600
H	-0.99750000	-3.92233400	-1.55382400
H	-0.63523900	-4.10853100	0.16181100
H	-2.32970100	-4.16757700	-0.39678800
C	-6.22620300	-1.02697300	0.25214500
H	-6.54516600	-0.63643000	1.22430800
H	-6.72622500	-0.45887300	-0.53938000
H	-6.52122000	-2.07533200	0.17686900
Pd	0.18782300	0.39020500	-0.15314500
C	4.27983400	-1.35808700	0.18491900
O	2.29035500	-0.18667700	-0.32509000
F	4.43191800	-1.97165600	-1.00820500
F	4.97528700	-0.19595200	0.13575800
F	4.84214900	-2.13184800	1.12197500
O	2.21287300	-1.71684200	1.35012300
C	2.77946800	-1.09008800	0.47552300

H	2.57133700	4.75325600	-1.00249500
H	1.18999000	4.88830800	0.13068000
H	2.85124700	4.60472200	0.73274000

a2-IN1'

C	0.37607600	0.14215600	2.25740200
O	-0.85149400	0.23119300	1.99433800
O	-3.34879600	-0.28268400	-1.24255900
C	-4.15295700	0.38769300	-0.50564800
O	-3.70226200	0.81878500	0.61046100
C	-5.57143100	0.62607100	-0.92400600
C	1.40216700	0.68264100	1.41244700
C	1.30027800	1.67495800	0.35639300
C	2.72529100	0.24305500	1.40311900
C	2.58209900	1.75867000	-0.23819000
C	0.28646400	2.53191000	-0.09681000
H	3.19110400	-0.52712100	2.00215400
C	2.87420400	2.63286500	-1.28689800
C	0.56853300	3.40690000	-1.14193100
H	-0.69663000	2.51838300	0.36093100
C	1.84326400	3.45318100	-1.73565200
H	3.86187800	2.67690300	-1.73562100
H	-0.21154300	4.06861500	-1.50714900
H	2.02894900	4.14429000	-2.55263100
N	3.42513500	0.86285800	0.42502900
C	0.72526500	-0.58896400	3.53062900
H	-0.03387300	-0.36711200	4.28556700
H	0.67322200	-1.66241900	3.31165500
H	1.71523600	-0.33558000	3.91626300
C	4.77966800	0.53531600	0.01291500
H	4.76669900	0.00835600	-0.94669400
H	5.37689000	1.44733900	-0.08007500
H	5.23555000	-0.10905200	0.76686100
Pd	-1.85981200	-0.09301300	0.19676900
C	1.43606500	-2.50578600	-1.15739200
O	-0.33023200	-1.01623800	-0.75265800
F	1.06922000	-2.53137100	-2.44681600
F	2.51527500	-1.67825900	-1.05571700
F	1.84438400	-3.73490200	-0.81316700
O	0.19265100	-2.50541800	0.89253200
C	0.30954000	-1.99735400	-0.21311200
H	-5.63799300	0.68240600	-2.01324600
H	-6.19020600	-0.21313700	-0.58469000
H	-5.94989000	1.54251000	-0.46513800

a2-TS1'

Imaginary Frequency: -37.0430

C	-1.15285400	-2.09729600	-1.03959300
O	-0.09307200	-1.44177400	-1.14116600
O	1.16186300	2.03396900	0.61290600
C	0.98113800	3.05417600	-0.18815900
O	0.33186200	2.98395800	-1.23752900
C	1.65743000	4.32616000	0.28199600
C	-2.35682000	-1.53816800	-0.47501000
C	-2.65307300	-0.13542000	-0.27278500
C	-3.40414600	-2.24367700	0.11067100
C	-3.86018800	-0.07746800	0.46325500
C	-2.04442600	1.06651200	-0.67506200
H	-3.55037900	-3.31134100	0.19889000
C	-4.44351200	1.12937200	0.85654900
C	-2.60900700	2.27600500	-0.26899000
H	-1.23825300	1.10709400	-1.41922600
C	-3.79038000	2.30494600	0.49242200
H	-5.37011100	1.15663400	1.42202300
H	-2.12228900	3.19633900	-0.57107400
H	-4.21200000	3.26085100	0.78796900
N	-4.29248700	-1.38758600	0.67901800
C	-1.13526800	-3.51100900	-1.56977600
H	-1.48351000	-3.50515300	-2.61058300
H	-0.11340700	-3.89460000	-1.54933400
H	-1.79435200	-4.17633100	-1.00495000
C	-5.48356900	-1.75936500	1.42543300
H	-5.41686300	-1.39663200	2.45633900
H	-6.37701500	-1.33617500	0.95475800
H	-5.57213000	-2.84710600	1.43771500
Pd	0.45731900	0.38587200	-0.23701700
C	4.25021500	-1.27530500	0.67176300
O	2.00374400	-0.62678100	0.58486100
F	4.41124400	-0.84640700	1.93898400
F	3.94868200	-2.59148300	0.71642400
F	5.42226500	-1.14367800	0.03763400
O	3.37198400	0.15094200	-1.06196800
C	3.12695500	-0.47831400	-0.05023200
H	1.54632600	4.45121200	1.36283800
H	2.72923100	4.25831500	0.06363100
H	1.23975200	5.18458000	-0.24841900

a2-IN2'

C	-1.29559700	-2.18353900	-0.89018500
O	-0.18075000	-1.62114600	-0.93105700
O	1.16607800	1.93598700	0.58051500
C	1.11859800	2.93528500	-0.26933200
O	0.49397700	2.91929300	-1.33139600
C	1.93504400	4.13181500	0.18759000
C	-2.48170800	-1.50655400	-0.42325600
C	-2.65582100	-0.08019100	-0.25498500
C	-3.62401100	-2.10205900	0.10423600
C	-3.89318500	0.10157500	0.40746100
C	-1.91179100	1.05566000	-0.62757300
H	-3.87550200	-3.14995700	0.19211000
C	-4.38040300	1.36297800	0.75725300
C	-2.38530200	2.31913700	-0.26587900
H	-1.09552800	1.02969800	-1.37241300
C	-3.59973300	2.46814200	0.42458200
H	-5.33210400	1.48412000	1.26596700
H	-1.80181100	3.18408600	-0.55898000
H	-3.94697000	3.46300900	0.68586500
N	-4.46034900	-1.15816800	0.60841700
C	-1.36329700	-3.61190500	-1.37464200
H	-1.68497600	-3.61921700	-2.42388700
H	-0.37183000	-4.06413700	-1.31182600
H	-2.08084700	-4.20966100	-0.80500300
C	-5.72495000	-1.40516400	1.28260300
H	-5.68736100	-1.03510700	2.31234200
H	-6.54384300	-0.90728900	0.75318200
H	-5.91641100	-2.47949000	1.29912900
Pd	0.41131700	0.25601900	-0.15756700
C	4.31558700	-1.21818600	0.60401500
O	2.03646600	-0.69224000	0.57302200
F	4.49173600	-0.78593600	1.86862400
F	4.07946800	-2.54715400	0.65136200
F	5.46219000	-1.02813000	-0.06160700
O	3.32788200	0.19084600	-1.08360800
C	3.13653100	-0.47066700	-0.08092900
H	1.82000100	4.30037800	1.26198800
H	2.99397700	3.92620400	-0.00555100
H	1.63551100	5.01876300	-0.37470700

a₂-TS2'

Imaginary Frequency: -1057.9565

C	1.26000700	-2.24206800	0.41256100
O	0.17418800	-1.79698400	-0.02464700

O	-1.18378600	2.08651300	-0.34579400
C	-0.90457400	2.64483700	0.76624000
O	0.07384600	2.30739700	1.50596700
C	-1.81782000	3.75408500	1.22383400
C	2.46636700	-1.45923600	0.41265800
C	2.57259100	-0.07392500	0.01788900
C	3.77154200	-1.94421200	0.50266300
C	3.94964000	0.18352000	-0.17501900
C	1.60812500	0.93328300	-0.21079300
H	4.12508000	-2.93468900	0.75346000
C	4.41864900	1.39882000	-0.67663800
C	2.09502400	2.12812600	-0.77715700
H	0.78569900	1.41833200	0.75495100
C	3.46234200	2.35938000	-1.00077300
H	5.47780600	1.59042500	-0.82089300
H	1.39052500	2.92656300	-0.98970100
H	3.78225800	3.31180900	-1.41311200
N	4.65635400	-0.97493800	0.15967000
C	1.24258600	-3.66127600	0.92921200
H	0.96839900	-3.64273600	1.99175100
H	0.47830100	-4.23050700	0.39578700
H	2.20968400	-4.16190600	0.83748100
C	6.10273600	-1.11490100	0.10502700
H	6.46459100	-0.93321400	-0.91224400
H	6.58167000	-0.40471200	0.78684700
H	6.37483200	-2.12923500	0.40219500
Pd	-0.38586000	0.16614100	-0.39306000
C	-4.50802300	-0.95272300	-0.25053200
O	-3.00908100	0.20518500	1.23183800
F	-5.43913600	-0.71872200	0.68691000
F	-4.94224100	-0.40775100	-1.40643800
F	-4.43340800	-2.28969700	-0.43087400
O	-2.24542900	-0.60084500	-0.75547800
C	-3.12736000	-0.37012600	0.15846400
H	-1.33233400	4.37435000	1.97868400
H	-2.14381500	4.35509300	0.37177400
H	-2.70343800	3.27638600	1.65879900

a₂-IN3'

C	1.27904500	-2.23041800	0.47706000
O	0.18165900	-1.79078600	0.05995800
O	-1.18202200	2.06665400	-0.32987400
C	-0.94964800	2.65670300	0.74523400
O	0.03270700	2.33224900	1.54477500

C	-1.84467100	3.78143700	1.15789500
C	2.48328000	-1.44932900	0.43833900
C	2.58044100	-0.05976600	0.03923700
C	3.78688800	-1.94188700	0.47304700
C	3.95160000	0.18783100	-0.20863500
C	1.60821300	0.93026500	-0.17904600
H	4.14516500	-2.93498200	0.70648300
C	4.41010800	1.39646100	-0.73391700
C	2.08552100	2.14352500	-0.71854300
H	0.59107800	1.62460200	1.08754100
C	3.44837600	2.36677400	-1.00461200
H	5.46221100	1.57270600	-0.93696200
H	1.38454800	2.94448100	-0.93967100
H	3.75544000	3.31685900	-1.43360900
N	4.66299000	-0.97800700	0.09113700
C	1.27432800	-3.64360300	1.01436400
H	1.05989300	-3.60946000	2.09017800
H	0.47812300	-4.21294500	0.53013700
H	2.23108100	-4.15387800	0.87712900
C	6.10328500	-1.12993100	-0.03218100
H	6.41833400	-0.95060900	-1.06555000
H	6.62090100	-0.42356800	0.62520300
H	6.38149800	-2.14664400	0.25158700
Pd	-0.37945400	0.17463100	-0.33808500
C	-4.49838600	-0.98128300	-0.30979800
O	-3.04882500	0.18197200	1.21864400
F	-5.46135300	-0.74957700	0.59591000
F	-4.89993700	-0.44488800	-1.48276700
F	-4.40862700	-2.31848200	-0.48175100
O	-2.23504900	-0.60539400	-0.75394400
C	-3.13626600	-0.38996300	0.13618600
H	-1.37849900	4.42764100	1.90273000
H	-2.13737800	4.34846900	0.27151600
H	-2.74967800	3.32840600	1.58048800

a₂'-IN1

C	0.95133200	-2.00810300	-1.48784500
O	-0.27752700	-1.94102100	-1.23864900
O	-2.81763700	-1.66845200	-0.01288600
C	-2.61254500	-2.52858100	0.96058400
O	-1.59768300	-2.61247900	1.64369700
C	-3.81555300	-3.44186000	1.16401000
C	1.97390500	-1.28122600	-0.78203500
C	1.97342600	-0.72936000	0.56567600

C	3.19452700	-0.91248500	-1.34876500
C	3.19913300	-0.03619300	0.71238800
C	1.10937000	-0.82644300	1.66892400
H	3.57199700	-1.09368600	-2.34551400
C	3.57125300	0.60813100	1.89436100
C	1.47376600	-0.18188000	2.84854500
H	0.19189900	-1.40785100	1.62357300
C	2.68028700	0.53375200	2.96059500
H	4.51561600	1.13643700	1.98474500
H	0.81083100	-0.24378700	3.70669200
H	2.92915900	1.02285000	3.89807400
N	3.91291500	-0.15879500	-0.48215500
C	1.33473400	-2.98101400	-2.58225800
H	0.53426300	-3.03668200	-3.32329800
H	2.28068000	-2.72816800	-3.06702400
H	1.45236300	-3.97515000	-2.13212600
C	5.20357000	0.45325600	-0.74580000
H	5.13159100	1.54331000	-0.67088800
H	5.94913800	0.09576100	-0.02772200
H	5.52711700	0.18718900	-1.75383600
Pd	-1.37179100	-0.37480300	-0.41938300
C	-1.23704600	3.61231800	-0.28586200
O	-0.28288200	1.44884700	-0.81850800
F	0.01909900	4.06651300	-0.16795300
F	-1.75337100	4.09088200	-1.43438900
F	-1.96383700	4.08366000	0.73435200
O	-2.27495900	1.46303500	0.12732100
C	-1.25898400	2.07643400	-0.31672900
H	-3.60176100	-4.15228400	1.96475200
H	-4.69729100	-2.84590200	1.42127700
H	-4.04216200	-3.97892000	0.23736500

a₂'-TS1

Imaginary Frequency: -485.9339

C	-2.13797500	1.38731500	-1.49556900
O	-0.88658600	1.47795900	-1.49849200
O	1.23210500	2.41701400	0.59312600
C	0.56513500	2.68398800	1.62902300
O	-0.44654100	2.03035600	2.05242400
C	1.00570300	3.87346600	2.47635100
C	-2.82726800	0.37432700	-0.74416300
C	-2.22648600	-0.46770200	0.25691100
C	-4.10598900	-0.13762100	-0.97140200
C	-3.16041300	-1.48275600	0.55389700

C	-0.98809300	-0.39358600	0.93511800
H	-4.87122400	0.19167300	-1.66092400
C	-2.87111400	-2.50672700	1.45672300
C	-0.68912500	-1.46561000	1.80376800
H	-0.63268800	0.70392300	1.33116500
C	-1.60926100	-2.49095100	2.06083900
H	-3.58704400	-3.29133000	1.68329400
H	0.26663200	-1.46404700	2.31887300
H	-1.34939200	-3.28100900	2.75921400
N	-4.30776200	-1.24364000	-0.21099200
C	-2.88853700	2.39947600	-2.32407000
H	-2.27039300	2.71596200	-3.16686800
H	-3.84674800	2.01741600	-2.68610900
H	-3.09024000	3.27926400	-1.69987500
C	-5.50409400	-2.07070800	-0.20199800
H	-5.26223400	-3.09354200	-0.50858100
H	-5.94509200	-2.09232900	0.79981100
H	-6.23223000	-1.65405300	-0.90017300
Pd	0.52038300	0.36599200	-0.47922900
C	4.22858600	-1.32602800	-0.35981300
O	2.61690000	-0.17112100	-1.76060900
F	4.99569200	-1.36362000	-1.45498400
F	4.87865600	-0.63469100	0.59352700
F	4.05826400	-2.58785900	0.08293400
O	2.02879500	-0.69932300	0.32233000
C	2.86448400	-0.67507500	-0.66031300
H	0.13375700	4.40997700	2.86286100
H	1.57759400	3.50756800	3.33780900
H	1.64178800	4.54600000	1.89566700

a₂'-IN2

C	-1.92147700	0.98448200	-1.70035300
O	-0.66306200	1.02068000	-1.70814800
O	-1.87142900	2.89607200	0.64557300
C	-1.05489700	3.12075200	1.51758200
O	0.01168500	2.33762000	1.76427100
C	-1.09660700	4.30105300	2.45918200
C	-2.62994000	-0.00676500	-0.95431100
C	-1.98946200	-0.97871500	-0.10625700
C	-3.99919900	-0.24254500	-0.85772600
C	-3.00931600	-1.76799900	0.46797200
C	-0.64952600	-1.21160900	0.20793400
H	-4.82657500	0.26788400	-1.33124900
C	-2.72557400	-2.80894700	1.35514200

C	-0.34932300	-2.24571300	1.09258600
H	0.02085900	1.59803500	1.11645900
C	-1.38089700	-3.02964800	1.65244200
H	-3.50600000	-3.41954500	1.79894100
H	0.68380500	-2.45045100	1.35427000
H	-1.11656000	-3.82926200	2.33910400
N	-4.23130800	-1.28706100	-0.01888300
C	-2.63682000	2.05599000	-2.47840700
H	-2.03244300	2.35381600	-3.33834900
H	-3.62848300	1.74064600	-2.81366000
H	-2.74653900	2.92212600	-1.81474600
C	-5.53351200	-1.82859800	0.33141600
H	-5.60170700	-2.88077600	0.03563600
H	-5.70056700	-1.75145900	1.41088100
H	-6.30887600	-1.26278400	-0.18842600
Pd	0.71234200	-0.08017800	-0.63084500
C	4.69635700	-0.50044400	0.10695400
O	2.95201900	0.69908900	-1.07463200
F	5.52782900	0.42039900	-0.39462000
F	4.85534600	-0.53289600	1.44298700
F	5.05294400	-1.70461000	-0.38421600
O	2.35437300	-0.93722400	0.31274100
C	3.23114900	-0.19702400	-0.25990100
H	-1.08124300	3.95528300	3.49773800
H	-0.20792300	4.92378400	2.31095700
H	-1.99585500	4.88876000	2.27215400

a₂'-IN3

C	-1.92147700	0.98448200	-1.70035300
O	-0.66306200	1.02068000	-1.70814800
O	-1.87142900	2.89607200	0.64557300
C	-1.05489700	3.12075200	1.51758200
O	0.01168500	2.33762000	1.76427100
C	-1.09660700	4.30105300	2.45918200
C	-2.62994000	-0.00676500	-0.95431100
C	-1.98946200	-0.97871500	-0.10625700
C	-3.99919900	-0.24254500	-0.85772600
C	-3.00931600	-1.76799900	0.46797200
C	-0.64952600	-1.21160900	0.20793400
H	-4.82657500	0.26788400	-1.33124900
C	-2.72557400	-2.80894700	1.35514200
C	-0.34932300	-2.24571300	1.09258600
H	0.02085900	1.59803500	1.11645900
C	-1.38089700	-3.02964800	1.65244200

H	-3.50600000	-3.41954500	1.79894100
H	0.68380500	-2.45045100	1.35427000
H	-1.11656000	-3.82926200	2.33910400
N	-4.23130800	-1.28706100	-0.01888300
C	-2.63682000	2.05599000	-2.47840700
H	-2.03244300	2.35381600	-3.33834900
H	-3.62848300	1.74064600	-2.81366000
H	-2.74653900	2.92212600	-1.81474600
C	-5.53351200	-1.82859800	0.33141600
H	-5.60170700	-2.88077600	0.03563600
H	-5.70056700	-1.75145900	1.41088100
H	-6.30887600	-1.26278400	-0.18842600
Pd	0.71234200	-0.08017800	-0.63084500
C	4.69635700	-0.50044400	0.10695400
O	2.95201900	0.69908900	-1.07463200
F	5.52782900	0.42039900	-0.39462000
F	4.85534600	-0.53289600	1.44298700
F	5.05294400	-1.70461000	-0.38421600
O	2.35437300	-0.93722400	0.31274100
C	3.23114900	-0.19702400	-0.25990100
H	-1.08124300	3.95528300	3.49773800
H	-0.20792300	4.92378400	2.31095700
H	-1.99585500	4.88876000	2.27215400

a₂^{''}-TS1

Imaginary Frequency: -83.7768

C	0.05268100	-1.50227000	2.25821300
O	1.07078500	-0.84656700	2.00009600
O	3.05713600	0.75575800	-0.23891800
C	3.91019900	-0.24308200	-0.17523100
O	3.63028700	-1.43534500	-0.12216300
C	5.35008900	0.25808000	-0.16586300
C	-0.78854500	-2.02256800	1.18977600
C	-0.47658800	-1.97478600	-0.21356600
C	-2.12720500	-2.38757300	1.27498900
C	-1.66798400	-2.27435200	-0.91338900
C	0.70518100	-1.68784800	-0.93204900
H	-2.75306000	-2.50850300	2.14909800
C	-1.73885700	-2.25532300	-2.30750000
C	0.62119600	-1.64486700	-2.33511500
H	1.69108000	-1.70733100	-0.45543900
C	-0.58044800	-1.91337600	-3.00875200
H	-2.65846300	-2.49069400	-2.83542000
H	1.52316800	-1.44115400	-2.90466600

H	-0.60725500	-1.88123100	-4.09381500
N	-2.65910500	-2.54326500	0.03035500
C	-0.35700300	-1.71099500	3.70451100
H	0.49757200	-1.50323800	4.35134800
H	-1.16342800	-1.01342600	3.96570800
H	-0.71905800	-2.72917500	3.88170500
C	-4.03854300	-2.88042600	-0.27629300
H	-4.51175700	-2.07460600	-0.84724200
H	-4.08942600	-3.80755600	-0.85722700
H	-4.58705800	-3.01960400	0.65713200
Pd	1.09855800	0.62338800	-0.05783300
C	-2.03115300	3.20085000	-0.02390400
C	-0.76457400	2.32774600	-0.03758400
O	-0.93190900	1.06981200	0.11733100
O	0.36080900	2.83842100	-0.21479200
F	-1.72828500	4.50118700	0.03216700
F	-2.75142300	2.97756400	-1.14138600
F	-2.80272500	2.89369400	1.03536800
H	6.02835400	-0.58776100	-0.29285700
H	5.50780200	0.99573300	-0.95797400
H	5.55596400	0.75165800	0.79023900

a₂^{''}-IN2

C	3.14047500	-1.47627000	-1.83049200
O	2.36347900	-2.38494800	-2.09798900
O	-1.89970500	-2.20039000	-0.62465800
C	-2.84604500	-2.69996600	0.14919100
O	-3.11165500	-2.29980600	1.27703900
C	-3.59301900	-3.83967900	-0.52808000
C	2.99411500	-0.70425900	-0.58632000
C	1.96069900	-0.87124400	0.40167000
C	3.80263000	0.31882100	-0.12057800
C	2.21063700	0.06489900	1.42882000
C	0.83401900	-1.72601400	0.50722400
H	4.68642700	0.75732300	-0.56314600
C	1.40585800	0.17211300	2.58228200
C	0.01469900	-1.61767100	1.66742900
H	0.69520100	-2.52865500	-0.20694900
C	0.32180300	-0.67221800	2.69408800
H	1.63035300	0.89638100	3.35939600
H	-0.75963800	-2.35227200	1.85691500
H	-0.31843200	-0.62829700	3.56884500
N	3.34116000	0.78145000	1.08448100
C	4.27817100	-1.11373700	-2.77330900

H	4.26034300	-1.79394600	-3.62664700
H	4.17272000	-0.08244100	-3.13190300
H	5.24909900	-1.19118600	-2.26874200
C	3.91323000	1.87428300	1.85506900
H	3.19390100	2.69420900	1.94963400
H	4.20183200	1.53182500	2.85422200
H	4.80246300	2.24236000	1.34034600
Pd	-1.08209100	-0.49864100	-0.00358500
C	-1.58073100	3.44603100	-0.65721000
C	-1.42148500	1.92870000	-0.46655500
O	-0.46462800	1.51720700	0.26533400
O	-2.23682900	1.13497300	-0.99882500
F	-2.36103100	3.72586000	-1.70553900
F	-2.13494400	3.98425100	0.44594800
F	-0.38136200	4.02399600	-0.84682300
H	-4.18472900	-4.37804500	0.21488500
H	-4.26202800	-3.42668100	-1.29139000
H	-2.89904100	-4.51920800	-1.03074500

a2''-TS2

Imaginary Frequency: -1059.8813

C	1.27869100	-0.19773900	2.38933300
O	0.62851800	0.83364000	2.24977300
O	-0.57122800	3.00875800	-0.15670200
C	0.53761500	3.58214200	0.09390200
O	1.67081800	3.02349200	0.05637000
C	0.46697800	5.04302300	0.48620800
C	1.91426800	-0.86772000	1.24751400
C	1.87296000	-0.48065300	-0.14077700
C	2.68495000	-2.02094200	1.30559800
C	2.64042000	-1.44320900	-0.84941300
C	1.26829100	0.59209800	-0.85865000
H	2.95213300	-2.62377000	2.16294500
C	2.82412000	-1.39525600	-2.23168000
C	1.47476800	0.62200400	-2.25812900
H	1.45117000	1.77205200	-0.33379000
C	2.23521900	-0.34185900	-2.93194200
H	3.40987700	-2.14877900	-2.75080100
H	1.04332900	1.44056900	-2.82814200
H	2.36865200	-0.27275500	-4.00746500
N	3.12367700	-2.37390400	0.06432400
C	1.44073900	-0.82195300	3.76942900
H	0.97501100	-1.81464200	3.80323200
H	2.49868500	-0.94102000	4.03255500

H	0.95729300	-0.17664800	4.50496400
C	3.95245500	-3.52132300	-0.26023600
H	3.43020200	-4.19196900	-0.95109800
H	4.89485900	-3.20158700	-0.71817000
H	4.17620000	-4.06836800	0.65757800
Pd	-0.74091100	0.99044400	-0.35128000
C	-3.63855200	-1.78754900	-0.05633400
C	-2.59532900	-0.66530300	-0.19307100
O	-1.39761100	-1.00994600	-0.45648000
O	-2.92741300	0.53091200	-0.01576000
F	-3.46895800	-2.42294400	1.12127800
F	-3.49705900	-2.69162000	-1.04081000
F	-4.88489300	-1.30329300	-0.09824500
H	-0.40918000	5.51716600	0.04032400
H	1.38286500	5.55879100	0.19143600
H	0.37302600	5.09917500	1.57691000

a2''-IN3

C	0.24618100	-1.12760800	1.93223500
O	-0.08815000	0.04550100	2.16646300
O	0.34336300	2.99611800	-0.06978200
C	0.94634100	3.23315600	0.99239600
O	1.12304100	2.38739100	1.97172400
C	1.54503200	4.59088600	1.23978600
C	1.30536800	-1.46181200	0.99040800
C	1.76991300	-0.69925200	-0.15505500
C	2.17421100	-2.53390100	1.12254100
C	2.93705800	-1.35763900	-0.62746500
C	1.27546200	0.39689900	-0.88551400
H	2.19073400	-3.31753600	1.86756800
C	3.66477900	-0.91544300	-1.73636100
C	2.00543200	0.86022500	-1.97658700
H	0.67804500	1.48598700	1.84348500
C	3.19013600	0.21518000	-2.39059700
H	4.55492900	-1.43372800	-2.07975600
H	1.64821000	1.71466900	-2.54406300
H	3.72562300	0.59808000	-3.25527500
N	3.15875800	-2.47026700	0.18027100
C	-0.51781600	-2.23917700	2.61600400
H	-1.39799800	-2.45058900	1.99416700
H	0.05239900	-3.16727400	2.70895500
H	-0.86677900	-1.90531400	3.59621100
C	4.26097500	-3.40205400	0.02946800
H	4.22782800	-3.88291700	-0.95443900

H	5.22112300	-2.88575800	0.13841400
H	4.18556100	-4.17220200	0.79972500
Pd	-0.51158300	1.13320400	-0.52020800
C	-3.83982200	-1.20431200	-0.42629900
C	-2.69130300	-0.18164300	-0.52240400
O	-1.54793500	-0.67386800	-0.81299800
O	-2.89528100	1.02286000	-0.28372400
F	-3.62777500	-2.02539000	0.63205900
F	-3.90205800	-1.96931000	-1.53002800
F	-5.02532100	-0.60990500	-0.25556800
H	1.39156800	5.23284500	0.37253200
H	2.61451700	4.48640300	1.44868500
H	1.08013500	5.03819000	2.12452300

b₂-IN1

C	-0.76713500	-0.71005800	1.53037400
O	0.33502100	-0.12165800	1.69622600
O	2.34366500	2.57254600	-0.70746600
C	1.54378400	3.45320700	-0.24739700
O	0.62654000	3.05765700	0.55699500
C	1.69668200	4.90069500	-0.60568000
C	-1.84491400	-0.21581400	0.71635500
C	-3.05633900	-0.88979900	0.26948800
C	-1.94453000	1.09983900	0.26214000
C	-3.81368900	0.07960700	-0.43631900
C	-3.56587900	-2.19623600	0.34985400
H	-1.26633500	1.92877400	0.41260700
C	-5.04515400	-0.19720100	-1.03251600
C	-4.79412700	-2.48238200	-0.23910700
H	-3.01436700	-2.98396400	0.84947700
C	-5.53010500	-1.49640000	-0.91989500
H	-5.60238500	0.56600700	-1.56738100
H	-5.18933800	-3.49220700	-0.17714900
H	-6.48437300	-1.75302600	-1.37031100
N	-3.10465900	1.28137800	-0.41077400
C	-0.92199600	-2.00299200	2.28810700
H	-0.71301300	-2.82212600	1.58748800
H	-0.17919000	-2.04207500	3.08725500
H	-1.92850500	-2.13283700	2.69367100
C	-3.55562900	2.52981600	-1.00246900
H	-2.79995400	3.29698000	-0.82573800
H	-3.69697400	2.41053400	-2.08173300
H	-4.50170600	2.84813900	-0.55196500
Pd	1.39448300	1.08492100	0.40076500

C	3.10831400	-2.67047300	-0.71298800
O	2.54559700	-0.50019500	-0.04428300
F	4.02239800	-2.21928700	-1.59251700
F	3.75094500	-2.98023700	0.43268400
F	2.57950600	-3.79942100	-1.20644600
O	0.83123700	-1.89168800	-0.61624500
C	2.00657100	-1.60615200	-0.44659600
H	0.72775400	5.40461000	-0.56920300
H	2.36025800	5.37995300	0.12385300
H	2.14726300	4.99850400	-1.59603000

b₂-TS0

Imaginary Frequency:		-1151.6002	
C	1.00943900	-1.78497700	-1.20649200
O	-0.22123400	-1.50108100	-1.15788500
O	-1.01114700	2.30918900	0.15647000
C	-0.33437600	3.09939300	-0.58406800
O	0.66178000	2.74442900	-1.28938700
C	-0.77362200	4.54522700	-0.61929700
C	1.96103700	-0.84972100	-0.68099400
C	3.27873600	-1.06141200	-0.14088600
C	1.51398800	0.43188600	-0.26387300
C	3.57083700	0.09830700	0.62737900
C	4.22835900	-2.09878300	-0.19219200
H	0.97756300	1.44966700	-0.92210900
C	4.78521000	0.25986900	1.30745800
C	5.42848200	-1.94434500	0.48733600
H	4.04018400	-3.00119500	-0.76394200
C	5.70539600	-0.77646400	1.22839400
H	5.00573200	1.15701600	1.87650200
H	6.17218600	-2.73466000	0.44537000
H	6.65613000	-0.68565700	1.74523900
N	2.48298800	0.95872900	0.55551200
C	1.39228300	-3.12876400	-1.75829900
H	1.73302200	-3.77771300	-0.94145300
H	0.52446100	-3.59057900	-2.23257600
H	2.21237100	-3.03906900	-2.47835200
C	2.43317200	2.26927300	1.19391700
H	1.39773100	2.50658800	1.43794900
H	3.00531200	2.23032500	2.12279700
H	2.84664000	3.04367000	0.54025900
Pd	-0.64269800	0.33046200	-0.28149400
C	-4.53521000	-1.08051400	0.58027900
O	-2.64370700	-0.02024200	-0.32863800

F	-5.25563800	0.05923400	0.59399500
F	-4.83384900	-1.74459600	-0.55571100
F	-4.93214000	-1.83313000	1.61522000
O	-2.33551900	-1.24335100	1.55608900
C	-3.01498800	-0.77814400	0.65378700
H	0.07688200	5.19744600	-0.82719900
H	-1.50302000	4.66112400	-1.42954000
H	-1.26120300	4.82053500	0.31775700

b₂-IN2

C	1.37150000	-2.08714900	-0.34358600
O	0.11961300	-1.82736900	-0.39167200
O	-0.71598100	2.23936200	0.03089500
C	-1.78222900	2.85049700	-0.20321700
O	-2.91037600	2.29840900	-0.53060300
C	-1.82707800	4.35195500	-0.10722600
C	2.26470100	-1.01517400	-0.15145800
C	3.69520200	-0.83971600	-0.02932500
C	1.65164300	0.25625700	-0.02962000
C	3.88233200	0.55263400	0.16483300
C	4.81965700	-1.67438000	-0.05871300
H	-2.84966500	1.26900500	-0.51495500
C	5.14235000	1.12557600	0.32585700
C	6.08442500	-1.10948300	0.10221800
H	4.71523700	-2.74564400	-0.20351300
C	6.24607200	0.27231000	0.29191400
H	5.26745800	2.19401400	0.47311900
H	6.96141200	-1.75035600	0.08075100
H	7.24328700	0.68481100	0.41469800
N	2.62110400	1.18132300	0.15940600
C	1.78399000	-3.52345200	-0.49549000
H	2.31106100	-3.85978300	0.40542900
H	0.90540600	-4.15089400	-0.65536100
H	2.47402200	-3.63385000	-1.34032100
C	2.44961400	2.61454900	0.34171400
H	1.38660300	2.84426700	0.31435200
H	2.86772900	2.92189400	1.30660600
H	2.96584500	3.15986900	-0.45638500
Pd	-0.32659400	0.16248800	-0.14556600
C	-4.50426200	-1.16097900	0.16958600
O	-2.42130000	-0.17250700	-0.35573700
F	-5.10954400	0.04444300	0.03536800
F	-4.65902000	-1.82623300	-0.99222200
F	-5.14375900	-1.83855900	1.12845000

O	-2.50282100	-1.54835500	1.44617200
C	-3.00166200	-0.97540400	0.50041100
H	-2.23885200	4.76516600	-1.03304700
H	-2.50146900	4.63944300	0.70657200
H	-0.83220000	4.75693100	0.07803400

b₂-IN1'

C	-0.99208200	-1.01742100	1.29120200
O	0.14976500	-0.50029200	1.37209900
O	2.06785700	2.58342900	-0.61289900
C	1.28860000	3.37180000	0.01829700
O	0.38425200	2.84379800	0.75903500
C	1.45266700	4.85869400	-0.07432900
C	-2.09976000	-0.46012200	0.55735700
C	-3.37304500	-1.07016900	0.19511500
C	-2.16432200	0.86154500	0.11115700
C	-4.12324000	-0.06237000	-0.46361500
C	-3.94870600	-2.34576200	0.32022600
H	-1.44396300	1.65944800	0.23257900
C	-5.40332200	-0.27451200	-0.97849500
C	-5.22606500	-2.56677500	-0.18668400
H	-3.41553100	-3.15930800	0.79815500
C	-5.94914200	-1.54522100	-0.82752800
H	-5.95254800	0.51669200	-1.47975200
H	-5.67226400	-3.55212400	-0.08813500
H	-6.94295400	-1.75099800	-1.21375300
N	-3.35462700	1.10201200	-0.48474300
C	-1.16561500	-2.31041400	2.05303600
H	-1.13865600	-3.15108300	1.34753400
H	-0.33546100	-2.42562000	2.75204200
H	-2.12049100	-2.34443100	2.58533900
C	-3.78133900	2.37462800	-1.04383200
H	-2.98518500	3.10703200	-0.90125500
H	-3.98400100	2.27165900	-2.11490200
H	-4.68740000	2.72802600	-0.54084000
Pd	1.15929300	0.92934800	0.25968700
C	3.81235800	-2.20915800	-0.74111800
O	2.09096900	-0.62193600	-0.60556400
F	2.98122500	-3.27358200	-0.68002300
F	4.03695400	-1.93772700	-2.04179900
F	4.97690000	-2.56403400	-0.18381000
O	3.71726100	-0.52347700	0.98077100
C	3.18682200	-0.99056600	-0.01031200
H	0.49188900	5.35662000	0.07760600

H	2.13924000	5.18929500	0.71403000
H	1.88283100	5.13155500	-1.04074500

b₂-TS0'

Imaginary Frequency: -1088.3883

C	-1.29780400	-2.04891800	0.63273000
O	-0.06273300	-1.94697100	0.38864300
O	1.14788300	1.88959800	-0.42057100
C	0.80944900	2.57835800	0.60484300
O	-0.11195900	2.24993800	1.41236800
C	1.58981100	3.84675900	0.84772800
C	-2.14463800	-0.90302500	0.45206300
C	-3.55097400	-0.81672600	0.15610200
C	-1.56000300	0.36136100	0.18244300
C	-3.76351800	0.50521900	-0.32298400
C	-4.64435300	-1.70146800	0.21309000
H	-0.75123700	1.12532400	0.87591300
C	-5.02888800	0.96828900	-0.70836700
C	-5.89660800	-1.24704700	-0.17521200
H	-4.52262500	-2.71866500	0.56962000
C	-6.08801000	0.07479400	-0.63000100
H	-5.18271600	1.98481300	-1.05533000
H	-6.74854700	-1.91863200	-0.12383100
H	-7.08228000	0.39949800	-0.92198600
N	-2.54729200	1.17382000	-0.32013700
C	-1.81790400	-3.39776600	1.04250500
H	-2.40445900	-3.83237900	0.22300600
H	-0.97983400	-4.06105300	1.26384400
H	-2.47418600	-3.31623400	1.91529400
C	-2.37783400	2.57352900	-0.69525800
H	-1.36617900	2.71886900	-1.07359100
H	-3.08473000	2.81368500	-1.49192300
H	-2.55001100	3.23452300	0.15996600
Pd	0.53351500	-0.05326700	-0.22632700
C	4.70896200	-0.83605800	-0.34718900
O	2.39281800	-0.70621800	-0.69062400
F	4.72012000	-2.17857400	-0.47334600
F	5.01773200	-0.30534500	-1.54864800
F	5.67609800	-0.49427500	0.51526000
O	3.22829600	0.31927400	1.16190800
C	3.32070700	-0.33242100	0.13450100
H	1.04321700	4.51751800	1.51225800
H	2.53489800	3.55814700	1.32245600
H	1.82767900	4.33765200	-0.09885200

b₂-IN2'

C	-1.25474500	-2.17306500	-0.06973600
O	-0.01910800	-1.90344300	-0.26868200
O	0.70242300	2.17367100	-0.56296100
C	1.37963600	2.90734500	0.19726300
O	2.11922400	2.52218000	1.17988100
C	1.35225500	4.40039500	-0.01755900
C	-2.16800200	-1.10261500	-0.01274800
C	-3.59626800	-0.94318200	0.15279000
C	-1.59715500	0.18222200	-0.19315300
C	-3.82675700	0.45262600	0.05710800
C	-4.68801000	-1.79485900	0.36408600
H	2.36635400	1.48820300	1.23861300
C	-5.09787600	1.01300600	0.16669000
C	-5.96380900	-1.24271200	0.47428600
H	-4.55027100	-2.86917500	0.44337800
C	-6.16840500	0.14292000	0.37725400
H	-5.25636400	2.08468100	0.09426100
H	-6.81552400	-1.89665400	0.63912700
H	-7.17302300	0.54547400	0.46835900
N	-2.59234700	1.09847600	-0.15766300
C	-1.63070000	-3.61969700	0.08091600
H	-2.36844800	-3.90049700	-0.68007400
H	-0.74545300	-4.25009500	-0.02010400
H	-2.09035400	-3.79060800	1.06174200
C	-2.47257200	2.53733600	-0.33459800
H	-1.44717800	2.76789300	-0.61552100
H	-3.15133000	2.87020500	-1.12683100
H	-2.73005000	3.06000100	0.59387000
Pd	0.37298100	0.11100300	-0.42506000
C	4.49945600	-1.21532400	0.10083800
O	2.42101500	-0.39755600	-0.72590700
F	4.37494600	-2.17371500	-0.82772000
F	5.50717900	-0.39754200	-0.27457200
F	4.84561200	-1.79687800	1.26016100
O	3.08834800	0.24733700	1.33800700
C	3.20289600	-0.38386800	0.26164300
H	1.05912500	4.89767900	0.91256900
H	2.36172700	4.74482400	-0.26508000
H	0.66556300	4.66517000	-0.82192200

b₂' -IN1

C	0.84840900	-1.50551500	-1.62019100
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O	-0.25776400	-0.93838300	-1.45325200
O	-2.60633300	0.23956000	-0.37059500
C	-2.81277200	-0.63679500	0.55744800
O	-2.02651200	-1.13480800	1.34913300
C	-4.30584800	-1.06406100	0.57927500
C	2.01360300	-1.29098200	-0.80032000
C	2.11996900	-0.82567800	0.57527500
C	3.32215000	-1.46290100	-1.25095300
C	3.50426300	-0.72388200	0.85552700
C	1.19762200	-0.57686900	1.60501400
H	3.67928500	-1.76564100	-2.22542000
C	4.00106000	-0.33106200	2.10058000
C	1.68706700	-0.18157000	2.84732200
H	0.13004400	-0.71561300	1.45851400
C	3.06660800	-0.04922000	3.09233700
H	5.06723600	-0.25924400	2.29388800
H	0.98274400	0.01736700	3.64981600
H	3.40976800	0.25974600	4.07565100
N	4.20789200	-1.10825000	-0.28808800
C	0.89154000	-2.52205800	-2.74089200
H	0.20092900	-2.22558900	-3.53334400
H	1.89465800	-2.66708800	-3.14908700
H	0.55698200	-3.48814100	-2.34146500
C	5.65477200	-1.10880800	-0.41357900
H	6.05170300	-0.09855900	-0.26849400
H	6.10266700	-1.77644700	0.33013200
H	5.92782100	-1.45719100	-1.41144300
Pd	-0.72905800	0.91558900	-0.62939300
C	0.90043300	4.49111400	-0.26707700
O	0.97112400	2.13881400	-0.86371500
F	-5.11677800	0.00303600	0.71404000
F	-4.63315500	-1.69099900	-0.57050800
F	-4.55565400	-1.90487700	1.59271700
O	-0.91060000	2.90055600	-0.05553000
C	0.30374700	3.12220100	-0.39435600
H	0.54123500	4.97107800	0.64706400
H	1.99073400	4.42846000	-0.26594700
H	0.58083800	5.10370500	-1.11822900

b₂' -TS1

Imaginary Frequency: -495.4066

C	1.61426300	1.15699000	-1.69624800
O	0.43063000	1.64014400	-1.82757200
O	-1.55344500	2.76115200	0.14112700

C	-0.97371100	3.19023200	1.16188200
O	0.03472700	2.61921500	1.74442800
C	-1.44740500	4.47113000	1.80686700
C	1.97792900	0.43494000	-0.53906100
C	3.09330900	-0.45788500	-0.28006000
C	1.12004000	0.44860200	0.60979500
C	2.84678300	-0.99627700	1.00779100
C	4.23253900	-0.88338100	-0.97928000
H	0.37753600	1.70099100	1.21885600
C	3.70125800	-1.91420700	1.61761700
C	5.09091000	-1.80292200	-0.37909000
H	4.45486100	-0.50714000	-1.97260000
C	4.83138500	-2.31207300	0.90425300
H	3.49546700	-2.31217300	2.60661000
H	5.97777400	-2.13192200	-0.91329400
H	5.51773000	-3.02860000	1.34619700
N	1.65872200	-0.42942300	1.49301800
C	2.54378200	1.38918500	-2.85679800
H	2.63757000	0.46574200	-3.44301000
H	2.13649200	2.16794300	-3.50491800
H	3.54308500	1.67206700	-2.51249100
C	1.12852900	-0.69600600	2.82202000
H	0.22426400	-0.10229900	2.95720400
H	0.88018800	-1.75771900	2.92689600
H	1.86047800	-0.42479600	3.59105500
Pd	-0.96217500	0.78003100	-0.65896600
C	-3.31253400	-2.45392400	-0.01558100
O	-1.69201300	-1.34524800	-1.44078600
F	-2.70600900	-3.17497400	0.95013100
F	-4.48455600	-2.01237000	0.46516800
F	-3.55026400	-3.25921600	-1.05665000
O	-2.39264400	-0.26455600	0.36149800
C	-2.40529600	-1.27961900	-0.42189800
H	-0.62452800	5.19286200	1.83478600
H	-2.29099400	4.88503400	1.25333000
H	-1.74217900	4.26923500	2.84205900

b₂' -IN2

C	1.08365500	-0.40041600	2.19157200
O	-0.16362600	-0.52254100	2.08376000
O	0.71531400	2.32780400	0.78443200
C	-0.01769500	2.68882300	-0.10484200
O	-0.90338900	1.96234300	-0.77550900
C	-0.02554000	4.14170500	-0.63291300

C	1.96655700	-0.80308900	1.14239300
C	1.52088600	-1.30162500	-0.13414100
C	3.35880600	-0.79270200	1.09637900
C	2.67477500	-1.57565600	-0.89961400
C	0.24400000	-1.50822700	-0.66234200
H	4.07669400	-0.48643700	1.84491100
C	2.59472900	-2.07071300	-2.20340000
C	0.15181800	-2.00159000	-1.96387800
H	-0.90745400	1.03051100	-0.43555800
C	1.31385600	-2.27756200	-2.71554200
H	3.47857200	-2.28333700	-2.79719100
H	-0.82535000	-2.17457700	-2.40442900
H	1.20629900	-2.66073600	-3.72685100
N	3.78560900	-1.25233400	-0.11004500
C	1.59646200	0.23199500	3.45937500
H	0.92782300	-0.01078000	4.28852400
H	2.61596600	-0.07891000	3.70252500
H	1.58666600	1.31991100	3.31860800
C	5.16947800	-1.38840800	-0.53134400
H	5.39470500	-2.43278700	-0.77195500
H	5.36134400	-0.77119500	-1.41532600
H	5.82492900	-1.06135200	0.27802900
Pd	-1.31934000	-1.11529500	0.46470200
C	-5.16627300	-1.52189200	-0.65743500
O	-3.55174700	-0.92391200	1.05000700
F	0.84311800	4.88965100	0.05463100
F	0.32226100	4.16818100	-1.93232600
F	-1.24893400	4.68359000	-0.51137000
O	-2.77735500	-1.57611900	-0.91307100
C	-3.77139100	-1.32271800	-0.12018700
H	-5.28849600	-2.55564900	-0.99748100
H	-5.90348900	-1.29452600	0.11455300
H	-5.32413000	-0.87115300	-1.52418800

b₂'-IN3

C	-1.75695200	2.16672300	0.00288100
O	-0.50377900	2.43360200	0.00013700
C	-2.13903500	0.81015500	0.00154100
C	-3.35626000	0.02680700	0.00307400
C	-1.05264600	-0.09311000	-0.00277800
C	-2.92917500	-1.32768200	-0.00043600
C	-4.72942600	0.30130600	0.00683500
C	-3.82297200	-2.39629100	-0.00017100
C	-5.63057700	-0.76294700	0.00710800

H	-5.09294900	1.32479600	0.00943100
C	-5.18542000	-2.09457700	0.00366800
H	-3.47832000	-3.42579900	-0.00285300
H	-6.69744100	-0.55819000	0.01001900
H	-5.91040700	-2.90319900	0.00397800
N	-1.51894800	-1.35804100	-0.00395700
C	-2.71674800	3.32162800	0.00699400
H	-3.36404400	3.27809900	-0.87713700
H	-3.36543200	3.27108500	0.88967800
H	-2.16974600	4.26610000	0.01095800
C	-0.72685300	-2.58144000	-0.00798200
H	-0.95289500	-3.17606300	0.88337600
H	-0.95822400	-3.17357500	-0.89962000
H	0.33009300	-2.31772000	-0.01078800
Pd	0.70409100	0.74876700	-0.00602500
C	4.48277100	-0.68239200	0.00510000
C	3.09101500	-0.02510700	-0.01180200
O	2.08610400	-0.81947600	-0.01235700
O	2.96573200	1.21594800	-0.01160100
F	4.59200500	-1.56785800	-1.00160700
F	4.66117400	-1.34247000	1.16534400
F	5.45271200	0.22793200	-0.11994200

b₂'-TS1

Imaginary Frequency: -97.3265

C	-0.99659700	-1.42559300	2.19794700
O	0.21367300	-1.39194600	2.42790500
O	2.61691900	-1.67135200	0.21377400
C	2.62997900	-2.66989600	-0.63135000
O	1.72287200	-2.96955900	-1.41041800
C	3.92965100	-3.45970900	-0.55892600
C	-1.49313700	-1.23496500	0.82746700
C	-2.67964700	-0.60506100	0.33006800
C	-0.75263100	-1.65531500	-0.29187500
C	-2.59462100	-0.65843700	-1.09374200
C	-3.78694100	0.03919300	0.92067200
H	0.05193900	-2.38273600	-0.37050700
C	-3.58132100	-0.10872500	-1.92360000
C	-4.76635300	0.57395400	0.10051500
H	-3.87805700	0.11239600	1.99948900
C	-4.66448400	0.50091500	-1.30812200
H	-3.50133300	-0.15571900	-3.00502000
H	-5.62813500	1.06410500	0.54374400
H	-5.44934200	0.93636900	-1.91977900

N	-1.42939000	-1.30945600	-1.43709800
C	-1.98221600	-1.66385800	3.32314600
H	-2.38000100	-0.69640800	3.65761400
H	-2.82820500	-2.28228600	3.00890800
H	-1.46140000	-2.12396400	4.16550400
C	-1.00162800	-1.64317200	-2.79029400
H	-1.73266200	-2.30311100	-3.26976000
H	-0.89929200	-0.72989000	-3.38568400
H	-0.03484800	-2.14413500	-2.72697100
Pd	1.22145800	-0.26195600	0.24218700
C	1.10397600	3.74759000	-0.08535100
C	1.23910500	2.22131000	0.04233300
O	0.18861100	1.54893000	0.31068400
O	2.34666300	1.66384300	-0.14905700
F	2.29039100	4.34823100	0.05380000
F	0.61045400	4.05167000	-1.30189000
F	0.26305900	4.22862400	0.84229100
H	4.16221700	-3.71735300	0.47838800
H	4.75227200	-2.84292200	-0.93676000
H	3.84164900	-4.36364400	-1.16432100

b₂''-IN2

C	2.85515100	0.78538200	-0.67503700
O	3.80962000	0.51511900	0.03116400
O	1.95617600	-1.83188700	-0.60427700
C	2.54756400	-2.33934100	0.46086300
O	2.18415000	-2.15241600	1.61900500
C	3.77862400	-3.15491100	0.10567900
C	1.50922000	1.05406200	-0.04341900
C	0.61044100	2.17917800	-0.34881300
C	1.28543000	0.76970600	1.34350700
C	-0.10714200	2.45878500	0.83712600
C	0.35567100	2.94969900	-1.49012500
H	1.82287500	0.05535300	1.95463800
C	-1.07529200	3.45662400	0.91673500
C	-0.60007000	3.96119100	-1.41908400
H	0.87714900	2.75906800	-2.42161700
C	-1.30860700	4.21001700	-0.23252000
H	-1.62940200	3.64326100	1.83092100
H	-0.80620200	4.56286300	-2.29920400
H	-2.05356100	4.99974800	-0.20903100
N	0.33528800	1.58256000	1.84230900
C	2.98035900	0.90858000	-2.17876600
H	2.11840100	0.47513800	-2.69473200

H	3.04970900	1.96833700	-2.45674400
H	3.89717300	0.40901900	-2.49745500
C	-0.30008500	1.43254000	3.14399600
H	-0.34568200	2.40116800	3.64975200
H	-1.31245900	1.03389900	3.02171900
H	0.29051200	0.74076300	3.74635600
Pd	0.29408600	-0.79038500	-0.23516100
C	-3.70112200	-1.37879900	-0.26658600
C	-2.17028300	-1.22990100	-0.25834000
O	-1.69317600	-0.08121900	0.02145600
O	-1.43550600	-2.20580900	-0.54100000
F	-4.06706900	-2.66328400	-0.30617100
F	-4.23000400	-0.81470100	0.83427800
F	-4.21162400	-0.75391500	-1.34455300
H	4.61123600	-2.46132000	-0.06030700
H	3.62554800	-3.72819200	-0.81225000
H	4.02873400	-3.81940000	0.93514100

b₂''-TS2

Imaginary Frequency: -834.2154

C	1.97175800	0.83989500	1.94731900
O	1.30123700	1.86241700	2.03174400
O	-0.65616800	2.89640600	-0.28877800
C	0.40072200	3.48901700	-0.67803800
O	1.46429600	2.91863900	-1.05748100
C	0.36793300	5.00269600	-0.65485700
C	1.93145900	0.01361300	0.71633200
C	2.65295200	-1.16816000	0.36896100
C	1.15699300	0.39754500	-0.41337800
C	2.27433200	-1.49044300	-0.97433500
C	3.58625100	-2.01121500	1.02165200
H	1.31737800	1.61762100	-0.77369900
C	2.79223800	-2.60700400	-1.65646400
C	4.08832700	-3.10936400	0.35041300
H	3.90291200	-1.81058000	2.03799300
C	3.69409000	-3.40607900	-0.97864100
H	2.48655400	-2.84062200	-2.67110800
H	4.79784800	-3.76342300	0.84865800
H	4.10659400	-4.28234400	-1.47051500
N	1.39237400	-0.54572900	-1.41670800
C	2.86239800	0.41465200	3.10034600
H	2.57562700	-0.57774000	3.46853000
H	3.91247100	0.36287100	2.78908800
H	2.75953300	1.14247700	3.90729400

C	0.77069300	-0.53427600	-2.73129200
H	1.51658500	-0.75646200	-3.50049000
H	-0.03915300	-1.27011800	-2.78360200
H	0.35828600	0.45939500	-2.91321700
Pd	-0.85521900	0.88306800	-0.13298300
C	-3.80560400	-1.80211600	0.38119600
C	-2.73769600	-0.70772700	0.21410400
O	-1.53035600	-1.08859500	0.04703900
O	-3.06052300	0.50295000	0.21252200
F	-3.38724200	-2.74464800	1.24094900
F	-4.03392900	-2.39099900	-0.81009700
F	-4.95692200	-1.29202000	0.82932700
H	-0.65518400	5.36682000	-0.76156400
H	1.01080900	5.40552800	-1.44002800
H	0.75706300	5.33381000	0.31492300

b₂''-IN3

C	1.62413700	0.77318700	1.99477100
O	0.66657200	1.55000300	2.05411800
O	-0.27439200	2.58495900	-0.86420500
C	0.77955700	3.23204600	-0.85805400
O	1.96522400	2.73424400	-0.57834600
C	0.79329900	4.69906800	-1.17845900
C	1.85544400	-0.05619900	0.80767400
C	2.94610400	-0.95995800	0.46857300
C	0.89716900	-0.18261200	-0.21736000
C	2.58310400	-1.57961300	-0.75485400
C	4.18102300	-1.30499900	1.04407100
H	1.88672100	1.78853500	-0.29081600
C	3.39400300	-2.51111600	-1.40682100
C	4.99414600	-2.23650500	0.40385400
H	4.50872600	-0.85942200	1.97658600
C	4.60820100	-2.83514700	-0.80798500
H	3.09126800	-2.96924300	-2.34351200
H	5.94709400	-2.50577700	0.85084400
H	5.26387200	-3.55868500	-1.28377300
N	1.33593500	-1.08621600	-1.14187600
C	2.58794000	0.67523200	3.16374000
H	2.71286100	-0.36385200	3.48866600
H	3.57848000	1.05229300	2.87960000
H	2.20244500	1.27659500	3.98933000
C	0.62633800	-1.53057000	-2.33158700
H	1.20241000	-1.29251300	-3.23281200
H	0.45830400	-2.61174600	-2.28875900

H	-0.33815000	-1.02424100	-2.37442300
Pd	-0.87830400	0.65120700	-0.26424300
C	-4.31327100	-1.37070800	0.38156000
C	-3.07417500	-0.48994800	0.13847800
O	-1.94193100	-1.08990000	0.13790700
O	-3.19088400	0.73353800	-0.07552100
F	-4.11776100	-2.19164100	1.42584700
F	-4.54769900	-2.12757700	-0.71005800
F	-5.39772200	-0.62570200	0.61937300
H	-0.14723500	4.98711200	-1.64814600
H	1.64182700	4.93908200	-1.82455300
H	0.91563400	5.25845000	-0.24359600

Pd(TFA)(OAc)

a₃-IN1

C	-1.53511400	-1.17073300	-1.63389500
O	-0.28935700	-1.00391900	-1.61345000
O	2.76032700	-0.10881800	1.05497300
C	3.34345200	0.20431300	-0.02638300
O	2.74206100	0.13187400	-1.13647800
C	4.78734700	0.72677800	0.02183800
C	-2.46433000	-0.27833700	-0.99634200
C	-2.25917600	1.07212000	-0.49858400
C	-3.79287100	-0.59403900	-0.71760400
C	-3.49079100	1.48183200	0.06771800
C	-1.19676700	1.98819800	-0.53241600
H	-4.32854800	-1.51470400	-0.90332400
C	-3.68682300	2.74562200	0.62860800
C	-1.38115400	3.24947800	0.02629900
H	-0.25098400	1.72480700	-0.99240000
C	-2.60733300	3.62360900	0.60611300
H	-4.64001500	3.03812500	1.05870600
H	-0.56123300	3.96155100	0.01222600
H	-2.71697300	4.61543400	1.03477400
N	-4.40157500	0.43128500	-0.07306900
C	-2.02062500	-2.37765100	-2.39845700
H	-3.05718600	-2.29443900	-2.73234300
H	-1.36670200	-2.53496600	-3.26031100
H	-1.90716600	-3.24077800	-1.73190000
C	-5.77266200	0.44853500	0.40710900
H	-5.79554700	0.58763900	1.49300000
H	-6.33399200	1.26049300	-0.06726700
H	-6.24916400	-0.50223800	0.16151000
Pd	1.01036800	-0.55682800	-0.05861900

C	-1.51574400	-2.33957000	2.85953700
O	-0.21726800	-0.99250400	1.44227100
F	5.44743200	0.40257600	-1.09733900
F	4.77117600	2.06983700	0.13177200
F	5.44459400	0.22384800	1.07386500
O	-0.95771200	-2.96083900	0.59271300
C	-0.86622500	-2.13390700	1.49354800
H	-1.99594600	-1.42056300	3.20756100
H	-2.24133800	-3.15375900	2.80109400
H	-0.74143100	-2.60169500	3.58918300

a₃-TS1

Imaginary Frequency: -57.1853

C	2.23510100	1.84423700	-0.78746800
O	0.99480700	1.93672500	-0.92647200
O	-2.13466200	-0.24987600	0.59810100
C	-2.46127000	-1.13848600	-0.27470100
O	-1.88649000	-1.35167900	-1.34381500
C	-3.65335100	-2.02233700	0.15727100
C	2.89037700	0.63502100	-0.35584700
C	2.35635500	-0.71272900	-0.36810500
C	4.13367800	0.55204300	0.26618300
C	3.30729900	-1.53188200	0.28517800
C	1.20478500	-1.30900600	-0.90630400
H	4.84175400	1.33603200	0.49639800
C	3.11978400	-2.90410600	0.46875000
C	0.99776600	-2.67295200	-0.71129800
H	0.51407400	-0.76589400	-1.55512600
C	1.94212000	-3.45881800	-0.02607700
H	3.85886600	-3.51821600	0.97434200
H	0.09348400	-3.12288400	-1.10602400
H	1.75683000	-4.52035600	0.10702800
N	4.38214400	-0.72304500	0.66094000
C	3.04601200	3.06865100	-1.14277800
H	3.95322000	3.15945300	-0.53896600
H	3.35443000	2.99722700	-2.19364300
H	2.42850600	3.96112100	-1.02471400
C	5.55401200	-1.18180200	1.38864900
H	5.26324700	-1.59190700	2.36134800
H	6.07914700	-1.95482300	0.81806200
H	6.22921500	-0.33895200	1.54670100
Pd	-0.55485400	0.74734400	-0.15364900
C	-2.28979100	4.21112900	1.46091000
O	-1.00571500	2.28741400	1.03381900

F	-4.22278400	-2.61070700	-0.90341700
F	-3.21093200	-2.99540400	0.98582900
F	-4.59270900	-1.31927600	0.80765800
O	-2.35149500	3.00838600	-0.63786600
C	-1.88698600	3.10655800	0.48658000
H	-1.42193700	4.60219800	1.99896400
H	-2.78829600	5.01051700	0.90911900
H	-2.98336800	3.79758400	2.20135700

a₃-IN2

C	-2.32904200	1.99810500	0.47509700
O	-1.08681100	2.13199900	0.46399000
O	1.95980300	-0.42070400	-0.57549800
C	2.41331200	-1.20058100	0.34936100
O	1.97153100	-1.39833100	1.47460800
C	3.64734100	-1.99907000	-0.14775000
C	-2.97321600	0.72442800	0.26211900
C	-2.36182500	-0.58547400	0.32942100
C	-4.26756900	0.52448100	-0.21054100
C	-3.32391200	-1.50628200	-0.15004900
C	-1.12063300	-1.07499700	0.77918500
H	-5.04190600	1.24872700	-0.42232900
C	-3.07056100	-2.87619100	-0.24900900
C	-0.85527700	-2.44211600	0.66990100
H	-0.43364300	-0.48434000	1.41349900
C	-1.81562800	-3.32786900	0.15287300
H	-3.82076900	-3.56797600	-0.62021800
H	0.10223300	-2.80853000	1.02109000
H	-1.58315300	-4.38606400	0.08543800
N	-4.48001500	-0.79155800	-0.46817000
C	-3.14788800	3.23840700	0.74329000
H	-4.07506700	3.25671000	0.16288600
H	-3.42130800	3.26454400	1.80572700
H	-2.55114700	4.12350500	0.51581500
C	-5.69460400	-1.37280700	-1.01756500
H	-5.48607900	-1.85631600	-1.97745900
H	-6.11001500	-2.11360000	-0.32665000
H	-6.43044700	-0.58168600	-1.17177200
Pd	0.41109500	0.74144000	-0.03327600
C	2.92819500	3.97043300	-0.96253100
O	1.34127800	2.23338800	-0.97543800
F	4.26478400	-2.61761600	0.86778200
F	3.24990900	-2.94630100	-1.02885600
F	4.54247900	-1.21021200	-0.76547400

O	2.34307500	2.68479900	1.00215800
C	2.17014000	2.89493000	-0.18898500
H	2.25929000	4.52297600	-1.62832400
H	3.40861900	4.64999500	-0.25586200
H	3.69460000	3.49233200	-1.58249400

a₃-TS2

Imaginary Frequency: -1319.1536

C	-2.07252800	2.07925600	0.50591700
O	-0.94096700	2.20815600	-0.01383100
O	2.05350400	-0.57955400	-0.68869900
C	2.08970200	-1.30595900	0.33821300
O	1.16135800	-1.48082800	1.17741300
C	3.36453800	-2.15125000	0.54115400
C	-2.77473400	0.82616900	0.52540700
C	-2.26842000	-0.43570700	0.03676600
C	-4.14756800	0.65706200	0.70842100
C	-3.38992600	-1.28416100	-0.11422800
C	-0.97094200	-0.88041700	-0.30243300
H	-4.89195900	1.36684900	1.04217200
C	-3.29351200	-2.55825400	-0.67613200
C	-0.90450100	-2.14463000	-0.92106200
H	0.08024900	-0.95572600	0.57999500
C	-2.03121400	-2.96384200	-1.10382800
H	-4.15885500	-3.20499500	-0.78645000
H	0.06610700	-2.53432000	-1.21455000
H	-1.91189700	-3.94048800	-1.56355300
N	-4.51912000	-0.59216200	0.33332000
C	-2.70835400	3.34384400	1.03910500
H	-1.94530200	3.92098300	1.56817200
H	-3.05860700	3.95609500	0.19950400
H	-3.54623400	3.14887800	1.71230900
C	-5.87087200	-1.12751900	0.35548100
H	-6.18453400	-1.41190800	-0.65425600
H	-5.92387600	-2.00611100	1.00658700
H	-6.55135300	-0.36363100	0.73591100
Pd	0.43517600	0.74098500	-0.55619500
C	3.45719900	3.70160900	-0.45483300
O	2.53719500	2.03408800	1.03236900
F	4.42196800	-1.60668900	-0.06546100
F	3.64202000	-2.30228800	1.84082000
F	3.15106900	-3.37491500	0.00768500
O	1.66055900	2.28103800	-1.03245400
C	2.49674800	2.58085800	-0.06776400

H	2.90513300	4.56291700	-0.84423300
H	4.04914600	3.99614700	0.41416200
H	4.12531100	3.35459800	-1.25091200

a₃-IN3

C	-2.37513300	2.05024100	-0.04156500
O	-1.13158000	2.11395500	-0.21679800
O	1.75104800	-0.83826200	-0.59620400
C	2.66784600	-0.95181500	0.28003300
O	2.94309400	-0.23062100	1.24707600
C	3.53205900	-2.21829900	0.04333900
C	-3.05254300	0.80089300	0.06133600
C	-2.39881700	-0.48541300	-0.01803900
C	-4.41259500	0.54737600	0.24397300
C	-3.41003800	-1.46261200	0.12080700
C	-1.05891800	-0.85542900	-0.19602800
H	-5.24088100	1.23441700	0.35002300
C	-3.13518000	-2.83027400	0.08698700
C	-0.77873000	-2.22385600	-0.23544800
H	2.72795900	1.37082100	1.27362800
C	-1.80028200	-3.18572700	-0.09456000
H	-3.91179100	-3.58141600	0.19451200
H	0.24139200	-2.56099900	-0.37453400
H	-1.53382200	-4.23879000	-0.12951800
N	-4.62984400	-0.79075700	0.28037500
C	-3.10331400	3.37020100	0.06451300
H	-2.76601100	3.89350700	0.96654200
H	-2.83702300	3.99622100	-0.79298800
H	-4.18903900	3.26066100	0.10574100
C	-5.91585900	-1.44387200	0.45486700
H	-6.14174800	-2.07697400	-0.40958100
H	-5.90839300	-2.06510800	1.35661400
H	-6.69434600	-0.68479200	0.55260700
Pd	0.28002700	0.59076800	-0.38220500
C	2.81125800	4.35363400	-0.02548000
O	2.87506100	2.37400400	1.25966400
F	4.15264500	-2.15160400	-1.15051900
F	4.46527300	-2.37360800	0.98997900
F	2.75392100	-3.32471100	0.04252200
O	1.67269000	2.33812400	-0.65420800
C	2.39183900	2.91736700	0.16568700
H	2.26975700	4.79441900	-0.86275800
H	2.62424700	4.92078800	0.89158100
H	3.88873600	4.39443000	-0.21965100

a₃-IN1'				C	2.41293500	1.09917500	-1.18702800
C	1.86372500	-0.95537800	1.53206500	O	1.25559600	1.45841700	-1.52085100
O	0.63411300	-1.21253200	1.61733600	O	-2.18526300	0.45577100	0.48207200
O	-2.70430400	-0.66588000	-0.80383900	C	-2.85420900	-0.34968300	-0.26857000
C	-2.98357800	0.22836800	0.04662700	O	-2.50201500	-0.78203400	-1.36701200
O	-2.20920700	0.47050200	1.01889700	C	-4.18760500	-0.81183600	0.36306100
C	-4.25929100	1.06911200	-0.11273600	C	2.67911600	-0.17393200	-0.57698100
C	2.43160000	0.17055200	0.83998400	C	1.78001500	-1.30521300	-0.47913500
C	1.83308500	1.40720400	0.36338100	C	3.80469000	-0.50743600	0.16872700
C	3.75705900	0.19751000	0.41408500	C	2.41453200	-2.25623600	0.35442300
C	2.85051900	2.09819900	-0.34218800	C	0.52522700	-1.61461500	-1.03110700
C	0.58494500	2.02993800	0.51696400	H	4.68674900	0.08238400	0.37673200
H	4.52130400	-0.55861100	0.52614200	C	1.82354700	-3.47705000	0.68655700
C	2.65506900	3.35065400	-0.92779400	C	-0.08326200	-2.82151400	-0.68581100
C	0.37850300	3.27574700	-0.06972800	H	0.06066700	-0.99349900	-1.80071100
H	-0.20908900	1.56619900	1.08774300	C	0.55816200	-3.73872700	0.16476900
C	1.39587800	3.92727400	-0.78995100	H	2.32297700	-4.19630400	1.32869800
H	3.45060000	3.85943700	-1.46401200	H	-1.06406700	-3.04569300	-1.09052700
H	-0.59116800	3.75373100	0.03562100	H	0.06346300	-4.67300200	0.41230400
H	1.20137600	4.89858300	-1.23539900	N	3.65403800	-1.73353300	0.73195900
N	4.00945800	1.32124800	-0.30026600	C	3.52161400	2.08713000	-1.44209300
C	2.76980000	-1.92082300	2.26329600	H	3.28872300	2.66694500	-2.33868200
H	2.21626700	-2.36382100	3.09459500	H	3.53459700	2.77720500	-0.58911600
H	3.02353900	-2.72178600	1.55916500	H	4.50169500	1.61609900	-1.54641500
H	3.68471900	-1.45270600	2.63344100	C	4.59579600	-2.38796000	1.62484800
C	5.26491400	1.66212300	-0.94595000	H	4.13934000	-2.55290000	2.60633400
H	5.12472600	1.75721500	-2.02780600	H	4.90994700	-3.35150700	1.21006600
H	5.65392200	2.60764200	-0.55306800	H	5.47398300	-1.75130300	1.74554500
H	5.99212500	0.87171300	-0.75169100	Pd	-0.47071200	0.87629100	-0.49253300
Pd	-0.89134500	-1.05470100	0.23632100	C	0.29144200	4.42292700	1.70225800
C	0.92398600	-4.18382400	-2.07328800	O	-0.52705100	2.68926100	0.35737300
O	-0.30390200	-2.59953300	-0.86765300	F	-4.83923200	0.20375200	0.95197800
F	-5.08145000	0.53954900	-1.02338800	F	-4.99444800	-1.35210400	-0.56042800
F	-4.90803100	1.15903200	1.05818100	F	-3.94088200	-1.75115800	1.30257300
F	-3.92573400	2.31380700	-0.50707900	O	1.54291200	2.40343800	1.24877400
O	1.96221600	-2.47937400	-0.71596800	C	0.51332200	3.04906800	1.07184700
C	0.92197800	-2.97926500	-1.13312100	H	-0.51656700	4.36016400	2.43852100
H	0.39499100	-3.93796400	-2.99937400	H	1.21044400	4.74952600	2.19292200
H	1.95335500	-4.47138000	-2.29603100	H	-0.01180300	5.14939200	0.94260700
H	0.39543900	-5.02205100	-1.60771700	a₃-IN2'			
a₃-TS1'				C	2.52173300	1.21450100	-1.04174600
Imaginary Frequency: -48.8038				O	1.37167100	1.58417300	-1.37515900
				O	-2.07395300	0.22379800	0.41115200

C	-2.82169800	-0.49312700	-0.35990000
O	-2.59316600	-0.87268700	-1.50344000
C	-4.12664500	-0.92852800	0.35579100
C	2.76910700	-0.09235800	-0.49153300
C	1.84043100	-1.20216200	-0.45545900
C	3.88187100	-0.49344100	0.23971700
C	2.44410600	-2.20989400	0.33246800
C	0.56846200	-1.44364700	-1.01225800
H	4.78172000	0.05805100	0.47507600
C	1.81253900	-3.42406400	0.60990800
C	-0.07722900	-2.64862300	-0.72083300
H	0.14116300	-0.81402200	-1.80846600
C	0.53764400	-3.62278200	0.08261300
H	2.28937600	-4.18713200	1.21779700
H	-1.06398700	-2.81992000	-1.13574600
H	0.01502400	-4.55153700	0.28910500
N	3.69642800	-1.74297900	0.73818900
C	3.62981300	2.22069800	-1.20832800
H	3.45269100	2.80473400	-2.11519300
H	3.56802400	2.90730700	-0.35438200
H	4.62362600	1.76910300	-1.24566800
C	4.61735300	-2.46848000	1.59822000
H	4.15417800	-2.66919400	2.56978100
H	4.90529700	-3.41809100	1.13538500
H	5.51284900	-1.86379600	1.75133800
Pd	-0.36733300	0.81281300	-0.47763200
C	-0.25960100	4.53332600	1.51007900
O	-0.76928700	2.65257200	0.20289600
F	-4.71706000	0.09643600	0.99300800
F	-5.00635300	-1.44273600	-0.51480900
F	-3.84540300	-1.88238400	1.27275000
O	1.18784900	2.60166600	1.34939600
C	0.14215300	3.14877800	1.00828400
H	-1.12933600	4.44293800	2.16944800
H	0.57240400	4.97572100	2.06162400
H	-0.54653200	5.17809800	0.67419700

a₃-TS2'

Imaginary Frequency: -1347.2526

C	-2.19966000	1.53926100	1.15594200
O	-1.04724900	1.90753600	0.84243000
O	2.30670100	-0.23653600	-0.37316700
C	2.38510900	-1.19661600	0.43205200
O	1.45358000	-1.66208600	1.15418000

C	3.73080700	-1.94980500	0.49539500
C	-2.73831700	0.26721900	0.75977700
C	-2.03621200	-0.76376300	0.03073700
C	-4.08580200	-0.08900300	0.75331200
C	-3.02378900	-1.66410500	-0.43394600
C	-0.67268400	-0.95769200	-0.28568800
H	-4.93777000	0.42824800	1.17298000
C	-2.72402700	-2.73421700	-1.27885500
C	-0.40007500	-2.00800400	-1.18382200
H	0.35548900	-1.12945700	0.64283500
C	-1.39422400	-2.87554600	-1.66686300
H	-3.48849200	-3.42060100	-1.63043400
H	0.62830100	-2.19545900	-1.47879400
H	-1.11677300	-3.68176000	-2.33949400
N	-4.26265500	-1.23565800	0.04982400
C	-3.04634000	2.54029600	1.91112300
H	-2.39282100	3.17567300	2.51273400
H	-3.56956300	3.18438400	1.19339000
H	-3.78766000	2.05944600	2.55493900
C	-5.53211100	-1.89516100	-0.20923500
H	-5.73003600	-1.93205500	-1.28554500
H	-5.52120100	-2.91580000	0.18690400
H	-6.33161300	-1.33485300	0.27882200
Pd	0.50530800	0.82297700	-0.06162600
C	1.92524800	4.68362200	-0.97066000
O	1.56425600	2.55115900	-0.01128000
F	4.74111900	-1.19638200	0.05472800
F	4.00113700	-2.34225100	1.74731400
F	3.64317000	-3.04735100	-0.28495700
O	0.28747300	3.09962600	-1.78129500
C	1.16991700	3.36003500	-0.96364200
H	1.81971500	5.18446200	-0.00247500
H	2.99382900	4.50249300	-1.12879000
H	1.53907600	5.32510000	-1.76552300

a₃-IN3'

C	2.42419100	1.97754200	-0.30933200
O	1.17073700	2.01238400	-0.38358500
O	-1.70699500	-0.94941400	0.00816900
C	-2.94253000	-0.80451900	-0.24725600
O	-3.57619500	0.20835100	-0.59213200
C	-3.75888400	-2.10588300	-0.03393100
C	3.12265600	0.75032300	-0.10484200
C	2.47215900	-0.53274100	0.01519500

C	4.49345100	0.51219900	-0.01388400
C	3.49459400	-1.49545400	0.17036000
C	1.12603200	-0.91558600	0.00222400
H	5.32377100	1.20360200	-0.05804100
C	3.21896100	-2.85666100	0.30996200
C	0.83958300	-2.27467100	0.13756400
H	-2.65651500	1.49155500	-0.55643300
C	1.87423300	-3.22170800	0.28757300
H	4.00350300	-3.59777000	0.42876900
H	-0.19088400	-2.61009700	0.12987900
H	1.61006800	-4.27077900	0.39117800
N	4.72007500	-0.81621200	0.14948200
C	3.14015400	3.29590800	-0.47827400
H	3.07879000	3.60510700	-1.52852100
H	2.62693000	4.05706000	0.11621500
H	4.19190100	3.24992600	-0.18653900
C	6.01977000	-1.45136900	0.28626900
H	6.09184400	-1.96879200	1.24866600
H	6.17598600	-2.17683000	-0.51898100
H	6.79939500	-0.68905500	0.23370500
Pd	-0.23078300	0.50799900	-0.17920800
C	-3.61491400	3.33369100	0.73247500
O	-1.86291500	2.10779600	-0.39806500
F	-3.02436700	-3.20606800	-0.28015500
F	-4.17734000	-2.16619500	1.24856600
F	-4.83929400	-2.14128500	-0.82615200
O	-1.25018900	3.80441700	0.93078900
C	-2.13620500	3.13184200	0.46867300
H	-4.11618800	3.65369200	-0.18845700
H	-4.08522600	2.39638500	1.04761300
H	-3.74395700	4.09771800	1.49975800

a₃'-IN1

C	0.85051800	-1.50426300	-1.62197000
O	-0.25631300	-0.93849100	-1.45453800
O	-2.60609800	0.23759800	-0.37274900
C	-2.81358600	-0.63591200	0.55776300
O	-2.02828400	-1.13108800	1.35216000
C	-4.30648700	-1.06381900	0.57861900
C	2.01509100	-1.28985800	-0.80123300
C	2.12022800	-0.82634700	0.57504400
C	3.32406800	-1.45994300	-1.25135100
C	3.50424700	-0.72365400	0.85626500
C	1.19700300	-0.57977300	1.60451400

H	3.68205000	-1.76100000	-2.22602800
C	3.99990500	-0.33207600	2.10216100
C	1.68529500	-0.18571400	2.84767100
H	0.12963000	-0.71920000	1.45717300
C	3.06456400	-0.05243900	3.09372000
H	5.06589300	-0.25953600	2.29623600
H	0.98025900	0.01152200	3.64995800
H	3.40683300	0.25551500	4.07766100
N	4.20890700	-1.10580100	-0.28747500
C	0.89510100	-2.51900400	-2.74424900
H	0.20485800	-2.22170900	-3.53671400
H	1.89860000	-2.66273600	-3.15196900
H	0.56087300	-3.48594000	-2.34662000
C	5.65586300	-1.10485500	-0.41210300
H	6.05177400	-0.09445400	-0.26530600
H	6.10392600	-1.77316500	0.33090400
H	5.92982800	-1.45153000	-1.41031000
Pd	-0.72897300	0.91480000	-0.62974200
C	0.89914700	4.49058500	-0.26392200
O	0.97093500	2.13870500	-0.86228300
F	-5.11819000	0.00334300	0.70808700
F	-4.63148500	-1.69509700	-0.56945500
F	-4.55761600	-1.90107400	1.59466100
O	-0.91151900	2.89934000	-0.05478900
C	0.30297500	3.12158400	-0.39268900
H	0.54337100	4.96753300	0.65316100
H	1.98947900	4.42881600	-0.26742800
H	0.57529900	5.10553500	-1.11174600

a₃'-TS1

Imaginary Frequency: -52.5844

C	0.55752600	-1.42634500	-1.48762800
O	-0.29893100	-0.51278700	-1.51260000
O	-2.45138000	-0.08029500	0.66020500
C	-2.03949900	-1.22370000	0.94232400
O	-0.90719300	-1.58756200	1.35800900
C	-3.02215000	-2.40583100	0.69501400
C	1.80528400	-1.26330600	-0.77755300
C	2.01889100	-0.31052300	0.27085100
C	3.06041600	-1.77087900	-1.10259400
C	3.40802000	-0.24314600	0.50288600
C	1.10789300	0.42103300	1.06525700
H	3.33905200	-2.49366000	-1.85751500
C	3.94194000	0.62333300	1.45776600

C	1.66078700	1.31335400	2.00686900	H	3.47857300	-2.28333500	-2.79719100
H	0.12387300	-0.11149600	1.27959700	H	-0.82534900	-2.17457600	-2.40442900
C	3.04685400	1.41810700	2.18566000	H	1.20630100	-2.66073600	-3.72685100
H	5.01074100	0.68573400	1.64098400	N	3.78561000	-1.25233300	-0.11004500
H	0.99293500	1.90068800	2.62939500	C	1.59646200	0.23199500	3.45937500
H	3.43995500	2.10485700	2.92913600	H	0.92782300	-0.01078000	4.28852400
N	4.02210100	-1.15865400	-0.35593500	H	2.61596600	-0.07890800	3.70252500
C	0.22670000	-2.69095700	-2.22840900	H	1.58666600	1.31991100	3.31860800
H	-0.28476300	-2.45667600	-3.16553200	C	5.16947900	-1.38840500	-0.53134400
H	1.10159900	-3.31882600	-2.41320300	H	5.39470700	-2.43278500	-0.77195500
H	-0.47776200	-3.24421100	-1.59402200	H	5.36134400	-0.77119300	-1.41532600
C	5.45405400	-1.39714600	-0.44169100	H	5.82492900	-1.06134900	0.27802900
H	5.97900000	-0.47824100	-0.72278500	Pd	-1.31934000	-1.11529600	0.46470200
H	5.84123500	-1.75140700	0.51928600	C	-5.16627300	-1.52189400	-0.65743500
H	5.64398100	-2.15868700	-1.20007500	O	-3.55174700	-0.92391500	1.05000700
Pd	-0.41338300	1.22275900	-0.37568100	F	0.84311500	4.88965100	0.05463200
C	-2.22527000	4.74290300	-0.49515800	F	0.32225800	4.16818100	-1.93232600
O	-1.56742000	2.67523800	-1.57877200	F	-1.24893700	4.68359000	-0.51137000
F	-4.27415900	-2.00935200	0.41844000	O	-2.77735400	-1.57612000	-0.91307100
F	-2.59461300	-3.14562300	-0.37392500	C	-3.77139000	-1.32272000	-0.12018700
F	-3.08131600	-3.24537500	1.74888800	H	-5.28849400	-2.55565200	-0.99748100
O	-0.78481700	3.03996100	0.43255300	H	-5.90348800	-1.29452800	0.11455300
C	-1.49536900	3.43668100	-0.57370200	H	-5.32413000	-0.87115500	-1.52418800
H	-1.67397100	5.45155600	0.12828300				
H	-2.37616500	5.14776100	-1.49863300	a₃'-IN3			
H	-3.20654400	4.57151600	-0.03716300	C	1.05659500	2.19500200	-0.00410800
				O	-0.19111100	2.04498100	-0.00432700
a₃'-IN2				C	1.94456300	1.07573800	-0.00533200
C	1.08365500	-0.40041700	2.19157200	C	1.50363900	-0.29864900	-0.00090200
O	-0.16362600	-0.52254000	2.08376000	C	3.33890200	1.04269600	-0.00707400
O	0.71531200	2.32780400	0.78443200	C	2.66210500	-1.10488000	0.00013300
C	-0.01769600	2.68882300	-0.10484200	C	0.22766900	-0.87052200	0.00199800
O	-0.90339000	1.96234300	-0.77550900	H	4.05548700	1.85268100	-0.00959400
C	-0.02554200	4.14170500	-0.63291300	C	2.59306800	-2.50003100	0.00408700
C	1.96655700	-0.80308700	1.14239300	C	0.14861200	-2.26402900	0.00589600
C	1.52088700	-1.30162500	-0.13414100	C	1.31461700	-3.05833600	0.00698800
C	3.35880600	-0.79270100	1.09637900	H	3.48118200	-3.12478500	0.00502000
C	2.67477600	-1.57565400	-0.89961400	H	-0.82581700	-2.74305100	0.00794400
C	0.24400100	-1.50822700	-0.66234200	H	1.21306400	-4.14062100	0.01015200
H	4.07669400	-0.48643500	1.84491100	N	3.76989000	-0.24609900	-0.00358900
C	2.59473000	-2.07071100	-2.20340000	C	1.56345600	3.61850500	0.01447500
C	0.15181800	-2.00159000	-1.96387800	H	1.30128500	4.07920400	0.97397500
H	-0.90745400	1.03051100	-0.43555800	H	2.64395600	3.69119400	-0.12809500
C	1.31385700	-2.27756200	-2.71554200	H	1.05618700	4.19029400	-0.76872700

C	5.15506600	-0.68316500	-0.00489200
H	5.36706100	-1.28215800	0.88712900
H	5.36379100	-1.28713500	-0.89432600
H	5.80849600	0.19145700	-0.00852900
Pd	-1.34492500	0.30431900	-0.00118800
C	-5.18578700	-0.92379300	-0.00066800
C	-3.79278000	-0.34125100	-0.00090300
O	-2.79602200	-1.16609900	0.00167900
O	-3.58691600	0.89785100	-0.00374800
H	-5.92931600	-0.12465800	-0.00028300
H	-5.32179700	-1.55840200	0.88156400
H	-5.3222300	-1.55756600	-0.88346900

a₃''-TS1

Imaginary Frequency: -91.9977

C	-1.25497400	-0.83949100	2.28765000
O	-0.07985700	-0.53966200	2.04726300
O	2.41106100	0.36814800	-0.14421100
C	2.87703300	-0.83605200	-0.07405200
O	2.28956400	-1.90608300	-0.03177200
C	4.43160700	-0.80758300	-0.06406100
C	-2.19491700	-1.07567700	1.19838200
C	-1.84094000	-1.16275800	-0.19374900
C	-3.58163600	-1.02887600	1.24216400
C	-3.04718500	-1.12321800	-0.93136800
C	-0.60889400	-1.26950800	-0.87342000
H	-4.24189900	-0.94116800	2.09466400
C	-3.06786000	-1.13990800	-2.32751200
C	-0.63300100	-1.26482500	-2.27708000
H	0.31180200	-1.54971800	-0.35436000
C	-1.84021000	-1.18978700	-2.99054100
H	-3.99989400	-1.11494500	-2.88488200
H	0.30491800	-1.36239700	-2.81567100
H	-1.82346100	-1.19825200	-4.07631300
N	-4.10009800	-1.05833600	-0.01988600
C	-1.73566300	-0.93422100	3.72380700
H	-0.89825400	-0.73832700	4.39574200
H	-2.52797600	-0.20037200	3.91717900
H	-2.14744600	-1.92899500	3.93045500
C	-5.50820500	-0.99902000	-0.36965500
H	-5.71476900	-0.11619300	-0.98423000
H	-5.80763200	-1.89559600	-0.92326000
H	-6.10052400	-0.93710600	0.54526300
Pd	0.47813300	0.87629400	-0.04309000

C	-1.40137200	4.38266300	-0.18645800
C	-0.64138000	3.09069900	-0.11763200
O	-1.26592800	1.97449000	0.03336100
O	0.62037000	3.05300500	-0.23056900
F	4.93638000	-2.04457700	0.03230400
F	4.90246800	-0.25263800	-1.19971000
F	4.89368600	-0.08522800	0.97425700
H	-0.81757500	5.18377900	0.27390800
H	-1.56897100	4.64528300	-1.23766800
H	-2.37062900	4.28102000	0.30744200

a₃''-IN2

C	2.47403200	-2.71840600	-1.18961300
O	1.32491100	-3.13942300	-1.23561100
O	-2.16483400	-0.41556300	-0.33843700
C	-3.13796000	-0.17551800	0.48635500
O	-3.16646000	0.58698700	1.43904200
C	-4.37548200	-1.04703200	0.13821200
C	2.83611700	-1.61926300	-0.28006500
C	1.94103400	-0.91004500	0.59650300
C	4.08597100	-1.05745700	-0.08268800
C	2.71072400	0.04861400	1.29100000
C	0.55005900	-1.00033000	0.85994700
H	5.03314000	-1.29901600	-0.54515600
C	2.16475100	0.91264800	2.26217400
C	-0.00519100	-0.12917200	1.83669900
H	-0.02898300	-1.80899500	0.42999400
C	0.81568600	0.81218800	2.52944200
H	2.78493100	1.63254200	2.78776900
H	-1.02580500	-0.27001600	2.17468100
H	0.35757900	1.45037100	3.27784000
N	4.01877800	-0.06031000	0.85594300
C	3.56383100	-3.31436200	-2.06864000
H	3.13487000	-4.12274300	-2.66335000
H	3.98231200	-2.55482800	-2.74042400
H	4.38763000	-3.70968200	-1.46163100
C	5.12837300	0.76308300	1.30777600
H	4.93830300	1.81856300	1.08694700
H	5.28414100	0.64513000	2.38531900
H	6.03543600	0.45182000	0.78656000
Pd	-0.54004100	0.76919000	-0.22448400
C	0.77811700	3.97968300	-2.16341900
C	0.26816800	2.75492100	-1.46318200
O	0.97091100	2.17128000	-0.55918900

O	-0.87832400	2.27235900	-1.72543600
F	-5.39660300	-0.78548100	0.96423400
F	-4.78712700	-0.81973100	-1.12302600
F	-4.07423400	-2.35773300	0.24889900
H	0.54519000	3.92099300	-3.23021800
H	0.26998100	4.86240600	-1.75832700
H	1.85438300	4.08696500	-2.01225600

a₃''-TS2

Imaginary Frequency: -1199.2703

C	-0.97278100	-0.85757300	2.29241500
O	0.18784600	-0.51223000	2.09131200
O	2.38566500	0.32139100	-0.18792700
C	2.49574600	-0.92364000	-0.24555400
O	1.58908400	-1.76875700	-0.49374400
C	3.91419300	-1.50600000	-0.05193200
C	-1.92558100	-1.04236600	1.19157400
C	-1.70292000	-0.83792800	-0.22104500
C	-3.23334000	-1.48828400	1.31824300
C	-2.91593500	-1.19071400	-0.87163100
C	-0.59221800	-0.40739100	-1.00144100
H	-3.78354000	-1.75370500	2.21082700
C	-3.07686900	-1.13194500	-2.25654500
C	-0.77679800	-0.36770500	-2.40145900
H	0.54003100	-1.09631300	-0.69520200
C	-1.98387700	-0.72305100	-3.01943700
H	-4.01657000	-1.40307900	-2.72967700
H	0.05690700	-0.06147600	-3.02826200
H	-2.07199800	-0.67785400	-4.10104100
N	-3.83446800	-1.58003900	0.09774000
C	-1.45949300	-1.11106100	3.71407200
H	-2.28187600	-0.43309100	3.97344900
H	-1.82598000	-2.13821100	3.83044000
H	-0.62889700	-0.94727700	4.40285500
C	-5.19381000	-2.01980000	-0.15962600
H	-5.76923300	-1.22924400	-0.65360400
H	-5.19894700	-2.91247600	-0.79475500
H	-5.67461300	-2.26231100	0.79006000
Pd	0.51962600	1.23033000	-0.26536300
C	-0.94240900	4.84696900	0.52453600
C	-0.33610500	3.50750900	0.21047800
O	-1.08779600	2.54460700	-0.19321000
O	0.90367300	3.28855800	0.35852700
F	4.72192700	-0.64047000	0.56661800

F	4.43771800	-1.78981600	-1.26114400
F	3.86892800	-2.63772800	0.66446500
H	-0.20583900	5.63750300	0.36239400
H	-1.24209800	4.86764200	1.57909400
H	-1.83064200	5.01642400	-0.08905600

a₃''-IN3

C	-0.94197900	-0.47194900	2.29434000
O	0.23606000	-0.22914100	2.03340500
O	2.16151700	-0.31628800	-0.38196100
C	1.98899100	-1.52430800	-0.32218600
O	0.85667900	-2.17431300	-0.41861100
C	3.18731300	-2.47921700	-0.14767100
C	-1.94898500	-0.62641100	1.24363600
C	-1.81955400	-0.35289000	-0.18108500
C	-3.19655600	-1.20064400	1.41782900
C	-3.02483300	-0.82240700	-0.78260300
C	-0.84403000	0.26390600	-1.00260600
H	-3.66690000	-1.55612100	2.32439200
C	-3.27582800	-0.74687600	-2.15372000
C	-1.09557300	0.31949200	-2.37893000
H	0.11995900	-1.51970400	-0.53947100
C	-2.28304200	-0.18044300	-2.94586300
H	-4.20360400	-1.11034100	-2.58519600
H	-0.36987300	0.79444100	-3.03332400
H	-2.43224600	-0.10383300	-4.01952300
N	-3.84277100	-1.32697200	0.22230800
C	-1.37742700	-0.63669800	3.74446200
H	-2.12910600	0.11560300	4.01155200
H	-1.82016000	-1.62469300	3.91919200
H	-0.50400600	-0.51980500	4.38843000
C	-5.16210800	-1.89538100	0.01650900
H	-5.83875800	-1.15349900	-0.42185700
H	-5.10973100	-2.76332400	-0.65009300
H	-5.56657200	-2.21496200	0.97897600
Pd	0.71027200	1.28915600	-0.29840200
C	0.65168900	5.21795100	0.51968600
C	0.77038500	3.74231900	0.23150200
O	-0.27694100	3.11808600	-0.19269300
O	1.85177700	3.11512000	0.39271100
F	4.31199700	-1.79223600	0.03861600
F	3.31667200	-3.23946000	-1.24901900
F	2.98421100	-3.28468900	0.90518400
H	1.60845800	5.61207000	0.86726700

H	-0.11801500	5.38544300	1.28053800
H	0.33800600	5.74744900	-0.38620000
b₃-IN1			
C	1.57539200	1.10791700	1.29131400
O	0.37820400	1.45873200	1.48219700
O	-3.04110600	0.32026600	-0.63124700
C	-2.94438700	-0.75336100	0.02513000
O	-2.01191600	-0.93210400	0.86647800
C	-3.95888300	-1.88713400	-0.18988200
C	1.98123300	-0.12827600	0.68111200
C	3.29281400	-0.54639700	0.20466700
C	1.13857000	-1.22648100	0.50132700
C	3.14651900	-1.88571500	-0.23980200
C	4.55138600	0.06148000	0.06723000
H	0.09543300	-1.33941800	0.76050800
C	4.19475400	-2.63003700	-0.78317200
C	5.60421400	-0.67284300	-0.47134000
H	4.71171500	1.09208000	0.36150900
C	5.43302600	-2.00437600	-0.88938900
H	4.05243800	-3.65433700	-1.11416400
H	6.57840200	-0.20409000	-0.57665400
H	6.27456100	-2.54924100	-1.30687800
N	1.81879600	-2.26442700	-0.03503700
C	2.61076100	2.08122100	1.79142400
H	2.94597900	2.67196000	0.92880100
H	2.14786600	2.76068400	2.50984800
H	3.47484300	1.58268200	2.23754600
C	1.26071200	-3.57295700	-0.33779700
H	0.19180900	-3.55991800	-0.11746900
H	1.40205300	-3.80750600	-1.39771100
H	1.74434200	-4.34734600	0.26701900
Pd	-1.27475400	1.04337500	0.32776900
C	-0.15063300	4.62929000	-1.63513100
O	-1.13737800	2.85595200	-0.45696900
F	-4.82064700	-1.59762200	-1.16715900
F	-3.30211500	-3.01904000	-0.51483000
F	-4.64543700	-2.11179300	0.94246400
O	0.99959300	2.55635700	-1.15657400
C	-0.02313100	3.22411700	-1.05493700
H	0.79025900	4.91218800	-2.11096300
H	-0.96188000	4.65835200	-2.36965100
H	-0.40016100	5.34342100	-0.84374000

b₃-TS0			
Imaginary Frequency: -1317.8262			
C	-1.77126800	1.81242400	-1.15674100
O	-0.59060400	2.25964900	-1.06312800
O	2.17007400	-0.53684000	0.28314300
C	1.98345800	-1.53869100	-0.44774800
O	0.98408200	-1.76444500	-1.19871600
C	3.02484600	-2.67561000	-0.36767200
C	-2.06317200	0.50229500	-0.66146700
C	-3.29824700	-0.08408100	-0.20596700
C	-0.99162400	-0.30429300	-0.19755700
C	-2.92294900	-1.21947800	0.56168100
C	-4.66389500	0.22705400	-0.33385700
H	0.07540000	-0.88889100	-0.86698100
C	-3.86591300	-2.05787400	1.16900900
C	-5.60097900	-0.59788300	0.27417700
H	-4.98970400	1.08723500	-0.90914800
C	-5.20694200	-1.72955100	1.01663800
H	-3.56917100	-2.93285100	1.73806500
H	-6.65834400	-0.37139100	0.17280100
H	-5.96481900	-2.35723100	1.47593800
N	-1.53426100	-1.30600100	0.56866900
C	-2.81519900	2.72697700	-1.73366900
H	-3.50707400	3.04302800	-0.94268200
H	-2.33571400	3.61182600	-2.15607700
H	-3.40176600	2.21444300	-2.50357200
C	-0.78518800	-2.36182900	1.24207600
H	0.18261600	-1.97051600	1.55668800
H	-1.33338700	-2.66891600	2.13468100
H	-0.63767600	-3.22678700	0.58790300
Pd	0.74468400	0.96622500	-0.13808600
C	3.26661200	4.03414700	1.17940700
O	2.18610800	2.37334700	-0.11606100
F	4.18216000	-2.25280900	0.14185800
F	2.52820100	-3.64195300	0.43561400
F	3.24933900	-3.20456100	-1.57617100
O	1.43323600	2.67097100	1.97989300
C	2.19843600	2.95714600	1.06012700
H	3.20836400	4.50061900	2.16464000
H	4.25870900	3.59311500	1.03631900
H	3.12862100	4.78988400	0.39933200
b₃-IN2			
C	2.05303700	2.12642000	0.34276300

O	0.80313600	2.39652300	0.38852400
O	-1.51857800	-0.99996700	-0.05837300
C	-2.76472100	-1.12987700	0.16903600
O	-3.61132800	-0.27445400	0.47532500
C	-3.25632200	-2.59867100	0.08810800
C	2.43250500	0.78518500	0.14086400
C	3.66425700	0.03827200	0.01591900
C	1.35597100	-0.12657300	0.01044600
C	3.26313700	-1.30642300	-0.18812300
C	5.03201500	0.33844400	0.05083400
H	-2.97033400	1.15445400	0.48667600
C	4.17761500	-2.34499300	-0.35409300
C	5.95352400	-0.69462500	-0.11498200
H	5.37574800	1.35714200	0.20440000
C	5.53379100	-2.01976300	-0.31473200
H	3.85331200	-3.36943900	-0.50797600
H	7.01626500	-0.47067000	-0.08905200
H	6.27406900	-2.80446000	-0.44054700
N	1.85429800	-1.36679800	-0.18709400
C	3.01513500	3.26785800	0.50793600
H	3.65299400	3.35469600	-0.37977300
H	2.46772100	4.20074000	0.65369300
H	3.67221100	3.08919600	1.36740000
C	1.12037700	-2.61205100	-0.38125400
H	0.05308800	-2.40519100	-0.37488400
H	1.40368800	-3.05906300	-1.34003800
H	1.36478100	-3.31508400	0.42247400
Pd	-0.40319900	0.74641800	0.14481700
C	-4.23523800	2.95904500	-0.61609600
O	-2.28786600	1.89803300	0.34492700
F	-2.46858200	-3.35150600	-0.70184200
F	-3.24277000	-3.14011000	1.32284400
F	-4.50711600	-2.66380600	-0.38634500
O	-1.94865500	3.66148500	-0.99883500
C	-2.72857600	2.90677100	-0.48366500
H	-4.50614400	3.72094900	-1.34753600
H	-4.63218500	1.98494900	-0.92162000
H	-4.68464600	3.20587500	0.35261000

b₃-IN1'

C	1.52822000	1.55261900	0.93509000
O	0.28147500	1.70757000	0.98368400
O	-2.89476300	-0.50879500	-0.64383700
C	-2.48278500	-1.43106800	0.11062400

O	-1.49034500	-1.26127300	0.88417600
C	-3.14770500	-2.81555800	0.07954300
C	2.20233900	0.38319300	0.43301600
C	3.61142400	0.18805300	0.11120300
C	1.58747600	-0.85404400	0.22749100
C	3.74486600	-1.16878700	-0.28297700
C	4.75816600	0.99914900	0.08005900
H	0.56348000	-1.14801200	0.40924100
C	4.95625400	-1.73321300	-0.68545300
C	5.97203400	0.44484100	-0.31658000
H	4.71432800	2.04651300	0.35527300
C	6.07460000	-0.90556800	-0.69405900
H	5.02603900	-2.77529900	-0.98218600
H	6.85913500	1.07127300	-0.33743400
H	7.03620000	-1.30696300	-0.99963600
N	2.48903500	-1.77003200	-0.18868300
C	2.33495200	2.71217700	1.47339900
H	2.75566400	3.28189800	0.63467500
H	1.67531100	3.37186600	2.03968600
H	3.16399700	2.37268700	2.10102900
C	2.19957800	-3.16835500	-0.46960800
H	1.13384500	-3.34563900	-0.31403800
H	2.45358200	-3.40712800	-1.50738100
H	2.77339800	-3.81910600	0.19820300
Pd	-1.32173600	0.75080600	0.07439700
C	-2.50130900	4.45999400	-1.46131600
O	-2.94448700	3.11627200	0.50439900
F	-4.19938500	-2.84071500	-0.74107900
F	-2.24430300	-3.72411000	-0.35063300
F	-3.54467400	-3.17299600	1.30984300
O	-1.48305400	2.37294800	-1.04529500
C	-2.33938400	3.25153900	-0.54917300
H	-1.52560800	4.88636300	-1.71414100
H	-2.97959100	4.15380200	-2.39801500
H	-3.12087400	5.20768100	-0.96251100

b₃-TS0'

Imaginary Frequency: -1318.5270

C	-1.70410100	-2.15938300	0.57228600
O	-0.52670400	-2.50185500	0.26163200
O	1.94792400	0.68723100	-0.66938800
C	1.82232700	1.48142700	0.29565400
O	0.90414100	1.48276500	1.17017500
C	2.82045600	2.65591300	0.36782500

C	-2.10359600	-0.79225800	0.41788900
C	-3.40809700	-0.20643100	0.23696600
C	-1.12933400	0.17704600	0.06813500
C	-3.17380800	1.10486100	-0.25752700
C	-4.73572000	-0.63837900	0.40952500
H	-0.02199700	0.65690500	0.73275400
C	-4.21633400	1.99333200	-0.54967900
C	-5.77158900	0.23772300	0.11372900
H	-4.95637800	-1.63276600	0.78280200
C	-5.51550900	1.54076800	-0.35960000
H	-4.02522100	2.99912400	-0.90931800
H	-6.79957700	-0.08331700	0.25437200
H	-6.34807300	2.20332700	-0.57673600
N	-1.80008100	1.29168500	-0.37168700
C	-2.63960800	-3.24156800	1.03375100
H	-3.40287600	-3.42388900	0.26667500
H	-2.07985900	-4.16356900	1.20048000
H	-3.15607400	-2.94498800	1.95281100
C	-1.18171100	2.53901800	-0.81004900
H	-0.22621400	2.32016600	-1.28674300
H	-1.83077600	3.01399900	-1.54826200
H	-1.02300400	3.22173700	0.03040200
Pd	0.66847800	-0.95001000	-0.41184300
C	4.19798300	-3.24356800	-0.49984600
O	3.12588900	-1.66558900	0.98798700
F	3.94074800	2.39772000	-0.30697200
F	2.22570500	3.73806600	-0.18688200
F	3.13038900	2.94901900	1.63404200
O	2.11662500	-2.22623000	-0.95133900
C	3.09046100	-2.29076700	-0.06635000
H	3.78730800	-4.24063400	-0.68877900
H	4.64780900	-2.89200700	-1.43440700
H	4.96001900	-3.29562000	0.28006800

b₃-IN2'

C	1.95000200	2.21594600	-0.01951200
O	0.70687400	2.47542000	-0.18561600
O	-1.54709900	-0.96684100	-0.57532500
C	-2.43531300	-1.25356200	0.29648000
O	-2.82852200	-0.60235600	1.26986100
C	-3.07318300	-2.64358200	0.03596100
C	2.35163500	0.86714200	-0.00018500
C	3.59388000	0.13806600	0.13390200
C	1.30706600	-0.07702800	-0.17384600

C	3.23396400	-1.22939300	0.02908000
C	4.94129300	0.46954000	0.32475500
H	-2.93146900	1.01735700	1.34135400
C	4.16874700	-2.25961700	0.10988200
C	5.88358400	-0.55526000	0.40630400
H	5.25445100	1.50601300	0.40963700
C	5.50429200	-1.90292600	0.30064700
H	3.87517900	-3.30162800	0.02952300
H	6.93066500	-0.30649400	0.55487700
H	6.25943800	-2.68058100	0.36874900
N	1.83960200	-1.31855400	-0.16031400
C	2.88886500	3.37890200	0.13882900
H	3.65297300	3.35904900	-0.64736700
H	2.33609300	4.31855200	0.08352200
H	3.40957000	3.31808400	1.10193900
C	1.14586900	-2.59017600	-0.32052100
H	0.09380400	-2.40063200	-0.51612900
H	1.58097700	-3.14250300	-1.16003600
H	1.24887600	-3.19055100	0.58999100
Pd	-0.45835500	0.77175700	-0.37530700
C	-3.66794000	3.86921900	-0.03173400
O	-3.27326900	1.96950600	1.31808400
F	-3.70503700	-2.65382300	-1.15238700
F	-2.11730300	-3.60056300	0.00505400
F	-3.95536900	-2.97249500	0.98432900
O	-2.17436800	2.09985200	-0.65073700
C	-2.96226300	2.55768600	0.18824100
H	-3.27496200	4.36277200	-0.92050900
H	-4.74202300	3.68888500	-0.14934100
H	-3.53900400	4.50826500	0.84731700

b₃' -IN1

C	1.28142700	0.51830600	1.77427300
O	0.04728900	0.77587900	1.81971900
O	-2.27548300	-0.60440600	0.72182600
C	-2.16007600	-1.53534900	-0.16114900
O	-1.45932600	-1.56846300	-1.16871400
C	-3.04488200	-2.75922000	0.19829800
C	1.98378400	0.03791700	0.61996400
C	3.41732100	-0.12092300	0.39731400
C	1.35637800	-0.48234400	-0.51765200
C	3.55403200	-0.72690600	-0.87886400
C	4.58829500	0.19790000	1.10398300
H	0.30195500	-0.61629700	-0.73462200

C	4.78885800	-1.02734400	-1.45434900
C	5.82618300	-0.10090600	0.53969000
H	4.54685400	0.67484000	2.07648000
C	5.92967000	-0.70801000	-0.72349300
H	4.85994700	-1.48924700	-2.43437500
H	6.73151400	0.14360100	1.08794600
H	6.90985100	-0.92686800	-1.13660400
N	2.27345400	-0.93992100	-1.39350200
C	2.02228100	0.73701400	3.07367700
H	2.63061900	1.64761800	2.99974600
H	1.29897100	0.86821900	3.88021700
H	2.69221300	-0.09788000	3.29935100
C	1.96172300	-1.59626800	-2.65617500
H	0.88011200	-1.72509900	-2.72136100
H	2.31162700	-0.99118400	-3.49921100
H	2.44385200	-2.57803400	-2.69583000
Pd	-1.35172700	1.16037700	0.34787900
C	-2.24858700	4.31478000	-1.83647000
O	-0.84336800	3.09513200	-0.27844900
F	-2.59965100	-3.33583900	1.33460700
F	-4.32584800	-2.39651400	0.38997000
F	-3.01369600	-3.68270200	-0.77283500
O	-2.60668000	2.05579800	-1.03996800
C	-1.87945400	3.10895600	-1.02856900
H	-2.94045500	4.93650700	-1.25599200
H	-1.35686200	4.90445500	-2.06109700
H	-2.75337700	4.00982900	-2.75642300

b₃' - TS1

Imaginary Frequency: -87.7000

C	-1.83063000	-1.19918800	1.80445100
O	-0.70513000	-1.77208600	1.78150200
O	2.45911900	-0.04173600	1.13875100
C	2.25061400	1.16858700	1.00471500
O	1.14685800	1.80731200	1.09084100
C	3.43544100	2.08326300	0.59209200
C	-2.06204700	-0.15064200	0.84615000
C	-3.24095500	0.36619200	0.22396100
C	-0.92819700	0.40833900	0.18413700
C	-2.77823300	1.21329400	-0.82969500
C	-4.62838500	0.19519000	0.40675800
H	0.05181800	0.86126200	0.72103500
C	-3.66426700	1.90016800	-1.67369300
C	-5.49974400	0.87343600	-0.42911900

H	-5.01191500	-0.44576500	1.19417200
C	-5.02149800	1.71804200	-1.45837500
H	-3.30324300	2.53969200	-2.47232300
H	-6.57113400	0.75913100	-0.29412600
H	-5.73512200	2.23120200	-2.09623400
N	-1.39863700	1.21447600	-0.82611100
C	-2.85562700	-1.66328900	2.79629100
H	-3.63548000	-2.23501400	2.27597600
H	-2.38480200	-2.31141900	3.53788000
H	-3.33811700	-0.81235800	3.28799600
C	-0.54402100	2.03762200	-1.67916900
H	0.41807000	2.16593600	-1.18129700
H	-0.39836100	1.55325200	-2.64991800
H	-1.00593600	3.01780600	-1.82252500
Pd	0.33845100	-1.34338700	0.03201500
C	3.05405800	-2.71302800	-2.48953600
O	1.56951600	-3.02559400	-0.59702100
F	4.61607900	1.44747900	0.62638400
F	3.24035400	2.51451000	-0.68344900
F	3.52895800	3.17552600	1.37508900
O	1.38166000	-1.15192200	-1.70777300
C	1.95349800	-2.30093100	-1.56226200
H	4.00254200	-2.32260900	-2.10222600
H	3.11790000	-3.80256200	-2.53633600
H	2.89072200	-2.29184300	-3.48485500

b₃' - IN2

C	-3.10234300	-1.43715200	0.97884100
O	-2.20945700	-2.35288900	0.89567400
O	4.46443600	-0.33277500	0.46219700
C	3.85126000	0.69232500	0.27372500
O	2.66220100	0.82799100	-0.29254300
C	4.40438200	2.07371600	0.68855600
C	-2.82733300	-0.19509600	0.37484500
C	-3.48883700	1.07625300	0.17354300
C	-1.56774300	-0.13041900	-0.26441800
C	-2.58078700	1.85174300	-0.59472100
C	-4.71620900	1.64121700	0.54145900
H	2.29051300	-0.06855000	-0.54632300
C	-2.86087400	3.15702100	-0.99344900
C	-5.00492900	2.94635100	0.14413500
H	-5.43502500	1.07770500	1.12922000
C	-4.09047000	3.69601200	-0.61282600
H	-2.15180400	3.73973800	-1.57331700

H	-5.95425500	3.39237600	0.42698800
H	-4.34042800	4.71162300	-0.90531300
N	-1.42896000	1.07788900	-0.84805300
C	-4.37229400	-1.76675700	1.70971500
H	-5.23615300	-1.62968000	1.04843500
H	-4.34582900	-2.79830100	2.06542000
H	-4.50319300	-1.09013600	2.56276200
C	-0.29075800	1.53872100	-1.63196900
H	0.32697100	0.67957500	-1.88981600
H	-0.64949500	2.01068800	-2.55151200
H	0.31075500	2.25566200	-1.06482100
Pd	-0.49220000	-1.75954900	-0.09509700
C	3.18479800	-3.04297000	-1.11837000
O	1.00198300	-3.42131100	-0.13464500
F	5.60196200	1.94819700	1.26379400
F	4.52700200	2.87071900	-0.39006000
F	3.56945600	2.67194000	1.55827200
O	1.38762300	-1.42787400	-0.97398700
C	1.79697000	-2.64636900	-0.71432200
H	3.90534800	-2.41422200	-0.58345100
H	3.35537300	-4.09546500	-0.88670700
H	3.32210900	-2.86741700	-2.19079400

b₃' –IN3

C	0.76248400	2.15345300	0.00008300
O	-0.51300300	2.25013200	0.00002200
C	1.32828000	0.86085300	0.00000300
C	2.64434200	0.25825900	0.00007200
C	0.37752500	-0.18425400	-0.00010700
C	2.41323800	-1.14384600	-0.00000400
C	3.96549900	0.72287700	0.00018000
C	3.44958100	-2.07472600	0.00003000
C	5.00863000	-0.20314400	0.00021700
H	4.18109100	1.78751700	0.00023400
C	4.75635800	-1.58417200	0.00014200
H	3.25356600	-3.14273700	-0.00003300
H	6.03586900	0.15072700	0.00030200
H	5.58831900	-2.28245900	0.00016900
N	1.02245400	-1.37049800	-0.00012600
C	1.56182100	3.42632300	0.00022400
H	2.21060300	3.46624300	0.88348300
H	2.21060800	3.46642900	-0.88302200
H	0.89404400	4.28977300	0.00031100
C	0.40527100	-2.68937500	-0.00023600

H	0.71142600	-3.24802900	-0.89144400
H	0.71117500	-3.24806500	0.89103500
H	-0.67788500	-2.56830800	-0.00038700
Pd	-1.48612400	0.40347700	-0.00017100
C	-5.05244400	-1.41566100	0.00095200
C	-3.75600200	-0.65070400	-0.00022900
O	-2.64533700	-1.31434200	-0.00036900
O	-3.71724900	0.60870100	-0.00029100
H	-5.89729000	-0.72488900	-0.00804500
H	-5.09637200	-2.06986800	-0.87618400
H	-5.10340300	-2.05400200	0.88944300

b₃'-TS1

Imaginary Frequency: -99.4607

C	-1.12597600	-0.67594900	2.34820100
O	-0.03576300	-0.13739600	2.54199200
O	2.37987100	0.23636500	0.30907300
C	2.82097600	-0.77762000	-0.35041200
O	2.21678700	-1.56527900	-1.07158800
C	4.34661900	-0.96315400	-0.11886900
C	-1.57727000	-0.95229200	0.97533200
C	-2.88647900	-0.95020900	0.38918200
C	-0.67193400	-1.25824400	-0.05392800
C	-2.70651300	-1.24722400	-0.99420500
C	-4.18861500	-0.69183300	0.86416700
H	0.35898000	-1.59035400	0.00109100
C	-3.78011800	-1.30709300	-1.89291900
C	-5.25154100	-0.76040400	-0.02209200
H	-4.36259800	-0.44967100	1.90758000
C	-5.04929500	-1.06489600	-1.38746500
H	-3.62651800	-1.53475100	-2.94305300
H	-6.26017000	-0.57402600	0.33493500
H	-5.90558600	-1.10691900	-2.05445600
N	-1.36134700	-1.44211600	-1.22774400
C	-2.01102700	-1.06047700	3.51593100
H	-2.77273100	-0.28217900	3.65784100
H	-2.53050500	-2.00850200	3.34707900
H	-1.40555300	-1.11053600	4.42334000
C	-0.76322600	-1.83619600	-2.49745300
H	-1.12997700	-2.82210100	-2.80307800
H	-1.01672600	-1.10447600	-3.27159800
H	0.31939400	-1.86530400	-2.37043900
Pd	0.50568000	0.95269600	0.13922800
C	-1.04184200	4.47960700	-0.79742900

C	-0.41990500	3.15137200	-0.49233800
O	-1.14051400	2.16526800	-0.08714800
O	0.83215200	2.95782400	-0.59434600
F	4.59875800	-1.20573200	1.18205000
F	4.82114700	-1.99205300	-0.83381900
F	5.02333000	0.14372900	-0.47734900
H	-0.48426000	4.98006500	-1.59295300
H	-2.08884700	4.35023200	-1.08176500
H	-0.99924200	5.10924500	0.09917700

b₃''-IN2

C	-0.59560200	-2.15416500	-0.43164500
O	-1.37523300	-2.63838200	0.36773500
O	-1.92138700	0.26646200	-0.57796700
C	-2.66971100	0.18041400	0.47958200
O	-2.36174200	0.34407700	1.64990000
C	-4.12666400	-0.18080000	0.08966100
C	0.54462000	-1.29924800	0.07014600
C	1.96059800	-1.42644800	-0.30323200
C	0.55883600	-0.82228500	1.41728200
C	2.71508300	-0.98182800	0.80736900
C	2.63503600	-1.87304400	-1.44640500
H	-0.29585600	-0.69536200	2.06989900
C	4.10781500	-0.94251500	0.80497100
C	4.02806100	-1.85241400	-1.45479100
H	2.08849200	-2.22071300	-2.31650500
C	4.75516800	-1.38975600	-0.34537500
H	4.67061100	-0.58198000	1.66006400
H	4.56167600	-2.19613100	-2.33591700
H	5.84048500	-1.38005000	-0.38299500
N	1.82629900	-0.62768000	1.83457100
C	-0.70898300	-2.41499300	-1.91884500
H	-0.35581100	-1.56899200	-2.51492500
H	-0.11354400	-3.29971200	-2.18093700
H	-1.75506600	-2.62296700	-2.15248400
C	2.21141100	0.05130300	3.06287500
H	2.99444900	-0.51703600	3.57279800
H	2.57690500	1.05820900	2.83603500
H	1.33943700	0.12188100	3.71493700
Pd	-0.00686600	0.83473800	-0.28177500
C	2.12376100	4.17632000	-0.71359900
C	1.28280000	2.94551400	-0.53745100
O	1.82091400	1.83788100	-0.16076700
O	0.03731000	2.95295300	-0.77659500

F	-4.15891900	-1.26643600	-0.70794600
F	-4.86932800	-0.43594700	1.17304000
F	-4.69811700	0.84198100	-0.57951500
H	1.56368400	5.05975500	-0.39622800
H	3.05509600	4.08779600	-0.14975000
H	2.36618200	4.29446000	-1.77624900

b₃''-TS2

Imaginary Frequency: -1112.0893

C	-0.73736300	-1.31743500	2.02926900
O	0.45130300	-1.06678200	2.20204800
O	2.39088200	0.15500500	-0.01340300
C	2.42520300	-1.03880100	-0.38755900
O	1.46321900	-1.75587100	-0.78662900
C	3.81677400	-1.71402600	-0.42661900
C	-1.40354200	-0.95424300	0.75821200
C	-2.74337500	-1.18125000	0.30928400
C	-0.68475600	-0.35035500	-0.30520000
C	-2.80776100	-0.67569200	-1.02689300
C	-3.91203100	-1.75491600	0.86419200
H	0.40867000	-1.06826600	-0.60010700
C	-3.98341700	-0.72595400	-1.79663200
C	-5.06866900	-1.79872100	0.10699800
H	-3.91357700	-2.15245500	1.87214500
C	-5.10525800	-1.28784300	-1.21301800
H	-4.01472800	-0.33047500	-2.80683600
H	-5.96990100	-2.23193200	0.53103600
H	-6.03333400	-1.33596400	-1.77552100
N	-1.57255500	-0.19301000	-1.36899900
C	-1.53468500	-2.01306300	3.11720400
H	-2.38227400	-1.39429300	3.43565000
H	-1.93768200	-2.96793800	2.75917500
H	-0.87838100	-2.19445200	3.97036200
C	-1.24775900	0.42650500	-2.64315700
H	-1.65935300	-0.16638500	-3.46582200
H	-1.64666200	1.44579000	-2.69148200
H	-0.16222100	0.47016500	-2.74418200
Pd	0.62551900	1.23836900	0.05320000
C	-0.41829900	5.02211400	0.66710600
C	0.04004600	3.61706300	0.40367200
O	-0.82761800	2.69862700	0.14284400
O	1.26245100	3.28910000	0.45559300
F	4.24411200	-1.75114000	-1.70417100
F	3.74385200	-2.97030000	0.03208900

F	4.71095500	-1.04139800	0.30110800
H	0.37666400	5.72818100	0.41655200
H	-1.32383200	5.24086500	0.09569400
H	-0.65219600	5.12788300	1.73309500

b₃''-IN3

C	-0.88900500	-0.64599500	2.13604400
O	0.31862200	-0.46440300	2.31699100
O	1.99251300	-0.70432100	-0.35087300
C	1.65832100	-1.88167600	-0.33841200
O	0.46310300	-2.38287900	-0.18588000
C	2.71777100	-2.98384800	-0.55724700
C	-1.51976200	-0.32520100	0.85061500
C	-2.88437400	-0.52760900	0.37978400
C	-0.85761000	0.43937700	-0.13585100
C	-2.96772600	0.11995100	-0.87914100
C	-4.02741800	-1.18706600	0.86228100
H	-0.20327200	-1.66285200	0.00909500
C	-4.12837300	0.12777300	-1.65553400
C	-5.19186700	-1.17881800	0.09830200
H	-4.01667900	-1.70146100	1.81675900
C	-5.24539600	-0.52984900	-1.14711400
H	-4.16276900	0.62689200	-2.61919600
H	-6.07645900	-1.68654800	0.47266000
H	-6.16722500	-0.54234800	-1.72148700
N	-1.72601400	0.69560400	-1.15695700
C	-1.74000700	-1.22072300	3.25438500
H	-2.62384000	-0.60035800	3.44068900
H	-2.09328900	-2.22576600	2.99116700
H	-1.13423800	-1.28486600	4.16035100
C	-1.44809800	1.46922100	-2.35732300
H	-1.49650300	0.83238500	-3.24810200
H	-2.17852500	2.27868800	-2.45723300
H	-0.45102600	1.90119600	-2.27221000
Pd	0.97555500	1.16266100	-0.02943000
C	1.99654700	4.98622700	0.47895100
C	1.70741900	3.52930100	0.24501100
O	0.47478000	3.15505400	0.11094700
O	2.61791700	2.65854500	0.20011700
F	2.43195400	-3.65650200	-1.68482600
F	2.70219900	-3.84289500	0.47091000
F	3.93313100	-2.45198700	-0.66545300
H	3.03780400	5.20461600	0.23304600
H	1.32180500	5.60925800	-0.11432400

H	1.82720800	5.21959400	1.53666900
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Pd(OAc)(OTf)_catalyst

Pd(OAc)(OTf)

O	2.67175400	0.16591900	1.08536700
C	3.33621100	0.31573800	0.00041800
O	2.67160200	0.16642800	-1.08471700
C	4.79818300	0.61580500	-0.00017000
Pd	0.96891800	-0.24158200	0.00022500
C	-2.60138700	0.85497000	0.00001800
O	-0.73149600	-0.66951800	-1.19601800
O	-0.73224400	-0.67033400	1.19595100
O	-2.66972300	-1.82498400	-0.00100000
F	-3.36243500	0.91982100	1.08900300
F	-3.36122500	0.92108300	-1.08967000
F	-1.72858600	1.86337500	0.00109900
S	-1.67902900	-0.76932900	-0.00025200
H	5.05389200	1.22628400	-0.86975200
H	5.35650900	-0.32572400	-0.06458600
H	5.07688300	1.12381000	0.92587600

Pd(OAc)(OTf)

a₄-IN1

C	1.03087600	-0.25807300	2.21009300
O	-0.10327700	0.29047500	2.21709600
O	-2.87274000	1.50891100	-0.57718200
C	-2.50652100	2.69257800	-0.26397900
O	-1.54774000	2.79558900	0.58049200
C	-3.18786100	3.89794900	-0.83032100
C	2.05001400	-0.03049600	1.22494600
C	2.22190800	1.03347900	0.24860400
C	3.07791800	-0.94119900	0.98501800
C	3.35187400	0.68056200	-0.53141200
C	1.59564600	2.26442200	0.00222400
H	3.26560500	-1.89251100	1.46239300
C	3.84863700	1.48364700	-1.55935500
C	2.08258800	3.07041400	-1.02381200
H	0.75235200	2.59457600	0.59505100
C	3.18960400	2.68552700	-1.80105200
H	4.71545100	1.19037900	-2.14386900
H	1.59734900	4.02140600	-1.22428600
H	3.54258600	3.33809700	-2.59428700
N	3.83851000	-0.54076500	-0.05982400
C	1.28378100	-1.22181300	3.34697900

H	0.66528000	-0.93447300	4.20028200
H	0.95711600	-2.21450000	3.01282000
H	2.33398800	-1.26564500	3.64447700
C	4.95589600	-1.27049200	-0.63477300
H	4.74833000	-1.52295100	-1.67966000
H	5.87023200	-0.66962200	-0.58693600
H	5.10682300	-2.19285900	-0.07136400
Pd	-1.46263200	0.70979400	0.71208500
C	-1.12035300	-2.04874000	-1.77293600
O	-1.99346400	-1.26947600	0.60787500
O	-1.94384000	-3.68539200	0.15854700
F	-2.35087100	-1.98123500	-2.28223900
F	-0.50743000	-0.86642600	-1.96653600
F	-0.42955700	-2.99404500	-2.42048600
O	0.23043100	-2.43761400	0.46803100
S	-1.17822200	-2.44841000	0.04409000
H	-4.02034800	4.17901100	-0.17439500
H	-2.48957500	4.73693800	-0.87951300
H	-3.59043100	3.67038700	-1.82015800

a₄-TS0

Imaginary Frequency: -1029.7394

C	-1.59963000	-1.95897600	-1.20540300
O	-0.42354300	-1.54435000	-1.13389200
O	1.12372500	2.17744500	-0.34910200
C	0.51631700	3.00900100	-1.11245600
O	-0.62269600	2.80644300	-1.62197700
C	1.24684200	4.29996300	-1.41053600
C	-2.69666600	-1.24980800	-0.60201300
C	-2.60808700	0.02152200	0.07310200
C	-3.94933900	-1.77704500	-0.29138000
C	-3.80250200	0.16142900	0.81868200
C	-1.60312400	1.01561500	0.13655700
H	-4.39072000	-2.71999900	-0.58372300
C	-4.01330900	1.22039700	1.70289100
C	-1.80635500	2.04149900	1.08232600
H	-1.12890100	1.66173200	-0.90210000
C	-2.98070400	2.14568000	1.84300900
H	-4.93295500	1.31691400	2.27216800
H	-1.05068300	2.81328300	1.18333800
H	-3.09467700	2.97199200	2.53800900
N	-4.61300500	-0.94364500	0.54806200
C	-1.80611200	-3.29379900	-1.88216300
H	-1.07181700	-3.40185500	-2.68365000

H	-1.62004200	-4.09449300	-1.15564300
H	-2.81505700	-3.40927300	-2.28636800
C	-5.92901200	-1.17510600	1.12311700
H	-5.86392100	-1.22712100	2.21476600
H	-6.61581600	-0.37006800	0.84277900
H	-6.32072200	-2.12150300	0.74639700
Pd	0.30896800	0.29707300	-0.47643400
C	3.81730800	-0.35094600	1.15248600
O	2.19270400	-0.46994900	-0.91214900
O	3.69635300	-2.40422700	-0.53254000
F	4.74058100	0.26654100	0.40829600
F	3.04972700	0.57854500	1.74392200
F	4.43508800	-1.06105000	2.10515800
O	1.74093800	-1.99055900	1.02467000
S	2.76681700	-1.47504900	0.10652600
H	1.90936400	4.12902800	-2.26692400
H	0.53718000	5.08776900	-1.66935800
H	1.86605800	4.59327300	-0.56035200

a₄-IN2

C	-1.61924500	-2.07880400	-0.66296100
O	-0.50597600	-1.51917200	-0.81617000
O	0.84395800	2.37693700	-0.20173800
C	1.96142700	2.84795200	-0.49716900
O	2.95643000	2.17935400	-1.00133700
C	2.24825000	4.30782500	-0.26900700
C	-2.76643000	-1.33846500	-0.24665600
C	-2.74892500	0.08127500	0.01033400
C	-4.07581100	-1.76638900	-0.03984400
C	-4.06772500	0.44725500	0.36137700
C	-1.72401000	1.03462000	-0.02853700
H	-4.50568500	-2.75471700	-0.12934500
C	-4.41449800	1.76231400	0.67696000
C	-2.06447300	2.35110900	0.28487600
H	2.75374900	1.17807400	-1.05477300
C	-3.38696300	2.70191900	0.62934000
H	-5.42713800	2.04624700	0.94647300
H	-1.30241200	3.12144400	0.27218300
H	-3.60829200	3.73894000	0.86785100
N	-4.85282200	-0.71197300	0.32018800
C	-1.67201300	-3.55267700	-0.97973800
H	-1.81203800	-3.68412300	-2.06000900
H	-0.71371700	-4.00438400	-0.71198800
H	-2.48716100	-4.06288800	-0.45988700

C	-6.27271100	-0.76150500	0.62593500
H	-6.45304600	-0.43512400	1.65554800
H	-6.83218200	-0.11227700	-0.05563800
H	-6.62876000	-1.78700800	0.51129200
Pd	0.09948600	0.41133600	-0.47811300
C	2.95902800	-0.88293200	1.44834300
O	2.17497400	-0.25853100	-0.98634800
O	4.41008000	-1.28761100	-0.73062500
F	3.36842500	0.39217400	1.57580300
F	1.71014500	-0.96970200	1.93900200
F	3.75760700	-1.66565400	2.17670500
O	2.32782400	-2.68867500	-0.39103700
S	3.00497600	-1.39491300	-0.34249100
H	3.00472200	4.40417400	0.51754600
H	2.66559800	4.74774700	-1.17964100
H	1.34079800	4.83412900	0.02705500

a₄-IN1'

C	-1.72145500	-2.23728000	-0.57027000
O	-0.55722800	-1.78673200	-0.56454900
O	0.96466800	1.81045500	0.63459000
C	1.12861000	2.71353900	-0.30623100
O	0.66047400	2.63013500	-1.44143300
C	1.97973400	3.88298800	0.15804300
C	-2.86242700	-1.39575700	-0.29394900
C	-2.87839000	0.04830500	-0.30075600
C	-4.10070100	-1.79661400	0.19861200
C	-4.12810000	0.44289200	0.23330900
C	-1.97579300	1.04222600	-0.73382500
H	-4.47862300	-2.79332800	0.37997400
C	-4.48101300	1.78342200	0.40190300
C	-2.32143400	2.38672100	-0.55324000
H	-1.14915200	0.83779800	-1.44209500
C	-3.55225900	2.74908700	0.01595300
H	-5.44380900	2.07000500	0.81439300
H	-1.62494700	3.14163900	-0.89842000
H	-3.79631400	3.79990100	0.13650000
N	-4.85356700	-0.71345700	0.52382300
C	-1.89360700	-3.70007400	-0.89467000
H	-2.12916200	-3.80340200	-1.96158600
H	-0.96050400	-4.22894800	-0.69237300
H	-2.71213900	-4.15510300	-0.32895900
C	-6.18310200	-0.73902700	1.11379800
H	-6.17413000	-0.25612600	2.09628300

H	-6.89840000	-0.22167200	0.46630800
H	-6.50015900	-1.77651600	1.23223900
Pd	0.14250400	0.12094900	0.00875400
C	4.15567300	-0.13687000	0.32608600
O	2.53282600	-1.39667900	-1.36227700
O	3.36293300	-2.64503200	0.68542200
F	5.29946600	-0.56044400	-0.22406300
F	3.80401600	1.01721800	-0.26197900
F	4.35664700	0.08574000	1.62731100
O	1.68367700	-0.85620700	0.94064100
S	2.83586200	-1.42780100	0.07059300
H	1.66212900	4.23012800	1.14567900
H	3.01791200	3.54552500	0.24435600
H	1.91890200	4.69396900	-0.57039800

a₄-TS0'

Imaginary Frequency: -821.7933

C	1.43354500	-2.19829300	0.11323300
O	0.45893500	-1.73348100	-0.51752300
O	-1.02580900	2.08418900	-0.55284000
C	-0.84887400	2.65597000	0.58479900
O	0.01407100	2.29850600	1.43005600
C	-1.76779700	3.81953600	0.88431200
C	2.59436700	-1.39479800	0.40105400
C	2.72205200	0.00831200	0.09978400
C	3.88746400	-1.86678800	0.62968200
C	4.10658500	0.29438500	0.08682600
C	1.77464600	1.02241000	-0.18001700
H	4.22392400	-2.86781200	0.86209300
C	4.60585200	1.53888200	-0.29947500
C	2.30020800	2.25190700	-0.63156500
H	0.87990400	1.37200000	0.67425600
C	3.67844700	2.50515200	-0.69051400
H	5.67087000	1.75097400	-0.30920400
H	1.60967600	3.05472800	-0.86958000
H	4.02972400	3.47950600	-1.01619000
N	4.78992200	-0.87006700	0.44787600
C	1.34977300	-3.65679200	0.48524400
H	0.43470000	-3.79077300	1.07262100
H	1.24027000	-4.26069300	-0.42172300
H	2.20765100	-4.00893600	1.06194200
C	6.23487200	-0.98833100	0.56999100
H	6.71849700	-0.74306200	-0.38105100
H	6.60991200	-0.31496600	1.34737700

H	6.48641400	-2.01529700	0.84030600
Pd	-0.16463800	0.23725700	-0.64684500
C	-4.05120400	-0.09767100	0.37623800
O	-2.04126100	-1.68454300	1.03884900
O	-3.59371400	-2.42309400	-0.81819400
F	-4.94088100	-0.65945300	1.20309000
F	-3.43483400	0.90080800	1.03971800
F	-4.70108400	0.42512700	-0.66714200
O	-2.00416500	-0.56353200	-1.21120900
S	-2.80842600	-1.37036400	-0.17564700
H	-1.88127800	4.45025800	-0.00111100
H	-2.75391000	3.41192800	1.13049400
H	-1.39051600	4.39862400	1.72820600

aa-IN2'

C	1.72257400	-2.23731200	-0.28332300
O	0.62914700	-1.68806900	-0.56838800
O	-0.64264500	2.26711200	-0.53920200
C	-1.48444300	2.82100900	0.19416000
O	-2.14804300	2.27708900	1.17036400
C	-1.80956400	4.27711100	-0.01902900
C	2.88814800	-1.46447600	-0.00017200
C	2.91980400	-0.02155900	-0.03079200
C	4.18593600	-1.88636600	0.28206600
C	4.25494300	0.36141800	0.22716900
C	1.92462600	0.93782200	-0.25682600
H	4.58396500	-2.88630900	0.38762600
C	4.65228600	1.69947400	0.25505600
C	2.32052600	2.27669900	-0.24437600
H	-2.07421400	1.26182000	1.27617600
C	3.65891200	2.64454300	0.00799500
H	5.67767400	1.99623800	0.45304100
H	1.59107600	3.05647600	-0.43204700
H	3.92089100	3.69937600	0.01145400
N	5.00078900	-0.80877700	0.41889100
C	1.73163700	-3.74585400	-0.29780900
H	0.81330800	-4.10786200	0.17268300
H	1.72721900	-4.09515700	-1.33739500
H	2.60079300	-4.16894500	0.21141000
C	6.42197100	-0.84452800	0.72025500
H	6.99343700	-0.36487300	-0.08125000
H	6.62565500	-0.32429700	1.66206600
H	6.74320300	-1.88372300	0.81226200
Pd	0.07372200	0.29348200	-0.53800500

C	-4.43066000	-0.74034900	0.04780500
O	-2.31124300	-0.27203100	1.57575200
O	-2.51697700	-2.53601000	0.51191100
F	-5.16695000	-1.19502000	1.06642100
F	-4.62524000	0.58308000	-0.06597400
F	-4.83284500	-1.33378100	-1.07951600
O	-1.99804500	-0.48074000	-0.86908000
S	-2.63086400	-1.08795800	0.35739900
H	-1.14745100	4.70974400	-0.76912200
H	-2.85003100	4.36535300	-0.34989700
H	-1.72088100	4.81764800	0.92827400

aa'-IN1

C	-1.64458200	0.67096800	1.95876700
O	-0.43059000	1.09972500	2.00543600
O	1.26817300	2.66876500	0.07615300
C	0.55535600	3.34811300	-0.69424700
O	-0.56279200	2.95359200	-1.21962700
C	0.98705300	4.74437300	-1.07420200
C	-2.22673700	0.27632600	0.73804800
C	-3.40637000	-0.52201400	0.45532800
C	-1.56154900	0.57258800	-0.49955500
C	-3.38765400	-0.72741200	-0.94674900
C	-4.43850300	-1.10312100	1.20643100
H	-0.86323100	1.93584700	-0.89187500
C	-4.36478300	-1.46462900	-1.61392900
C	-5.41844700	-1.84469400	0.54871800
H	-4.48631800	-0.98182300	2.28374700
C	-5.38484400	-2.02309300	-0.84418500
H	-4.33302500	-1.60836500	-2.68954500
H	-6.22371000	-2.29285800	1.12382200
H	-6.16124800	-2.60770800	-1.32907900
N	-2.26752600	-0.05973200	-1.46731700
C	-2.35279500	0.59608000	3.28400200
H	-3.37992500	0.96428900	3.20346700
H	-2.39310000	-0.44815100	3.62026700
H	-1.80459900	1.17643500	4.02903900
C	-1.95937400	-0.00080500	-2.88917700
H	-1.76952300	-1.00695000	-3.27765500
H	-2.79111000	0.44597400	-3.44511400
H	-1.06458400	0.60728500	-3.02226400
Pd	0.70729000	0.55657500	0.45400500
C	3.94000900	-1.35999300	0.19244000
O	1.89903500	-0.19827800	-1.07507700

O	1.34105300	-1.72754500	0.72446700
F	4.78060000	-1.09069800	-0.80603000
F	3.95383700	-0.34998700	1.06761400
F	4.32103700	-2.48060600	0.80663500
O	2.28227600	-2.66816800	-1.44820000
S	2.21691600	-1.58367800	-0.48343100
H	1.92931500	4.99617300	-0.58625800
H	1.10067100	4.80606600	-2.16164100
H	0.20989800	5.45906900	-0.78432000

a₄'-TS1

Imaginary Frequency: -383.9977

C	-2.14857100	1.38584800	-1.61085200
O	-0.89555000	1.32158300	-1.55516600
O	1.23625400	2.16302700	0.55186700
C	0.54761800	2.66384800	1.48144200
O	-0.56931600	2.21226600	1.90123300
C	1.09420300	3.89734400	2.19333700
C	-2.99128300	0.53505900	-0.81829700
C	-2.54506800	-0.26584600	0.29049300
C	-4.30726200	0.14736500	-1.07833500
C	-3.60302300	-1.13881800	0.61922800
C	-1.34390100	-0.25869600	1.03617000
H	-0.87823100	0.81538300	1.32532700
C	-3.47939500	-2.09453500	1.62833100
C	-1.21482900	-1.26505800	2.01840600
C	-2.25735400	-2.15514200	2.30777600
H	-4.28972700	-2.77249200	1.87951000
H	-0.29499200	-1.31655900	2.59278800
H	-2.12603400	-2.89630500	3.09048200
N	-4.67356000	-0.85115700	-0.23565100
C	-2.72578300	2.40829900	-2.55610700
H	-3.70942900	2.11790800	-2.93462800
H	-2.83893700	3.35636900	-2.01508200
H	-2.03794900	2.57154500	-3.38840000
C	-5.95413600	-1.54131100	-0.23036500
H	-5.81245800	-2.60775900	-0.43327400
H	-6.44589400	-1.42361100	0.74057400
H	-6.59360000	-1.11454900	-1.00502800
Pd	0.29759000	0.12069400	-0.39695100
C	4.13129500	-0.43552900	-0.07449700
O	2.10827900	-0.76309800	-1.81603900
O	1.61931300	-1.14238300	0.53861100
F	5.11265700	-0.65215500	-0.95571000

F	3.84048100	0.85917500	-0.04346000
F	4.52906500	-0.83672200	1.13547400
O	3.07441100	-2.81397600	-0.65414900
S	2.63828100	-1.42724000	-0.59068300
H	-4.99171900	0.48935300	-1.84257800
H	0.28127300	4.58763000	2.43867400
H	1.56244900	3.58945700	3.13625700
H	1.84649500	4.39661700	1.57763300

a₄'-IN2

C	2.03420200	0.91211100	1.79077500
O	0.78717800	0.74545000	1.85870600
O	1.60965100	3.03335100	-0.31296800
C	0.74798100	3.19579700	-1.15488200
O	-0.19546200	2.28049700	-1.44484200
C	0.58984300	4.43381700	-2.00497700
C	2.83949300	0.13100200	0.90783800
C	2.30494300	-0.83916500	-0.01222700
C	4.21945000	0.13441800	0.71773800
C	3.39552300	-1.38606500	-0.72231300
C	1.00156900	-1.25804100	-0.28110700
H	-0.07737000	1.50451100	-0.85481100
C	3.22044700	-2.36318000	-1.70489700
C	0.80862600	-2.23286100	-1.25785100
C	1.91094500	-2.77247100	-1.95518400
H	4.05546400	-2.78829100	-2.25330500
H	-0.19290600	-2.58393000	-1.48483100
H	1.73019400	-3.53125400	-2.71157200
N	4.55616800	-0.76410700	-0.24491500
C	2.61990200	1.99695200	2.65344400
H	3.66481400	1.80673200	2.91261500
H	2.56068000	2.93300200	2.08535200
H	2.02628400	2.10576800	3.56399400
C	5.90149400	-1.04725600	-0.71664600
H	6.15373100	-2.09844800	-0.54211100
H	5.98176100	-0.83532700	-1.78788800
H	6.61078900	-0.41741700	-0.17658200
Pd	-0.46000300	-0.46561500	0.75866700
C	-3.91980000	0.23809100	-0.73048100
O	-2.64321000	-0.00613100	1.60442800
O	-2.02397200	-1.54387500	-0.17690300
F	-4.94234400	0.91971400	-0.20953000
F	-2.98066800	1.10048000	-1.13675200
F	-4.34794700	-0.46723100	-1.77978800

O	-4.28561400	-1.82668300	0.91630900
S	-3.21547700	-0.90946400	0.55700300
H	4.98555100	0.72219000	1.20444100
H	0.59746700	4.16589500	-3.06634300
H	-0.37664100	4.90462400	-1.79572100
H	1.39710000	5.13401400	-1.78815000

a₄'-IN3

C	-2.08942800	2.18383000	0.08907000
O	-0.84677200	2.10164000	-0.09653800
C	-2.91208500	1.02014900	0.14189000
C	-2.40699500	-0.32214100	-0.01115100
C	-4.28959900	0.90265700	0.33453000
C	-3.50995400	-1.19580500	0.09649300
C	-1.12186600	-0.82222100	-0.22761300
H	-5.03865300	1.66734900	0.48808300
C	-3.36944700	-2.58138600	-0.00761400
C	-0.96474400	-2.20304500	-0.33520300
C	-2.07867100	-3.06252500	-0.22504900
H	-4.21500500	-3.25735000	0.07425800
H	0.02081300	-2.62413600	-0.50619400
H	-1.92287900	-4.13422800	-0.31358000
N	-4.64865700	-0.40590900	0.30863400
C	-2.65069400	3.57633100	0.24493300
H	-2.45555000	4.14528900	-0.67073900
H	-3.72357400	3.58517400	0.44812100
H	-2.12580400	4.08538800	1.05998400
C	-5.99645700	-0.92565700	0.47246000
H	-6.29900000	-1.48495400	-0.41884300
H	-6.04490400	-1.58921100	1.34202500
H	-6.68690500	-0.09341800	0.62131700
Pd	0.36316400	0.44660600	-0.36738700
C	3.82979100	-0.33662700	1.00971700
O	1.88601300	-1.00062200	-0.67785500
O	2.55931400	1.33797100	-0.63743900
S	3.09700100	-0.05826900	-0.68000300
O	4.14296300	-0.38716400	-1.63609300
F	2.91283900	-0.08948600	1.95347000
F	4.86924600	0.48190100	1.18799900
F	4.24049600	-1.60198000	1.12337600

a₄''-TS1

Imaginary Frequency: -78.9736

C	-0.46821700	-2.41274600	-1.74737100
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O	-1.45008200	-1.68885700	-1.52878000
O	-3.04663100	0.61882500	0.27199400
C	-3.83723400	-0.31747300	0.75383600
O	-3.50032600	-1.43819900	1.11470900
C	-5.28398200	0.16011600	0.80585500
C	0.59336500	-2.54142000	-0.76084400
C	0.56551300	-1.99143900	0.56822500
C	1.90804100	-2.93466300	-0.98777300
C	1.88834000	-2.04160100	1.06500300
C	-0.46318800	-1.44579400	1.36821200
H	2.35295000	-3.36749300	-1.87376700
C	2.23562800	-1.52688600	2.31495800
C	-0.10241400	-0.90542200	2.61569900
H	-1.52118700	-1.61533400	1.14413300
C	1.22294700	-0.93624200	3.07482500
H	3.25447100	-1.57369300	2.68843300
H	-0.88205000	-0.49510000	3.25071400
H	1.46480300	-0.51862500	4.04750600
N	2.68506500	-2.64588400	0.09228500
C	-0.34246500	-3.11328900	-3.08680100
H	-1.33346000	-3.20498700	-3.53610400
H	0.28010900	-2.50824600	-3.75871700
H	0.11614300	-4.10281100	-2.99272800
C	4.11567300	-2.87469200	0.20489100
H	4.64499500	-1.92596600	0.34197500
H	4.33523600	-3.53277000	1.05234500
H	4.47358800	-3.34852300	-0.71094000
Pd	-1.14958800	0.40106800	-0.18450000
C	1.64823500	2.89970300	0.34514600
O	0.83522700	0.68077600	-0.88644200
O	-0.67154800	2.58132900	-0.94619100
F	1.62327100	4.23113500	0.28734300
F	1.04949900	2.49595900	1.47074000
F	2.91681000	2.48024300	0.35126600
O	1.48082700	2.66934600	-2.30693700
S	0.76491500	2.19235700	-1.13509300
H	-5.34669500	1.16885300	1.22326200
H	-5.87183100	-0.53842800	1.40430800
H	-5.68754300	0.19679500	-0.21202600

a₄''-IN2

C	-3.93348300	0.85654200	-1.39191600
O	-3.47396800	1.98913200	-1.47491400
O	0.78013400	2.76693900	-0.35210500

C	1.65651600	3.35664600	0.44331700
O	2.18966100	2.82592100	1.41009800
C	1.94222900	4.78659200	0.00980000
C	-3.43909800	-0.08000200	-0.36936000
C	-2.38066900	0.17257700	0.57210200
C	-3.87737000	-1.36750700	-0.11030900
C	-2.24296300	-0.98630200	1.36663500
C	-1.52084200	1.27543500	0.80614400
H	-4.65326700	-1.94426100	-0.59452600
C	-1.30539100	-1.08996500	2.41628300
C	-0.56417800	1.17181800	1.85842000
H	-1.69393700	2.21370600	0.29319500
C	-0.48122800	-0.01154100	2.65634000
H	-1.23263300	-1.99098100	3.01777600
H	-0.00333300	2.04556300	2.17048500
H	0.24767000	-0.04753900	3.45909600
N	-3.16845600	-1.91345000	0.92864000
C	-5.02147100	0.37841400	-2.34093000
H	-5.30075900	1.20085700	-3.00179700
H	-4.66448400	-0.46423900	-2.94576700
H	-5.90710500	0.03914600	-1.78981000
C	-3.32285100	-3.26246700	1.45066100
H	-2.40256100	-3.83717300	1.30459900
H	-3.56676200	-3.23715200	2.51769800
H	-4.13618300	-3.75697600	0.91684200
Pd	0.57410200	0.81205000	-0.09251400
C	3.14249600	-1.95918900	-0.10778600
O	0.54514700	-1.34117700	-0.22727900
O	2.04187000	-0.01310700	-1.58129200
F	4.26386800	-1.99473700	-0.82559700
F	3.28321800	-1.09150000	0.89642100
F	2.89311300	-3.17301300	0.39030900
O	1.61631300	-2.43457700	-2.25076500
S	1.72248200	-1.43936500	-1.19795000
H	2.57371100	4.77069200	-0.88550200
H	2.46759500	5.30935300	0.81142000
H	1.01758700	5.31057600	-0.24790300

a₄''-TS2

Imaginary Frequency: -1042.7459

C	2.20966800	0.42561100	2.12057500
O	1.49604200	1.40481800	1.92698700
O	-0.50802900	2.89837300	-0.40513500
C	0.57878400	3.51847300	-0.64543500

O	1.68659600	2.97296100	-0.91041700
C	0.51476600	5.03018800	-0.58170400
C	2.53317600	-0.51226300	1.03683900
C	2.06910000	-0.47693700	-0.32643200
C	3.35780200	-1.62481700	1.13645200
C	2.65789500	-1.59171400	-0.98165700
C	1.21343500	0.39120600	-1.06665700
H	3.89695700	-2.00256700	1.99459100
C	2.42882600	-1.88562900	-2.32570500
C	0.99895400	0.07269900	-2.42964000
H	1.46278600	1.65820600	-0.91963700
C	1.59436700	-1.03201000	-3.04960200
H	2.88538400	-2.74934400	-2.80103500
H	0.36605700	0.72843100	-3.02159900
H	1.40587700	-1.23142100	-4.10023900
N	3.44155300	-2.27530100	-0.05820800
C	2.77714700	0.14801700	3.50561700
H	2.36239800	-0.78320800	3.91102800
H	3.86852300	0.04438200	3.47977400
H	2.50853800	0.97363100	4.16690100
C	4.21189400	-3.47611100	-0.33099900
H	3.55534800	-4.29031900	-0.65602200
H	4.95958700	-3.28815300	-1.10915700
H	4.72523300	-3.78300100	0.58216300
Pd	-0.57920800	0.89612200	-0.08880900
C	-3.55855800	-1.38697200	-0.38282800
O	-1.03688400	-1.12825900	0.45190300
O	-2.56403500	0.67289700	1.00283800
S	-2.43402300	-0.82823900	0.99429100
O	-2.83846600	-1.56923300	2.17749000
F	-3.23847300	-0.76011700	-1.52032400
F	-4.82346300	-1.10445100	-0.06817500
F	-3.42951000	-2.70409300	-0.55936100
H	-0.49144500	5.38170800	-0.81623300
H	1.24989500	5.46816700	-1.25954900
H	0.75959600	5.33783800	0.44149600

a₄''-IN3

C	1.43727400	-0.65020100	2.24580800
O	0.90413600	0.46765700	2.34505600
O	0.05126500	2.84680200	-0.35439200
C	0.88768200	3.40061300	0.38237300
O	1.51872500	2.83265100	1.37323400
C	1.24380500	4.84669700	0.17210400

C	2.18656600	-1.05229200	1.06510100
C	2.08512100	-0.54042800	-0.29147100
C	3.26140500	-1.92913800	1.07011800
C	3.15186100	-1.13166000	-1.02182000
C	1.16884200	0.26811300	-0.98891800
H	3.68212000	-2.49612800	1.88897100
C	3.37941900	-0.88324000	-2.37837300
C	1.39958900	0.54306400	-2.33391900
H	1.23790900	1.87607900	1.56014200
C	2.49638000	-0.02172500	-3.01801100
H	4.20257400	-1.34658600	-2.91364300
H	0.71040000	1.17873400	-2.88228200
H	2.63586100	0.20457700	-4.07162300
N	3.85222300	-1.96942300	-0.15722700
C	1.25468200	-1.63313600	3.38077600
H	0.35591200	-2.22583200	3.16453500
H	2.09006000	-2.33057600	3.48863100
H	1.09062500	-1.09214300	4.31528200
C	5.01881100	-2.75292400	-0.52084400
H	4.77305700	-3.46217500	-1.31878200
H	5.82971300	-2.10113300	-0.86389700
H	5.36054500	-3.31110200	0.35301600
Pd	-0.52873800	0.84274000	-0.17799200
C	-3.77462100	-1.07903400	-0.85409500
O	-1.29599400	-1.14158500	0.10866500
O	-2.69460400	0.74334500	0.76863500
S	-2.68387200	-0.74804800	0.61870900
O	-3.20541900	-1.56677500	1.70436800
F	-3.33793300	-0.38577000	-1.91267700
F	-5.02698700	-0.70782100	-0.57732300
F	-3.75650100	-2.38118400	-1.14925300
H	0.72232400	5.23941300	-0.70059000
H	2.32643000	4.94235400	0.04228800
H	0.96780000	5.42119400	1.06259100

b4-IN1

C	-0.73934100	-0.65227800	1.45341900
O	0.35045800	-0.02476700	1.55804300
O	2.03776800	3.02518800	-0.62651000
C	1.20335800	3.77998600	-0.02842200
O	0.36076900	3.21073900	0.75871400
C	1.22491400	5.26632400	-0.20450100
C	-1.88100700	-0.20718500	0.70452200
C	-3.07417300	-0.94685400	0.31390900

C	-2.07683500	1.10246200	0.26262700
C	-3.91721700	-0.01990500	-0.34938900
C	-3.50533200	-2.27999600	0.41094300
H	-1.44528400	1.97020000	0.39493000
C	-5.15814100	-0.36314000	-0.88843900
C	-4.74252600	-2.63264900	-0.12036400
H	-2.88792700	-3.03760700	0.87877900
C	-5.56398300	-1.68765200	-0.76001400
H	-5.78125000	0.36895000	-1.39312400
H	-5.07712500	-3.66323600	-0.04546700
H	-6.52254400	-1.99617000	-1.16649200
N	-3.27655300	1.22023100	-0.35063800
C	-0.79543800	-1.94946300	2.21848400
H	-0.58814600	-2.76483700	1.51402800
H	-0.01096600	-1.95410600	2.97689400
H	-1.77365500	-2.11739400	2.67557100
C	-3.82662500	2.44178600	-0.91439600
H	-3.11465400	3.25421700	-0.76010100
H	-4.00126200	2.32012600	-1.98842300
H	-4.77253500	2.69685300	-0.42522400
Pd	1.24835200	1.35548900	0.33295000
C	2.72302900	-2.66421200	0.00396800
O	2.50427500	-0.08457500	-0.38201600
O	2.71069900	-1.52820000	-2.39603700
F	4.04664100	-2.53958800	0.10970500
F	2.18011800	-2.56528100	1.22899500
F	2.43496500	-3.87487100	-0.48876400
O	0.56452900	-1.53214500	-1.05653000
S	2.02230900	-1.35706400	-1.12052000
H	1.87087800	5.70660900	0.56436700
H	1.63196600	5.52254200	-1.18528300
H	0.21964500	5.67716600	-0.08219100

b4-TS0

Imaginary Frequency: -985.7497

C	1.04709000	-1.63991300	-1.40952600
O	-0.15380300	-1.24791400	-1.39666900
O	-0.64218200	2.54694200	0.07750600
C	0.12991600	3.30428800	-0.60670900
O	1.11702200	2.89499200	-1.28956900
C	-0.19142500	4.78190000	-0.58652700
C	2.04320800	-0.82509700	-0.77216000
C	3.28858400	-1.18320300	-0.15205300
C	1.67621600	0.46733600	-0.30859000

C	3.61599500	-0.09912300	0.71015000	H	-2.49392300	1.90930700	-0.57928600
C	4.14723500	-2.29844400	-0.20066700	C	5.39834100	0.69936900	0.30666000
H	1.30556100	1.52846600	-0.95818400	C	6.04613100	-1.64332900	0.14511200
C	4.78398500	-0.08799800	1.48624900	H	4.47965300	-3.09746700	-0.13237400
C	5.29733200	-2.29169900	0.57356000	C	6.38295100	-0.28923100	0.30261900
H	3.92809000	-3.14455500	-0.84311400	H	5.65914700	1.74613500	0.42894400
C	5.61353200	-1.19674600	1.40748900	H	6.83366500	-2.39160900	0.14655900
H	5.03508600	0.75056700	2.12710400	H	7.42422400	-0.00529400	0.42371700
H	5.97261600	-3.14130200	0.53618800	N	2.90645700	1.07533300	0.11825200
H	6.52466500	-1.22316800	1.99763600	C	1.46449800	-3.49917000	-0.41641400
N	2.61710200	0.85714700	0.61652100	H	1.94306900	-3.87409500	0.49620700
C	1.34331200	-2.97291000	-2.03362800	H	0.50959000	-4.00783900	-0.55935800
H	1.58445000	-3.70075600	-1.24829900	H	2.13245400	-3.72699800	-1.25547900
H	0.46634000	-3.32547500	-2.57942100	C	2.92402700	2.52279400	0.26930900
H	2.20559600	-2.90853800	-2.70556300	H	1.90075400	2.88971600	0.23596800
C	2.62884000	2.13268400	1.32557900	H	3.38036100	2.79167300	1.22810300
H	1.60099800	2.44337200	1.51271100	H	3.50667000	2.97732900	-0.53969200
H	3.12815200	1.99641100	2.28645000	Pd	-0.13652800	0.44010800	-0.18801900
H	3.15040900	2.90012100	0.74523000	C	-3.82145700	-1.76006200	-0.18645300
Pd	-0.45428100	0.56680400	-0.42935600	O	-2.29497500	0.36879300	-0.40643600
C	-3.58090400	-1.77952400	0.41299800	O	-4.30944500	0.56605100	1.02840100
O	-2.50469900	0.40746300	-0.57810200	F	-4.51827700	-1.36574300	-1.25676100
O	-4.52407300	0.66703000	0.84850200	F	-2.82367700	-2.55332500	-0.58295900
F	-4.31005600	-1.92369000	-0.69697800	F	-4.62680800	-2.44650300	0.63063200
F	-2.43207400	-2.45901300	0.26505400	O	-2.31987000	-0.79793000	1.80642500
F	-4.25316300	-2.29942500	1.44599000	S	-3.15585400	-0.27918200	0.72352100
O	-2.29477800	0.02207600	1.87980700	H	-1.53574600	5.16568200	0.67840600
S	-3.22134600	0.01773200	0.73885700	H	0.02238100	5.07068300	-0.18477600
H	-0.94236400	4.97800600	-1.36069000	H	-1.51765600	5.28210600	-1.08316200
H	-0.62144400	5.06536400	0.37624800				
H	0.70081900	5.36987900	-0.80867800	b4-IN1'			
b4-IN2				C	-1.12715500	-0.16729900	1.89587100
C	1.24795100	-2.01719000	-0.31113100	O	0.05884400	0.21540900	2.09251500
O	0.04209900	-1.59346600	-0.37760500	O	2.86510200	1.87173800	-0.42191700
O	-0.24092300	2.55503700	-0.06003500	C	2.23773800	2.96721000	-0.24449300
C	-1.20440300	3.31251900	-0.31023400	O	1.16840500	2.92047200	0.46658000
O	-2.40047500	2.92481200	-0.63540000	C	2.74457600	4.25840300	-0.80763000
C	-1.03404000	4.80467100	-0.22674500	C	-1.96862300	0.29279100	0.82527700
C	2.27260400	-1.06636800	-0.14287800	C	-3.23899100	-0.23897400	0.35157600
C	3.71287300	-1.07228800	-0.01262100	C	-1.72686100	1.44393000	0.07390200
C	1.82941000	0.27646200	-0.05705100	C	-3.68135500	0.63868200	-0.67031400
C	4.07601400	0.28863300	0.14908300	C	-4.02477500	-1.36606500	0.64242800
C	4.72038300	-2.04530200	-0.01259000	H	-0.90965000	2.14857100	0.14615900
				C	-4.86708300	0.44808600	-1.38193000

C	-5.21031500	-1.56409200	-0.05924000
H	-3.71708000	-2.08659200	1.39096400
C	-5.63191600	-0.66789600	-1.05757000
H	-5.18027500	1.13676100	-2.16079500
H	-5.81961700	-2.43492200	0.16451400
H	-6.56116300	-0.85296100	-1.58819100
N	-2.73557200	1.65667800	-0.80273500
C	-1.65197800	-1.15409900	2.90468000
H	-1.55826600	-2.15470500	2.46289500
H	-1.02809100	-1.11993400	3.79989100
H	-2.69955300	-0.97381000	3.15864600
C	-2.83658300	2.77361600	-1.72716900
H	-1.96110100	3.41354800	-1.60534000
H	-2.87207700	2.41107400	-2.75974700
H	-3.73923900	3.35916200	-1.52331500
Pd	1.48335800	0.86343400	0.76326800
C	2.00563200	-2.01565400	-1.62307900
O	0.12106100	-2.17067000	0.22799700
O	2.26483600	-3.46462900	0.59676000
F	1.48021800	-3.01486800	-2.33868300
F	1.49285000	-0.85430300	-2.07039500
F	3.32709600	-1.99660900	-1.80279900
O	2.28212600	-1.01249300	0.80862500
S	1.58784500	-2.24257800	0.17676700
H	3.32470700	4.07120300	-1.71411400
H	1.91167400	4.93540000	-1.01288000
H	3.40042200	4.73531900	-0.06958700

H	4.57990800	-2.61794500	-0.45429800
C	5.64960700	-0.26323200	1.78411200
H	4.64639300	1.56688900	2.32111800
H	6.45158200	-2.14216100	1.07962300
H	6.49126400	-0.07978700	2.44529300
N	2.39939500	1.11677400	0.62085800
C	2.14175500	-3.01422600	-1.86970300
H	2.42147400	-3.64731300	-1.01786000
H	1.41042800	-3.55110400	-2.47647300
H	3.04706200	-2.81693000	-2.45325100
C	2.10564600	2.40497900	1.23924700
H	1.02495600	2.52252600	1.31815100
H	2.52804200	2.41691600	2.24564600
H	2.52722000	3.22858000	0.65441000
Pd	-0.44871600	0.16689600	-0.64230800
C	-3.77983500	-0.26185400	1.31369900
O	-1.86299200	-2.04275900	0.87955200
O	-4.01333500	-2.23556900	-0.45599500
F	-4.34595000	-0.96634100	2.29978700
F	-2.87294500	0.57202000	1.84930300
F	-4.72042600	0.46282900	0.70201000
O	-2.40715800	-0.40640900	-0.92983700
S	-2.94847900	-1.41560800	0.11284500
H	-1.58774700	4.57075600	-0.17753800
H	-0.21363800	5.08103900	-1.22431400
H	-1.66796700	4.34776400	-1.93142400

b₄-IN2'

b₄-TS0'

Imaginary Frequency: -1058.3425

C	1.53601700	-1.73707900	-1.36432300
O	0.28977400	-1.58610500	-1.48564800
O	-1.06493100	2.09451600	-0.28117100
C	-0.39610300	2.95401500	-0.95254700
O	0.71090800	2.71522000	-1.52494600
C	-0.99635100	4.33713800	-1.06501000
C	2.29012000	-0.71194700	-0.69454300
C	3.51731400	-0.78679800	0.04726500
C	1.63916900	0.50311400	-0.35008600
C	3.55062000	0.38266400	0.85766700
C	4.57438500	-1.71277800	0.14335200
H	1.12939200	1.44750500	-1.09788400
C	4.61960400	0.66341300	1.72106100
C	5.62609200	-1.44063600	1.00445900

C	1.80448200	-2.05324700	-0.52953500
O	0.54644300	-1.89858400	-0.70032400
O	-0.69847400	2.05441100	-0.23204100
C	-1.71951200	2.60386300	-0.69520300
O	-2.68634500	1.99128300	-1.31643100
C	-1.91958800	4.08633000	-0.54701800
C	2.56886500	-0.91711000	-0.19720500
C	3.95371400	-0.61813700	0.09224400
C	1.82817100	0.28436500	-0.08550600
C	3.98278200	0.77182800	0.37129200
C	5.15033800	-1.34404300	0.14931300
H	-2.58288600	0.98237100	-1.25952200
C	5.15683500	1.44766800	0.69867000
C	6.32943000	-0.67598100	0.47679000
H	5.16615400	-2.41017000	-0.05671500
C	6.33495500	0.70187800	0.74803900

H	5.16152000	2.51284200	0.90874800
H	7.26180100	-1.23154600	0.52330300
H	7.26864300	1.19586800	1.00051700
N	2.67440700	1.28330700	0.25524200
C	2.35816000	-3.43864900	-0.69602600
H	2.82359300	-3.77085200	0.23965700
H	1.55961900	-4.13080700	-0.96846200
H	3.13395000	-3.44704900	-1.47076600
C	2.34760200	2.68128700	0.49273100
H	1.27425800	2.81382100	0.37688900
H	2.64536900	2.96623300	1.50757100
H	2.87809600	3.31870300	-0.22351500
Pd	-0.10229900	0.02640300	-0.42252200
C	-4.01423500	-0.22232800	0.95622800
O	-2.06028800	-2.01271600	1.09793600
O	-3.84770200	-2.31407300	-0.67886100
F	-4.74137300	-0.83292600	1.89057700
F	-3.24887900	0.71681500	1.54684900
F	-4.83337900	0.39217800	0.09191100
O	-2.15724600	-0.49295800	-0.87936200
S	-2.93566600	-1.45557900	0.06780500
H	-0.98974000	4.57298800	-0.25203800
H	-2.29488400	4.50709200	-1.48371300
H	-2.68035700	4.26221500	0.22223700

b₄'-IN1

C	-1.54057900	-0.00828600	1.87707000
O	-0.35226000	0.42196700	1.93894800
O	1.18157300	2.57011300	0.78039300
C	0.59189600	3.34973700	-0.09325300
O	-0.13681300	2.97244500	-1.01202800
C	0.91978400	4.81838300	0.13225000
C	-2.33413800	-0.07183500	0.68862700
C	-3.60410000	-0.74917300	0.44872200
C	-2.03582200	0.62517100	-0.48990100
C	-3.98093600	-0.42008400	-0.87882500
C	-4.43930000	-1.61037200	1.17792200
H	-1.22441200	1.31792100	-0.70074300
C	-5.14138500	-0.90092700	-1.48511200
C	-5.60316700	-2.09259000	0.58343700
H	-4.19334200	-1.90987100	2.19037000
C	-5.95439400	-1.74310900	-0.73145900
H	-5.40073200	-0.63418500	-2.50508300
H	-6.25110000	-2.75670300	1.14828500

H	-6.86713800	-2.13811000	-1.16747700
N	-3.00388000	0.42879300	-1.40586200
C	-2.11205800	-0.46438500	3.19955800
H	-3.14379800	-0.12647200	3.33135700
H	-2.10674200	-1.56146200	3.23817600
H	-1.48429300	-0.08972100	4.01002000
C	-3.03472100	1.03812300	-2.72847300
H	-2.96358600	0.26873000	-3.50419600
H	-3.96573400	1.59793500	-2.86224800
H	-2.18817000	1.72095000	-2.81524000
Pd	1.05251600	0.61176200	0.44789100
C	3.98125000	-1.67626300	0.03538000
O	2.60024300	0.36924400	-1.01884400
O	1.31142300	-1.46017000	-0.12685100
F	5.10726300	-1.34445200	-0.59385200
F	3.93697300	-1.06589000	1.22121400
F	3.93957700	-2.99641100	0.21420300
O	2.63346100	-1.84972900	-2.26824900
S	2.52065000	-1.15314800	-1.00094900
H	0.84521500	5.07342300	1.19304500
H	1.95204000	5.00906500	-0.18181600
H	0.24351800	5.43976000	-0.45789200

b₄'-TS1

Imaginary Frequency: -497.0656

C	-1.64458200	0.67096800	1.95876700
O	-0.43059000	1.09972500	2.00543600
O	1.26817300	2.66876500	0.07615300
C	0.55535600	3.34811300	-0.69424700
O	-0.56279200	2.95359200	-1.21962700
C	0.98705300	4.74437300	-1.07420200
C	-2.22673700	0.27632600	0.73804800
C	-3.40637000	-0.52201400	0.45532800
C	-1.56154900	0.57258800	-0.49955500
C	-3.38765400	-0.72741200	-0.94674900
C	-4.43850300	-1.10312100	1.20643100
H	-0.86323100	1.93584700	-0.89187500
C	-4.36478300	-1.46462900	-1.61392900
C	-5.41844700	-1.84469400	0.54871800
H	-4.48631800	-0.98182300	2.28374700
C	-5.38484400	-2.02309300	-0.84418500
H	-4.33302500	-1.60836500	-2.68954500
H	-6.22371000	-2.29285800	1.12382200
H	-6.16124800	-2.60770800	-1.32907900

N	-2.26752600	-0.05973200	-1.46731700	H	-3.12550000	1.93643600	2.18651300
C	-2.35279500	0.59608000	3.28400200	H	-3.15282900	0.55083500	3.28877700
H	-3.37992500	0.96428900	3.20346700	H	-1.98766800	1.87878400	3.57291500
H	-2.39310000	-0.44815100	3.62026700	C	-0.27405600	-2.61420000	-1.50862600
H	-1.80459900	1.17643500	4.02903900	H	-0.42907200	-3.67683800	-1.29592900
C	-1.95937400	-0.00080500	-2.88917700	H	-0.52907900	-2.41751500	-2.55507900
H	-1.76952300	-1.00695000	-3.27765500	H	0.77014700	-2.35773100	-1.33452500
H	-2.79111000	0.44597400	-3.44511400	Pd	1.01302100	-0.18646900	0.86890300
H	-1.06458400	0.60728500	-3.02226400	C	4.06920100	0.79387600	-1.12755400
Pd	0.70729000	0.55657500	0.45400500	O	2.46293500	-1.17910300	-0.32279600
C	3.94000900	-1.35999300	0.19244000	O	3.16297500	0.40706200	1.36432400
O	1.89903500	-0.19827800	-1.07507700	F	4.41925100	0.13582000	-2.23333300
O	1.34105300	-1.72754500	0.72446700	F	2.98906800	1.53957400	-1.38167600
F	4.78060000	-1.09069800	-0.80603000	F	5.07013600	1.58326400	-0.74125400
F	3.95383700	-0.34998700	1.06761400	O	4.88409900	-1.22388700	0.42601000
F	4.32103700	-2.48060600	0.80663500	S	3.68648700	-0.42788300	0.22805400
O	2.28227600	-2.66816800	-1.44820000	H	-4.59738400	4.46565400	-1.63296800
S	2.21691600	-1.58367800	-0.48343100	H	-2.94042500	4.41558100	-2.30836100
H	1.92931500	4.99617300	-0.58625800	H	-4.16309700	3.30256600	-2.92266100
H	1.10067100	4.80606600	-2.16164100				
H	0.20989800	5.45906900	-0.78432000				
				b₄'-IN3			
				C	-1.86720100	2.17000200	0.14535700
b₄'-IN2				O	-0.61193500	2.38631500	-0.00638500
C	-1.49787100	0.59711800	1.93547800	C	-2.31549400	0.83763800	0.07200300
O	-0.25548400	0.84968200	2.12050600	C	-3.56125000	0.10643600	0.16626300
O	-3.90938200	2.72680100	0.13799900	C	-1.28766600	-0.10297200	-0.16753900
C	-3.42039500	2.80829000	-0.97178200	C	-3.21017600	-1.25577900	-0.02551500
O	-2.44418200	1.98732800	-1.41032500	C	-4.90512300	0.43300700	0.38519600
C	-3.81198600	3.81754000	-2.02231900	C	-4.15058400	-2.28329800	-0.00445600
C	-1.82644000	-0.31436600	0.90383200	C	-5.85285900	-0.58974600	0.40759300
C	-3.00893700	-0.96000000	0.36310400	H	-5.21064900	1.46431100	0.53577600
C	-0.70141800	-0.87867900	0.25327400	C	-5.48263000	-1.93038600	0.21554600
C	-2.52238200	-1.88661200	-0.59553500	H	-3.86412200	-3.31984600	-0.15309800
C	-4.39109400	-0.84989700	0.56097100	H	-6.89758600	-0.34486500	0.57675300
H	-2.25250600	1.34580700	-0.69420500	H	-6.24256900	-2.70587700	0.23800700
C	-3.36697400	-2.70282000	-1.34544700	N	-1.81597600	-1.34134400	-0.22620900
C	-5.24143200	-1.66758900	-0.18193700	C	-2.75266800	3.35797600	0.38735700
H	-4.79580300	-0.13151200	1.26630200	H	-3.51474800	3.42695100	-0.39809300
C	-4.73856900	-2.58292600	-1.12103200	H	-3.27750300	3.24930500	1.34400100
H	-2.97847500	-3.40588700	-2.07562000	H	-2.15962600	4.27413200	0.39980100
H	-6.31499100	-1.59147600	-0.03524200	C	-1.10114600	-2.58984000	-0.45932300
H	-5.42671700	-3.20507800	-1.68566600	H	-1.23410800	-3.26187700	0.39494200
N	-1.11362700	-1.80605800	-0.63218100	H	-1.48608300	-3.07762800	-1.36083900
C	-2.49727200	1.28784600	2.80977700	H	-0.04169800	-2.37271400	-0.58935900

Pd	0.49150400	0.67523600	-0.33646900	F	-0.73512800	2.25549300	1.47327100
C	3.79896700	-0.57855800	0.99989200	F	0.47522400	3.68718300	0.36532900
O	1.77749000	-0.97734400	-0.69487100	F	-1.66244800	4.02512600	0.60784900
O	2.68933400	1.26204200	-0.59909100	O	-1.01533900	3.14429800	-2.22067800
O	4.08953800	-0.58770800	-1.65689100	S	-1.04883900	2.16715300	-1.14839600
F	4.91664300	0.12179700	1.18686300	H	-4.87572000	-2.34624300	1.27745600
F	4.07062200	-1.88223900	1.07374200	H	-4.04893500	-3.61792200	2.22159600
F	2.91240500	-0.25927600	1.94866400	H	-4.18248000	-3.73468800	0.43580500
S	3.09411900	-0.18369900	-0.68041300				

b₄''-TS1

Imaginary Frequency:		-94.5179	
C	1.14624100	-2.39671400	-1.57998300
O	-0.04059700	-2.43587000	-1.91009100
O	-2.58788000	-1.77483400	-0.03797900
C	-2.72969000	-2.30172300	1.15359700
O	-1.92274700	-2.21518900	2.07980600
C	-4.04367700	-3.05866900	1.28427900
C	1.55193200	-1.65028900	-0.37971800
C	2.72058500	-0.87196200	-0.10053200
C	0.71622400	-1.55482900	0.74908100
C	2.52861400	-0.31341400	1.19908700
C	3.88987300	-0.54088700	-0.81719100
H	-0.11516000	-2.18105200	1.06109000
C	3.46918200	0.53896000	1.79328100
C	4.82357600	0.29289300	-0.22546900
H	4.06211800	-0.93445700	-1.81364300
C	4.61501600	0.82799600	1.06716300
H	3.30766200	0.95859500	2.78111600
H	5.73203600	0.54778100	-0.76302300
H	5.36684300	1.48354300	1.49694700
N	1.31990900	-0.75642600	1.69079200
C	2.19402200	-3.11414100	-2.40468900
H	2.66730300	-2.39082300	-3.08211200
H	2.97969500	-3.55476200	-1.78396400
H	1.70983600	-3.87985200	-3.01437400
C	0.77157100	-0.45966800	3.00880000
H	1.44735000	-0.81783800	3.79254100
H	0.63136800	0.62038400	3.11701000
H	-0.19507500	-0.95743200	3.09440700
Pd	-1.14171500	-0.50400600	-0.48429700
C	-0.71997600	3.10146800	0.43218300
O	0.05523300	1.10377700	-1.16202000
O	-2.32938100	1.41597300	-0.88675900

b₄''-IN2

C	3.19810100	-0.16722100	-0.13101300
O	3.77675600	-0.81009300	0.72584200
O	1.45054000	-2.27693600	-0.60407000
C	1.51536800	-3.01203000	0.49141800
O	0.94868200	-2.74837000	1.54760600
C	2.42272500	-4.21801700	0.31995200
C	1.90991500	0.54615600	0.21202400
C	1.57973800	1.94521800	-0.10976100
C	1.24843300	0.29138600	1.46134100
C	0.72621200	2.40846600	0.91762300
C	1.91916000	2.81731500	-1.15082000
H	1.31862800	-0.60722100	2.06177200
C	0.18898000	3.69242000	0.93187400
C	1.39972000	4.11062200	-1.14076500
H	2.56029700	2.49561800	-1.96403400
C	0.54410700	4.54214500	-0.11511600
H	-0.48031600	4.02372400	1.71914300
H	1.65452400	4.79376600	-1.94531900
H	0.14754000	5.55271600	-0.13789800
N	0.55210900	1.37234100	1.85347800
C	3.75068500	-0.01805500	-1.53239900
H	2.96124300	-0.06818700	-2.28834600
H	4.25524400	0.95224800	-1.62764800
H	4.48613900	-0.80586000	-1.70623800
C	-0.41969600	1.39486100	2.93880200
H	-0.28488800	2.29941300	3.53780400
H	-1.43580800	1.36879900	2.53272400
H	-0.26188100	0.51921900	3.57009400
Pd	0.24016200	-0.69862700	-0.51786300
C	-3.37204600	-0.47423100	0.45558100
O	-1.32110500	0.78004400	-0.67371400
O	-1.70841400	-1.50287000	-1.37782300
F	-2.55604400	-0.94259300	1.40969900
F	-3.88786200	0.68887200	0.86968100

F	-4.35265100	-1.34733500	0.24519200
O	-3.36049000	0.29457800	-2.10249700
S	-2.41211400	-0.19565100	-1.11839700
H	2.31843700	-4.65678800	-0.67562400
H	2.19502400	-4.95744000	1.09025800
H	3.46027100	-3.88467600	0.43868000

F	-2.99490100	-0.99139300	-1.48169500
S	-2.60894700	-0.70891600	1.11689200
H	0.84882800	5.09351500	-2.31120400
H	0.97111700	5.33835200	-0.55816700
H	-0.63676300	5.20344200	-1.30202600

b₄''-TS2

Imaginary Frequency: -880.1271

C	2.54804200	1.13636800	1.58538200
O	1.92319700	2.19025400	1.60708300
O	-0.49704700	2.85306000	-0.43007400
C	0.45389800	3.35354300	-1.11198100
O	1.43813600	2.71159700	-1.58146100
C	0.39346200	4.84738000	-1.34983500
C	2.27642700	0.12687300	0.53153100
C	2.92386800	-1.10998600	0.24118300
C	1.29248100	0.34748400	-0.47257400
C	2.29010400	-1.63183600	-0.93393900
C	3.97757300	-1.85818900	0.82358800
H	1.38007700	1.49120400	-1.05707400
C	2.67649500	-2.85340200	-1.51719200
C	4.34850100	-3.05867700	0.25109700
H	4.48564500	-1.50518600	1.71275600
C	3.70222000	-3.55329500	-0.91051500
H	2.17943100	-3.24037000	-2.40062900
H	5.14882100	-3.64115200	0.69777700
H	4.01823100	-4.50538500	-1.32712300
N	1.33031500	-0.74890400	-1.33919400
C	3.61389700	0.85681100	2.62811000
H	3.39166500	-0.06626000	3.17656100
H	4.59838900	0.73720200	2.16004600
H	3.64685400	1.69476800	3.32678900
C	0.46033100	-0.91811900	-2.49323700
H	1.01531500	-1.38677100	-3.31049100
H	-0.41094400	-1.53097500	-2.24077100
H	0.11740500	0.06581100	-2.81881200
Pd	-0.62026100	0.90872000	0.12054500
C	-3.52084600	-1.44547700	-0.33341800
O	-1.14460600	-1.03512700	0.80272400
O	-2.74222800	0.78104900	0.93737500
O	-3.16664700	-1.32456000	2.30722900
F	-4.80594500	-1.10248700	-0.27682200
F	-3.40985200	-2.77405300	-0.30379900

b₄''-IN3

C	2.20860700	1.19528400	1.69958000
O	1.26711200	1.99171400	1.75612300
O	-0.18664200	2.38570400	-1.10730100
C	0.84694700	2.97980600	-1.43819000
O	2.06678100	2.51825600	-1.26605400
C	0.79006600	4.33313200	-2.08600800
C	2.22575000	0.11675400	0.70572500
C	3.24237000	-0.87307800	0.37826000
C	1.09292800	-0.20515200	-0.06628200
C	2.66130200	-1.73616500	-0.58600100
C	4.56774300	-1.11969400	0.77535400
H	2.04953400	1.66580800	-0.75966900
C	3.34613200	-2.81199500	-1.15537300
C	5.25635300	-2.19338200	0.21742900
H	5.05968700	-0.48927700	1.50759500
C	4.65551700	-3.03207500	-0.73747500
H	2.87856000	-3.45485300	-1.89488600
H	6.27984300	-2.38639900	0.52650600
H	5.21866500	-3.86140400	-1.15555400
N	1.35572400	-1.30474500	-0.83048900
C	3.37303100	1.33225800	2.66297400
H	3.56818400	0.38832800	3.18432900
H	4.28891800	1.60601200	2.12417500
H	3.14035000	2.11374400	3.38883000
C	0.44118700	-1.97834700	-1.74052600
H	0.79160900	-1.88990500	-2.77518600
H	0.36982000	-3.03854400	-1.47729000
H	-0.54727900	-1.52844900	-1.65317300
Pd	-0.65815600	0.67066500	0.02711200
C	-3.86449900	-1.24299400	-0.39713400
O	-1.62111800	-0.94387600	1.00860100
O	-2.88236900	1.07191900	0.51498400
O	-3.83499500	-0.59677900	2.18930200
F	-5.08575700	-0.74740300	-0.58849900
F	-3.94862100	-2.54237800	-0.11156300
F	-3.15070200	-1.09134800	-1.52556700
S	-3.03347600	-0.33930000	1.00679600

H	1.50784700	4.39130700	-2.90842500
H	1.07163400	5.08698100	-1.34147300
H	-0.22168500	4.53666200	-2.43685300

H	-1.84695100	-4.43176800	2.60753000
H	-0.51410900	-5.13726400	1.64166000

Pd(OTf)(OAc)

a₅-IN1

C	-2.08832000	-1.16110600	-1.36777900
O	-0.86924900	-1.41680000	-1.56044600
O	2.75921600	-1.03042800	0.51393700
O	2.00595300	0.24941800	-1.38199400
C	2.99217900	1.63717500	0.69383100
C	-2.59961000	0.03727300	-0.76386000
C	-1.96961600	1.32008000	-0.49640700
C	-3.88625700	0.12541800	-0.23551000
C	-2.92835800	2.10085000	0.19684800
C	-0.73950100	1.90703100	-0.82546000
H	-4.65570400	-0.63242000	-0.19090200
C	-2.69123900	3.41615200	0.59987300
C	-0.49022000	3.21608400	-0.42099800
H	0.00685500	1.36377900	-1.38996700
C	-1.44906900	3.96154800	0.28761600
H	-3.44211800	3.99465900	1.12967400
H	0.47004700	3.66568000	-0.65465600
H	-1.22247700	4.98034700	0.58830900
N	-4.08358600	1.33092300	0.34920500
C	-3.04961500	-2.21721000	-1.86811300
H	-2.57910900	-2.76111200	-2.69053600
H	-3.21530000	-2.92237700	-1.04504700
H	-4.00723400	-1.80600100	-2.19538300
C	-5.28343500	1.75881100	1.04721700
H	-5.05497900	1.98841200	2.09319500
H	-5.70611400	2.64997900	0.57110800
H	-6.02134900	0.95529200	1.01415300
Pd	0.80729600	-1.26236700	-0.35883700
C	-0.84830000	-4.25822800	2.20205800
O	0.31340600	-2.80235100	0.78572300
F	3.98785500	1.65593300	1.57742100
F	3.05233500	2.73282000	-0.06998200
F	1.82504300	1.61312700	1.33797200
O	-1.90010500	-2.39005900	1.08745200
O	4.50686400	0.14382700	-0.92066300
S	3.15640000	0.12749500	-0.39184100
C	-0.87598000	-3.03385500	1.28961200
H	-0.13610800	-4.10060900	3.01807200

a₅-TS1

Imaginary Frequency: -42.7123

C	-2.74700800	-0.95306500	-1.08880900
O	-1.64521400	-1.46486200	-1.41863100
O	1.95159700	-0.89676000	0.51825000
O	2.39858700	0.31993700	-1.58541000
C	3.60379300	1.14434700	0.66134600
C	-2.84548800	0.37154500	-0.54926500
C	-1.81314600	1.38687300	-0.54047600
C	-3.91156400	0.89360300	0.17706200
C	-2.31549400	2.46739100	0.22163300
C	-0.54015300	1.49949100	-1.12567100
H	-4.85697800	0.43418500	0.43076400
C	-1.57943300	3.63194500	0.44889300
C	0.20977600	2.65085600	-0.88712700
H	-0.16771600	0.77247500	-1.85279000
C	-0.30405300	3.70166600	-0.10780800
H	-1.97833600	4.45321700	1.03664200
H	1.20098000	2.72665100	-1.31806100
H	0.30091300	4.58783600	0.05752600
N	-3.60321700	2.12832900	0.64690900
C	-3.96681100	-1.81525500	-1.28079100
H	-3.82569300	-2.44975500	-2.15945800
H	-4.03642000	-2.46902100	-0.40233900
H	-4.88861000	-1.23821100	-1.38205100
C	-4.44519700	2.95852500	1.49280600
H	-3.95691600	3.13949200	2.45586300
H	-4.64557700	3.91909900	1.00692700
H	-5.39236200	2.44507600	1.66675800
Pd	0.14911100	-1.05889600	-0.44590500
C	-0.96702900	-4.45862600	1.79964200
O	0.00829800	-2.85756500	0.39900400
F	4.15774500	0.69401600	1.78746700
F	4.50485900	1.86292600	-0.01736900
F	2.57023400	1.93949500	0.97405500
O	-1.96007100	-2.29075900	1.38034300
O	4.21106600	-1.12770300	-0.56200200
S	3.03609000	-0.28176400	-0.39381900
C	-1.03799200	-3.07129200	1.16588400
H	-0.13872700	-4.48877100	2.51506800
H	-1.90596300	-4.66672100	2.31643200

H	-0.77349600	-5.22065400	1.03935900
a₅-IN2			
C	2.86967300	1.03875600	-1.01918700
O	1.75828200	1.55497500	-1.29016300
O	-1.80271400	0.49135600	0.51862300
O	-2.51016500	-0.45687300	-1.67845300
C	-3.80362200	-1.16331100	0.54969900
C	2.98102500	-0.30614700	-0.52521100
C	1.92898600	-1.29879900	-0.49880300
C	4.05720200	-0.86157900	0.16054100
C	2.42580200	-2.39629600	0.24059400
C	0.62491800	-1.36712700	-1.02978100
H	5.02190700	-0.42890600	0.38742100
C	1.65764200	-3.53364000	0.49924200
C	-0.15655300	-2.49264600	-0.75412400
H	0.26662500	-0.67367200	-1.80686100
C	0.35499700	-3.55859200	0.00371800
H	2.05227100	-4.36834900	1.07085000
H	-1.16665000	-2.52900200	-1.14288200
H	-0.27277200	-4.42198600	0.20008300
N	3.73540000	-2.09553900	0.62466200
C	4.07911100	1.91640300	-1.20389200
H	3.94226200	2.53570700	-2.09432500
H	4.12539600	2.58877000	-0.33778800
H	5.01212400	1.35436500	-1.28309200
C	4.58348700	-2.95487200	1.43565600
H	4.12293100	-3.13146000	2.41302300
H	4.74322400	-3.91550800	0.93534400
H	5.54867600	-2.46708900	1.58184900
Pd	-0.02969200	0.94364600	-0.39666500
C	0.47970300	4.56992800	1.66661000
O	-0.22237100	2.79516700	0.30445300
F	-4.15648400	-0.71777200	1.75616700
F	-4.89459900	-1.58040000	-0.10079600
F	-2.97312400	-2.20919400	0.70111600
O	1.69827400	2.48627900	1.46930100
O	-3.96468400	1.26116700	-0.52522700
S	-2.98207700	0.18595300	-0.43768400
C	0.73035600	3.16275300	1.13457200
H	-0.39387300	4.55706200	2.32686400
H	1.35554600	4.90616200	2.22518600
H	0.26215800	5.26045000	0.84679900

a₅-TS2			
Imaginary Frequency: -1294.4944			
C	-2.58911000	1.26489000	1.19984500
O	-1.53004600	1.83647200	0.86145900
O	2.16862500	0.24518300	-0.43861400
O	1.33322700	-1.29201600	1.31260800
C	3.64045600	-1.88236100	0.10498400
C	-2.92324100	-0.06188400	0.75641800
C	-2.06770900	-0.93340600	-0.01292100
C	-4.18348700	-0.65770300	0.77339200
C	-2.88479400	-1.99220400	-0.47185500
C	-0.69944000	-0.86618900	-0.36238300
H	-5.10342700	-0.31698800	1.22810700
C	-2.41225000	-2.97438400	-1.34473600
C	-0.25830500	-1.83256600	-1.28855600
H	0.32858400	-0.96638000	0.62059500
C	-1.08828900	-2.86310900	-1.76304400
H	-3.04559600	-3.78400600	-1.69507200
H	0.77843400	-1.81728200	-1.60692800
H	-0.68503500	-3.59509000	-2.45668200
N	-4.16737400	-1.80572500	0.04966100
C	-3.52012300	2.04079800	2.10378400
H	-3.35664400	1.72884500	3.14305700
H	-3.29609600	3.10594700	2.02300300
H	-4.57255900	1.86699600	1.86167800
C	-5.30319600	-2.67977400	-0.19560300
H	-5.52044000	-2.73125100	-1.26755800
H	-5.09666700	-3.68868400	0.17597300
H	-6.17735500	-2.28358600	0.32419300
Pd	0.15824100	1.06352900	-0.13651000
C	0.87124600	5.07144300	-1.15185300
O	-0.38853900	3.15424200	-1.92248900
F	4.70948600	-1.33849100	-0.47130400
F	4.02335600	-2.68602100	1.09543900
F	2.96312600	-2.59505100	-0.80165700
O	0.88768000	2.95356000	-0.08805000
S	2.56506800	-0.52440900	0.79562000
O	3.34254600	0.14269800	1.82493200
C	0.39129000	3.62891700	-1.09337200
H	1.96208600	5.09820200	-1.24585800
H	0.41447900	5.57909000	-2.00400300
H	0.61173100	5.59264400	-0.22426700

a₅-IN3

C	-1.20177800	-0.82425200	2.00404600	O	-2.40374000	-0.17436500	-1.09277100
O	-0.19738400	-0.06676900	1.95963900	O	-1.61721600	-2.05703900	0.37803200
O	0.38161200	-2.51387300	-0.06326300	C	-3.35098800	-0.32618600	1.36615300
O	1.14864800	-0.75333100	-1.70621000	C	2.35838100	-1.16276500	-0.66563300
C	2.99688000	-1.96761300	-0.21661300	C	2.16038900	-0.64316700	0.67951700
C	-2.29287100	-0.66999500	1.09575100	C	3.73860300	-1.21534900	-0.85708200
C	-2.31904900	0.30051600	0.03071600	C	3.45077100	-0.38515800	1.20260700
C	-3.49333000	-1.37370700	1.01583600	C	1.04466800	-0.46204500	1.51235500
C	-3.54663700	0.14124700	-0.64711600	H	4.29929100	-1.51231400	-1.73239600
C	-1.38962400	1.25669400	-0.38585400	C	3.66306300	0.10406400	2.49405600
H	-3.86399100	-2.18680900	1.62482100	C	1.24715900	0.03149700	2.79768500
C	-3.89074100	0.93174600	-1.74598300	H	0.05119100	-0.74454900	1.18457100
C	-1.72222000	2.05239300	-1.48232900	C	2.53653600	0.32300500	3.28093000
H	0.73953500	-0.13563400	-1.03680200	H	4.66178700	0.29487100	2.87525500
C	-2.95674800	1.88745600	-2.14554800	H	0.38708800	0.18045500	3.44384000
H	-4.83316300	0.81307400	-2.27190300	H	2.65753500	0.70393300	4.29097100
H	-1.02260800	2.80557900	-1.83166300	N	4.39008000	-0.73573000	0.23115300
H	-3.18392500	2.52267000	-2.99748500	C	1.74347600	-2.55914800	-2.71855100
N	-4.24192700	-0.89626000	-0.01266400	H	1.24473700	-2.33315900	-3.66361800
C	-1.17231900	-1.92630700	3.03131000	H	2.81810000	-2.67832200	-2.87410000
H	-0.61946600	-2.77128000	2.60262700	H	1.35441400	-3.51760800	-2.35140100
H	-0.63584900	-1.58582200	3.92020700	C	5.82854700	-0.59374100	0.37433500
H	-2.17176700	-2.26901800	3.31119800	H	6.09530200	0.45603500	0.53548600
C	-5.55218700	-1.38125200	-0.41283500	H	6.18847500	-1.18606500	1.22226900
H	-6.29166200	-0.57589500	-0.35213500	H	6.31577000	-0.94761200	-0.53613900
H	-5.52094100	-1.75882000	-1.44018300	Pd	-0.57525000	0.73624300	-1.06872500
H	-5.85385700	-2.19142900	0.25361500	C	0.53878000	4.47283900	-0.52284200
Pd	0.30034400	1.42590000	0.60852400	O	0.96647800	2.14484800	-1.06373000
C	3.25077700	4.02747500	-0.25806300	F	-4.34919400	0.49593100	1.04079600
O	1.14468400	2.90556600	-0.54190200	F	-3.76298200	-1.15490900	2.33088900
F	3.31897900	-3.09868600	0.41298600	F	-2.32689100	0.40848100	1.84614100
F	3.94550600	-1.65960900	-1.09648600	O	-1.08618500	2.67658800	-0.55109000
F	2.86966800	-0.98206200	0.67140200	S	-2.78202700	-1.30657900	-0.11064500
O	2.39327500	2.25727100	1.16050400	O	-3.95651400	-2.02471000	-0.59304800
S	1.37160300	-2.22500000	-1.09542500	C	0.12789400	3.04594700	-0.71102100
O	1.61238000	-3.11873000	-2.21114800	H	-0.05711000	4.93132100	0.27027600
C	2.22902800	3.00219700	0.16353700	H	1.60399100	4.52990100	-0.28771800
H	3.53829600	3.85864700	-1.30096400	H	0.35378000	5.02519700	-1.45171000
H	2.81311600	5.02984000	-0.19707400				
H	4.13008200	3.96986900	0.38586900				
				as⁺-TS1			
				Imaginary Frequency:	-540.5502		
as⁺-IN1				C	-2.01453300	0.80504300	1.99956400
C	1.40376700	-1.50037300	-1.69301600	O	-0.91620200	1.36272300	1.77275400
O	0.25647200	-1.00731200	-1.80356900	O	2.32280300	-0.13838400	1.29565900

O	0.49353200	-1.75340300	0.78204400	C	3.56862400	0.17392100	0.38532400
C	2.84714800	-2.17229600	-0.30069700	C	2.52019500	-0.58412500	-0.25333600
C	-2.73921700	0.11403100	0.96500100	C	4.67195700	-0.67588000	0.47845400
C	-2.19676000	-0.22009900	-0.32161700	C	3.04457200	-1.86741000	-0.51993700
C	-4.08556500	-0.24889100	0.92714900	C	1.20710200	-0.25794500	-0.60531600
C	-3.25316300	-0.74123900	-1.09580900	H	5.65572700	-0.49706700	0.89030400
C	-0.87909900	-0.15364900	-0.82926600	C	2.28852000	-2.86342300	-1.14100500
H	-4.85007900	-0.15426400	1.68618000	C	0.44453000	-1.24553900	-1.22922000
C	-3.06072600	-1.13967400	-2.41972800	H	-2.47865300	0.33144300	-1.07239100
C	-0.70640500	-0.53269700	-2.17835600	C	0.98228500	-2.52411700	-1.48892400
H	-0.05252700	-0.73143600	-0.06690300	H	2.68739300	-3.85210100	-1.34587800
C	-1.77287900	-1.01378500	-2.95109000	H	-0.57959600	-1.04748100	-1.52444700
H	-3.87220800	-1.53817900	-3.02171400	H	0.35303400	-3.26583200	-1.97286500
H	0.29077600	-0.49592100	-2.60514400	N	4.36710800	-1.88526500	-0.05540700
H	-1.59486800	-1.31593700	-3.97871900	C	4.53902700	2.29762100	1.46264800
N	-4.40083300	-0.74829300	-0.29656200	H	4.20190400	2.64657800	2.44456200
C	-2.53925400	0.87488100	3.41073400	H	5.44971400	1.70785900	1.58611500
H	-2.15470700	1.77099500	3.90193700	H	4.76590500	3.18627000	0.86390300
H	-3.63213900	0.86574000	3.45057800	C	5.25748500	-3.03133200	-0.14001300
H	-2.17261400	-0.00094600	3.96122700	H	4.83912100	-3.87949600	0.41169900
C	-5.71341400	-1.20943200	-0.72179300	H	5.40207100	-3.32376900	-1.18515300
H	-6.06773300	-0.61935900	-1.57322000	H	6.22443000	-2.76779100	0.29253200
H	-5.67164500	-2.26487200	-1.00941200	Pd	0.54214500	1.54625000	-0.19315900
H	-6.41674000	-1.09606700	0.10497900	C	-3.14035700	3.17039900	-0.82574500
Pd	0.21888000	1.42689000	0.02565200	O	-0.85462300	3.38958600	-0.05263600
C	3.18997700	3.59063800	-1.44634000	F	-3.32290400	-2.20179800	2.19555400
O	1.48480900	3.20054400	0.23284300	F	-2.28916900	-2.84852400	0.39187600
F	4.16737800	-2.01740500	-0.15725100	F	-1.69623000	-1.00258400	1.38237400
F	2.58645800	-3.46507700	-0.52668500	O	-1.44553100	1.44596900	-0.89480000
F	2.45329900	-1.46819000	-1.38302600	S	-3.96261000	-0.83524900	0.05197800
O	1.51276000	1.85356600	-1.49565900	O	-4.99720700	-1.77204700	-0.34691900
S	1.95005800	-1.56150300	1.20871700	C	-1.74240500	2.68210400	-0.56556800
O	2.33821200	-2.46121100	2.29333700	H	-3.84400200	2.60151600	-0.20822600
C	2.00766500	2.87063100	-0.87090200	H	-3.21246700	4.23300100	-0.58910100
H	3.16073700	3.56135600	-2.53858600	H	-3.40737300	3.00169400	-1.87450400
H	3.21126800	4.62232200	-1.08776900				
H	4.10473000	3.08634500	-1.11322700	as³-IN3			
				C	1.05658800	2.19499800	-0.00410100
as³-IN2				O	-0.19111900	2.04497300	-0.00431700
C	3.42082900	1.52874600	0.80138000	C	1.94456000	1.07574000	-0.00529800
O	2.33994000	2.15187800	0.63252800	C	1.50364100	-0.29864800	-0.00090200
O	-4.26228900	0.37580100	0.81112500	C	3.33889900	1.04270500	-0.00704800
O	-3.07697000	-0.49644300	-1.22368700	C	2.66211100	-1.10487200	0.00011100
C	-2.73164900	-1.79023200	1.07323500	C	0.22767400	-0.87052400	0.00198000

H	4.05547800	1.85269500	-0.00952700
C	2.59308200	-2.50002300	0.00402600
C	0.14862500	-2.26403200	0.00584000
C	1.31463300	-3.05833400	0.00691400
H	3.48119700	-3.12477500	0.00493500
H	-0.82580200	-2.74305900	0.00787600
H	1.21308500	-4.14062000	0.01004900
N	3.76989200	-0.24608700	-0.00362000
C	1.56343300	3.61850400	0.01439300
H	1.30079300	4.07943200	0.97365100
H	2.64399800	3.69116300	-0.12769500
H	1.05654000	4.19010600	-0.76919500
C	5.15507000	-0.68314700	-0.00473400
H	5.36698100	-1.28203000	0.88738100
H	5.36388300	-1.28722600	-0.89407300
H	5.80849700	0.19147600	-0.00842500
Pd	-1.34492300	0.30431100	-0.00119300
C	-5.18580200	-0.92377200	-0.00057300
H	-5.92931400	-0.12462000	-0.00109000
H	-5.32207000	-1.55754300	0.88222700
H	-5.32200600	-1.55838100	-0.88280300
C	-3.79278300	-0.34125700	-0.00091500
O	-2.79603600	-1.16611300	0.00164600
O	-3.58690100	0.89784500	-0.00373500

as''-TS1

Imaginary Frequency: -89.9543

C	-2.20603000	-0.82373200	-2.23532600
O	-0.96867200	-0.80325600	-2.22124200
O	1.76874000	0.36949100	-1.05348100
O	3.28928600	2.31998700	-1.14080000
C	4.22804800	0.04126800	-0.12956000
C	-2.96487500	-0.01640800	-1.29119700
C	-2.39599900	0.95009000	-0.38931500
C	-4.28639600	-0.18372300	-0.89593400
C	-3.40449600	1.28951000	0.54311600
C	-1.12318400	1.55158200	-0.28444300
H	-5.04808600	-0.83718000	-1.30004300
C	-3.17582800	2.16983300	1.60178900
C	-0.88380800	2.41261100	0.79872700
H	-0.41028600	1.49308100	-1.10247700
C	-1.89272700	2.70576900	1.72942900
H	-3.95923500	2.42850900	2.30836200
H	0.09805100	2.86039700	0.90795200

H	-1.67833400	3.37982000	2.55307500
N	-4.55958000	0.59002400	0.19241000
C	-2.93684400	-1.73596000	-3.20292600
H	-2.23671400	-2.08298300	-3.96517200
H	-3.32789300	-2.61114400	-2.66786800
H	-3.78214200	-1.22686200	-3.67834100
C	-5.82555200	0.65636500	0.90175000
H	-6.54337300	-0.00446700	0.41222900
H	-5.70040700	0.33459200	1.94112300
H	-6.22135300	1.67754500	0.89036400
Pd	0.30950600	-0.57112100	0.00422400
C	-0.37140300	-3.48764000	2.61980000
O	-0.98058500	-1.71546100	1.08583300
O	1.14976800	-2.16423900	1.27734000
F	5.23313200	0.63579900	0.52219500
F	3.84426100	-1.04052400	0.55469800
F	4.65309700	-0.33472500	-1.33841100
O	2.36579400	1.52054500	1.08106700
S	2.80861000	1.23499900	-0.29066300
C	-0.03933100	-2.42450400	1.61667800
H	-0.33038400	-3.05483400	3.62634200
H	-1.37968600	-3.87243900	2.44802800
H	0.36335200	-4.29448100	2.56425300

as''-IN2

C	-3.32734400	-2.25301900	1.38443600
O	-2.29511000	-2.90690200	1.46111100
O	1.73584200	-1.14752000	0.26965000
O	3.63810800	-2.52328700	-0.47431500
C	4.14349300	-0.01561300	0.27321900
C	-3.45434100	-1.16406500	0.40108600
C	-2.44062800	-0.73234800	-0.52636100
C	-4.55056200	-0.35176300	0.17092900
C	-2.99053100	0.32854800	-1.28019600
C	-1.11451300	-1.15165200	-0.79476200
H	-5.51903600	-0.34480800	0.65188500
C	-2.28427000	0.98682300	-2.30877600
C	-0.39502400	-0.48841400	-1.82772500
H	-0.71749900	-2.03843000	-0.31409100
C	-0.99788900	0.56964500	-2.57573700
H	-2.73927400	1.79209300	-2.87764500
H	0.55601600	-0.88672800	-2.16568400
H	-0.42333700	1.03824500	-3.36795600
N	-4.28019200	0.54281900	-0.83383000

C	-4.50976900	-2.54049400	2.29756000
H	-4.25428100	-3.37421400	2.95386900
H	-4.75571000	-1.66264500	2.90762200
H	-5.40239600	-2.79956500	1.71486100
C	-5.18908900	1.55978400	-1.33791800
H	-6.13254500	1.49255800	-0.79334100
H	-4.76669600	2.55926100	-1.19128200
H	-5.38693800	1.40740100	-2.40407800
Pd	0.40103700	0.39259500	0.14682200
C	-0.29346800	3.84005700	1.99239600
O	-0.79130600	2.05528600	0.42737500
O	1.02195600	1.84076000	1.62817400
F	5.33447400	-0.00238900	-0.33252800
F	3.62212300	1.21983500	0.22797900
F	4.30312200	-0.37283100	1.54807900
O	2.80832600	-0.62620100	-1.93791400
S	3.01739100	-1.21009200	-0.60590900
C	-0.00548200	2.52426600	1.33528500
H	0.38261600	4.60025000	1.58443600
H	-1.32603100	4.14379300	1.80723900
H	-0.10300600	3.76601800	3.06668400

as''-TS2

Imaginary Frequency: -1139.5326

C	-1.98844900	0.28472800	2.17488600
O	-0.89977800	0.84824500	2.13265100
O	2.22929800	0.80990200	-0.08539800
O	1.48687300	-1.28445800	1.01284600
C	3.91691800	-1.20779000	-0.05795300
C	-2.41453700	-0.66172600	1.13492900
C	-1.70764400	-1.05084000	-0.06214800
C	-3.59135100	-1.39623000	1.14589900
C	-2.51760000	-2.02569900	-0.70661900
C	-0.45963500	-0.68917800	-0.64549200
H	-4.39230700	-1.39531300	1.87268300
C	-2.15063100	-2.64435900	-1.90224800
C	-0.10837400	-1.33226600	-1.85383500
H	0.57629900	-0.96410700	0.28140100
C	-0.92475300	-2.29315700	-2.46635500
H	-2.79168800	-3.38123000	-2.37810000
H	0.84528500	-1.08839700	-2.31440700
H	-0.60470900	-2.76471200	-3.39090300
N	-3.66582200	-2.21154000	0.05511500
C	-2.94090400	0.55047000	3.33428300

H	-3.88871000	0.96946200	2.97465900
H	-3.17027900	-0.37382400	3.87831000
H	-2.47022000	1.25936100	4.01763200
C	-4.74473700	-3.13124700	-0.25822600
H	-5.20225000	-2.87774400	-1.22075600
H	-4.37576800	-4.16190800	-0.30042300
H	-5.50654900	-3.06319000	0.52074700
Pd	0.18064200	1.28460600	-0.49260600
C	-2.03429400	4.52767700	-1.12877100
O	-1.64141500	2.15025300	-0.97379600
O	0.09271600	3.46291500	-0.66925300
S	2.62713900	-0.25820200	0.89443700
O	3.22295000	0.14102300	2.15565300
F	4.33273400	-2.24654000	0.66459800
F	4.94604500	-0.40717300	-0.32620000
F	3.38666700	-1.64956700	-1.20331300
C	-1.14136700	3.33639500	-0.92208400
H	-1.44948000	5.37209700	-1.50076000
H	-2.84196500	4.28324000	-1.82345300
H	-2.48068900	4.81222200	-0.16854700

as-TS2'

Imaginary Frequency: -1308.1378

C	-1.90353500	1.65993000	1.35900200
O	-0.75870700	1.85608400	0.89419500
O	1.90449500	-0.73724600	-1.10074700
O	0.92219400	-2.07230600	0.74738100
C	3.38188300	-1.11812800	1.12645800
C	-2.72337600	0.55307500	0.95284800
C	-2.33447500	-0.49665300	0.04168600
C	-4.09647500	0.41527300	1.15406800
C	-3.52012600	-1.18351500	-0.30604700
C	-1.08937800	-0.86329600	-0.51630400
H	-4.77000800	1.01359500	1.75232400
C	-3.53853900	-2.20171300	-1.26135800
C	-1.13915800	-1.85233300	-1.51966800
H	-0.01505000	-1.36757500	0.27927400
C	-2.32841900	-2.50940300	-1.87924700
H	-4.45243500	-2.72572900	-1.52499600
H	-0.21578000	-2.15787000	-2.00314900
H	-2.30007200	-3.28210300	-2.64176500
N	-4.57555200	-0.61472900	0.41242000
C	-2.42342800	2.70107400	2.32552000
H	-1.58232900	3.12474600	2.87868200

H	-2.89292100	3.51461300	1.75855600
H	-3.15683400	2.29308800	3.02592400
C	-5.96392100	-1.03951400	0.33152500
H	-6.33384800	-0.93950400	-0.69414100
H	-6.06327600	-2.08314100	0.64703000
H	-6.56826400	-0.41193200	0.98893800
Pd	0.39505400	0.64919900	-0.37475700
C	2.28653300	4.30112600	-1.27209100
O	0.27946200	3.07845700	-1.84486200
F	4.48341900	-0.73832200	0.48450200
F	2.83357400	-0.07129100	1.74067900
F	3.68711100	-2.05238900	2.02806100
O	1.73957400	2.16775700	-0.40015000
S	2.18151700	-1.84011200	-0.10953000
O	2.79543300	-3.04353600	-0.64539400
C	1.32909600	3.11933800	-1.20189400
H	2.43901400	4.72332900	-0.27310800
H	3.26391100	3.96858000	-1.63792300
H	1.88333700	5.06443900	-1.94083400

a₅-TS2''

Imaginary Frequency: -1317.9965

C	-2.46979000	1.86677400	0.38012100
O	-1.41369200	2.15806700	-0.22615000
O	2.07163600	-0.15299000	-0.73024600
O	1.09772200	-1.12977300	1.31934600
C	3.24419200	-2.30862000	0.24606600
C	-2.94902400	0.51547900	0.47836000
C	-2.25513300	-0.64904500	-0.01594300
C	-4.26043400	0.11351700	0.73611800
C	-3.21393000	-1.68418800	-0.09614800
C	-0.91368900	-0.86021800	-0.41081300
H	-5.10181800	0.68799700	1.09812000
C	-2.91743900	-2.93077600	-0.65037000
C	-0.65462000	-2.10195900	-1.02773000
H	0.11795800	-0.84786900	0.55502300
C	-1.62576100	-3.11187300	-1.14136200
H	-3.65675300	-3.72407400	-0.71000900
H	0.35314800	-2.31623000	-1.36624000
H	-1.35793400	-4.06009400	-1.59827900
N	-4.42381300	-1.19107800	0.40130800
C	-3.23757600	3.03003600	0.96102400
H	-3.34714300	3.80990000	0.20168800
H	-4.21913400	2.75415900	1.35169200

H	-2.63855400	3.45239800	1.77622400
C	-5.65670000	-1.95497300	0.50714600
H	-5.96383200	-2.32062200	-0.47811800
H	-5.52172500	-2.80873000	1.17911200
H	-6.44239800	-1.31122800	0.90658700
Pd	0.20986200	0.94201000	-0.66953900
C	2.22439200	4.64820900	-0.37106900
O	1.17630100	3.04941200	1.10820200
F	4.35382500	-2.06486700	-0.44749000
F	3.55206500	-2.93203300	1.38200600
F	2.43636600	-3.09335700	-0.47738300
O	1.18630700	2.65744800	-1.11166400
S	2.40590700	-0.68998700	0.64243600
O	3.32865100	0.04817600	1.48334000
C	1.46746000	3.36605100	-0.04287500
H	1.70063700	5.21598100	-1.14680400
H	2.33152300	5.25342400	0.53152300
H	3.21715900	4.39900000	-0.76180500

a₅-TS2'''

Imaginary Frequency: -1319.5051

C	-1.95587100	2.13108500	0.49265600
O	-0.90514900	2.15504200	-0.18848000
O	1.75040600	-0.96292800	-1.11990200
O	0.76276600	-1.76844500	1.00580300
C	3.36573300	-1.18306600	1.03674000
C	-2.76639000	0.95133800	0.60876100
C	-2.44889500	-0.33064100	0.02845000
C	-4.11373100	0.89856800	0.96975700
C	-3.65202200	-1.07155700	0.00688000
C	-1.24716700	-0.86761300	-0.48602300
H	-4.74002500	1.65855000	1.41633400
C	-3.74136400	-2.32496400	-0.60100000
C	-1.37572700	-2.10462400	-1.15310400
H	-0.17315100	-1.17314300	0.38287800
C	-2.58603700	-2.81672700	-1.20660600
H	-4.66695900	-2.89284700	-0.61522200
H	-0.49191700	-2.56278500	-1.58847600
H	-2.61530500	-3.78018800	-1.70676600
N	-4.64439100	-0.29971000	0.61929300
C	-2.35818400	3.44352800	1.12252000
H	-1.50614900	3.81171800	1.70304900
H	-2.55808500	4.17974400	0.33631100
H	-3.23094600	3.36127100	1.77366100

C	-6.02417300	-0.71604500	0.81422000
H	-6.49301900	-0.94225700	-0.14896100
H	-6.06927500	-1.60523200	1.45132300
H	-6.57657300	0.09280100	1.29575900
Pd	0.29583600	0.58311900	-0.78533100
C	3.08281300	3.79841300	-0.76571600
O	1.79229400	2.59030000	0.88142300
F	4.45150700	-1.15497800	0.26446500
F	3.06238800	0.04243600	1.43818700
F	3.58889900	-1.96604400	2.09346100
O	1.66008300	1.99138600	-1.29332700
S	1.95633800	-1.90346000	0.04534200
O	2.33193800	-3.26504400	-0.30297300
C	2.10356300	2.72409600	-0.29934600
H	2.59163700	4.47080600	-1.47744600
H	3.44249500	4.36791300	0.09384600
H	3.92903000	3.33757400	-1.28608500

b₅-IN1

C	1.68062200	0.97038300	1.39165500
O	0.44144000	1.21082400	1.45784000
O	-2.59600500	0.14762700	-1.24377600
O	-1.65125700	-1.24599300	0.48633500
C	-4.31422300	-0.95245200	0.50183100
C	2.26699300	-0.15333000	0.71853200
C	3.66023100	-0.40754300	0.37701300
C	1.55922600	-1.28939500	0.31946600
C	3.69553500	-1.69521300	-0.21641100
C	4.86277300	0.31222600	0.46622000
H	0.50847400	-1.51601100	0.43190100
C	4.86684100	-2.28625900	-0.69244500
C	6.03737100	-0.26909500	-0.00308200
H	4.88858000	1.31282800	0.88151300
C	6.04423300	-1.55444600	-0.57289600
H	4.86247100	-3.27435000	-1.14249000
H	6.96839700	0.28602000	0.06677600
H	6.97745000	-1.97871300	-0.93127300
N	2.39466700	-2.20160800	-0.22471100
C	2.55385300	1.95316900	2.12700300
H	2.94044700	2.66369100	1.38476800
H	1.94613100	2.50747700	2.84502300
H	3.39607000	1.47121600	2.62944500
C	2.00741700	-3.51025700	-0.72850300
H	0.92696300	-3.62324200	-0.62603100

H	2.27517700	-3.60226900	-1.78591100
H	2.50842200	-4.30226400	-0.16209300
Pd	-1.00383500	0.80875000	0.05811200
C	0.13428300	4.56044500	-1.56187500
O	1.37536200	2.57254100	-0.96399800
F	-4.17236800	0.11962300	1.28179700
F	-5.36364400	-0.78582700	-0.30045800
F	-4.49575400	-2.03368800	1.25996900
O	-0.86551100	2.66165400	-0.61672600
O	-2.99765800	-2.36410700	-1.35520600
S	-2.78172700	-1.18468300	-0.53623500
C	0.29449600	3.14668600	-1.01120200
H	1.11349200	4.95164100	-1.84431500
H	-0.52559300	4.54704500	-2.43536300
H	-0.32806900	5.20976800	-0.81172200

b₅-TS1

Imaginary Frequency: -17.8668

C	1.93679000	1.56459000	1.29401600
O	0.71629000	1.86429100	1.39225300
O	-1.68634900	-0.40661400	-1.05823600
O	-1.47830000	-1.99978300	0.84019800
C	-3.90048600	-1.06932500	0.25912100
C	2.32232200	0.25362100	0.83533100
C	3.52062100	-0.19917300	0.16876200
C	1.45872400	-0.85894300	0.90267600
C	3.30569500	-1.56805300	-0.14275700
C	4.72385700	0.40731400	-0.23445800
H	0.54034200	-0.99561800	1.46972400
C	4.25623200	-2.34734900	-0.81014700
C	5.67166800	-0.36287100	-0.89465600
H	4.91562200	1.45661500	-0.03784600
C	5.44242800	-1.72517000	-1.17796500
H	4.07456600	-3.39257100	-1.03822500
H	6.60754500	0.09261800	-1.20414000
H	6.20467500	-2.29654100	-1.69912700
N	2.04795300	-1.93455700	0.32345500
C	2.94116500	2.62314900	1.64293100
H	3.18169900	3.18025700	0.72707600
H	2.49328000	3.32705900	2.34819300
H	3.86292700	2.20251000	2.05226800
C	1.49015100	-3.28314800	0.25918000
H	0.45521600	-3.25067900	0.60022900
H	1.50852600	-3.63457800	-0.77641600

H	2.07718700	-3.96434400	0.88379700
Pd	-0.51555100	0.73850100	0.17758200
C	-1.80625500	4.43438100	-1.32536700
O	0.24563900	3.14766000	-1.26750800
F	-3.71538200	-0.07168700	1.13098800
F	-4.65243300	-0.63642200	-0.75226300
F	-4.52660400	-2.07597300	0.87590400
O	-1.62137600	2.33939400	-0.27682600
O	-2.53829100	-2.72460600	-1.34020900
S	-2.25569600	-1.66655800	-0.37772100
C	-0.93432000	3.23975100	-0.95387300
H	-1.17847100	5.21667300	-1.75608600
H	-2.55838400	4.12255100	-2.05768000
H	-2.33660100	4.81320200	-0.44698300

b₅-IN2

C	1.95354900	1.64327000	1.27814200
O	0.73560500	1.94974600	1.36500000
O	-1.53976600	-0.52141100	-1.01533400
O	-1.48593500	-2.01391200	0.98273500
C	-3.84418000	-1.06603900	0.20177000
C	2.32278100	0.31749300	0.83770200
C	3.49600400	-0.14661400	0.14027500
C	1.45475500	-0.79225400	0.94741200
C	3.26858500	-1.51980800	-0.14469900
C	4.68657300	0.45377700	-0.30985700
H	0.56842200	-0.92489900	1.56530200
C	4.19720600	-2.30895100	-0.83307400
C	5.61120100	-0.32636700	-0.98893900
H	4.88561000	1.50517300	-0.13223700
C	5.37051900	-1.69289200	-1.24664000
H	4.00696500	-3.35647100	-1.04240500
H	6.53755900	0.12260700	-1.33431900
H	6.11505100	-2.27174600	-1.78487800
N	2.02887200	-1.87844600	0.36603400
C	2.96944600	2.69566400	1.61088000
H	3.22351700	3.23402900	0.68757100
H	2.52792300	3.41752900	2.30187300
H	3.88378400	2.26958500	2.03141100
C	1.47456800	-3.23035000	0.34339500
H	0.46077600	-3.20057300	0.74274600
H	1.43427700	-3.58958100	-0.68894500
H	2.10098600	-3.90268700	0.93850700
Pd	-0.44839300	0.73389300	0.18017200

C	-2.10654300	4.28497300	-1.30446400
O	0.04112600	3.16428500	-1.31156500
F	-3.69378300	-0.03726100	1.04229400
F	-4.51615900	-0.66092100	-0.87567200
F	-4.53533800	-2.03212200	0.81490600
O	-1.71437900	2.22438800	-0.24057600
O	-2.42235400	-2.82949400	-1.22064500
S	-2.17639500	-1.72833300	-0.29582000
C	-1.13034700	3.16772600	-0.95372200
H	-1.55970100	5.10780300	-1.76870000
H	-2.85974300	3.90475600	-2.00262300
H	-2.63071500	4.63399000	-0.41010600

b₅-TS2

Imaginary Frequency: -1272.4776

C	1.71894900	1.59384500	1.48868700
O	0.52564200	1.98425200	1.30871500
O	-1.76727200	-0.65725400	-1.05204000
O	-0.61373200	-2.04067100	0.66471500
C	-3.21300700	-1.55920800	1.03971200
C	2.18499500	0.44174100	0.78496600
C	3.50965900	0.01041600	0.42120200
C	1.24873100	-0.28332000	-0.00002100
C	3.32647800	-0.94761300	-0.61350200
C	4.81798200	0.33082500	0.82594200
H	0.16808600	-1.09376800	0.45682600
C	4.40113800	-1.60736200	-1.22250300
C	5.88579400	-0.31487100	0.21691500
H	4.99794000	1.05846600	1.61050300
C	5.68023100	-1.27505600	-0.79527700
H	4.24749000	-2.34921200	-1.99931700
H	6.89975300	-0.08142700	0.52830900
H	6.53739700	-1.76476100	-1.24776900
N	1.96379900	-1.07759200	-0.85929800
C	2.58816800	2.41911200	2.39499200
H	3.36681700	2.91963900	1.80564400
H	1.98404500	3.17603600	2.89831300
H	3.08816600	1.78578400	3.13576200
C	1.39447800	-1.99481800	-1.84172900
H	0.40803500	-1.63604000	-2.13420000
H	2.03334900	-2.00719100	-2.72765700
H	1.31358400	-3.00827800	-1.43547600
Pd	-0.53086100	0.88232200	-0.09801800
C	-3.16203400	3.82103800	-1.45044900

O	-2.02933300	2.22771800	-0.10621900
F	-4.34633000	-1.29602500	0.39566100
F	-3.37077100	-2.63243900	1.81217200
F	-2.86653500	-0.51472900	1.79060800
O	-1.22417700	2.55904400	-2.17054700
S	-1.87510500	-1.90720100	-0.21792300
O	-2.24572200	-3.12323800	-0.92063600
C	-2.04062500	2.81025400	-1.28330200
H	-4.13111500	3.31542200	-1.38023500
H	-3.12222600	4.56632000	-0.64958000
H	-3.07278400	4.31058600	-2.42210200

b₅-IN3

C	-0.77197500	-1.45160300	-1.02034200
O	0.22834200	-0.63509600	-1.17813400
O	2.12442600	-2.78781400	0.56765400
O	2.77363700	-1.29254900	-1.34189500
C	3.54506200	-0.59502800	1.11007400
C	-1.93420500	-0.92548200	-0.44998900
C	-3.26361400	-1.38775000	-0.08488900
C	-1.85165300	0.45049500	-0.09766200
C	-3.91385300	-0.25471400	0.46725200
C	-3.96714300	-2.59576900	-0.15104400
H	1.78283600	-1.08689700	-1.30721600
C	-5.22247800	-0.29028300	0.94067200
C	-5.27971300	-2.64273400	0.31980500
H	-3.50711500	-3.49164200	-0.55583800
C	-5.90191900	-1.50667200	0.85827600
H	-5.69984100	0.59012800	1.35957100
H	-5.82896900	-3.57851800	0.27018200
H	-6.92432200	-1.57270100	1.21835300
N	-3.01913000	0.83878700	0.44043000
C	-0.56496000	-2.86919200	-1.45302900
H	-1.50270700	-3.42466100	-1.49811200
H	-0.08313100	-2.88979800	-2.43629000
H	0.11373200	-3.35986200	-0.74430900
C	-3.34646100	2.17170200	0.93113200
H	-2.48034100	2.81846200	0.79498600
H	-4.19823300	2.57517400	0.37350300
H	-3.60634100	2.12376200	1.99375500
Pd	-0.14513900	1.31368800	-0.49100500
C	1.36863400	4.98470900	-0.08195800
O	1.58895900	2.67229600	-0.78009500
F	3.95943800	-1.04947100	2.29324800

F	4.46869100	0.20731700	0.59077700
F	2.40409100	0.08660500	1.27643800
O	-0.32571000	3.27950600	0.11349700
S	3.24084200	-2.04791500	-0.01679300
O	4.52674800	-2.66537300	-0.27755500
C	0.87734600	3.57610200	-0.26389400
H	1.19854300	5.30939200	0.94927500
H	2.43036200	5.04601200	-0.32692100
H	0.80277200	5.65616400	-0.73741800

b₅⁺-IN1

C	-1.78892600	1.01909400	-1.56823800
O	-0.56620800	1.32268200	-1.65203300
O	1.63580700	-0.48075000	-1.22895600
O	1.25312600	-1.69643900	0.92354000
C	3.69886800	-1.73836900	-0.12984900
C	-2.38226300	0.22681000	-0.53257000
C	-3.79042000	-0.04640600	-0.25929500
C	-1.65816100	-0.54074100	0.38733300
C	-3.81197300	-0.96549400	0.82183300
C	-5.02106500	0.38976300	-0.77671800
H	-0.59126500	-0.67400000	0.49714300
C	-4.98964000	-1.45954700	1.38323100
C	-6.20278300	-0.09932500	-0.22508400
H	-5.06933800	1.10060200	-1.59335100
C	-6.19180000	-1.01468900	0.84110800
H	-4.97132600	-2.16148900	2.21124300
H	-7.15406500	0.23648300	-0.62785500
H	-7.13073300	-1.37661100	1.24933200
N	-2.49066700	-1.24665700	1.17587800
C	-2.64475600	1.55670500	-2.69235000
H	-3.27384000	2.37422200	-2.31802300
H	-1.99792200	1.94656700	-3.47984400
H	-3.30347800	0.78204200	-3.09605700
C	-2.06587000	-2.19354900	2.19989400
H	-0.97903600	-2.28210000	2.16013900
H	-2.37348100	-1.84537600	3.19143800
H	-2.51403900	-3.17331600	2.00831600
Pd	1.00802200	1.26108200	-0.32690700
C	2.36478700	3.83611800	2.31918000
O	2.47960700	1.77506800	1.04778000
F	4.34514800	-1.74341500	-1.29813800
F	4.03930200	-0.64262800	0.55354300
F	4.05498200	-2.81896700	0.57307700

O	0.72471500	3.02625200	0.72342400
O	1.60796200	-2.95713600	-1.24024900
S	1.86059500	-1.77568600	-0.42024600
C	1.83536000	2.83983200	1.33709000
H	1.53943200	4.37663600	2.78862100
H	2.97539500	3.33134100	3.07158000
H	2.99671200	4.55926700	1.79006100

b₅'-TS1

Imaginary Frequency: -820.8557

C	1.93847300	1.09243800	1.85243900
O	0.82447100	1.69057200	1.85075400
O	-2.28964600	0.00118400	1.40471900
O	-0.69421200	-1.82680000	0.83831700
C	-3.09813500	-1.93015900	-0.21758300
C	2.20212700	0.18386800	0.77195000
C	3.39205000	-0.34118700	0.17883900
C	1.09560400	-0.16250500	-0.05587000
C	2.96630900	-0.97306900	-1.02934700
C	4.76348200	-0.34148200	0.50376500
H	0.08985100	-0.79513000	0.43416500
C	3.86610700	-1.62018400	-1.88954600
C	5.65111600	-0.97338700	-0.35180000
H	5.12108000	0.13233700	1.41235800
C	5.20646700	-1.60763100	-1.53546700
H	3.52916200	-2.10380700	-2.80061400
H	6.70970600	-0.98860700	-0.11020600
H	5.93250700	-2.09369900	-2.18043600
N	1.59785100	-0.83433100	-1.14736000
C	2.91204100	1.38899500	2.95386600
H	3.77337100	1.93559000	2.54843700
H	2.43189600	2.00155500	3.71898600
H	3.28749800	0.46015200	3.39682400
C	0.78397300	-1.44439200	-2.19275800
H	-0.26667800	-1.28712500	-1.95490400
H	1.00914500	-0.98245200	-3.15922300
H	0.98464100	-2.51890900	-2.24537400
Pd	-0.21817400	1.48013900	0.06234900
C	-2.99329000	3.17532400	-2.18846700
O	-1.30965200	1.51870300	-1.66914400
F	-4.38449700	-1.61295800	-0.04911500
F	-2.63588200	-1.26469200	-1.29699200
F	-2.99931500	-3.24094100	-0.45890600
O	-1.50714600	3.19072100	-0.27231100

O	-2.60429400	-2.31989400	2.36123700
S	-2.11784000	-1.45677500	1.29051600
C	-1.88837600	2.62495100	-1.34039200
H	-3.05643900	4.25887300	-2.06507900
H	-2.83416300	2.91387400	-3.23766900
H	-3.94169500	2.73159300	-1.86326800

b₅'-IN2

C	-2.34755900	-1.68647200	1.40152000
O	-1.28031500	-2.38721800	1.29446800
O	3.60225100	0.02366000	0.58413500
O	1.38416800	0.66512000	1.60504600
C	2.59295100	2.44456700	0.04383800
C	-2.51950100	-0.60467400	0.51269500
C	-3.50715800	0.41630400	0.23387200
C	-1.46140800	-0.43870500	-0.40799900
C	-2.98329500	1.15343900	-0.86135700
C	-4.74742300	0.78970100	0.76646700
H	1.09167600	-0.07531300	1.01249600
C	-3.65411600	2.23544400	-1.42757700
C	-5.42544900	1.87093700	0.20472200
H	-5.17882100	0.25080600	1.60496500
C	-4.88773000	2.58568300	-0.87782300
H	-3.23702800	2.78883700	-2.26338400
H	-6.38762100	2.16715100	0.61288000
H	-5.43810800	3.42438300	-1.29393900
N	-1.73839100	0.59968300	-1.22318900
C	-3.33264700	-2.07375000	2.46668100
H	-4.31378800	-2.27537600	2.02066400
H	-2.98367200	-2.96069800	2.99840300
H	-3.46024700	-1.24915900	3.17847600
C	-0.90952600	1.08876600	-2.31707400
H	-0.03375700	0.44687000	-2.40738300
H	-1.47836000	1.06670700	-3.25241700
H	-0.58750000	2.11588000	-2.11804600
Pd	-0.01067500	-1.74518600	-0.22223200
C	3.54184500	-2.35772000	-1.92595500
O	1.41683400	-1.25343700	-1.62344700
F	3.76378600	2.91008900	-0.38690200
F	1.90598600	1.94575100	-0.99020400
F	1.89574000	3.42938500	0.60322900
O	1.81869600	-2.99357600	-0.34376000
O	3.43632300	1.72660600	2.48019800
S	2.90946100	1.09308100	1.28903800

C	2.20305400	-2.22258200	-1.26478800
H	3.90571200	-3.38290300	-1.83084300
H	3.48414000	-2.06318200	-2.97700800
H	4.24032400	-1.68440900	-1.41604900

H	0.46014500	-4.11295300	2.99843400
H	-1.29470400	-4.01050200	2.62266200
H	-0.20923400	-4.97382100	1.59748300

b₅''-TS1

Imaginary Frequency: -94.2050

C	-2.06065900	-0.73709400	-2.21875300
O	-0.97637000	-1.24379700	-2.50956700
O	1.76613400	0.18345600	-0.97184400
O	2.59266300	2.50273300	-0.68031300
C	4.18956900	0.47814800	0.03002400
C	-2.14504500	0.26573700	-1.14299900
C	-3.20702200	0.59456900	-0.22827000
C	-1.11374800	1.18962400	-0.90346200
C	-2.74631400	1.70182500	0.53851400
C	-4.47583400	0.05342600	0.05381300
H	-0.22525500	1.37583600	-1.49173600
C	-3.50969100	2.27279300	1.56293200
C	-5.24169100	0.62808600	1.05780900
H	-4.85438800	-0.79830900	-0.50191400
C	-4.76306100	1.72497300	1.80565700
H	-3.13832400	3.10793800	2.14817500
H	-6.22529400	0.22416800	1.27886900
H	-5.38492500	2.14559600	2.59055700
N	-1.48418600	2.05273300	0.08775500
C	-3.31698400	-1.13077200	-2.96622700
H	-3.86352600	-1.87597000	-2.37288800
H	-3.98533300	-0.28042100	-3.13088900
H	-3.03908900	-1.59188700	-3.91628900
C	-0.67683000	3.15113000	0.60806300
H	-1.27364000	4.06797100	0.62803600
H	-0.31793700	2.91666300	1.61431800
H	0.19072200	3.29480800	-0.03680900
Pd	0.26455000	-0.95233900	-0.17758400
C	-0.28715000	-4.06296700	2.20286100
O	-0.99511400	-2.27942400	0.72178400
O	1.14113600	-2.41794300	1.13946000
F	4.71656600	0.44382500	-1.19522200
F	4.95349300	1.24155700	0.81714200
F	4.14662500	-0.75969200	0.52701700
O	1.94181500	1.12711400	1.33693300
S	2.47247600	1.19408500	-0.03149100
C	-0.02738700	-2.87353500	1.33310000

b₅''-IN2

C	-2.05129500	0.29224200	2.28924900
O	-1.48581900	0.12977500	3.35808100
O	1.51498700	-0.00801700	0.97715000
O	2.78111800	-2.12659300	0.82871600
C	3.78263700	0.03883000	-0.37994800
C	-1.58821000	-0.47899500	1.07159700
C	-2.37221100	-0.85654200	-0.12902000
C	-0.74061500	-1.61703800	1.30208600
C	-1.88756300	-2.11194900	-0.55391300
C	-3.38702700	-0.24576100	-0.87396700
H	-0.05301200	-1.75085800	2.12433200
C	-2.35497800	-2.77196500	-1.68517400
C	-3.87925000	-0.90276400	-2.00290400
H	-3.76850900	0.73036900	-0.60071300
C	-3.37102900	-2.14580400	-2.40785200
H	-1.95054200	-3.72943100	-1.99670600
H	-4.66775900	-0.43567700	-2.58577600
H	-3.76862700	-2.62664400	-3.29637900
N	-0.89431500	-2.53232600	0.35779500
C	-3.22900100	1.23265500	2.14011000
H	-3.03775900	1.97586300	1.35876300
H	-4.12819500	0.67242300	1.85517400
H	-3.40137300	1.73052700	3.09633500
C	-0.09439300	-3.74401600	0.19257100
H	-0.75074200	-4.61876600	0.19689200
H	0.45119700	-3.67825600	-0.75178100
H	0.62930700	-3.80426900	1.00458300
Pd	-0.14933800	0.99591500	0.26990200
C	-0.91044200	4.45973800	-1.52500200
O	-1.51648900	2.36469000	-0.47336800
O	0.62159000	2.79410700	-0.65940100
F	4.44633500	0.38433200	0.72452200
F	4.58703300	-0.68042700	-1.16939700
F	3.40264100	1.14133900	-1.03000400
O	1.58231400	-1.23772900	-1.20537400
S	2.28798700	-0.97942400	0.05933000
C	-0.57439500	3.15438300	-0.86870000
H	-0.06311600	4.80899300	-2.11885400
H	-1.79978500	4.34998200	-2.15122800

H	-1.12818600	5.20557200	-0.75132400
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b₅''-TS2

Imaginary Frequency: -1104.0201			
C	-1.16722400	0.21063100	2.24037400
O	0.02915600	0.46528100	2.33696000
O	1.94232800	-0.43340600	-1.27801500
O	0.78343100	-2.13117200	0.11288000
C	3.27089900	-1.44149500	0.82802600
C	-1.75297300	-0.15287400	0.93034200
C	-3.08297500	-0.54502000	0.57679200
C	-0.95624200	-0.20749500	-0.24177100
C	-3.06386800	-0.79480900	-0.83064300
C	-4.30141000	-0.73022900	1.27232800
H	-0.01203500	-1.22216100	0.00785900
C	-4.20273100	-1.21785900	-1.53846200
C	-5.42357100	-1.13521900	0.57242500
H	-4.36680100	-0.55448300	2.33952000
C	-5.37562900	-1.37792000	-0.82181700
H	-4.16590100	-1.40540700	-2.60682900
H	-6.36286000	-1.27217400	1.10028000
H	-6.27787100	-1.69551200	-1.33668000
N	-1.79395900	-0.57641400	-1.29603400
C	-2.06009100	0.26518300	3.46591500
H	-2.88669500	0.96988900	3.31654700
H	-2.49660800	-0.71896500	3.67490100
H	-1.46172800	0.58244300	4.32198500
C	-1.38194700	-0.76791000	-2.67866800
H	-1.62203700	-1.78371700	-3.01101900
H	-1.88711500	-0.04814000	-3.33213200
H	-0.30539700	-0.61305600	-2.75032800
Pd	0.61070200	1.08827500	-0.57625600
C	0.63556800	5.01859900	-0.05366000
O	-0.38006400	2.82815600	-0.09461400
O	1.71517300	2.95465200	-0.72989200
S	2.10257300	-1.76582900	-0.59255100
O	2.67538900	-2.83190000	-1.39305500
F	4.46415800	-1.12436400	0.32901500
F	2.81016000	-0.43863100	1.56852600
F	3.37104500	-2.54343500	1.56878700
C	0.67005000	3.54190200	-0.31706800
H	1.39472200	5.52328900	-0.65539100
H	-0.35778000	5.42029300	-0.26956700
H	0.85362400	5.19727000	1.00590300

b₅-TS2'

Imaginary Frequency: -1277.9105			
C	1.72204000	2.07416400	0.70158200
O	0.55678700	2.36856100	0.30121200
O	-1.62809900	-0.90827200	-1.14843600
O	-0.56842100	-1.74399800	0.94100900
C	-3.23988200	-1.61489300	0.91255300
C	2.22340000	0.75411000	0.48239300
C	3.57195100	0.25557600	0.39057900
C	1.34741600	-0.21890700	-0.06602400
C	3.46748600	-1.00541600	-0.25576100
C	4.84573800	0.72874500	0.75344000
H	0.21982800	-0.87668500	0.52954700
C	4.58471000	-1.80820400	-0.51766100
C	5.95633300	-0.06151400	0.48780800
H	4.96641400	1.68676000	1.24820100
C	5.82795100	-1.31749400	-0.13970100
H	4.49087200	-2.77799600	-0.99526200
H	6.94329300	0.29025900	0.77379200
H	6.71606800	-1.91332400	-0.32818100
N	2.12630500	-1.24484300	-0.54045600
C	2.52955600	3.17408700	1.33069300
H	3.36325400	3.44701600	0.67162000
H	1.89821500	4.05035200	1.48762800
H	2.95423200	2.84417100	2.28488000
C	1.63981800	-2.46159600	-1.18402000
H	0.70807300	-2.24630200	-1.70620200
H	2.37652400	-2.78992400	-1.92024500
H	1.47298600	-3.25895000	-0.45336300
Pd	-0.46240900	0.82260100	-0.60095500
C	-3.63730700	3.59377500	-0.86681400
O	-1.88966700	2.05754500	-1.26040000
F	-4.28684300	-1.66251800	0.09159800
F	-3.36291400	-2.54895600	1.85470000
F	-3.14537400	-0.41719400	1.46637000
O	-2.53823100	2.33381900	0.88266200
S	-1.69967000	-1.97850000	-0.08433800
O	-1.80576200	-3.34557600	-0.56773400
C	-2.63173700	2.59313400	-0.31030400
H	-4.29417400	3.93407700	-0.06390100
H	-3.10791500	4.45078500	-1.29728400
H	-4.22778600	3.13799700	-1.66780200

b₅-TS2''

Imaginary Frequency: -1285.6414			
C	1.94024700	2.12964300	0.53672000
O	0.80874500	2.55292700	0.15898400
O	-1.96044400	-0.47554000	-0.75230400
O	-0.79069000	-1.31952000	1.25817000
C	-2.64777000	-2.88385300	0.12703500
C	2.24714100	0.73977700	0.40170000
C	3.51408100	0.06489800	0.27690700
C	1.22148800	-0.14507100	-0.02549300
C	3.21202700	-1.21085700	-0.26970600
C	4.85807000	0.38952500	0.53577300
H	0.06912400	-0.61576800	0.68925800
C	4.19912300	-2.16823200	-0.53475500
C	5.84048100	-0.55491200	0.26824600
H	5.13060500	1.35291400	0.95367400
C	5.51570400	-1.82113200	-0.26043900
H	3.95170000	-3.14514100	-0.93742800
H	6.87992400	-0.31759200	0.47533600
H	6.30809300	-2.53818400	-0.45349800
N	1.83775100	-1.29141700	-0.46307900
C	2.92073500	3.14912400	1.04437800
H	3.74661000	3.25873500	0.33034500
H	2.42161400	4.11260600	1.16117100
H	3.34799800	2.83143500	2.00148800
C	1.16529300	-2.46729200	-0.99812500
H	0.19213300	-2.17338600	-1.38512100
H	1.76090100	-2.87304100	-1.81987100
H	1.03592000	-3.23588400	-0.22952100
Pd	-0.47817100	1.09398200	-0.53136500
C	-3.42482300	4.09042200	-0.57062000
O	-2.28971300	2.70816000	1.06112900
F	-3.82376700	-2.85110100	-0.49189100
F	-1.73657500	-3.42917900	-0.68657800
F	-2.73785400	-3.61515400	1.23478600
O	-1.79150600	2.47540400	-1.12390900
O	-3.22565700	-0.65611200	1.46054000
S	-2.17224300	-1.13785700	0.59052700
C	-2.44366400	3.01996500	-0.11276500
H	-3.94008600	4.50480900	0.29796300
H	-2.89378100	4.88556800	-1.10430700
H	-4.15417900	3.65973400	-1.26448200

Pd(TFA)(OTf)_{catalyst}

Pd(TFA)(OTf)

O	1.95642400	-0.02921100	1.09282000
C	2.59341100	0.07661500	0.00001200
O	1.95625300	-0.02927900	-1.09269300
C	4.11457900	0.28314900	-0.00007600
Pd	0.20913400	-0.35037000	0.00007600
C	-3.28059700	0.95031600	-0.00003000
O	-1.48947900	-0.68190400	-1.19228800
O	-1.48969900	-0.68193500	1.19230400
O	-3.49372200	-1.72976700	-0.00019700
F	-4.03331900	1.05479700	1.08954900
F	-4.03345500	1.05483600	-1.08948900
F	-2.34829900	1.90224400	-0.00007900
S	-2.45234100	-0.72669800	-0.00002800
F	4.48897200	0.95848000	1.09000200
F	4.48914400	0.95675200	-1.09114300
F	4.71859200	-0.91594700	0.00093100

Pd(TFA)(OTf)

a₆-IN1

C	1.63379700	0.25944400	2.20103600
O	0.42583400	-0.09664100	2.30928900
O	-2.72897900	-0.79600600	-0.27101500
C	-3.14810200	0.31135600	0.17483700
O	-2.45338600	0.96360900	1.01409800
C	-4.47988100	0.89863300	-0.31377200
C	2.14946300	1.14218300	1.19892400
C	1.48697100	2.07437100	0.29925200
C	3.49700100	1.14807700	0.83227100
C	2.49012500	2.57243600	-0.56871600
C	0.18853900	2.59261200	0.18813300
H	4.30784400	0.54966700	1.22279400
C	2.23720200	3.52196500	-1.55962700
C	-0.07603300	3.53549700	-0.80231800
H	-0.59993500	2.28324800	0.86170600
C	0.93096200	3.99021000	-1.67186600
H	3.02320500	3.88724600	-2.21354800
H	-1.08335400	3.92968000	-0.90018400
H	0.69094400	4.72577400	-2.43388000
N	3.70269900	1.97094500	-0.21876400
C	2.55750000	-0.33459700	3.23905000
H	1.98874300	-0.52672100	4.15188300
H	2.90873800	-1.29969300	2.85308000
H	3.41519100	0.30331900	3.46285000

C	4.96475000	2.17837800	-0.91004200
H	4.87780000	1.87321500	-1.95767100
H	5.25385800	3.23359300	-0.86701200
H	5.73792200	1.57730900	-0.42867600
Pd	-0.99307200	-0.57304400	0.90411600
C	0.81112200	-2.25735900	-1.88183200
O	-0.13321300	-2.39162000	0.59611000
O	1.43056000	-4.14800500	-0.10608800
F	-0.19800600	-2.99363700	-2.34397700
F	0.47068700	-0.95766400	-1.95690300
F	1.89026500	-2.45851800	-2.64472700
F	-5.17544600	-0.00301400	-1.00892800
F	-5.21223500	1.30955400	0.73100600
F	-4.23129500	1.95980300	-1.10328100
O	2.29166600	-1.80035700	0.26627700
S	1.20158500	-2.70806300	-0.11808500

a₆-TS1

Imaginary Frequency: -59.7414

C	2.29535600	-0.34457400	-1.95185100
O	1.16738400	0.09346400	-2.30219000
O	-2.16370600	0.40841500	0.02505800
C	-2.97131800	-0.46434300	-0.47260400
O	-2.70423100	-1.20394400	-1.42452200
C	-4.32344000	-0.60691300	0.25583700
C	2.45051200	-1.28516400	-0.88001200
C	1.41031500	-2.07757000	-0.26052000
C	3.58661100	-1.45223600	-0.09415900
C	1.97795900	-2.65899200	0.89690200
C	0.07625100	-2.37484100	-0.59269200
H	4.55925600	-0.99037300	-0.19320400
C	1.24487100	-3.47703300	1.75903200
C	-0.67109600	-3.16932300	0.27997100
H	-0.34835100	-2.11269200	-1.56434600
C	-0.09333100	-3.70731800	1.44257200
H	1.69129000	-3.91515900	2.64649000
H	-1.70919300	-3.37700600	0.04310800
H	-0.69563400	-4.32696600	2.09965600
N	3.31394900	-2.25486700	0.96499800
C	3.48351200	0.20365600	-2.69458800
H	3.19403900	0.43605000	-3.72225500
H	3.76235600	1.14572200	-2.20517200
H	4.33743500	-0.47745700	-2.68883700
C	4.23320800	-2.59702700	2.03920500

H	3.85553500	-2.22229600	2.99589200
H	4.35888700	-3.68277800	2.10256000
H	5.20277800	-2.13883500	1.83748100
Pd	-0.49459200	0.20028200	-1.06679600
C	0.37159300	2.67792500	1.71937400
O	-0.11660500	2.21304400	-0.84797300
O	1.34171700	4.11853000	-0.30731000
F	-0.71501500	3.44314300	1.79763400
F	0.04777400	1.41855100	2.05138800
F	1.28890900	3.12540000	2.58492600
F	-4.61670800	0.46102600	1.00581800
F	-5.31294200	-0.79803700	-0.62736600
F	-4.26609000	-1.68988500	1.06302200
O	2.20152200	1.76338100	0.03731000
S	1.07982300	2.71565700	-0.00214500

a₆-IN2

C	2.66543800	0.49323300	-1.59174300
O	1.50367400	0.64102800	-2.03918800
O	-1.87385600	-0.47548800	-0.00328000
C	-2.57673200	-1.37646300	-0.61333300
O	-2.30171700	-1.97704600	-1.64401300
C	-3.86554800	-1.73083200	0.17219300
C	2.95069100	-0.52110300	-0.60894200
C	2.06814900	-1.60760500	-0.25817100
C	3.98994900	-0.54845800	0.31391700
C	2.61246800	-2.21704700	0.89605500
C	0.87316900	-2.12215300	-0.81641100
H	4.83385600	0.12039000	0.41417600
C	1.98770400	-3.28939100	1.53434400
C	0.23836400	-3.18993800	-0.16078400
H	0.57208500	-1.90273300	-1.85066800
C	0.78460100	-3.75510300	0.99943600
H	2.41265500	-3.74717100	2.42264300
H	-0.68257000	-3.57947600	-0.57952700
H	0.27223800	-4.57997100	1.48396400
N	3.79447700	-1.54576400	1.21564500
C	3.71856900	1.44553800	-2.08313300
H	3.51744700	1.70454400	-3.12560800
H	3.61844200	2.36459800	-1.49066700
H	4.73222200	1.05141500	-1.98096500
C	4.63561900	-1.83772300	2.36697700
H	4.07052200	-1.70365700	3.29483700
H	5.00818000	-2.86586100	2.31669800

H	5.48534600	-1.15322300	2.36846400
Pd	-0.19680900	-0.00547000	-0.98129900
C	-0.98942000	2.89032000	1.52570900
O	-0.80138000	1.96287700	-0.94945000
O	-0.11655600	4.30374100	-0.56272300
F	-2.25675200	3.23166300	1.29613700
F	-0.95243400	1.65784400	2.04847200
F	-0.45696600	3.74671500	2.40655400
F	-4.42960800	-0.65838200	0.74478700
F	-4.76864800	-2.30782800	-0.63011600
F	-3.55282600	-2.61327000	1.15056300
O	1.32481200	2.41966100	0.32144400
S	-0.00196300	2.94091200	-0.05185500

Pd	0.18922700	-0.14379700	-0.36323500
C	3.50550700	-1.56536400	1.15659500
O	1.92601900	-1.14896900	-0.90379000
O	3.04938200	-3.35705100	-0.75920600
F	4.54444800	-1.05511700	0.49013800
F	2.90336500	-0.57790200	1.83954200
F	3.95398000	-2.47537700	2.02958100
F	2.95284000	3.60870000	-0.47433200
F	1.46136500	4.55597800	-1.74051400
F	1.24884000	4.62433300	0.42888900
O	1.16905900	-2.77517200	0.83775900
S	2.29295000	-2.35506200	-0.01265200

a₆-IN3

C	-2.38117200	-1.95724800	-0.68117300
O	-1.15955000	-1.69082800	-0.81021900
O	1.09981100	1.75090800	-0.15181400
C	2.30364600	1.89814500	-0.40015800
O	3.14463800	1.03414200	-0.84557400
C	2.92986300	3.28505100	-0.13624900
C	-3.31481800	-0.96071300	-0.26958700
C	-2.95000500	0.40699700	0.00807500
C	-4.69316200	-1.05149500	-0.08270900
C	-4.14045500	1.08591700	0.35018100
C	-1.72272700	1.07771000	-0.00738000
H	-5.35378700	-1.90089200	-0.19073900
C	-4.15208300	2.44265900	0.67905600
C	-1.72345300	2.43483300	0.31766600
H	2.70057100	0.08742700	-0.93529600
C	-2.92296100	3.09820500	0.65337600
H	-5.06526300	2.96757300	0.94194500
H	-0.79594800	2.99578500	0.31998900
H	-2.88241300	4.15523100	0.90194800
N	-5.18815100	0.15810500	0.28423500
C	-2.79241100	-3.36747300	-1.02244100
H	-2.94281300	-3.44523000	-2.10650500
H	-1.98159800	-4.04790800	-0.75133800
H	-3.71719700	-3.66551500	-0.52168300
C	-6.58062400	0.46024200	0.57324200
H	-6.68749100	0.81353200	1.60405800
H	-6.95162700	1.23288500	-0.10803800
H	-7.17808200	-0.44404000	0.44395800
Pd	-0.10758000	0.02967500	-0.45191000
C	2.25444600	-2.08760700	1.43600800

a₆-TS2

Imaginary Frequency: -1246.9895

C	-2.04509900	-1.91858200	-1.40774500
O	-0.81813200	-1.71944400	-1.27106300
O	1.30602800	1.58152000	-0.00110600
C	0.80980800	2.56819700	-0.61025400
O	-0.32946600	2.63249200	-1.14882300
C	1.65097200	3.86394600	-0.61136100
C	-3.02741000	-1.11794700	-0.72982200
C	-2.74485000	0.01727700	0.11200600
C	-4.36756600	-1.44308600	-0.51991000
C	-3.92766600	0.27800100	0.84239600
C	-1.57924800	0.78876800	0.32942500
H	-4.95716300	-2.24256800	-0.94718800
C	-3.98352600	1.23584200	1.85576700
C	-1.63629000	1.70421200	1.40239300
H	-0.99197900	1.54323600	-0.62919200
C	-2.80823300	1.92844900	2.14098700
H	-4.89510400	1.42763300	2.41366700
H	-0.76151300	2.30530200	1.62985300
H	-2.80276500	2.66687900	2.93672500
N	-4.90913300	-0.61667600	0.40828400
C	-2.44182600	-3.10212300	-2.25748200
H	-1.73188200	-3.20025500	-3.08213500
H	-2.36874300	-4.01402800	-1.65215400
H	-3.45717200	-3.01721400	-2.65236000
C	-6.27176200	-0.67308900	0.91642500
H	-6.26835100	-0.87522600	1.99229500
H	-6.78787100	0.27404600	0.73035200
H	-6.80868800	-1.47497800	0.40696900

O	1.79487500	-1.07481700	-0.94953700
O	3.72510100	-2.60480100	-0.70977600
F	2.91560100	-0.94894700	1.70557500
F	0.98580000	-1.94431000	1.85524600
F	2.81884000	-3.08778700	2.11327600
F	1.97684100	4.20130600	0.06889600
F	3.70768300	3.22052800	0.95576400
F	3.67901700	3.66674800	-1.17792700
O	1.36156900	-3.51988000	-0.61966400
S	2.30945600	-2.43360200	-0.39389500

a₆-IN1'

C	-1.50131600	-0.47514200	2.21099200
O	-0.23808900	-0.50449500	2.13869000
O	2.63499200	0.04880000	-0.76943900
C	3.29168800	-0.66564100	0.04471700
O	2.73583200	-1.10635900	1.09707400
C	4.74817000	-1.04256800	-0.26211700
C	-2.35713500	-0.98475000	1.18688500
C	-2.06231300	-1.92171600	0.11611600
C	-3.65499300	-0.52323400	0.95179500
C	-3.20893200	-1.95429900	-0.71156800
C	-0.98884800	-2.77391400	-0.18002200
H	-4.21690600	0.22853200	1.48833600
C	-3.30606700	-2.77139700	-1.83856400
C	-1.07464400	-3.59139800	-1.30432800
H	-0.11276300	-2.80906300	0.45912000
C	-2.21441600	-3.58569400	-2.12830400
H	-4.19310600	-2.77852600	-2.46441600
H	-0.24577400	-4.24936500	-1.54850300
H	-2.24852500	-4.23299500	-2.99955900
N	-4.15493900	-1.07424300	-0.17460500
C	-2.06049900	0.15318700	3.46181500
H	-1.95767600	1.24001100	3.35878900
H	-3.10475300	-0.11073300	3.64107400
H	-1.45146500	-0.15694400	4.31598400
C	-5.42012600	-0.72931000	-0.80327600
H	-5.24127800	-0.23040100	-1.76086500
H	-6.01852200	-1.63072400	-0.96874700
H	-5.97017100	-0.05212900	-0.14798200
Pd	0.95770800	-0.14114600	0.50061000
C	-0.00106600	3.37429700	-0.96492300
O	-1.01480800	2.41601700	1.29985400
O	-2.44234500	2.29642400	-0.78424500

F	-0.40855100	4.61723900	-0.69324900
F	1.24471300	3.21211500	-0.50053800
F	-0.00242700	3.18982700	-2.28562800
F	5.45541000	-1.13973300	0.86974900
F	4.77267700	-2.23473500	-0.88657300
F	5.31591500	-0.13090900	-1.05737500
O	-0.49583600	0.80875500	-0.56232600
S	-1.13648000	2.15292800	-0.13929200

a₆-TS1'

Imaginary Frequency: -58.2448

C	-1.70121800	1.24591700	-1.61818500
O	-1.09376600	0.15778600	-1.81034000
O	1.88731300	-1.42078900	0.46880200
C	2.91738600	-1.32643100	-0.29961600
O	2.89664800	-0.84933600	-1.43928400
C	4.25590500	-1.77721500	0.31894300
C	-1.13122900	2.31720700	-0.85608100
C	0.25720100	2.47226200	-0.48013600
C	-1.83821800	3.27431400	-0.13302100
C	0.30452300	3.50548000	0.48381300
C	1.45600600	1.86451700	-0.89416200
H	-2.90439800	3.44843200	-0.09050400
C	1.49642800	3.90998500	1.08771700
C	2.64882500	2.24441400	-0.27316100
H	1.49759500	1.20604800	-1.76420400
C	2.66465300	3.24956500	0.70834300
H	1.51970000	4.70199200	1.82996600
H	3.57312900	1.75715200	-0.56519700
H	3.60654400	3.52898900	1.17009000
N	-0.99909300	3.97391900	0.66976200
C	-3.07233300	1.34994500	-2.23046200
H	-3.72122600	0.62363800	-1.73078800
H	-3.49756400	2.35232500	-2.15500800
H	-3.01194800	1.06220700	-3.28516000
C	-1.38641200	4.99680500	1.62906500
H	-1.13669100	4.67696000	2.64567600
H	-0.87213800	5.93828800	1.41071900
H	-2.46368700	5.15724200	1.56289100
Pd	0.42145200	-0.58407100	-0.61195100
C	-3.50667400	-2.22470000	0.21597800
O	-2.35508700	0.04951000	0.95720300
O	-2.10836500	-1.96574400	2.46312700
F	-4.66241200	-1.93327200	0.82382100

F	-3.56964000	-1.77633600	-1.05090900
F	-3.34260100	-3.54619300	0.19577600
F	4.99135200	-2.43683400	-0.58647000
F	4.94475000	-0.67648600	0.69772000
F	4.08920000	-2.55840100	1.39064900
O	-0.91461200	-1.89430300	0.27376100
S	-2.10777400	-1.39282100	1.12107900

a₆-IN2'

C	-1.77085100	1.71951800	-1.29310200
O	-1.38098000	0.56720900	-1.59950200
O	1.68520800	-1.31997500	0.35549800
C	2.66828500	-1.64492600	-0.42317300
O	2.80235700	-1.38730200	-1.61253500
C	3.80569000	-2.36473800	0.34529400
C	-0.88861200	2.62992700	-0.61012400
C	0.53940400	2.45787300	-0.49823500
C	-1.22393500	3.67661200	0.24146900
C	0.98960600	3.40015000	0.45523800
C	1.47480900	1.59717400	-1.12410700
H	-2.19796900	4.08514400	0.47346300
C	2.32856000	3.48565600	0.83720400
C	2.82009700	1.67702800	-0.72243300
H	1.24451900	1.07544100	-2.06121400
C	3.23316400	2.59804100	0.24830400
H	2.66390200	4.20912900	1.57429900
H	3.53951800	1.01270200	-1.18765200
H	4.27793800	2.63485500	0.53930100
N	-0.11820300	4.13477200	0.88390000
C	-3.18651100	2.08079300	-1.64526500
H	-3.84854800	1.45850900	-1.03316300
H	-3.40984800	3.13782900	-1.48806000
H	-3.37332500	1.81944500	-2.69164800
C	-0.08856500	5.16865300	1.90819300
H	0.25556200	4.75108600	2.85968500
H	0.57828900	5.98339100	1.60851200
H	-1.09597900	5.56638900	2.04023000
Pd	0.23354600	-0.35141000	-0.61012700
C	-3.68904300	-1.89971000	0.11229100
O	-2.24337800	0.03182200	1.21941500
O	-2.14047100	-2.28262600	2.23621300
F	-4.76115100	-1.68236200	0.88385000
F	-3.80792200	-1.14725000	-0.99607100
F	-3.65813400	-3.18382400	-0.24210800

F	4.53991100	-3.11464500	-0.48624700
F	4.61958100	-1.42760900	0.88933000
F	3.35188900	-3.14515800	1.33397500
O	-1.06887800	-1.83601300	0.02346300
S	-2.15067300	-1.43012900	1.05190700

a₆-TS2'

Imaginary Frequency: -1129.1855

C	1.97144000	-2.31405900	0.21056100
O	0.96026500	-2.05839400	-0.48215600
O	-1.12033100	1.47738700	-0.80427800
C	-1.00457100	2.13526000	0.26856400
O	-0.11705400	1.99390100	1.14883900
C	-2.01127100	3.29092300	0.46275000
C	2.97468900	-1.31537500	0.47089700
C	2.88709800	0.06078700	0.05752500
C	4.31265500	-1.54257300	0.79874700
C	4.20238100	0.57703500	0.08597400
C	1.79980800	0.86913700	-0.35323800
H	4.79541300	-2.45041400	1.13342200
C	4.50778500	1.85535800	-0.38260400
C	2.13998700	2.13184600	-0.88913100
H	0.84416500	1.19771900	0.50933200
C	3.45697900	2.61446600	-0.89942800
H	5.52039700	2.24703700	-0.36122600
H	1.34478600	2.78591600	-1.23447000
H	3.65866400	3.60701600	-1.29023800
N	5.04621000	-0.42385200	0.57615300
C	2.09882500	-3.73504900	0.69414500
H	1.22175700	-3.94516800	1.31700100
H	2.05656800	-4.41812100	-0.16028000
H	3.00692600	-3.91929400	1.27175300
C	6.48083100	-0.28396600	0.77886200
H	6.97500200	-0.03166000	-0.16473900
H	6.68821500	0.49981000	1.51424400
H	6.88208000	-1.22968500	1.14689700
Pd	0.03784900	-0.23780300	-0.76807400
C	-3.74583600	-1.03412400	0.32887500
O	-1.49831900	-2.18273600	1.13136500
O	-2.91935100	-3.39218300	-0.57904900
F	-4.51072200	-1.60944200	1.26335400
F	-3.29305000	0.13676400	0.81620600
F	-4.49061000	-0.78695400	-0.75078500
F	-3.16056900	3.05663000	-0.17183500

F	-2.26410100	3.49295200	1.75970200
F	-1.46106800	4.41558100	-0.04502800
O	-1.65324400	-1.36235100	-1.23570600
S	-2.31737200	-2.15312500	-0.09093800

a₆-IN3'

C	2.27078900	-2.39061400	-0.28475500
O	1.09442800	-2.00627600	-0.51002400
O	-0.72070500	1.73606100	-0.43718400
C	-1.66114600	2.18245800	0.23181900
O	-2.40550100	1.61524500	1.10616600
C	-2.01917100	3.66528800	-0.02835100
C	3.31956400	-1.45928200	-0.03194800
C	3.13447200	-0.02801900	-0.02406200
C	4.67582900	-1.68704100	0.19944700
C	4.40427200	0.54592000	0.20680700
C	2.00265300	0.77700900	-0.19413000
H	5.22248600	-2.61763300	0.26666400
C	4.59541000	1.92733900	0.26543000
C	2.18682100	2.16026900	-0.14707300
H	-2.27650600	0.57219000	1.26070800
C	3.46307300	2.71746900	0.08011300
H	5.57022700	2.37109500	0.44256800
H	1.34444500	2.82868700	-0.28290300
H	3.56202900	3.79911100	0.11230200
N	5.32321800	-0.50324100	0.34211000
C	2.49934100	-3.88089300	-0.32974800
H	1.70392800	-4.37761400	0.23335100
H	2.42552400	-4.22325600	-1.36869400
H	3.47233700	-4.17404000	0.07078200
C	6.74384400	-0.33085300	0.59816100
H	7.20861300	0.24471000	-0.20899900
H	6.89868700	0.19581500	1.54550200
H	7.21975500	-1.31152500	0.65499700
Pd	0.26299900	-0.12896500	-0.45869700
C	-4.11315800	-1.83744100	-0.04581300
O	-2.28189200	-0.83017000	1.59353900
O	-1.93616700	-3.16330000	0.75625700
F	-4.83469800	-2.35944800	0.94889900
F	-4.54452000	-0.59167200	-0.28790600
F	-4.27889400	-2.57764100	-1.14393400
F	-2.66546200	3.76225400	-1.20144900
F	-2.79355800	4.17177800	0.93337200
F	-0.89363400	4.39695500	-0.10169500

O	-1.69512800	-1.17007200	-0.78733500
S	-2.31693300	-1.79337900	0.43166700

a₆'-IN1

C	-0.61329200	-1.65742900	1.97174000
O	0.44893100	-1.08045800	1.61584800
O	2.63091100	-0.09924000	0.10219400
C	2.95386800	-1.27490000	-0.34295300
O	2.23971000	-2.16640700	-0.76768600
C	4.49305100	-1.47295900	-0.26372400
C	-1.77139300	-1.83086500	1.14207100
C	-1.89866500	-1.85868300	-0.30886900
C	-3.07271000	-1.91269700	1.64498100
C	-3.28521800	-1.92560000	-0.58454700
C	-0.98969400	-1.92564700	-1.37734700
H	0.08270100	-1.96930100	-1.21011900
C	-3.80098900	-1.99402800	-1.88017100
C	-1.49818700	-1.98748900	-2.67258800
C	-2.88204800	-2.00927600	-2.92482000
H	-4.86913300	-2.04170400	-2.06882400
H	-0.80545700	-2.03139500	-3.50779800
H	-3.23988300	-2.05688700	-3.94910400
N	-3.97030500	-1.94364500	0.63408400
C	-0.58251200	-2.22733100	3.37212800
H	-1.57602300	-2.44810300	3.76764200
H	-0.02229900	-3.17056600	3.33933700
H	-0.04850900	-1.54651500	4.03963000
C	-5.41685500	-1.96650100	0.77310600
H	-5.85731300	-1.07869700	0.30804600
H	-5.83064400	-2.86128400	0.29662700
H	-5.67478700	-1.97801900	1.83363400
Pd	0.70130200	0.38839000	0.19325800
C	-0.42321200	3.93726100	0.45036700
O	-1.21085700	1.39039500	0.13920500
O	0.72404700	2.08012200	-1.11387500
F	-1.60413500	4.31937900	0.93827000
F	0.36465900	3.54525300	1.45328200
F	0.14595000	4.95255800	-0.19432900
F	4.89715400	-1.47346200	1.02301800
F	4.85433400	-2.63875800	-0.81364200
F	5.14398300	-0.48558900	-0.90521300
O	-1.54809400	3.01485300	-1.79437600
S	-0.68620500	2.52222000	-0.73793700
H	-3.41465500	-1.88517500	2.67027800

a₆'-TS1			
Imaginary Frequency: -88.5250			
C	-2.06440500	0.91584700	-1.51475700
O	-0.81707900	0.77161000	-1.50486000
O	1.11556400	1.80606300	0.54749900
C	0.10506200	2.43331300	0.92976400
O	-0.94466400	1.99681100	1.47290800
C	0.07722500	3.95973500	0.63228100
C	-2.92521200	0.02355300	-0.78101600
C	-2.48479600	-0.81668300	0.29106400
C	-4.22193100	-0.38802600	-1.09167100
C	-3.51639400	-1.74101600	0.55152500
C	-1.31062400	-0.78331600	1.08159300
H	-0.92028800	0.26913200	1.32407700
C	-3.37598700	-2.72750600	1.52745400
C	-1.16734400	-1.81328500	2.04135300
C	-2.17380100	-2.76268100	2.24901600
H	-4.16133700	-3.45005700	1.72916900
H	-0.27173700	-1.83773800	2.65407800
H	-2.03888900	-3.52817300	3.00677000
N	-4.57468800	-1.44574700	-0.31440000
C	-2.60259100	2.05979000	-2.32642000
H	-3.67496500	1.97774100	-2.51750200
H	-2.41514200	2.97215500	-1.74602400
H	-2.05050100	2.14672300	-3.26580600
C	-5.83319200	-2.17451300	-0.37836600
H	-5.65317000	-3.22351100	-0.63422400
H	-6.35235900	-2.12245900	0.58387300
H	-6.46609900	-1.72601700	-1.14587500
Pd	0.34554300	-0.46467800	-0.34748100
C	4.15987800	-0.73640900	0.09210400
O	2.16760600	-1.03446600	-1.70705800
O	1.69990200	-1.72201600	0.56528300
F	5.13807400	-0.72780400	-0.81571400
F	3.73839900	0.49941300	0.31279800
F	4.61092600	-1.27336900	1.22748200
F	-0.73829900	4.19594500	-0.44112400
F	-0.41770900	4.67119300	1.66225700
F	1.28321800	4.45886300	0.32658400
O	3.31520800	-3.11653500	-0.78733400
S	2.76312100	-1.79241200	-0.55709000
H	-4.89672800	-0.02650800	-1.85575400

a₆'-IN2			
C	-1.48283500	2.08395900	-0.12781200
O	-0.46305000	1.36261600	-0.29129100
O	2.30250500	2.39351200	-1.63195200
C	2.74621600	2.37589800	-0.51150000
O	3.09939800	1.32061600	0.21311500
C	2.94614200	3.66922400	0.30973800
C	-2.77579000	1.50359900	0.03577300
C	-3.01931000	0.08263600	0.01832200
C	-4.01483500	2.11248900	0.23694100
C	-4.40476700	-0.10428100	0.21151700
C	-2.17431300	-1.01529500	-0.14723800
H	2.87716900	0.48933100	-0.27447500
C	-4.98161300	-1.37588600	0.24640400
C	-2.73148300	-2.29141500	-0.11592200
C	-4.11947900	-2.45897300	0.07944000
H	-6.04677400	-1.52430500	0.39426500
H	-2.10017800	-3.16496400	-0.24413400
H	-4.52653700	-3.46612600	0.09848600
N	-4.98240400	1.16614800	0.34158500
C	-1.25773700	3.57419600	-0.14426100
H	-2.10218900	4.13384200	0.26439200
H	-0.35054500	3.80892900	0.41773700
H	-1.08902200	3.89395200	-1.17990000
C	-6.39975700	1.41271100	0.55370700
H	-6.98449600	1.00914700	-0.27928200
H	-6.73237600	0.94096700	1.48400900
H	-6.57079900	2.48867600	0.61976200
Pd	-0.26711800	-0.68177400	-0.42639900
C	2.45505100	-2.92427600	1.03019000
O	2.07800500	-1.02538000	-0.80777700
O	0.35719700	-2.72419300	-0.60627900
F	3.76072100	-2.66547400	1.12215000
F	1.79598200	-2.18148000	1.92593700
F	2.23711200	-4.21464700	1.28282200
F	1.96839300	3.76748300	1.24567600
F	4.12582700	3.68627000	0.94608200
F	2.86796200	4.74440300	-0.48010000
O	2.58855400	-3.38388100	-1.59975000
S	1.86510200	-2.51341000	-0.68953900
H	-4.26942300	3.16084500	0.31158200
a₆'-IN3			
C	-2.08930600	2.18384500	0.08910200

O	-0.84666100	2.10161900	-0.09651200
C	-2.91198700	1.02017600	0.14190100
C	-2.40691700	-0.32212500	-0.01110900
C	-4.28949900	0.90271800	0.33456300
C	-3.50990100	-1.19576200	0.09653700
C	-1.12180400	-0.82223200	-0.22763200
H	-5.03855700	1.66744300	0.48793500
C	-3.36942800	-2.58134600	-0.00756900
C	-0.96472800	-2.20306000	-0.33525900
C	-2.07867500	-3.06251200	-0.22506500
H	-4.21499400	-3.25729400	0.07435100
H	0.02080500	-2.62417800	-0.50630800
H	-1.92291600	-4.13421900	-0.31361000
N	-4.64858500	-0.40584100	0.30869200
C	-2.65057800	3.57636500	0.24479400
H	-2.45653400	4.14483200	-0.67142500
H	-3.72323800	3.58517500	0.44914200
H	-2.12486100	4.08595000	1.05897000
C	-5.99639400	-0.92556300	0.47252100
H	-6.29865400	-1.48542700	-0.41851900
H	-6.04505000	-1.58858200	1.34248500
H	-6.68693100	-0.09326900	0.62065900
Pd	0.36326200	0.44656200	-0.36750700
C	3.82940600	-0.33652200	1.00991900
O	1.88605000	-1.00070600	-0.67814800
O	2.55943900	1.33786900	-0.63772900
S	3.09707500	-0.05839700	-0.68004200
O	4.14329000	-0.38746100	-1.63578700
F	2.91215900	-0.08933600	1.95339000
F	4.86874000	0.48211000	1.18838100
F	4.24017600	-1.60183200	1.12386000

a₆''-TS1

Imaginary Frequency: -81.8450

C	0.26044100	-2.46760500	-1.76262300
O	-0.75431800	-1.76717800	-1.62755300
O	-2.55919000	0.47042100	-0.01101200
C	-3.32797800	-0.48834000	0.40606100
O	-3.04355300	-1.60711900	0.79658400
C	-4.81259400	-0.02398500	0.37292800
C	1.25188100	-2.54106800	-0.70116600
C	1.10631000	-1.96346500	0.60710600
C	2.59643500	-2.87904700	-0.82554700
C	2.39142100	-1.93933600	1.19575000

C	-0.00075300	-1.44700100	1.31791500
H	3.12127100	-3.31116100	-1.66703200
C	2.62521500	-1.37628300	2.45068300
C	0.24587100	-0.85696500	2.57213500
H	-1.02623100	-1.68423600	1.02656700
C	1.53556400	-0.81226600	3.12055600
H	3.61559000	-1.36588600	2.89633200
H	-0.59355600	-0.46847000	3.14112300
H	1.68949000	-0.35824400	4.09464200
N	3.28087900	-2.52992800	0.29727600
C	0.49646900	-3.18949300	-3.07412600
H	-0.46326300	-3.35640400	-3.56772600
H	1.10875300	-2.55879000	-3.73176800
H	1.01300100	-4.14399300	-2.93306200
C	4.70882900	-2.69312600	0.51665900
H	5.18504800	-1.71913600	0.66919300
H	4.89394400	-3.32417300	1.39221900
H	5.15148300	-3.16839900	-0.36045200
Pd	-0.61088400	0.34412800	-0.32994700
C	2.04726300	2.92585700	0.40860200
O	1.39062100	0.67662900	-0.86869100
O	-0.15514600	2.53127300	-1.06412200
F	1.99398200	4.25449000	0.33786300
F	1.36844700	2.51108400	1.48275700
F	3.31992000	2.53587500	0.51735400
F	-5.62427300	-0.99588000	0.80471500
F	-4.98822300	1.05300700	1.16293600
F	-5.17950200	0.30844500	-0.87788200
O	2.09939400	2.67216200	-2.24947200
S	1.30357100	2.18991000	-1.13428600

a₆''-IN2

C	2.69932200	-3.09648000	-1.38820500
O	1.58017100	-3.58619100	-1.47302400
O	-2.05162200	-1.21815800	-0.33131600
C	-3.06414300	-1.05964600	0.47331400
O	-3.15597400	-0.32955600	1.44413800
C	-4.23560700	-1.99226100	0.06026400
C	2.99243300	-2.07856400	-0.36383200
C	2.05216400	-1.52825900	0.57549200
C	4.19890300	-1.45286400	-0.10214100
C	2.75312500	-0.59451100	1.37057400
C	0.66965400	-1.73275400	0.80957700
H	5.15925800	-1.57414500	-0.58389000

C	2.14544000	0.13067100	2.41816400
C	0.04776100	-0.99172700	1.85932800
H	0.14805300	-2.53421600	0.29976100
C	0.80399200	-0.07719400	2.65666400
H	2.71537400	0.83134600	3.02069700
H	-0.95657500	-1.24534100	2.17960500
H	0.30149600	0.45252900	3.45899200
N	4.06259700	-0.56656900	0.93610200
C	3.81616800	-3.51266800	-2.33150900
H	3.44468100	-4.29417800	-2.99654100
H	4.15403200	-2.65913300	-2.93208300
H	4.68293000	-3.89097200	-1.77577200
C	5.10867600	0.29785400	1.46200100
H	4.84396100	1.35014600	1.31724800
H	5.26489900	0.10788100	2.52873600
H	6.03831500	0.09132100	0.92918600
Pd	-0.52505500	0.04731800	-0.09553100
C	-0.43073800	3.81229200	-0.10085400
O	0.99032700	1.54751000	-0.23397400
O	-1.01083800	1.64833400	-1.57529300
F	-1.20530600	4.62555000	-0.81419100
F	-1.13683700	3.28449600	0.90065700
F	0.60069800	4.49694000	0.39765600
F	-5.29644800	-1.80190400	0.85225700
F	-4.60835700	-1.76320000	-1.21071800
F	-3.85992500	-3.28352300	0.16251700
O	0.98477100	3.08502200	-2.25407000
S	0.21474400	2.45061600	-1.20015900

a₆^{''}-TS2

Imaginary Frequency: -1185.1810

C	-1.14894400	1.81086000	2.16877500
O	-1.46651900	0.63345300	2.02859900
O	-1.60655300	-1.88122900	-0.09055900
C	-2.72153000	-1.36277400	-0.34075400
O	-2.96029300	-0.18082200	-0.70832800
C	-3.94657300	-2.30340900	-0.25108600
C	-0.67521000	2.61272500	1.03223000
C	-0.46265100	2.17523600	-0.32308000
C	-0.35993800	3.96494800	1.05639900
C	-0.03183800	3.31667500	-1.05258500
C	-0.60289200	0.92970700	-1.00398500
H	-0.38509600	4.65835500	1.88604700
C	0.27076400	3.27290300	-2.41289000

C	-0.28716400	0.91081800	-2.38456000
H	-1.81267300	0.39134900	-0.81682800
C	0.12714400	2.05347800	-3.07794700
H	0.60550400	4.15834800	-2.94596600
H	-0.39384500	-0.02279000	-2.93053500
H	0.34572900	1.99319600	-4.13975100
N	0.02341900	4.39620900	-0.17778000
C	-1.23479300	2.47483100	3.53462600
H	-0.23684500	2.76894300	3.88257900
H	-1.85703400	3.37724900	3.50327200
H	-1.66453500	1.76544200	4.24384800
C	0.41831800	5.74920100	-0.53167600
H	1.44573900	5.76409100	-0.91049400
H	-0.25067400	6.16005200	-1.29537800
H	0.36347900	6.37841300	0.35852400
Pd	0.10446300	-0.74355600	0.02230400
C	3.67015400	-1.82479200	-0.48235500
O	2.02811000	0.11677100	0.33473700
O	1.54182100	-2.12576200	1.11410600
F	-4.23735700	-2.75069700	-1.48822500
F	-5.01254400	-1.64792900	0.22456500
F	-3.70179100	-3.35415400	0.53509500
S	2.66720400	-1.14065000	0.93236500
O	3.59505400	-0.92725900	2.02952900
F	2.88287700	-2.03055000	-1.54377000
F	4.22412700	-2.98024600	-0.11570800
F	4.62843300	-0.95595700	-0.81040600

a₆^{''}-IN3

C	-0.78200600	1.48980800	2.25270400
O	-0.75705000	0.24566900	2.33742600
O	-0.90229400	-2.18988800	-0.37726400
C	-1.90789300	-2.28068900	0.33394000
O	-2.27895900	-1.52718600	1.31192800
C	-2.90156200	-3.43299100	0.06808900
C	-1.28094400	2.17933700	1.07802100
C	-1.36302700	1.70098900	-0.29238400
C	-1.91619100	3.41425300	1.09740800
C	-2.08971100	2.68549600	-1.01507900
C	-0.82483800	0.61540500	-1.00637200
H	-2.09429300	4.08160000	1.92925200
C	-2.36561900	2.58197800	-2.38113400
C	-1.11247100	0.48797900	-2.36193900
H	-1.61331500	-0.77457900	1.57234500

C	-1.88152100	1.45771200	-3.03884600	H	-2.59036100	2.64123600	-2.04478200
H	-2.92550900	3.34680400	-2.91034700	H	-4.69323400	2.95385900	-3.29338500
H	-0.71810200	-0.35384700	-2.92382700	N	-6.53503100	-0.58998400	-0.90555000
H	-2.07578200	1.33130300	-4.10024300	C	-3.86888200	-2.76607800	1.90211300
N	-2.41645900	3.71300500	-0.13202200	H	-4.93071900	-2.99456800	2.01850100
C	-0.22212400	2.28545800	3.40749400	H	-3.36712200	-3.63241100	1.45499600
H	0.85140200	2.42405000	3.22135000	H	-3.41747000	-2.60104300	2.88459600
H	-0.66868200	3.27856100	3.50492200	C	-7.90445800	-0.70451900	-1.37638100
H	-0.33677600	1.72355900	4.33704800	H	-8.46021500	0.21412000	-1.16067100
C	-3.17154600	4.90297900	-0.48362100	H	-7.92185100	-0.88384500	-2.45656200
H	-2.65084800	5.47168600	-1.26145900	H	-8.39002300	-1.54072400	-0.86961900
H	-4.16804300	4.63210000	-0.84849300	Pd	-1.72279300	0.72499600	0.29466900
H	-3.27813000	5.53263600	0.40173800	C	-0.48358800	-0.22521800	4.08586300
Pd	0.48337700	-0.61202300	-0.19552500	O	0.13251600	0.61148000	1.63880900
C	4.23790500	-0.16931700	-0.81351600	O	1.98009800	-0.15469800	3.10144600
O	1.97836700	0.88403300	0.11999900	F	-0.33052600	1.00021100	4.58883900
O	2.47921400	-1.41035500	0.76835700	F	-1.77035400	-0.40089600	3.75444100
F	-4.11594000	-2.92625900	-0.19909000	F	-0.15867200	-1.12602800	5.02298900
F	-2.99171900	-4.21373200	1.15501300	F	2.59840800	4.44111100	-1.09087300
F	-2.50533100	-4.17390300	-0.96667600	F	4.26413900	3.40130200	-0.14705600
S	3.08163800	-0.04308500	0.64141200	F	3.68420100	2.90529600	-2.18552600
O	3.86698700	0.48557300	1.74722800	O	0.36975200	-1.82373100	2.12671000
F	3.57340800	-0.61525500	-1.88606300	S	0.63142400	-0.45396000	2.61164700
F	5.22561100	-1.01934000	-0.52679100	C	0.06401700	-1.28364100	-0.99002800
F	4.75296000	1.03119700	-1.08712000	H	-0.27527400	-1.66814000	-0.03301300
a6-TS3				C	-0.69464000	-1.70114600	-2.23360100
Imaginary Frequency: -87.7162				C	5.29401700	0.17931800	-1.30146800
C	-3.61578700	-1.54576100	1.04935200	C	5.83658300	0.16962700	-0.01146800
O	-2.44588700	-1.08700500	1.07094500	C	5.32289900	-0.73357500	0.92094000
O	1.88052600	1.25629400	-1.15444900	C	4.26388300	-1.60412700	0.62398900
C	2.23453100	2.17738700	-0.44671300	C	3.74677900	-1.50912400	-0.67480600
O	1.90206000	2.43331300	0.79305200	C	4.23281300	-0.65190500	-1.67429300
C	3.21387200	3.24932200	-0.97762000	H	5.68507900	0.87328200	-2.04053100
C	-4.41284700	0.17224400	-0.63922000	H	5.74022100	-0.76319000	1.92361900
C	-5.94449700	-1.37377500	0.03147900	I	2.06496800	-2.77919200	-1.17518500
C	-5.61698500	0.37114800	-1.35082800	F	-0.09344400	-1.25428700	-3.35119500
C	-3.30585900	1.00062900	-0.86048400	F	-0.77079000	-3.05659900	-2.32307800
H	-6.49582500	-2.18473800	0.48734500	F	-1.95523000	-1.24764300	-2.23323500
C	-5.75682200	1.37069900	-2.31499600	H	0.57911900	-0.32417400	-1.00787800
C	-3.43081200	1.98915500	-1.83668400	C	3.68217100	-0.57786800	-3.07663900
H	1.23656800	1.75616100	1.12939500	H	3.78882500	-1.53401800	-3.60280600
C	-4.63613800	2.16593500	-2.54680200	H	2.62302000	-0.30556900	-3.07732400
H	-6.68246300	1.52419800	-2.86132500	H	4.21661600	0.18404300	-3.64920000
				C	3.77960500	-2.57725500	1.66958900

H	2.70824400	-2.47519600	1.86029300
H	3.97660800	-3.61278400	1.36367200
H	4.29771800	-2.39999900	2.61463100
C	6.93223000	1.13862500	0.35974400
H	7.74416400	1.12704800	-0.37663200
H	6.53503400	2.16019700	0.39217200
H	7.35680300	0.91058700	1.34164300
C	-4.62938500	-0.95722100	0.23648700
C	-1.35025300	3.45483600	0.46480300
C	-0.80557800	4.82818600	0.09818200
O	-2.11679900	3.28220400	1.41061000
O	-0.93679600	2.49779900	-0.33777800
H	0.27615200	4.78756700	-0.05289300
H	-1.04853100	5.54379700	0.88600800
H	-1.25806500	5.16203900	-0.84325700

a₆-IN4

C	-2.74183900	1.71015800	0.21239500
O	-1.49177100	1.56572100	0.27816500
O	3.12124500	-1.42038000	1.46256900
C	3.79847500	-1.27054500	0.47135800
O	3.72373200	-0.31423700	-0.43546200
C	4.91474900	-2.26841200	0.09027000
C	-3.14264800	-0.70251000	-0.43050400
C	-4.98984700	0.61219900	-0.27248700
C	-4.29117300	-1.48364800	-0.68911800
C	-1.88360300	-1.29670600	-0.45609900
H	-5.70912800	1.40894900	-0.14226900
C	-4.21427600	-2.84853100	-0.96770300
C	-1.78168200	-2.65694000	-0.71593600
H	2.96651700	0.30539100	-0.22936300
C	-2.94226700	-3.41661000	-0.97115200
H	-5.09706700	-3.44789700	-1.16638000
H	-0.81357900	-3.14284700	-0.72127200
H	-2.83562100	-4.47830100	-1.17374200
N	-5.40409800	-0.63762900	-0.58875000
C	-3.25247700	3.07841600	0.58064700
H	-4.26721600	3.26128500	0.22009000
H	-3.23894900	3.17740500	1.67279300
H	-2.56844000	3.82853600	0.17597200
C	-6.78242300	-1.05664500	-0.79552900
H	-6.91370800	-1.43909500	-1.81268700
H	-7.05030700	-1.84056400	-0.08021600
H	-7.44251100	-0.20011100	-0.64892700

Pd	-0.32425900	-0.06208800	-0.21940500
C	1.21012100	3.78246100	-0.76630100
O	1.51344700	1.23262000	-0.13222100
O	3.16663300	2.83714200	0.75518000
F	1.96848600	3.62652100	-1.85384800
F	-0.07483000	3.58522300	-1.11126100
F	1.33945700	5.03556300	-0.31805300
F	4.61261500	-2.86969400	-1.08549700
F	6.09568700	-1.64710400	-0.05583900
F	5.04224800	-3.21781500	1.02032000
O	0.81358200	2.81068300	1.68341500
S	1.73866800	2.59149800	0.56562000
C	0.00066700	-0.38776200	1.80035600
H	0.13588800	0.64221300	2.13281700
C	-1.05078700	-1.08047800	2.62013000
F	-0.66984400	-1.04066700	3.91797500
F	-2.26175500	-0.47468600	2.54690800
F	-1.22572900	-2.37609200	2.29770000
H	0.93901500	-0.94432900	1.77141000
C	-3.59893800	0.63826800	-0.16071900
C	0.90826700	-1.15575100	-2.17521000
C	1.82459500	-1.90851800	-3.09882600
O	0.13725000	-0.24742200	-2.54472800
O	0.93313900	-1.49980900	-0.91149000
H	1.85006000	-1.41836700	-4.07355200
H	1.45916100	-2.93524700	-3.21668200
H	2.82721800	-1.95800900	-2.66652600

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Imaginary Frequency: -305.2682

C	-2.52595400	1.91878700	-0.13052100
O	-1.28884300	1.76732500	-0.25409000
O	2.68093500	-1.21251900	1.39254300
C	3.52000400	-1.32645700	0.52900500
O	3.71626700	-0.55883600	-0.52822100
C	4.53611100	-2.49026700	0.52807500
C	-3.01129600	-0.56969100	-0.30417500
C	-4.81039400	0.80965400	-0.37416800
C	-4.17908100	-1.33700200	-0.51363100
C	-1.75531400	-1.20552100	-0.20094000
H	-5.49997600	1.64250700	-0.38460200
C	-4.14229800	-2.72136000	-0.67737100
C	-1.71896800	-2.59866000	-0.39848500
H	3.02773900	0.16218400	-0.55041100

C	-2.88771800	-3.33367000	-0.63287000	O	0.48736400	2.66509800	0.32410500
H	-5.04302200	-3.30482600	-0.84041100	C	1.62075300	3.10002300	0.34846800
H	-0.76466900	-3.11057600	-0.35517800	O	2.73654000	2.46784200	0.05692200
H	-2.81616600	-4.40822300	-0.77054500	C	1.91757000	4.55878200	0.76406700
N	-5.26472600	-0.45709400	-0.54345200	C	-2.29367200	-0.73808900	0.19969800
C	-3.01218100	3.31646400	0.15009100	C	-2.40407200	-2.73378500	-0.91857900
H	-3.95495800	3.53311100	-0.36135500	C	-2.61579200	-1.80076600	1.10825900
H	-3.17693300	3.42358900	1.22967700	C	-2.43942800	0.62287200	0.64621200
H	-2.24516100	4.03056200	-0.15357000	H	-2.29939000	-3.55104900	-1.61881400
C	-6.64945600	-0.84931100	-0.76181600	C	-2.89859900	-1.58071500	2.45325900
H	-6.75967800	-1.32983700	-1.73919300	C	-2.70179300	0.80950400	2.00538000
H	-6.97466400	-1.54334600	0.01939800	H	2.54120800	1.51939200	-0.19756100
H	-7.28054400	0.04033000	-0.73018000	C	-2.90372900	-0.26017300	2.89102000
Pd	-0.18313700	0.03404700	-0.58924100	H	-3.11487000	-2.39960300	3.13064100
C	1.60989500	3.92658600	-0.33921300	H	-2.77819500	1.82469600	2.38207800
O	1.66552600	1.29685100	-0.64619400	H	-3.10848200	-0.04663500	3.93576300
O	3.32765800	2.32083300	0.88144300	N	-2.65896500	-2.98445200	0.39500100
F	2.49702300	4.10592500	-1.32051100	C	-1.78750400	-1.10560900	-3.66538000
F	0.37552600	3.98596400	-0.86491100	H	-2.12656000	-2.13980300	-3.77971900
F	1.73821400	4.91545500	0.55292400	H	-2.60808600	-0.45314200	-3.99190700
F	4.33424700	-3.27970800	-0.55414400	H	-0.91002500	-0.92096000	-4.28783500
F	5.79920200	-2.03892400	0.47894800	C	-2.67662500	-4.30660100	1.00905300
F	4.39405100	-3.24544000	1.62150800	H	-1.74544600	-4.44633700	1.56646300
O	0.89531800	2.19445200	1.56331500	H	-3.53912300	-4.39987400	1.67524100
S	1.91459000	2.29307000	0.50727600	H	-2.75600500	-5.06044100	0.22404900
C	-0.60907900	-0.84384400	1.46693300	Pd	0.01914700	-0.29713900	0.06576600
H	-0.01222300	0.03530700	1.73395300	C	3.81358600	-2.04048100	-0.39415900
C	-1.70448200	-0.92937200	2.50848700	O	2.05995700	-0.08651600	-0.45441400
F	-1.10801200	-1.02961900	3.71473400	O	3.53584900	-0.34881500	-2.43537900
F	-2.47497000	0.18269600	2.53116700	F	4.68767800	-1.22284300	0.19886300
F	-2.52830800	-1.98879200	2.38861500	F	3.11146900	-2.68270000	0.54813200
H	0.01264000	-1.73447000	1.46254600	F	4.47883400	-2.93930900	-1.12480800
C	-3.42353000	0.80548000	-0.23892100	F	2.68403700	4.58255600	1.86901500
C	1.04648100	-1.44986100	-2.41983200	F	2.56681100	5.20924700	-0.21599900
C	1.93879900	-2.49333000	-3.04782500	F	0.77848700	5.21138900	1.02500300
O	0.44413300	-0.57793900	-3.05004500	O	1.68035700	-2.02294100	-1.99569900
O	0.94649600	-1.53804600	-1.10553300	S	2.67439100	-1.06686900	-1.50031800
H	2.07941400	-2.26399700	-4.10573500	C	-2.46187100	1.82939000	-0.27177800
H	1.47834500	-3.48305800	-2.94767700	H	-1.65629400	1.82382600	-1.00667000
H	2.90189100	-2.52159600	-2.53152300	C	-3.76718400	1.96228200	-1.03569900
a₆-IN5				F	-3.78432000	3.09900100	-1.75730800
C	-1.48282500	-0.78686800	-2.23668500	F	-3.94661100	0.93288000	-1.90971000
O	-0.58669500	0.04850200	-1.95557600	F	-4.84168600	1.97560800	-0.22149300
				H	-2.33656700	2.73911300	0.31974700

C	-2.18045400	-1.38542000	-1.12054500
C	0.61252200	-1.92251200	2.27178000
C	1.32595700	-2.14836000	3.59396000
O	0.13362400	-2.83938100	1.60770600
O	0.59669200	-0.65425600	1.92150300
H	0.96793400	-3.07356100	4.05151800
H	1.19110600	-1.30403300	4.27428400
H	2.39772800	-2.25168900	3.38897600

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Imaginary Frequency: -143.1507

C	-3.75780900	-1.92250100	1.03777100
O	-2.59115100	-1.47536800	1.16391700
O	2.10205500	1.16517000	-0.37964200
C	2.38845900	1.85076300	0.57983800
O	1.84518200	1.83834700	1.77443900
C	3.55931500	2.85803500	0.52284900
C	-4.51430200	0.04943400	-0.36560200
C	-6.07947500	-1.54915600	0.05830500
C	-5.72360000	0.39814900	-1.00880600
C	-3.38683900	0.87328300	-0.47074000
H	-6.64628500	-2.41094700	0.38319600
C	-5.85164500	1.55474300	-1.77904700
C	-3.50191400	2.02449200	-1.25022400
H	1.15381200	1.11311900	1.82734600
C	-4.71636700	2.35431600	-1.88682000
H	-6.78111000	1.82313200	-2.27180600
H	-2.65592200	2.69039500	-1.36574600
H	-4.76419900	3.26545400	-2.47694300
N	-6.66056200	-0.60314200	-0.72134000
C	-4.03039600	-3.27027100	1.66103500
H	-5.08613800	-3.41330500	1.90561600
H	-3.72584500	-4.05864100	0.96133600
H	-3.42158300	-3.37314000	2.56181000
C	-8.03788700	-0.60392100	-1.18459100
H	-8.56656900	0.27873800	-0.80984400
H	-8.07139400	-0.59975600	-2.27907000
H	-8.53954200	-1.50116700	-0.81725500
Pd	-1.77473400	0.33415900	0.55418900
C	-0.13399900	-1.93727200	3.84012500
O	0.03423300	-0.15347300	1.87587400
O	2.09503200	-1.37754100	2.51928900
F	0.18466300	-1.02398100	4.75949000
F	-1.46809100	-1.99314200	3.73358700

F	0.31303100	-3.13473000	4.23930000
F	3.25747500	4.02412000	1.10331900
F	4.63024300	2.33589700	1.16410100
F	3.91777300	3.09250200	-0.74962800
O	0.26145700	-2.56779400	1.27583400
S	0.66673600	-1.50056300	2.21533700
C	-0.05276700	-0.95170800	-1.38743300
H	-0.10410700	-1.66452500	-0.56656200
C	-1.11419500	-1.07291100	-2.47628100
C	5.55143600	0.09251400	-1.00944800
C	5.95822200	-0.65668600	0.10012200
C	5.23923000	-1.80708900	0.42701100
C	4.10592200	-2.21635500	-0.29003000
C	3.73525900	-1.39619500	-1.36426700
C	4.42691600	-0.24217700	-1.76868700
H	6.10437500	0.98777600	-1.28093200
H	5.54776900	-2.40724200	1.27842500
I	1.97316100	-1.94772600	-2.49248200
F	-1.38626500	0.11294200	-3.03083400
F	-0.74192400	-1.90699900	-3.48794900
F	-2.24922400	-1.59547700	-1.97845000
H	0.37152100	0.02768600	-1.18238500
C	4.02351800	0.63883000	-2.92428200
H	3.92167800	0.07510600	-3.85803700
H	3.07182400	1.13449600	-2.71086700
H	4.77394200	1.41732900	-3.08179500
C	3.38774400	-3.47983100	0.11217100
H	2.35634700	-3.28253200	0.41903000
H	3.36863000	-4.20732700	-0.70843000
H	3.89664800	-3.94388700	0.96048700
C	7.12976800	-0.20281600	0.93493900
H	7.99792000	0.03898900	0.31091400
H	6.86517300	0.70510100	1.49086000
H	7.42945600	-0.96557500	1.65942500
C	-4.75245300	-1.20423900	0.31041500
C	-1.05253300	3.04768400	0.85675700
C	-0.45321100	4.37007700	0.31181500
O	-1.66318400	3.04454700	1.91106700
O	-0.85214600	2.07439000	0.02143000
F	0.79011500	4.20345900	-0.19233900
F	-0.39365500	5.31655700	1.25259800
F	-1.23305200	4.83313000	-0.69708200

a₆'-IN4

C	-3.03848500	1.68414100	-0.00821200
O	-1.77904400	1.64644300	0.07363900
O	2.93217000	-0.67737100	1.93947500
C	3.73009300	-0.59106700	1.03200500
O	3.64266200	0.14473000	-0.05952200
C	5.06543100	-1.36840000	1.05303700
C	-3.24925300	-0.82373300	-0.20665900
C	-5.19311900	0.35270400	-0.29193000
C	-4.33107600	-1.72277600	-0.33794000
C	-1.94901400	-1.31514200	-0.12215900
H	-5.97149300	1.10302900	-0.30879600
C	-4.14684700	-3.10437300	-0.38433300
C	-1.74006100	-2.68882200	-0.15330200
H	2.79721900	0.67203000	-0.05524500
C	-2.83569800	-3.56592800	-0.28865100
H	-4.97800700	-3.79483500	-0.48608400
H	-0.74047300	-3.09956600	-0.08177500
H	-2.64482600	-4.63450600	-0.31689300
N	-5.50607600	-0.95934600	-0.39134300
C	-3.64477400	3.05730600	0.10467200
H	-4.67747400	3.09334700	-0.24877400
H	-3.61500900	3.36958200	1.15549100
H	-3.02847600	3.76069000	-0.46121200
C	-6.84527100	-1.51241600	-0.53666400
H	-6.92412900	-2.06968100	-1.47527400
H	-7.06898800	-2.18242500	0.29918200
H	-7.57007500	-0.69677200	-0.54378400
Pd	-0.48779200	0.05925000	-0.08250700
C	0.75702400	3.81948300	-1.34485400
O	1.23887100	1.47000500	-0.22584400
O	2.72804500	3.34796300	0.37019000
F	1.57306500	3.53861700	-2.36153600
F	-0.48868300	3.43515100	-1.67829300
F	0.75053700	5.13956200	-1.13643400
F	5.27871700	-2.00428800	-0.11178700
F	6.08777400	-0.51794200	1.26106800
F	5.06209000	-2.27523600	2.03630700
O	0.35356900	3.29735900	1.24040900
S	1.33227900	2.95323000	0.20167400
C	-0.18543100	0.14849800	1.96594300
H	-0.15098800	1.23197800	2.08784500
C	-1.20777800	-0.47146800	2.87839700
F	-1.27724900	-1.81065500	2.78896800
F	-0.85566300	-0.16791700	4.14774800

F	-2.45521500	0.01953600	2.68297700
H	0.79670600	-0.32327500	2.03911500
C	-3.80907300	0.50402700	-0.17647000
C	0.92160200	-1.41521600	-1.68772700
C	1.86648100	-2.47482500	-2.29032300
O	0.20585700	-0.70461400	-2.39456200
O	0.89967800	-1.40252700	-0.39186600
F	3.03292000	-2.52335100	-1.63699300
F	2.09785900	-2.23183500	-3.58150000
F	1.26913000	-3.68377600	-2.18165500

ag'-TS4

Imaginary Frequency: -282.2576

C	-2.88139000	1.79323200	-0.25853200
O	-1.63002700	1.77328900	-0.33556800
O	2.52061500	-0.28084700	1.73997900
C	3.45808100	-0.43785100	0.98931500
O	3.64437500	0.10826200	-0.19852400
C	4.65102100	-1.33620900	1.38510600
C	-3.06990700	-0.73517600	-0.16560100
C	-5.01553800	0.40419600	-0.41736900
C	-4.13407800	-1.65331200	-0.31343900
C	-1.75310500	-1.20515000	0.02413300
H	-5.79616800	1.14381000	-0.53056900
C	-3.93192400	-3.03235700	-0.32834000
C	-1.54890300	-2.59761400	-0.01849400
H	2.87328400	0.69518900	-0.41059800
C	-2.61728100	-3.48511700	-0.19672100
H	-4.75357700	-3.73205000	-0.44525500
H	-0.54600200	-2.99322400	0.08916200
H	-2.41627000	-4.55145700	-0.22168900
N	-5.31350800	-0.91664700	-0.45755700
C	-3.52632500	3.14983100	-0.15722700
H	-4.49851400	3.18373400	-0.65726900
H	-3.67720600	3.38834000	0.90329900
H	-2.85559600	3.89811900	-0.58260200
C	-6.63628500	-1.49188700	-0.66031500
H	-6.65773800	-2.07908100	-1.58370100
H	-6.90201800	-2.13586400	0.18349500
H	-7.36719300	-0.68518000	-0.73461200
Pd	-0.31331500	0.17481100	-0.40535500
C	0.90944000	4.21394600	-0.96896500
O	1.30287200	1.59978400	-0.76823700
O	2.83907200	3.09868800	0.46358100

F	1.75628300	4.30821700	-1.99510200
F	-0.32706000	4.01060100	-1.45376200
F	0.91331900	5.36448500	-0.28762900
F	4.23241200	-2.32074000	2.19467500
F	5.25315600	-1.88961800	0.32259400
F	5.56313500	-0.60255000	2.05158000
O	0.45513200	2.80877300	1.26222000
S	1.43360200	2.83004700	0.16724600
C	-0.68963500	-0.55938900	1.70685000
H	-0.14938500	0.37406300	1.89422600
C	-1.82375800	-0.61074500	2.70760900
F	-1.27172200	-0.53455400	3.93589200
F	-2.66721300	0.43755000	2.57604300
F	-2.56321000	-1.73501500	2.67520400
H	-0.01876300	-1.40803600	1.79434700
C	-3.64099200	0.57935300	-0.25653000
C	1.12591100	-1.66158400	-1.86948200
C	2.04534600	-2.89900400	-2.02236900
O	0.55604800	-1.16723900	-2.82496900
O	1.01971400	-1.31751800	-0.61503100
F	2.33118700	-3.13432000	-3.30414500
F	3.19186100	-2.76498300	-1.34062700
F	1.39319500	-3.98356200	-1.52920600

a₆⁺-IN5

C	-1.60297300	0.54359900	2.50714000
O	-0.95027200	-0.44675700	2.08496900
O	-0.36637100	-2.72542300	-0.63444100
C	0.58637400	-3.47727900	-0.68219900
O	1.78936000	-3.28852500	-0.18520400
C	0.49917500	-4.84969800	-1.38747700
C	-2.03467900	1.25874300	0.08657700
C	-1.73412200	2.91224500	1.64322200
C	-1.89236300	2.53257000	-0.56175700
C	-2.49965400	0.13437200	-0.68735800
H	-1.50596900	3.49188900	2.52714600
C	-2.00753000	2.69188600	-1.93856500
C	-2.58407400	0.32319100	-2.06980400
H	1.84216700	-2.39475300	0.25965800
C	-2.31987900	1.55681100	-2.68252900
H	-1.85873500	3.65332700	-2.41710100
H	-2.88795000	-0.51559200	-2.68800900
H	-2.39590700	1.63565300	-3.76232400
N	-1.69776000	3.49481100	0.41293600

C	-1.99196200	0.61936800	3.94766800
H	-2.04009400	1.65678800	4.29251900
H	-2.99818800	0.19198000	4.05096200
H	-1.29172200	0.04633500	4.55819500
C	-1.26783200	4.86139400	0.13764900
H	-0.27734500	4.83492200	-0.32625600
H	-1.98447900	5.35411300	-0.52573600
H	-1.22018300	5.41321700	1.07765600
Pd	-0.03044500	0.08862900	0.24953400
C	3.99195700	0.53344000	1.38870100
O	1.78667400	-0.78719800	0.83861100
O	2.95550700	-1.36744100	2.95364600
F	4.69455600	-0.37832300	0.71324100
F	3.63385200	1.51657200	0.55769500
F	4.74948700	1.04056900	2.36474900
F	-0.73022000	-5.04349500	-1.87954500
F	1.37920600	-4.91174100	-2.40118800
F	0.77463600	-5.84171900	-0.52404900
O	1.71179600	0.83542900	2.74491700
S	2.47952500	-0.25535000	2.13683700
C	-3.02126800	-1.16017200	-0.09446700
H	-2.37144300	-1.57103500	0.67902700
C	-4.40564100	-1.01273400	0.51240800
F	-4.87606400	-2.20555000	0.92118500
F	-4.39181100	-0.19464600	1.60174300
F	-5.29543700	-0.49318700	-0.35624300
H	-3.08753300	-1.91735500	-0.87894700
C	-1.94422800	1.55122700	1.52992200
C	1.21590000	1.85746500	-1.55761200
C	1.79487400	2.16156800	-2.96489400
O	1.12266000	2.75414900	-0.73344500
O	0.81751100	0.62664400	-1.47210100
F	2.56979200	3.25274500	-2.93563500
F	2.51025100	1.14454200	-3.46273600
F	0.76646500	2.40651100	-3.81484400

a₆⁺-TS3

Imaginary Frequency: -169.9971

C	-3.70927500	1.70408300	0.09215500
O	-2.46223400	1.70116600	-0.14271300
O	0.13522700	-1.22138600	-1.57007100
C	1.03878800	-1.00729900	-2.40108700
O	1.51931200	0.11625100	-2.78313700
C	1.62580700	-2.24294600	-3.12235900

C	-3.93006900	-0.76455800	-0.34709800
C	-5.85638100	0.32433200	0.17585600
C	-4.99900100	-1.68745000	-0.33805200
C	-2.63977300	-1.19940300	-0.64008000
H	-6.62755100	1.03665500	0.43556300
C	-4.80994800	-3.04149600	-0.61267200
C	-2.42515300	-2.54791000	-0.91452400
H	1.09865400	0.91118000	-2.25590100
C	-3.50828400	-3.45084500	-0.89954500
H	-5.62935100	-3.75277800	-0.60565200
H	-1.43450500	-2.91862600	-1.14960500
H	-3.31747500	-4.49667500	-1.11996100
N	-6.16400200	-0.97548300	-0.01413000
C	-4.28423100	3.02857600	0.51588700
H	-4.04034200	3.19748800	1.57216200
H	-3.81565500	3.82977100	-0.06074900
H	-5.36866900	3.07071200	0.39571400
C	-7.49545400	-1.56599700	0.08755400
H	-7.78412900	-2.00634200	-0.87121800
H	-7.50324300	-2.34042000	0.85992700
H	-8.21149400	-0.78752000	0.35413400
Pd	-1.23156100	0.19797600	-0.74067600
C	0.14799200	4.39205700	-0.91982700
O	0.27801700	1.77357100	-1.34284100
O	2.41316900	2.95467500	-0.88274600
F	0.22849900	4.57442600	-2.23618000
F	-1.13735500	4.32477200	-0.55920100
F	0.73315800	5.40407900	-0.28570100
F	0.81066000	-2.55668800	-4.13853900
F	2.84700100	-2.00155700	-3.59773300
F	1.67853600	-3.27913700	-2.27421500
O	0.72807200	2.58112600	0.96710100
S	1.02444400	2.81245800	-0.45708300
C	-0.17548900	-0.33247700	1.43562800
H	0.18009400	0.69494700	1.38475800
C	-1.25851900	-0.68531600	2.44278200
C	4.36025000	-1.85830500	-0.67304400
C	5.04274700	-0.68511700	-1.02459700
C	4.92192500	0.42716500	-0.18962600
C	4.13467300	0.41909700	0.97139500
C	3.45401700	-0.77703700	1.24951500
C	3.55450600	-1.94314300	0.46702500
H	4.46131800	-2.74077500	-1.29940000
H	5.44906900	1.34265000	-0.44150000

I	2.15117600	-0.81752900	2.96885000
F	-1.61167500	-1.97483900	2.33814200
F	-0.85338400	-0.46720800	3.70984500
F	-2.35786000	0.07322600	2.26197600
H	0.25596400	-1.13085400	0.85318000
C	2.86599500	-3.24761600	0.79351900
H	3.13596000	-3.60782300	1.79201200
H	1.77251000	-3.16186700	0.76618400
H	3.14937500	-4.01634800	0.07102600
C	4.07599500	1.65277200	1.83751900
H	3.05678000	2.04212900	1.92116100
H	4.44270900	1.44560200	2.84950800
H	4.69460900	2.44353600	1.40801400
C	5.88449600	-0.63802300	-2.27529300
H	6.36139100	0.33731600	-2.40275100
H	6.67173300	-1.40088100	-2.25102800
H	5.27085500	-0.83433000	-3.16228200
C	-4.48276800	0.52311200	-0.01758600

ae⁺⁺-IN4

C	1.62503200	-2.27343700	-0.43452600
O	0.47985000	-1.73945400	-0.24978200
O	-0.79130200	2.15373700	-0.11154200
C	-1.95407300	2.56214900	-0.35156600
O	-3.00964300	1.87927100	-0.54569700
C	-2.13803700	4.09717000	-0.47102800
C	2.77374900	-0.05039000	-0.60524400
C	4.09874200	-1.87018500	-0.92803400
C	4.09481800	0.37491200	-0.86763000
C	1.78767600	0.89929200	-0.36425100
H	4.51905500	-2.86011800	-1.04279100
C	4.44334800	1.72328500	-0.89623700
C	2.10342900	2.25558500	-0.37638100
H	-2.82967400	0.84034100	-0.47087100
C	3.42719600	2.64964800	-0.65097400
H	5.45743600	2.05347300	-1.09597600
H	1.35292100	3.01150600	-0.18067700
H	3.66046900	3.70957600	-0.66447000
N	4.87317400	-0.77890800	-1.06128300
C	1.63028100	-3.77456300	-0.38418300
H	1.63810100	-4.08658500	0.66804500
H	0.71122000	-4.15827500	-0.83343000
H	2.50081800	-4.20226500	-0.88567200
C	6.30368700	-0.77223400	-1.36722200

H	6.48025700	-0.24144400	-2.30676900
H	6.85327700	-0.28089500	-0.55969900
H	6.65146200	-1.80123500	-1.46442400
Pd	-0.06569600	0.19159900	-0.13010700
C	-3.05615000	-2.88766900	-0.94483300
O	-2.18922900	-0.45613500	-0.34449200
O	-4.32329100	-1.17426000	0.69729300
F	-3.72919700	-2.39145300	-1.97852900
F	-1.81838000	-3.21565300	-1.34189100
F	-3.66942000	-3.96581600	-0.47290600
F	-2.19097000	4.40537200	-1.77231600
F	-3.26390200	4.47312300	0.12664500
F	-1.10014600	4.72553200	0.08819400
O	-2.11406800	-2.16848100	1.46319600
S	-2.96458100	-1.60712500	0.40981200
C	-0.07531400	0.15919900	1.96670000
H	-0.76364600	-0.68214400	2.08435300
C	1.23061000	-0.05788000	2.69929200
F	2.08320200	0.97060600	2.58953300
F	0.90465500	-0.19446400	3.99767400
F	1.87004300	-1.17713200	2.30809100
H	-0.50049000	1.13602000	2.19105300
C	2.77507300	-1.48714900	-0.64955500

a₆''-TS4

Imaginary Frequency: -249.0420

C	1.56688400	-2.22597500	-0.79633800
O	0.40490200	-1.75940000	-0.60086400
O	-0.99096100	2.06245600	-0.01904000
C	-2.08999300	2.49254800	-0.43158700
O	-3.04912500	1.83300500	-0.95909800
C	-2.33193700	4.02019800	-0.34380000
C	2.66814000	0.02743900	-0.55852800
C	4.01635700	-1.65813400	-1.26083800
C	3.96194700	0.53566400	-0.81134000
C	1.66040700	0.88605200	-0.08909100
H	4.45109200	-2.59730600	-1.57507100
C	4.27163600	1.88359300	-0.65115800
C	1.95814400	2.25433700	0.05130700
H	-2.86258100	0.81412500	-0.94388000
C	3.24236800	2.73462200	-0.23039800
H	5.26535500	2.27329200	-0.84713300
H	1.19449700	2.94750600	0.38535200
H	3.44642500	3.79328900	-0.10765300

N	4.75954500	-0.53514500	-1.23666800
C	1.65600600	-3.72076000	-0.91903200
H	1.81888100	-4.14339400	0.08100600
H	0.71461200	-4.11669100	-1.30421100
H	2.48458500	-4.02993300	-1.56119200
C	6.16843800	-0.42801600	-1.61632100
H	6.27572900	0.25171600	-2.46617600
H	6.75399700	-0.05564000	-0.77141500
H	6.53549500	-1.41542600	-1.89828200
Pd	-0.21383500	0.13925900	-0.25740900
C	-3.15604900	-3.02981400	-0.42597400
O	-2.21260500	-0.56200300	-0.72834300
O	-4.22092900	-0.83090700	0.71386700
F	-3.90050700	-2.85051500	-1.51132700
F	-1.97087300	-3.54001700	-0.77526300
F	-3.76451000	-3.85447800	0.41786200
F	-2.22216900	4.52939000	-1.57678500
F	-3.54616600	4.26598500	0.13744500
F	-1.41217900	4.58086900	0.44660200
O	-1.94142200	-1.61264200	1.51494300
S	-2.90587400	-1.38855600	0.43033800
C	0.68245700	0.35908300	1.82206000
H	-0.17997900	-0.28298500	2.03142400
C	1.89516600	-0.23477600	2.51003700
F	3.01627700	0.49123300	2.39087600
F	1.58523800	-0.30000200	3.81738100
F	2.15566800	-1.48588400	2.07959200
H	0.51261900	1.39474800	2.09839500
C	2.69952300	-1.37099500	-0.86870400

a₆''-IN5

C	1.08861100	-2.41580600	-0.92416900
O	0.05629300	-1.95564400	-0.36843700
O	-0.64956800	2.11068500	0.18450600
C	-1.67156300	2.74232700	-0.14831200
O	-2.77280300	2.27957500	-0.61481200
C	-1.60069100	4.28445800	-0.03543600
C	2.33848400	-0.25843900	-0.55250500
C	3.00830400	-1.48546700	-2.33988800
C	3.20900900	0.51492800	-1.36212100
C	1.84164400	0.25871200	0.70205000
H	3.15578600	-2.23693100	-3.10420300
C	3.52643600	1.83114500	-1.05270400
C	2.17081700	1.63194200	0.95813200

H	-2.75617900	1.25682000	-0.64463500
C	2.95030800	2.39472400	0.10048200
H	4.18922000	2.42126100	-1.67838800
H	1.83085600	2.07079900	1.89088400
H	3.17117300	3.42661600	0.35139000
N	3.61256400	-0.28045100	-2.43879200
C	1.12060800	-3.87911600	-1.24331600
H	1.69203000	-4.39982000	-0.46317600
H	0.10651300	-4.28088300	-1.26792000
H	1.62824600	-4.06699600	-2.19496800
C	4.51511800	0.14626100	-3.50825800
H	4.09324300	1.00651500	-4.03550200
H	5.49124200	0.41090600	-3.09233400
H	4.64077400	-0.67658500	-4.21285400
Pd	-0.27706300	0.07839600	-0.03943300
C	-3.62671000	-2.54168200	-0.45526200
O	-2.28115000	-0.25172400	-0.53020900
O	-4.32511000	-0.30934800	0.87787600
F	-4.33656900	-2.13204000	-1.50103200
F	-2.53968600	-3.19232600	-0.88046100
F	-4.35607100	-3.34363900	0.31024400
F	-0.87451900	4.73615200	-1.07111900
F	-2.81005200	4.82674000	-0.07040700
F	-0.98687200	4.61666500	1.10357800
O	-2.21576100	-1.53084200	1.61709500
S	-3.11705800	-1.06031700	0.56673700
C	1.68496900	-0.63344300	1.94231800
H	1.15001300	-1.56383000	1.74797900
C	3.04431500	-1.01173000	2.52814500
F	3.75970600	0.07857800	2.86813400
F	2.88268100	-1.76915400	3.62034800
F	3.77768800	-1.71526000	1.63325100
H	1.13063500	-0.10106600	2.72049300
C	2.17773700	-1.51846100	-1.21583000

b₆-IN1

C	-1.62898600	0.08620600	-1.88861900
O	-0.41556300	0.31722300	-2.16700700
O	3.00366300	-0.15398800	0.12312100
C	2.86264900	-1.37382100	-0.16599900
O	1.87591600	-1.75941700	-0.87174200
C	3.86735300	-2.42334900	0.33155500
C	-2.07974600	-0.80449000	-0.85995100
C	-3.40777400	-0.95132900	-0.27882100

C	-1.28860500	-1.79379300	-0.26883600
C	-3.32346000	-2.02917800	0.63792700
C	-4.63218300	-0.27422400	-0.39564400
H	-0.25733600	-2.05265200	-0.46298700
C	-4.40243400	-2.46275400	1.40976700
C	-5.71560500	-0.70022600	0.36738300
H	-4.74236400	0.57729100	-1.05671700
C	-5.60706900	-1.78337500	1.25745200
H	-4.30851900	-3.29154300	2.10478100
H	-6.66428400	-0.17911200	0.27822400
H	-6.47122000	-2.08876500	1.83978200
N	-2.01632600	-2.52094300	0.60637500
C	-2.61887400	0.81149900	-2.75991300
H	-2.94156400	1.70700300	-2.21280400
H	-2.12262800	1.13682400	-3.67636300
H	-3.49440700	0.20048200	-2.99233100
C	-1.52861300	-3.65277200	1.37947200
H	-1.64986600	-3.45927400	2.45002500
H	-2.07879000	-4.56182800	1.11548400
H	-0.46906800	-3.79923400	1.16290600
Pd	1.22024200	0.26526600	-0.95235700
C	0.60893100	2.84353800	1.72574900
O	-1.29350100	2.27080300	-0.02691800
O	0.00094900	4.42693100	-0.33455500
F	-0.25315600	3.41637000	2.56935900
F	0.72531700	1.54210100	2.04748000
F	1.80092200	3.42541600	1.85035100
F	4.79864600	-1.87112800	1.10900000
F	3.21136000	-3.36464700	1.03692300
F	4.46238800	-3.01674100	-0.71411200
O	1.10132000	2.28053300	-0.81334500
S	-0.02136600	3.00403600	-0.01892600

b₆-TS1

Imaginary Frequency: -46.1359

C	0.91695300	-2.04499500	-1.78025500
O	-0.03950300	-1.40282600	-2.29938500
O	-0.91793300	1.86042600	-0.01324000
C	-0.15601000	2.80824400	-0.42913400
O	0.62442000	2.74251000	-1.38524900
C	-0.18525400	4.09100600	0.42987800
C	1.87829300	-1.32256100	-0.98200700
C	2.69353600	-1.72715300	0.13492200
C	2.08620400	0.06589400	-1.15014800

C	3.34618900	-0.55149800	0.59407000
C	2.90067100	-2.93614800	0.82316800
H	1.80869600	0.70484800	-1.98180400
C	4.21325300	-0.55320600	1.69094600
C	3.76479500	-2.94320100	1.90894000
H	2.39450200	-3.84586200	0.51888500
C	4.41518600	-1.76668400	2.33689800
H	4.70282600	0.35368500	2.03062900
H	3.94008000	-3.87044100	2.44582900
H	5.08066000	-1.80879400	3.19388200
N	2.96216500	0.51315500	-0.21580700
C	0.97203100	-3.52365200	-1.99031500
H	0.36834300	-3.97963100	-1.19308700
H	0.49793100	-3.77457500	-2.94249400
H	1.99054100	-3.91648200	-1.94850700
C	3.45831900	1.88141900	-0.09664100
H	3.23552700	2.26722000	0.90257500
H	4.53912300	1.90723600	-0.26647700
H	2.94225200	2.50564900	-0.82540800
Pd	-0.51954900	0.24799800	-1.15231700
C	-2.97439400	-0.95474000	1.64946100
O	-1.35572900	-2.45772200	0.18177400
O	-3.82231600	-2.44112300	-0.40003200
F	-3.20171300	-1.92379600	2.54265400
F	-1.92090800	-0.23276000	2.05348800
F	-4.04507600	-0.16483300	1.57708900
F	-1.28229000	4.18752600	1.18549700
F	0.89473600	4.07261400	1.25046600
F	-0.09609200	5.18111400	-0.34373200
O	-2.43963000	-0.45577500	-0.89534600
S	-2.61546200	-1.72011800	-0.00955300

b₆-IN2

C	0.41779500	-2.79869300	-1.07915800
O	-0.48869200	-2.29619100	-1.78382500
O	0.07959900	1.35236300	0.06035700
C	0.66274900	2.24030700	-0.67739800
O	1.00611300	2.15652700	-1.84935500
C	1.03767300	3.51195200	0.12731900
C	1.45078200	-1.86342500	-0.61528700
C	2.25566300	-1.85436600	0.58720800
C	1.95547600	-0.81272400	-1.44529100
C	3.18397200	-0.79522500	0.43405800
C	2.24303400	-2.59791200	1.77764600

H	1.77081300	-0.63093100	-2.49575000
C	4.10600100	-0.46326700	1.42992700
C	3.16754700	-2.28183600	2.76494600
H	1.52481100	-3.39671300	1.93146300
C	4.08550800	-1.22673800	2.59228200
H	4.80299100	0.35921800	1.30932500
H	3.17726300	-2.84875000	3.69058700
H	4.78762100	-0.99849400	3.38849500
N	2.99217400	-0.20670400	-0.81421600
C	0.37038000	-4.24186400	-0.69379000
H	-0.24669000	-4.32704200	0.21153800
H	-0.13187400	-4.80906700	-1.48163300
H	1.36283900	-4.65009700	-0.48891200
C	3.78886700	0.89642500	-1.34579700
H	3.70333800	1.76313400	-0.68632100
H	4.83619300	0.59012200	-1.42908100
H	3.39651900	1.17529900	-2.32246900
Pd	-0.33396600	-0.35525300	-0.91464700
C	-3.48612600	0.52409000	1.31884600
O	-2.52732900	-1.81017800	0.48180000
O	-4.56049400	-0.85207800	-0.69542100
F	-4.32784200	-0.01677700	2.20721600
F	-2.31567100	0.76210100	1.92171600
F	-3.99512000	1.67673700	0.88031900
F	0.21069600	3.75891300	1.14780800
F	2.28860000	3.33410900	0.64078100
F	1.07492200	4.58867100	-0.66490800
O	-2.32485800	0.17153200	-1.03249500
S	-3.24359300	-0.66050300	-0.09699400

b₆-TS2

Imaginary Frequency: -1278.0478

C	1.77637400	-1.91949500	-1.46361800
O	0.51841000	-1.86547400	-1.56749600
O	-1.13274600	1.59856300	-0.05840600
C	-0.49125100	2.52572200	-0.61728300
O	0.61123000	2.43087600	-1.23379100
C	-1.05047400	3.95656600	-0.44958200
C	2.44581800	-0.89094500	-0.71841700
C	3.69466400	-0.89899800	-0.01066200
C	1.67907800	0.21205700	-0.25439500
C	3.62653700	0.19098900	0.90190300
C	4.84729600	-1.70820200	-0.02263500
H	1.09349200	1.22332100	-0.94906300

C	4.68550800	0.51069300	1.76400800
C	5.88907900	-1.39984800	0.83823800
H	4.93154600	-2.55016800	-0.70132500
C	5.80988700	-0.30016100	1.72105500
H	4.63481200	1.35571400	2.44242000
H	6.78705900	-2.01033200	0.83223000
H	6.64683700	-0.08470100	2.37843700
N	2.39591500	0.81432100	0.75631200
C	2.47801000	-3.09782200	-2.07214400
H	2.84640400	-3.75542000	-1.27443800
H	1.77980900	-3.66006200	-2.69459400
H	3.33987700	-2.77580500	-2.66618500
C	1.98740900	2.00157700	1.50172100
H	0.90475000	1.99263600	1.62808300
H	2.44522800	1.96992600	2.49175000
H	2.29147100	2.91826300	0.98704300
Pd	-0.35852200	-0.27430600	-0.57599500
C	-3.66625700	-1.14446300	1.28300800
O	-1.54987900	-2.66533700	0.77838400
O	-3.64709600	-3.02037300	-0.60948200
F	-4.14666400	-1.96507900	2.22253200
F	-2.86631900	-0.23926000	1.87092200
F	-4.68213000	-0.50642200	0.69868600
F	-2.34826500	3.94854100	-0.15086900
F	-0.37626000	4.54463500	0.56322900
F	-0.86048300	4.67561900	-1.56001500
O	-2.25286000	-0.99129400	-0.93382400
S	-2.69413100	-2.12184800	0.03228800

b₆-IN3

C	1.62695300	-2.30953500	-0.29077400
O	0.37656600	-2.03215100	-0.33894800
O	-0.40323100	2.04798100	0.00863400
C	-1.47371800	2.65050000	-0.15940000
O	-2.64119100	2.16054800	-0.37518000
C	-1.44729400	4.19534500	-0.15130500
C	2.53160300	-1.24421400	-0.13098800
C	3.96365300	-1.07289700	-0.02373200
C	1.93054800	0.03498300	-0.03426100
C	4.15902000	0.32204300	0.13469300
C	5.08224100	-1.91544100	-0.04178300
H	-2.61403200	1.11652800	-0.35413600
C	5.42324900	0.89225500	0.27192000
C	6.35077900	-1.35362500	0.09549000

H	4.97026400	-2.98916000	-0.15947800
C	6.52111800	0.03167100	0.25015600
H	5.55584500	1.96289500	0.39235400
H	7.22418100	-1.99937200	0.08304500
H	7.52140500	0.44124700	0.35527400
N	2.90111200	0.96153400	0.12416500
C	2.01433900	-3.75472900	-0.40797400
H	2.53985700	-4.07604800	0.49926700
H	1.12480400	-4.37123100	-0.54797600
H	2.69846200	-3.89725900	-1.25272100
C	2.75383400	2.40369600	0.27272000
H	1.69965100	2.66643600	0.24060700
H	3.17958200	2.72276100	1.22993000
H	3.28278600	2.91624000	-0.53794000
Pd	-0.04030600	-0.04166000	-0.13014200
C	-3.44523900	-2.63320900	-0.30360800
O	-2.19783200	-0.31663100	-0.29570900
O	-4.20613700	-0.51785200	1.14440800
F	-4.20252400	-2.21720000	-1.32227300
F	-2.35773400	-3.23894200	-0.78427200
F	-4.14114900	-3.50144400	0.43549000
F	-0.26894000	4.64194500	0.29989600
F	-1.62577200	4.64229500	-1.40436000
F	-2.42121300	4.67788200	0.62519900
O	-2.05421500	-1.70002000	1.78466500
S	-2.96367000	-1.18526700	0.76325800

b₆-IN1'

C	-1.42928500	0.31710000	1.43158000
O	-0.46579400	-0.49581900	1.55646200
O	3.06607800	-0.85738400	-0.57271800
C	3.38848800	0.17433300	0.07618600
O	2.56724600	0.70427400	0.89344300
C	4.76081800	0.83520900	-0.11853000
C	-1.38031600	1.55613200	0.71457900
C	-2.47525600	2.41690100	0.28407800
C	-0.20413800	2.22077900	0.35454600
C	-1.87568800	3.55133300	-0.31813700
C	-3.87703600	2.33831600	0.29882200
H	0.82335500	1.94554500	0.54524400
C	-2.60937000	4.60016200	-0.87421300
C	-4.61887300	3.38043700	-0.25010500
H	-4.38766100	1.47880400	0.71673100
C	-3.99639300	4.50126300	-0.82718000

H	-2.12203800	5.45637900	-1.33040500
H	-5.70330500	3.32229600	-0.23873800
H	-4.60451100	5.29568100	-1.24927500
N	-0.48929400	3.39640500	-0.24462200
C	-2.68980100	-0.10186000	2.14145400
H	-3.34446200	-0.58296400	1.40367800
H	-2.44549200	-0.84193600	2.90519600
H	-3.21608300	0.74772000	2.58270700
C	0.48795400	4.36244600	-0.72290300
H	0.36093900	4.52764100	-1.79749200
H	0.37129900	5.31585200	-0.19750600
H	1.49056500	3.97232600	-0.53956100
Pd	1.15771000	-0.79740200	0.36580900
C	-1.98246000	-3.63587300	0.01205800
O	0.31281500	-2.44705100	-0.44651700
O	-1.00304500	-3.18020500	-2.41667500
F	-1.36802900	-4.81654500	0.07408500
F	-2.03914700	-3.10943900	1.24570700
F	-3.23176900	-3.81140200	-0.43260100
F	5.51212400	0.14754500	-0.97760600
F	4.58231800	2.08306000	-0.59581600
F	5.40030600	0.92049100	1.05699500
O	-1.78786200	-1.20097800	-1.04614700
S	-1.07886200	-2.48361600	-1.13803300

b₆-TS1'

Imaginary Frequency: -42.1552

C	0.88232400	1.79774700	-1.40495200
O	1.22175000	0.62336400	-1.72828300
O	-0.95597000	-2.05497400	0.43650200
C	-2.02745400	-2.27273700	-0.23880600
O	-2.28107900	-1.81503500	-1.35887900
C	-3.10067800	-3.10649800	0.49403100
C	-0.46559100	2.02180300	-0.94364100
C	-1.01826900	2.99493200	-0.03616500
C	-1.51951500	1.13980700	-1.27932500
C	-2.38252000	2.63975400	0.14082100
C	-0.49910400	4.08860100	0.67954600
H	-1.56566300	0.39508700	-2.06660200
C	-3.24189000	3.35346200	0.98133100
C	-1.35016900	4.80331900	1.51058000
H	0.54470600	4.36950700	0.59115200
C	-2.70566900	4.44181500	1.65867500
H	-4.28097600	3.06767100	1.10819800

H	-0.96536300	5.65401800	2.06458900
H	-3.34082400	5.02076700	2.32229800
N	-2.65246400	1.51728700	-0.63712000
C	1.91504500	2.87571300	-1.47714800
H	2.40954500	2.90682200	-0.49617500
H	2.67235800	2.60704200	-2.21716700
H	1.48422300	3.85542600	-1.69698000
C	-3.95893900	0.87690200	-0.76331900
H	-4.30052600	0.54105600	0.22021500
H	-4.68424300	1.58062100	-1.18304100
H	-3.85960000	0.00251300	-1.40559300
Pd	0.15318300	-0.76163300	-0.63504300
C	4.29628100	-0.52774000	0.07458100
O	1.87484900	-1.56245400	0.19014900
O	3.11567300	-1.29356200	2.33115400
F	4.79432300	-1.74372700	-0.14913200
F	4.04826300	0.06580400	-1.10185900
F	5.19997900	0.20289100	0.73784900
F	-2.59997600	-3.84164800	1.48942000
F	-4.01370900	-2.24938500	1.01671600
F	-3.73888200	-3.91488700	-0.36267800
O	2.21037000	0.74237100	1.12740700
S	2.73558400	-0.63355000	1.08727800

b₆-IN2'

C	-0.40811900	-2.49559000	-0.88974400
O	-1.28162700	-1.70611100	-1.31899900
O	0.76405300	1.39446800	0.48135400
C	1.37190400	2.18974900	-0.33781600
O	1.36571100	2.17871000	-1.56178200
C	2.29405900	3.19496200	0.40021400
C	0.92288800	-1.90973100	-0.68006000
C	1.96977000	-2.23532900	0.26704900
C	1.48918700	-0.96499300	-1.59417700
C	3.09403500	-1.45834400	-0.10354500
C	2.03932000	-3.05672400	1.40219800
H	1.10642000	-0.63403600	-2.55027300
C	4.28811700	-1.48294000	0.62024700
C	3.22987000	-3.09727100	2.11772700
H	1.18381100	-3.64174200	1.72390700
C	4.33818600	-2.31858500	1.73154200
H	5.13844200	-0.87157100	0.33744200
H	3.30484900	-3.73008900	2.99647400
H	5.24995600	-2.36421900	2.31937900

N	2.77619500	-0.72524400	-1.24715300
C	-0.75683500	-3.90854500	-0.54909300
H	-1.12456600	-3.92411700	0.48634700
H	-1.57709800	-4.24244500	-1.18959400
H	0.10223800	-4.57864300	-0.63080800
C	3.69535100	0.17258200	-1.94244200
H	4.02265500	0.96200500	-1.26224200
H	4.55915600	-0.39205000	-2.30660600
H	3.16983200	0.63914500	-2.77424600
Pd	-0.37147100	0.01401000	-0.43306600
C	-4.47110500	0.13652300	-0.13164300
O	-2.04660400	1.14459600	0.01055700
O	-3.50598400	1.36310900	2.02386400
F	-4.95836500	1.28874700	-0.59602900
F	-4.09326500	-0.62484800	-1.16758900
F	-5.43104400	-0.50423200	0.54473500
F	1.87870200	3.49383300	1.63397200
F	3.53276000	2.63211500	0.50442500
F	2.42298000	4.32891200	-0.29678200
O	-2.52989600	-0.88660600	1.37809200
S	-3.02201900	0.44871100	0.99558200

C	-1.20210000	-3.42793600	2.11963700
H	-1.43456400	-4.18410700	1.35896200
H	-0.30964900	-3.74024500	2.66467700
H	-2.05742700	-3.36634700	2.80093100
C	-2.59647100	1.49289800	-1.46196900
H	-1.57528900	1.80536700	-1.68095100
H	-3.10458400	1.30267900	-2.40858600
H	-3.11808800	2.28640100	-0.91830100
Pd	0.48425700	0.10681700	0.41000400
C	3.60821900	-2.15926600	-0.41160300
O	2.53184000	0.02224500	0.60365300
O	4.57223400	0.29012800	-0.79181600
F	4.31948600	-2.32765200	0.70554100
F	2.45086900	-2.83104500	-0.29185700
F	4.28973600	-2.66480200	-1.44444600
F	0.99477100	4.73691800	-0.14985500
F	-1.12176100	4.66874200	-0.66924000
F	-0.50907400	4.98214500	1.40111500
O	2.34744600	-0.32123500	-1.85775000
S	3.26615700	-0.35350200	-0.71011100

b₆-TS1'

Imaginary Frequency: -1232.9372

C	-0.95338700	-2.10579400	1.45502000
O	0.23342300	-1.66651100	1.44328000
O	0.58577100	2.12178600	-0.14740600
C	-0.26853700	2.80918700	0.47008700
O	-1.23099400	2.38355400	1.17413700
C	-0.20504800	4.34044100	0.26815900
C	-1.96853100	-1.35117100	0.77986600
C	-3.20566300	-1.75951100	0.17598300
C	-1.62137100	-0.07487300	0.25870200
C	-3.54860700	-0.72213700	-0.73651900
C	-4.04688800	-2.88410400	0.27867100
H	-1.32855500	1.06565800	0.91001500
C	-4.71670800	-0.76524700	-1.51138200
C	-5.19579100	-2.93193100	-0.49568300
H	-3.81521000	-3.69448600	0.96160600
C	-5.52821900	-1.88230100	-1.38034700
H	-4.98160800	0.03823600	-2.19037400
H	-5.85809500	-3.78895500	-0.41847100
H	-6.43837800	-1.95080700	-1.96849700
N	-2.56461300	0.25443300	-0.68789000

b₆-IN2'

C	-1.62755500	-2.30939300	-0.29050600
O	-0.37714200	-2.03223800	-0.33888300
O	0.40346500	2.04781100	0.00825900
C	1.47397900	2.65014500	-0.16024300
O	2.64119700	2.15999800	-0.37704400
C	1.44848200	4.19500900	-0.15045500
C	-2.53200600	-1.24386600	-0.13093100
C	-3.96401700	-1.07228500	-0.02357700
C	-1.93072600	0.03524600	-0.03456600
C	-4.15913000	0.32271600	0.13459100
C	-5.08274100	-1.91465400	-0.04142200
H	2.61390400	1.11599900	-0.35565700
C	-5.42325800	0.89315700	0.27181800
C	-6.35117400	-1.35260600	0.09587000
H	-4.97094000	-2.98840100	-0.15901300
C	-6.52126500	0.03274600	0.25031100
H	-5.55568300	1.96384000	0.39207100
H	-7.22469000	-1.99820100	0.08358700
H	-7.52147500	0.44251000	0.35544100
N	-2.90111600	0.96199300	0.12376800
C	-2.01525300	-3.75453300	-0.40741800
H	-2.69706100	-3.89743100	-1.25399400

H	-1.12562200	-4.37153900	-0.54454700
H	-2.54349800	-4.07484800	0.49857500
C	-2.75359600	2.40418900	0.27171000
H	-1.69939500	2.66678900	0.23905900
H	-3.28283000	2.91647500	-0.53892600
H	-3.17888900	2.72369400	1.22897900
Pd	0.04012500	-0.04178400	-0.13051300
C	3.44497700	-2.63374800	-0.30335100
O	2.05397400	-1.69967000	1.78450000
O	4.20588900	-0.51776200	1.14378100
F	4.14082200	-3.50172100	0.43611100
F	2.35741600	-3.23961700	-0.78373700
F	4.20228200	-2.21822400	-1.32220100
F	0.26772900	4.64194500	0.29408500
F	2.41793800	4.67547000	0.63301400
F	1.63526800	4.64377200	-1.40156400
O	2.19759900	-0.31721400	-0.29647700
S	2.96343700	-1.18534600	0.76288600

b₆⁺-IN1

C	-1.63751500	-0.19769600	1.84966200
O	-0.40371400	0.09021000	1.88558200
O	0.04974400	2.52718900	-1.16114300
C	0.81805600	2.78703100	-0.24371900
O	1.34742800	1.99138100	0.62746800
C	1.25658500	4.25461500	0.01079900
C	-2.44352200	-0.23642400	0.67049200
C	-3.78647900	-0.77502400	0.47884500
C	-2.08583500	0.35655100	-0.54887200
C	-4.14281200	-0.47704700	-0.86098300
C	-4.70262500	-1.49490200	1.26189200
H	-1.20631200	0.93919300	-0.80425900
C	-5.35938900	-0.85301400	-1.43020400
C	-5.92252200	-1.87143400	0.70484200
H	-4.47722600	-1.76631600	2.28685900
C	-6.25142700	-1.55463000	-0.62408300
H	-5.60212800	-0.61308200	-2.46077000
H	-6.63344900	-2.42551000	1.31090300
H	-7.20985400	-1.86477500	-1.02940700
N	-3.08303100	0.22445100	-1.44340900
C	-2.24306000	-0.50070300	3.19975900
H	-3.23076900	-0.04479800	3.30992700
H	-2.35466700	-1.58712000	3.31133300
H	-1.57152600	-0.14337300	3.98247100

C	-3.06964000	0.76487800	-2.79647500
H	-3.10554000	-0.04681100	-3.53016700
H	-3.93115800	1.42308400	-2.94538500
H	-2.15169700	1.33825800	-2.93370600
Pd	0.99255800	0.03040300	0.39324000
C	3.62106000	-2.59808200	0.09725900
O	2.47400800	-0.45856500	-1.05994300
O	0.99090800	-2.06656000	-0.06271300
F	4.76899400	-2.43574700	-0.55545300
F	3.65840900	-1.92250300	1.24632700
F	3.42171200	-3.89120200	0.34616000
F	0.74427300	4.69109300	1.17952100
F	2.59485100	4.35830900	0.07499200
F	0.81818200	5.06148700	-0.96335100
O	2.22885400	-2.73108400	-2.18870200
S	2.22106400	-1.96104200	-0.96102600

b₆⁺-TS1

Imaginary Frequency: -103.3278

C	-2.37482200	-0.49425900	2.15604500
O	-1.15543500	-0.73284000	2.39624200
O	1.44537300	1.25145300	1.50616000
C	1.14900400	2.24606800	0.83060400
O	-0.01434200	2.67878300	0.53002000
C	2.29121500	3.04956100	0.15569800
C	-2.68952500	0.04481300	0.85936500
C	-3.83629700	-0.02931100	0.01595800
C	-1.60466900	0.58555200	0.09262200
C	-3.40137100	0.43673200	-1.26612000
C	-5.17017000	-0.46204800	0.17434900
H	-0.87389100	1.46230700	0.46582400
C	-4.27168400	0.50090800	-2.36572200
C	-6.02226000	-0.39999100	-0.91361800
H	-5.52783600	-0.82524000	1.13239300
C	-5.57626200	0.07775400	-2.17048900
H	-3.93387700	0.85337100	-3.33440600
H	-7.05413400	-0.72027900	-0.80684000
H	-6.27453100	0.10724900	-3.00161600
N	-2.07171100	0.78736600	-1.18716800
C	-3.39326400	-0.82033500	3.20484100
H	-4.10181300	0.00519700	3.32881300
H	-3.96294100	-1.70752100	2.89798000
H	-2.89453600	-1.03570400	4.15165500
C	-1.27746500	1.39793000	-2.25233700

H	-0.88686500	0.62418900	-2.92024800
H	-1.89698700	2.09944500	-2.81647400
H	-0.44805300	1.93848100	-1.79370200
Pd	-0.03801500	-0.74844600	0.66497500
C	3.61916600	-1.31441800	-0.52639000
O	1.00876200	-0.95715400	-1.11684700
O	1.49261400	-2.44704500	0.71730900
F	3.98980800	-0.87345100	-1.72866300
F	3.57422500	-0.30764700	0.33186900
F	4.48197900	-2.23825000	-0.10171000
F	2.23264700	2.85237200	-1.18834000
F	2.17455900	4.37275000	0.37498800
F	3.50574300	2.66301700	0.56984100
O	2.07765000	-3.19014100	-1.64966000
S	1.93680800	-2.11511400	-0.68365900

b₆⁺-IN2

C	-1.65657400	-0.52704500	2.10429700
O	-0.39867300	-0.40020900	2.34013300
O	-1.78160800	2.45206300	1.08845200
C	-1.06612400	2.84179100	0.19980900
O	-0.02090900	2.20436900	-0.32907700
C	-1.26166400	4.20328500	-0.50358500
C	-2.03153200	-1.05825700	0.85480300
C	-3.24246200	-1.39538900	0.13573000
C	-0.94024900	-1.38062300	0.01736100
C	-2.80481300	-1.91838000	-1.10933300
C	-4.61768300	-1.31491900	0.38746700
H	0.09330400	1.34045400	0.12577400
C	-3.68859300	-2.36177900	-2.09133500
C	-5.50857500	-1.75792500	-0.58882300
H	-4.99050100	-0.90916800	1.32293200
C	-5.05234900	-2.27560500	-1.81207700
H	-3.33529500	-2.75855200	-3.03800800
H	-6.57682100	-1.69889300	-0.40124300
H	-5.77050800	-2.61192400	-2.55397400
N	-1.39438600	-1.89194400	-1.14336900
C	-2.60361000	-0.07192900	3.16992700
H	-2.95743000	0.93245000	2.90591700
H	-3.46972700	-0.73669400	3.24063300
H	-2.09107300	-0.01987200	4.13277000
C	-0.59654700	-2.35643900	-2.27163900
H	-0.80459600	-3.41385000	-2.46434300
H	-0.84081800	-1.77496900	-3.16662800

H	0.45949600	-2.23291700	-2.03491800
Pd	0.81042500	-1.01870600	0.80291000
C	3.92484500	0.44528900	-0.76714000
O	2.21171100	-1.60136600	-0.67584200
O	2.97792600	-0.73253200	1.44679800
F	4.24339800	0.19389900	-2.03628700
F	2.88489200	1.28568500	-0.73027600
F	4.96292300	0.99846300	-0.14414300
F	-0.15991100	4.96024300	-0.37345900
F	-1.49767500	4.01739700	-1.81425300
F	-2.29699400	4.85360300	0.03095100
O	4.62195300	-2.02677200	-0.01241000
S	3.47048700	-1.14952900	0.08692300

b₆⁺-IN3

C	-1.86713700	2.17000000	0.14533900
O	-0.61187600	2.38628900	-0.00634200
C	-2.31546200	0.83763200	0.07199700
C	-3.56125300	0.10647600	0.16625900
C	-1.28767200	-0.10301400	-0.16747300
C	-3.21020400	-1.25575800	-0.02545700
C	-4.90512000	0.43310900	0.38506900
C	-4.15066200	-2.28323300	-0.00445100
C	-5.85290100	-0.58960700	0.40744200
H	-5.21061600	1.46443700	0.53556800
C	-5.48270700	-1.93026400	0.21546700
H	-3.86422700	-3.31979900	-0.15301300
H	-6.89763000	-0.34467800	0.57651900
H	-6.24267500	-2.70572600	0.23793100
N	-1.81598300	-1.34140600	-0.22599400
C	-2.75256800	3.35800200	0.38733000
H	-3.51472200	3.42692200	-0.39805200
H	-3.27731800	3.24940000	1.34402900
H	-2.15951300	4.27415200	0.39965700
C	-1.10119400	-2.58994000	-0.45901800
H	-1.23407300	-3.26187800	0.39534000
H	-1.48624100	-3.07782800	-1.36043100
H	-0.04175300	-2.37286300	-0.58917100
Pd	0.49148800	0.67515100	-0.33646500
C	3.79898900	-0.57843800	0.99987600
O	1.77756000	-0.97746700	-0.69482500
O	2.68924300	1.26199200	-0.59923800
O	4.08956000	-0.58777200	-1.65690700
F	4.91663300	0.12199900	1.18674300

F	4.07071600	-1.88210800	1.07381100
F	2.91241200	-0.25912700	1.94861600
S	3.09411200	-0.18376500	-0.68045700

b₆^{''}-IN1

C	1.28839300	-1.31583900	-1.83970200
O	0.05856400	-1.07449500	-2.02679500
O	-2.40650700	-1.28817100	-0.58309900
C	-2.31713000	-1.77478800	0.61155000
O	-1.52597100	-1.49216400	1.50292900
C	-3.38267100	-2.88064500	0.84035400
C	2.00370900	-1.05342500	-0.63010300
C	3.44178900	-1.03400400	-0.38424500
C	1.39393200	-0.84113800	0.61418000
C	3.60088300	-0.79237500	1.00408300
C	4.59759300	-1.15391800	-1.17186500
H	0.34257000	-0.86931200	0.88278000
C	4.84634500	-0.68058900	1.62219500
C	5.84630500	-1.04923200	-0.56382300
H	4.53592000	-1.32143200	-2.24115400
C	5.97323200	-0.81716000	0.81638600
H	4.93671800	-0.49153100	2.68742800
H	6.74152500	-1.14562900	-1.17124800
H	6.96138000	-0.73816500	1.25953600
N	2.32771400	-0.69669400	1.57359400
C	1.98848900	-1.93694700	-3.02457300
H	2.56029400	-1.16258900	-3.55265400
H	2.68332000	-2.72297000	-2.71691500
H	1.24205300	-2.33785700	-3.71273700
C	2.04685500	-0.49205400	2.98807100
H	2.55076300	-1.25792300	3.58538500
H	2.39253600	0.49727000	3.30493200
H	0.96969300	-0.56627100	3.14393300
Pd	-1.16090100	0.22247900	-1.02047900
C	-0.31458700	3.21662400	1.04034300
O	-0.16384900	2.08963000	-1.39215500
O	-2.26236500	1.87415900	-0.23719500
F	0.10865800	2.06318900	1.57264900
F	0.73319700	4.01028200	0.82575800
F	-1.16186400	3.80444600	1.87984900
F	-3.10612400	-3.95033900	0.06713200
F	-3.39001500	-3.28078700	2.11803700
F	-4.61385400	-2.44358900	0.52740900
O	-1.59461000	4.17942200	-1.09770500

S	-1.17876400	2.89102100	-0.58280400
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b₆^{''}-TS1

Imaginary Frequency: -101.2179

C	0.36042400	-2.52026500	-1.72787900
O	-0.60293300	-1.88247100	-2.15837500
O	-2.60741000	-0.05046100	-0.44886700
C	-3.12811200	-0.44599900	0.66605700
O	-2.57572200	-0.82233000	1.69183700
C	-4.68039700	-0.43596000	0.57584300
C	0.96246600	-2.15287100	-0.43697500
C	2.32467700	-2.12637000	-0.00189900
C	0.18089700	-1.66825900	0.63070900
C	2.31118500	-1.60020800	1.32524800
C	3.56448400	-2.43914500	-0.59892300
H	-0.88153600	-1.77863400	0.81796100
C	3.48653800	-1.39972500	2.06145300
C	4.72416800	-2.25123200	0.13301300
H	3.61281400	-2.82591000	-1.61162300
C	4.68533500	-1.73619800	1.45017500
H	3.46196000	-0.99624600	3.06864500
H	5.68435700	-2.49718700	-0.31030800
H	5.61638200	-1.59675900	1.99170600
N	1.00362100	-1.35105800	1.68410700
C	0.92667700	-3.67956300	-2.51800000
H	1.80111200	-3.32864400	-3.08224000
H	1.25273500	-4.49992400	-1.87207600
H	0.17947500	-4.02627500	-3.23475100
C	0.55166200	-0.86388000	2.98232400
H	0.84246900	-1.56217900	3.77390200
H	0.99290700	0.11709900	3.18375800
H	-0.53423800	-0.76833100	2.95260600
Pd	-0.65420000	0.25757100	-0.68931800
C	1.55361300	2.98421000	0.59236000
O	1.27147000	0.95448500	-1.12582400
O	-0.56398800	2.52020100	-0.98685400
F	0.96307900	2.24531300	1.54287900
F	2.87217500	2.80842600	0.65901700
F	1.25926100	4.26630500	0.78818500
F	-5.09513400	-1.34728900	-0.32476100
F	-5.22649400	-0.73733200	1.75978000
F	-5.13327700	0.77036800	0.19526400
O	1.61856100	3.28628200	-2.06292400
S	0.93883600	2.45544600	-1.08837400

				Imaginary Frequency: -1119.6640			
b₆''-IN2				C	-2.16022600	1.14080200	1.88984400
C	1.80147300	2.30228200	-0.02089900	O	-2.19851700	-0.07026400	2.07732200
O	2.60099900	2.32203500	0.89564900	O	-0.99492100	-2.24451000	0.06021000
O	2.17844200	-0.34938800	-0.65978900	C	-2.11625400	-2.09403600	-0.47901800
C	2.80266400	-0.75103900	0.41021300	O	-2.60920400	-1.03790900	-0.96618200
O	2.34253900	-1.00111300	1.51118900	C	-2.98640400	-3.36662600	-0.62392300
C	4.32270500	-0.88466500	0.13017100	C	-1.51055000	1.68138700	0.67018700
C	0.38734000	1.82692700	0.24691700	C	-1.42554200	3.01349400	0.16897800
C	-0.84275000	2.55460500	-0.11017400	C	-0.90906500	0.81899900	-0.28802500
C	0.07373800	1.16818700	1.48800300	C	-0.72799600	2.93152300	-1.07996000
C	-1.80138700	2.24738600	0.88095600	C	-1.86142900	4.28645000	0.61402400
C	-1.19804100	3.41462200	-1.15508500	H	-1.79896000	-0.10176500	-0.68509900
H	0.75742600	0.60658500	2.11228300	C	-0.46123200	4.06736600	-1.86736600
C	-3.10034100	2.74457800	0.85487000	C	-1.58957000	5.39846100	-0.15794900
C	-2.49254100	3.93140600	-1.18600200	H	-2.39342200	4.39636300	1.55127600
H	-0.48949200	3.66781500	-1.93626600	C	-0.89387900	5.28984600	-1.38910000
C	-3.43161100	3.59858700	-0.19745300	H	0.07664900	3.99158600	-2.80656300
H	-3.82989600	2.48318600	1.61434500	H	-1.91127200	6.37855600	0.18129300
H	-2.78166100	4.59776100	-1.99292100	H	-0.69388000	6.18891600	-1.96481500
H	-4.43492700	4.00996800	-0.25199400	N	-0.43072300	1.62034800	-1.32817600
N	-1.20047200	1.39932900	1.83371700	C	-2.77894900	2.09385100	2.89292100
C	2.15845800	2.77745300	-1.41227500	H	-2.03986800	2.82040300	3.25058100
H	1.60427300	2.24228300	-2.18815500	H	-3.60476200	2.65492200	2.43888900
H	1.93517800	3.84905800	-1.49927200	H	-3.15913600	1.51551200	3.73686700
H	3.23136700	2.63768900	-1.55899400	C	0.29074200	1.12546400	-2.49126900
C	-1.92320500	0.71167900	2.89654500	H	0.01082500	1.70428700	-3.37535900
H	-2.49667900	1.43568200	3.48120700	H	1.37261700	1.18863100	-2.33637500
H	-2.59906800	-0.03360500	2.46576800	H	0.01989500	0.08064600	-2.65457600
H	-1.20294800	0.21420500	3.54759500	Pd	0.33783800	-0.70284200	0.32669700
Pd	0.18248500	-0.20769000	-0.54089500	C	3.99236700	-0.62579800	-0.54325400
C	-2.36511800	-2.72715800	0.49059900	O	1.95992300	0.60012500	0.67586100
O	-1.94455700	-0.36203400	-0.64270700	O	2.19340700	-1.77492600	1.08182700
O	-0.55026900	-2.18138500	-1.41057400	F	-2.88833200	-3.81050000	-1.89158200
F	-1.41074300	-2.47670600	1.39619200	F	-4.26991200	-3.08735400	-0.36835400
F	-3.53493800	-2.28782200	0.97133200	F	-2.58088300	-4.33343600	0.20046100
F	-2.43557300	-4.03497900	0.26933100	O	3.91457900	-0.18654200	2.08935400
F	4.81829600	0.26808900	-0.36047900	F	4.82651600	-1.65796200	-0.45026400
F	4.99153600	-1.18858200	1.24674000	F	4.68537800	0.49868900	-0.72204400
F	4.54830300	-1.85527000	-0.77639400	F	3.17913700	-0.80802700	-1.59444100
O	-3.01957700	-2.18277400	-2.04497800	S	2.98340500	-0.49358300	1.02033900
S	-1.98033900	-1.82666300	-1.09735100				
				b₆''-IN3			
b₆''-TS2				C	2.09197900	-0.10715700	2.08061700

O	1.25319900	0.76182500	2.33864900
O	0.13314100	2.13371100	-0.28310700
C	1.27155500	2.55287800	-0.45596600
O	2.39266800	1.88856600	-0.41063500
C	1.49621600	4.04033100	-0.80845300
C	2.02146000	-0.86420900	0.82550600
C	2.90206000	-1.87417000	0.25276200
C	0.87908900	-0.81921700	-0.00026300
C	2.23994500	-2.37169100	-0.89822600
C	4.16675100	-2.39706700	0.57043500
H	2.23740900	0.94023800	-0.13464300
C	2.78931200	-3.35159700	-1.72772600
C	4.71931400	-3.37949200	-0.24669800
H	4.71530800	-2.04833600	1.43836800
C	4.04132100	-3.85315100	-1.38348500
H	2.26354600	-3.71202500	-2.60648400
H	5.69564300	-3.78752200	-0.00103700
H	4.49937800	-4.61906000	-2.00239000
N	1.01312800	-1.71156700	-1.01995800
C	3.21422000	-0.39385200	3.05863500
H	3.26312900	-1.46150900	3.30074800
H	4.18236800	-0.10963800	2.62729800
H	3.04696400	0.18479900	3.96894400
C	0.04919800	-1.98820800	-2.07609700
H	0.45391200	-1.69560000	-3.05134100
H	-0.18549100	-3.05712400	-2.09199800
H	-0.86648500	-1.43102000	-1.88149700
Pd	-0.71743800	0.26699700	0.32509700
C	-4.15308100	-0.83065400	-0.71163400
O	-1.99013100	-1.36873400	0.75189700
O	-2.85782500	0.89364200	0.87612800
F	2.04965800	4.12537500	-2.02896400
F	2.32735200	4.59606000	0.08233100
F	0.34168200	4.70099500	-0.80580500
O	-4.19034300	-0.99534700	1.95213700
F	-5.24830900	-0.07695400	-0.76815500
F	-4.48526900	-2.11598000	-0.82609400
F	-3.33966100	-0.49877300	-1.72825700
S	-3.28163800	-0.54789900	0.91354900

b₆-TS3

Imaginary Frequency: -129.9729

C	-3.58924900	-1.70424300	0.43379700
O	-2.36080600	-1.62179000	0.79492700

O	1.80501300	1.62229500	-0.83514000
C	2.18912300	2.22943300	0.14493600
O	1.94390200	1.97893600	1.40601500
C	3.08018000	3.48361700	0.00025900
C	-5.50620600	-0.20776700	-0.62604500
C	-3.40321000	0.61234600	-0.11803000
C	-5.40064100	1.15592000	-1.00038700
C	-6.71374900	-0.87930000	-0.85297200
C	-6.45330200	1.85724900	-1.58384900
C	-7.77264500	-0.18519500	-1.43793100
H	1.31866400	1.19841100	1.50044600
C	-7.64611600	1.16538000	-1.79898600
H	-6.35807100	2.90358400	-1.85679900
H	-8.71381700	-0.69825600	-1.61467100
H	-8.48856700	1.68253800	-2.24893300
N	-4.10393700	1.61283200	-0.68407600
C	-4.26325400	-3.04075700	0.56775900
H	-5.11603100	-2.96342800	1.25279900
H	-4.65141300	-3.37440800	-0.40196300
H	-3.55766100	-3.77783900	0.95552700
C	-3.64528500	2.96834000	-0.95387800
H	-3.88890800	3.23514400	-1.98700600
H	-4.13092800	3.67543300	-0.27326700
H	-2.56697400	3.00159000	-0.80896800
Pd	-1.64307600	0.35033600	0.71960800
C	0.12896300	-2.61221700	2.75613300
O	0.28054200	-0.15416100	1.68685900
O	-0.45660200	-0.37999700	4.08169600
F	-1.14977400	-2.89335000	2.99047100
F	0.41675600	-2.94527000	1.47452900
F	0.89074200	-3.36644000	3.55362100
F	2.37194500	4.59120200	0.29286500
F	4.13711700	3.43299400	0.83233700
F	3.53737300	3.59619000	-1.25360700
O	1.94711300	-0.78455000	3.37411600
S	0.51246900	-0.80058600	3.07511700
C	0.00859700	-0.85948900	-1.20826300
H	-0.33974600	-1.57703400	-0.47882300
C	-0.69923000	-0.81597200	-2.54779800
C	5.24077900	0.77925800	-1.55991000
C	5.84085800	0.56784400	-0.31410900
C	5.37549300	-0.48449300	0.47789300
C	4.31809900	-1.31615700	0.08232000
C	3.75090700	-1.02896800	-1.16674900

C	4.17722100	-0.00314900	-2.02359900
H	5.59001500	1.59303400	-2.18987100
H	5.83368900	-0.66863400	1.44574500
I	2.08380000	-2.25732000	-1.82000000
F	-1.89528500	-0.21144600	-2.46478200
F	0.02193500	-0.14926300	-3.46860300
F	-0.91534500	-2.06745100	-3.01699500
H	0.57228500	0.01973400	-0.90410400
C	3.55337100	0.30441200	-3.36122800
H	3.59634300	-0.55617200	-4.03875200
H	2.50415900	0.59381100	-3.24992600
H	4.07865400	1.13517100	-3.83906600
C	3.88018400	-2.44159400	0.98536100
H	2.82262300	-2.36907700	1.24661500
H	4.04426800	-3.41809500	0.51319000
H	4.44472800	-2.41732700	1.91978700
C	6.93871200	1.48177600	0.17193100
H	7.64392400	1.72421900	-0.63052600
H	6.50947400	2.42569900	0.52896100
H	7.49842500	1.03526900	0.99901900
C	-4.21486700	-0.54953100	-0.06798300
C	-1.48102100	2.96248500	1.61219200
C	-0.89587700	4.35940500	1.74780000
O	-2.37538300	2.54281700	2.34174600
O	-0.95932700	2.26756600	0.62008500
H	-6.83268700	-1.92261700	-0.57598700
H	0.19574900	4.32493800	1.71304400
H	-1.23111200	4.98339900	0.91045100
H	-1.23074600	4.80777100	2.68478400

b₆-IN4

C	-2.56323800	1.86202100	-0.02721400
O	-1.29236700	1.97697900	0.10848800
O	2.92093700	-1.50623600	1.51150300
C	3.56084600	-1.63519200	0.49185800
O	3.61468400	-0.82177500	-0.54584500
C	4.44936100	-2.87298000	0.23800800
C	-4.40568600	-0.02817500	-0.35409400
C	-2.15393800	-0.47341700	-0.24696900
C	-4.16842400	-1.42358300	-0.43110900
C	-5.72490700	0.43925200	-0.40343800
C	-5.19731200	-2.35616400	-0.54954200
C	-6.75974000	-0.48587600	-0.52471300
H	2.97949100	-0.06060200	-0.42432600

C	-6.50126900	-1.86500400	-0.59613300
H	-4.99829000	-3.42159600	-0.60467600
H	-7.78654500	-0.13444100	-0.56514700
H	-7.32912400	-2.56128300	-0.69018600
N	-2.77679700	-1.65608200	-0.36247900
C	-3.37186700	3.12190200	0.04904200
H	-3.88343100	3.29104000	-0.90601200
H	-4.13892700	3.03084500	0.82683500
H	-2.72372200	3.97247400	0.26535500
C	-2.18674600	-2.99008100	-0.35261800
H	-2.56733300	-3.55103300	0.50578600
H	-2.45123200	-3.51550700	-1.27566700
H	-1.10582000	-2.89639500	-0.27603100
Pd	-0.29080900	0.20611700	-0.25638700
C	2.14054000	3.54494700	0.45378900
O	1.68439400	1.08409900	-0.33367700
O	0.78962600	2.93794100	-1.76515700
F	1.03751600	3.47312200	1.21973100
F	3.19097400	3.16248700	1.18436900
F	2.31025000	4.80967800	0.06517500
F	3.97350100	-3.56546300	-0.82326200
F	5.71419700	-2.51590900	-0.03248800
F	4.44871100	-3.68336000	1.29859600
O	3.27319000	2.41908500	-1.67762400
S	1.95987700	2.44888600	-1.04146800
C	0.08790800	0.10894200	1.77891000
H	0.19958100	1.16197300	2.03052700
C	-0.91996100	-0.56940200	2.66421300
F	-1.16106100	-1.84878800	2.29975700
F	-0.43481600	-0.59505300	3.92412800
F	-2.10883000	0.07010600	2.70716100
H	1.03673400	-0.43172000	1.76309700
C	-3.09644300	0.57536000	-0.22760200
C	0.58114800	-1.36396100	-2.08092700
C	1.31228100	-2.35726400	-2.93910400
O	-0.06452500	-0.39450800	-2.52857600
O	0.63362300	-1.54263300	-0.78441100
H	-5.94379200	1.50130100	-0.35154100
H	2.31908700	-2.51408800	-2.54315000
H	0.78888700	-3.32003300	-2.91306000
H	1.35538600	-1.99482900	-3.96740500

b₆-TS4

Imaginary Frequency: -278.4020

C	-2.12165600	2.05086100	0.79981400
O	-0.85221400	2.00223600	0.82709500
O	2.21398300	-1.80238200	1.39308900
C	3.08872500	-1.92359200	0.56200600
O	3.55980600	-1.01446100	-0.26402200
C	3.80491700	-3.27281500	0.33056300
C	-4.15819600	0.61950800	-0.09802400
C	-2.00386400	-0.19723800	-0.08228200
C	-4.09950300	-0.65266400	-0.73291200
C	-5.39236200	1.28806700	-0.01906500
C	-5.22855100	-1.26675600	-1.28286000
C	-6.51569800	0.67870600	-0.56095900
H	3.02672100	-0.16723500	-0.19643100
C	-6.43517900	-0.58396100	-1.18511700
H	-5.17011300	-2.23611700	-1.76638600
H	-7.47654700	1.18125000	-0.50443400
H	-7.33433100	-1.03143500	-1.59773500
N	-2.78249900	-1.11547500	-0.71467500
C	-2.79420200	3.31104600	1.25405100
H	-3.30002300	3.78286400	0.40235500
H	-3.55386400	3.09203400	2.01295700
H	-2.05234600	4.00407300	1.65392200
C	-2.35759700	-2.34173200	-1.38605900
H	-2.88672600	-3.19893400	-0.96343600
H	-2.58219200	-2.25886900	-2.45406900
H	-1.28596800	-2.46290500	-1.24696700
Pd	-0.09358800	0.36042800	-0.23241000
C	2.77541800	3.36124100	0.81315700
O	1.92381300	1.10158900	-0.19327500
O	1.01426900	3.20463500	-1.18044400
F	1.78216200	3.34737800	1.71161900
F	3.83545700	2.73328300	1.33277200
F	3.10288300	4.62999200	0.55174600
F	3.53373200	-3.72458300	-0.91421900
F	5.13589100	-3.14368000	0.44684100
F	3.38516500	-4.18896800	1.20798100
O	3.41338100	2.49320900	-1.62232000
S	2.23719700	2.52117200	-0.75891400
C	-0.82864800	-0.81748200	1.58490400
H	-0.88092700	0.03765300	2.25308900
C	-1.77547600	-1.89726600	2.06682800
F	-1.74169300	-3.00781600	1.30479700
F	-1.36197700	-2.24445300	3.30456400
F	-3.06040900	-1.50725200	2.17375700

H	0.17674300	-1.24538200	1.54280100
C	-2.81322200	0.90576700	0.30885200
C	0.76832700	-0.84935600	-2.45594600
C	1.50902000	-1.81665500	-3.34833300
O	0.31419400	0.23482400	-2.82296500
O	0.62426700	-1.25732600	-1.20670400
H	-5.47104400	2.26011100	0.45679500
H	2.40420800	-2.18444700	-2.83968200
H	0.87154500	-2.68117500	-3.56818000
H	1.77582500	-1.31933700	-4.28247700

b6-IN5

C	1.34432500	2.59882300	0.48774900
O	0.10456400	2.67430900	0.38202500
O	-1.06358800	-1.53637900	-1.57536600
C	-1.59733400	-2.43691700	-0.95838900
O	-2.43134900	-2.35106600	0.04962600
C	-1.34314800	-3.91641800	-1.32567300
C	3.00637800	0.55836000	0.95337200
C	1.60231500	0.47527600	-0.89472800
C	3.27897200	-0.59168100	0.18144500
C	3.72192400	0.78873700	2.13383500
C	4.26339600	-1.51139800	0.54739700
C	4.71543800	-0.11446400	2.49674000
H	-2.47703100	-1.41054900	0.39378300
C	4.98183300	-1.24954700	1.71167400
H	4.47714900	-2.39270800	-0.04755800
H	5.28462200	0.05215600	3.40583000
H	5.76058700	-1.94077600	2.01952800
N	2.42313600	-0.60227400	-0.92965200
C	2.18969500	3.79200800	0.79331900
H	2.72020500	3.64492300	1.74106400
H	2.94701300	3.91259600	0.01015500
H	1.56274900	4.68285400	0.86098400
C	2.35666600	-1.68439100	-1.91554800
H	2.84264200	-1.38482900	-2.84697800
H	2.86393800	-2.55710100	-1.50570800
H	1.31367000	-1.95116600	-2.09555600
Pd	-0.13109000	0.52829400	0.83530900
C	-3.60222700	1.64734700	-0.42383300
O	-2.18744800	0.08636900	1.14445100
O	-2.58373500	2.42471000	1.91068100
F	-2.49437200	2.09636700	-1.04647500
F	-4.03587200	0.55794700	-1.06932500

F	-4.53730600	2.59520600	-0.48606400	H	-4.95642400	-3.16972900	1.79852800
F	-0.96561700	-4.62469100	-0.24570200	H	-4.49791700	-3.85830400	0.23622600
F	-2.45082000	-4.47872600	-1.83346300	H	-3.36259700	-3.94929500	1.61777100
F	-0.36482700	-4.00531000	-2.24355500	C	-3.81649400	2.36502300	-1.39769700
O	-4.46242900	0.71088000	1.90875300	H	-4.21353600	2.49841700	-2.40772200
S	-3.22005300	1.23320500	1.35245100	H	-4.20517600	3.15280400	-0.74545900
C	0.81959700	0.90535700	-2.10725100	H	-2.73140100	2.42323000	-1.42656300
H	-0.02725300	1.53101300	-1.82516600	Pd	-1.65495600	0.12424900	0.61757000
C	1.67733400	1.71495300	-3.07104300	C	0.24853000	-2.64563400	2.79287700
F	2.74089000	1.01436100	-3.52570300	O	0.21014400	-0.17580800	1.73230200
F	0.95736700	2.10641700	-4.13175900	O	-1.18656600	-0.60183600	3.76575100
F	2.16738000	2.82759900	-2.46797700	F	-0.85819900	-3.27880900	3.17446400
H	0.40819300	0.04077200	-2.63054100	F	0.44200500	-2.87945100	1.47388800
C	1.88885400	1.22958300	0.30515200	F	1.29154400	-3.16412100	3.44862600
C	0.47630900	-1.62150500	2.45753900	F	2.99220800	4.28667100	0.66362200
C	0.66238500	-3.09904700	2.76300900	F	4.51646700	2.75403600	0.92238800
O	0.59731500	-0.73400400	3.29048200	F	3.79621900	3.24962300	-1.07287100
O	0.20557600	-1.40371600	1.17803100	O	1.34604900	-0.47401900	3.90075600
H	3.49850000	1.64096300	2.76736900	S	0.12823000	-0.78843200	3.15712600
H	0.37909800	-3.28788900	3.80090800	C	0.05482600	-0.98041200	-1.20481800
H	0.07462400	-3.72224600	2.08558700	H	-0.33288700	-1.75600200	-0.55957800
H	1.72141900	-3.35673700	2.64257400	C	-0.56994500	-0.80958800	-2.57823200
b₆'-TS3				C	5.46933400	0.38866500	-1.46365100
Imaginary Frequency: -140.1218				C	6.08169300	0.05979400	-0.25015000
C	-3.50998500	-2.01497400	0.72513000	C	5.55710400	-1.00053500	0.49247900
O	-2.27573600	-1.82151500	1.02028000	C	4.43248700	-1.72772500	0.07770900
O	2.03670600	1.31691800	-0.61547200	C	3.86413400	-1.33235900	-1.14075900
C	2.34690100	2.00585000	0.33692800	C	4.34264800	-0.28688900	-1.94494800
O	1.90749700	1.92619300	1.56807900	H	5.86020600	1.21435600	-2.05220100
C	3.42451400	3.10641300	0.20685900	H	6.02310000	-1.27427500	1.43530200
C	-5.52193600	-0.79147000	-0.49787000	I	2.12272400	-2.42557500	-1.83971000
C	-3.44303800	0.18170400	-0.21254000	F	-1.73216500	-0.13799100	-2.52760700
C	-5.49129800	0.49845700	-1.08612400	F	0.24175500	-0.13366800	-3.41007500
C	-6.70420000	-1.53895400	-0.56457100	F	-0.82923300	-2.01543100	-3.13506500
C	-6.59645500	1.05615300	-1.72588900	H	0.64812800	-0.15882600	-0.80710900
C	-7.81381400	-0.98913800	-1.20503500	C	3.71059900	0.14868200	-3.24184900
H	1.25588400	1.16826200	1.65696700	H	3.66193900	-0.67018500	-3.96868300
C	-7.76228000	0.29161100	-1.77817600	H	2.69393400	0.51584900	-3.07496500
H	-6.56184600	2.04989200	-2.16091800	H	4.28924800	0.96124400	-3.68807400
H	-8.73628700	-1.56030900	-1.25870500	C	3.92647300	-2.86233100	0.93360600
H	-8.64360500	0.69739400	-2.26609600	H	2.88228200	-2.72411800	1.22491000
N	-4.20556500	1.05039900	-0.90187400	H	3.99686200	-3.82397900	0.41077600
C	-4.11223400	-3.33313100	1.11818400	H	4.51806700	-2.93681800	1.84921500
				C	7.25774400	0.85864200	0.25408100

H	7.98074000	1.05542500	-0.54521600	F	1.43634100	-1.15173000	4.61674700
H	6.91588600	1.82884000	0.63386300	F	1.05930600	-1.87167600	2.59693000
H	7.77673300	0.34356100	1.06772500	F	2.66763600	-0.45151800	2.96241900
C	-4.19874200	-0.98914000	0.05410500	F	1.62920500	4.82289400	-1.76120100
C	-1.51136300	2.93867500	0.87920600	F	3.44488700	4.39553400	-0.63506900
C	-0.98805600	4.33374400	0.44821900	F	3.16051600	3.52514200	-2.60934800
O	-2.34738700	2.84943400	1.76060600	O	0.90835100	1.78463400	3.63266600
O	-1.00981600	1.99825800	0.13608900	S	0.25586000	0.61054900	3.06543000
H	-6.76423200	-2.52893300	-0.12231400	C	-0.34749200	-0.77665400	-0.88335700
F	0.31928400	4.32067400	0.12412400	H	0.11592400	-1.55695600	-0.28200300
F	-1.67386000	4.73891900	-0.65203900	C	-0.99562800	-1.32572300	-2.12699200
F	-1.17227400	5.24575300	1.40590900	C	4.75625700	0.60977300	-1.22896000
b₆'-IN4				C	5.31955900	0.75649100	0.04194600
C	-2.91265300	-2.22141300	1.28701000	C	5.24870400	-0.32651600	0.91896000
O	-1.74573900	-1.70267600	1.42791800	C	4.63625300	-1.53936000	0.56908600
O	1.48537300	1.71246200	-1.56328700	C	4.08992100	-1.62976400	-0.71813400
C	1.82196500	2.64413600	-0.86428800	C	4.13168200	-0.57486400	-1.64251900
O	1.63559700	2.80088600	0.42906700	H	4.78206500	1.44503800	-1.92498300
C	2.53518700	3.87118000	-1.47422300	H	5.67208300	-0.23276800	1.91625200
C	-5.16836500	-1.80507100	-0.05793800	I	3.12003100	-3.48357400	-1.30198800
C	-3.34151000	-0.41918600	-0.21198500	F	-1.71154600	-0.39981600	-2.79843700
C	-5.41245000	-0.75581100	-0.97931600	F	-0.01470500	-1.75522800	-2.94935600
C	-6.17316700	-2.75289800	0.17384000	F	-1.80816200	-2.37473800	-1.88654000
C	-6.61631200	-0.62632300	-1.67016700	H	0.30910500	0.06799700	-1.10553100
C	-7.37911000	-2.63130800	-0.51266500	C	3.54305100	-0.65234300	-3.02976000
H	1.15190500	2.01791100	0.81273500	H	4.03780300	-1.42447800	-3.63115600
C	-7.59902000	-1.58311500	-1.42255900	H	2.47705100	-0.90033800	-3.00467200
H	-6.78882100	0.18526400	-2.36946800	H	3.65034600	0.30708100	-3.54256500
H	-8.16602100	-3.35960600	-0.34039400	C	4.57949700	-2.65720100	1.58119600
H	-8.55081400	-1.51425500	-1.94043900	H	3.54451000	-2.90115300	1.84591600
N	-4.26816100	0.06928200	-1.04962700	H	5.03954500	-3.57450900	1.19741700
C	-3.19550900	-3.47363200	2.05948900	H	5.10232900	-2.36925300	2.49777700
H	-3.96934700	-3.27363200	2.81069500	C	5.98488200	2.05207500	0.44575400
H	-3.57300300	-4.25490200	1.39027300	H	6.92926300	2.19920600	-0.09429000
H	-2.29081100	-3.81916400	2.56203200	H	5.34565700	2.91266000	0.22143500
C	-4.17315100	1.23205300	-1.92795000	H	6.20892500	2.06877900	1.51682200
H	-4.41727000	0.92982900	-2.94993600	C	-3.82391400	-1.58133600	0.42760800
H	-4.87295300	2.00601400	-1.59842400	C	-2.08425000	2.70979600	0.43988800
H	-3.15856900	1.61946900	-1.89873700	C	-2.11795300	4.20111700	0.04310200
Pd	-1.57771200	0.13621800	0.51194300	O	-2.65750700	2.28371700	1.44001600
C	1.43424100	-0.81021200	3.32693400	O	-1.45294900	1.95950400	-0.40923500
O	0.25881500	0.68221900	1.50304900	H	-6.02321400	-3.56654700	0.87660600
O	-1.04570700	0.16272300	3.56237800	F	-0.91557600	4.61948900	-0.37303100
				F	-2.99544100	4.35031400	-0.97672600

F	-2.51839200	4.96098400	1.06100700
b₆'-TS4			
Imaginary Frequency:		-244.0623	
C	2.36302200	2.02205000	-0.93318200
O	1.09444600	2.05216600	-1.02762700
O	-2.25151100	-0.95985000	-1.87102700
C	-3.25050900	-1.08545700	-1.19233600
O	-3.65982400	-0.31047300	-0.21189800
C	-4.23059700	-2.26144600	-1.40119600
C	4.26572700	0.44205100	0.00948200
C	2.07231900	-0.23568300	-0.12150600
C	4.09936500	-0.83991600	0.60250600
C	5.54026500	1.03432300	0.00658300
C	5.16012800	-1.53767900	1.18702000
C	6.59711100	0.34089800	0.58047400
H	-2.98671700	0.40668000	-0.03815500
C	6.40972400	-0.92979800	1.16361200
H	5.01883800	-2.51154900	1.64322600
H	7.58848700	0.78367200	0.58290900
H	7.25865800	-1.44289800	1.60498700
N	2.75682300	-1.22088400	0.50956400
C	3.12834100	3.25412700	-1.30763000
H	3.58551700	3.68338700	-0.40709100
H	3.93439200	3.01257300	-2.00927800
H	2.45454500	3.99147900	-1.74677400
C	2.23281900	-2.43810700	1.12945500
H	2.80289100	-3.29979400	0.77488600
H	2.32111600	-2.35413000	2.21640700
H	1.18929200	-2.56021900	0.85820200
Pd	0.19304700	0.43471200	-0.05836700
C	-2.10278100	3.99242600	-0.25682700
O	-1.65225400	1.45014400	0.22285800
O	-0.22787300	3.09419100	1.42262000
F	-1.21779500	3.97712600	-1.26023200
F	-3.30998800	3.68321800	-0.73802900
F	-2.13897600	5.21852000	0.27088100
F	-3.88407700	-2.97067200	-2.48127100
F	-4.20526200	-3.07468100	-0.33055200
F	-5.48685700	-1.81574600	-1.56652400
O	-2.67375700	2.79992400	2.05612400
S	-1.61058600	2.77004000	1.06027700
C	0.88026200	-0.72655900	-1.87724700
H	1.05653600	0.14178800	-2.50571800

C	1.75522700	-1.87897200	-2.32724100
F	1.58782500	-2.99138900	-1.58963000
F	1.36826900	-2.16464100	-3.58910500
F	3.07088000	-1.59872600	-2.36823500
H	-0.16349700	-1.04916900	-1.89977600
C	2.95996600	0.82413900	-0.44804000
C	-0.73116900	-1.11748200	2.06252700
C	-1.49388900	-2.33168200	2.65110400
O	-0.20834700	-0.28291500	2.77522200
O	-0.68752000	-1.18947900	0.75807100
H	5.70074800	2.01264400	-0.43444800
F	-1.73063500	-2.16720200	3.95269900
F	-0.72618300	-3.44061400	2.49734300
F	-2.65700000	-2.54171600	2.01977300

b₆'-IN5			
C	0.42941500	3.02639600	0.54832200
O	-0.76628100	2.74278100	0.33240000
O	-0.82211300	-1.12259000	-2.06393200
C	-1.13947800	-2.23619800	-1.69514600
O	-1.98300700	-2.56133800	-0.74359400
C	-0.55878200	-3.49443000	-2.37867900
C	2.52191400	1.48410300	1.15526400
C	1.43935600	1.16353400	-0.87744100
C	3.17873600	0.49186200	0.39754000
C	2.99653600	1.81358900	2.43034600
C	4.30500500	-0.18093800	0.87156500
C	4.13308300	1.16484300	2.90112800
H	-2.25949800	-1.75050700	-0.23040100
C	4.77661100	0.17988400	2.13140600
H	4.79686200	-0.95315800	0.29105300
H	4.51982800	1.40977700	3.88521800
H	5.65475700	-0.31850400	2.53022500
N	2.50553700	0.33078600	-0.82262500
C	0.86286800	4.39745800	0.94629200
H	1.46237400	4.36066900	1.86207600
H	1.50701000	4.80293300	0.15559400
H	-0.00725700	5.03978300	1.09247500
C	2.82280200	-0.73846700	-1.77194300
H	3.66403400	-0.45317900	-2.40859500
H	3.06351500	-1.63583200	-1.19943200
H	1.94818200	-0.96257600	-2.38071200
Pd	-0.42577000	0.60011600	0.58944700
C	-4.34649300	1.10797600	0.06179900

O	-2.29272200	-0.34899400	0.79266800	H	-8.49134100	-0.79809500	0.33905900
O	-2.89682200	1.56998100	2.25112500	H	-7.80908100	-3.11566200	-0.18011000
F	-3.52988700	1.90238700	-0.64819600	N	-3.40748200	-1.66370900	-0.59076900
F	-4.76812200	0.11370900	-0.72691200	C	-4.40057500	2.95273700	0.45571100
F	-5.39647200	1.82159700	0.47022600	H	-4.84600900	2.77260200	1.44201900
F	0.52337000	-3.15799900	-3.10556100	H	-3.82567500	3.87961800	0.48388300
F	-0.19298900	-4.41997700	-1.48417200	H	-5.22003100	3.04751500	-0.26570400
F	-1.46959200	-4.03326600	-3.20763800	C	-2.70071500	-2.91258100	-0.85930100
O	-4.35406700	-0.51420500	2.17597100	H	-2.78167600	-3.57373100	0.00905100
S	-3.43596800	0.41508600	1.53074800	H	-3.14795100	-3.40458400	-1.72758200
C	0.73894600	1.48760300	-2.16814400	H	-1.65473200	-2.70128200	-1.06726200
H	-0.21565000	1.97691700	-1.97135800	Pd	-1.15796400	0.48848900	-0.67348400
C	1.56671300	2.43875900	-3.02245000	C	0.62597000	4.38432100	-1.04202200
F	2.75361000	1.90334400	-3.37912900	O	0.50501100	1.73833300	-1.32639600
F	0.90581400	2.76562900	-4.14211300	O	2.74663900	2.73064800	-0.97455200
F	1.83347900	3.58631600	-2.34747800	F	0.72087100	4.48756300	-2.36538700
H	0.51324800	0.58599500	-2.73952300	F	-0.65445900	4.43796900	-0.67822900
C	1.35918400	1.88125800	0.37582200	F	1.30297200	5.36690300	-0.45798800
C	0.79229700	-1.60005300	1.87892600	F	0.32964700	-2.65484800	-4.03006300
C	1.47163300	-2.99376400	1.78553200	F	2.44585900	-2.40023800	-3.57576300
O	0.71036500	-1.00454300	2.93332800	F	1.14701300	-3.44247000	-2.16893200
O	0.40716700	-1.22336700	0.68996500	O	1.08098800	2.61508700	0.93277700
H	2.48370300	2.54159500	3.05101000	S	1.36790700	2.75842400	-0.50157100
F	1.82897000	-3.44410300	2.98896500	C	-0.21157700	-0.14822000	1.45449300
F	2.59835900	-2.90379300	1.02465700	H	0.29668000	0.81394700	1.43461900
F	0.66554800	-3.89700200	1.20733900	C	-1.31085800	-0.36965800	2.47992200
b₆''-TS3				C	4.12081300	-2.22758100	-0.74380500
Imaginary Frequency: -126.9684				C	4.91462500	-1.14432800	-1.14881100
C	-3.51956700	1.80127100	0.08680200	C	4.95979300	-0.01398800	-0.33026700
O	-2.25746500	2.05733900	-0.04065100	C	4.23238100	0.08318100	0.86495900
O	-0.08484600	-1.14988800	-1.53591500	C	3.43151700	-1.02239500	1.19825100
C	0.85443600	-1.10865700	-2.35634900	C	3.36579600	-2.20369400	0.43266300
O	1.53148300	-0.09132100	-2.73558300	H	4.09504000	-3.12550700	-1.35580500
C	1.22229200	-2.43901200	-3.05482300	H	5.57589200	0.83118200	-0.62276500
C	-5.17106900	-0.27358000	-0.06976200	I	2.21184700	-0.89140700	2.96720100
C	-2.90100800	-0.42988200	-0.44259900	F	-2.00555000	-1.48958200	2.19868000
C	-4.80401400	-1.60905600	-0.36740700	F	-0.81804100	-0.50325800	3.72489900
C	-6.51537200	0.02296400	0.18661700	F	-2.16147000	0.66853100	2.50448400
C	-5.72803200	-2.65241900	-0.41383700	H	0.16831800	-1.01381800	0.93331800
C	-7.44572600	-1.01257400	0.14125500	C	2.55349100	-3.41867600	0.81572700
H	1.23618400	0.76570300	-2.22974600	H	2.82793900	-3.79085500	1.80848900
C	-7.05884800	-2.33173900	-0.15402000	H	1.47569000	-3.21279700	0.83711000
H	-5.43346700	-3.67185900	-0.63997600	H	2.71657800	-4.22543100	0.09740400
				C	4.35800500	1.32504200	1.71185000

H	3.39405300	1.82465800	1.84812300
H	4.75649300	1.08823700	2.70515100
H	5.03409000	2.03876400	1.23649800
C	5.70135300	-1.21409800	-2.43340800
H	6.22206300	-0.27501800	-2.63807700
H	6.45019500	-2.01452200	-2.39356200
H	5.04218900	-1.43054000	-3.28211000
C	-3.93644900	0.48021400	-0.11754200
H	-6.83315500	1.03445400	0.41860100

b₆''-IN4

C	1.33274800	-2.42225200	-0.24470100
O	0.10721900	-2.05935400	0.00179400
O	-0.44412700	1.99716200	-0.32711100
C	-1.49153800	2.66215100	-0.50740300
O	-2.69720600	2.24585400	-0.52349200
C	-1.31280500	4.17606800	-0.79078400
C	3.70287200	-1.31519700	-0.67609000
C	1.79002100	-0.08882900	-0.30183800
C	3.98102900	0.07475600	-0.69975400
C	4.74499000	-2.22575900	-0.89074500
C	5.25964000	0.58464000	-0.92693100
C	6.02415400	-1.72556700	-1.11737200
H	-2.74596600	1.21535600	-0.39218900
C	6.27868000	-0.34113800	-1.13471700
H	5.46112000	1.65029600	-0.94015900
H	6.84449100	-2.41678200	-1.28267600
H	7.28895500	0.01293300	-1.31287600
N	2.78379000	0.79257400	-0.46356300
C	1.57420900	-3.89559000	-0.31556700
H	2.26928200	-4.19047500	0.48065300
H	0.63808500	-4.44382000	-0.19949500
H	2.03785900	-4.15388800	-1.27458900
C	2.74677300	2.25501000	-0.39411700
H	3.35892600	2.59009600	0.44735800
H	3.14930300	2.66565900	-1.32383700
H	1.72356800	2.59170200	-0.25869200
Pd	-0.19502900	-0.07524900	-0.09825100
C	-3.57091000	-2.44126600	-0.96326000
O	-2.31898900	-0.21950000	-0.23518800
O	-4.55472300	-0.60113300	0.75025000
F	-4.14484300	-1.78214200	-1.96461700
F	-2.39178900	-2.92623200	-1.36572100
F	-4.35025200	-3.43279400	-0.55618200

F	-1.19663400	4.33050900	-2.11527700
F	-2.35618900	4.86219600	-0.34484900
F	-0.19656400	4.61150300	-0.19731400
O	-2.56604900	-2.00351800	1.49806400
S	-3.29597600	-1.27060700	0.46688200
C	-0.27747600	-0.01749700	2.00412800
H	-0.59026500	-1.04257900	2.19807300
C	0.98126500	0.41116100	2.72362800
F	1.42565300	1.61118900	2.30284800
F	0.65195200	0.51286300	4.02159400
F	1.98047300	-0.47407700	2.60645600
H	-1.07845400	0.70981600	2.12504000
C	2.28455100	-1.41436300	-0.41277800
H	4.56906100	-3.29639900	-0.87940800

b₆''-TS4

Imaginary Frequency: -204.4461

C	1.37558700	-2.11469400	-0.93263600
O	0.13388700	-1.89902900	-0.70228300
O	-0.68455500	2.08542300	0.00373800
C	-1.70916300	2.72993600	-0.31506600
O	-2.81515300	2.27780400	-0.76614500
C	-1.63238100	4.27371200	-0.20663500
C	3.66217800	-0.77791900	-0.89662100
C	1.68400200	0.14750300	-0.17986000
C	3.85198300	0.58036700	-0.50210200
C	4.76165800	-1.51692200	-1.37042300
C	5.10020100	1.20825900	-0.55452900
C	5.99831700	-0.89383400	-1.42766500
H	-2.81456500	1.24477200	-0.80372000
C	6.16598400	0.45149100	-1.02334000
H	5.24017600	2.23749100	-0.24298400
H	6.86051600	-1.44784600	-1.78471500
H	7.15201600	0.90153200	-1.07934100
N	2.62790400	1.11245300	-0.08048000
C	1.75584700	-3.46372900	-1.44688200
H	2.39592000	-3.96230600	-0.70761200
H	0.86575500	-4.06965500	-1.62217600
H	2.33035100	-3.36849400	-2.37539100
C	2.48846700	2.46739400	0.45516200
H	2.95431000	2.52334200	1.44438700
H	2.98672000	3.16951800	-0.21741100
H	1.43528100	2.73182600	0.51800100
Pd	-0.30398900	0.04103200	-0.28931600

C	-3.66286400	-2.56775300	-0.61723600
O	-2.37720600	-0.23430000	-0.70414100
O	-4.43681400	-0.32385800	0.68103000
F	-4.36073100	-2.19589300	-1.68379700
F	-2.54670300	-3.18814400	-0.99965100
F	-4.38646100	-3.36971000	0.15237700
F	-1.30190900	4.75164600	-1.41315200
F	-2.79930000	4.77568100	0.17382200
F	-0.68414600	4.61342600	0.67370900
O	-2.30993400	-1.48377300	1.45046200
S	-3.21297700	-1.04990800	0.37754600
C	0.54146200	-0.09466400	1.81863500
H	-0.44590200	-0.52472200	2.01143500
C	1.60831500	-0.96278700	2.45902700
F	2.85536600	-0.48182300	2.31874800
F	1.31493500	-0.96765900	3.77235400
F	1.58606200	-2.22818600	2.01622200
H	0.63163900	0.95237300	2.09383200
C	2.27294800	-1.04541200	-0.68045100
H	4.65251600	-2.55180500	-1.67638600

b₆''-IN5

C	0.53797400	-1.93222300	-1.65569500
O	-0.67924700	-1.74233700	-1.44400400
O	0.39627700	1.91863800	0.18462900
C	-0.20184500	2.99371000	0.38805300
O	-1.45291300	3.24109200	0.25621800
C	0.66860000	4.19698000	0.82405800
C	2.59866000	-0.30298200	-1.27734800
C	1.56280900	-1.22915400	0.59817500
C	3.35138500	-0.04044800	-0.11867200
C	3.04270900	0.17528400	-2.51407400
C	4.54001200	0.68342600	-0.13915000
C	4.23958200	0.89024500	-2.55331800
H	-1.97650500	2.40206400	-0.01659900
C	4.97522200	1.14195300	-1.38384700
H	5.11143300	0.88550500	0.76022200
H	4.60697800	1.26343500	-3.50377500
H	5.90037600	1.70567500	-1.44633600
N	2.69415000	-0.63002800	0.98619200
C	1.03670600	-2.91909400	-2.64822900
H	1.68096000	-3.64375300	-2.13591700
H	0.20019600	-3.42817400	-3.13059900
H	1.65620200	-2.41757000	-3.40112300

C	3.23948500	-0.53271900	2.34399500
H	4.25352300	-0.93936400	2.34639900
H	3.26146700	0.51742800	2.64725400
H	2.63436100	-1.10579200	3.04068300
Pd	-0.40011100	0.15196800	-0.57265600
C	-4.47716200	-0.64529200	-0.60909500
O	-2.35396200	0.93316200	-0.44747200
O	-3.97412300	1.05272700	1.44151500
F	-5.13864900	0.31282800	-1.24607400
F	-3.80495500	-1.39352600	-1.48690000
F	-5.31729500	-1.40526000	0.08211000
F	1.35931000	4.61923700	-0.24385700
F	-0.07539400	5.18716100	1.29630100
F	1.52968100	3.79062100	1.76655500
O	-2.46543500	-0.97325900	1.14969100
S	-3.25876700	0.12495100	0.57941800
C	0.71086700	-2.07546300	1.50303300
H	-0.32232000	-2.11303300	1.15045800
C	1.23776700	-3.50850100	1.58609500
F	2.50147200	-3.53913100	2.05850200
F	0.46673300	-4.25062600	2.37748700
F	1.25571000	-4.07216600	0.35180800
H	0.67141700	-1.66586700	2.51525700
C	1.40064800	-1.01764500	-0.83764100
H	2.47345200	0.00901600	-3.42380500

Pd(OTf)(TFA)

a₇-IN1

C	1.86069000	0.62218200	1.82893300
O	0.89706300	-0.17706500	1.99123600
O	-2.15498000	-1.93274700	-0.24317200
O	-2.32232700	-0.18842700	1.40151600
C	-3.64000700	0.20584800	-0.91270500
C	1.85138900	1.77137600	0.97153500
C	0.75521400	2.50639000	0.36048300
C	3.02188700	2.36405700	0.49763500
C	1.34796200	3.49635800	-0.46279300
C	-0.64159000	2.48560700	0.48302800
H	4.04856200	2.07930000	0.68020600
C	0.60380400	4.42664300	-1.19020800
C	-1.39316700	3.40588300	-0.24334500
H	-1.13597600	1.77934000	1.13764300
C	-0.78191000	4.36030900	-1.07547700
H	1.08087300	5.17628100	-1.81422600

H	-2.47573600	3.38013400	-0.16590000
H	-1.39764800	5.06344900	-1.62859300
N	2.73559200	3.36683800	-0.36406100
C	3.08654400	0.30633800	2.65624600
H	2.77286100	-0.19797700	3.57346400
H	3.70154000	-0.39482600	2.07970800
H	3.67520000	1.19219500	2.90368100
C	3.70119800	4.17003000	-1.09546800
H	3.56248900	4.04326500	-2.17399900
H	3.58617800	5.22924200	-0.84255000
H	4.70894100	3.84809500	-0.82750200
Pd	-0.46258900	-1.03337400	0.70749400
C	2.73643100	-3.21465200	-1.16516000
O	0.86208400	-2.24805500	-0.16555300
F	2.72914300	-4.29334300	-0.35867800
F	2.05824100	-3.52272400	-2.28521000
F	4.00758400	-2.95778200	-1.50423900
F	-4.45413600	-0.39262600	-1.77720100
F	-4.26439700	1.24642700	-0.35329700
F	-2.54877800	0.63367900	-1.54672500
O	2.77207400	-0.99643500	-0.22654200
O	-4.39749100	-1.58532700	0.92290200
S	-3.16486900	-1.00791100	0.42610400
C	2.09826700	-1.99017500	-0.44451000

a7-TS1

Imaginary Frequency: -45.6705

C	-2.34318400	1.16837300	-1.40483900
O	-1.65624100	0.17046100	-1.75470800
O	1.44043500	-1.51770500	0.34140200
O	2.65031500	-0.54483000	-1.57267200
C	3.92513400	-0.75777000	0.78235600
C	-1.78151000	2.25483100	-0.66088100
C	-0.37462200	2.52273400	-0.45388800
C	-2.47395000	3.17869100	0.11745800
C	-0.29827000	3.59078500	0.46960100
C	0.81355400	1.99257700	-0.98743400
H	-3.53964200	3.28550700	0.26658600
C	0.91872900	4.11636400	0.90769300
C	2.03397000	2.50029600	-0.53985900
H	0.81155900	1.29663600	-1.83099200
C	2.08360800	3.54574100	0.39777500
H	0.96342400	4.93619800	1.61817500
H	2.95108700	2.07972900	-0.93455800

H	3.04757600	3.92329900	0.72428800
N	-1.60477900	3.96443100	0.79950900
C	-3.79533800	1.14644500	-1.79994100
H	-3.89956600	0.64931800	-2.76777200
H	-4.32472300	0.53911000	-1.05480900
H	-4.24065300	2.14268000	-1.84220200
C	-1.95668400	5.00112900	1.75736500
H	-1.56078800	4.75375200	2.74750200
H	-1.55111100	5.96709000	1.43951700
H	-3.04364100	5.07554500	1.81863700
Pd	-0.03925300	-0.56018100	-0.68422400
C	-3.15486300	-2.98728600	0.90297600
O	-1.24414400	-2.06127800	-0.08676200
F	-3.74879400	-3.44292300	-0.21976700
F	-2.40330000	-3.97351100	1.41243500
F	-4.11609300	-2.68968700	1.78819800
F	4.06369800	-1.56564500	1.83218000
F	5.11675500	-0.56668600	0.20762700
F	3.45589200	0.42574300	1.20201800
O	-2.71442100	-0.61723300	0.89124700
O	3.29422300	-2.84769500	-0.72377200
S	2.76435400	-1.51684500	-0.46241200
C	-2.30971800	-1.72314300	0.56659200

a7-IN2

C	-2.76393200	0.69059600	-1.26870000
O	-1.91020400	-0.17821400	-1.57653400
O	1.66652200	-0.72793600	0.38251400
O	2.81786000	0.07430400	-1.67982300
C	4.14952700	-0.01407600	0.63992800
C	-2.39010300	1.90116700	-0.59242100
C	-1.04150000	2.39100300	-0.42301400
C	-3.20592500	2.73160300	0.17140100
C	-1.11517200	3.47949900	0.47488900
C	0.21432800	2.01572400	-0.94838400
H	-4.27379500	2.68106300	0.33447400
C	0.01933000	4.17513500	0.89794000
C	1.35542300	2.69782900	-0.50857100
H	0.31112600	1.38255000	-1.84391800
C	1.25590100	3.75757100	0.40586600
H	-0.05037700	5.00782900	1.59144300
H	2.31987500	2.39535000	-0.89690200
H	2.15697100	4.26934400	0.72822900
N	-2.45861900	3.66358400	0.81413300

C	-4.19511800	0.37637900	-1.60967800
H	-4.23300000	-0.12846700	-2.57869800
H	-4.56268800	-0.33200300	-0.85616400
H	-4.83595500	1.26040800	-1.62582300
C	-2.95260100	4.66258900	1.75011400
H	-2.51492600	4.50434900	2.74086800
H	-2.70019200	5.66904600	1.40138300
H	-4.03774200	4.57502700	1.82398900
Pd	-0.07636600	-0.37434700	-0.60434200
C	-2.11272700	-3.79810400	0.82405600
O	-0.63898300	-2.25152900	-0.14498100
F	-2.58301900	-4.33283700	-0.32244100
F	-1.07362000	-4.53798900	1.23803000
F	-3.08200600	-3.88070800	1.74644800
F	4.22280300	-0.68254500	1.79014500
F	5.35338200	0.00234800	0.06082600
F	3.78298700	1.25334200	0.89741800
O	-2.39798900	-1.41232400	1.03441900
O	3.41440700	-2.18487400	-0.70845400
S	2.93120200	-0.82309000	-0.51539500
C	-1.70960000	-2.31526700	0.58278700

a7-TS2

Imaginary Frequency: -1311.3480

C	0.91259400	-2.64644700	1.19685500
O	-0.15765000	-2.08110300	0.87546500
O	-0.90856400	1.84211600	-0.38936800
O	0.89507000	2.09018900	1.28559700
C	0.00762400	4.28206300	0.03159000
C	2.19147800	-2.18036400	0.73855300
C	2.41475700	-0.98663300	-0.03887100
C	3.39016600	-2.89495600	0.71960600
C	3.73212300	-1.07730300	-0.54292400
C	1.58445800	0.11046300	-0.36726700
H	3.63390100	-3.84807700	1.16804500
C	4.24972100	-0.14651300	-1.44553200
C	2.10168500	1.00128900	-1.33185000
H	1.16928700	1.03223500	0.60556800
C	3.40210100	0.88290100	-1.84996700
H	5.26178000	-0.22310800	-1.83164600
H	1.49802800	1.84807600	-1.63846500
H	3.75826800	1.61638900	-2.56703500
N	4.30954400	-2.24405700	-0.03458200
C	0.78567700	-3.85778200	2.08915700

H	0.79753400	-3.52748600	3.13561200
H	-0.17243700	-4.34634900	1.90004800
H	1.60004900	-4.57297200	1.94921500
C	5.66139000	-2.70010000	-0.32066200
H	5.79050100	-2.85617500	-1.39651100
H	6.39356700	-1.96374500	0.02549300
H	5.83639800	-3.64423500	0.19795800
Pd	-0.47536200	-0.23962100	-0.03406300
C	-4.33260800	-1.93516600	-0.51433500
O	-2.18701100	-2.06033500	-1.60443500
F	-4.76596000	-2.72457100	-1.50812200
F	-4.48121000	-2.61287800	0.64591900
F	-5.13209900	-0.85289100	-0.46423300
F	-1.07242500	4.81737200	-0.52872600
F	0.47786900	5.09465800	0.97504000
F	0.94883900	4.10031200	-0.90132800
O	-2.46757000	-0.66153500	0.15514100
S	-0.45490600	2.64993000	0.80812100
O	-1.41045900	2.93806600	1.86173100
C	-2.84686300	-1.53806200	-0.71589000

a7-IN3

C	-2.19596800	-2.53015600	-0.68451600
O	-0.96811800	-2.35471500	-0.50059800
O	1.29826000	1.18787800	0.26050700
O	-0.07947500	2.56804600	-1.32924100
C	1.93603400	3.73621600	-0.00492800
C	-3.15903200	-1.51169900	-0.39066000
C	-2.83202900	-0.22655200	0.17853700
C	-4.54733100	-1.56392200	-0.47902400
C	-4.05529600	0.43377800	0.42464300
C	-1.59908400	0.35560100	0.51185800
H	-5.19203200	-2.35350500	-0.84006500
C	-4.11222300	1.69870500	1.02041300
C	-1.66298400	1.60898300	1.14332100
H	-0.75198500	2.20640000	-0.68845900
C	-2.89587700	2.26459900	1.38437800
H	-5.05140100	2.20963200	1.20799800
H	-0.75534100	2.07925000	1.51396200
H	-2.88730800	3.23325500	1.87692800
N	-5.08509000	-0.40875500	-0.00260800
C	-2.61103400	-3.89416900	-1.18315200
H	-1.84392100	-4.27742300	-1.86012300
H	-2.67645500	-4.58207700	-0.33106800

H	-3.57821600	-3.87863100	-1.69195500
C	-6.50288100	-0.09391100	0.07340200
H	-6.79849100	0.08338400	1.11258700
H	-6.72811400	0.79905600	-0.51873700
H	-7.07767900	-0.93417100	-0.32015300
Pd	0.07502900	-0.64456400	0.06160800
C	3.78902700	-2.74156100	0.33941500
O	2.20207800	-1.63910100	1.77474600
F	4.47376900	-2.99482700	1.46594600
F	3.51905500	-3.92705800	-0.25128800
F	4.60253000	-2.05017200	-0.48876300
F	3.13491900	3.54134600	0.52494900
F	1.98015800	4.71676400	-0.89909000
F	1.05536900	4.03528900	0.95127100
O	1.81880600	-1.70993900	-0.45159500
S	1.39787300	2.15920800	-0.85311100
O	2.22995200	1.94640700	-2.01317500
C	2.48451400	-1.95290400	0.61977000

a₇⁺-IN1

C	0.99290900	-2.11028500	-1.70217200
O	-0.07404500	-1.45153000	-1.80453700
O	-2.52010100	-0.16661900	-1.11436700
O	-2.12682400	-2.18563600	0.33597700
C	-3.54619100	-0.18186600	1.31934300
C	1.97623300	-1.93898900	-0.66681500
C	1.84912400	-1.41826700	0.68712800
C	3.33850100	-2.17827600	-0.85970500
C	3.16171100	-1.34738600	1.21226800
C	0.76757100	-1.09947100	1.52371800
H	3.85406500	-2.53262500	-1.74143000
C	3.43805800	-0.91052100	2.50987800
C	1.03492800	-0.65549800	2.81558400
H	-0.25537800	-1.24033900	1.19410600
C	2.35157000	-0.54952300	3.30081400
H	4.45306300	-0.86224600	2.89234400
H	0.20346800	-0.39792500	3.46488000
H	2.52295300	-0.20065400	4.31491900
N	4.04571800	-1.80907200	0.23378300
C	1.17549000	-3.17649800	-2.75796900
H	0.58555600	-4.05047900	-2.45324800
H	0.78173500	-2.82516300	-3.71459900
H	2.21282100	-3.49974300	-2.86661500
C	5.49141300	-1.85834500	0.37576200

H	5.89157700	-0.85389100	0.54765700
H	5.76956600	-2.50196400	1.21675300
H	5.92748900	-2.26295500	-0.53935500
Pd	-0.57158400	0.38060700	-1.02831400
C	1.26016900	3.81780300	-0.24939500
O	1.22807800	1.49622200	-0.96240200
F	2.35021700	3.96915200	-1.01362200
F	0.44478300	4.85919300	-0.44013200
F	1.64248800	3.79937300	1.04030200
F	-4.37614800	0.80474200	0.98425700
F	-4.11632600	-0.93748500	2.26171900
F	-2.41743300	0.35360700	1.82538700
O	-0.70686000	2.40520300	-0.45199600
S	-3.12588100	-1.23130000	-0.16015900
O	-4.39390600	-1.71102900	-0.69536100
C	0.54869200	2.49949300	-0.58620700

a₇⁺-TS1

Imaginary Frequency: -199.0635

C	2.30375800	-0.47727100	2.13952100
O	1.05908000	-0.62286700	2.13995100
O	-1.32586700	1.60610000	1.35108600
O	0.74102300	2.29537800	0.14721200
C	-1.56776900	3.07166000	-0.82722700
C	3.06517100	-0.52484900	0.91796200
C	2.48811400	-0.47098500	-0.39200400
C	4.42815000	-0.76579100	0.73403500
C	3.52315100	-0.71973200	-1.31555300
C	1.17464600	-0.16851800	-0.82663700
H	5.21417400	-0.88816400	1.46670000
C	3.27767500	-0.76741400	-2.68816500
C	0.93503700	-0.25811900	-2.21962200
H	0.76756800	0.88630700	-0.34597700
C	1.96426500	-0.54719200	-3.12304700
H	4.06982700	-0.96605300	-3.40420800
H	-0.06205500	-0.04217100	-2.58956300
H	1.74907000	-0.58116800	-4.18651300
N	4.70562100	-0.89362800	-0.58883200
C	2.96476300	-0.23726100	3.47082600
H	2.99467500	0.84521500	3.65009200
H	2.37306800	-0.69691300	4.26501100
H	3.99107200	-0.61363200	3.50055100
C	6.01135400	-1.17510700	-1.16804400
H	5.98435500	-2.11460400	-1.72911200

H	6.31260600	-0.36378800	-1.83808900
H	6.74581600	-1.26223900	-0.36571300
Pd	-0.25709800	-0.84338300	0.55671100
C	-3.89085200	-2.32778400	-0.27740800
O	-2.11522800	-1.92572700	1.33245900
F	-4.69143300	-2.50068600	0.77801000
F	-4.47852500	-1.48500100	-1.13781800
F	-3.73199600	-3.51766900	-0.89306900
F	-2.83019200	3.39551400	-0.53606200
F	-1.01529700	4.06799700	-1.52845700
F	-1.58020500	1.96659800	-1.60436400
O	-1.78437900	-1.25465600	-0.74797000
S	-0.60194300	2.73098000	0.72379500
O	-0.53065200	4.00174000	1.44198700
C	-2.51494500	-1.79630200	0.15657500

a7'-IN2

C	2.00312400	0.30847600	2.00614000
O	0.75106900	0.16680900	2.00836500
O	1.41452400	2.55582900	-0.02843700
O	-0.07030700	1.39980000	-1.71254800
C	-1.12775300	3.36703300	-0.25503800
C	2.82603300	-0.38224700	1.06711100
C	2.30976300	-1.23295800	0.02574800
C	4.21360200	-0.39081700	0.92871500
C	3.41690900	-1.72533600	-0.69789200
C	1.00958100	-1.58509100	-0.34063500
H	4.97167000	0.12098100	1.50552400
C	3.26283200	-2.58417600	-1.78829800
C	0.83830100	-2.44246500	-1.42635800
H	-0.02793900	0.66806400	-1.04030100
C	1.95717500	-2.93148600	-2.13387600
H	4.11110500	-2.96515000	-2.34851800
H	-0.16069300	-2.73517600	-1.73309000
H	1.79312200	-3.59641600	-2.97720400
N	4.56979400	-1.18611800	-0.11241100
C	2.57432200	1.27362200	3.01091500
H	2.49971700	2.28264700	2.58698500
H	1.97957100	1.24605600	3.92710000
H	3.62220700	1.06854400	3.24373500
C	5.92691400	-1.44001900	-0.56907300
H	6.15333400	-2.50970200	-0.51257600
H	6.04857700	-1.10357800	-1.60375300
H	6.62679600	-0.89430900	0.06624000

Pd	-0.48021000	-0.86270200	0.71380300
C	-4.37277000	-1.72451900	-0.10484700
O	-2.79208400	-0.55353000	1.31562600
F	-5.31673700	-1.09394400	0.60238400
F	-4.57320200	-1.46556000	-1.40966500
F	-4.51463200	-3.05128800	0.08497900
F	-0.86835600	4.50003900	0.39731300
F	-2.07378400	3.57704600	-1.16384200
F	-1.53198100	2.43497400	0.60959600
O	-1.99798100	-1.73146200	-0.39757800
S	0.44091100	2.79512900	-1.08873000
O	0.70401600	3.68835800	-2.19886900
C	-2.96079800	-1.28247400	0.32374600

a7'-IN3

C	2.00823500	2.16504600	0.00075600
O	0.74998200	2.14956500	-0.00080100
C	2.76677000	0.95628500	0.00115700
C	2.17483000	-0.35926700	-0.00006000
C	4.14928400	0.76567900	0.00260400
C	3.23453100	-1.29136200	0.00066800
C	0.84650100	-0.79069500	-0.00177200
H	4.95198100	1.49033900	0.00391600
C	3.00824000	-2.66954800	-0.00019200
C	0.60478700	-2.16383700	-0.00267600
C	1.67596700	-3.08233800	-0.00186600
H	3.82035600	-3.39010100	0.00039300
H	-0.41666400	-2.53049600	-0.00405900
H	1.45355900	-4.14603100	-0.00258300
N	4.43190000	-0.56219000	0.00225700
C	2.66219600	3.52594000	0.00244700
H	2.32917100	4.08208600	0.88534600
H	3.75316900	3.47796600	0.00098900
H	2.32682800	4.08546700	-0.87737800
C	5.75985700	-1.15300400	0.00362900
H	5.89955200	-1.77318100	0.89515600
H	5.90069700	-1.77444400	-0.88682500
H	6.50724000	-0.35737100	0.00350900
Pd	-0.57661300	0.55256900	-0.00288900
C	-4.53440700	-0.41420200	0.00234000
O	-2.17370800	-0.78372000	-0.00499500
O	-2.85678000	1.33628000	-0.00508400
F	-5.42342200	0.58509800	-0.04774900
F	-4.76403200	-1.12836700	1.12222100

F	-4.74564700	-1.22161100	-1.05524700
C	-3.08729700	0.11461400	-0.00492600

a₇''-TS1

Imaginary Frequency: -92.3872

C	-0.81161600	-1.48599900	2.23714300
O	0.17732300	-0.77935900	1.99195000
O	3.01696000	-1.66843300	0.45044500
O	3.36129100	0.43811500	1.80879400
C	4.73311800	0.16250600	-0.47863600
C	-1.59653000	-2.05288500	1.15054900
C	-1.22803900	-2.00133700	-0.23595800
C	-2.93878700	-2.42114200	1.17853000
C	-2.38853000	-2.29420700	-0.98808400
C	-0.01452200	-1.70925000	-0.90025200
H	-3.60035500	-2.54258700	2.02585500
C	-2.39818300	-2.25959900	-2.38258700
C	-0.03858900	-1.64214200	-2.30768200
H	0.93779400	-1.76169400	-0.37695300
C	-1.21149300	-1.90064300	-3.03050300
H	-3.29201700	-2.49262100	-2.95377800
H	0.88538900	-1.42566000	-2.83475400
H	-1.19448100	-1.85185400	-4.11487900
N	-3.41735100	-2.57167100	-0.08663600
C	-1.23830400	-1.69068100	3.67592300
H	-1.69193500	-2.67380200	3.83510700
H	-0.36810400	-1.57230500	4.32503500
H	-1.97156300	-0.92161000	3.95182600
C	-4.78254300	-2.91357200	-0.45237000
H	-5.36951600	-3.05495200	0.45680300
H	-5.23236600	-2.10830000	-1.04218900
H	-4.80416800	-3.84045400	-1.03496800
Pd	0.21895100	0.62332000	-0.04030200
C	-2.94081100	3.14542100	-0.06986600
O	-1.75852900	1.06438700	0.15995500
O	-0.53973600	2.84629800	-0.32023000
F	-2.68449800	4.45389300	-0.11306300
F	-3.68823400	2.81596100	-1.14168400
F	-3.65705800	2.87862400	1.03642800
F	5.77857200	-0.40367800	0.13214800
F	4.62539500	-0.34051700	-1.71264100
F	4.93103500	1.47891300	-0.55612800
O	2.19481700	0.53090200	-0.42755200
S	3.19764400	-0.21184900	0.51188800

C	-1.64104200	2.32359200	-0.07610600
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a₇''-IN2

C	2.48030100	-2.86796200	-1.62979800
O	1.38707600	-3.39945700	-1.48856200
O	-3.52412500	-2.71075100	-0.31745700
O	-2.34804500	-0.84235300	-1.58497300
C	-4.32687000	-0.20124200	0.09571400
C	2.96768800	-1.89357800	-0.63583800
C	2.24020300	-1.42329600	0.51176200
C	4.19428700	-1.25400600	-0.59437100
C	3.08256300	-0.52190500	1.20088400
C	0.94211100	-1.67833500	1.01879300
H	5.03334600	-1.32416500	-1.27274700
C	2.70522300	0.11495300	2.40160100
C	0.55222800	-1.02255000	2.22675200
H	0.33731400	-2.46792200	0.58868400
C	1.44961900	-0.14721500	2.90926400
H	3.38231500	0.78981000	2.91635700
H	-0.36289000	-1.33722700	2.71811300
H	1.12988000	0.31271300	3.83849300
N	4.27044300	-0.43503900	0.50387700
C	3.36637600	-3.18648200	-2.82269900
H	4.34715000	-3.55678200	-2.49961700
H	2.87670600	-3.94679400	-3.43352100
H	3.53430700	-2.28893500	-3.43061900
C	5.39593200	0.41802600	0.85491700
H	6.19394900	0.26723100	0.12606200
H	5.09744400	1.47119500	0.84011600
H	5.77601400	0.16432900	1.84974200
Pd	-0.44794700	0.11723100	0.50214400
C	0.69229900	3.69777100	-0.95730500
O	0.98192700	1.56090300	0.11555900
O	-1.06318700	2.06348000	-0.53970600
F	-0.24281400	4.38129700	-1.61768400
F	1.12103900	4.44150100	0.08093700
F	1.73686200	3.48412600	-1.77733800
F	-5.23741500	-0.18723500	-0.87991200
F	-4.90607500	-0.59398000	1.23342300
F	-3.83877700	1.03340700	0.25951500
O	-1.98865200	-1.15505200	0.85672100
S	-2.95055100	-1.37203100	-0.35815500
C	0.14478100	2.35840800	-0.43959200

a7''-TS2

Imaginary Frequency: -1201.9159

C	-1.08934200	-0.58667900	2.29281600
O	-0.06645900	0.03428800	2.02484400
O	2.31573700	0.27035600	-1.23038400
O	2.15874800	-1.78159100	0.15403500
C	3.75962200	0.17139200	1.03513700
C	-1.68544900	-1.53456400	1.33986900
C	-1.26311300	-1.82234900	-0.00655100
C	-2.76702200	-2.36753300	1.59284500
C	-2.12891000	-2.84274200	-0.49001600
C	-0.22874100	-1.33617000	-0.86039700
H	-3.36690600	-2.45574600	2.48838300
C	-2.02383700	-3.38051900	-1.77209300
C	-0.15049300	-1.88962000	-2.16181600
H	1.01422200	-1.56111800	-0.26411600
C	-1.01207200	-2.89942000	-2.60467500
H	-2.70580800	-4.15227100	-2.11786700
H	0.62652400	-1.53165500	-2.83205300
H	-0.90108000	-3.30547600	-3.60543600
N	-3.04021600	-3.15205700	0.51298800
C	-1.77511200	-0.39460800	3.63782500
H	-2.78010800	0.02321000	3.50136900
H	-1.87828500	-1.34525700	4.17471700
H	-1.18003800	0.29419700	4.23981400
C	-4.09069700	-4.15176800	0.41970000
H	-4.78464500	-3.90776500	-0.39166800
H	-3.66500300	-5.14471900	0.23968500
H	-4.64425400	-4.17228000	1.36020500
Pd	0.27828200	0.65963800	-0.77110800
C	-2.29330900	3.70303800	-0.24089300
O	-1.65143500	1.39443200	-0.43202400
O	-0.04070900	2.89603100	-0.66541300
S	3.11848200	-0.74995500	-0.45747200
O	4.26924900	-1.30360200	-1.14894300
F	4.65545400	1.06746400	0.62415200
F	4.33910700	-0.69496400	1.86516000
F	2.75752300	0.78741700	1.65210400
C	-1.24011600	2.60307200	-0.45770300
F	-1.72181500	4.90193900	-0.09512800
F	-3.02567000	3.43936200	0.85658700
F	-3.12673900	3.75108500	-1.29783400

a7'-IN3

C	-1.43682000	0.07937800	2.00182800
O	-0.16103100	0.28524100	2.02793400
O	2.12251600	-0.76606900	-1.10834800
O	1.55412400	-1.47662900	1.23527700
C	3.91682300	-0.37470000	0.77812900
C	-2.07188700	-0.88046100	1.18349500
C	-1.65922900	-1.51233400	-0.06706900
C	-3.25388900	-1.53055200	1.57932900
C	-2.59840100	-2.54400600	-0.31149400
C	-0.69894900	-1.22692400	-1.05069000
H	-3.84824000	-1.38327500	2.47032300
C	-2.55636700	-3.36972800	-1.43385000
C	-0.62458800	-2.06731100	-2.16196300
H	0.43287800	-0.39135400	1.54409500
C	-1.53287400	-3.12653100	-2.34524400
H	-3.28654400	-4.15547600	-1.59862400
H	0.14103000	-1.89679000	-2.91180100
H	-1.44514200	-3.75051400	-3.22995700
N	-3.54494300	-2.52596300	0.72561100
C	-2.19563800	1.00447600	2.89899700
H	-2.22342600	1.97712500	2.38862200
H	-3.22569100	0.68784500	3.06708200
H	-1.67004900	1.13943500	3.84808400
C	-4.65370500	-3.46105700	0.84575300
H	-5.30440300	-3.38562700	-0.03093000
H	-4.27511100	-4.48475900	0.92403700
H	-5.23020900	-3.22124800	1.74075400
Pd	0.39249900	0.40080800	-1.00149400
C	-1.28936100	4.05248300	-0.29791900
O	-1.22471300	1.70439200	-0.70566600
O	0.71214800	2.80250000	-0.84565800
F	-0.53326200	5.14570300	-0.41577200
F	-1.70972200	3.97321600	0.99353600
F	-2.37946500	4.19803400	-1.06940900
S	2.57939500	-1.50414300	0.14762100
O	3.20338700	-2.79124600	-0.12569000
F	4.87643200	-0.24062900	-0.13700900
F	4.44184500	-0.87903600	1.89823900
F	3.39180000	0.82804500	1.04647400
C	-0.51442300	2.77093000	-0.66121800

a7'-TS2'

Imaginary Frequency: -1247.5636

C	1.55375700	-1.95351900	1.40706000
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O	0.41101500	-1.69623000	0.96186800
O	-1.05805500	1.64755600	-1.07130700
O	0.43306100	2.60264100	0.66748300
C	-2.19371600	2.75258100	1.11731500
C	2.72871200	-1.27108900	0.94732300
C	2.74966900	-0.18964100	-0.00610900
C	4.05336000	-1.67984600	1.11204100
C	4.09385900	-0.04346600	-0.41688800
C	1.72791300	0.61705700	-0.55672100
H	4.45969700	-2.47239300	1.72536100
C	4.46970900	0.83834900	-1.43177000
C	2.11807800	1.45208500	-1.62589300
H	1.01511800	1.54407200	0.22277800
C	3.45334500	1.56783900	-2.04609300
H	5.50386700	0.94592000	-1.74503900
H	1.36948700	2.07321300	-2.10840400
H	3.69960100	2.25008800	-2.85399600
N	4.86827300	-0.95376300	0.30869300
C	1.63866400	-3.08645600	2.40296500
H	0.75229200	-3.06501400	3.04159100
H	1.62992700	-4.03986000	1.86058300
H	2.53808800	-3.03826700	3.02141000
C	6.30842000	-1.11563000	0.17688000
H	6.56706200	-1.39501300	-0.84949400
H	6.82188700	-0.18416100	0.43535200
H	6.64212900	-1.90390200	0.85381100
Pd	-0.22057000	-0.15434100	-0.26832700
C	-3.58648900	-2.73654700	-0.55593900
O	-1.36246700	-2.63368500	-1.47612300
F	-3.75812500	-3.79743600	-1.35744300
F	-3.71184900	-3.15986200	0.72222300
F	-4.58505000	-1.86553400	-0.79942900
F	-3.36984400	2.81628100	0.50266600
F	-2.09804700	1.61345300	1.79963500
F	-2.06270600	3.78461900	1.95104800
O	-2.08848000	-0.97749400	-0.10855900
S	-0.83734200	2.84112800	-0.16539800
O	-0.93277900	4.14117400	-0.80705800
C	-2.19547200	-2.08373100	-0.76985800

a₇-TS2''

Imaginary Frequency: -1335.1180

C	1.07591000	-2.78172700	0.45010200
O	0.07841200	-2.30190200	-0.13784900

O	-0.97679000	1.70860100	-0.67169600
O	0.46820200	1.86360600	1.32572100
C	-0.42858200	4.13010000	0.21869600
C	2.33347600	-2.08974300	0.50110100
C	2.56999800	-0.77260200	-0.03317200
C	3.59043300	-2.65355600	0.73058000
C	3.96976200	-0.63669300	-0.16669700
C	1.69314000	0.26648400	-0.42517000
H	3.84969200	-3.63284500	1.10861600
C	4.55160500	0.47575900	-0.77692600
C	2.29728300	1.34765900	-1.10398600
H	0.99574900	0.96490600	0.55090500
C	3.68821600	1.45402300	-1.26903600
H	5.62796900	0.57677200	-0.87995500
H	1.67133500	2.16546300	-1.44360200
H	4.10065800	2.32571600	-1.76819200
N	4.56525800	-1.79582900	0.34047900
C	0.88959500	-4.15654400	1.04238500
H	1.78883000	-4.54872900	1.52149200
H	0.08523500	-4.09441200	1.78374300
H	0.55594700	-4.84784400	0.26180400
C	5.99837500	-2.04040200	0.40405800
H	6.43598700	-1.99774900	-0.59846600
H	6.48531000	-1.29443600	1.04017100
H	6.17242400	-3.03223600	0.82471200
Pd	-0.33981900	-0.33170100	-0.57983400
C	-4.23648000	-2.02044100	-0.20890100
O	-2.42729900	-1.51168200	1.29482500
F	-4.10516200	-3.12913900	-0.97341700
F	-4.91882600	-2.36333600	0.89312300
F	-4.97846200	-1.13298300	-0.89805600
F	-1.44824400	4.64408700	-0.46247200
F	-0.22287900	4.83769700	1.32718000
F	0.67488900	4.17053100	-0.53797800
O	-2.25013100	-0.97480300	-0.90570200
S	-0.83105700	2.36903000	0.68510500
O	-1.98494100	2.42337100	1.56187600
C	-2.83753800	-1.44886400	0.14584800

a₇-TS2'''

Imaginary Frequency: -1312.3621

C	1.54949900	-2.35104000	0.65092400
O	0.52307300	-2.04917700	-0.00266700
O	-0.92604100	1.70726100	-1.09447700

O	0.35597600	2.26635600	0.95171100
C	-2.29817200	2.53322900	1.08286200
C	2.71712200	-1.51620600	0.66133100
C	2.82376200	-0.24333900	-0.00530500
C	4.01993000	-1.90153500	0.98611900
C	4.20312700	0.04227100	-0.11206300
C	1.85108000	0.63721900	-0.53262200
H	4.37283300	-2.79908000	1.47514100
C	4.67834800	1.14659500	-0.82098600
C	2.35486700	1.70735300	-1.30561700
H	1.02658700	1.34108400	0.33619600
C	3.72960800	1.96007300	-1.44038100
H	5.73925900	1.36369600	-0.90258000
H	1.65539000	2.40528600	-1.75680200
H	4.05912200	2.81890500	-2.01711700
N	4.90546700	-0.98023700	0.53403600
C	1.50542400	-3.68224900	1.35978300
H	0.60059600	-3.70518900	1.97572100
H	1.41431700	-4.48577100	0.62066200
H	2.37840400	-3.86462500	1.98981400
C	6.35343800	-1.04606200	0.66472900
H	6.82379500	-1.05538900	-0.32369000
H	6.72507600	-0.18614200	1.23091900
H	6.62240300	-1.96177600	1.19395900
Pd	-0.09162400	-0.20746800	-0.67742300
C	-3.76989100	-2.38054100	-0.39811200
O	-2.13257300	-1.61668700	1.19107900
F	-4.43641400	-2.83898300	0.67191000
F	-4.60339200	-1.58221600	-1.09396100
F	-3.46650900	-3.44094100	-1.17961000
F	-3.36772500	2.81195600	0.34202400
F	-2.37366500	1.29136200	1.54337700
F	-2.21894100	3.39083100	2.10037500
O	-1.90349300	-1.09688500	-1.01207600
S	-0.77394500	2.72472800	0.01951800
O	-0.71797600	4.11226700	-0.41170000
C	-2.47649600	-1.62820400	0.01878700

b₇-IN1

C	1.65488100	0.22384300	1.60120900
O	0.41689600	0.48168500	1.67812500
O	-2.60133000	-0.12044700	-1.14704900
O	-1.68785900	-1.74512500	0.37872500
C	-4.35045900	-1.41078900	0.43993000

C	2.23833800	-0.77657900	0.75819600
C	3.63596700	-0.98715800	0.40250600
C	1.52699400	-1.82151500	0.16035700
C	3.66986700	-2.15576600	-0.39930500
C	4.84233300	-0.30603000	0.63119400
H	0.47348800	-2.05506700	0.22111800
C	4.84357500	-2.67162600	-0.95057200
C	6.01956000	-0.81349600	0.08852300
H	4.86982700	0.60989800	1.20959400
C	6.02489000	-1.98400500	-0.69031900
H	4.83842400	-3.56882300	-1.56190900
H	6.95394000	-0.28884200	0.26536200
H	6.96034300	-2.35196700	-1.10102300
N	2.36402500	-2.63829000	-0.51412100
C	2.52075300	1.04820600	2.51687400
H	2.93550000	1.87339600	1.92308700
H	1.90270500	1.47718500	3.30814400
H	3.34390200	0.47058100	2.94416100
C	1.97650200	-3.84159800	-1.23494500
H	0.89450200	-3.96373600	-1.16470800
H	2.25688300	-3.75625100	-2.28954000
H	2.46756300	-4.71983400	-0.80336300
Pd	-1.01293600	0.31288800	0.23155100
C	0.19385200	4.29486900	-0.70818300
O	1.44879600	2.25168400	-0.44867600
F	1.36859900	4.83500600	-1.05685000
F	-0.68487900	4.52188200	-1.70035200
F	-0.24708800	4.93014400	0.39654200
F	-4.18452900	-0.45376000	1.35199800
F	-5.39407700	-1.12084100	-0.33204500
F	-4.54822400	-2.57933100	1.04772800
O	-0.81660100	2.25255800	-0.17979500
O	-3.05347500	-2.58884900	-1.59265700
S	-2.82215300	-1.53284900	-0.62529300
C	0.34705100	2.77235600	-0.42735200

b₇-TS1

Imaginary Frequency: -24.7715

C	1.69722300	1.54859200	1.53646000
O	0.45626300	1.40896400	1.73048700
O	-1.18542600	-1.17062600	-0.99307800
O	-0.48425400	-2.75997500	0.77517800
C	-3.07624200	-2.63972700	0.17013500
C	2.44072700	0.47875700	0.92328600

C	3.64559200	0.49207500	0.12953800
C	1.98720700	-0.85942500	0.94090900
C	3.84902000	-0.84609400	-0.30092500
C	4.54022900	1.48856600	-0.30039500
H	1.22617000	-1.32361300	1.56145500
C	4.92401200	-1.22041500	-1.11309900
C	5.61082300	1.12104000	-1.10376300
H	4.40181900	2.52608800	-0.01601300
C	5.80249300	-0.21776100	-1.50404600
H	5.06473800	-2.24791800	-1.43215700
H	6.31319900	1.87921900	-1.43647800
H	6.64895300	-0.46820400	-2.13629800
N	2.82856200	-1.63734900	0.21769700
C	2.31826400	2.85271000	1.93178900
H	2.21952400	3.54010100	1.08003000
H	1.75639800	3.28323800	2.76439300
H	3.37443500	2.75165500	2.19146600
C	2.72627800	-3.08603000	0.05816900
H	1.77128200	-3.41631400	0.46663900
H	2.75656100	-3.33680000	-1.00586900
H	3.55542300	-3.58206600	0.57285700
Pd	-0.40350400	0.11174300	0.39026600
C	-2.65896300	3.52918400	-0.67120000
O	-0.33121500	2.88881600	-0.72760900
F	-2.24522400	4.65364000	-1.26844200
F	-3.61873300	2.97628800	-1.43189400
F	-3.20182700	3.86113200	0.51712600
F	-3.24028200	-1.70374800	1.11061500
F	-3.91309500	-2.40716300	-0.83824300
F	-3.33492700	-3.83964700	0.69606500
O	-1.90038700	1.42196400	0.02570700
O	-1.21415100	-3.60887900	-1.49645000
S	-1.31755000	-2.60774400	-0.44293300
C	-1.47104800	2.54738900	-0.46021100

b7-IN2

C	1.37355900	-2.43972800	-1.23390700
O	0.19862000	-2.21247600	-1.61839700
O	-0.19702300	1.16627300	0.70567600
O	0.00944600	2.43420800	-1.44219400
C	-1.96183900	3.10367900	0.23756700
C	2.14599000	-1.28617000	-0.77933200
C	3.15822800	-1.17650600	0.24618600
C	2.05997300	-0.00325500	-1.39874600

C	3.61505800	0.16467700	0.20858600
C	3.67568900	-2.05574100	1.21175500
H	1.57257800	0.27678600	-2.32351800
C	4.57800600	0.65036300	1.09765200
C	4.64383700	-1.58226500	2.08699300
H	3.32690400	-3.08102900	1.28075700
C	5.08743300	-0.24510300	2.03070900
H	4.90624900	1.68389100	1.07093100
H	5.06009900	-2.24878700	2.83595900
H	5.83679700	0.09566700	2.73873400
N	2.95105400	0.83510200	-0.81413300
C	1.88877300	-3.84367400	-1.19955700
H	1.61329300	-4.28708700	-0.23268600
H	1.39314800	-4.42891000	-1.97836500
H	2.97479300	-3.88726400	-1.31064600
C	3.19303700	2.22724800	-1.19097400
H	2.54257900	2.48261500	-2.02594500
H	2.93937100	2.88382100	-0.35450200
H	4.24303800	2.35386800	-1.47168900
Pd	-0.15972000	-0.47640000	-0.49769100
C	-3.95414300	-1.98690400	0.56416000
O	-1.64072600	-2.59573400	0.89567500
F	-4.22805800	-3.07615500	1.29313700
F	-4.51721400	-0.92451700	1.16824200
F	-4.53138900	-2.13619900	-0.64468900
F	-2.78037400	2.28841100	-0.42397100
F	-2.27666900	3.10048900	1.53286700
F	-2.08877900	4.34424400	-0.24500900
O	-2.15974400	-0.71736800	-0.26927800
O	0.63124300	3.49945700	0.76286800
S	-0.19659200	2.55298500	0.01251600
C	-2.42123500	-1.79061700	0.41281500

b7-TS2

Imaginary Frequency: -1297.9925

C	-1.47650800	-1.76647100	1.48197800
O	-0.22105100	-1.69524400	1.31551300
O	0.96513100	1.51365800	-1.07580200
O	-0.57223100	2.48788000	0.62288700
C	2.04163700	2.96777700	0.93378900
C	-2.31821200	-0.84970800	0.77944000
C	-3.70129500	-0.93097300	0.39381300
C	-1.69808800	0.17132300	0.00782500
C	-3.86497600	0.03080400	-0.64078600

C	-4.80767600	-1.70950800	0.78080900
H	-0.99224800	1.32378700	0.45634600
C	-5.09896500	0.25627900	-1.26509500
C	-6.02782600	-1.49575200	0.15553500
H	-4.72010600	-2.45534000	1.56376200
C	-6.17290200	-0.52182300	-0.85528600
H	-5.21758600	1.00609400	-2.04020500
H	-6.89101900	-2.08421800	0.45202700
H	-7.14347100	-0.37746600	-1.32033500
N	-2.64082900	0.64841400	-0.86906900
C	-1.99323800	-2.86443300	2.36528300
H	-2.51772700	-3.61047600	1.75493300
H	-1.16040100	-3.35030600	2.87652800
H	-2.70618000	-2.47091600	3.09768200
C	-2.43763600	1.71581300	-1.84489700
H	-1.39365100	1.72280400	-2.15629400
H	-3.05671000	1.51505500	-2.72166000
H	-2.70400200	2.69095900	-1.42495200
Pd	0.37759500	-0.28080700	-0.04981700
C	3.86799800	-2.60327400	-0.57713500
O	2.29082000	-0.94918500	-0.00997100
F	4.75419500	-1.68631100	-1.01191300
F	4.17847300	-2.90780500	0.69999900
F	4.01711200	-3.70989300	-1.31585900
F	3.17850300	3.09770600	0.26104600
F	1.81615200	4.05752900	1.66376000
F	2.09784500	1.89924000	1.72546900
O	1.56185500	-2.67059500	-1.28840100
S	0.64169500	2.76627400	-0.29094400
O	0.54950700	3.99092700	-1.06479500
C	2.41762600	-2.06102500	-0.66621400

b₇-IN3

C	-2.51704100	-2.29092200	0.35545400
O	-1.24006500	-2.40021900	0.41305200
O	0.76470000	1.17364400	-0.26823200
O	2.54016700	0.76619000	1.44416400
C	2.83306500	2.74427100	-0.32040300
C	-3.05516100	-1.01745100	0.09820300
C	-4.36355300	-0.41829300	-0.04904400
C	-2.09334800	0.00926600	-0.06814100
C	-4.11717900	0.95552700	-0.29897600
C	-5.68785900	-0.87106400	0.00001200
H	2.31893800	-0.71762900	0.89816100

C	-5.14292700	1.87824700	-0.49489500
C	-6.72004000	0.04518500	-0.19651200
H	-5.91369100	-1.91649500	0.18821500
C	-6.45304000	1.40217100	-0.44032200
H	-4.93698100	2.92765800	-0.68035100
H	-7.75051600	-0.29647200	-0.15963900
H	-7.27751400	2.09339500	-0.58788600
N	-2.72300000	1.17635500	-0.30705600
C	-3.32805900	-3.53560000	0.56886200
H	-3.94720700	-3.73761700	-0.31327800
H	-2.67008900	-4.38663000	0.75305600
H	-4.00468400	-3.40426900	1.42161900
C	-2.12594200	2.48802400	-0.53492800
H	-1.04594200	2.37798000	-0.59270500
H	-2.50754000	2.90292700	-1.47311700
H	-2.38017700	3.16328000	0.28834600
Pd	-0.25089600	-0.62778800	0.11022400
C	4.04908800	-2.01142200	-0.31957200
O	1.81805900	-1.48809600	0.46318400
F	4.30938300	-0.82872000	-0.90861300
F	4.47360200	-1.94642800	0.95582700
F	4.71711000	-2.97014200	-0.95406300
F	2.13722600	3.63225500	-1.03422800
F	3.73396400	3.38283800	0.42569600
F	3.45856800	1.90411500	-1.14742300
O	2.02953700	-3.10228100	-1.08510200
S	1.68129500	1.79701100	0.79289200
O	1.02833000	2.76776200	1.66280500
C	2.52572600	-2.28057900	-0.37029500

b₇'-IN1

C	-1.03148000	-3.03258500	-0.26542000
O	0.21629200	-3.00750900	-0.35208100
O	2.22461600	-0.55236000	-1.09140800
O	2.89462800	-1.39365400	1.16446500
C	3.90061700	0.92322000	0.32634200
C	-1.64628000	-1.84181000	0.34469200
C	-2.91138100	-1.17643800	0.09710400
C	-1.09004000	-1.22168400	1.51054100
C	-3.02152400	-0.16047900	1.07719000
C	-3.90567700	-1.30038500	-0.88322800
H	-0.27944100	-1.57014800	2.13959700
C	-4.08437800	0.74464000	1.09714900
C	-4.98108800	-0.42104600	-0.85216300

H	-3.83743000	-2.05525000	-1.65981600
C	-5.06508800	0.59159400	0.12211000
H	-4.14064500	1.54161900	1.83051700
H	-5.76147800	-0.50359400	-1.60208200
H	-5.90825800	1.27543600	0.10668900
N	-1.92278300	-0.24217200	1.93524400
C	-1.82160900	-4.17839400	-0.81473600
H	-2.18787400	-3.90854700	-1.81456900
H	-1.17472200	-5.05258300	-0.91624400
H	-2.68936800	-4.40351700	-0.18809100
C	-1.61687400	0.71901300	2.98968300
H	-0.74203200	0.37149800	3.54117800
H	-1.39575400	1.69058700	2.53992000
H	-2.46552000	0.80420700	3.67398800
Pd	0.35543800	-0.85164500	-0.27217700
C	-1.02907100	3.11521300	-0.62920400
O	0.06870900	1.12471400	-0.05847900
F	-1.76856100	3.16777800	0.51592100
F	0.08313100	3.83522000	-0.42618600
F	-1.74273700	3.69493600	-1.59707400
F	4.20290800	1.60382800	-0.78067700
F	2.90955400	1.55172400	0.97003000
F	4.97456000	0.88367500	1.12347800
O	-1.22564300	1.08963100	-1.92645000
O	4.53103000	-1.41773300	-0.77548500
S	3.38765600	-0.81624900	-0.09683000
C	-0.71569600	1.63280000	-0.96377400

b₇'-TS1

Imaginary Frequency:	-687.3474		
C	-2.27642800	-0.44073700	2.13580300
O	-1.06334500	-0.64368600	2.43097700
O	1.52178000	1.41867300	1.49284400
O	-0.27932700	2.45612100	0.12400400
C	2.20063500	2.72874300	-0.70764800
C	-2.57335800	-0.16001100	0.75755800
C	-3.73214500	-0.29981900	-0.06100400
C	-1.45703100	0.13299500	-0.08523200
C	-3.27206700	-0.12321800	-1.40412400
C	-5.09796000	-0.57059500	0.16609500
H	-0.75760200	1.16959600	0.13067600
C	-4.14406800	-0.17966100	-2.50304400
C	-5.95181100	-0.63617300	-0.92086500
H	-5.47799600	-0.71251700	1.17263700

C	-5.47915000	-0.44085400	-2.24180600
H	-3.78600200	-0.03613900	-3.51707800
H	-7.00727700	-0.83590500	-0.76279700
H	-6.18153100	-0.49968300	-3.06788500
N	-1.91448600	0.11161400	-1.38590000
C	-3.30719800	-0.53610500	3.21866300
H	-3.94390900	-1.41354900	3.04637300
H	-2.81888000	-0.63674200	4.18947800
H	-3.95288800	0.34887900	3.21247400
C	-1.10592000	0.45221000	-2.55272400
H	-0.11550800	0.75313900	-2.21544000
H	-1.01423300	-0.41757900	-3.21046000
H	-1.56839700	1.27946400	-3.09935500
Pd	0.14510200	-0.90383200	0.77245100
C	3.47708000	-2.60154600	-0.65349300
O	1.41823800	-1.34427100	-0.78620300
F	3.25775400	-3.00681400	-1.91461200
F	4.41382400	-1.63952800	-0.67218600
F	3.93595500	-3.63580000	0.05852000
F	3.47698300	2.82053500	-0.33202700
F	2.05381700	1.61166600	-1.45113000
F	1.88858000	3.78290700	-1.46680400
O	1.89874500	-2.25666600	1.16456100
O	1.22806700	3.93035800	1.45483000
S	1.09641600	2.64117500	0.78621400
C	2.18155500	-2.04918300	-0.03708800

b₇'-IN2

C	-1.74596900	0.35659400	1.89853600
O	-0.47584200	0.41576600	2.07597300
O	-1.39610900	2.84338700	-0.01037300
O	0.07230300	1.54372800	-1.60124300
C	1.18581100	3.53177300	-0.21783200
C	-2.22236400	-0.50523100	0.88822700
C	-3.48840600	-0.92778500	0.32735600
C	-1.20308100	-1.18795300	0.18939600
C	-3.15459300	-1.86176200	-0.68876500
C	-4.83844800	-0.63116200	0.55357500
H	-0.01231600	0.86391300	-0.88786100
C	-4.11703300	-2.50186200	-1.46775900
C	-5.80695200	-1.26802900	-0.22007100
H	-5.13200000	0.08731700	1.31273300
C	-5.45323300	-2.19202800	-1.21732600
H	-3.84262400	-3.21259700	-2.24102900

H	-6.85608900	-1.04299400	-0.05136700
H	-6.23059600	-2.67091100	-1.80523300
N	-1.75161800	-1.99184100	-0.74342500
C	-2.60413000	1.23159700	2.75823900
H	-3.52400300	0.71815500	3.05387000
H	-2.05040400	1.54998000	3.64383800
H	-2.87800200	2.12140000	2.17727400
C	-1.04569200	-2.86602100	-1.67277200
H	0.02616800	-2.77403300	-1.50127600
H	-1.35269500	-3.90473300	-1.51289900
H	-1.27708300	-2.57937000	-2.70373900
Pd	0.60857100	-0.77695300	0.79432600
C	4.28120200	-2.05957500	-0.28000800
O	1.88532700	-1.89668600	-0.41467100
F	4.37280700	-3.34550100	0.10943800
F	4.36849200	-2.01780400	-1.61959300
F	5.30812400	-1.38203400	0.23963400
F	0.97056600	4.69979800	0.38309300
F	1.52865500	2.61532800	0.69054400
F	2.15601000	3.65702200	-1.11657700
O	2.88120000	-0.65810500	1.12887900
O	-0.58997700	3.83788400	-2.21920100
S	-0.39374300	2.99678600	-1.05703400
C	2.93613400	-1.47706400	0.18911300

b7'-IN3

C	1.75695600	2.16672400	0.00239200
O	0.50381000	2.43359600	0.00000800
C	2.13906000	0.81015500	0.00129200
C	3.35625200	0.02676900	0.00265200
C	1.05264600	-0.09309100	-0.00237000
C	2.92912800	-1.32771200	-0.00033800
C	4.72942700	0.30124300	0.00590500
C	3.82291200	-2.39633500	-0.00012700
C	5.63055800	-0.76302700	0.00613400
H	5.09295900	1.32473100	0.00818800
C	5.18536500	-2.09464700	0.00316300
H	3.47824100	-3.42583800	-0.00244900
H	6.69742900	-0.55830000	0.00864600
H	5.91033400	-2.90328600	0.00341200
N	1.51891500	-1.35803500	-0.00333900
C	2.71684500	3.32156500	0.00602100
H	3.36385500	3.27254400	0.89003700
H	3.36580600	3.27632700	-0.87678500

H	2.16997300	4.26611900	0.00736900
C	0.72674700	-2.58138700	-0.00708300
H	0.95731700	-3.17328900	-0.89908800
H	0.95349400	-3.17627600	0.88391200
H	-0.33018700	-2.31759700	-0.00894100
Pd	-0.70409200	0.74882800	-0.00516400
C	-4.48277000	-0.68234100	0.00438400
O	-2.08623600	-0.81936700	-0.01036200
O	-2.96569700	1.21614800	-0.01011400
F	-4.59592700	-1.55407100	-1.01399300
F	-4.65644000	-1.35823300	1.15609500
F	-5.45327900	0.22940800	-0.10444200
C	-3.09105800	-0.02490800	-0.01012400

b7''-TS1

Imaginary Frequency: -90.2864

C	-1.85360500	-0.71910400	2.45053500
O	-0.81269900	-0.18361500	2.83573500
O	1.94568100	-0.81481400	0.94249000
O	3.03957200	-2.71761400	-0.22038100
C	4.32112700	-0.36499000	-0.13297200
C	-1.93084000	-1.29876500	1.09806800
C	-3.01701900	-1.39641700	0.16521500
C	-0.83221400	-1.95096900	0.50490000
C	-2.51058900	-2.09630700	-0.96819800
C	-4.34661600	-0.92965700	0.14069100
H	0.09344800	-2.26391400	0.96946500
C	-3.28881400	-2.33917700	-2.10563900
C	-5.12383900	-1.18507700	-0.97796200
H	-4.75945600	-0.37982800	0.98013200
C	-4.59977700	-1.88098800	-2.08983300
H	-2.88564400	-2.85966200	-2.96830100
H	-6.15218800	-0.83770800	-1.00710200
H	-5.23407600	-2.05482200	-2.95408500
N	-1.19318900	-2.44098600	-0.71889900
C	-3.05863800	-0.79592600	3.36194800
H	-3.74701500	0.02011100	3.10418400
H	-3.60219600	-1.73877700	3.25212000
H	-2.73743100	-0.65333600	4.39575200
C	-0.32502600	-3.18345300	-1.62717200
H	-0.84171500	-4.08233800	-1.97589500
H	-0.04255400	-2.55972900	-2.48012200
H	0.58458400	-3.47029600	-1.09825300
Pd	0.33252700	0.36234800	0.56365300

C	-0.91075000	3.96935700	-0.69083600
O	-1.13327000	1.72127400	0.16131200
O	0.91869200	2.43758400	-0.20881600
F	-1.44395100	3.80760300	-1.91509900
F	-1.88188000	4.37155100	0.14403100
F	0.02888000	4.91566800	-0.75220100
F	4.92419500	-0.72457500	1.00030300
F	5.11316700	-0.65260300	-1.16824000
F	4.07895600	0.94615600	-0.11112800
O	2.07558700	-0.78814500	-1.54346500
S	2.71768000	-1.29379400	-0.32054600
C	-0.31429600	2.63620000	-0.21189700

b₇''-IN2

C	-0.33357900	-2.89447400	-0.81919300
O	-1.04938200	-3.61490200	-0.15254400
O	-1.96606700	-0.63116800	-0.84390700
O	-4.17693900	-1.55735900	-0.24525000
C	-3.75238300	1.03946100	0.18820300
C	0.60629100	-1.93630300	-0.10664900
C	2.06545000	-1.88569500	-0.30607300
C	0.42239900	-1.66857700	1.29548400
C	2.63778200	-1.55165600	0.94120700
C	2.90676800	-2.08967400	-1.40514400
H	-0.51391200	-1.70598800	1.84048800
C	4.00739500	-1.39737100	1.12809400
C	4.28316000	-1.95066000	-1.23006900
H	2.50221600	-2.33766900	-2.38052100
C	4.82603100	-1.60711100	0.01774500
H	4.42799100	-1.12532500	2.09070300
H	4.94665300	-2.10543700	-2.07541500
H	5.90141400	-1.50023500	0.12272100
N	1.59883100	-1.42512700	1.88606000
C	-0.29342300	-2.96208300	-2.32976700
H	-0.13085500	-1.97936100	-2.78150200
H	0.52225400	-3.62708000	-2.64330500
H	-1.23539400	-3.38422100	-2.68509600
C	1.77786100	-0.94017100	3.24866300
H	2.51753000	-1.55685900	3.76674600
H	2.11539100	0.10094300	3.23222700
H	0.82395400	-1.00429400	3.77378900
Pd	-0.13518200	0.11116400	-0.33922900
C	1.97500600	3.54729100	-0.25399300
O	1.60881600	1.18473100	0.03833600

O	-0.10929200	2.36989800	-0.68600500
F	2.61981100	3.60470500	0.92490800
F	2.89438100	3.48343700	-1.23435800
F	1.25970700	4.66329100	-0.40820200
F	-4.14990600	1.35803600	-1.04373400
F	-4.78601700	1.14162900	1.02699200
F	-2.79286600	1.89284900	0.57375800
O	-2.55201800	-0.87097000	1.58419700
S	-3.09628000	-0.70390000	0.22810800
C	1.07838900	2.29917400	-0.30539400

b₇''-TS2

Imaginary Frequency: -1128.5842

C	0.24490300	1.86317200	2.33307400
O	-0.29346400	0.83940800	2.74056000
O	-1.93524700	-1.19080700	0.84909000
O	-4.13215400	-0.17482200	1.54813900
C	-3.83547600	-0.98168100	-0.99367100
C	0.50601400	2.03296400	0.88329000
C	1.12892400	3.09368000	0.16136000
C	0.05996500	1.06862100	-0.06244500
C	1.09844400	2.71398900	-1.21939400
C	1.71472300	4.33706900	0.50544900
H	-1.33520200	1.08814000	0.01699800
C	1.62949100	3.53155700	-2.23461300
C	2.24400100	5.13051400	-0.49323400
H	1.75761700	4.66584500	1.53681100
C	2.20233600	4.73032300	-1.85292500
H	1.60679200	3.22808900	-3.27599500
H	2.70290700	6.08067400	-0.23675600
H	2.63398200	5.37967700	-2.60910400
N	0.46594000	1.50568500	-1.32577400
C	0.64793900	2.95695300	3.30150500
H	1.73122100	3.12497200	3.26773500
H	0.15630900	3.90442300	3.05099100
H	0.36138200	2.65452800	4.31025800
C	0.24133400	0.77827500	-2.56640400
H	0.04716100	1.48263800	-3.37944200
H	1.11094900	0.16058600	-2.81465100
H	-0.63055100	0.13402500	-2.44419400
Pd	0.11111700	-0.93309200	0.32664500
C	3.44493800	-3.12490100	-0.12522700
O	2.09264500	-1.13753900	-0.21744800
O	1.09637100	-2.97896900	0.49988300

F	3.84877900	-3.00249200	-1.40311100
F	4.38866700	-2.58934400	0.66798800
F	3.32468000	-4.42248600	0.16415200
F	-4.31060000	-2.19494600	-0.73279700
F	-4.81656400	-0.19321700	-1.42434200
F	-2.89062600	-1.07050300	-1.94231600
O	-2.54573000	1.08515800	0.04528000
S	-3.08131600	-0.26680200	0.55493600
C	2.11032200	-2.38634700	0.07372600

b₇''-IN3

C	2.00283200	0.30838300	2.00598500
O	0.75073800	0.16709800	2.00803300
O	1.41583400	2.55527700	-0.02953000
O	-0.07042700	1.39990300	-1.71287100
C	-1.12624500	3.36754900	-0.25466000
C	2.82568500	-0.38274500	1.06719900
C	2.30934900	-1.23347600	0.02589100
C	4.21327100	-0.39170300	0.92902800
C	3.41648100	-1.72626900	-0.69749300
C	1.00912700	-1.58533700	-0.34061800
H	4.97137900	0.12000100	1.50586800
C	3.26234200	-2.58529200	-1.78774700
C	0.83779300	-2.44287600	-1.42620000
H	-0.02800200	0.66816500	-1.04063200
C	1.95664700	-2.93232900	-2.13345100
H	4.11059900	-2.96660500	-2.34776000
H	-0.16122900	-2.73539300	-1.73302900
H	1.79254600	-3.59739000	-2.97666600
N	4.56941400	-1.18723500	-0.11194400
C	2.57422200	1.27354600	3.01064200
H	3.62162100	1.06727700	3.24462500
H	2.50136100	2.28237100	2.58592500
H	1.97853000	1.24736300	3.92624600
C	5.92655100	-1.44176000	-0.56820200
H	6.15288500	-2.51140500	-0.51058800
H	6.04832200	-1.10639400	-1.60321400
H	6.62642600	-0.89543200	0.06658900
Pd	-0.48062400	-0.86232900	0.71345600
C	-4.37330300	-1.72406500	-0.10468500
O	-1.99847000	-1.73092300	-0.39797100
O	-2.79245600	-0.55239400	1.31487300
S	0.44171900	2.79502700	-1.08926400
O	0.70456300	3.68819000	-2.19951200

F	-2.07271700	3.57789200	-1.16292900
F	-0.86600800	4.50049000	0.39747700
F	-1.53033200	2.43571100	0.61025500
C	-2.96124400	-1.28159700	0.32318000
F	-5.31719300	-1.08864400	0.59833300
F	-4.51689500	-3.04966300	0.09210100
F	-4.57224000	-1.47185100	-1.41100500

b₇-TS2'

Imaginary Frequency: -1304.8449

C	-1.53919300	-2.15772100	0.89035800
O	-0.31869900	-2.11979700	0.55033000
O	0.86141800	1.51937200	-1.10789400
O	-0.44859600	2.15582200	0.90920000
C	2.16631200	2.72894700	0.93375600
C	-2.38594100	-1.05656700	0.55130000
C	-3.80969000	-0.98016000	0.36127800
C	-1.79233600	0.08736900	-0.04718700
C	-4.02977900	0.20526600	-0.39245700
C	-4.91452300	-1.77600800	0.71639300
H	-0.95865000	1.06656100	0.54248700
C	-5.31272300	0.62726500	-0.76649200
C	-6.18470400	-1.36494300	0.33810200
H	-4.78568200	-2.68740000	1.29059800
C	-6.38242000	-0.17498200	-0.39418400
H	-5.47184300	1.54378600	-1.32482800
H	-7.04585200	-1.96558100	0.61556700
H	-7.39062100	0.11998100	-0.66918200
N	-2.80053500	0.80203200	-0.64730300
C	-2.02325900	-3.40402100	1.57260900
H	-2.70765500	-3.94813400	0.90964500
H	-1.17426300	-4.04633200	1.81260200
H	-2.57312300	-3.15395500	2.48632200
C	-2.64286000	2.06041800	-1.37194500
H	-1.66064100	2.08489100	-1.84274500
H	-3.40054900	2.11252200	-2.15627800
H	-2.74965400	2.91921200	-0.70225900
Pd	0.24564700	-0.42170100	-0.44934900
C	4.08620400	-2.24385100	-0.46960400
O	2.02656900	-1.22366400	-0.95191100
F	3.76563400	-3.41496400	-1.05803400
F	4.73681700	-1.48869600	-1.37656100
F	4.93013300	-2.50302600	0.53719400
F	3.18189000	3.04386100	0.13570800

F	1.99931500	3.67767100	1.85246600
F	2.38575600	1.56000800	1.51769000
O	2.64843000	-1.31801900	1.23157500
S	0.61365900	2.62797100	-0.10514200
O	0.37401100	3.94353000	-0.67371100
C	2.80874700	-1.52446300	0.04218300

F	-0.37862600	4.92053900	-0.83549600
O	-2.37417600	-1.30218000	-0.41182100
O	-1.79795900	2.49595700	-1.91748100
S	-0.86321000	2.34700600	-0.81839700
C	-2.79512600	-1.67746200	0.75507900

b7-TS2''

Imaginary Frequency: -1291.0763			
C	1.52059500	-2.23817200	-1.35074200
O	0.25474900	-2.17407200	-1.30390800
O	-1.20913800	1.39799300	0.30930900
O	0.60130400	2.08802300	-1.23541900
C	-0.76703000	4.00166400	0.04351900
C	2.28441400	-1.22154300	-0.69853500
C	3.61337600	-1.24131300	-0.14896400
C	1.58330900	-0.11889500	-0.13539200
C	3.65797100	-0.16248200	0.77646200
C	4.75483000	-2.04897700	-0.30715000
H	0.97243500	0.95985300	-0.81933900
C	4.80863700	0.14629300	1.51403000
C	5.89240500	-1.75102000	0.42957100
H	4.75885800	-2.88150400	-1.00282800
C	5.92020000	-0.66423100	1.32967500
H	4.83499600	0.98244800	2.20501100
H	6.78257300	-2.36118600	0.30866100
H	6.82894700	-0.45773200	1.88703800
N	2.42020200	0.46659300	0.78260400
C	2.12735100	-3.42883700	-2.03476500
H	2.60979400	-4.07573000	-1.29112300
H	1.34897500	-3.99775900	-2.54619400
H	2.89442900	-3.11482400	-2.75075200
C	2.10272200	1.63022800	1.60165800
H	1.02182000	1.70956000	1.69949500
H	2.53481400	1.49107200	2.59558300
H	2.50046900	2.54731500	1.15592200
Pd	-0.49094900	-0.57137800	-0.24391700
C	-4.24222000	-2.22936000	0.69116800
O	-2.18585100	-1.63930500	1.81502800
F	-4.67473500	-2.58995600	1.90610200
F	-5.08782100	-1.30255500	0.20217800
F	-4.29981000	-3.31117700	-0.11189100
F	-1.97037900	4.30284100	0.51662700
F	0.10975600	3.95330300	1.05086900

b7-TS2'''

Imaginary Frequency: -1302.6449			
C	-1.23879100	-2.52956600	0.68248000
O	-0.02434700	-2.38281500	0.35406200
O	1.01373800	1.52531400	-0.68578900
O	-0.46591200	1.81788900	1.27636400
C	0.53191600	4.01345800	0.10246500
C	-2.14949800	-1.44856000	0.46255700
C	-3.57227700	-1.44796700	0.24907600
C	-1.62599800	-0.20726400	0.00784400
C	-3.86181400	-0.20560200	-0.37799400
C	-4.62584900	-2.34988200	0.48807800
H	-0.88875300	0.76029000	0.73397800
C	-5.16312400	0.16803100	-0.73956100
C	-5.91428400	-1.98590400	0.12311300
H	-4.44540400	-3.30739900	0.96502600
C	-6.18127000	-0.73975400	-0.48322600
H	-5.37299400	1.12689100	-1.20208900
H	-6.73657900	-2.66943000	0.31280800
H	-7.20238100	-0.48581100	-0.75150200
N	-2.67422100	0.49634500	-0.53506500
C	-1.64907000	-3.87091300	1.21731900
H	-2.29543300	-4.37851400	0.49029800
H	-0.76333500	-4.48344000	1.39409000
H	-2.21724600	-3.75770900	2.14681800
C	-2.59168900	1.82670200	-1.12421000
H	-1.57192500	2.00313100	-1.45928000
H	-3.25797600	1.87219900	-1.98917400
H	-2.87856700	2.59796000	-0.40260200
Pd	0.45436700	-0.53326000	-0.39905200
C	4.43912400	-1.96511200	-0.34091000
O	2.82928000	-1.25278600	1.31021100
F	5.26498100	-2.14735800	0.69635200
F	4.27317600	-3.15481700	-0.95712700
F	5.03665400	-1.12837400	-1.21118900
F	1.60961600	4.48001800	-0.51743200
F	-0.51516000	4.06521100	-0.72774800
F	0.27291800	4.74543600	1.18173600

O	2.30104900	-1.16081400	-0.89552100
O	2.00433500	2.30825000	1.53386400
S	0.86883100	2.25437800	0.63597400
C	3.06982000	-1.40334000	0.12647700

Pd(OTf)₂-catalyst

Pd(OTf)₂

O	-1.60214100	-0.64503100	1.19244800
O	-1.60231700	-0.64549400	-1.19258600
C	-3.66462000	0.63198800	-0.00000500
Pd	-0.00019700	-0.00027600	-0.00007000
C	3.66544100	-0.63144500	0.00000700
O	1.60173000	0.64400700	-1.19245800
O	1.60220700	0.64462700	1.19260300
O	3.37751400	2.04415500	-0.00038500
F	4.42346600	-0.59366600	1.08995200
F	4.42440400	-0.59342200	-1.08922200
F	2.92446500	-1.73796800	-0.00045800
S	2.54136000	0.86471200	0.00005300
S	-2.54173700	-0.86495400	-0.00002000
O	-3.37910800	-2.04351800	0.00035600
F	-4.42197500	0.59557400	1.09042500
F	-2.92292500	1.73811900	-0.00171100
F	-4.42442400	0.59395700	-1.08866900

Pd(OTf)₂

a₈-IN1

C	-1.43173600	-0.21926700	2.31754800
O	-0.18684900	-0.04653500	2.16872500
O	2.40177900	0.38126700	-1.05447500
O	2.15906900	-1.48437400	0.43753200
C	4.61006200	-0.38826200	0.28296600
C	-2.28533600	-0.93029100	1.41649800
C	-1.99735000	-1.87327000	0.34525800
C	-3.66239500	-0.69783600	1.36231100
C	-3.23221100	-2.13369700	-0.29854200
C	-0.86109000	-2.57755300	-0.07877500
H	-4.25754900	-0.01643000	1.95345200
C	-3.36312400	-3.02340600	-1.36546000
C	-0.97923600	-3.46297800	-1.14745400
H	0.09442300	-2.45518800	0.41440200
C	-2.21076600	-3.67877600	-1.79032800
H	-4.32128200	-3.20451100	-1.84290500
H	-0.09890800	-4.00044200	-1.48727100

H	-2.26790800	-4.37513400	-2.62162700
N	-4.22269900	-1.38444000	0.34455700
C	-1.99965100	0.41171300	3.56756500
H	-1.22646800	0.42797500	4.33946400
H	-2.25384600	1.45085500	3.32462600
H	-2.88577900	-0.10536200	3.94146800
C	-5.61977200	-1.33540000	-0.05534300
H	-5.70725000	-0.96076500	-1.08007300
H	-6.06708900	-2.33319000	0.00086200
H	-6.15932500	-0.66444400	0.61507200
Pd	0.94987800	0.28399800	0.49999800
C	-1.34478800	2.13751300	-1.76488400
O	0.30682800	2.20353700	0.31454700
O	-1.06204000	4.19657900	-0.09290200
F	-0.40776500	2.63522800	-2.56921100
F	-1.27656100	0.79397800	-1.79607900
F	-2.55041800	2.51171900	-2.20560700
F	5.43582500	0.22458600	-0.56013400
F	4.26696200	0.44442000	1.26474900
F	5.20143500	-1.46572200	0.79445000
O	-2.17145900	2.08800500	0.75081600
S	-1.10481800	2.74124600	-0.02004000
O	3.50746200	-1.82570900	-1.69752200
S	3.08083100	-0.92294400	-0.64775400

a₈-TS1

Imaginary Frequency: -54.4954

C	-2.07589100	-0.00167900	2.22726900
O	-0.81882600	0.08659200	2.29939200
O	1.79483900	-0.27095300	-0.82829200
O	2.21832300	-2.13324600	0.71057200
C	4.21376500	-0.40161000	0.28910500
C	-2.73090200	-0.75784000	1.20243300
C	-2.12822300	-1.74246200	0.32964600
C	-4.01278000	-0.53207500	0.70817800
C	-3.08124000	-2.03306700	-0.67308200
C	-0.89995400	-2.42782700	0.32863800
H	-4.76269900	0.16788800	1.04998600
C	-2.82681800	-2.93765800	-1.70601500
C	-0.62874400	-3.31446000	-0.71583300
H	-0.21490100	-2.38242500	1.17696800
C	-1.57887100	-3.55929200	-1.72194100
H	-3.56516700	-3.14968900	-2.47326900
H	0.32550900	-3.83011400	-0.73391300

H	-1.34301700	-4.25741600	-2.51899800
N	-4.22426300	-1.27289400	-0.40737000
C	-2.85279700	0.76613800	3.26146200
H	-2.28239600	0.80164500	4.19285400
H	-2.95254900	1.79480100	2.89182600
H	-3.84401200	0.34499300	3.44308700
C	-5.41725900	-1.24646800	-1.23968000
H	-5.16845300	-0.90053400	-2.24793700
H	-5.86107400	-2.24536800	-1.30125900
H	-6.14367700	-0.56162800	-0.79927900
Pd	0.45200600	-0.13005200	0.69152900
C	-0.31651400	2.72203900	-1.73236300
O	0.60420400	1.92015700	0.62595800
O	-0.34126900	4.18592500	0.50157300
F	0.89333000	3.16971800	-2.06060300
F	-0.44849400	1.45618400	-2.15624700
F	-1.24427500	3.47469800	-2.33451300
F	4.71736000	0.41020900	-0.63756700
F	3.77627700	0.31973000	1.32509300
F	5.15994500	-1.24458500	0.70718900
O	-1.88581300	2.18735000	0.33509700
S	-0.56573000	2.79799100	0.11134700
O	3.32474700	-2.10435500	-1.57859300
S	2.80013300	-1.38157100	-0.43019200

a8-IN2

C	-2.42013600	0.59917400	1.98851700
O	-1.18454200	0.49384000	2.18814700
O	1.40208500	-0.83871400	-0.71818100
O	1.93091800	-2.65913800	0.90661600
C	3.84340800	-0.88702400	0.35118000
C	-3.06591100	-0.19496300	0.97663000
C	-2.47678600	-1.34721300	0.33992600
C	-4.22303800	0.09764600	0.26315100
C	-3.30055700	-1.66888400	-0.76274300
C	-1.33042400	-2.13532300	0.60885600
H	-4.92405400	0.90983200	0.39942300
C	-2.99752300	-2.71780200	-1.63180000
C	-1.01990800	-3.17855000	-0.28114600
H	-0.84336300	-2.12859400	1.59072300
C	-1.83592100	-3.45446600	-1.38577500
H	-3.63284400	-2.95404200	-2.48021000
H	-0.13819600	-3.77888400	-0.08804600
H	-1.56966800	-4.26503500	-2.05623300

N	-4.36661500	-0.76600000	-0.77532100
C	-3.16455500	1.61353700	2.80804100
H	-2.71398000	1.68318900	3.80121800
H	-3.02643800	2.58475500	2.31455100
H	-4.23109300	1.39255500	2.89064000
C	-5.41467600	-0.72600300	-1.78486700
H	-4.98260200	-0.54349700	-2.77385700
H	-5.96572300	-1.67172100	-1.80018800
H	-6.10668600	0.08314000	-1.54626400
Pd	0.10157300	-0.23750800	0.70573900
C	0.78760700	2.78806500	-1.65538100
O	0.99990000	1.61544800	0.71304500
O	0.65803900	4.06009000	0.68936100
F	2.11379400	2.90186700	-1.70796000
F	0.41825600	1.64601300	-2.24912600
F	0.23161500	3.81383000	-2.31125900
F	4.27658900	-0.07600100	-0.61224800
F	3.44585200	-0.16069500	1.39993000
F	4.83765500	-1.69544500	0.73023000
O	-1.24528700	2.52785600	0.02603100
S	0.20044100	2.80037000	0.11148000
O	2.91729600	-2.65625200	-1.43067900
S	2.42443200	-1.92315900	-0.27003400

a8-TS2

Imaginary Frequency: -1307.4765

C	2.02797000	-1.50095300	1.77492200
O	0.81636600	-1.37170100	1.48811300
O	-1.15906700	1.43355500	-0.88022200
O	0.51731700	2.76504700	0.37621100
C	-2.01177900	2.89787200	1.22236600
C	3.06665000	-0.89402000	0.99041300
C	2.85426400	-0.03303000	-0.14325800
C	4.42620200	-1.21063100	0.99786100
C	4.09856300	0.07677000	-0.80418300
C	1.70062700	0.60470200	-0.65757700
H	4.98267200	-1.84433200	1.67474200
C	4.23465400	0.73988100	-2.02477500
C	1.84415700	1.20697500	-1.92866400
H	1.10619100	1.63959400	0.03023600
C	3.08075100	1.28468300	-2.58754200
H	5.19229400	0.81772600	-2.53083600
H	0.98080500	1.68023800	-2.38571300
H	3.14185700	1.79001400	-3.54634500

N	5.04492700	-0.63502800	-0.06171800
C	2.34317200	-2.39812300	2.94742100
H	1.57874100	-2.26028400	3.71595600
H	2.29023800	-3.44287200	2.61742000
H	3.33164200	-2.20742200	3.37199400
C	6.45237700	-0.76790500	-0.40931900
H	6.55844800	-1.24581900	-1.38837500
H	6.93274200	0.21517000	-0.43480700
H	6.94785200	-1.38502900	0.34196600
Pd	-0.10455600	-0.14780200	0.09467700
C	-3.22458100	-2.00848900	-1.29922800
O	-1.88644500	-1.01425500	0.73313500
O	-3.01458100	-3.19812500	1.07514100
F	-4.32551400	-1.35330000	-0.92133800
F	-2.53254100	-1.23411800	-2.15154500
F	-3.58243900	-3.12960000	-1.93563200
F	-3.27015400	2.79863900	0.80927000
F	-1.73317000	1.91249300	2.07390100
F	-1.82290900	4.07311200	1.82198000
O	-0.95692400	-3.03998500	-0.39655400
S	-2.16576000	-2.42505500	0.17252900
O	-1.16618800	3.93160500	-1.11211500
S	-0.87860500	2.79046400	-0.25998900

a₈-IN3

C	2.35111000	-2.15252300	1.05539400
O	1.13938800	-1.94941300	0.79905600
O	-0.93461100	1.34353800	-0.89038500
O	0.20683300	3.09266600	0.50153800
C	-2.02425200	2.05048400	1.55415700
C	3.37349100	-1.26133600	0.60138900
C	3.12310600	-0.10139100	-0.21828500
C	4.75537700	-1.34827600	0.75305800
C	4.38148700	0.45300000	-0.53763900
C	1.93437400	0.45324900	-0.71436600
H	5.35144000	-2.07602100	1.28638600
C	4.51298100	1.57328700	-1.36462600
C	2.06835600	1.55400300	-1.57293000
H	0.94043200	2.51772200	0.16436800
C	3.33599700	2.10329600	-1.88151000
H	5.47950900	2.00194200	-1.61014900
H	1.19498700	1.97588400	-2.06192900
H	3.38670500	2.95708100	-2.55143400
N	5.35844400	-0.32986800	0.08508100

C	2.66821600	-3.41059700	1.82580700
H	1.89499100	-3.57454900	2.58050000
H	2.64101400	-4.26395400	1.13722300
H	3.65047600	-3.37678300	2.30324400
C	6.79122200	-0.09123100	0.00295000
H	7.12484600	-0.13518700	-1.03879700
H	7.03812100	0.89209300	0.41596900
H	7.31501900	-0.85834400	0.57593500
Pd	0.21372400	-0.36341900	-0.15012800
C	-3.89876200	-1.14093900	-0.75917600
O	-1.64951900	-1.17016800	0.58124200
O	-2.82459600	-3.34852500	0.23713500
F	-4.58802900	-0.91068100	0.36771000
F	-3.59054600	0.04635700	-1.31103700
F	-4.67955100	-1.81334600	-1.61163200
F	-3.16432900	1.45064800	1.27028600
F	-1.21870500	1.25169900	2.23957100
F	-2.24436700	3.16863900	2.24093500
O	-1.63838100	-2.19847000	-1.67918100
S	-2.35519600	-2.11494600	-0.39445400
O	-1.96466700	3.63133100	-0.64193600
S	-1.20105400	2.54824500	-0.06670700

a₈'-IN1

C	-1.26539200	-1.29351300	2.20296600
O	-0.15013200	-0.72284800	2.06947800
O	2.42062700	-0.09663300	0.98770200
O	1.85966500	-2.52955500	0.66556700
C	3.47554000	-1.36395700	-1.07790900
C	-2.19509800	-1.56436000	1.14202300
C	-1.98784200	-1.72722500	-0.29049900
C	-3.57828300	-1.61203500	1.33712800
C	-3.27448300	-1.82881500	-0.87087600
C	-0.86155400	-1.88625800	-1.11271700
H	-4.14609400	-1.49425500	2.24952900
C	-3.47828500	-2.01595000	-2.23973600
C	-1.05517200	-2.06401600	-2.47951700
H	0.13685300	-1.91974700	-0.69338200
C	-2.34450900	-2.11610200	-3.04015700
H	-4.47487200	-2.08863100	-2.66433000
H	-0.18730200	-2.17534900	-3.12250800
H	-2.45841600	-2.25596300	-4.11103200
N	-4.22076500	-1.74239600	0.15414300
C	-1.56863500	-1.73719300	3.61604700

H	-1.01395500	-2.66681000	3.79693800
H	-1.20753200	-0.99069000	4.32759300
H	-2.62718500	-1.94518500	3.78354700
C	-5.66105000	-1.76724200	-0.04069400
H	-5.97343400	-0.93032500	-0.67351100
H	-5.96427300	-2.70616400	-0.51531900
H	-6.15524600	-1.68434000	0.92894100
Pd	0.53264400	0.49539600	0.57488300
C	-0.34231300	4.09020800	0.18269600
O	-1.22918400	1.56000800	-0.00387100
O	-1.04271000	2.94475900	-2.13563000
F	-1.56814200	4.58250500	0.35913200
F	0.19028100	3.78586800	1.36661300
F	0.41985100	4.98781400	-0.43520700
F	4.39159400	-0.40575300	-1.20700500
F	3.98373100	-2.52216400	-1.50657800
F	2.41077600	-1.05344400	-1.84249200
O	0.96502300	1.99374600	-0.88058700
S	-0.45440200	2.55252400	-0.87119400
S	2.93710300	-1.53399000	0.69673000
O	4.14690800	-1.78512800	1.46967200

as'-TS1

Imaginary Frequency: **-108.0341**

C	2.41348200	-0.30859000	2.16097000
O	1.19156800	-0.57261000	2.07917200
O	-1.09526400	1.48156800	1.42317500
O	0.75588000	2.39207200	0.03550500
C	-1.70396300	2.77163500	-0.79191300
C	3.25447200	-0.27458400	0.99137700
C	2.76054200	-0.25539000	-0.35160200
C	4.64173300	-0.40467200	0.89501300
C	3.86859000	-0.41564200	-1.20758700
C	1.45665800	-0.05289800	-0.86957300
H	5.38605500	-0.47051700	1.67684900
C	3.71424100	-0.47678100	-2.59256900
C	1.31400600	-0.15675200	-2.27671600
H	0.93920600	0.94870000	-0.42628000
C	2.41727100	-0.36025600	-3.11159100
H	4.56313400	-0.61014900	-3.25685400
H	0.32829300	-0.01801000	-2.70907400
H	2.27415800	-0.40731500	-4.18651800
N	5.01254600	-0.50041300	-0.40721600
C	2.95904400	-0.01782400	3.53341600

H	2.88330900	1.06263400	3.71143000
H	2.35693000	-0.52978800	4.28656000
H	4.00977600	-0.30444400	3.63233800
C	6.37098100	-0.67576400	-0.90175900
H	6.45384700	-1.61220900	-1.46234300
H	6.64920400	0.15978000	-1.55156300
H	7.05710700	-0.70805000	-0.05390900
Pd	0.01705400	-0.89810400	0.41252900
C	-3.80126300	-1.13981500	-0.04229600
O	-1.66092500	-2.21586900	1.21829000
O	-2.77562200	-3.53063900	-0.65814100
F	-4.68336000	-1.68992400	0.79294200
F	-3.45272600	0.06137900	0.39617000
F	-4.33933300	-1.04034400	-1.25891900
F	-2.98147700	2.88761600	-0.41839000
F	-1.38118400	3.81567300	-1.56268000
F	-1.58125200	1.64766300	-1.53451200
O	-1.33287200	-1.48806300	-1.06071100
S	-2.30649000	-2.25662900	-0.14210200
S	-0.58982400	2.66264200	0.69229100
O	-0.66439900	3.96782600	1.34621500

as'-IN2

C	2.13491300	0.47053900	1.98780600
O	0.92152600	0.12771400	2.01424100
O	1.23868300	2.67971500	0.05507500
O	-0.10019900	1.33892000	-1.61382000
C	-1.40536200	3.08480900	-0.06917500
C	3.03257600	-0.05212400	1.01110300
C	2.63209800	-0.94912700	-0.04203200
C	4.39707100	0.17628100	0.83425600
C	3.78160200	-1.22869700	-0.81162000
C	1.39885800	-1.50712600	-0.38090900
H	5.07686700	0.79337600	1.40552200
C	3.73760600	-2.07351500	-1.92259700
C	1.33765700	-2.35559900	-1.48516800
H	0.07491700	0.60933000	-0.96428400
C	2.49841000	-2.62883400	-2.24003100
H	4.61850300	-2.29201000	-2.51816800
H	0.39480500	-2.81193400	-1.76912700
H	2.42031100	-3.29186900	-3.09697300
N	4.84653400	-0.51910300	-0.24117200
C	2.56714100	1.48978400	3.00787400
H	2.33142300	2.48425700	2.60958800

H	2.00046100	1.34975700	3.93142100
H	3.63816700	1.44249100	3.22001900
C	6.21197200	-0.53035000	-0.74229200
H	6.61459900	-1.54826000	-0.72510200
H	6.24241700	-0.15125100	-1.76881700
H	6.83108000	0.10793500	-0.10948000
Pd	-0.15223900	-1.08232900	0.74785100
C	-3.74253300	-0.76490400	-0.62202800
O	-2.35427500	-1.08441700	1.64506000
O	-3.68497700	-3.05807400	0.73799000
F	-4.81900300	-0.30714200	0.01825900
F	-2.96276700	0.26914600	-0.96373400
F	-4.12132000	-1.40817200	-1.72665400
F	-1.31650500	4.25178100	0.56865800
F	-2.41080500	3.12025000	-0.93595900
F	-1.60401100	2.10584100	0.81491000
O	-1.54454600	-2.24173600	-0.33348900
S	-2.80440100	-1.92771600	0.49265400
S	0.20294900	2.78489200	-0.96771300
O	0.28311100	3.73063300	-2.06218400

aa'-IN3

C	-2.08943000	2.18381600	0.08927400
O	-0.84678700	2.10164200	-0.09634500
C	-2.91206900	1.02011400	0.14206100
C	-2.40695000	-0.32214300	-0.01114300
C	-4.28955700	0.90257500	0.33482200
C	-3.50988600	-1.19584400	0.09649000
C	-1.12182700	-0.82218500	-0.22775100
H	-5.03862300	1.66724000	0.48844800
C	-3.36936500	-2.58140800	-0.00780000
C	-0.96469000	-2.20299400	-0.33551400
C	-2.07859700	-3.06250200	-0.22538300
H	-4.21490100	-3.25739900	0.07407600
H	0.02086100	-2.62404500	-0.50663100
H	-1.92279800	-4.13419300	-0.31405700
N	-4.64858500	-0.40600000	0.30883600
C	-2.65083500	3.57632700	0.24456500
H	-2.46008100	4.14336900	-0.67325500
H	-3.72284200	3.58498000	0.45231900
H	-2.12267400	4.08750600	1.05612700
C	-5.99638100	-0.92578900	0.47255300
H	-6.29913200	-1.48448400	-0.41906000
H	-6.04468400	-1.58991300	1.34168800

H	-6.68675900	-0.09361800	0.62212100
Pd	0.36319200	0.44668300	-0.36738600
C	3.82964100	-0.33674600	1.00979000
O	1.88602100	-1.00050300	-0.67807600
O	2.55941000	1.33807200	-0.63731000
S	3.09704500	-0.05818500	-0.67998100
O	4.14310300	-0.38702900	-1.63597800
F	4.86909000	0.48174200	1.18826300
F	4.24030600	-1.60212600	1.12334300
F	2.91258800	-0.08969500	1.95347200

aa''-TS1

Imaginary Frequency: -94.1974

C	0.10991000	-2.20972000	-1.80573400
O	-0.84196900	-1.50511500	-1.43720800
O	-2.11513200	0.51153200	1.15771400
O	-4.25245100	-0.15894300	2.15963700
C	-4.17425900	0.19281700	-0.48672200
C	1.24555100	-2.43051300	-0.92429400
C	1.30888200	-2.02564700	0.45291800
C	2.54952300	-2.75015100	-1.29213200
C	2.66820700	-2.07682600	0.84009300
C	0.33047300	-1.61055000	1.38376800
H	2.93364200	-3.06881600	-2.25191800
C	3.09521800	-1.68580400	2.10893600
C	0.76907800	-1.18623700	2.65199900
H	-0.72465100	-1.80012200	1.20497500
C	2.12656200	-1.21344900	3.00063000
H	4.14001400	-1.73574400	2.40111400
H	0.03147400	-0.86547000	3.38113700
H	2.43175800	-0.88910300	3.99068800
N	3.40125200	-2.54721200	-0.25073500
C	0.11219400	-2.77697400	-3.21011400
H	0.62943100	-3.73961900	-3.26662000
H	-0.91919100	-2.88900100	-3.55140700
H	0.61470900	-2.07151000	-3.88462500
C	4.84220200	-2.74150700	-0.27066600
H	5.14001800	-3.09330700	-1.25991800
H	5.35691400	-1.79823800	-0.06108100
H	5.14036600	-3.48631400	0.47458600
Pd	-0.44996900	0.41632300	0.04563900
C	2.50482800	2.73802100	0.31759400
O	1.30692200	0.75925600	-1.01632400
O	-0.06074000	2.67560500	-0.45843800

F	2.55303800	4.06015800	0.46043500
F	2.13344000	2.17797500	1.47226700
F	3.71192300	2.28041500	-0.02391600
F	-4.63325100	1.42759300	-0.28260800
F	-3.29833000	0.21648600	-1.50153900
F	-5.19070400	-0.61038200	-0.80802500
O	1.75061900	2.92817200	-2.23999200
S	1.27913600	2.30180900	-1.01845600
O	-2.94501400	-1.82371700	0.76401900
S	-3.34400100	-0.44483500	1.05572800

a₈^{''}-IN2

C	-1.29498100	-3.68484200	1.42548600
O	-0.07682600	-3.74967700	1.33381000
O	2.36484700	0.60052000	-1.11127100
O	4.66687200	-0.11780100	-1.57139300
C	3.74033800	-0.44256800	0.91431000
C	-2.07061300	-2.85051500	0.48771600
C	-1.52970400	-2.02958400	-0.56874000
C	-3.43812500	-2.67934600	0.43650800
C	-2.62758000	-1.39975400	-1.20906000
C	-0.22840700	-1.76859100	-1.02653600
H	-4.21392500	-3.11127700	1.05333100
C	-2.48085300	-0.51498500	-2.30183600
C	-0.06240000	-0.84925300	-2.10831000
H	0.62799900	-2.29897300	-0.62723100
C	-1.20548000	-0.25358300	-2.74615900
H	-3.34393500	-0.05950600	-2.77724200
H	0.89494200	-0.82430300	-2.61785500
H	-1.04477900	0.40305000	-3.59507200
N	-3.77699900	-1.81406100	-0.58086100
C	-2.04918300	-4.44823800	2.50185400
H	-2.79506500	-5.12046400	2.06023400
H	-1.33607800	-5.03379300	3.08457700
H	-2.57848300	-3.75704600	3.16924500
C	-5.12506800	-1.36775000	-0.90155300
H	-5.83240800	-1.88808000	-0.25385700
H	-5.22110700	-0.28966600	-0.73701400
H	-5.36800000	-1.59768600	-1.94370100
Pd	0.46300000	0.53837700	-0.43914300
C	-1.56405500	3.61927200	0.28123700
O	-1.42695600	0.95098000	0.41550200
O	0.52971500	2.16847000	1.12084300
F	-1.16910500	4.74009500	0.87763600

F	-1.05787800	3.56692300	-0.95402300
F	-2.89665200	3.59146700	0.21231600
F	4.20927400	0.75769000	1.25184800
F	2.59276800	-0.66531600	1.57717300
F	4.62579900	-1.37887800	1.25572000
O	-1.56015900	2.25868500	2.58588100
S	-0.97113600	2.14922100	1.26480300
O	2.86746400	-1.85729800	-1.16656300
S	3.42807200	-0.52482200	-0.92098100

a₈^{''}-TS2

Imaginary Frequency: -1255.5213

C	0.19809900	1.63736500	2.34481300
O	-0.57057600	0.70915700	2.11901700
O	-1.98764400	-1.06161000	-1.16824700
O	-2.64144700	1.24272800	-0.52210600
C	-3.90959500	-0.77821000	0.69209800
C	0.77155600	2.43613200	1.25038200
C	0.61987700	2.22552700	-0.16449000
C	1.54527900	3.58051700	1.39054500
C	1.31753300	3.28613700	-0.80764700
C	-0.04833500	1.25455100	-0.96918600
H	1.88464500	4.06932000	2.29361400
C	1.39327700	3.40971400	-2.19387500
C	0.05775700	1.39260000	-2.37578000
H	-1.40363600	1.26794400	-0.67906300
C	0.74197100	2.45387100	-2.97697400
H	1.94208500	4.22420200	-2.65828900
H	-0.43561000	0.65904300	-3.00784000
H	0.77826500	2.53094100	-4.05923400
N	1.87532800	4.09713400	0.17371300
C	0.58180000	1.99151900	3.77275000
H	1.65241100	1.81441400	3.93343400
H	0.37890000	3.04576300	3.99590500
H	0.01049500	1.36175100	4.45670100
C	2.66160200	5.29555600	-0.06758400
H	3.56279200	5.05646200	-0.64202400
H	2.07412400	6.03953900	-0.61602300
H	2.96022000	5.72168100	0.89185000
Pd	-0.08093700	-0.69628900	-0.32061800
C	3.00230400	-2.83781100	-0.60285000
O	1.89528800	-0.66489800	0.48490800
O	0.57590000	-2.69828500	0.51832000
S	1.95905800	-2.16572400	0.78855400

O	2.62618800	-2.54025500	2.02328700
F	3.06838400	-4.16532500	-0.50620900
F	4.23152800	-2.32384500	-0.52595100
F	2.46108300	-2.50684300	-1.77975100
S	-3.16442500	-0.14936500	-0.90145500
O	-4.21326100	-0.17029800	-1.90584000
F	-4.45954300	-1.96826500	0.45740900
F	-4.84607200	0.07729600	1.09994600
F	-2.96619500	-0.89272700	1.61921200

a₈''-IN3

C	0.14312900	1.41816300	2.25477100
O	-0.46042900	0.27561500	2.23990200
O	-1.71718000	-1.30924700	-1.19617600
O	-2.59836800	-0.15728800	0.85655600
C	-3.06234300	-2.74839200	0.54982900
C	-0.00551500	2.40569800	1.25397500
C	-0.40244000	2.31175400	-0.14880500
C	0.08017600	3.77744700	1.54462900
C	-0.58321100	3.64421800	-0.59394100
C	-0.48092300	1.27424600	-1.09181700
H	0.30752300	4.26191800	2.48404200
C	-0.94636600	3.97397700	-1.89925900
C	-0.87555500	1.58420800	-2.39191400
H	-1.20118900	0.14520300	1.54894300
C	-1.11402300	2.91462900	-2.78594000
H	-1.08266400	5.00304100	-2.21569900
H	-0.98898900	0.78987200	-3.12238300
H	-1.41082200	3.11658000	-3.81099000
N	-0.29047000	4.50400000	0.47642500
C	1.06273400	1.57686600	3.42180200
H	1.93419000	0.93729400	3.21716800
H	1.41872000	2.59970700	3.54978600
H	0.59116500	1.20907200	4.33729200
C	-0.39264200	5.95484900	0.42055100
H	0.27481300	6.34836000	-0.35230400
H	-1.42084400	6.25096600	0.19129100
H	-0.10536100	6.37204500	1.38711400
Pd	0.13740400	-0.53540200	-0.66333300
C	4.00883800	-1.44164100	-0.71294100
O	2.02295600	0.15712800	0.04917800
O	1.63013100	-2.24600900	0.21713900
S	2.62853100	-1.17605200	0.50840200
O	3.25131900	-1.12139100	1.82846100

F	4.60418200	-2.60916100	-0.46555000
F	4.90304800	-0.45605200	-0.60194600
F	3.51752200	-1.45069700	-1.95529300
S	-2.91403200	-1.08506100	-0.27142400
O	-4.16233500	-0.84712800	-0.98239400
F	-3.26138900	-3.69595900	-0.36589500
F	-4.08873300	-2.73615000	1.40435200
F	-1.93637500	-3.01257400	1.22271500

a₈-TS2'

Imaginary Frequency: -1277.8224

C	-2.04794600	-2.12455300	-1.40627200
O	-0.82043200	-1.92774400	-1.26802100
O	1.28321400	1.43409300	0.04943300
O	-0.58358500	2.38476800	-1.26701000
C	1.13222600	4.06289300	-0.08133500
C	-3.02846000	-1.34163600	-0.70553800
C	-2.73667700	-0.22758800	0.15737000
C	-4.37267100	-1.65770900	-0.50392200
C	-3.91675200	0.03332700	0.89017500
C	-1.55967500	0.52537400	0.38618400
H	-4.97040100	-2.44168700	-0.94836600
C	-3.95771500	0.97256700	1.92197300
C	-1.60133800	1.41679200	1.48229700
H	-1.07859400	1.37176400	-0.58253200
C	-2.77301900	1.64437600	2.22093000
H	-4.86578300	1.16491100	2.48559500
H	-0.71683200	1.99783400	1.71659800
H	-2.75943100	2.36677100	3.03121800
N	-4.90708600	-0.84318600	0.43886500
C	-2.44554500	-3.28525200	-2.28616800
H	-1.73909000	-3.35989800	-3.11625100
H	-2.36885200	-4.21286100	-1.70561600
H	-3.46276900	-3.19097600	-2.67395100
C	-6.27175800	-0.89432000	0.94300600
H	-6.27305300	-1.11744000	2.01468000
H	-6.77659500	0.06195600	0.77393100
H	-6.81626400	-1.68009800	0.41684400
Pd	0.19334400	-0.37701200	-0.32514900
C	3.50502700	-1.76085300	1.18456800
O	1.92400800	-1.38569700	-0.88397300
O	3.02525300	-3.60368100	-0.67768800
F	4.55042600	-1.28366200	0.50549700
F	2.91263900	-0.74560200	1.83615700

F	3.93984900	-2.64918900	2.08603200
F	2.39645700	4.18091100	0.31034200
F	0.80995100	5.07445300	-0.88375000
F	0.33066800	4.07892000	0.99010800
O	1.15335500	-2.94949700	0.90163200
S	2.28335000	-2.56965400	0.03803100
O	1.75627400	2.54487700	-2.19979700
S	0.92694100	2.45869400	-1.01197200

F	-4.87077700	-1.06054000	-0.98403000
F	-1.52018500	4.52900300	-0.52685300
F	-0.42082600	4.78013400	1.33591400
F	0.63388800	4.21823700	-0.48125300
O	-1.92830400	-1.12087500	-1.15686000
S	-2.58141700	-2.04653400	-0.10607400
S	-0.79700100	2.28484900	0.62397600
O	-1.99833700	2.23234200	1.43405800

a₈-TS2''

Imaginary Frequency: -1212.6804

C	1.46566000	-2.71360700	0.25302000
O	0.51903100	-2.27769400	-0.44327900
O	-0.82420900	1.65233000	-0.75811600
O	0.49705400	1.85841700	1.31807600
C	-0.50693400	4.08041600	0.20708300
C	2.65030900	-1.92807400	0.47283900
C	2.82243600	-0.58017200	0.00439800
C	3.92451400	-2.39621500	0.80213000
C	4.21139900	-0.32465100	0.00244600
C	1.89746400	0.40164900	-0.43108500
H	4.22831200	-3.36578000	1.17225100
C	4.74466200	0.84987400	-0.52996100
C	2.46360400	1.54731600	-1.04016900
H	1.14959900	1.00600700	0.51929000
C	3.84840100	1.76951300	-1.07779000
H	5.81338100	1.04282000	-0.53637100
H	1.80078000	2.32138100	-1.41024000
H	4.22941400	2.68556100	-1.51861400
N	4.85523100	-1.44854900	0.52961400
C	1.30474500	-4.11374200	0.78050800
H	0.42690200	-4.11095400	1.43746600
H	1.08076000	-4.79403500	-0.04707800
H	2.17474300	-4.47249500	1.33435200
C	6.29284000	-1.57788000	0.72050900
H	6.81452800	-1.46302900	-0.23488300
H	6.65449500	-0.81945200	1.42187700
H	6.51018700	-2.56738100	1.12596400
Pd	-0.05161800	-0.32678000	-0.73437200
C	-4.18619600	-1.14365000	0.16188200
O	-1.88322000	-2.00058700	1.18943800
O	-2.94725100	-3.34869700	-0.66532500
F	-4.92418400	-1.80999800	1.05945500
F	-3.95526400	0.08866500	0.62171800

a₈-TS2'''

Imaginary Frequency: -1230.4398

C	1.70853800	-2.34443900	0.51798500
O	0.74193100	-2.00034500	-0.20296200
O	-0.61694200	1.81004000	-1.11056800
O	0.62279800	2.30492100	0.97914600
C	-2.03970400	2.46137800	1.09821400
C	2.88330700	-1.52433700	0.62910600
C	3.03143300	-0.23597800	0.00883300
C	4.16622700	-1.92934100	1.00687800
C	4.41551100	0.04291400	-0.02365000
C	2.09033300	0.67155800	-0.53657400
H	4.48703400	-2.84435300	1.48565300
C	4.92796300	1.15936100	-0.68534100
C	2.63624400	1.75305600	-1.27034900
H	1.31188000	1.35925700	0.32626600
C	4.01610800	1.99565300	-1.33275100
H	5.99293000	1.37010200	-0.71388500
H	1.96000300	2.46560200	-1.73322000
H	4.38053300	2.86365900	-1.87321000
N	5.07915000	-1.00273200	0.62645300
C	1.57965300	-3.68524600	1.18977800
H	0.67061800	-3.65900200	1.80118700
H	1.42889000	-4.45997200	0.43087100
H	2.43727000	-3.93996300	1.81583300
C	6.51920100	-1.08405300	0.82695000
H	7.03767700	-1.07040500	-0.13689000
H	6.86734200	-0.24356800	1.43537300
H	6.75446200	-2.01638900	1.34279300
Pd	0.16175400	-0.12420300	-0.77408300
C	-4.07764700	-1.33886300	-0.17714200
O	-1.84008100	-1.76789200	1.20612200
O	-2.39994400	-3.33411400	-0.69371300
F	-4.81685300	-2.07535800	0.66198400
F	-4.12220300	-0.06105300	0.22439300

F	-4.60116900	-1.42323500	-1.40346400
F	-3.11450300	2.63928600	0.33759600
F	-2.01052800	1.22319700	1.57417600
F	-2.05078100	3.33342800	2.10709800
O	-1.70296600	-0.97423600	-1.16988000
S	-2.32580700	-1.96958700	-0.16796200
S	-0.51220500	2.77014400	0.06557700
O	-0.50652600	4.17690500	-0.30160100

b₈-IN1

C	1.57128200	-0.32584800	1.93446700
O	0.33638300	-0.06008000	2.04372800
O	-2.64563500	0.20132900	-0.85080600
O	-1.76578800	-1.77912000	0.19231400
C	-4.42368800	-1.41607000	0.36791900
C	2.16637400	-1.04436200	0.84854900
C	3.57241900	-1.17473500	0.48790700
C	1.46091600	-1.84792600	-0.05342000
C	3.61749200	-2.05381900	-0.62282500
C	4.77891500	-0.62047900	0.94419800
H	0.40339500	-2.06738700	-0.09225900
C	4.80235600	-2.41218600	-1.26719200
C	5.96716600	-0.97353200	0.31080700
H	4.79833700	0.08307900	1.76804500
C	5.98327700	-1.86131700	-0.77932800
H	4.80620600	-3.08768500	-2.11709500
H	6.90210400	-0.54736100	0.66260600
H	6.92740000	-2.11402200	-1.25247500
N	2.30932400	-2.44884700	-0.91417300
C	2.41294100	0.15764600	3.08473500
H	2.86645300	1.11011500	2.78079100
H	1.77098900	0.34899800	3.94685800
H	3.20549500	-0.54814700	3.34464200
C	1.93156000	-3.37806800	-1.96857000
H	0.84666600	-3.49455500	-1.96689800
H	2.24620400	-2.99096500	-2.94281200
H	2.39922700	-4.35386800	-1.80222700
Pd	-1.05335100	0.21060200	0.58406700
C	0.23936300	3.01611800	-1.56138500
O	1.71354300	2.13537000	0.45775700
O	0.46385900	4.31881900	0.75803000
F	1.27900100	3.62542300	-2.13634100
F	0.14369500	1.76866600	-2.05512400
F	-0.87783200	3.68119000	-1.85069900

F	-4.22690700	-0.73201700	1.49352100
F	-5.46204800	-0.91207800	-0.29159300
F	-4.64509500	-2.69735200	0.65315400
O	-0.79040700	2.20706400	0.74267600
S	0.50021800	2.94210600	0.28093900
O	-3.16159200	-2.05845200	-1.91534000
S	-2.90434700	-1.29213300	-0.71190000

b₈-TS1

Imaginary Frequency: -33.2306

C	-2.01426600	0.50812800	-2.03126600
O	-0.78908000	0.62467700	-2.32470000
O	1.52044700	-0.65639800	0.79933100
O	1.31972200	-2.66403100	-0.62627700
C	3.76992000	-1.71665700	-0.15502400
C	-2.40340000	-0.52196800	-1.10153300
C	-3.49875900	-0.60699000	-0.16995000
C	-1.60625100	-1.67311100	-0.89273000
C	-3.29987000	-1.80684300	0.56465100
C	-4.58933900	0.22003900	0.15450800
H	-0.80850100	-2.07592700	-1.50790500
C	-4.16634600	-2.21701900	1.58224500
C	-5.45418300	-0.18575800	1.16086100
H	-4.75342000	1.15814000	-0.36457200
C	-5.24697800	-1.39069300	1.86499300
H	-4.00094100	-3.13614100	2.13467700
H	-6.30460200	0.43826300	1.41789700
H	-5.94183000	-1.67388500	2.64981500
N	-2.14896600	-2.43038500	0.09104200
C	-2.97656200	1.47612700	-2.63901100
H	-2.99745700	2.35813300	-1.98356700
H	-2.59943700	1.80275800	-3.61146100
H	-3.98390100	1.06421800	-2.73239800
C	-1.64543300	-3.72409500	0.54551400
H	-0.67849700	-3.90690700	0.07705600
H	-1.50783300	-3.70072200	1.63016900
H	-2.35208600	-4.51819900	0.28423300
Pd	0.40255200	0.00107400	-0.77505500
C	0.92279800	3.06055700	1.59830100
O	-0.97673600	2.74809800	-0.22897300
O	0.96518400	4.28293300	-0.77737000
F	0.30039000	4.08166100	2.19615000
F	0.53595400	1.91723300	2.17736300
F	2.23966000	3.20285000	1.74294300

F	3.66795400	-0.95050000	-1.24537800
F	4.49346600	-1.08616200	0.76622000
F	4.36252300	-2.86758700	-0.47913300
O	1.32056500	1.84061800	-0.71882300
S	0.46635700	3.03636000	-0.20698800
O	2.23568000	-2.85813000	1.72840300
S	2.06740100	-2.07363000	0.51297000

b₈-IN2

C	1.68875200	-2.13450300	-1.56950600
O	0.61555600	-1.86535500	-2.16617400
O	-0.23705200	1.13989200	0.52203700
O	0.14799900	2.66440200	-1.42231200
C	-2.06512000	3.01763600	0.04186600
C	2.31138100	-1.01869700	-0.85516200
C	3.10424200	-0.98504600	0.35160700
C	2.29243100	0.31982300	-1.36355700
C	3.50776600	0.36296500	0.52153400
C	3.45956200	-1.94204100	1.31627700
H	1.98446500	0.67040500	-2.33997300
C	4.26444700	0.78149800	1.61881300
C	4.22463600	-1.53393200	2.40050600
H	3.13939600	-2.97483600	1.22528700
C	4.61984000	-0.18875100	2.54921000
H	4.55236200	1.81911100	1.74899500
H	4.51460200	-2.25909600	3.15437900
H	5.20684500	0.09867000	3.41624300
N	3.02450400	1.11506300	-0.54677600
C	2.20726400	-3.53436900	-1.55044000
H	1.68407700	-4.06866000	-0.74487000
H	1.94313400	-4.02983600	-2.48855100
H	3.28438300	-3.57848000	-1.37505100
C	3.27901600	2.54199200	-0.74202100
H	2.78069100	2.86536200	-1.65461000
H	2.85639100	3.10783300	0.09232400
H	4.35694800	2.71549600	-0.81445800
Pd	0.01812800	-0.32306400	-0.86737400
C	-2.94407100	-1.51135400	1.46210500
O	-1.14730900	-2.90147600	0.08211800
O	-3.50210800	-2.72716600	-0.84637000
F	-3.35903700	-2.56020900	2.18065400
F	-1.94282600	-0.90849500	2.11346400
F	-3.95357200	-0.65170200	1.31800000
F	-2.72900600	2.23686500	-0.80785400

F	-2.53822200	2.84312000	1.27520100
F	-2.22044000	4.29568500	-0.31620000
O	-1.99716800	-0.75525100	-0.89054800
S	-2.35226600	-2.10276400	-0.20152900
O	0.40848000	3.49142600	0.95251200
S	-0.24953600	2.60082900	-0.00471800

b₈-TS2

Imaginary Frequency: -1309.6534

C	-1.89730100	-1.29492600	1.84992300
O	-0.63185700	-1.30348000	1.85781200
O	1.05947700	1.33476100	-0.89011300
O	-0.61913500	2.66510300	0.38140100
C	1.95911200	3.06431000	0.98142200
C	-2.56639300	-0.50690200	0.85701800
C	-3.87170200	-0.61821600	0.27354400
C	-1.76651100	0.31296600	0.01214500
C	-3.80844500	0.11504600	-0.94553600
C	-5.07509700	-1.26192300	0.62197000
H	-1.10090800	1.49701700	0.35896200
C	-4.91726600	0.25203700	-1.79346000
C	-6.16642800	-1.13878100	-0.22347300
H	-5.15745400	-1.83281200	1.54074700
C	-6.08900300	-0.38738200	-1.41766100
H	-4.86641800	0.83014200	-2.70997000
H	-7.10282800	-1.62288500	0.03704300
H	-6.96576900	-0.30868200	-2.05337700
N	-2.52796900	0.62681600	-1.09091700
C	-2.60542500	-2.16817200	2.84267800
H	-3.08521600	-3.00369700	2.31728500
H	-1.88726600	-2.56991100	3.55946900
H	-3.38761400	-1.60721500	3.36534200
C	-2.10886300	1.47216100	-2.20621400
H	-1.03139700	1.38185500	-2.33866700
H	-2.59925300	1.12309400	-3.11705700
H	-2.37256700	2.51941600	-2.02705300
Pd	0.24098700	-0.22600500	0.33280800
C	3.22992900	-1.97690200	-1.38966000
O	1.11280600	-3.04541000	-0.19759200
O	3.34073900	-3.11321500	1.02036600
F	3.54320600	-3.10005700	-2.04221900
F	2.41344400	-1.24206800	-2.16351700
F	4.34405900	-1.28049300	-1.15627800
F	3.18069900	3.02335500	0.46473900

F	1.71576900	4.27152400	1.48514400
F	1.83457000	2.14420100	1.93578500
O	2.10811100	-0.97226000	0.76915400
S	2.36759500	-2.39446800	0.20608900
O	0.82391900	3.79051600	-1.35577100
S	0.72173100	2.72109400	-0.37962500

b₈-IN3

C	1.41688800	-2.43700000	0.62376000
O	0.19351300	-2.05961800	0.53587100
O	-0.20628700	1.79757400	-0.96696400
O	-2.39371400	2.30365800	0.13734500
C	-0.20043900	3.37146500	1.17385500
C	2.41377600	-1.53218500	0.21868200
C	3.85722600	-1.50694800	0.12391400
C	1.93125500	-0.28622300	-0.25388500
C	4.17249000	-0.23194000	-0.40959600
C	4.89971000	-2.39393100	0.41996500
H	-2.53124800	0.80257100	0.05111000
C	5.48244400	0.17838600	-0.64943500
C	6.21329300	-1.99193200	0.18223100
H	4.69546500	-3.37930700	0.82813000
C	6.50271000	-0.72299600	-0.34503200
H	5.70674600	1.15966600	-1.05545900
H	7.02863400	-2.67283000	0.40920700
H	7.53572200	-0.43678100	-0.51895300
N	2.97383700	0.48048700	-0.63054400
C	1.67886500	-3.81832600	1.14907300
H	2.32918800	-3.77212200	2.03047600
H	0.73885300	-4.30560000	1.41371700
H	2.19676400	-4.41663300	0.38989100
C	2.94287500	1.82688000	-1.19179000
H	1.90906500	2.11549300	-1.36454600
H	3.41038400	2.53285500	-0.49771100
H	3.49134700	1.83777300	-2.13864900
Pd	-0.02342300	-0.15489800	-0.19692100
C	-3.93578400	-2.20837200	0.45404300
O	-2.40204800	-1.95567400	-1.74240800
O	-4.32127000	-0.29930000	-1.42234100
F	-4.77827000	-3.07635900	-0.10300900
F	-2.94470300	-2.86066700	1.05215600
F	-4.58252600	-1.45349600	1.33768000
F	1.03659600	3.77049500	0.85550400
F	-0.84242700	4.36419900	1.78334300

F	-0.11463700	2.32374900	2.00610800
O	-2.27502700	-0.20561100	0.04276700
S	-3.24585000	-1.12535700	-0.90339900
O	-1.18801100	4.06420900	-1.20900100
S	-1.11200900	2.87800500	-0.37397300

b₈'-IN1

C	-2.00431100	-0.69196900	1.77447800
O	-0.74727400	-0.59018600	1.90857200
O	1.01106400	1.55095700	1.25453600
O	0.19606900	2.41647100	-0.94774100
C	2.58737300	3.21755800	-0.07912300
C	-2.75539500	-0.30272600	0.62446200
C	-4.15727100	-0.55585800	0.30121500
C	-2.26684400	0.51728100	-0.40306400
C	-4.41184400	0.12970600	-0.91384500
C	-5.20409700	-1.29660000	0.87250900
H	-1.30048300	0.98956800	-0.51887400
C	-5.64881500	0.11245100	-1.55790800
C	-6.44475800	-1.31790500	0.23956600
H	-5.06522600	-1.85414500	1.79140700
C	-6.66915100	-0.62164300	-0.96009100
H	-5.81089900	0.64610500	-2.48923800
H	-7.25572500	-1.88842100	0.68287300
H	-7.64761700	-0.65993300	-1.42927200
N	-3.23515800	0.77939400	-1.29814700
C	-2.70269200	-1.27220000	2.98171900
H	-2.99079000	-2.31036700	2.77237200
H	-2.01651200	-1.26797100	3.83018600
H	-3.60872100	-0.71068800	3.22620200
C	-3.08307300	1.64491300	-2.46189900
H	-2.08708200	2.08952800	-2.43616000
H	-3.20423900	1.06622300	-3.38316500
H	-3.83401900	2.44020800	-2.43407300
Pd	0.73017000	-0.33150900	0.52987500
C	3.30122300	-2.94355900	-0.10285200
O	2.30625600	-0.56913500	-0.89289100
O	2.07748600	-2.57027900	-2.46060700
F	4.49907800	-2.71191400	-0.63195800
F	3.27130800	-2.50200700	1.15472200
F	3.03977100	-4.24852600	-0.12556600
F	3.25724900	3.50558000	1.03779200
F	3.17786800	2.19124100	-0.69490300
F	2.59795300	4.28069400	-0.88775800

O	0.70691400	-2.26728500	-0.33277600
S	2.00796800	-2.04905600	-1.11126500
O	0.29293900	3.91634600	1.09061400
S	0.82333400	2.78693700	0.33507100

O	1.56477700	-2.47824800	0.95786100
S	2.05570900	-2.32760900	-0.46244600
O	1.11355100	3.87355500	1.57316500
S	0.93946700	2.60146800	0.88185000

b₈'-TS1

Imaginary Frequency:		-615.7963	
C	-2.38418400	-0.50246300	2.12960300
O	-1.16579400	-0.76706500	2.34484700
O	1.28886600	1.35012100	1.57863900
O	-0.42467700	2.48598100	0.18265600
C	2.08374700	2.66046100	-0.58381300
C	-2.73734500	-0.11978500	0.78953000
C	-3.93380400	-0.17730100	0.01940500
C	-1.64988000	0.19197900	-0.08679800
C	-3.52825400	0.06250700	-1.33269900
C	-5.29649700	-0.42065100	0.29469800
H	-0.93121400	1.20114700	0.15257000
C	-4.45073600	0.09425400	-2.39114100
C	-6.19915700	-0.39927400	-0.75307700
H	-5.63497200	-0.60828900	1.30852500
C	-5.77969500	-0.14269300	-2.08227500
H	-4.13444500	0.28352400	-3.41146000
H	-7.25232500	-0.57698000	-0.55804100
H	-6.52006600	-0.13480700	-2.87659600
N	-2.16569200	0.25654000	-1.36508400
C	-3.36060200	-0.63763200	3.25701700
H	-4.03927100	-1.47746800	3.05934400
H	-2.82762500	-0.82379600	4.19100200
H	-3.97007400	0.26834500	3.34617900
C	-1.39509000	0.63396900	-2.54662700
H	-0.39478700	0.92582000	-2.23052700
H	-1.32216500	-0.21556500	-3.23244900
H	-1.87549300	1.47697400	-3.05161800
Pd	-0.05706700	-0.95598800	0.61656400
C	3.64513500	-1.34916200	-0.35334900
O	1.05401100	-1.34709200	-1.10736900
O	2.35117800	-3.52178600	-1.23246000
F	4.01859900	-1.00516000	-1.58543400
F	3.46526100	-0.26300800	0.38602600
F	4.57758100	-2.12432300	0.19900400
F	3.35489200	2.63420900	-0.17918900
F	1.86780200	1.58829400	-1.37674200
F	1.87446600	3.76443500	-1.30536700

b₈'-IN2

C	-1.69412400	-0.17043900	2.06564700
O	-0.44112900	-0.14733800	2.32028100
O	-2.09790400	2.98481800	0.82154600
O	-1.53884900	1.56536100	-1.17016500
C	0.36002600	3.19145100	-0.24455800
C	-2.09912300	-0.79662600	0.85925500
C	-3.33650800	-1.17053600	0.19444200
C	-1.03279100	-1.39653000	0.13681300
C	-2.93956300	-1.96926900	-0.90890300
C	-4.69915700	-0.91492900	0.39054700
H	-1.72751500	0.89211100	-0.46983900
C	-3.85356200	-2.51408400	-1.80859400
C	-5.62027100	-1.46246200	-0.50117400
H	-5.03787400	-0.29660200	1.21615400
C	-5.20504700	-2.25090800	-1.58646600
H	-3.53219100	-3.12040100	-2.64952300
H	-6.67952500	-1.27119000	-0.35665200
H	-5.94596400	-2.66023500	-2.26655700
N	-1.53162800	-2.08129000	-0.90811200
C	-2.62179600	0.47630300	3.04778200
H	-3.52112200	-0.13055000	3.19401300
H	-2.11158400	0.62631500	4.00120300
H	-2.92682100	1.45316000	2.65240000
C	-0.77254300	-2.82374200	-1.90894200
H	0.28918600	-2.74161600	-1.68007200
H	-1.07009200	-3.87696100	-1.89412400
H	-0.96491800	-2.40934300	-2.90364800
Pd	0.73331900	-1.06067300	0.88920000
C	3.88390000	-0.00947500	-0.87368300
O	2.08514800	-1.94551000	-0.48165900
O	4.48261700	-2.37765400	0.22059800
F	4.19184700	-0.45480000	-2.09123900
F	2.87822800	0.86777700	-0.96546900
F	4.94337400	0.58832000	-0.33258900
F	0.61474400	4.39748800	0.25594800
F	0.76557800	2.25475300	0.61647300
F	0.99175500	3.03854700	-1.40374900
O	2.91341600	-0.81878800	1.49083500

S	3.37070800	-1.44579200	0.20118800
O	-1.86208000	4.00024100	-1.51221200
S	-1.48314600	3.03610200	-0.50062200

b₈'-IN3

C	-1.86710400	2.17001500	0.14535800
O	-0.61183600	2.38633100	-0.00642500
C	-2.31540100	0.83762500	0.07225000
C	-3.56120500	0.10647200	0.16636900
C	-1.28761000	-0.10299600	-0.16733500
C	-3.21017000	-1.25573700	-0.02548900
C	-4.90505500	0.43309300	0.38529800
C	-4.15062600	-2.28321300	-0.00454100
C	-5.85284400	-0.58961900	0.40756200
H	-5.21054000	1.46440800	0.53591200
C	-5.48267000	-1.93025400	0.21543100
H	-3.86421800	-3.31976300	-0.15325300
H	-6.89756500	-0.34469500	0.57669700
H	-6.24263600	-2.70571900	0.23783100
N	-1.81592400	-1.34136800	-0.22602100
C	-2.75250900	3.35808300	0.38704200
H	-3.51451100	3.42696500	-0.39849400
H	-3.27745000	3.24963500	1.34365100
H	-2.15937600	4.27418500	0.39934900
C	-1.10122300	-2.58992000	-0.45922800
H	-1.23457400	-3.26212600	0.39484200
H	-1.48598100	-3.07742100	-1.36097500
H	-0.04170400	-2.37293900	-0.58886800
Pd	0.49153600	0.67515200	-0.33650400
C	3.79881600	-0.57840200	0.99996400
O	1.77755900	-0.97754000	-0.69488900
O	2.68931500	1.26189600	-0.59940900
O	4.08963400	-0.58797800	-1.65682400
F	4.91646600	0.12199500	1.18693800
F	4.07046100	-1.88206200	1.07410900
F	2.91212100	-0.25893500	1.94857400
S	3.09413700	-0.18384300	-0.68047700

b₈''-TS1

Imaginary Frequency: -87.0075			
C	0.15124300	-3.18320600	-0.17776000
O	-0.41716700	-3.77443800	0.71840600
O	-1.79954000	-1.24604100	-0.69817200
O	-3.76801800	-2.33069300	0.32630700

C	-3.85207600	0.30877900	-0.03866700
C	0.96079900	-1.94351600	0.16663600
C	2.39106300	-1.76632900	-0.14216000
C	0.78713600	-1.31253400	1.45153300
C	2.95008200	-1.01896600	0.91758800
C	3.21524600	-2.16715000	-1.19864600
H	-0.11583500	-1.31121100	2.05146700
C	4.28812200	-0.64370100	0.95443900
C	4.56284600	-1.80881600	-1.16957600
H	2.81775300	-2.73197200	-2.03495200
C	5.09141800	-1.05624800	-0.11007800
H	4.69750700	-0.05507200	1.76886600
H	5.21295500	-2.11176100	-1.98455300
H	6.14298200	-0.78618900	-0.11747200
N	1.93357100	-0.76021400	1.86287600
C	0.14032100	-3.66967200	-1.60952400
H	0.14074400	-2.84290900	-2.32547300
H	1.03047100	-4.28648900	-1.79135000
H	-0.74378200	-4.29235000	-1.75951300
C	2.07274000	0.14875800	2.99448400
H	2.94983300	-0.12838500	3.58485300
H	2.17992500	1.17661500	2.63358900
H	1.18069800	0.07419900	3.61790900
Pd	-0.08355000	-0.16522300	-0.55684000
C	0.57386600	3.34994300	0.49906700
O	1.56763100	1.15280000	-0.61263300
O	-0.57239800	1.89819900	-1.44904600
F	-0.08620000	2.59519300	1.38725200
F	1.77539200	3.65121100	1.00393300
F	-0.10893700	4.46539800	0.26856400
F	-4.32554300	0.17290600	-1.27719600
F	-4.87071800	0.45514000	0.81168900
F	-3.07582300	1.39851600	0.01842800
O	1.50535700	3.26859900	-2.00914800
S	0.79921300	2.39733700	-1.08923600
O	-2.25600800	-0.85357600	1.73872400
S	-2.86384900	-1.19551500	0.44408300

b₈''-IN2

C	0.15124300	-3.18320600	-0.17776000
O	-0.41716700	-3.77443800	0.71840600
O	-1.79954000	-1.24604100	-0.69817200
O	-3.76801800	-2.33069300	0.32630700
C	-3.85207600	0.30877900	-0.03866700

C	0.96079900	-1.94351600	0.16663600
C	2.39106300	-1.76632900	-0.14216000
C	0.78713600	-1.31253400	1.45153300
C	2.95008200	-1.01896600	0.91758800
C	3.21524600	-2.16715000	-1.19864600
H	-0.11583500	-1.31121100	2.05146700
C	4.28812200	-0.64370100	0.95443900
C	4.56284600	-1.80881600	-1.16957600
H	2.81775300	-2.73197200	-2.03495200
C	5.09141800	-1.05624800	-0.11007800
H	4.69750700	-0.05507200	1.76886600
H	5.21295500	-2.11176100	-1.98455300
H	6.14298200	-0.78618900	-0.11747200
N	1.93357100	-0.76021400	1.86287600
C	0.14032100	-3.66967200	-1.60952400
H	0.14074400	-2.84290900	-2.32547300
H	1.03047100	-4.28648900	-1.79135000
H	-0.74378200	-4.29235000	-1.75951300
C	2.07274000	0.14875800	2.99448400
H	2.94983300	-0.12838500	3.58485300
H	2.17992500	1.17661500	2.63358900
H	1.18069800	0.07419900	3.61790900
Pd	-0.08355000	-0.16522300	-0.55684000
C	0.57386600	3.34994300	0.49906700
O	1.56763100	1.15280000	-0.61263300
O	-0.57239800	1.89819900	-1.44904600
F	-0.08620000	2.59519300	1.38725200
F	1.77539200	3.65121100	1.00393300
F	-0.10893700	4.46539800	0.26856400
F	-4.32554300	0.17290600	-1.27719600
F	-4.87071800	0.45514000	0.81168900
F	-3.07582300	1.39851600	0.01842800
O	1.50535700	3.26859900	-2.00914800
S	0.79921300	2.39733700	-1.08923600
O	-2.25600800	-0.85357600	1.73872400
S	-2.86384900	-1.19551500	0.44408300

b₈''-TS2

Imaginary Frequency:	-1132.6585		
C	1.44721900	-0.74952500	2.29013300
O	0.90236000	0.33971900	2.42928500
O	0.12305400	2.02428200	-1.26572600
O	2.42339000	1.57984400	-0.44202600
C	1.20803500	3.80818200	0.43122100

C	1.60269100	-1.32722000	0.93230700
C	2.27211000	-2.50264100	0.48201600
C	1.08729800	-0.65717100	-0.21170900
C	2.09874600	-2.54517200	-0.93862900
C	3.01936700	-3.53577400	1.10000200
H	1.82270200	0.52776100	-0.27243300
C	2.64838100	-3.56728400	-1.73453000
C	3.54270800	-4.54618000	0.31738400
H	3.17639100	-3.54467700	2.17195700
C	3.35960700	-4.56161300	-1.08901000
H	2.51153100	-3.58046900	-2.81087800
H	4.10861500	-5.34696600	0.78388900
H	3.78806600	-5.37383700	-1.66907300
N	1.37372300	-1.45248500	-1.32636200
C	1.96282100	-1.51427200	3.49187100
H	1.52477700	-2.51833500	3.53398800
H	3.05274400	-1.62714800	3.44177700
H	1.70027300	-0.96382300	4.39697700
C	1.03683400	-1.13251900	-2.70697700
H	1.94320600	-1.09211500	-3.32039100
H	0.35699200	-1.88652800	-3.11768600
H	0.54389700	-0.16081700	-2.73340300
Pd	-0.64907100	0.40159900	-0.14212400
C	-3.98181700	-1.23550000	-0.61059500
O	-1.74453400	-1.10976800	0.84773000
O	-2.77978800	0.99674900	0.25916300
O	-3.94389600	-0.50527300	1.96007700
F	-5.14402800	-0.62595900	-0.83470600
F	-4.19788300	-2.51004900	-0.28715100
F	-3.23352800	-1.18318500	-1.71892500
S	-3.09536800	-0.38027100	0.79056400
S	1.47596100	2.64961500	-1.01114200
O	2.02264500	3.42808200	-2.10596300
F	0.41672800	4.79978300	0.03053900
F	0.63757700	3.14908300	1.43364900
F	2.38476200	4.29502900	0.81720700

b₈''-IN3

C	1.98027800	0.14350200	2.24308600
O	0.87874800	0.75346900	2.60854900
O	-0.62810200	1.63066200	-1.16322000
O	0.07793600	2.69711200	0.99021400
C	-2.20423200	3.47561100	-0.11744000
C	2.32662000	-0.10444800	0.91510700

C	3.64948600	-0.41305100	0.36841600
C	1.41305800	-0.11234800	-0.19103600
C	3.47393300	-0.53648000	-1.02610800
C	4.94352000	-0.53000600	0.89119900
H	0.46248800	1.29688000	1.87927100
C	4.52065200	-0.79603900	-1.90629900
C	6.00220800	-0.79654200	0.02195900
H	5.13818100	-0.41604700	1.95145400
C	5.79644900	-0.93114100	-1.35838500
H	4.35816800	-0.88955400	-2.97506500
H	7.00570800	-0.89866600	0.42442400
H	6.63908900	-1.13724500	-2.01131100
N	2.10671000	-0.35116700	-1.31603000
C	2.83273000	-0.25086500	3.40868900
H	3.38746100	-1.17059200	3.21489200
H	3.54941600	0.55114200	3.63202400
H	2.19501200	-0.37545700	4.28741800
C	1.55739900	-0.46936700	-2.66375700
H	2.16102900	0.13107800	-3.34973700
H	1.56889700	-1.51527800	-2.98724000
H	0.53838500	-0.08663700	-2.66631400
Pd	-0.54817300	-0.14813600	-0.13049300
C	-2.50845000	-3.32555300	-0.60977300
O	-0.70272700	-2.00873100	0.85315300
O	-2.70345000	-0.79164000	0.23815900
O	-2.88847100	-2.66964600	1.95457400
F	-3.81299800	-3.43888200	-0.84918500
F	-2.00858200	-4.51356500	-0.27177400
F	-1.89226600	-2.88692600	-1.71464600
S	-2.23687100	-2.11509800	0.78287500
S	-0.43842800	2.94576600	-0.37847900
O	0.20590800	3.97454600	-1.18251000
F	-2.80536400	3.64372500	-1.29494800
F	-2.84957000	2.53697400	0.58056900
F	-2.22574200	4.62382000	0.56103500

b₈-TS2'

Imaginary Frequency:	-1273.6706		
C	-0.57962900	-2.31460900	1.60636800
O	0.52568400	-1.69683600	1.58587700
O	0.31703100	2.03943100	-0.27928100
O	-1.68107800	1.91967000	1.18113900
C	-1.24241000	4.18248900	-0.18108400
C	-1.66298000	-1.79086200	0.82908900

C	-2.79014200	-2.43420800	0.21888500
C	-1.47114500	-0.52906000	0.19615600
C	-3.22041900	-1.55120200	-0.81272900
C	-3.47071000	-3.65402900	0.40077600
H	-1.48289200	0.69984900	0.82298400
C	-4.32221200	-1.83772400	-1.63215400
C	-4.55168500	-3.94274100	-0.41721400
H	-3.17026300	-4.35130600	1.17570900
C	-4.97429900	-3.04323100	-1.42224300
H	-4.65208800	-1.14973700	-2.40338100
H	-5.09128800	-4.87524600	-0.28173100
H	-5.82795100	-3.30204300	-2.04136700
N	-2.39187100	-0.44178800	-0.82316800
C	-0.65036800	-3.59373200	2.38710200
H	-0.74804300	-4.44155800	1.69718100
H	0.26068800	-3.71961300	2.97459900
H	-1.52574400	-3.59700300	3.04551700
C	-2.55242000	0.69084200	-1.72878000
H	-1.61653700	1.24461200	-1.77125900
H	-2.78312700	0.31327600	-2.72772000
H	-3.35712300	1.35135500	-1.39159200
Pd	0.55817400	-0.01706700	0.38012000
C	3.86427300	-1.83481000	-0.51634600
O	2.59476700	0.18858400	0.60297000
O	4.56795700	0.71375200	-0.82337500
F	4.62781700	-1.97110600	0.56918400
F	2.77976700	-2.61876000	-0.38290500
F	4.55103400	-2.23675200	-1.58967100
F	-0.27677800	4.95970200	-0.65475400
F	-1.96801600	3.70160400	-1.19578700
F	-2.03083800	4.87785600	0.63332800
O	2.38569200	-0.08217000	-1.85778700
S	3.33766700	-0.06205500	-0.73435900
S	-0.46679700	2.78259500	0.78340600
O	0.25563900	3.37766400	1.89188900

b₈-TS2''

Imaginary Frequency:	-1299.3752		
C	-1.49323000	-1.48416400	1.71253500
O	-0.23748500	-1.36403100	1.58846800
O	0.87193900	1.70968600	-1.00643100
O	-0.79035300	2.70178100	0.55809000
C	1.77708800	3.34518400	0.94414000
C	-2.33880400	-0.68921500	0.87436900

C	-3.68025300	-0.88991300	0.40786300	O	-1.16179800	1.42424800	0.10399600
C	-1.71659400	0.28240200	0.03993800	O	0.74265400	2.29849600	-1.22094200
C	-3.81455800	-0.05359900	-0.73745800	C	-0.84087200	4.05697500	0.03482100
C	-4.77221600	-1.68630500	0.80411300	C	2.48914500	-0.97542800	-0.73827900
H	-1.14913600	1.47756300	0.44471000	C	3.73954700	-0.99586900	-0.03625500
C	-5.01168700	0.03265000	-1.46326000	C	1.67510500	0.04870700	-0.17587100
C	-5.95062500	-1.61102300	0.07831500	C	3.62495000	-0.00099300	0.97577800
H	-4.70449700	-2.33651700	1.66992000	C	4.92883300	-1.74572400	-0.12393200
C	-6.06975600	-0.75869300	-1.04252300	H	1.13314600	1.15075100	-0.84984000
H	-5.11133900	0.68720200	-2.32251200	C	4.66990200	0.28543500	1.86642100
H	-6.80337200	-2.21272000	0.37808100	C	5.95675900	-1.47209200	0.76460200
H	-7.01001000	-0.72232700	-1.58436000	H	5.05054400	-2.51384700	-0.88021900
N	-2.61351400	0.60477500	-0.95164800	C	5.82965100	-0.46552600	1.74846000
C	-2.00181600	-2.50632800	2.68557200	H	4.57851000	1.05858300	2.62202200
H	-2.47269900	-3.33300500	2.13861100	H	6.88226700	-2.03659300	0.70244200
H	-1.17297800	-2.90028400	3.27617200	H	6.65782900	-0.27658500	2.42484000
H	-2.75914200	-2.06903900	3.34518800	N	2.36958400	0.57789900	0.88942500
C	-2.39225400	1.58155800	-2.01609300	C	2.57806100	-3.06821200	-2.26166000
H	-1.32958600	1.61644200	-2.25330000	H	2.99043900	-3.76495100	-1.52080600
H	-2.93543500	1.26085000	-2.90709000	H	1.88798300	-3.61174500	-2.90922700
H	-2.73742800	2.57535700	-1.71368500	H	3.41262700	-2.67009100	-2.84868600
Pd	0.35675100	-0.05725000	0.11015500	C	1.91218300	1.66123000	1.75166500
C	2.69013100	-3.19530600	-0.21958900	H	0.82541900	1.70392200	1.71984700
O	2.32624600	-0.63300200	0.28876700	H	2.22576100	1.45229400	2.77728000
O	4.24004300	-1.25355100	-1.17248300	H	2.32749400	2.62188000	1.43133500
F	3.42361300	-3.31316300	0.88929400	Pd	-0.33397500	-0.47331700	-0.51429200
F	1.40895700	-3.47054900	0.07885800	C	-3.59501800	-1.49328000	1.32196800
F	3.11732000	-4.08120500	-1.12405900	O	-1.38870000	-2.87985900	0.81447600
F	2.93284900	3.50420600	0.31298800	O	-3.46482000	-3.37357300	-0.56364800
F	1.45803600	4.45807500	1.60118600	F	-4.01927800	-2.33885100	2.26614100
F	1.85904600	2.32682300	1.79957400	F	-2.84768400	-0.53951000	1.90302900
O	1.84919400	-1.43024900	-2.01950000	F	-4.64962500	-0.92042500	0.74054200
S	2.82165800	-1.47394800	-0.91695100	F	-2.09559300	4.26100800	0.41661600
S	0.44407600	2.98995500	-0.31903400	F	-0.05135000	3.98866400	1.11090700
O	0.32379300	4.15427400	-1.17811800	F	-0.43377600	5.04980100	-0.74942200
b₈-TS2'''				O	-2.19473600	-1.26162700	-0.89834700
Imaginary Frequency: -1294.5004				S	-2.56953100	-2.41311400	0.07008800
C	1.84832100	-1.96318000	-1.55688300	O	-1.60365500	2.62764500	-2.10202400
O	0.58690400	-1.94264400	-1.64270700	S	-0.76463800	2.45897200	-0.93129400