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Supplementary Information

Chiral Bisoxazoline Catalyzed Decarboxylative Aldol Reactions between *β*-Carbonyl Acids and Trifluoroacetaldehyde Hemiacetals as well as Trifluoroacetaldehyde: Mechanism, Origin of Enantioselectivity and Role of Catalyst

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1. Structures of catalyst and reactants

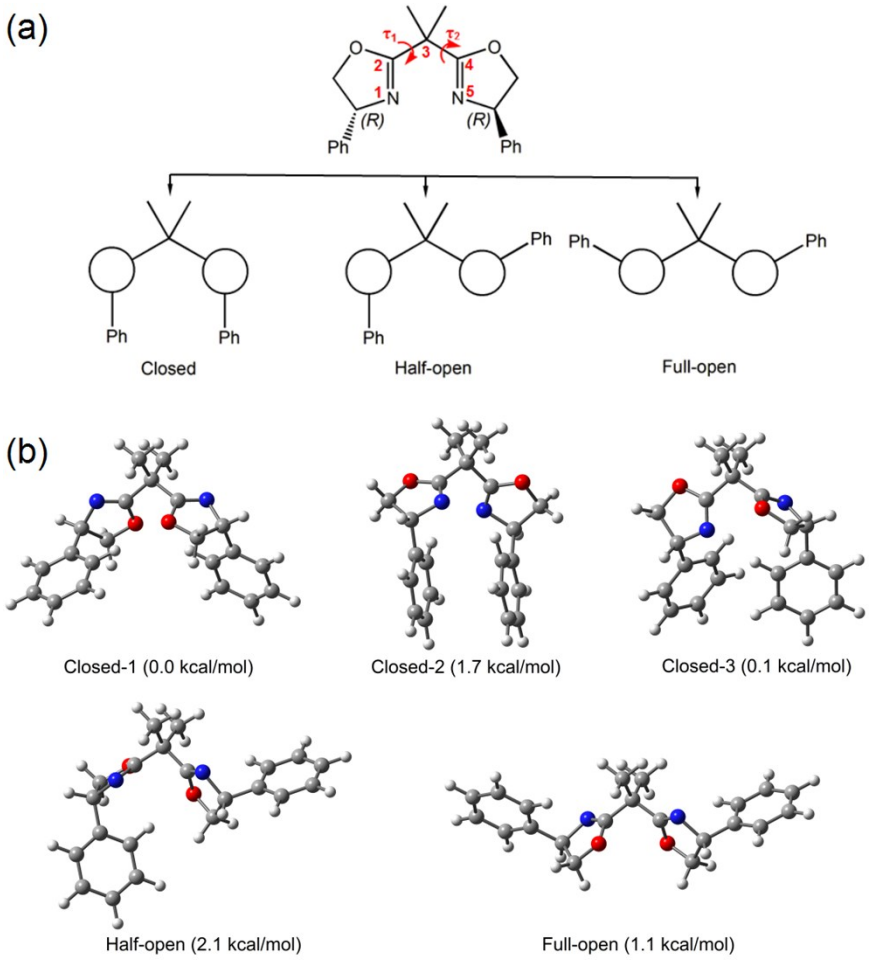

Fig. S1. (a) **Box** with two rotatable C-C single bonds (τ_1 is the torsion angle of N1-C2-C3-C4 and τ_2 is the torsion angle of N5-C4-C3-C2) and three types of conformations; (b) Optimized geometries of five conformations (closed-1, closed-2, closed-3, half-open, full-open. The value in the parenthesis is the relative Gibbs free energy compared to that of conformation closed-1.) at the local minima on the potential energy surface for **Box**.

As a flexible molecule, **Box** has multiple conformations, and the conformation with lower energy has larger Boltzmann distribution, so such conformation would contribute significantly during the reaction process. Herein, two rotable C-C single bonds of **Box** (τ_1 and τ_2, Fig. S1a) were taken into account because their rotations would affect the binding between reactants and

Box. The variations of the two torsion angles (τ_1 and τ_2) lead to three types of conformations (closed, half-open, full-open, Fig. S1a), in which the benzene rings of **Box** have distinctive orientations. Five stable conformations were found for **Box**, as shown in Fig. 1b. Due to the much higher conformation energies of three conformations (closed-2, half-open, full-open), two more stable conformations (closed-1 and closed-3) were chosen as starting structures which are termed as $\mathbf{Box}_{c\text{-}1}$ and $\mathbf{Box}_{c\text{-}3}$, respectively. With respect to ***β*-CA**, it has four possible structures (***β*-CA$_1$**, ***β*-CA$_2$**, ***β*-CA$_3$**, ***β*-CA$_4$**) considering its enol-keto tautomerization and the rotation of carboxyl group, as shown in Fig. S2a. The most stable one is ***β*-CA$_1$**, so it is taken into account in the reaction process. **TMH** used in the experiment is racemic, so both (*S*)- and (*R*)-**TMH** participate in the reaction process, and their optimized structures are shown in Fig. S2b.

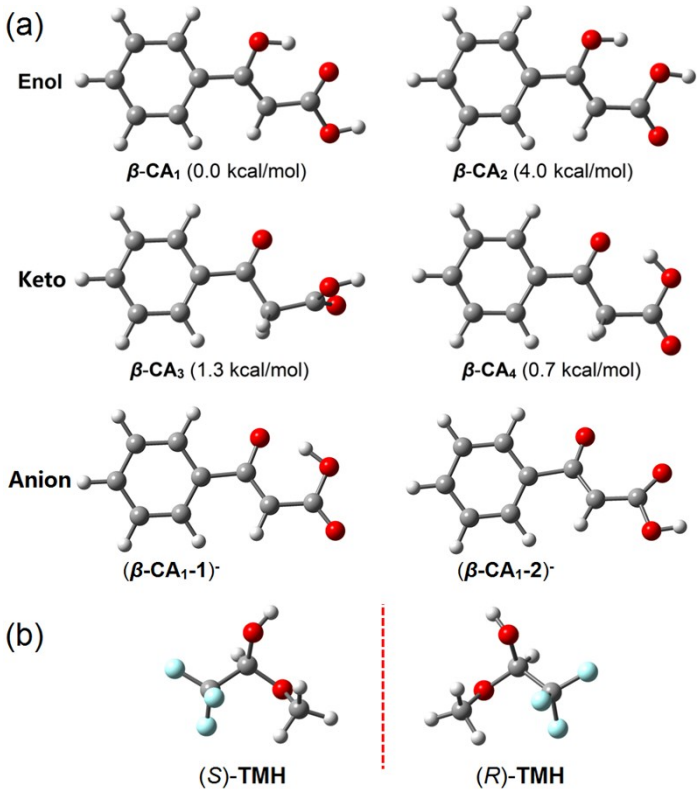

Fig. S2. (a) Optimized geometries of four possible structures (***β*-CA$_1$**, ***β*-CA$_2$**, ***β*-CA$_3$**, ***β*-CA$_4$**. The value in the parenthesis is the relative Gibbs free energy compared to that of ***β*-CA$_1$**.) of ***β*-CA** and its two possible anions; (b) Optimized geometries of (*S*)- and (*R*)-**TMH**.

2. QTAIM analyses of the intermediate IM1-1 in the reaction of *β*-CA$_1$ and TMH catalyzed by Box in Scheme 1a.

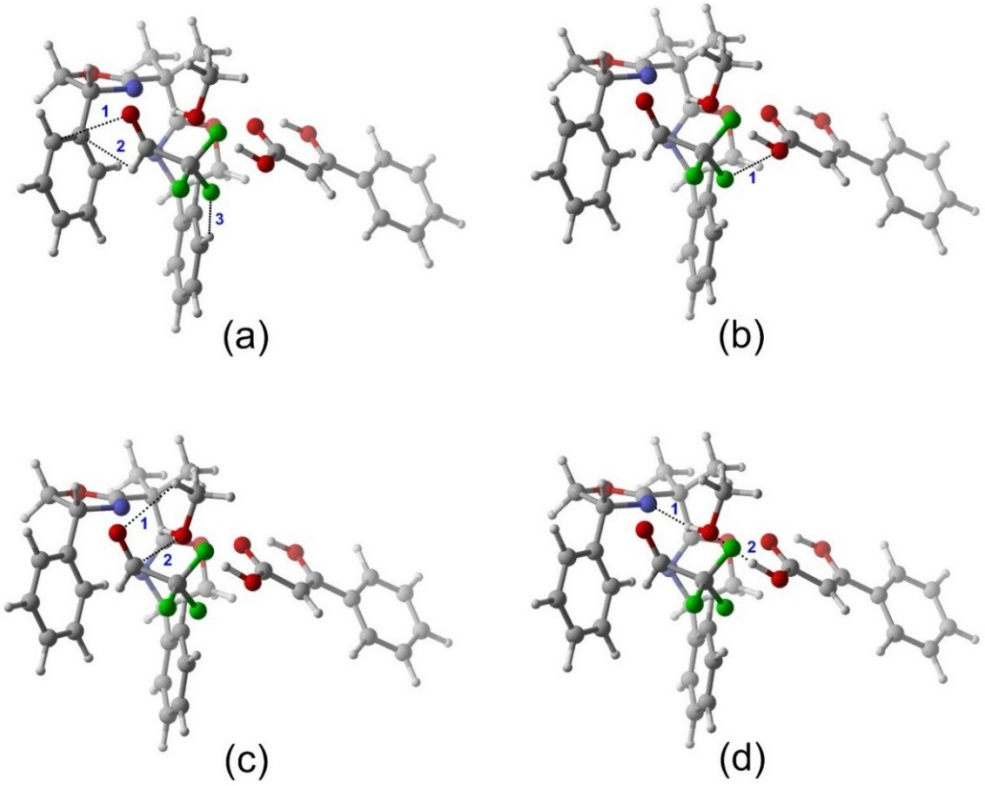

Fig. S3. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and CF_3CHO in **IM1-1**, (b) the interaction between ***β*-CA$_1$** and CF_3CHO in **IM1-1**, (c) the interaction between MeOH and CF3CHO (d) the interaction between MeOH and **Box**, between MeOH and ***β*-CA$_1$** in **IM1-1**.

Table S1. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and Its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **IM1-1**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.47	lp···π	0.0081	0.0273	-0.0052	0.0060	0.0008
	2	3.01	C-H···π	0.0103	0.0345	-0.0059	0.0072	0.0013
	3	2.66	C-H···F	0.0071	0.0281	-0.0050	0.0060	0.0010
(b)	1	3.03	lp···lp	0.0076	0.0367	-0.0065	0.0079	0.0014
(c)	1	2.83	C-H···O	0.0092	0.0312	-0.0058	0.0068	0.0010
	2	1.92	lp···π	0.0211	0.0698	-0.0163	0.0169	0.0006
(d)	1	2.85	O-H···N	0.0387	0.1072	-0.0331	0.0299	-0.0032
	2	3.18	O-H···O	0.0468	0.1467	-0.0466	0.0416	-0.0050

3. The optimized structures for the four transition states and intermediates without removal of MeOH during nucleophilic addition.

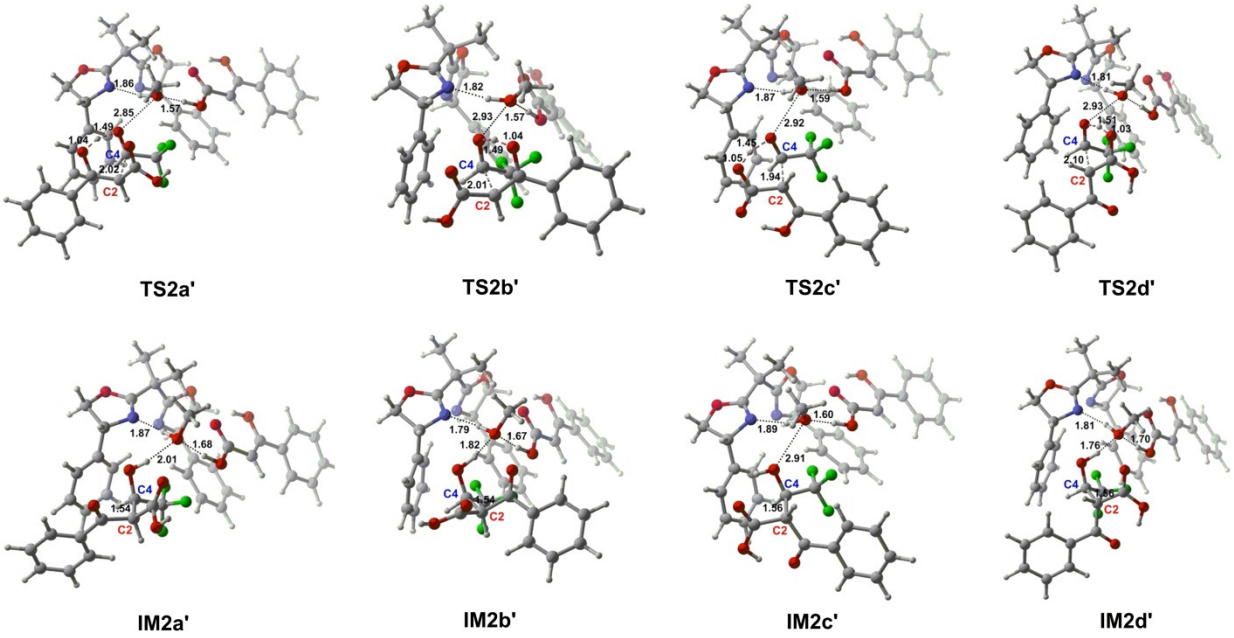

Fig. S4. The optimized structures for the four transition states and intermediates without removal of MeOH during nucleophilic addition.

4. The optimized structures for the four transition states and intermediates in the path of IM1-1→IM2X→TS2X→IM3X (X=a, b, c, g).

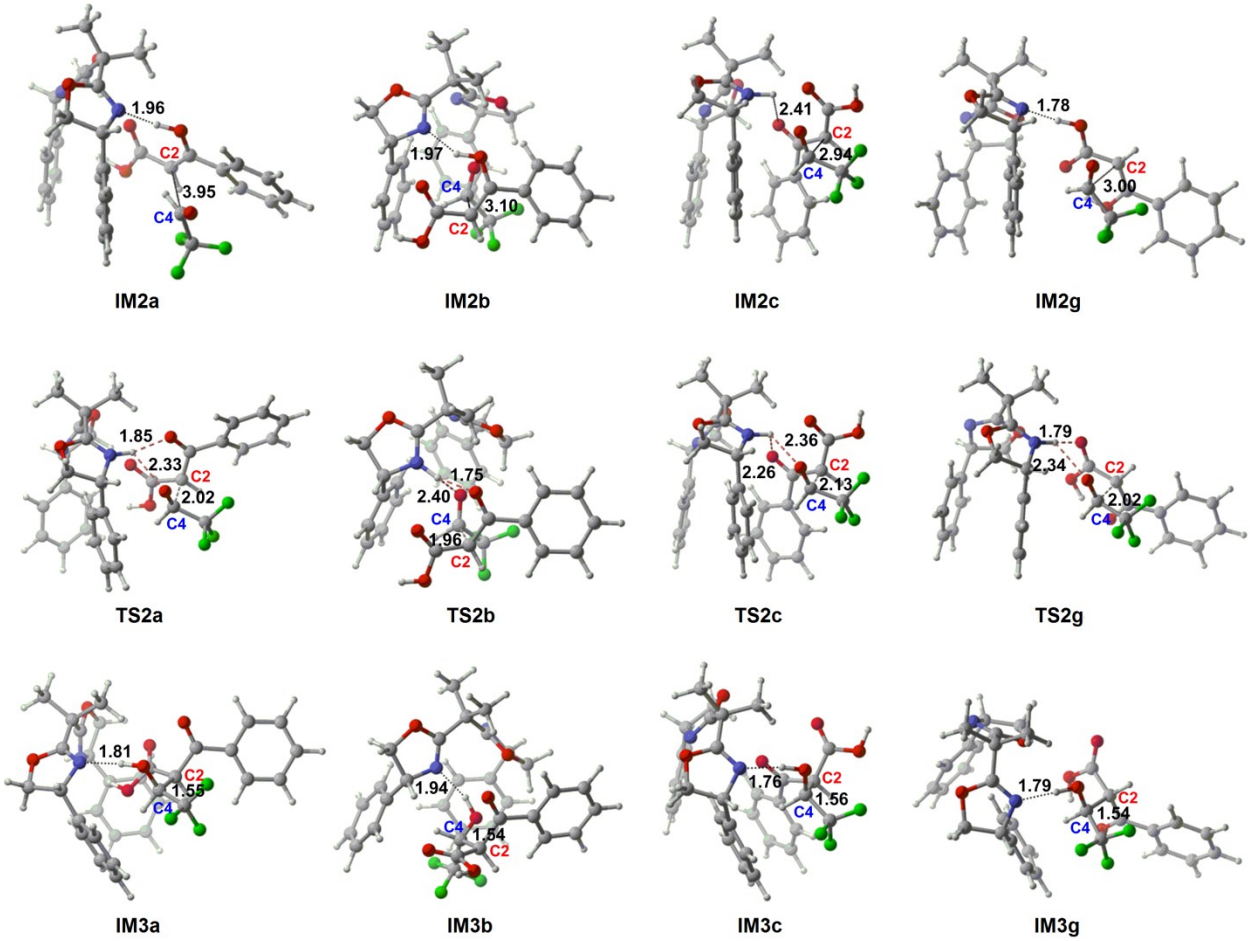

Fig. S5. The optimized structures for the four transition states and intermediates in the path of **IM1-1→IM2X→TS2X→IM3X** (**X=a**, **b**, **c**, **g**).

5. The optimized structures for the three transition states TS3e', TS3f', TS3h'.

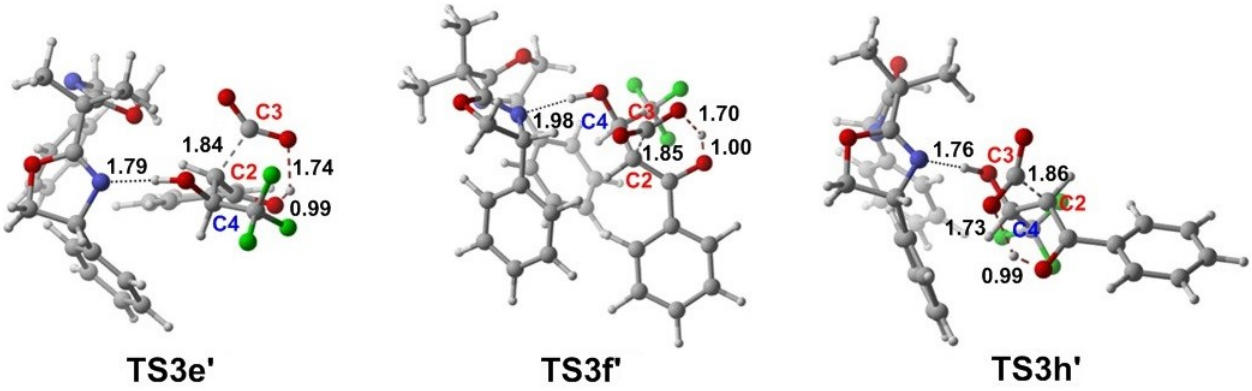

Fig. S6. The optimized structures for the three transition states **TS3e'**, **TS3f'**, **TS3h'**.

6. The optimized structures for the transition state TS_T'.

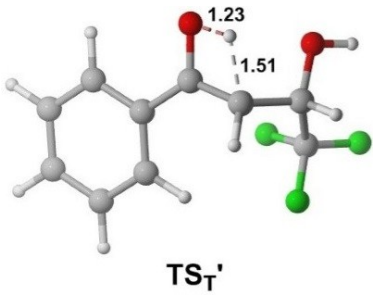

Fig. S7. The optimized structures for the transition state $\mathbf{TS_T'}$.

7. QTAIM analyses of the intermediate IM2X (X=d, e, f, h) in the reaction of *β*-CA$_1$ and TMH catalyzed by Box in Scheme 1a.

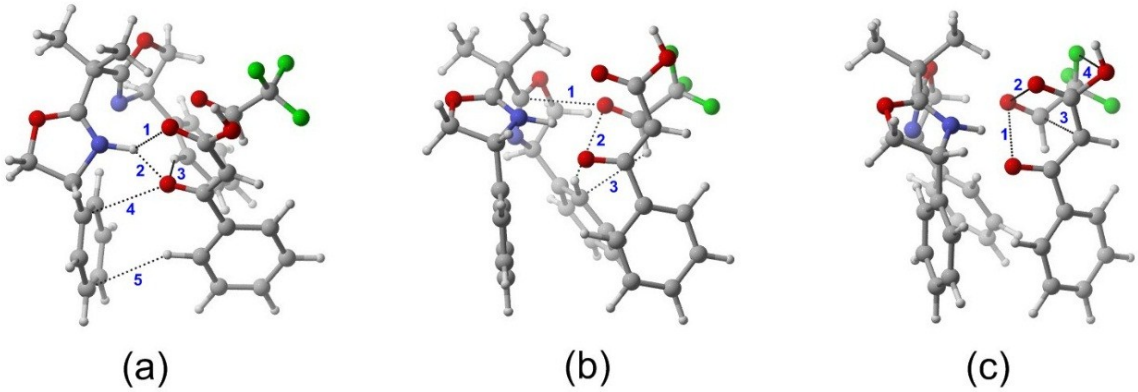

Fig. S8. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **IM2d**, (b) the interaction between **Box** and CF_3CHO in **IM2d**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **IM2d**.

Table S2. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **IM2d**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	2.29	N-H···O	0.0129	0.0553	-0.0090	0.0114	0.0024
	2	1.58	N-H···O	0.0627	0.1151	-0.0703	0.0496	-0.0207
	3	2.42	C-H···O	0.0101	0.0379	-0.0058	0.0077	0.0019
	4	2.96	lp···π	0.0099	0.0383	-0.0064	0.0080	0.0016
	5	2.82	C-H···π	0.0066	0.0220	-0.0036	0.0045	0.0009
(b)	1	2.85	lp···π	0.0098	0.0418	-0.0067	0.0086	0.0019
	2	2.63	C-H···O	0.0083	0.0318	-0.0051	0.0065	0.0014
	3	2.77	C-H···π	0.0072	0.0249	-0.0043	0.0053	0.0010
(c)	1	2.95	lp···lp	0.0095	0.0427	-0.0064	0.0085	0.0021
	2	3.08	lp···lp	0.0069	0.0301	-0.0041	0.0058	0.0017
	3	2.76	π···π	0.0192	0.0438	-0.0103	0.0106	0.0003
	4	2.93	lp···lp	0.0078	0.0393	-0.0052	0.0075	0.0023

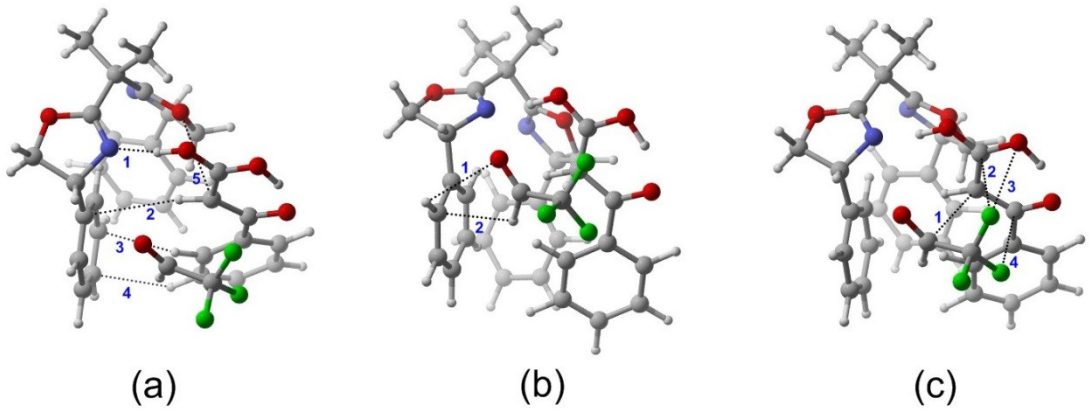

Fig. S9. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **IM2e**, (b) the interaction between **Box** and CF_3CHO in **IM2e**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **IM2e**.

Table S3. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **IM2e**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.65	O-H···N	0.0608	0.0568	-0.0588	0.0365	-0.0223
	2	2.97	C-H···π	0.0051	0.0145	-0.0022	0.0029	0.0007
	3	2.76	C-H···π	0.0079	0.0249	-0.0042	0.0052	0.0010
	4	2.82	C-H···π	0.0063	0.0206	-0.0033	0.0042	0.0009
	5	3.12	lp···π	0.0082	0.0316	-0.0051	0.0065	0.0014
(b)	1	2.76	C-H···O	0.0073	0.0291	-0.0045	0.0059	0.0014
	2	2.66	C-H···π	0.0085	0.0262	-0.0047	0.0056	0.0009
(c)	1	2.82	π···π	0.0150	0.0387	-0.0082	0.0090	0.0008
	2	2.94	lp···π	0.0081	0.0328	-0.0052	0.0067	0.0015
	3	2.91	lp···lp	0.0080	0.0409	-0.0055	0.0079	0.0024
	4	2.91	lp···π	0.0086	0.0341	-0.0053	0.0069	0.0016

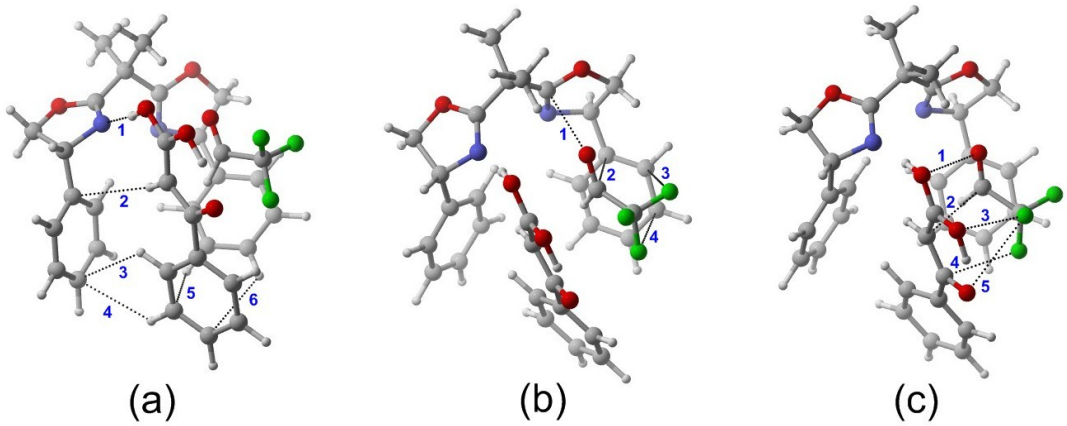

Fig. S10. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **IM2f**, (b) the interaction between **Box** and CF_3CHO in **IM2f**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **IM2f**.

Table S4. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **IM2f**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.65	O-H···N	0.0606	0.0581	-0.0588	0.0367	-0.0221
	2	2.80	C-H···π	0.0060	0.0176	-0.0029	0.0036	0.0007
	3	2.80	C-H···π	0.0075	0.0254	-0.0042	0.0053	0.0011
	4	2.78	C-H···π	0.0066	0.0206	-0.0034	0.0043	0.0009
	5	2.80	C-H···π	0.0066	0.0201	-0.0033	0.0042	0.0009
	6	3.21	C-H···π	0.0033	0.0108	-0.0014	0.0020	0.0006
(b)	1	2.87	lp···π	0.0105	0.0408	-0.0068	0.0085	0.0105
	2	3.10	π···π	0.0115	0.0366	-0.0071	0.0081	0.0115
	3	3.24	lp···π	0.0060	0.0226	-0.0032	0.0044	0.0060
	4	3.18	lp···π	0.0059	0.0224	-0.0032	0.0044	0.0059
(c)	1	3.11	lp···lp	0.0061	0.0288	-0.0036	0.0054	0.0018
	2	2.81	π···π	0.0156	0.0427	-0.0090	0.0098	0.0008
	3	2.90	lp···lp	0.0077	0.0410	-0.0053	0.0078	0.0025
	4	2.92	lp···π	0.0080	0.0358	-0.0054	0.0072	0.0018
	5	3.11	lp···lp	0.0055	0.0270	-0.0035	0.0051	0.0016

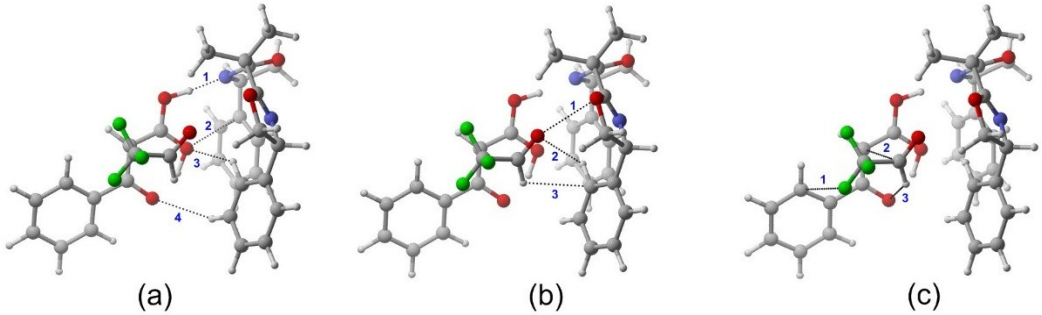

Fig. S11. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **IM2h**, (b) the interaction between **Box** and CF_3CHO in **IM2h**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **IM2h**.

Table S5. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **IM2h**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.59	O-H···N	0.0698	0.0467	-0.0689	0.0403	-0.0286
	2	3.08	lp···π	0.0088	0.0337	-0.0054	0.0069	0.0015
	3	2.38	C-H···O	0.0106	0.0426	-0.0066	0.0086	0.0020
	4	2.63	C-H···O	0.0065	0.0253	-0.0036	0.0050	0.0014
(b)	1	2.97	lp···lp	0.0075	0.0385	-0.0053	0.0075	0.0022
	2	2.68	C-H···O	0.0087	0.0336	-0.0055	0.0069	0.0014
	3	2.72	C-H···π	0.0083	0.0260	-0.0046	0.0055	0.0009
(c)	1	3.05	lp···π	0.0068	0.0303	-0.0042	0.0059	0.0017
	2	2.98	π···π	0.0129	0.0352	-0.0071	0.0080	0.0009
	3	2.64	C-H···O	0.0077	0.0301	-0.0047	0.0061	0.0014

8. The intermolecular complexes formed between two conformations of Box (Box_{c-1} and Box_{c-3}) and CF_3CHO, and the calculated interaction energies and relative Gibbs free energies.

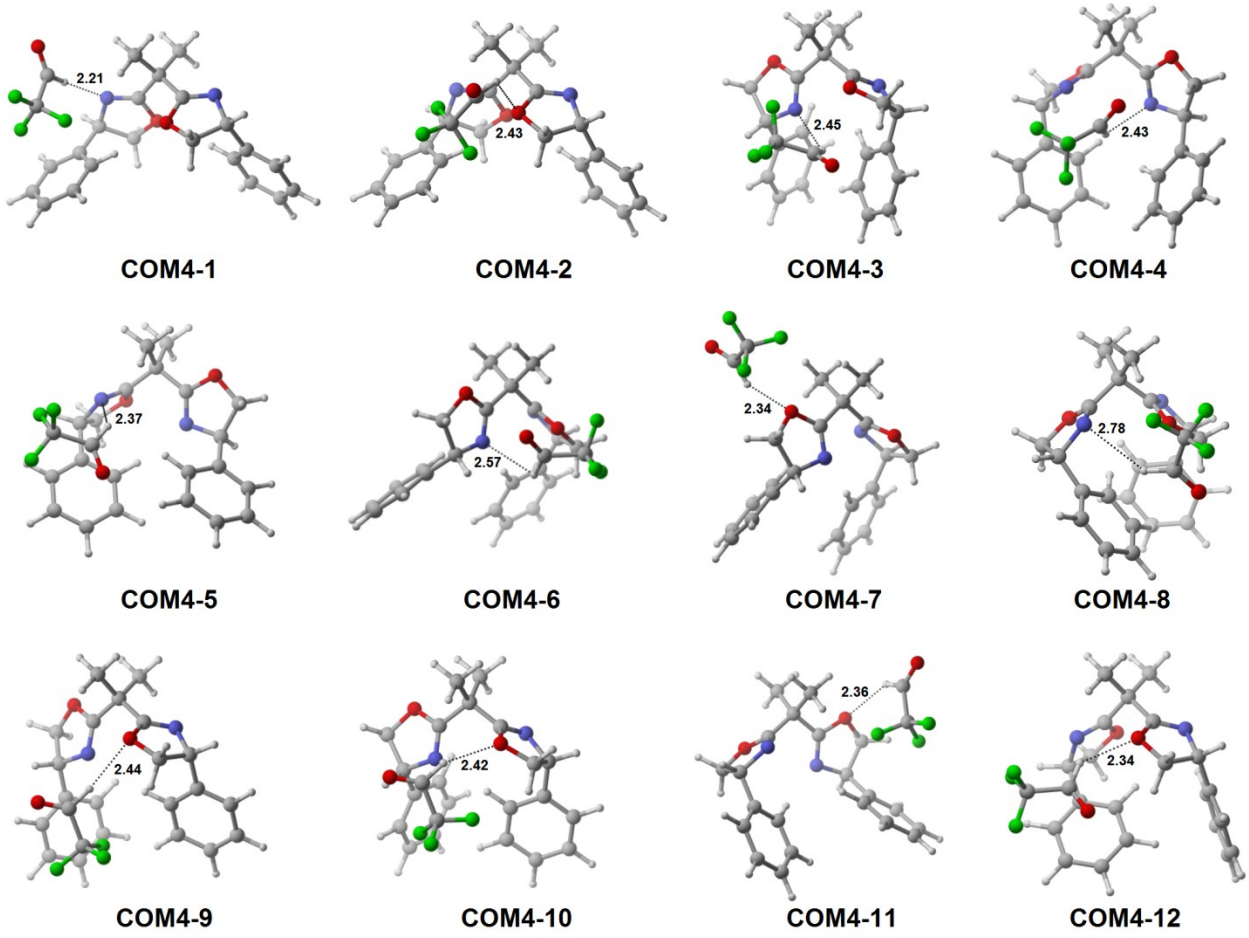

Fig. S12. The intermolecular complexes formed between two conformations of **Box** (**Box_{c-1}** and **Box_{c-3}**) and CF_3CHO.

Table S6. The interaction energies (ΔE_{int}, in kcal/mol) and relative Gibbs free energies (ΔG, in kcal/mol) for the complexes formed between two conformations of **Box** (**Box**$_{c-1}$ and **Box**$_{c-3}$) and CF_3CHO at the M06-2X/6-311G(d,p) level of theory.

Complex[a]	Interaction	ΔE_{int}[b]	ΔG[c]
COM4-1	C-H···N	-7.7	3.2
COM4-2	C-H···O	-6.0	5.3
COM4-3	C-H···N	-11.8	2.6
COM4-4	C-H···N	-11.3	3.0
COM4-5	C-H···N	-11.9	1.6
COM4-6	C-H···N	-11.1	1.2
COM4-7	C-H···N	-10.2	3.2
COM4-8	C-H···O	-9.9	3.1
COM4-9	C-H···O	-12.2	2.0
COM4-10	C-H···O	-5.8	6.1
COM4-11	C-H···O	-5.7	5.2
COM4-12	C-H···O	-12.8	2.0

[a] The complexes formed between two conformations of **Box** (**Box**$_{c-1}$ and **Box**$_{c-3}$) and CF_3CHO are shown in Fig. S12.

[b] The interaction energy (ΔE_{int}) is the energy difference between the total energy of the complex and the sum of total energies of **Box**$_{c-1}$ and CF_3CHO.

[c] The relative Gibbs free energies (ΔG) is the free energy difference between the total free energy of the complex and the sum of total free energies of **Box**$_{c-1}$ and CF_3CHO.

9. The intermolecular complexes formed between two conformations of Box (Box_{c-1} and Box_{c-3}), *β*-CA_1 and CF_3CHO (*Si*- and *Re*-faces)., and the calculated interaction energies and relative Gibbs free energies.

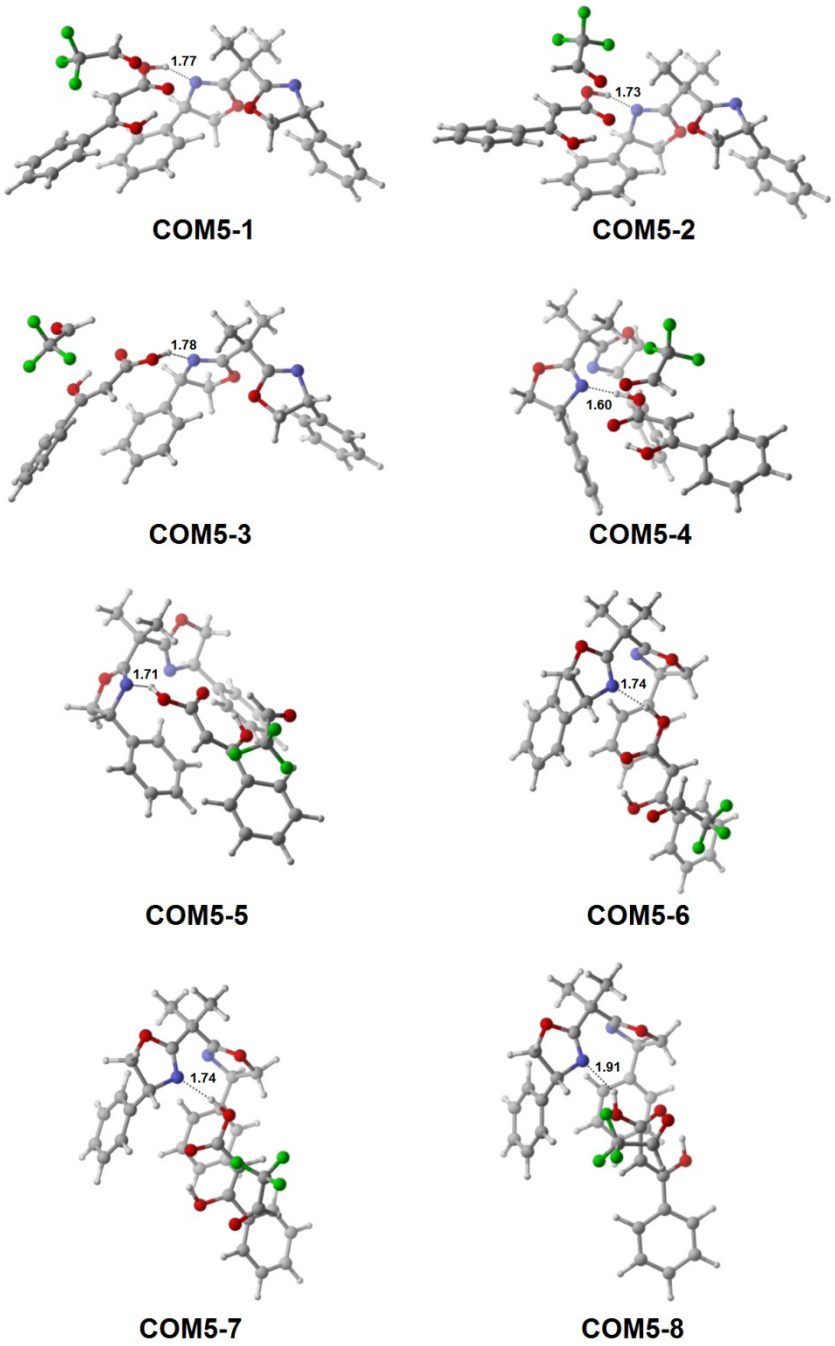

Fig. S13. The tertiary complexes formed between two conformations of **Box** (**Box_{c-1}** and **Box_{c-3}**), ***β*-CA_1** and CF_3CHO (*Si*- and *Re*-faces).

Table S7. The interaction energies (ΔE_{int}, in kcal/mol) and relative Gibbs free energies (ΔG, in kcal/mol) for the tertiary complexes formed between two conformations of **Box** (**Box**$_{c\text{-}1}$ and **Box**$_{c\text{-}3}$), ***β*-CA$_1$** and CF_3CHO at the M06-2X/6-311G(d,p) level of theory.

Complex[a]	ΔE_{int}[b]	ΔG[c]
COM5-1	-22.4	1.3
COM5-2	-21.9	2.2
COM5-3	-22.3	1.1
COM5-4	-23.5	1.3
COM5-5	-25.3	0.9
COM5-6	-25.9	-0.2
COM5-7	-26.4	0.4
COM5-8	-22.2	2.1

[a] The tertiary complexes formed between two conformations of **Box** (**Box**$_{c\text{-}1}$ and **Box**$_{c\text{-}3}$), ***β*-CA$_1$** and CF_3CHO (*Si*- and *Re*-faces) are shown in Fig. S13.

[b] The interaction energy (ΔE_{int}) is the energy difference between the total energy of the tertiary complex and the sum of total energies of **Box**$_{c\text{-}1}$, ***β*-CA$_1$** and CF_3CHO (*Si*- and *Re*-faces).

[c] The relative Gibbs free energies (ΔG) is the free energy difference between the total free energy of the tertiary complex and the sum of total free energies of **Box**$_{c\text{-}1}$, ***β*-CA$_1$** and CF_3CHO (*Si*- and *Re*-faces).

10. The optimized structures for the twelve transition states and intermediates in the nucleophilic addition of *β*-CA$_1$ in secondary complexes between Box and *β*-CA$_1$ to either *Si*- or *Re*-face of CF$_3$CHO.

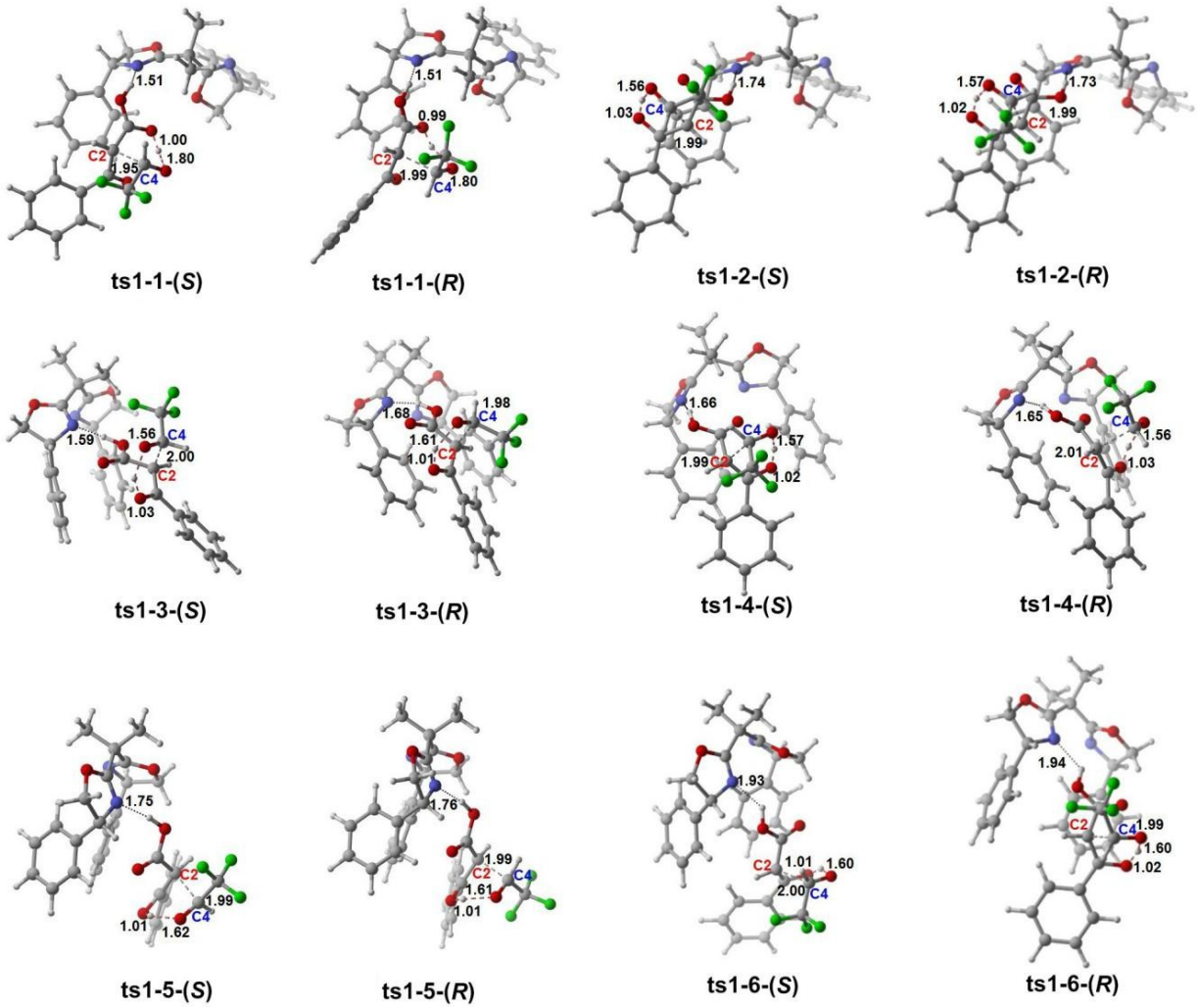

Fig. S14. The optimized structures for the twelve transition states in the nucleophilic addition of ***β*-CA$_1$** in secondary complexes between **Box** and ***β*-CA$_1$** to either *Si*- or *Re*-face of CF$_3$CHO.

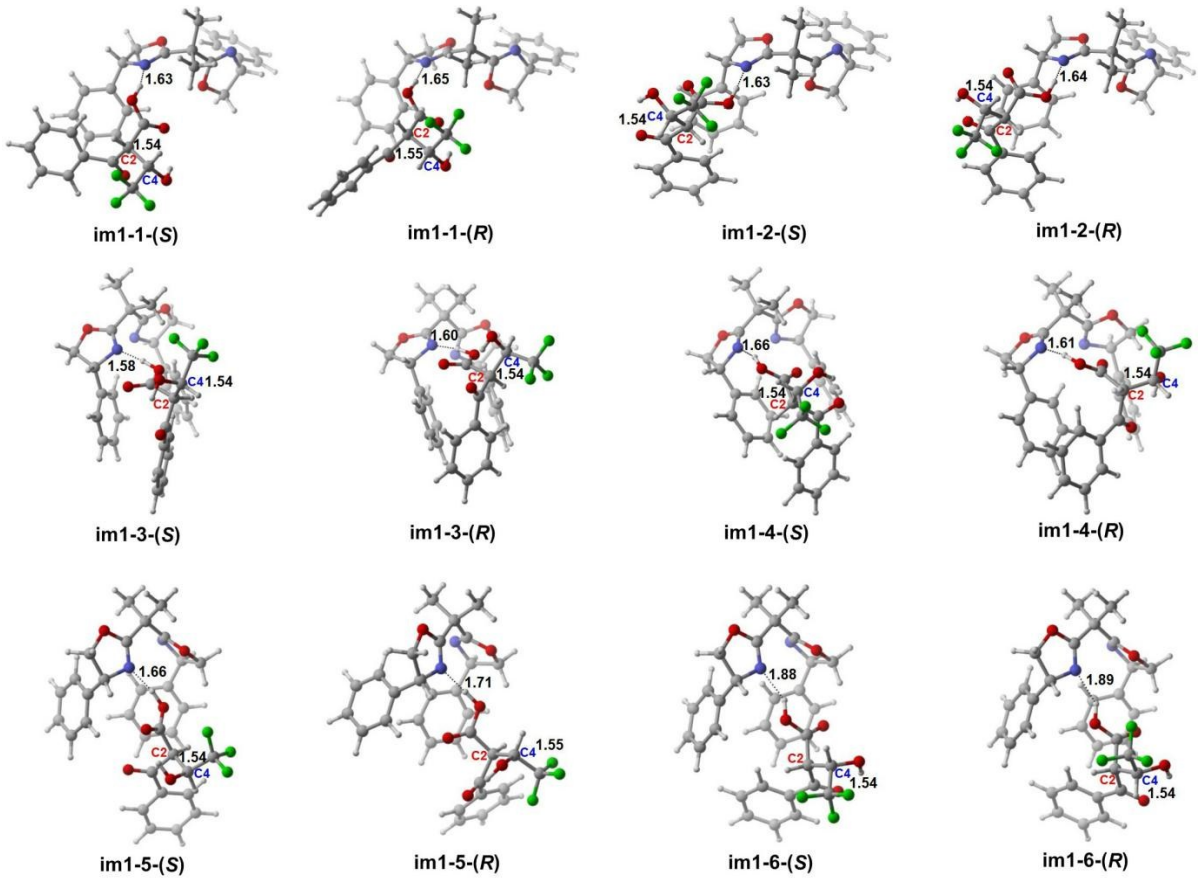

Fig. S15. The optimized structures for the twelve intermediates in the nucleophilic addition of ***β*-CA$_1$** in secondary complexes between **Box** and ***β*-CA$_1$** to either *Si*- or *Re*-face of CF_3CHO.

11. The optimized structures for the twelve transition states and intermediates for the direct decarboxylation in the third step (step C).

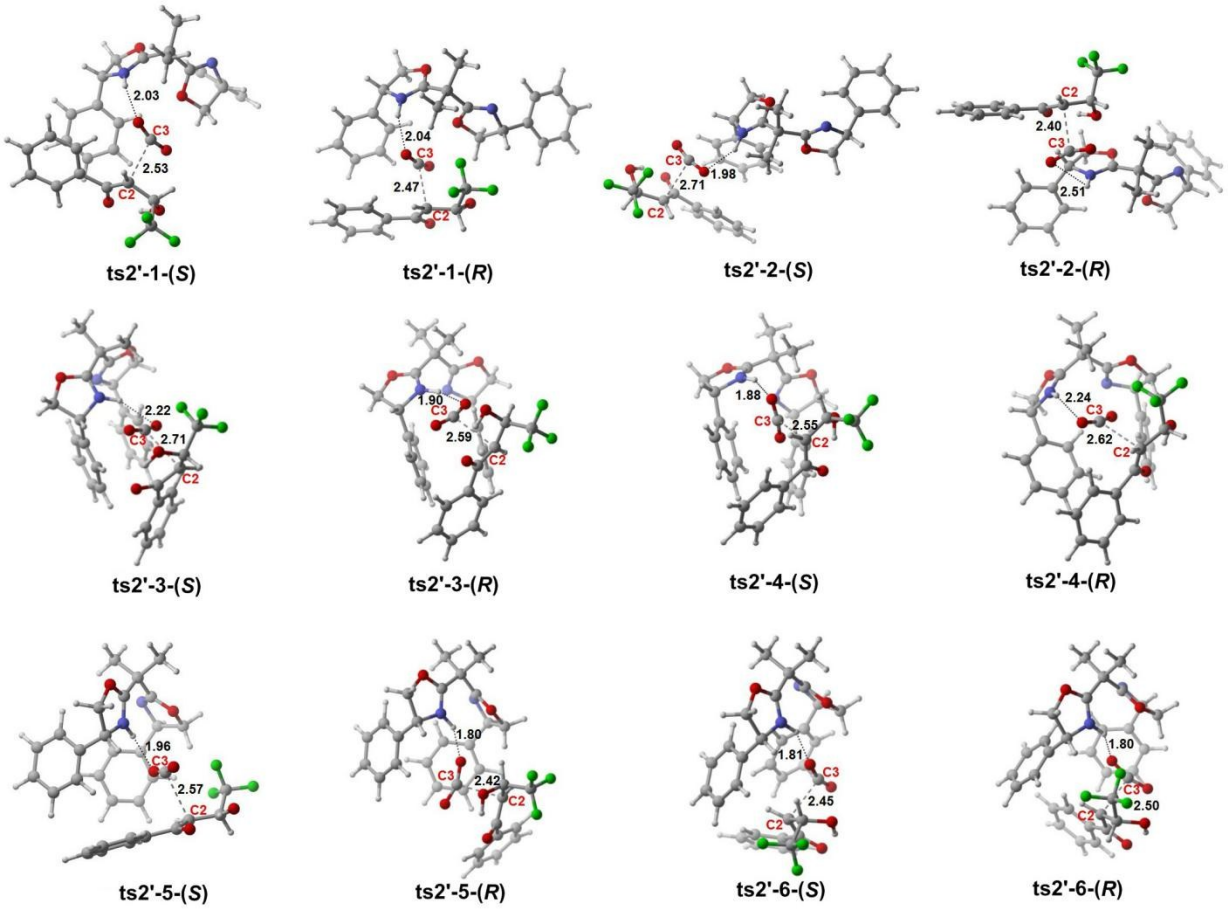

Fig. S16. The optimized structures for the twelve transition states for the direct decarboxylation in the third step (step C).

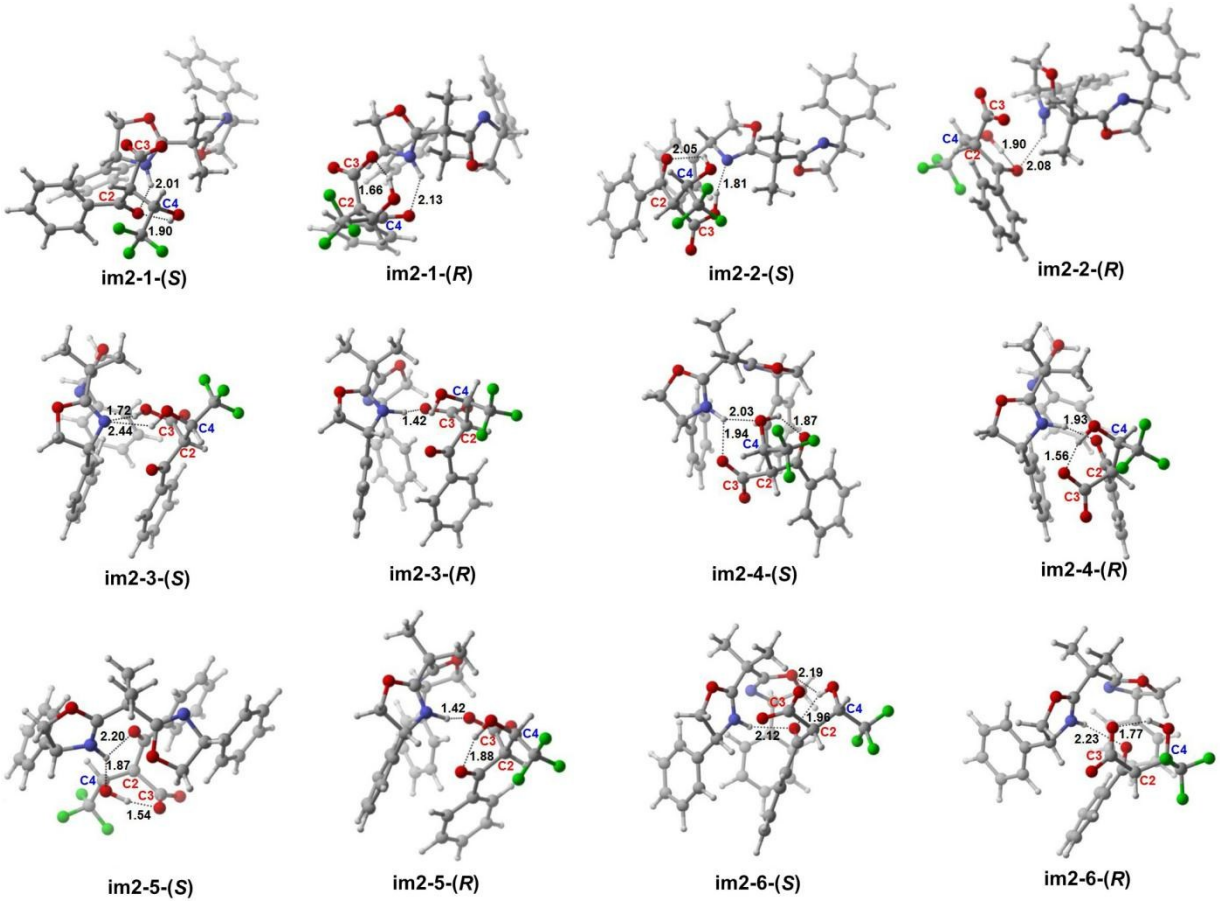

Fig. S17. The optimized structures for the twelve intermediates formed with a six-membered ring during the decarboxylation in the third step (step C).

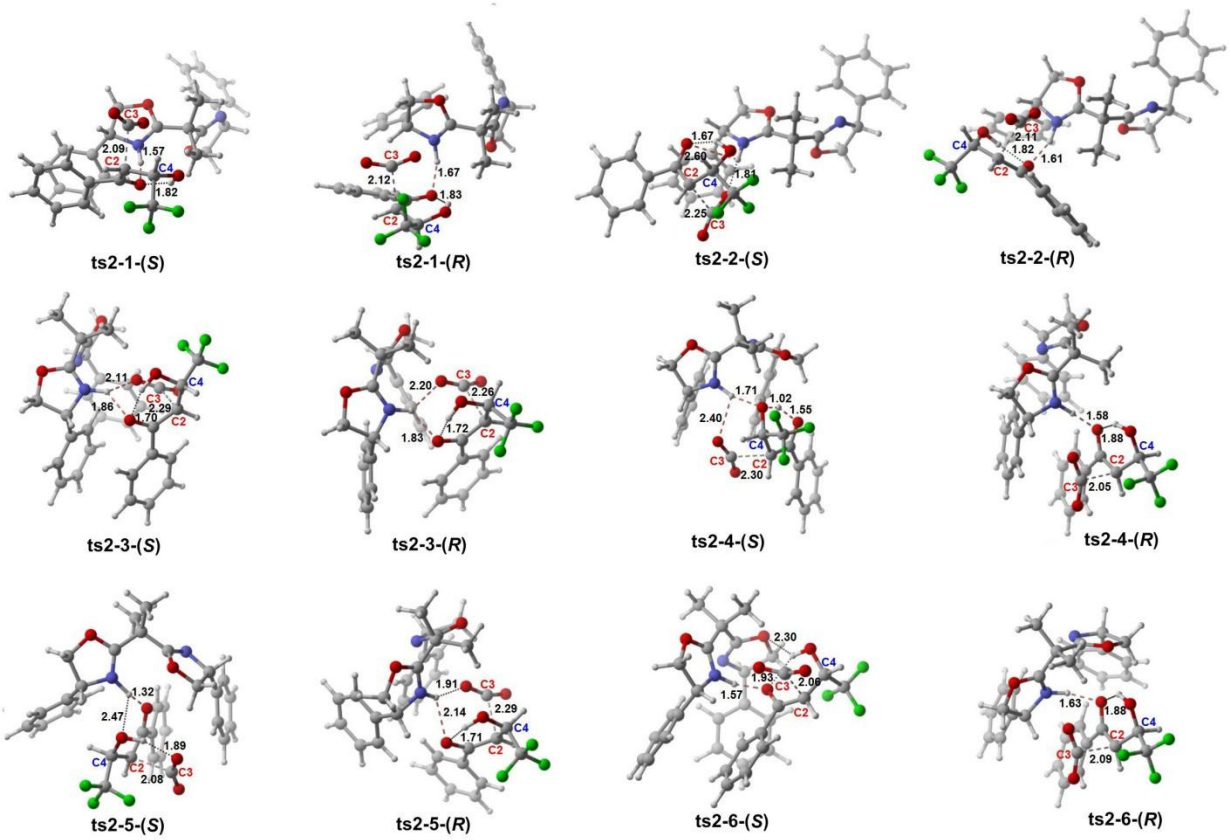

Fig. S18. The optimized structures for the twelve transition states for the decarboxylation in the third step (step C).

12. The optimized structures for the twelve intermediates as HB complexes (the Box•enol-P complexes) after the decarboxylation in the fourth step (step D).

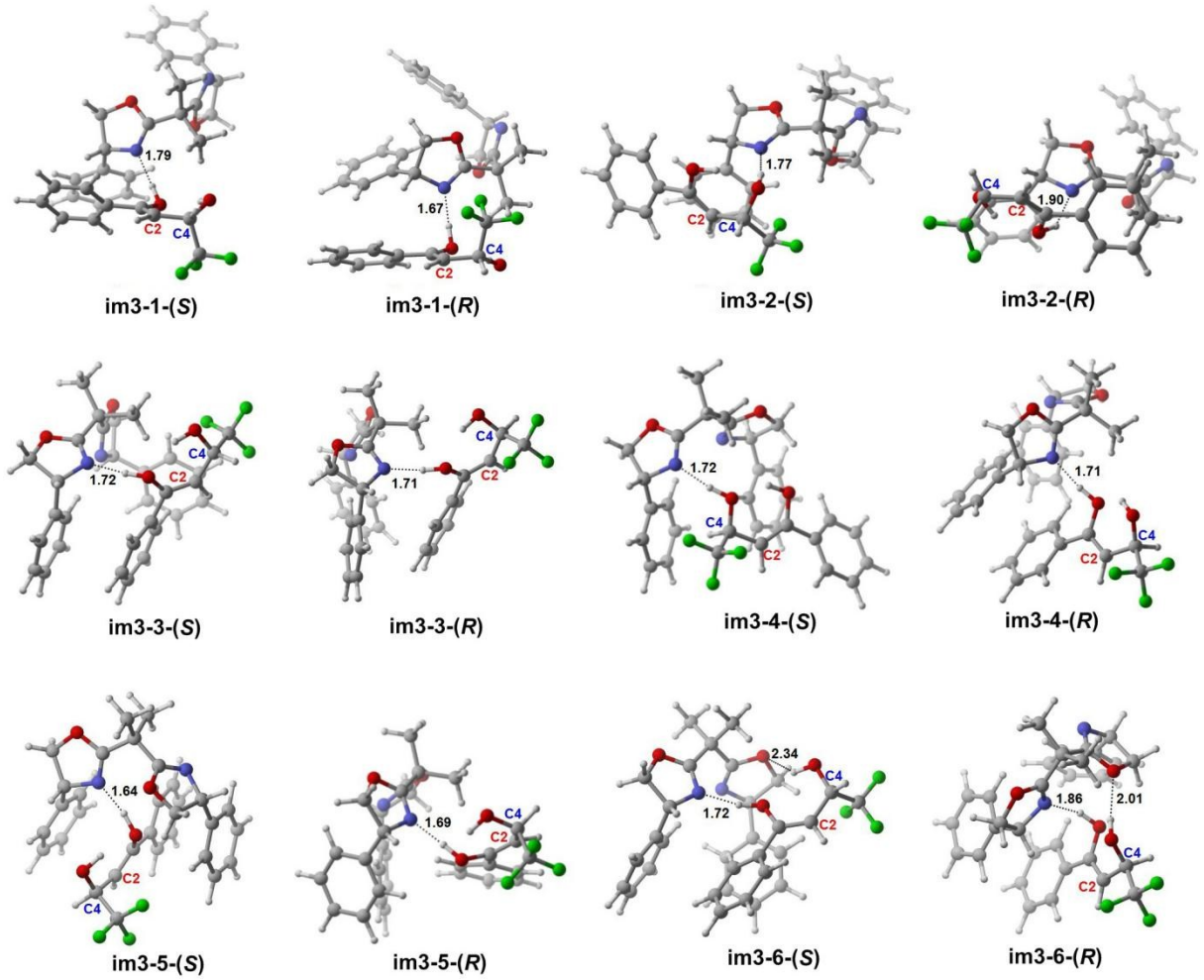

Fig. S19. The optimized structures for the twelve intermediates as HB complexes (the **Box•**enol-**P** complexes) after the decarboxylation in the fourth step (step D).

13. The distortion/interaction analyses for the origin of enantioselectivity in the reaction of *β*-CA_1 and TMH catalyzed by Box in Scheme 1a.

Table S8. The out-of-plane distortion distance of C2 atom (d_{C2}, in Å) in the transition state **TS2X** (**X**=**a**, **b**, **c**, **d**, **e**, **f**, **g**, **h**) and the relative distortion energy (in kcal/mol).

	TS2a	**TS2b**	**TS2c**	**TS2d**	**TS2e**	**TS2f**	**TS2g**	**TS2h**
d_{C2}	0.245	0.265	0.249	0.113	0.325	0.136	0.245	0.286
$\Delta E_{dist}'$	-1.7	-1.6	-3.2	-7.1	/	/	/	/
ΔE_{dist}	/	/	/	/	0.3	-6.6	-2.5	0.0

Table S9. The out-of-plane distortion distance of C4 atom (d_{C4}, in Å) and the F-C-C-O dihedral angel (τ, in º) in CF_3CHO in the transition state **TS2X** (**X=a**, **b**, **c**, **d**, **e**, **f**, **g**, **h**) and the relative distortion energy (in kcal/mol).

	TS2a	**TS2b**	**TS2c**	**TS2d**	**TS2e**	**TS2f**	**TS2g**	**TS2h**
d_{C4}	0.262	0.289	0.232	0.110	0.285	0.135	0.250	0.280
τ(F-C-C-O)	53.4	46.1	48.3	36.1	57.2	56.5	59.3	57.5
$\Delta E_{dist}(CF_3CHO)$	-2.4	0.5	-5.7	-7.7	0.4	-11.7	-3.3	0.0

Table S10. The distances between N and O atoms in different oxazoline rings (d_1, (N-H$^+$···O); d_2,(N···O); in Å), the sum of their distance (d_1+d_2), and ΔE_{dist}(**Box**·H$^+$) in **TS2X** (**X**=**a**, **b**, **c**, **d**, **e**, **f**, **g**, **h**), in kcal/mol.

	TS2a	**TS2b**	**TS2c**	**TS2d**	**TS2e**	**TS2f**	**TS2g**	**TS2h**
d_2	3.17	3.45	3.03	3.50	3.80	3.54	3.37	3.15
d_1	4.15	3.71	4.37	4.22	2.97	4.19	3.26	4.36
(d_1+ d_2)	7.32	7.16	7.40	7.72	6.77	7.73	6.63	7.51
ΔE_{dist}(**Box**·H$^+$)	2.5	2.8	2.4	1.0	4.6	3.4	1.9	0.0

14. QTAIM analyses of the transition state TS2X (X=a, b, c, d, e, f, g, h).

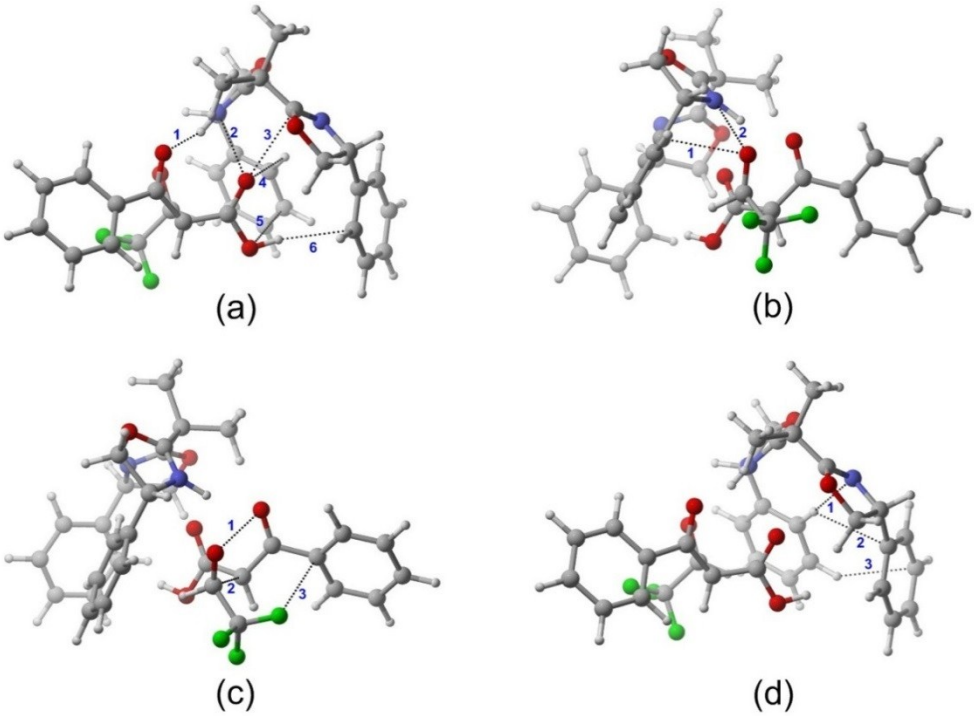

Fig. S20. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2a**, (b) the interaction between **Box** and CF_3CHO in **TS2a**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2a**, (d) the interaction between two phenyl rings in **Box** in **TS2a**.

Table S11. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of**TS2a**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.85	N-H···O	0.0309	0.0913	-0.0280	0.0254	-0.0026
	2	2.86	lp···lp	0.0132	0.0555	-0.0095	0.0117	0.0022
	3	2.79	lp···π	0.0112	0.0477	-0.0080	0.0100	0.0020
	4	2.60	C-H···O	0.0093	0.0346	-0.0057	0.0072	0.0015
	5	3.39	lp···π	0.0052	0.0180	-0.0025	0.0035	0.0010
	6	2.50	O-H···π	0.0089	0.0260	-0.0047	0.0056	0.0009
(b)	1	2.84	lp···π	0.0139	0.0544	-0.0101	0.0119	0.0018
	2	2.86	lp···lp	0.0133	0.0576	-0.0097	0.0120	0.0023
(c)	1	2.67	lp···lp	0.0171	0.0773	-0.0142	0.0168	0.0026
	2	2.02	π···π	0.0840	0.0226	-0.0552	0.0304	-0.0248
	3	2.98	lp···π	0.0080	0.0335	-0.0049	0.0067	0.0018
(d)	1	2.46	C-H···N	0.0104	0.0345	-0.0058	0.0072	0.0014
	2	3.06	C-H···π	0.0045	0.0145	-0.0022	0.0029	0.0007
	3	2.63	C-H···π	0.0092	0.0292	-0.0051	0.0062	0.0011

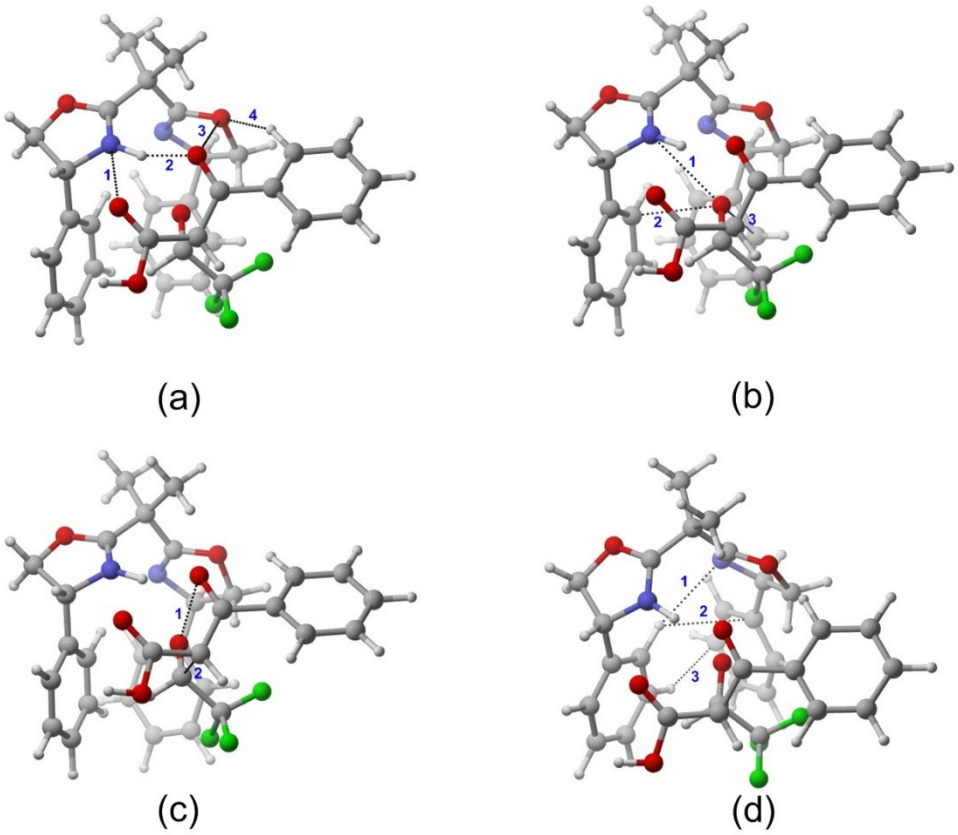

Fig. S21. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2b**, (b) the interaction between **Box** and CF_3CHO in **TS2b**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2b**, (d) the interaction between two phenyl rings in **Box** in **TS2b**.

Table S12. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **TS2b**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	2.87	lp···lp	0.0118	0.0531	-0.0086	0.0109	0.0023
	2	1.75	N-H···O	0.0395	0.1021	-0.0388	0.0322	-0.0066
	3	3.26	lp···lp	0.0049	0.0195	-0.0026	0.0037	0.0011
	4	2.45	C-H···O	0.0086	0.0346	-0.0051	0.0069	0.0018
(b)	1	2.96	lp···lp	0.0120	0.0479	-0.0080	0.0100	0.0020
	2	2.80	lp···π	0.0133	0.0516	-0.0091	0.0110	0.0019
	3	3.38	lp···π	0.0053	0.0183	-0.0027	0.0036	0.0009
(c)	1	2.70	lp···lp	0.0165	0.0762	-0.0139	0.0165	0.0026
	2	1.96	π···π	0.0957	-0.0018	-0.0663	0.0329	-0.0334
(d)	1	2.67	C-H···N	0.0069	0.0224	-0.0034	0.0045	0.0011
	2	3.13	C-H···π	0.0039	0.0124	-0.0018	0.0024	0.0006
	3	2.73	C-H···π	0.0078	0.0247	-0.0041	0.0052	0.0011

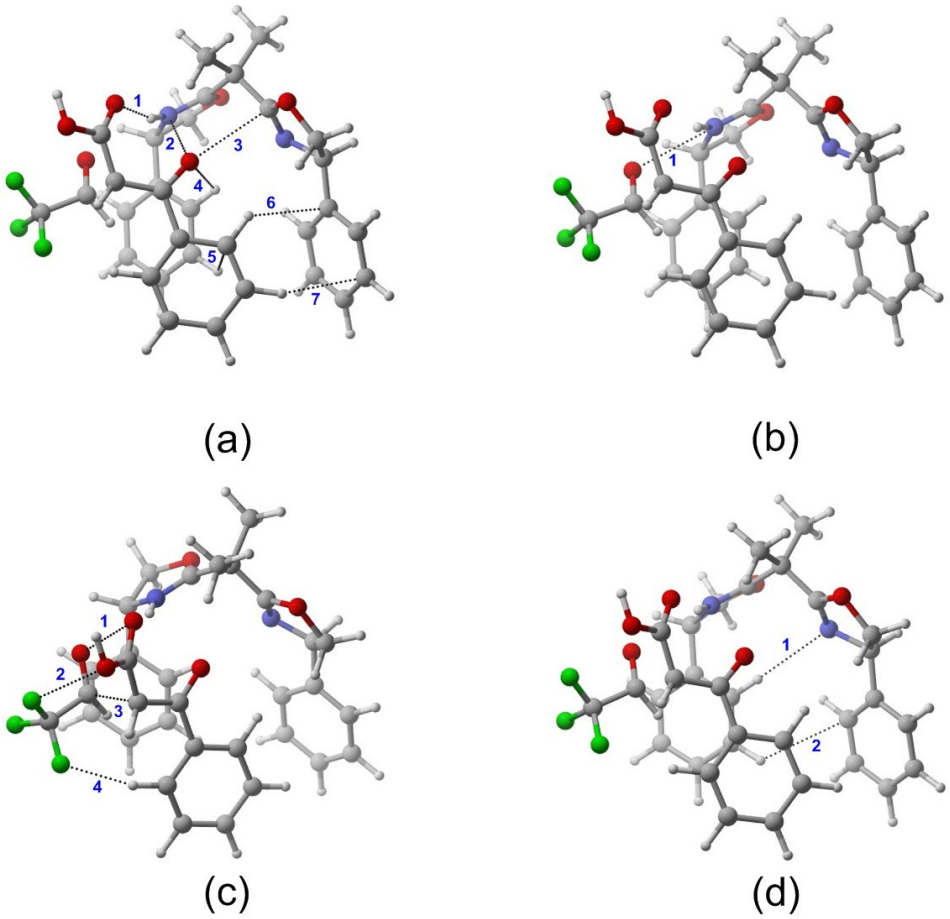

Fig. S22. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2c**, (b) the interaction between **Box** and CF_3CHO in **TS2c**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2c**, (d) the interaction between two phenyl rings in **Box** in **TS2c**.

Table S13. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **TS2c**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.91	N-H···O	0.0267	0.0860	-0.0232	0.0224	-0.0008
	2	2.80	lp···lp	0.0156	0.0660	-0.0116	0.0141	0.0025
	3	3.03	lp···π	0.0071	0.0279	-0.0043	0.0056	0.0013
	4	2.52	C-H···O	0.0099	0.0371	-0.0060	0.0077	0.0016
	5	2.83	C-H···π	0.0071	0.0222	-0.0037	0.0047	0.0010
	6	2.85	C-H···π	0.0061	0.0180	-0.0030	0.0037	0.0008
	7	2.72	C-H···π	0.0079	0.0248	-0.0041	0.0052	0.0011
(b)	1	2.86	lp···lp	0.0125	0.0552	-0.0092	0.0115	0.0023
(c)	1	2.72	lp···lp	0.0152	0.0704	-0.0124	0.0150	0.0026
	2	2.89	lp···lp	0.0082	0.0415	-0.0055	0.0079	0.0024
	3	2.13	π···π	0.0671	0.0445	-0.0401	0.0256	-0.0145
	4	2.27	C-H···F	0.0111	0.0499	-0.0076	0.0100	0.0024
(d)	1	2.64	C-H···N	0.0077	0.0246	-0.0039	0.0050	0.0012
	2	2.96	C-H···π	0.0054	0.0175	-0.0027	0.0035	0.0008

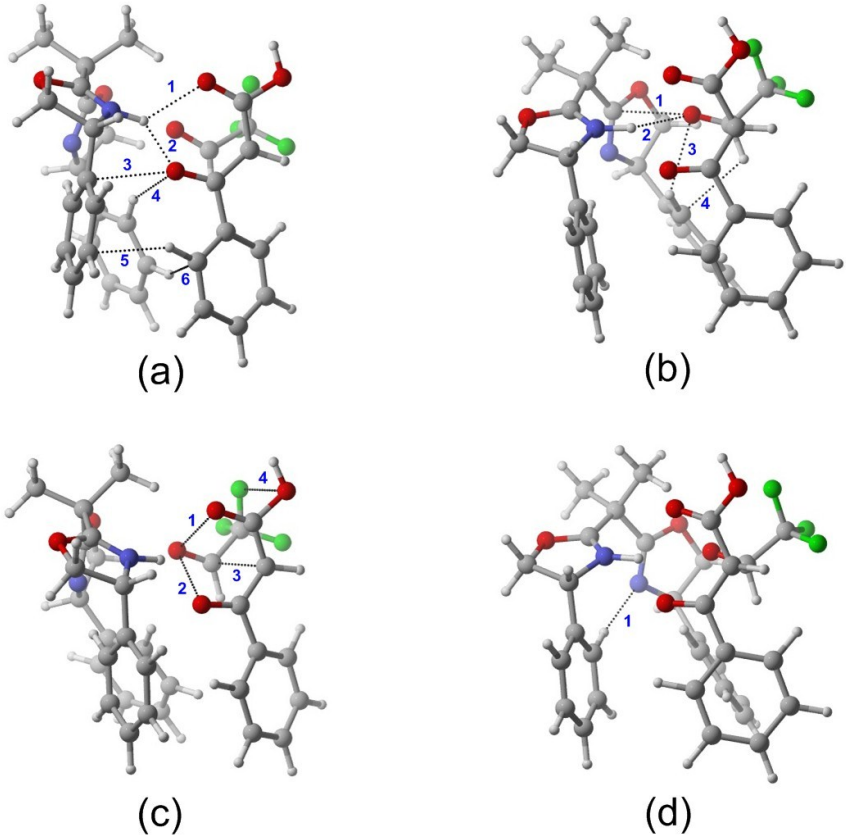

Fig. S23. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2d**, (b) the interaction between **Box** and CF_3CHO in **TS2d**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2d**, (d) the interaction between two phenyl rings in **Box** in **TS2d**.

Table S14. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **TS2d**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	2.18	N-H···O	0.0156	0.0658	-0.0114	0.0139	0.0025
	2	1.79	N-H···O	0.0376	0.1242	-0.0374	0.0342	-0.0032
	3	2.86	lp···π	0.0112	0.0453	-0.0077	0.0095	0.0018
	4	2.63	C-H···O	0.0067	0.0236	-0.0034	0.0047	0.0013
	5	2.80	C-H···π	0.0065	0.0209	-0.0033	0.0043	0.0010
	6	2.63	C-H···π	0.0091	0.0294	-0.0051	0.0062	0.0011
(b)	1	2.77	lp···π	0.0115	0.0489	-0.0082	0.0102	0.0020
	2	2.48	N-H···O	0.0076	0.0300	-0.0045	0.0060	0.0015
	3	2.49	C-H···O	0.0104	0.0403	-0.0066	0.0083	0.0017
	4	2.78	C-H···π	0.0075	0.0275	-0.0048	0.0059	0.0011
(c)	1	2.93	lp···lp	0.0096	0.0420	-0.0063	0.0084	0.0021
	2	2.94	lp···lp	0.0101	0.0458	-0.0071	0.0093	0.0022
	3	2.54	π···π	0.0300	0.0504	-0.0158	0.0142	-0.0016
	4	2.89	lp···lp	0.0086	0.0437	-0.0059	0.0084	0.0025
(d)	1	2.38	C-H···N	0.0129	0.0428	-0.0076	0.0091	0.0015

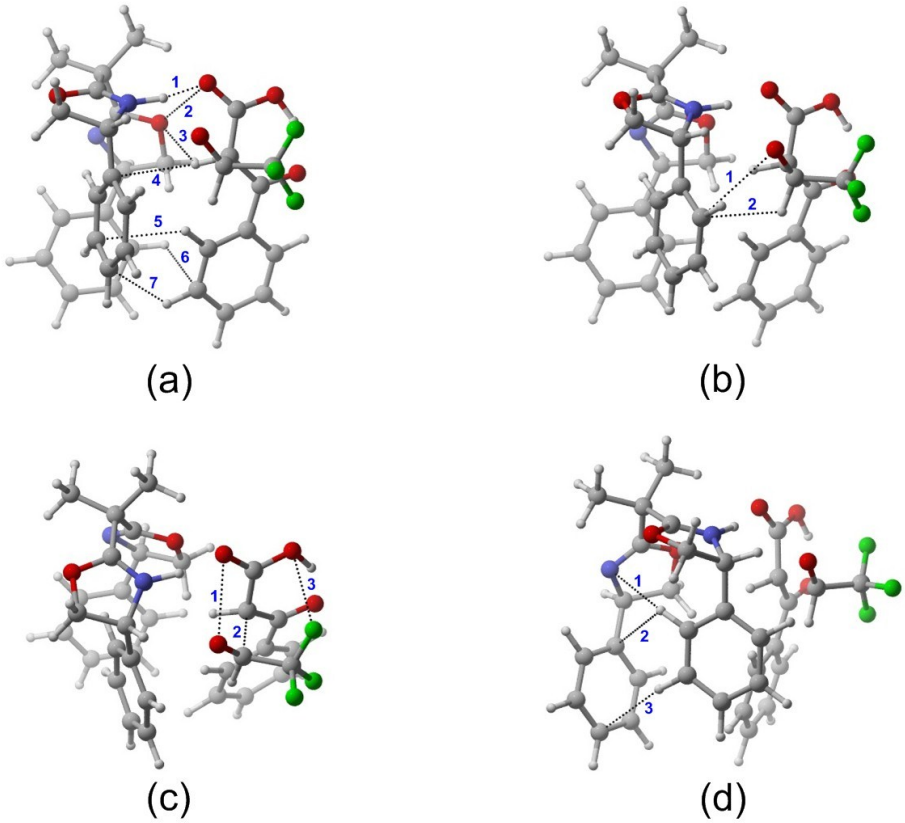

Fig. S24. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2e**, (b) the interaction between **Box** and CF_3CHO in **TS2e**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2e**, (d) the interaction between two phenyl rings in **Box** in **TS2e**.

Table S15. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **TS2e**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.47	N-H···O	0.0834	0.0810	-0.0966	0.0584	-0.0382
	2	3.01	lp···lp	0.0082	0.0367	-0.0052	0.0072	0.0020
	3	2.66	C-H···O	0.0076	0.0299	-0.0048	0.0061	0.0013
	4	3.03	C-H···π	0.0046	0.0130	-0.0020	0.0026	0.0006
	5	2.77	C-H···π	0.0079	0.0256	-0.0043	0.0054	0.0011
	6	3.07	C-H···π	0.0053	0.0160	-0.0025	0.0033	0.0008
	7	2.75	C-H···π	0.0071	0.0230	-0.0038	0.0048	0.0010
(b)	1	3.03	lp···π	0.0105	0.0407	-0.0071	0.0086	0.0015
	2	2.67	C-H···π	0.0085	0.0278	-0.0051	0.0060	0.0009
(c)	1	2.83	lp···lp	0.0126	0.0598	-0.0099	0.0124	0.0025
	2	1.92	π···π	0.1012	-0.0124	-0.0731	0.0350	-0.0381
	3	2.81	lp···lp	0.0103	0.0536	-0.0075	0.0105	0.0030
(d)	1	2.85	C-H···N	0.0066	0.0203	-0.0033	0.0042	0.0009
	2	3.18	C-H···π	0.0040	0.0128	-0.0019	0.0025	0.0008
	3	2.75	C-H···π	0.0074	0.0246	-0.0041	0.0051	0.0010

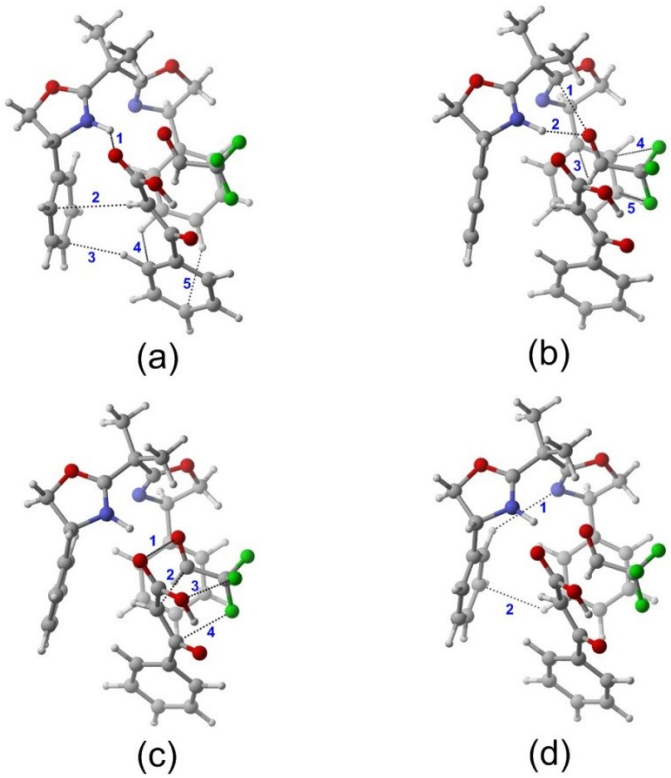

Fig. S25. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2f**, (b) the interaction between **Box** and CF_3CHO in **TS2f**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2f**, (d) the interaction between two phenyl rings in **Box** in **TS2f**.

Table S16. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **TS2f**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.78	N-H···O	0.0380	0.1210	-0.0377	0.0340	-0.0037
	2	2.99	C-H···π	0.0052	0.0156	-0.0024	0.0031	0.0007
	3	2.68	C-H···π	0.0082	0.0244	-0.0041	0.0051	0.0010
	4	3.04	C-H···π	0.0058	0.0185	-0.0029	0.0038	0.0009
	5	2.80	C-H···π	0.0069	0.0216	-0.0035	0.0045	0.0010
(b)	1	2.84	lp···π	0.0114	0.0436	-0.0075	0.0092	0.0114
	2	2.12	N-H···O	0.0164	0.0696	-0.0123	0.0148	0.0164
	3	2.64	C-H···π	0.0111	0.0378	-0.0071	0.0083	0.0111
	4	3.32	lp···π	0.0046	0.0164	-0.0023	0.0032	0.0046
	5	3.35	lp···π	0.0041	0.0146	-0.0020	0.0028	0.0041
(c)	1	2.83	lp···lp	0.0126	0.0598	-0.0099	0.0124	0.0025
	2	1.92	π···π	0.1012	-0.0124	-0.0731	0.0350	-0.0381
	3	2.81	lp···lp	0.0103	0.0536	-0.0075	0.0105	0.0030
	4	2.86	lp···π	0.0118	0.0498	-0.0080	0.0103	0.0023
(d)	1	2.96	C-H···N	0.0047	0.0145	-0.0021	0.0029	0.0008
	2	2.89	C-H···π	0.0059	0.0194	-0.0031	0.0040	0.0009

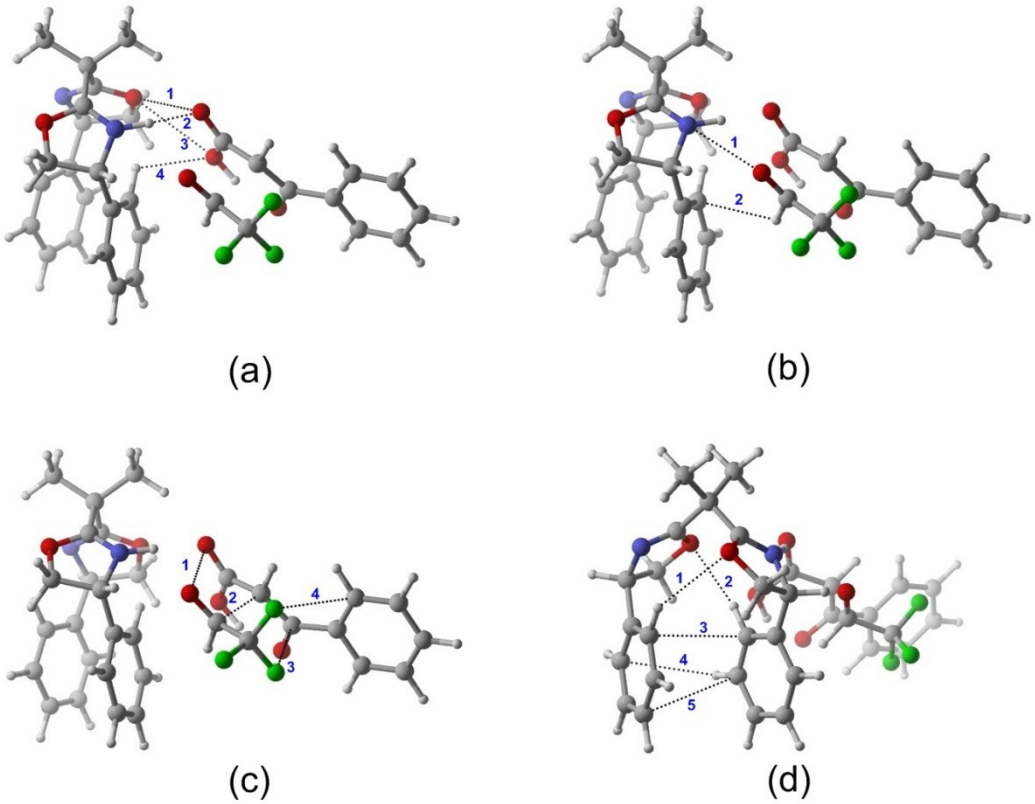

Fig. S26. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2g**, (b) the interaction between **Box** and CF_3CHO in **TS2g**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2g**, (d) the interaction between two phenyl rings in **Box** in **TS2g**.

Table S17. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **TS2g**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	3.06	lp···lp	0.0073	0.0304	-0.0043	0.0060	0.0017
	2	1.79	N-H···O	0.0340	0.1027	-0.0326	0.0291	0.0035
	3	3.16	lp···lp	0.0049	0.0225	-0.0029	0.0043	0.0014
	4	2.51	C-H···O	0.0104	0.0405	-0.0066	0.0084	0.0018
(b)	1	2.83	lp···lp	0.0134	0.0595	-0.0101	0.0125	0.0024
	2	2.73	C-H···π	0.0084	0.0269	-0.0049	0.0058	0.0009
(c)	1	2.79	lp···lp	0.0142	0.0654	-0.0114	0.0139	0.0025
	2	2.02	π···π	0.0818	0.0272	-0.0540	0.0304	-0.0236
	3	2.78	lp···π	0.0112	0.0510	-0.0081	0.0104	0.0023
	4	3.13	lp···π	0.0062	0.0263	-0.0037	0.0051	0.0014
(d)	1	2.77	C-H···O	0.0049	0.0185	-0.0025	0.0036	0.0011
	2	2.43	C-H···O	0.0098	0.0380	-0.0059	0.0077	0.0018
	3	3.32	π···π	0.0067	0.0193	-0.0032	0.0040	0.0008
	4	3.10	C-H···π	0.0053	0.0167	-0.0025	0.0034	0.0009
	5	3.51	π···π	0.0054	0.0160	-0.0024	0.0032	0.0008

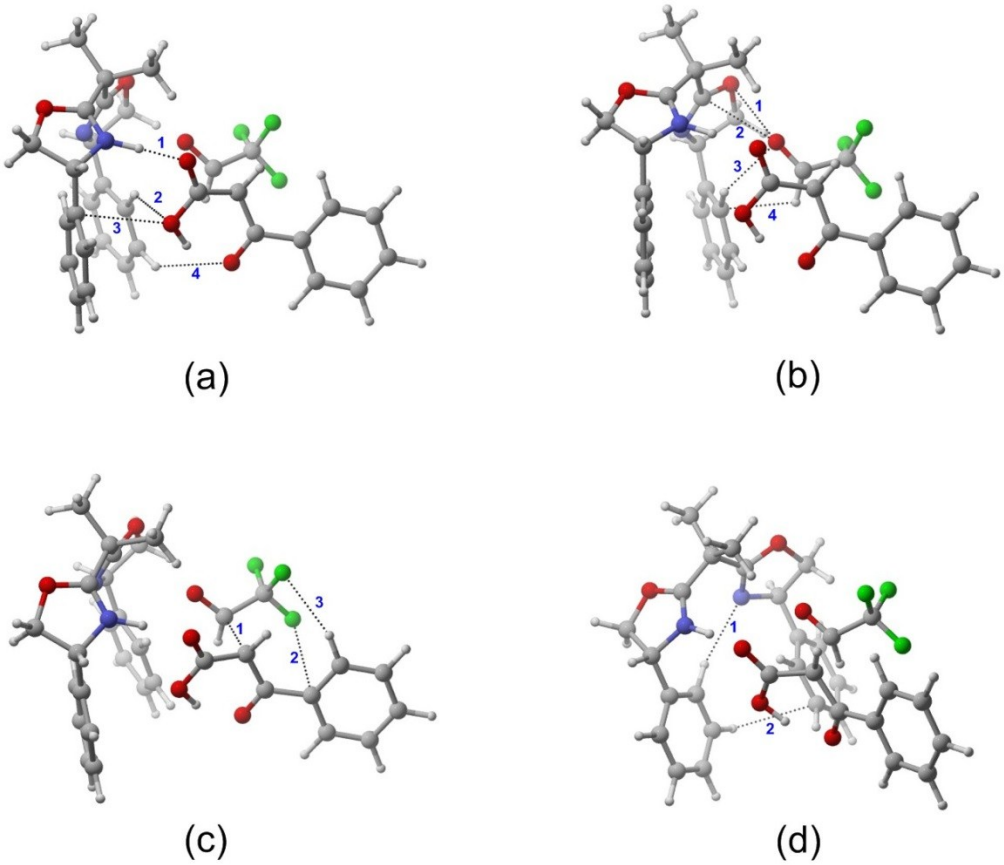

Fig. S27. The interacting atoms numbered with dash lines in which the bond paths and BCPs appeared for (a) the interaction between **Box** and ***β*-CA$_1$** in **TS2h**, (b) the interaction between **Box** and CF_3CHO in **TS2h**, (c) the interaction between ***β*-CA$_1$** and CF_3CHO in **TS2h**, (d) the interaction between two phenyl rings in **Box** in **TS2h**.

Table S18. Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (*d*, in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (*V*, in a.u.), the Electronic Kinetic Energy Density (G, in a.u.) and the Electronic Energy Density (H, in a.u.) at the BCPs of **TS2h**.

	BCP	*d*	Classification	ρ	$\nabla^2\rho$	*V*	*G*	*H*
(a)	1	1.56	N-H···O	0.0656	0.0934	-0.0727	0.0480	-0.0247
	2	2.62	C-H···O	0.0070	0.0261	-0.0038	0.0051	0.0013
	3	3.20	lp···π	0.0069	0.0255	-0.0038	0.0051	0.0013
	4	2.89	C-H···O	0.0040	0.0145	-0.0019	0.0028	0.0009
(b)	1	2.91	lp···lp	0.0091	0.0384	-0.0062	0.0079	0.0017
	2	2.93	lp···π	0.0091	0.0448	-0.0067	0.0090	0.0023
	3	2.36	C-H···O	0.0134	0.0520	-0.0090	0.0110	0.0020
	4	2.65	C-H···π	0.0096	0.0345	-0.0065	0.0075	0.0010
(c)	1	1.95	π···π	0.0968	-0.0021	-0.0681	0.0338	-0.0343
	2	2.96	lp···π	0.0094	0.0411	-0.0062	0.0082	0.0020
	3	2.64	C-H···F	0.0056	0.0236	-0.0033	0.0046	0.0013
(d)	1	2.51	C-H···N	0.0101	0.0331	-0.0054	0.0068	-0.0083
	2	2.94	C-H···π	0.0063	0.0190	-0.0031	0.0039	-0.0048

15. Investigations of the uncatalyzed reaction

For the uncatalyzed reaction between ***β*-CA$_1$** and CF_3CHO, because both *Si*- and *Re*-faces of the C2 atom of ***β*-CA$_1$** can attack the *Si*- as well as *Re*-face of the C4 atom of CF_3CHO, so four paths (denoted as **Path(C2$_{Re}$C4$_{Re}$)**, **Path(C2$_{Re}$C4$_{Si}$)**, **Path(C2$_{Si}$C4$_{Re}$)** and **Path(C2$_{Si}$C4$_{Si}$)**) can occur. The products generated via **Path(C2$_{Re}$C4$_{Re}$)** and **Path(C2$_{Si}$C4$_{Si}$)** are enantiomers, and those generated via **Path(C2$_{Re}$C4$_{Si}$)** and **Path(C2$_{Si}$C4$_{Re}$)** are also enantiomers, so the overall ee value should be 0.0%. Herein we only considered **Path(C2$_{Re}$C4$_{Re}$)** and **Path(C2$_{Re}$C4$_{Si}$)** because the paths generated the enantiomeric products have the same free energy profiles. The attacks of *Re*-face of C2 atom in ***β*-CA$_1$** on *Si*- and *Re*-faces of C4 atom in CF_3CHO via transition states **^{uncat}TS1-*S*** and **^{uncat}TS1-*R*** lead to the diastereoisomeric intermediates **^{uncat}IM1-*S*** and **^{uncat}IM1-*R***, respectively. Subsequently, the decarboxylation reactions of **^{uncat}IM1-*S*** and **^{uncat}IM1-*R*** via transition states **^{uncat}TS2-*S*** and **^{uncat}TS2-*R*** yield enantiomers (*S*)-enol-**P** and (*R*)-enol-**P**, respectively. With the assistance of ***β*-CA$_1$**, (*S*)-enol-**P** and (*R*)-enol-**P** go through transition states **^{uncat}TS$_T$-*S*** and **^{uncat}TS$_T$-*R*** to tautomerize to final products (*S*)-**P** and (*R*)-**P**. Without the assistance of ***β*-CA$_1$**, the tautomerization (*S*)-enol-**P** or (*R*)-enol-**P** via transition state **^{uncat}TS$_T$-*S*'** or **^{uncat}TS$_T$-*R*'** with the four-membered ring structure is much less favorable due to the even higher energy barrier (55.9 kcal/mol). The optimized structures for the transition states, intermediates and products are depicted in Fig. S28, and the free energy profiles are shown in Fig. S29.

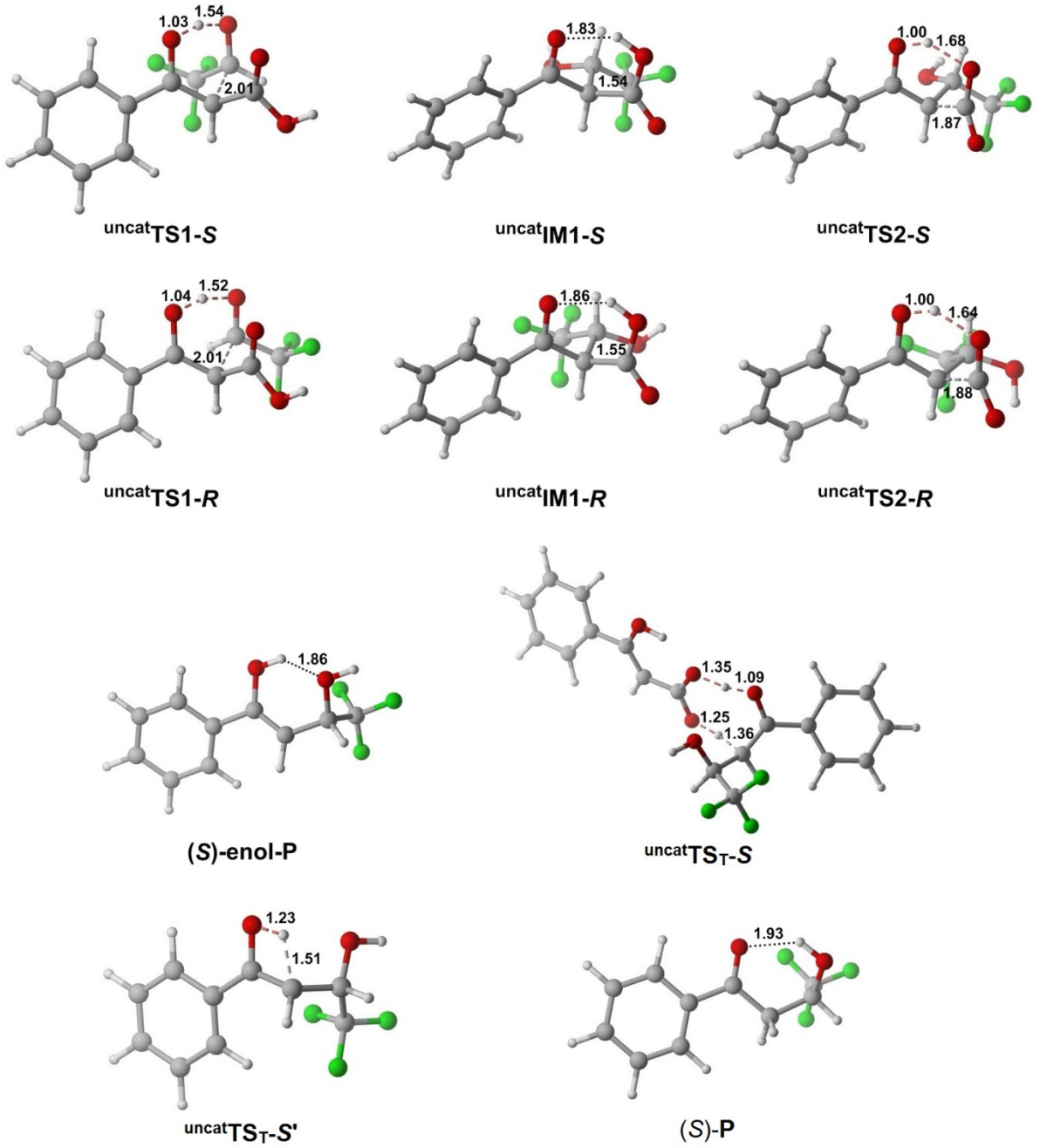

Fig. S28. The optimized structures for the transition states, intermediates and products in the uncatalyzed reaction. For the tautomerization process, only (*S*)-enol-**P**, ^{uncat}**TS$_T$-*S***, ^{uncat}**TS$_T$-*S*'**, (*S*)-**P** are displayed. Distances are in Å.

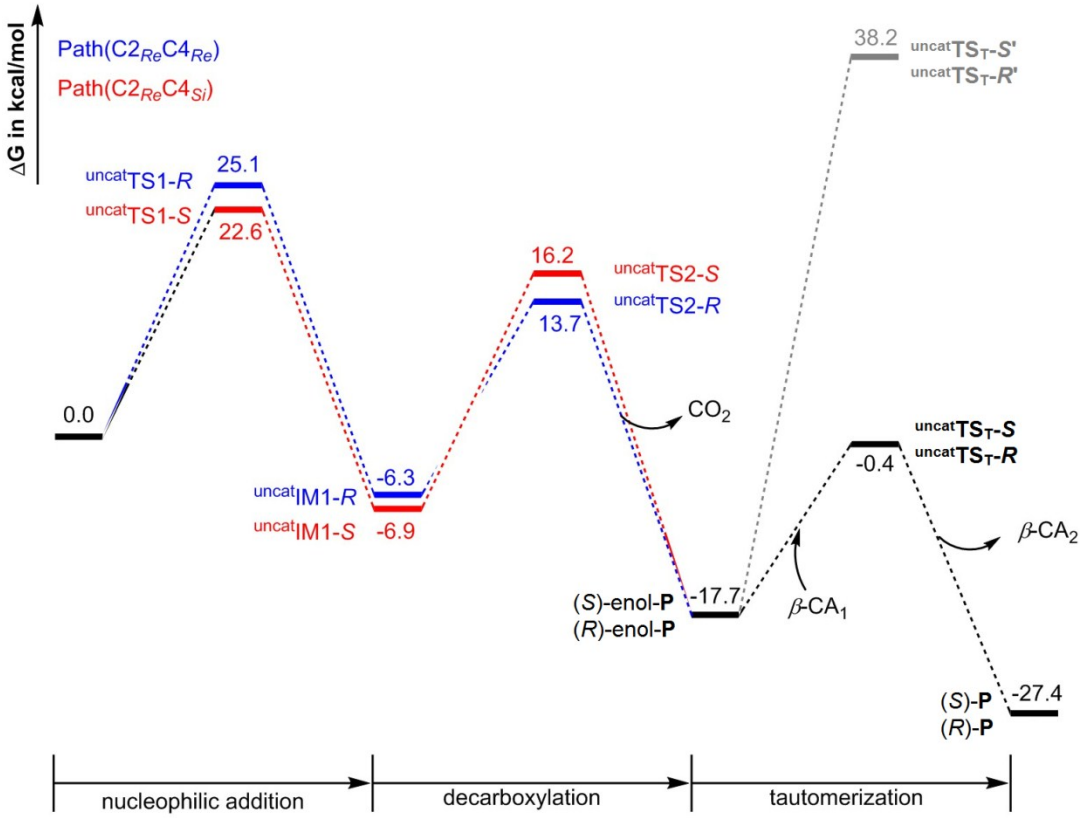

Fig. S29. The free energy profiles for **Path(C2$_{Re}$C4$_{Re}$)** and **Path(C2$_{Re}$C4$_{Si}$)**.

16. Cartesian coordinates of all the optimized structures of the reactant, intermediates, transition states and products in the reaction reaction of *β*-CA_1 and TMH catalyzed by Box in Scheme 1a.

(*S*)-TMH

C	0.34753800	0.63305400	-0.57197400
C	-0.83568200	-0.15918000	-0.00757600
O	1.47556900	-0.14633100	-0.76838100
C	2.00360100	-0.77618400	0.39873400
H	3.01528700	-1.08429000	0.14631000
H	2.02695000	-0.08007100	1.23846200
H	1.41224400	-1.65558100	0.66469200
F	-1.97318500	0.52021000	-0.18009300
F	-0.71100800	-0.41232300	1.29840700
F	-0.95762800	-1.33111100	-0.63780000
O	0.53351900	1.68789000	0.31619300
H	1.10532300	2.33725500	-0.10355900
H	0.05113100	0.97310300	-1.56813200

(*R*)-TMH

C	-0.34753800	0.63305400	-0.57197400
C	0.83568200	-0.15918000	-0.00757600
O	-1.47556900	-0.14633100	-0.76838100
C	-2.00360100	-0.77618400	0.39873400
H	-3.01528700	-1.08429000	0.14631000
H	-2.02695000	-0.08007100	1.23846200
H	-1.41224400	-1.65558100	0.66469200
F	1.97318500	0.52021000	-0.18009300
F	0.71100800	-0.41232300	1.29840700
F	0.95762800	-1.33111100	-0.63780000
O	-0.53351900	1.68789000	0.31619300
H	-1.10532300	2.33725500	-0.10355900
H	-0.05113100	0.97310300	-1.56813200

CF_3CHO

C	-1.06110300	-0.58379300	-0.00065700
C	0.35783200	0.00155600	-0.00014700
F	1.01905700	-0.42695200	1.07979000
F	0.34914900	1.32406200	0.00060400
F	1.02006000	-0.42578000	-1.07963900
O	-2.02291900	0.11715800	-0.00005900
H	-1.09140800	-1.68580700	-0.00149700

Box (Closed-1)

C	-0.00004600	2.49557700	0.00001200
C	1.02528300	1.59334800	0.64034600
O	0.50840300	0.67655800	1.50015300
C	2.83837200	0.49945900	1.23830700
C	1.63801700	0.01033400	2.09205800
H	3.64258600	0.87451900	1.87340500
H	1.70998800	0.32454200	3.13426400
C	-1.02538200	1.59340700	-0.64038700
O	-0.50850200	0.67667600	-1.50024200
C	-2.83845400	0.49948600	-1.23829800
C	-1.63811200	0.01041000	-2.09211000
H	-3.64271600	0.87451100	-1.87335600
H	-1.71013200	0.32461900	-3.13431100
N	2.27481200	1.61285300	0.45411700
N	-2.27490400	1.61287400	-0.45410900
C	-0.66069300	3.35866900	1.08049100
H	-1.13504300	2.73527800	1.83752700
H	0.09463200	3.99142200	1.55052400
H	-1.42548000	3.99019500	0.62801500
C	0.66062000	3.35875200	-1.08039000
H	1.13492800	2.73541800	-1.83749900
H	-0.09468600	3.99158900	-1.55034300
H	1.42544100	3.99019000	-0.62785300
H	1.47543900	-1.06450600	2.03375400
H	-1.47549600	-1.06442300	-2.03380700
C	3.39046500	-0.57830500	0.32891200
C	4.59873900	-1.20192600	0.62840600
C	2.66833400	-0.99101300	-0.79232900
C	5.08264800	-2.23038000	-0.17529900
H	5.16795300	-0.87831100	1.49377600
C	3.15108500	-2.01777100	-1.59473400
H	1.73272700	-0.49915500	-1.04109000
C	4.35859300	-2.64060600	-1.28843800
H	6.02635500	-2.70529800	0.06558700
H	2.58672200	-2.33042700	-2.46549900
H	4.73427800	-3.43825700	-1.91812200
C	-3.39045000	-0.57833300	-0.32890200
C	-4.59863400	-1.20211900	-0.62844900
C	-2.66833100	-0.99091500	0.79238700
C	-5.08244600	-2.23061700	0.17524400
H	-5.16783800	-0.87858800	-1.49385800
C	-3.15099400	-2.01772700	1.59478800
H	-1.73280300	-0.49892700	1.04119900
C	-4.35839400	-2.64072800	1.28843600
H	-6.02607800	-2.70566900	-0.06567400

H	-2.58663100	-2.33028500	2.46558900
H	-4.73402100	-3.43841600	1.91810900

Box (Closed-2)

C	-2.95326700	0.05762900	0.11663400
C	-2.00805000	1.21759500	-0.12018700
O	-2.13268300	2.28178400	0.70530900
C	-0.33042800	2.47416600	-0.78993300
C	-1.21416900	3.27105700	0.20066500
H	-0.20703700	3.01443500	-1.72969100
H	-1.79649200	4.04954300	-0.29552000
C	-2.07484500	-1.17786800	0.13422600
O	-2.22188500	-2.04733600	-0.89078600
C	-0.47279200	-2.62562200	0.56994400
C	-1.35544300	-3.15716900	-0.58449100
H	-0.41577600	-3.34516400	1.38823400
H	-1.98079000	-3.99735000	-0.27804100
N	-1.11257700	1.24420400	-1.01474200
N	-1.20297100	-1.42206100	1.01927400
C	-3.66127000	0.18121800	1.47156900
H	-2.93637800	0.20846700	2.28401900
H	-4.26067700	1.09145800	1.49844000
H	-4.31717900	-0.67955000	1.61446800
C	-3.97157200	0.01663600	-1.03085800
H	-3.46608300	-0.07862900	-1.99081100
H	-4.64682100	-0.83059800	-0.90200600
H	-4.55839600	0.93734900	-1.02509700
H	-0.66328200	3.68793500	1.04123300
H	-0.79458000	-3.41247000	-1.48136000
C	1.03501100	2.13191200	-0.22746200
C	2.19066100	2.66251500	-0.79201000
C	1.14317500	1.28891300	0.88207400
C	3.44188400	2.36604500	-0.25459600
H	2.11417500	3.30980000	-1.65991600
C	2.38817900	0.99633100	1.42080700
H	0.25592600	0.82383500	1.30167700
C	3.54106800	1.53577600	0.85461000
H	4.33512000	2.78240000	-0.70568000
H	2.46169500	0.32413000	2.26774300
H	4.51315600	1.29626200	1.26975300
C	0.92957700	-2.25396200	0.13364900
C	2.04449200	-2.76263900	0.79225000
C	1.11162700	-1.38176800	-0.94280000
C	3.32925400	-2.41567900	0.37891900
H	1.90896500	-3.43431500	1.63385900
C	2.39062800	-1.03701100	-1.35701600
H	0.24828600	-0.93832500	-1.43104300
C	3.50287400	-1.55557200	-0.69832000
H	4.19063700	-2.81712400	0.90006300

H	2.52071400	-0.34144400	-2.17798900
H	4.50064900	-1.27626200	-1.01628400

Box (Closed-3)

C	1.19575400	-2.52640800	0.46094500
C	-0.19520900	-2.25666600	-0.06199500
O	-1.14327900	-3.12667300	0.35665600
C	-1.99789300	-1.37750300	-0.97525900
C	-2.37296500	-2.71009900	-0.26783700
H	-2.24496800	-1.42158800	-2.03793700
H	-2.67801300	-3.48721700	-0.96881900
C	2.02634900	-1.31318100	0.11500900
O	2.49527400	-1.26462700	-1.15149100
C	2.99088100	0.66887800	0.10745000
C	3.20860600	-0.02041500	-1.26726100
H	3.94350500	0.89320000	0.59193300
H	4.25607900	-0.24577200	-1.46830200
N	-0.54035300	-1.30226800	-0.81820500
N	2.27540100	-0.35072200	0.89766500
C	1.13534800	-2.70614800	1.98362600
H	0.72807200	-1.81705500	2.46460900
H	0.51245100	-3.56675800	2.22627900
H	2.14264800	-2.86964100	2.36886300
C	1.75205400	-3.79123500	-0.21328500
H	1.79494500	-3.66872100	-1.29508400
H	2.75972400	-3.99209700	0.15583900
H	1.11439500	-4.64237300	0.02885200
H	-3.12703600	-2.58771000	0.50823700
H	2.78171700	0.54223700	-2.09658100
C	-2.67409400	-0.16226700	-0.37152600
C	-3.87510000	0.30294500	-0.90638200
C	-2.12942900	0.48464700	0.73750200
C	-4.52813900	1.39187600	-0.33886700
H	-4.29792500	-0.18678600	-1.77797400
C	-2.77960800	1.57625000	1.30362200
H	-1.17831900	0.15443700	1.14106000
C	-3.98060500	2.03147100	0.76907400
H	-5.45880900	1.74562100	-0.76660500
H	-2.33802100	2.07902300	2.15594100
H	-4.48389500	2.88444300	1.20842300
C	2.17331100	1.94048200	0.01948800
C	2.71710800	3.17189800	0.37202300
C	0.85129000	1.87907400	-0.42743900
C	1.95353600	4.33341900	0.27877400
H	3.74126800	3.22447500	0.72696100
C	0.08659200	3.03568800	-0.51350400
H	0.41836300	0.91875300	-0.69592300
C	0.63711900	4.26683300	-0.16226700
H	2.38645600	5.28721700	0.55687100

H	-0.94369500	2.97152100	-0.84633900
H	0.04032600	5.16887400	-0.22920400

Box (Half-open)

C	0.04800200	2.09167700	0.33269500
C	0.74329900	0.75320900	0.33612200
O	0.46610600	-0.02963700	-0.74400600
C	2.03597500	-0.98831000	0.71102900
C	1.07489700	-1.30245900	-0.46054200
H	1.93827500	-1.72555800	1.50872600
H	0.28324500	-1.99628500	-0.16876000
C	-1.42393400	1.79663500	0.11715400
O	-1.92958600	2.08113000	-1.10617700
C	-3.47382800	1.01474400	0.31016900
C	-3.33731100	1.78914000	-1.02395600
H	-4.28599500	1.41478900	0.91902600
H	-3.87878200	2.73631300	-1.01320700
N	1.55637200	0.32118600	1.20063900
N	-2.18306500	1.26650700	0.98022700
C	0.24073700	2.78387900	1.68322500
H	-0.18756400	2.18046900	2.48186600
H	1.30482000	2.92085500	1.87577900
H	-0.25203900	3.75787800	1.66726800
C	0.62931700	2.93489000	-0.81254800
H	0.50990300	2.43213000	-1.77157600
H	0.12147800	3.89919600	-0.86101100
H	1.69108100	3.10636500	-0.62422800
H	1.57776500	-1.65467400	-1.35921700
H	-3.61912700	1.20577700	-1.89856500
C	3.48837900	-0.89589200	0.29394900
C	4.45959300	-1.68805000	0.89736400
C	3.86670400	-0.00856200	-0.71612800
C	5.79172300	-1.60062600	0.49969100
H	4.17371600	-2.37565300	1.68627500
C	5.19302400	0.07987800	-1.11600200
H	3.11467300	0.61474200	-1.19180800
C	6.16027400	-0.71728300	-0.50708100
H	6.53937700	-2.22124200	0.97915700
H	5.47579000	0.77153900	-1.90070700
H	7.19593600	-0.64676800	-0.81719600
C	-3.68107300	-0.47353300	0.12167600
C	-4.79781400	-1.11672800	0.64431900
C	-2.73977100	-1.21605900	-0.59619300
C	-4.98000500	-2.48496500	0.45423200
H	-5.52901600	-0.54648100	1.20755800
C	-2.92114500	-2.57928500	-0.78860700
H	-1.86128700	-0.72016000	-1.00049600
C	-4.04277600	-3.21801200	-0.26236800
H	-5.85277300	-2.97549400	0.86868500

H	-2.18813500	-3.14716300	-1.35020900
H	-4.18224800	-4.28209000	-0.41114400

Box (Full-open)

C	0.00001627	0.77515809	0.00047518
C	-1.20380327	-0.10898729	-0.19653261
O	-1.35305156	-1.07687417	0.74492167
C	-3.13069669	-0.99353809	-0.78644208
C	-2.47647635	-1.86532257	0.31323569
H	-3.34263206	-1.58053982	-1.68109174
H	-2.09624460	-2.80961792	-0.07975957
C	1.20387349	-0.10904824	0.19694163
O	1.35299491	-1.07655307	-0.74492756
C	3.13087789	-0.99381584	0.78617673
C	2.47646266	-1.86519719	-0.31369618
H	3.34301745	-1.58113696	1.68056627
H	2.09626769	-2.80962399	0.07901909
N	-2.08563025	0.00458852	-1.09525791
N	2.08582455	0.00415756	1.09559588
C	0.22913994	1.64306551	-1.24333696
H	0.40018195	1.02125777	-2.12229302
H	-0.65002409	2.26085271	-1.42571945
H	1.09602980	2.28631877	-1.07849238
C	-0.22913655	1.64231719	1.24479184
H	-0.40025725	1.01999070	2.12336563
H	0.65004566	2.25995001	1.42761847
H	-1.09597714	2.28572517	1.08029455
H	-3.12254808	-2.04713799	1.17016353
H	3.12239818	-2.04671910	-1.17078768
C	-4.39969640	-0.30206970	-0.33517856
C	-5.59359090	-0.46735227	-1.02955029
C	-4.38031976	0.51349398	0.79846961
C	-6.75584369	0.16943512	-0.60054229
H	-5.61493458	-1.09520781	-1.91402562
C	-5.53698931	1.14826875	1.22971690
H	-3.45150583	0.64874277	1.34575464
C	-6.72946870	0.97754421	0.52902940
H	-7.67928498	0.03481209	-1.15118235
H	-5.51100898	1.77864751	2.11064987
H	-7.63200998	1.47466446	0.86374572
C	4.39975236	-0.30215702	0.33487507
C	5.59389333	-0.46789726	1.02872528
C	4.38001453	0.51404724	-0.79829749
C	6.75602573	0.16905673	0.59965557
H	5.61551308	-1.09623729	1.91285024
C	5.53656967	1.14899717	-1.22960705
H	3.45101205	0.64965840	-1.34517741
C	6.72928968	0.97780297	-0.52945864
H	7.67965308	0.03406977	1.14989344

H	5.51030216	1.77986101	-2.11018405
H	7.63173613	1.47505635	-0.86423128

***β*-CA$_1$**

C	2.83152000	-1.43088500	-0.17563400
C	1.46390000	-1.20272600	-0.22958300
C	0.95775400	0.08590300	-0.03746900
C	1.84201800	1.14265100	0.19315300
C	3.20993500	0.90926900	0.25121300
C	3.70737100	-0.37665200	0.06908800
H	3.21562700	-2.43129400	-0.33281200
H	0.79345000	-2.02524400	-0.44546900
H	1.44751800	2.14082400	0.33025000
H	3.88802200	1.73304600	0.43769900
H	4.77472700	-0.55737700	0.11089700
C	-0.49509400	0.35785400	-0.07579700
O	-0.79281300	1.63653400	-0.27840300
C	-1.44581900	-0.59942500	0.10378700
H	-1.77390100	1.71864500	-0.26456800
H	-1.18277200	-1.62362500	0.31067500
C	-2.84431700	-0.23885800	0.05808300
O	-3.27390200	0.89372900	-0.12705000
O	-3.67682600	-1.26976400	0.24429200
H	-4.57795200	-0.92175200	0.20158300

***β*-CA$_2$**

C	2.83394500	1.40730500	0.22680000
C	1.46542300	1.18417800	0.28656600
C	0.94890200	-0.09125500	0.04195800
C	1.82524400	-1.14161400	-0.24262500
C	3.19372000	-0.91295400	-0.30678400
C	3.70107100	0.36106300	-0.07480900
H	3.22515800	2.39759300	0.42528100
H	0.80155800	1.99805900	0.55044600
H	1.42518000	-2.13155100	-0.41807600
H	3.86467400	-1.73158700	-0.53685700
H	4.76891300	0.53767800	-0.12097000
C	-0.50763700	-0.35603300	0.08338000
O	-0.78465000	-1.63858900	0.33565500
C	-1.42860200	0.61332800	-0.14281200
H	-1.74600000	-1.76983500	0.31804300
H	-1.09822200	1.60989600	-0.38962800
C	-2.87400700	0.45183200	-0.11466200
O	-3.68281300	1.32153400	-0.30532400
O	-3.27594700	-0.82847600	0.15423300
H	-4.24233700	-0.84110500	0.15316800

***β*-CA$_3$**

C	2.85268000	-1.37387200	-0.07122200
C	1.47729300	-1.17475200	-0.03559100
C	0.95983400	0.12002900	0.02849300
C	1.83005600	1.21259000	0.05771000
C	3.20136900	1.01227700	0.02098300
C	3.71353000	-0.28205100	-0.04357300
H	3.25120000	-2.37964500	-0.12008500
H	0.81709500	-2.03354200	-0.05670300
H	1.40850600	2.20881800	0.10876000
H	3.87336200	1.86139700	0.04281200
H	4.78523600	-0.43879100	-0.07191000
C	-0.50932000	0.39387800	0.07094400
O	-0.94175100	1.51836000	0.14097000
C	-1.45671200	-0.80238400	0.03170500
H	-1.27456400	-1.37942600	-0.87750000
H	-1.27750800	-1.43919000	0.89916900
C	-2.88443600	-0.32258800	0.06756900
O	-3.57826100	-0.29797800	1.04411900
O	-3.29244500	0.08776900	-1.14053700
H	-4.18943000	0.43641600	-1.04306100

***β*-CA$_4$**

C	-2.79899300	-1.44514500	0.02444300
C	-1.43379500	-1.18788900	0.03759900
C	-0.97149400	0.13023400	0.00821000
C	-1.88736000	1.18571100	-0.03419700
C	-3.24855900	0.92552800	-0.04959700
C	-3.70483100	-0.39061800	-0.02008900
H	-3.15491800	-2.46744300	0.04851100
H	-0.74050300	-2.01906100	0.07307100
H	-1.51100000	2.20074300	-0.05500700
H	-3.95575400	1.74487200	-0.08415800
H	-4.76891000	-0.59407100	-0.03167900
C	0.47936300	0.46531100	0.02635000
O	0.84091100	1.62824500	0.03684500
C	1.47914300	-0.67404800	0.03982100
H	1.32263100	-1.26521900	0.94739300
H	1.27186600	-1.35257200	-0.79082000
C	2.97486400	-0.35604400	-0.01927300
O	3.76902600	-1.25049900	-0.09050500
O	3.34718700	0.91602000	0.02383000
H	2.54956600	1.48437900	0.05173200

(β-CA_1-1)$^-$

C	-2.81017500	1.41208000	0.16349700
C	-1.43775000	1.19482400	0.21126600
C	-0.91158800	-0.08730900	0.03313300
C	-1.79597800	-1.14755600	-0.17359100
C	-3.16823200	-0.93284100	-0.22812500
C	-3.68164600	0.34999200	-0.06206700
H	-3.20124000	2.41275900	0.30959700
H	-0.77232800	2.02597200	0.40942500
H	-1.37369300	-2.13854600	-0.28322200
H	-3.83958800	-1.76748600	-0.39722200
H	-4.75153100	0.52075900	-0.10016400
C	0.56658900	-0.39490700	0.07507500
O	0.87775900	-1.61826700	0.25200900
C	1.47924300	0.63305500	-0.10344100
H	2.43923700	-1.40683600	0.21008500
H	1.16790200	1.64778700	-0.29780700
C	2.91264200	0.39842700	-0.08135200
O	3.28965600	-0.87839700	0.12460400
O	3.75916100	1.26554000	-0.23374600

(β-CA$_1$-2)$^-$

C	-2.74147300	-1.46995100	-0.22849500
C	-1.38766200	-1.15114500	-0.28561200
C	-0.94851900	0.15262000	-0.04481600
C	-1.90342500	1.13053800	0.23896700
C	-3.25510300	0.81574800	0.30932200
C	-3.68068900	-0.48954500	0.07630800
H	-3.06395800	-2.48600800	-0.42837500
H	-0.66942100	-1.91997800	-0.54368000
H	-1.54823800	2.14272400	0.39090500
H	-3.98000200	1.58878800	0.54052100
H	-4.73488700	-0.73879400	0.12380300
C	0.51505500	0.59725300	-0.11275400
O	0.70705200	1.80649100	-0.30788500
C	1.47723200	-0.41382400	0.08211500
H	4.50768800	-1.09049300	0.27377900
H	1.16223200	-1.41736600	0.32446700
C	2.88012900	-0.19445500	0.05307600
O	3.58485700	-1.36272000	0.32814700
O	3.53225700	0.81344100	-0.17152300

H_2O

O	0.00000000	0.00000000	0.11829200
H	0.00000000	0.75558100	-0.47316900
H	0.00000000	-0.75558100	-0.47316900

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15437300
O	0.00000000	0.00000000	-1.15437300

MeOH

C	0.66209000	-0.01966700	0.00000300
H	1.08506700	0.98450000	-0.00102600
H	1.02394100	-0.54346100	0.89134500
H	1.02378600	-0.54520100	-0.89037200
O	-0.74684600	0.12238500	0.00000300
H	-1.13056400	-0.75691700	0.00001600

COM1-(*S*)-1

C	0.97653900	-1.67313700	1.41503500
C	0.43503700	-0.30825000	1.75187300
O	1.36589400	0.64866700	1.94816900
C	-0.82799300	1.48431000	2.07604000
C	0.65079300	1.83667200	2.34802800
H	-1.45770000	1.70565800	2.93836000
H	0.85081600	2.00860800	3.40560700
C	1.92442400	-1.48173900	0.25667500
O	1.40180700	-0.78371100	-0.78339700
C	3.63798500	-1.42172300	-1.11851800
C	2.38214700	-0.85752300	-1.83441700
H	4.06084900	-2.25963100	-1.67472400
H	2.00223600	-1.52964500	-2.60499900
N	-0.78451800	0.02072800	1.85968400
N	3.11123000	-1.90597700	0.17086800
C	1.72645200	-2.23324300	2.62876300
H	2.53477100	-1.56662400	2.92841500
H	1.03035000	-2.35967900	3.46001400
H	2.15831900	-3.20043200	2.37244400
C	-0.16470000	-2.59921300	0.97501600
H	-0.68520800	-2.19058100	0.10766100
H	0.24737800	-3.57858200	0.72457000
H	-0.88288800	-2.71670800	1.78844400
H	1.01657300	2.67290900	1.75517100
H	2.52725800	0.14051900	-2.24394200
C	-1.41933700	2.12009100	0.83691200
C	-2.70402100	2.65266200	0.85409500
C	-0.71066500	2.07148000	-0.36669900
C	-3.28049500	3.13588000	-0.31841000
H	-3.26756300	2.66594100	1.78071300
C	-1.28305500	2.55669000	-1.53488800
H	0.27612400	1.61704900	-0.39556700
C	-2.57197400	3.08816500	-1.51263800
H	-4.28818200	3.53225700	-0.29931700
H	-0.73282100	2.50647800	-2.46673400
H	-3.02332300	3.45434200	-2.42673400
C	4.71311700	-0.37578700	-0.90891700
C	5.85035700	-0.36819700	-1.71249600
C	4.55111000	0.62243300	0.05336000
C	6.81412400	0.62521100	-1.56594600
H	5.98534300	-1.14718300	-2.45581400
C	5.51331900	1.61450700	0.20021600
H	3.67503500	0.61510100	0.69465700
C	6.64655100	1.61938500	-0.60911700
H	7.69670700	0.61793600	-2.19450400

H	5.38259300	2.38385900	0.95220600
H	7.39683600	2.39181400	-0.48982100
C	-3.24257700	-0.64267000	-0.38213800
C	-4.71129300	-0.42516400	-0.74519700
O	-2.65035000	-1.60677500	-1.20531900
C	-3.12928000	-2.93868100	-1.04885100
H	-2.35366700	-3.59229000	-1.44519700
H	-3.30070600	-3.16858900	0.00415200
H	-4.05265000	-3.09173800	-1.61306700
F	-5.19633700	0.66495800	-0.13864400
F	-5.48918300	-1.45587600	-0.38748900
F	-4.85826800	-0.25261100	-2.06416500
O	-3.21654200	-0.94921300	0.96167200
H	-2.33747100	-0.69494900	1.32088300
H	-2.71776600	0.28796800	-0.61973500

COM1-(*S*)-2

C	0.91211000	-2.13347400	0.43675100
C	0.32130400	-0.87510600	1.02067300
O	1.16769800	-0.12830200	1.75446500
C	-0.96012200	0.85341500	1.54027700
C	0.37992900	0.94324200	2.31447400
H	-1.81412100	0.85876200	2.21977800
H	0.26243800	0.74803800	3.38083300
C	2.09201000	-1.69284800	-0.39520900
O	1.79545200	-0.74790600	-1.32373800
C	4.07534100	-1.32330100	-1.26904200
C	3.00227300	-0.55230100	-2.08431400
H	4.63837400	-2.00396800	-1.90945300
H	2.84848600	-0.97405600	-3.07840400
N	-0.86876200	-0.45959500	0.88173200
N	3.28190500	-2.10536400	-0.30291300
C	1.37524800	-3.05161800	1.57299700
H	2.10298200	-2.54782700	2.20785700
H	0.51379400	-3.35210500	2.17252800
H	1.84447000	-3.94043000	1.15149600
C	-0.11100200	-2.83177700	-0.46702900
H	-0.41823900	-2.18504800	-1.28940900
H	0.33419000	-3.73925100	-0.87808200
H	-0.99659200	-3.10409500	0.10875300
H	0.91160400	1.87914100	2.15621300
H	3.19632300	0.51640200	-2.15390100
C	-1.14099900	1.97437800	0.53674300
C	-1.65844800	3.19327100	0.97730300
C	-0.76921500	1.83342400	-0.79764000
C	-1.79923400	4.26012700	0.09874100
H	-1.96575000	3.30115900	2.01286800
C	-0.92225600	2.89965200	-1.68109800
H	-0.36475300	0.89095700	-1.14974000
C	-1.43457500	4.11321600	-1.23762100
H	-2.20510000	5.20072500	0.45200400
H	-0.63917600	2.77855200	-2.72010900
H	-1.55243600	4.94000200	-1.92774200
C	5.04338000	-0.40316000	-0.55497100
C	6.33762300	-0.23107700	-1.03889800
C	4.63191300	0.32055900	0.56545800
C	7.21270800	0.65626300	-0.41879900
H	6.66540500	-0.79784300	-1.90429300
C	5.50524400	1.20632700	1.18493100
H	3.62966900	0.18120400	0.95873800
C	6.79730900	1.37726500	0.69446700
H	8.21875400	0.77868000	-0.80214200

H	5.17959000	1.76180200	2.05660400
H	7.47744500	2.06573900	1.18151600
C	-3.97138700	-0.68259800	0.27361000
C	-5.32497500	-1.23816300	-0.17130100
O	-4.00278000	0.70157900	0.44605300
C	-4.22875000	1.46160100	-0.74035800
H	-3.86470900	2.46676000	-0.53633000
H	-3.67514000	1.03936400	-1.57999000
H	-5.29556400	1.49461300	-0.97794900
F	-5.36770500	-2.56432100	0.00414500
F	-5.58520800	-0.99601000	-1.46052800
F	-6.32002800	-0.70294600	0.54605900
O	-3.04875100	-1.11860800	-0.65326200
H	-2.17203800	-0.96651900	-0.23497800
H	-3.78097400	-1.08457600	1.27551600

COM1-(*S*)-3

C	0.97275100	0.95237900	2.55125700
C	1.63343300	-0.13926600	1.74712800
O	0.76434600	-0.86037800	0.97682200
C	3.01894500	-1.47282500	0.66736400
C	1.56372000	-1.80490600	0.23284700
H	3.49904000	-2.33813500	1.12843700
H	1.24803200	-2.81157000	0.50991600
C	0.36625200	1.88943600	1.53177700
O	1.26486100	2.43690500	0.67420500
C	-0.95505600	3.10539000	0.25171400
C	0.52285200	3.35193100	-0.15312600
H	-1.43100300	4.03084300	0.58044300
H	0.86041800	4.36342000	0.07275200
N	2.86107200	-0.41557300	1.68166700
N	-0.85476200	2.18962900	1.40710500
C	-0.12308600	0.36618600	3.44747100
H	-0.92002600	-0.09423200	2.86410300
H	0.31158900	-0.37504000	4.12138300
H	-0.57065100	1.16285000	4.04202200
C	2.02378700	1.70337800	3.37569500
H	2.81080300	2.09691200	2.73476600
H	1.54471200	2.52519200	3.91112600
H	2.47480100	1.02350400	4.09927400
H	1.37883800	-1.63932000	-0.82714100
H	0.72622400	3.11467800	-1.19658900
C	3.87105000	-0.99288800	-0.48808200
C	4.79705900	-1.84490300	-1.08358500
C	3.69629000	0.29391000	-1.00024300
C	5.53804300	-1.42363300	-2.18429700
H	4.94376600	-2.84240700	-0.68225600
C	4.43739200	0.71487200	-2.09758100
H	2.99096600	0.96994600	-0.52608000
C	5.35866800	-0.14296500	-2.69350900
H	6.25831700	-2.09382900	-2.63822500
H	4.30088800	1.71713500	-2.48644400
H	5.93724700	0.18874900	-3.54729800
C	-1.78755800	2.49275600	-0.85218000
C	-2.90878200	3.15155600	-1.34692200
C	-1.43000100	1.25529900	-1.39193800
C	-3.66689500	2.58579300	-2.36878500
H	-3.19518400	4.10967800	-0.92622800
C	-2.18919600	0.68526400	-2.40565500
H	-0.56609900	0.72007700	-1.00219300
C	-3.30889800	1.35195300	-2.89743500
H	-4.54061900	3.10579000	-2.74335300

H	-1.91679500	-0.28954600	-2.78918100
H	-3.90445200	0.90384300	-3.68370900
C	-2.03450100	-1.57525200	0.36282700
C	-3.53781700	-1.84600000	0.27788600
O	-1.36512800	-1.91659400	-0.81048100
C	-1.44220700	-3.28834000	-1.19023900
H	-0.64147500	-3.45338300	-1.90881900
H	-1.30338100	-3.93974800	-0.32543700
H	-2.40311300	-3.50785900	-1.66252400
F	-4.18502000	-1.18712600	1.24171700
F	-3.83295800	-3.14569100	0.41126400
F	-4.02870400	-1.44442400	-0.89877700
O	-1.58713200	-2.27230700	1.47884200
H	-0.72481000	-1.89233700	1.69161400
H	-1.90512600	-0.49419500	0.47096100

COM1-(*S*)-4

C	0.28602000	3.40211000	-0.00032000
C	1.28126100	2.46924600	0.63928300
O	0.72943400	1.52052800	1.45989300
C	3.02907000	1.28595800	1.22683000
C	1.85421800	0.94920400	2.16615300
H	3.92881400	1.53672200	1.79037300
H	1.93818800	1.46294900	3.12624700
C	-0.73789300	2.53272700	-0.68896300
O	-0.20762100	1.54041100	-1.44566200
C	-2.55652200	1.53107200	-1.40624300
C	-1.32191500	0.92752300	-2.12560800
H	-3.26814900	1.92684900	-2.13496600
H	-1.27009900	1.21715700	-3.17620800
N	2.53618100	2.46939900	0.50099100
N	-1.99448700	2.64823900	-0.62888400
C	-0.38470600	4.25264900	1.08397100
H	-0.86333400	3.61966200	1.83124200
H	0.36419200	4.88187600	1.56858000
H	-1.14737200	4.88562300	0.63077700
C	0.98464900	4.27779300	-1.04695700
H	1.43775000	3.66474600	-1.82609200
H	0.25435100	4.95211300	-1.49748600
H	1.77054500	4.86453900	-0.57103600
H	1.66909800	-0.11450300	2.30761600
H	-1.23322400	-0.14979400	-2.01503400
C	3.31890800	0.14101100	0.26735600
C	3.76152600	-1.07527700	0.79328900
C	3.06121700	0.23509900	-1.09863600
C	3.90764900	-2.18825000	-0.02308500
H	3.95966700	-1.16042600	1.85737600
C	3.21356700	-0.88097200	-1.91940900
H	2.71121900	1.17105600	-1.51375000
C	3.62530600	-2.09540600	-1.38437500
H	4.22390100	-3.13223700	0.40357500
H	2.99172900	-0.80147400	-2.97694900
H	3.72089600	-2.96753200	-2.01967200
C	-3.27860900	0.53909900	-0.50952700
C	-3.70899400	-0.67323000	-1.04931200
C	-3.50033200	0.79535000	0.84004600
C	-4.32932000	-1.62363100	-0.25083300
H	-3.54148000	-0.88546000	-2.10108900
C	-4.12770200	-0.15523400	1.64128500
H	-3.17047100	1.73676000	1.26144500
C	-4.53836500	-1.36807500	1.10191900
H	-4.64279700	-2.56741200	-0.68104400

H	-4.29106800	0.05371900	2.69233000
H	-5.01966500	-2.10991500	1.72818800
C	0.32853100	-1.67247900	0.36824900
C	-0.08983300	-2.78156800	-0.59728900
O	0.70406500	-2.17537000	1.61297400
C	-0.33128600	-2.82787200	2.34895700
H	-0.00289100	-2.85029600	3.38583200
H	-1.27019600	-2.27759300	2.26718800
H	-0.47082800	-3.85134400	1.99214100
F	-0.12531800	-2.31489000	-1.85464700
F	-1.29930700	-3.28362300	-0.32696600
F	0.78274200	-3.79356900	-0.56712300
O	-0.73767400	-0.78964900	0.41991100
H	-0.40780000	0.07170600	0.71781500
H	1.22983500	-1.22066600	-0.05114500

COM1-(*R*)-1

C	0.02501100	3.03268100	0.30935500
C	0.07203500	2.12012800	1.51835700
O	-1.03932300	2.09157800	2.27686500
C	0.50100900	0.43113900	2.88448100
C	-0.76537000	1.17555900	3.35739800
H	1.23984100	0.34435400	3.68157100
H	-0.59307700	1.76364400	4.25977300
C	-0.67005300	2.17886100	-0.73853500
O	0.14933500	1.39869100	-1.48035900
C	-2.13329700	1.05508500	-1.94030900
C	-0.70031600	0.55470500	-2.27905100
H	-2.59403500	1.52603700	-2.81370700
H	-0.42043300	0.68319500	-3.32308600
N	1.01176000	1.31750700	1.81478000
N	-1.91854600	2.08772500	-0.91675100
C	-0.81090000	4.28082400	0.60447000
H	-1.83255300	4.01240100	0.86350900
H	-0.36321600	4.83779600	1.42966800
H	-0.82818500	4.91878500	-0.28031000
C	1.44603900	3.39441900	-0.13325000
H	2.05262100	2.50744500	-0.30719800
H	1.40408700	3.97256600	-1.05781500
H	1.92027000	4.00207300	0.63905000
H	-1.63082000	0.52862300	3.48387700
H	-0.53201100	-0.48161000	-1.97482900
C	0.21555600	-0.93500800	2.29486200
C	0.82534900	-2.08087600	2.79071300
C	-0.68464700	-1.04549900	1.23155100
C	0.53384700	-3.32617000	2.23726900
H	1.53040500	-2.00191600	3.61171200
C	-0.97501700	-2.28290200	0.67625900
H	-1.17709000	-0.15817300	0.84134700
C	-0.36088400	-3.42822100	1.18050800
H	1.01210400	-4.21521800	2.63196400
H	-1.68608500	-2.35061700	-0.14121700
H	-0.58200900	-4.39658500	0.74790100
C	-3.04544500	-0.05661700	-1.45970600
C	-3.25269200	-1.16389800	-2.28616800
C	-3.66898300	-0.01351500	-0.21530700
C	-4.05899700	-2.21634700	-1.87084700
H	-2.77743400	-1.20374600	-3.26200300
C	-4.47380400	-1.07069200	0.20284900
H	-3.51035400	0.84632500	0.42483300
C	-4.67016400	-2.17334000	-0.61990700
H	-4.20944900	-3.06970300	-2.52139900

H	-4.94620600	-1.03092100	1.17723400
H	-5.29512800	-2.99488400	-0.29121400
C	2.38014400	-0.56368200	-0.40938300
C	3.01692900	-0.32429900	-1.77687200
O	2.22843500	-1.93000500	-0.17403300
C	3.38095300	-2.63670300	0.26357400
H	3.01447000	-3.57537000	0.67619800
H	3.90569700	-2.07801200	1.03984700
H	4.06423600	-2.84518200	-0.56333400
F	3.07971600	0.98145700	-2.06228900
F	4.26341900	-0.81026100	-1.86070600
F	2.29452400	-0.90772300	-2.74632800
O	3.13779600	0.10818300	0.53075700
H	2.50890000	0.63299300	1.06960700
H	1.36626300	-0.16353900	-0.46397300

COM1-(*R*)-2

C	0.56990800	-1.75856000	0.24591100
C	0.16097600	-0.43087300	0.83076600
O	1.09615300	0.16762700	1.59373300
C	-0.85621800	1.46622300	1.36531000
C	0.49097700	1.36374500	2.12577400
H	-1.69205900	1.56625000	2.06002400
H	0.36054200	1.22554100	3.19893000
C	1.86960600	-1.51674500	-0.48145900
O	1.82519400	-0.50181800	-1.38366700
C	3.94581000	-1.50189300	-1.20572300
C	3.09702100	-0.52115400	-2.05842800
H	4.42051600	-2.25611700	-1.83508700
H	2.93561300	-0.88195300	-3.07507500
N	-0.94823200	0.16471600	0.67610000
N	2.95176900	-2.14985100	-0.33090600
C	0.77783200	-2.76467400	1.38390900
H	1.53458100	-2.41052800	2.08300600
H	-0.16633800	-2.91700500	1.91022900
H	1.11319400	-3.71503400	0.96890900
C	-0.48670400	-2.25370200	-0.74867100
H	-0.64538000	-1.52770100	-1.54682100
H	-0.15049200	-3.19641200	-1.18449500
H	-1.43325000	-2.41804800	-0.23143700
H	1.15906600	2.20049400	1.93085600
H	3.49435300	0.49206600	-2.07681800
C	-0.90178700	2.60179700	0.36595200
C	-1.73315100	3.69732000	0.57772000
C	-0.08361200	2.56884900	-0.76528400
C	-1.74539800	4.75745500	-0.32448100
H	-2.38004400	3.71925000	1.44835500
C	-0.09627200	3.62656700	-1.66537200
H	0.55339900	1.70774400	-0.94758500
C	-0.92603200	4.72379100	-1.44614300
H	-2.39981300	5.60372000	-0.15342900
H	0.53716200	3.59355900	-2.54384100
H	-0.93730800	5.54544900	-2.15212700
C	5.01035300	-0.79924900	-0.38904100
C	6.34447600	-0.84493000	-0.78543100
C	4.65846100	-0.05593300	0.73876600
C	7.31884800	-0.15385600	-0.07094500
H	6.62435100	-1.42880800	-1.65630700
C	5.63113900	0.63381500	1.45260800
H	3.62294500	-0.02717800	1.06341500
C	6.96324400	0.58757100	1.04970100
H	8.35435600	-0.20056000	-0.38654700

H	5.35091700	1.20526200	2.32975900
H	7.72008200	1.12307400	1.61026000
C	-3.96103100	-0.95669500	0.29518800
C	-5.43338500	-0.57367100	0.13468700
O	-3.78967700	-2.34446100	0.31931500
C	-4.10478200	-3.01950900	-0.89520900
H	-3.62654300	-3.99559800	-0.83676900
H	-3.71805100	-2.46937600	-1.75492600
H	-5.18467700	-3.15293000	-0.99882000
F	-5.61874500	0.70977700	0.46570300
F	-5.87366000	-0.73261800	-1.11835600
F	-6.21465400	-1.31338600	0.93081900
O	-3.27469900	-0.31655700	-0.71087200
H	-2.37311300	-0.13556000	-0.36306000
H	-3.65267500	-0.62006300	1.29082700

COM1-(*R*)-3

C	0.81172300	0.70991600	2.37692300
C	1.61167200	-0.23220300	1.51450500
O	0.87213700	-0.95386200	0.61310000
C	3.19199200	-1.36859200	0.46959700
C	1.82050100	-1.69917400	-0.18173700
H	3.63411700	-2.25621100	0.92772800
H	1.55685500	-2.75579300	-0.12760000
C	0.27245500	1.80368400	1.48370500
O	1.13933000	2.25721200	0.54447400
C	-0.93754700	3.38103400	0.53065300
C	0.46800800	3.33686900	-0.13360500
H	-1.11263600	4.34807100	1.00695500
H	1.04381400	4.24812800	0.02485800
N	2.85888300	-0.40716000	1.53242500
N	-0.86533000	2.34448600	1.57621400
C	-0.35324400	-0.03491700	3.03774600
H	-1.04433100	-0.41752000	2.28607300
H	0.02675800	-0.86240100	3.64111800
H	-0.90461100	0.65167400	3.67920400
C	1.73097200	1.35555100	3.42282200
H	2.55613100	1.87866200	2.94066600
H	1.15135400	2.05880900	4.02266500
H	2.14724800	0.58559800	4.07340500
H	1.75118400	-1.34564400	-1.21040400
H	0.42601200	3.10023700	-1.19624500
C	4.17481000	-0.78171700	-0.51903300
C	5.19735500	-1.56376100	-1.04839100
C	4.03099800	0.53981400	-0.94478100
C	6.06641400	-1.03771900	-2.00031600
H	5.31838500	-2.58830200	-0.71204100
C	4.90030700	1.06538700	-1.89250900
H	3.24378500	1.15517100	-0.51981400
C	5.91869300	0.27762700	-2.42399200
H	6.86070300	-1.65379200	-2.40466800
H	4.78751500	2.09375000	-2.21504800
H	6.59649900	0.69050400	-3.16146700
C	-2.06374300	3.09987500	-0.43952400
C	-2.87717400	4.12515200	-0.91456900
C	-2.27678600	1.79686400	-0.88648000
C	-3.89172400	3.85165700	-1.82849300
H	-2.72372000	5.14049400	-0.56313600
C	-3.29703000	1.51885900	-1.78756100
H	-1.66577700	0.98526200	-0.50770800
C	-4.10531800	2.54828900	-2.26429100
H	-4.52149400	4.65565000	-2.19079900

H	-3.46048900	0.49384400	-2.10090500
H	-4.90252000	2.33444600	-2.96629000
C	-1.80051600	-2.37193900	-0.16892100
C	-2.78354400	-3.47344800	-0.56773500
O	-2.40678400	-1.12617700	-0.08844600
C	-3.44187200	-0.97601700	0.88403500
H	-3.50889100	0.09183700	1.08787700
H	-3.19425500	-1.51484300	1.80011200
H	-4.39422300	-1.33754400	0.48855200
F	-2.12490700	-4.57156800	-0.95131600
F	-3.60101200	-3.81906200	0.43061300
F	-3.54322900	-3.07289200	-1.59289200
O	-1.21334000	-2.79121900	1.01495900
H	-0.45925600	-2.20198900	1.16282800
H	-1.07584700	-2.28188000	-0.98504000

COM1-(*R*)-4

C	0.59247900	3.35179900	0.10107900
C	1.48024300	2.27407000	0.67021000
O	0.82001300	1.27376300	1.34051600
C	3.13274800	0.94914900	1.25874300
C	1.85945200	0.54169600	2.03189400
H	3.96177400	1.13284200	1.94302700
H	1.87908300	0.89208200	3.06552100
C	-0.55605400	2.66073800	-0.58862000
O	-0.18287800	1.66361000	-1.43220900
C	-2.51161800	1.91434100	-1.25552800
C	-1.39443300	1.21579500	-2.07626000
H	-3.21610800	2.42362100	-1.91558000
H	-1.36676800	1.55353500	-3.11286000
N	2.73842600	2.21158900	0.60838700
N	-1.78636700	2.91085000	-0.45126500
C	0.07110800	4.22378200	1.24982500
H	-0.45698500	3.61964000	1.98806600
H	0.91031800	4.73055400	1.72932300
H	-0.62372800	4.96632900	0.85785100
C	1.37192600	4.18519300	-0.92317900
H	1.72375600	3.56052100	-1.74452000
H	0.72446700	4.97036900	-1.31741000
H	2.23829300	4.63920800	-0.44248000
H	1.62167800	-0.51989400	1.98930300
H	-1.42343300	0.12991000	-2.02031900
C	3.55537500	-0.08627800	0.23336900
C	4.49813200	-1.05218600	0.58570800
C	2.98225500	-0.12753100	-1.03719100
C	4.86190900	-2.04889900	-0.31292600
H	4.95392200	-1.02034000	1.57046000
C	3.34856900	-1.12261400	-1.93811200
H	2.24513400	0.61304400	-1.32738100
C	4.28710500	-2.08505700	-1.57982200
H	5.59871400	-2.79052600	-0.02773900
H	2.89449500	-1.14707100	-2.92153800
H	4.57183900	-2.85684200	-2.28488300
C	-3.28310200	0.95379700	-0.37092400
C	-4.38564400	0.27766500	-0.89323700
C	-2.89383500	0.70103900	0.94271400
C	-5.08400800	-0.64259600	-0.12169700
H	-4.70032400	0.47624400	-1.91306400
C	-3.59906000	-0.21516000	1.71956700
H	-2.04675100	1.23272700	1.36324200
C	-4.69135100	-0.89218500	1.18958900
H	-5.93663300	-1.16249000	-0.54196100

H	-3.29521300	-0.39592300	2.74474700
H	-5.23637300	-1.60610900	1.79516100
C	-0.53974900	-1.86424500	0.61941900
C	-1.34911500	-2.88977000	-0.17458700
O	0.45478400	-2.45537200	1.39372800
C	1.49884300	-3.11929800	0.67702100
H	2.33284600	-3.21039700	1.37034100
H	1.80964600	-2.53372200	-0.18961400
H	1.17729200	-4.11478000	0.36203700
F	-2.44115900	-2.31951300	-0.69248200
F	-0.65552200	-3.41879100	-1.19070700
F	-1.74303700	-3.89627700	0.61167900
O	-0.07163900	-0.96130100	-0.32083400
H	0.10684900	-0.10682000	0.09972500
H	-1.23003100	-1.40663200	1.33232800

COM1-(*S*)-5

C	2.66415000	-1.55624400	-0.80247100
C	2.83414200	-0.05936400	-0.66177700
O	3.19983900	0.58172700	-1.79631100
C	2.78627500	2.04099900	0.00826000
C	3.35365400	1.96911400	-1.43306800
H	3.49001300	2.52800500	0.68518200
H	4.41526300	2.21434000	-1.47728900
C	1.89590400	-2.01025700	0.41437700
O	2.58133100	-2.09097500	1.56445000
C	0.27171100	-2.45239400	1.85999300
C	1.63910000	-2.49978200	2.57813500
H	-0.27698400	-3.38824500	1.97583900
H	1.90910700	-3.50504200	2.90116200
N	2.64123900	0.62344800	0.38538500
N	0.65396500	-2.27534800	0.44158100
C	1.85461200	-1.85022300	-2.07294500
H	0.90553600	-1.31142700	-2.06369000
H	2.42656000	-1.54036300	-2.94697100
H	1.64757300	-2.91952600	-2.13719600
C	4.04788000	-2.22361600	-0.85935800
H	4.61244300	-2.02458900	0.05115500
H	3.93381900	-3.30329200	-0.97519900
H	4.59997400	-1.83716400	-1.71696900
H	2.79758800	2.57244200	-2.14834600
H	1.71403900	-1.80398600	3.41180400
C	1.43996800	2.72918100	0.10645900
C	1.26299400	3.86515900	0.89073800
C	0.35228300	2.21139400	-0.59883600
C	0.01494900	4.48252700	0.96558700
H	2.10200400	4.26984900	1.44744700
C	-0.89219900	2.82255300	-0.52621200
H	0.46261700	1.31602400	-1.20336200
C	-1.06285900	3.96240500	0.25801300
H	-0.11239100	5.36676700	1.57915500
H	-1.72348600	2.39656400	-1.07589100
H	-2.03392000	4.43955400	0.31875500
C	-0.61807500	-1.28871400	2.24397900
C	-1.98112200	-1.46963000	2.45484200
C	-0.08298800	0.00233600	2.26555800
C	-2.80645100	-0.37150500	2.68763000
H	-2.40546200	-2.46699800	2.40982500
C	-0.90691300	1.09738000	2.48886000
H	0.97117400	0.15825500	2.05268800
C	-2.27231000	0.91166300	2.69969200
H	-3.86933200	-0.51976500	2.83488800

H	-0.48663300	2.09714000	2.47096600
H	-2.91740400	1.76736600	2.86130800
C	-1.87074500	-0.68138400	-1.06153800
C	-3.38787600	-0.51911800	-1.15472100
O	-1.23137200	0.01836300	-2.09685800
C	-1.43302900	-0.47732400	-3.41785300
H	-0.60356800	-0.10128700	-4.01471200
H	-1.42828000	-1.56837200	-3.42528400
H	-2.37420900	-0.11004400	-3.83328400
F	-3.99359800	-0.97691000	-0.05589800
F	-3.90965600	-1.17720400	-2.19854400
F	-3.72122400	0.77253200	-1.29284000
O	-1.61525200	-2.03232300	-1.05896400
H	-0.75144400	-2.17515300	-0.60282500
H	-1.54542700	-0.17876600	-0.14098500

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C	2.52676500	-1.99868100	-0.15761000
C	2.80540600	-0.61687800	-0.70572800
O	3.13052400	-0.56652100	-2.01618300
C	2.95730500	1.56097300	-1.01580800
C	3.42015700	0.81932400	-2.29618500
H	3.73447600	2.23055700	-0.64438200
H	4.49320800	0.91115100	-2.46727800
C	1.73447800	-1.78693200	1.11381000
O	2.42929400	-1.68556400	2.25308100
C	0.11033400	-1.32664000	2.55931700
C	1.47336000	-1.40884700	3.29958300
H	-0.58977000	-2.07589900	2.93448600
H	1.52070300	-2.22362300	4.02065200
N	2.74421600	0.46465500	-0.05147100
N	0.47146800	-1.65948100	1.17015300
C	1.69439900	-2.80128600	-1.16910300
H	0.76785900	-2.28662800	-1.42619300
H	2.27513400	-2.94879500	-2.07905500
H	1.44646600	-3.77457500	-0.74261200
C	3.86360400	-2.70239300	0.12418900
H	4.45516300	-2.14025500	0.84589200
H	3.68172100	-3.70265100	0.52162700
H	4.42301500	-2.79347500	-0.80783600
H	2.86919500	1.10832600	-3.18915600
H	1.75581600	-0.46938500	3.77210400
C	1.66545000	2.33586100	-1.18594800
C	1.61280900	3.71350400	-0.99270000
C	0.49802500	1.65197500	-1.52719600
C	0.40923700	4.40015100	-1.14563200
H	2.51393000	4.25274700	-0.71930500
C	-0.70570900	2.32877800	-1.66646300
H	0.51331300	0.57622900	-1.66639700
C	-0.75068200	3.70914200	-1.47951000
H	0.37897200	5.47307100	-0.99554400
H	-1.60017100	1.76695000	-1.90965300
H	-1.68770200	4.24256600	-1.58789700
C	-0.54056600	0.03846500	2.63915200
C	-1.66222700	0.24674700	3.43726700
C	0.00350900	1.10832300	1.92673800
C	-2.23089000	1.51402600	3.53232500
H	-2.09905500	-0.58616300	3.97857300
C	-0.57522800	2.36948900	2.00634800
H	0.87708200	0.95310500	1.30109200
C	-1.69199700	2.57578000	2.81314700
H	-3.10368900	1.66726100	4.15650700

H	-0.15391600	3.18490500	1.42816500
H	-2.14324600	3.55900800	2.87735500
C	-2.34013400	-1.55162200	-0.60574300
C	-3.10046200	-1.51773000	-1.93377400
O	-3.12129800	-1.11332800	0.46075400
C	-3.41995800	0.28100500	0.47209500
H	-3.90907700	0.47301400	1.42380800
H	-2.50542200	0.87559400	0.40903500
H	-4.09739300	0.54776500	-0.34404600
F	-2.47267800	-2.26965900	-2.84683200
F	-3.20493500	-0.28155600	-2.44275700
F	-4.34018300	-1.99760800	-1.79595100
O	-1.19096600	-0.82073500	-0.81231200
H	-0.55440200	-1.07693500	-0.09845700
H	-2.13420200	-2.60668400	-0.39054700

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C	0.31288800	-3.12297100	-0.21688900
C	0.90509900	-2.14080600	0.76558200
O	1.74520000	-2.66737100	1.67772000
C	1.54657700	-0.32237600	1.86088400
C	2.12097700	-1.58247400	2.55472000
H	0.90992000	0.24949100	2.53709900
H	1.66720700	-1.76675800	3.52821800
C	-0.41929100	-2.29607400	-1.24553800
O	-1.63019500	-1.82444400	-0.86564700
C	-0.90423500	-0.96421600	-2.91444400
C	-2.15523500	-1.14198100	-2.02337700
H	-1.13103100	-1.18265000	-3.95964900
H	-2.90339700	-1.79167100	-2.48209400
N	0.69904200	-0.88933900	0.79440900
N	0.03320200	-1.96407700	-2.37954600
C	1.44978700	-3.90999100	-0.88127600
H	2.13350500	-3.23895700	-1.40139400
H	1.99622700	-4.47322000	-0.12499400
H	1.03121900	-4.60142900	-1.61346100
C	-0.64438500	-4.06717600	0.52837300
H	-1.44560700	-3.51033500	1.01430000
H	-1.08914000	-4.76954900	-0.17907500
H	-0.09057100	-4.63017700	1.28037900
H	3.20611700	-1.57540100	2.64093500
H	-2.59906900	-0.20690200	-1.69320400
C	2.59206600	0.59023200	1.25688400
C	2.64382000	1.93834500	1.59609700
C	3.51597800	0.08311200	0.34038700
C	3.61368700	2.77061300	1.04069100
H	1.92095900	2.33993900	2.29839500
C	4.48262500	0.90938400	-0.21693200
H	3.47519600	-0.96637900	0.06032500
C	4.53556000	2.25714900	0.13672000
H	3.64551200	3.81864100	1.31361300
H	5.19368800	0.50633800	-0.92806000
H	5.29010700	2.90230900	-0.29701600
C	-0.32469100	0.43865200	-2.80640200
C	-1.05984000	1.51035800	-3.31665300
C	0.88111700	0.69470800	-2.15917400
C	-0.61082500	2.81457200	-3.16100000
H	-1.99949700	1.32179600	-3.82785500
C	1.32949700	2.00343700	-1.99442800
H	1.46191900	-0.12736200	-1.76170300
C	0.58493800	3.06547000	-2.49180500
H	-1.19621500	3.63682600	-3.55548800

H	2.26088800	2.18372400	-1.46869300
H	0.93079300	4.08393100	-2.36007700
C	-1.98437700	0.45612400	1.34528600
C	-3.45344000	0.86113100	1.22498800
O	-1.43216300	0.88714400	2.55702800
C	-1.30924800	2.29886500	2.70762400
H	-0.60924500	2.45920000	3.52640600
H	-0.92309100	2.75361000	1.79362500
H	-2.26977000	2.75148500	2.96681100
F	-4.05134500	0.16758400	0.24514900
F	-3.61464400	2.15959600	0.94731800
F	-4.11618200	0.60754500	2.35846700
O	-1.35024500	0.95066600	0.22606800
H	-0.55271200	0.39881500	0.10136900
H	-1.95515700	-0.63640700	1.38557800

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C	-2.72721900	2.03395500	-0.60976400
C	-1.34542200	2.41989100	-0.13939000
O	-1.26963800	3.61835100	0.46493900
C	0.80101800	2.49954600	0.39988500
C	0.12108200	3.84386900	0.76834900
H	1.61204700	2.66395300	-0.31498700
H	0.46948700	4.67461300	0.15537100
C	-2.73835600	0.54374000	-0.84924800
O	-2.07658800	0.12180300	-1.95088200
C	-2.99907700	-1.63933500	-0.68066700
C	-2.23873100	-1.31019600	-1.99315600
H	-3.93811500	-2.15704100	-0.88630200
H	-2.81086700	-1.55842500	-2.88673300
N	-0.27546300	1.74510900	-0.26212700
N	-3.30498800	-0.31146500	-0.10986600
C	-3.75775100	2.39676400	0.46608700
H	-3.54144000	1.88335900	1.40267400
H	-3.75224200	3.47306000	0.63373500
H	-4.74766300	2.08632600	0.13136900
C	-3.01924700	2.79005800	-1.91993700
H	-2.29250600	2.53115500	-2.68929600
H	-4.01718900	2.52738700	-2.27603200
H	-2.98594700	3.86476600	-1.73573900
H	0.20418700	4.09273600	1.82464800
H	-1.24509900	-1.75257700	-2.04518200
C	1.34735000	1.74477400	1.59604300
C	2.65844100	1.97752900	2.01268400
C	0.55957500	0.83408700	2.29850700
C	3.17388400	1.31668500	3.12148100
H	3.28216700	2.67234800	1.45866700
C	1.07709200	0.17079500	3.40716700
H	-0.45309500	0.62648400	1.97051200
C	2.38263500	0.41067100	3.82141300
H	4.19527600	1.50065000	3.43237700
H	0.45784400	-0.54230700	3.93873900
H	2.78568400	-0.11135500	4.68082600
C	-2.19537800	-2.45301000	0.31039300
C	-2.71412800	-3.60932600	0.88617400
C	-0.91634000	-2.02934100	0.66968000
C	-1.96507700	-4.33372300	1.80987100
H	-3.70940200	-3.94401000	0.61304000
C	-0.16321100	-2.75039800	1.58750300
H	-0.49634500	-1.13503700	0.21929500
C	-0.68950000	-3.90548700	2.16216300
H	-2.37789000	-5.23277000	2.25216400

H	0.83779300	-2.41059300	1.82855800
H	-0.10493800	-4.47209100	2.87745500
C	1.96714300	-0.47671500	-1.11499500
C	3.13922600	-0.35873800	-2.09183100
O	2.00671000	-1.67111100	-0.40107700
C	1.80812100	-2.85428800	-1.16725400
H	1.55946100	-3.64033300	-0.45692500
H	0.98236100	-2.72855800	-1.87057300
H	2.71713300	-3.12463400	-1.71131700
F	3.27253700	0.91493600	-2.49120000
F	2.98131400	-1.10705900	-3.18900300
F	4.29114100	-0.72357500	-1.51861700
O	0.81215800	-0.29424000	-1.85221600
H	0.23777600	0.34719400	-1.38438500
H	2.11185300	0.30221800	-0.36168300

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C	-0.81707900	-2.53210500	0.21030600
C	-0.18115400	-1.57181100	1.18445600
O	1.11223300	-1.85888300	1.52843200
C	0.34648600	0.16234400	2.43552000
C	1.45817300	-0.90569000	2.56237000
H	-0.03708700	0.43768500	3.41958400
H	1.42717600	-1.42967700	3.51841700
C	-2.21984800	-2.03072800	-0.03498800
O	-3.10551900	-2.27396400	0.95678400
C	-4.00649800	-1.00686600	-0.81865800
C	-4.35292200	-1.69693600	0.52904000
H	-4.62814300	-1.39034600	-1.63019000
H	-5.08022000	-2.50139600	0.41947200
N	-0.70036100	-0.53063700	1.67509300
N	-2.60471300	-1.39834700	-1.06013500
C	-0.02089200	-2.51127900	-1.10274700
H	-0.02230600	-1.51438300	-1.54427100
H	1.00696300	-2.83473100	-0.93478200
H	-0.48790500	-3.19047500	-1.81681900
C	-0.83907900	-3.94562100	0.81418800
H	-1.38579700	-3.95951100	1.75680700
H	-1.32586300	-4.63155700	0.11846500
H	0.18179200	-4.28841000	0.98520800
H	2.45574400	-0.52284700	2.35324500
H	-4.68459300	-0.99492300	1.29307600
C	0.81878200	1.41328300	1.71408200
C	1.73674900	2.24620000	2.35560900
C	0.41059500	1.72195800	0.41937200
C	2.26454100	3.35071200	1.70303000
H	2.04872800	2.01848500	3.37103800
C	0.94322800	2.82967900	-0.23734500
H	-0.32243000	1.09835800	-0.08090800
C	1.87476900	3.64007700	0.39729400
H	2.98132300	3.98633200	2.20979300
H	0.62638300	3.05319600	-1.24915600
H	2.29135900	4.49750500	-0.11745100
C	-4.13082400	0.50109200	-0.77410000
C	-5.04239700	1.17180100	-1.58295300
C	-3.31830900	1.23322300	0.09507900
C	-5.14657700	2.56004100	-1.52836100
H	-5.67076500	0.60807000	-2.26471200
C	-3.41594700	2.61789600	0.14433300
H	-2.59935500	0.71398800	0.72392200
C	-4.33210100	3.28487000	-0.66698800
H	-5.85879400	3.07278700	-2.16406200

H	-2.77122300	3.17771100	0.81229000
H	-4.40679400	4.36516400	-0.62876700
C	2.91127100	-0.47271200	-0.57333500
C	3.31755900	-0.23238500	-2.02785500
O	3.43971800	0.46877800	0.29716000
C	4.86142100	0.54207600	0.35084100
H	5.10112900	1.09488200	1.25686500
H	5.30223100	-0.45559100	0.39587100
H	5.25494800	1.08161800	-0.51425200
F	2.51619300	-0.92085100	-2.84850000
F	4.57480000	-0.60999000	-2.28368200
F	3.21208000	1.06181600	-2.34347300
O	3.27855400	-1.78078600	-0.28116500
H	2.66351400	-2.09814500	0.39430400
H	1.82826700	-0.32552800	-0.52563800

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C	0.34259500	-1.70954400	0.26019700
C	0.25605000	-0.28309500	0.74741300
O	1.34673000	0.50063500	0.48734800
C	-0.40440200	1.67450400	1.52798100
C	1.09232900	1.76731000	1.13555500
H	-0.54515200	1.95061000	2.57399700
H	1.74797400	1.83617900	2.00459100
C	-1.07368300	-2.23891000	0.26117300
O	-1.52865800	-2.70642200	1.44346300
C	-3.16134200	-2.71623100	-0.26035400
C	-2.88510500	-3.12851900	1.21096300
H	-3.47015300	-3.57511100	-0.85957600
H	-2.93654400	-4.20635300	1.36603100
N	-0.71557700	0.25043600	1.35115000
N	-1.84873400	-2.24046500	-0.73905500
C	0.90862600	-1.74082300	-1.16554000
H	0.31604600	-1.12355000	-1.84071500
H	1.94215700	-1.39581800	-1.15847700
H	0.88549000	-2.76609000	-1.53700900
C	1.24395100	-2.51347000	1.21285600
H	0.85482000	-2.48710300	2.23018000
H	1.28168900	-3.55412400	0.88308500
H	2.25485100	-2.10317800	1.18773700
H	1.31202300	2.56522300	0.42825100
H	-3.52917700	-2.61713300	1.92499500
C	-1.30953200	2.53464000	0.66734600
C	-1.69603600	3.79706800	1.11594300
C	-1.73644600	2.09827800	-0.58675200
C	-2.48963500	4.61748000	0.32137900
H	-1.37850100	4.13726100	2.09647100
C	-2.53107900	2.91762200	-1.38143600
H	-1.48154000	1.10122900	-0.93090000
C	-2.90756700	4.17882800	-0.93130000
H	-2.78670700	5.59473100	0.68298200
H	-2.86913400	2.56104400	-2.34706700
H	-3.53081900	4.81363200	-1.54963400
C	-4.20061000	-1.62346400	-0.39536500
C	-5.38639700	-1.83868400	-1.09115400
C	-3.96643900	-0.37620300	0.18750500
C	-6.33201900	-0.82209500	-1.20468800
H	-5.57051500	-2.80354600	-1.55230000
C	-4.90479600	0.64113200	0.06806900
H	-3.03729400	-0.19892000	0.72281700
C	-6.09171300	0.41945300	-0.62739400
H	-7.25177700	-0.99942700	-1.74967700

H	-4.70152300	1.61122800	0.50864100
H	-6.82360600	1.21303400	-0.72126200
C	4.36375100	0.09278000	-0.03762500
C	5.81141300	0.52780600	-0.27410700
O	4.24573200	-1.28421400	0.12292900
C	4.63725900	-2.08146400	-0.99382900
H	4.15714900	-3.04930900	-0.85998200
H	4.30373800	-1.63076500	-1.93020400
H	5.72175400	-2.21225600	-1.01283300
F	5.93848000	1.84464800	-0.08384600
F	6.23260200	0.25572800	-1.51292900
F	6.63508800	-0.09043600	0.57795900
O	3.63530700	0.60147000	-1.10061900
H	2.70822800	0.60350500	-0.82308400
H	4.05324500	0.51761200	0.92163300

COM1-(*S*)-11

C	0.43009500	-1.90220800	0.19969500
C	-1.00398200	-2.19722500	-0.17878300
O	-1.52120000	-3.33246200	0.34228400
C	-3.06845800	-2.10698600	-0.94966300
C	-2.84768100	-3.45402600	-0.21007800
H	-3.37529000	-2.27456800	-1.98342800
H	-2.85512300	-4.30902300	-0.88656400
C	0.62675800	-0.42985900	-0.07825800
O	1.06343400	-0.10658400	-1.33317000
C	0.53496100	1.77875300	-0.00872400
C	0.98088400	1.33293700	-1.42884500
H	1.30882400	2.37410500	0.48387500
H	1.96203000	1.71141500	-1.71985800
N	-1.73425100	-1.48559600	-0.92905900
N	0.36905300	0.50980700	0.72262800
C	0.65630400	-2.17810300	1.69158200
H	-0.00920300	-1.56837500	2.30243100
H	0.47487700	-3.23182200	1.90215100
H	1.68688200	-1.92188400	1.94081000
C	1.34586200	-2.78490800	-0.66416000
H	1.18644300	-2.59256900	-1.72569100
H	2.38919300	-2.58795100	-0.41572900
H	1.12877300	-3.83406700	-0.45847600
H	-3.54533600	-3.61728400	0.60957200
H	0.24475900	1.57681400	-2.19372100
C	-4.07997100	-1.19919200	-0.27900100
C	-5.28846900	-0.89611600	-0.90029800
C	-3.81141200	-0.66350900	0.98231500
C	-6.22404400	-0.07962700	-0.26864900
H	-5.49941000	-1.29931500	-1.88535900
C	-4.74261700	0.14924100	1.61483700
H	-2.85733500	-0.86400600	1.46080400
C	-5.95351100	0.44154900	0.99118500
H	-7.16052700	0.14981400	-0.76318000
H	-4.51833600	0.56749400	2.58868400
H	-6.67769500	1.07980200	1.48315800
C	-0.75861100	2.56480600	-0.01284700
C	-0.78783000	3.90917400	0.34471300
C	-1.94261000	1.92811800	-0.38939600
C	-1.98853600	4.61510000	0.32411100
H	0.12827100	4.40622000	0.64675500
C	-3.14176100	2.62853200	-0.40091000
H	-1.92421100	0.87595900	-0.65773200
C	-3.16650400	3.97582100	-0.04610000
H	-2.00302700	5.66169000	0.60472100

H	-4.05704100	2.11420600	-0.67544300
H	-4.10149100	4.52362000	-0.05365500
C	3.89452700	0.06170300	-0.04663000
C	5.21742300	0.81417300	0.11138500
O	3.74767600	-0.96582600	0.87786300
C	4.72599000	-2.00335600	0.81422200
H	4.30335800	-2.85279000	1.34789300
H	4.93118300	-2.28049300	-0.22145100
H	5.65111200	-1.69151700	1.30422900
F	5.15649900	1.98553400	-0.53157500
F	6.25813900	0.13620000	-0.38006200
F	5.46810600	1.06593200	1.39898800
O	3.85204900	-0.35414000	-1.36824000
H	2.92270000	-0.50457800	-1.59634000
H	3.10078500	0.77397500	0.20029200

COM1-(*R*)-5

C	2.33309500	2.13187600	0.19250000
C	2.73222600	0.75977600	0.68987700
O	3.00131100	0.67984900	2.01313500
C	3.08697700	-1.40304900	0.91826700
C	3.43397500	-0.67693600	2.24276500
H	3.93460900	-1.98585100	0.55492700
H	4.50660300	-0.66011200	2.44038800
C	1.60189100	1.90076200	-1.11020400
O	2.34998500	1.81503400	-2.21782000
C	0.06803500	1.35550300	-2.62176800
C	1.45089700	1.50198500	-3.30342300
H	-0.65876900	2.05249200	-3.04356800
H	1.48823500	2.32403000	-4.01683500
N	2.81156500	-0.29109600	-0.01075200
N	0.34676300	1.73465400	-1.22019800
C	1.39615200	2.80093800	1.20807300
H	0.51001900	2.19480200	1.39908800
H	1.92822300	2.95358100	2.14652700
H	1.06794500	3.76640600	0.82018200
C	3.60021300	2.97548700	-0.01942600
H	4.26216900	2.50671800	-0.74660000
H	3.32916100	3.97006700	-0.37872400
H	4.12476900	3.07937500	0.93144700
H	2.89659400	-1.06503900	3.10581200
H	1.79581800	0.58177400	-3.77242800
C	1.86710700	-2.29807000	1.01327400
C	1.96781000	-3.67714300	0.85022900
C	0.61625400	-1.73317100	1.26403000
C	0.83358500	-4.48173700	0.94509100
H	2.93488800	-4.12493700	0.64513500
C	-0.51820500	-2.52832900	1.34543200
H	0.51161000	-0.65843000	1.36721300
C	-0.40963600	-3.90869100	1.19123800
H	0.92245700	-5.55429600	0.81712300
H	-1.48200500	-2.05739100	1.49931400
H	-1.29319400	-4.53334500	1.25017600
C	-0.51004800	-0.04317800	-2.63437000
C	-1.82758100	-0.27167800	-3.01732200
C	0.26195100	-1.10352600	-2.15476300
C	-2.37285300	-1.54970300	-2.92501900
H	-2.43652600	0.55349200	-3.37211300
C	-0.28271600	-2.37633600	-2.05846100
H	1.27581000	-0.92252600	-1.80705400
C	-1.60216300	-2.60147300	-2.44429300
H	-3.40346200	-1.71768500	-3.21402700

H	0.31478900	-3.18563600	-1.65271600
H	-2.03101300	-3.59290400	-2.35676800
C	-2.35520200	1.48747400	0.71931700
C	-3.67703800	0.72494400	0.84336300
O	-2.14606000	2.34519500	1.80003200
C	-1.96922100	1.70689400	3.06023700
H	-1.53950600	2.45457100	3.72386700
H	-1.28868200	0.85649600	2.97537700
H	-2.92628800	1.37052600	3.46811400
F	-4.03584100	0.21480100	-0.33969900
F	-3.60329400	-0.29313200	1.71251900
F	-4.66474400	1.52799900	1.25539200
O	-1.37107400	0.53776600	0.55676100
H	-0.69742500	0.92022100	-0.05288800
H	-2.44653000	2.14320500	-0.15295100

COM1-(*R*)-6

C	-1.74890400	-2.58482400	-0.36073400
C	-0.39497900	-2.52475300	0.30330700
O	0.43912900	-3.52736000	-0.05147700
C	1.38138600	-2.05482900	1.51286400
C	1.71568700	-3.20221800	0.53101700
H	1.33585400	-2.43578200	2.53972800
H	2.11056000	-4.09629900	1.00902400
C	-2.52551200	-1.35633800	0.05065500
O	-3.17652800	-1.42211500	1.22462200
C	-3.40587000	0.67766500	0.18175200
C	-3.92451000	-0.19490600	1.34740700
H	-4.23035900	1.05334500	-0.42627500
H	-4.98219000	-0.43832400	1.24664900
N	0.01119100	-1.65973600	1.13298000
N	-2.62229800	-0.28315000	-0.62212900
C	-1.55912100	-2.60715500	-1.88541000
H	-1.00951100	-1.73251000	-2.23076500
H	-1.00451500	-3.50287000	-2.16348400
H	-2.53459100	-2.62246000	-2.37390300
C	-2.47574400	-3.85832400	0.10727800
H	-2.59896800	-3.86525700	1.18991500
H	-3.46225700	-3.91049400	-0.35727400
H	-1.89856000	-4.73202700	-0.19515900
H	2.37810500	-2.87378800	-0.27126500
H	-3.73254600	0.22823000	2.33129200
C	2.35712400	-0.89842300	1.48028000
C	3.72467500	-1.13133000	1.33046500
C	1.90926400	0.41102600	1.63305100
C	4.62363300	-0.07090200	1.32223200
H	4.09635100	-2.14496900	1.21722700
C	2.80538000	1.47307300	1.61496000
H	0.84903700	0.59535900	1.73737300
C	4.16596300	1.23573300	1.46132300
H	5.68249700	-0.26534600	1.19869900
H	2.43064100	2.48681000	1.69696000
H	4.86640500	2.06199600	1.43992000
C	-2.52572700	1.83980500	0.59144300
C	-2.64301300	3.07178200	-0.04535700
C	-1.56018000	1.67340700	1.58505000
C	-1.82199900	4.13495100	0.31817500
H	-3.38315500	3.20064900	-0.82818500
C	-0.74715400	2.73734400	1.95533700
H	-1.43601700	0.70085000	2.05610100
C	-0.87883800	3.97105700	1.32475100
H	-1.92396800	5.09064800	-0.18259400

H	-0.00502500	2.60324900	2.73448200
H	-0.24262000	4.79894200	1.61476800
C	0.33287200	0.86198500	-1.33488400
C	1.58605700	0.21630000	-1.94352600
O	0.56375200	2.17543500	-0.94290600
C	0.79311100	3.09315700	-2.00093600
H	0.73318100	4.08629200	-1.55896400
H	0.03130400	2.99008400	-2.77582400
H	1.78589000	2.95198100	-2.44039300
F	1.49744200	-1.12676500	-1.83236600
F	1.73285500	0.49158200	-3.24554800
F	2.70937200	0.59379700	-1.33338000
O	-0.67289100	0.71577500	-2.27471200
H	-1.47687100	0.41384800	-1.79741100
H	0.11275200	0.31693400	-0.41217400

COM1-(*R*)-7

C	-3.46581100	0.39966400	-0.36775900
C	-2.53466200	1.45642000	0.18201500
O	-3.02561200	2.21868500	1.17292700
C	-0.78005300	2.71048700	0.68307900
C	-2.02137900	3.21289700	1.45955700
H	-0.34507000	3.51612400	0.08804900
H	-2.38496300	4.17238400	1.09052600
C	-2.62402800	-0.81989700	-0.68667900
O	-2.04210000	-0.83805800	-1.90515700
C	-1.59718000	-2.77176200	-0.62838000
C	-1.26329000	-2.05348900	-1.96127000
H	-2.20419400	-3.66323700	-0.80799000
H	-1.57879300	-2.61409000	-2.83944200
N	-1.34683600	1.68386600	-0.20937500
N	-2.44511700	-1.80003400	0.09345300
C	-4.53165200	0.02811100	0.66884000
H	-4.07492200	-0.35638600	1.57952600
H	-5.13562100	0.90206400	0.91079800
H	-5.17408300	-0.74922600	0.25382300
C	-4.12167700	0.95998400	-1.64280200
H	-3.36911800	1.21952200	-2.38579000
H	-4.79454800	0.21303700	-2.06795300
H	-4.70339900	1.84850300	-1.39029400
H	-1.87585800	3.25028900	2.53693400
H	-0.21499600	-1.77057800	-2.04658700
C	0.29161600	2.11234600	1.57362700
C	1.41935400	2.86349200	1.90306500
C	0.15158600	0.82637900	2.09552300
C	2.39225300	2.34202000	2.74890200
H	1.53963800	3.85979900	1.48863400
C	1.12077700	0.30814500	2.94724300
H	-0.70313500	0.21407600	1.82391800
C	2.24183300	1.06367600	3.27543800
H	3.26900600	2.93095800	2.99019200
H	1.00388100	-0.69506800	3.33958200
H	3.00061200	0.65379900	3.93125100
C	-0.38890300	-3.18018000	0.18469600
C	-0.28450700	-4.47617900	0.68406400
C	0.62804100	-2.26312700	0.45531600
C	0.81981200	-4.85841200	1.43995900
H	-1.07394200	-5.19205600	0.48004900
C	1.73385600	-2.64385500	1.20683500
H	0.56580600	-1.25075900	0.06720500
C	1.83204800	-3.94214700	1.70129400
H	0.88942000	-5.87064600	1.82058100

H	2.51788000	-1.92149000	1.39950000
H	2.69661200	-4.23821600	2.28372600
C	1.64021700	1.27674400	-1.59053900
C	2.85278900	0.47129800	-1.10993900
O	1.90293000	1.96047100	-2.77382100
C	2.15743400	1.13552900	-3.90574500
H	2.09595400	1.78434800	-4.77666300
H	1.41062100	0.34368700	-3.98442300
H	3.15762600	0.69602700	-3.85487100
F	2.72837300	0.19445900	0.19626400
F	2.98906900	-0.69558600	-1.75124100
F	3.99058900	1.15513800	-1.27121000
O	0.58890900	0.38798800	-1.67364800
H	-0.22109100	0.81024600	-1.30650000
H	1.47418900	2.05240400	-0.83709100

COM1-(*R*)-8

C	-3.30368100	-1.06665400	-0.35025800
C	-2.71858300	0.30625100	-0.58877300
O	-3.60146000	1.32298700	-0.60044500
C	-1.37432700	2.05545600	-0.82109900
C	-2.84779800	2.50403600	-0.95602500
H	-0.78211500	2.32907900	-1.69508100
H	-3.11005400	2.77154500	-1.98003300
C	-2.14040500	-1.97539000	-0.02974200
O	-1.37960500	-2.34282400	-1.08581800
C	-0.51162900	-3.04756200	0.98399900
C	-0.34336100	-3.19390500	-0.55239800
H	-0.56342700	-4.02482200	1.46768000
H	-0.53187600	-4.21007900	-0.90086100
N	-1.49033000	0.58331200	-0.75561400
N	-1.80284400	-2.35551700	1.12822600
C	-4.26603000	-1.00356000	0.84211500
H	-3.75081500	-0.66082800	1.73953400
H	-5.09024900	-0.32806800	0.61465700
H	-4.65981500	-2.00115900	1.03922900
C	-4.03584700	-1.52639300	-1.62237000
H	-3.35255900	-1.57564100	-2.46976200
H	-4.46282000	-2.51774400	-1.45919400
H	-4.84485100	-0.83088300	-1.84973100
H	-3.12711900	3.30368500	-0.27326000
H	0.61242300	-2.82806800	-0.92209400
C	-0.68209000	2.57049100	0.42587200
C	0.53639800	3.23936400	0.34012800
C	-1.26614300	2.37297300	1.67962900
C	1.15488300	3.72368900	1.49153300
H	1.00964600	3.35895000	-0.62833000
C	-0.64970500	2.85273700	2.82760100
H	-2.20922000	1.83804300	1.75773500
C	0.56124500	3.53698600	2.73404200
H	2.10285900	4.24263500	1.41411900
H	-1.10974800	2.69181100	3.79507200
H	1.04198100	3.91266600	3.62938100
C	0.61135300	-2.24513300	1.61401000
C	1.75773500	-2.89466000	2.06991500
C	0.54584500	-0.85543500	1.68955900
C	2.82715400	-2.16688500	2.57993500
H	1.81450000	-3.97791100	2.02436700
C	1.61518600	-0.12482600	2.19925400
H	-0.34311700	-0.33868400	1.34830200
C	2.76023500	-0.77840000	2.64227400
H	3.71334000	-2.68426700	2.92831200

H	1.54514700	0.95744900	2.24652400
H	3.59526300	-0.21033200	3.03462500
C	1.57017300	0.35722100	-1.44134800
C	2.94584200	-0.29290400	-1.31555800
O	1.62657800	1.55400600	-2.16752900
C	1.92578800	1.43594200	-3.55722100
H	1.53106600	2.33120600	-4.03441200
H	1.44713800	0.55251900	-3.98104300
H	3.00435200	1.38508300	-3.72040600
F	2.89699000	-1.34933300	-0.50019600
F	3.42086400	-0.72391200	-2.49419600
F	3.83778000	0.57058100	-0.81648900
O	0.73296600	-0.59320300	-1.98431300
H	-0.15738400	-0.43740000	-1.60927300
H	1.26770800	0.65228100	-0.43201600

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C	0.22411100	-0.59770600	-2.37946800
C	0.34807100	0.61695000	-1.48756900
O	1.39752400	1.45328900	-1.74756200
C	0.05701400	2.17411800	0.05127600
C	1.17976800	2.62031500	-0.91724200
H	0.48208400	1.92665700	1.02800500
H	2.11446300	2.85887400	-0.41295300
C	-0.36808700	-1.69434900	-1.53281700
O	0.40664800	-2.06268900	-0.48076900
C	-1.64230100	-3.21293800	-0.58030500
C	-0.26681700	-3.17203500	0.14060200
H	-1.85198400	-4.21207400	-0.96590500
H	0.32850900	-4.06921600	-0.03318400
N	-0.43868000	0.92699000	-0.55089500
N	-1.47172400	-2.28067400	-1.71120900
C	-0.71742300	-0.23929000	-3.53584400
H	-1.70033500	0.03554100	-3.15401000
H	-0.29767400	0.59335300	-4.10392800
H	-0.83154900	-1.10012700	-4.19542100
C	1.59265200	-1.05640000	-2.90816100
H	2.27050700	-1.32484100	-2.09708500
H	1.45047300	-1.93444500	-3.54060600
H	2.04653600	-0.26644800	-3.50766300
H	0.86776200	3.43975300	-1.56650700
H	-0.34461300	-2.97343400	1.20812600
C	-1.01931700	3.21930300	0.21978300
C	-0.90511800	4.17444800	1.22861100
C	-2.10385000	3.27726600	-0.65434100
C	-1.85563100	5.18180600	1.35736600
H	-0.07037200	4.12446900	1.92058500
C	-3.05778000	4.28023100	-0.52240900
H	-2.20561100	2.52300300	-1.42650100
C	-2.93447800	5.23644800	0.48114000
H	-1.75808200	5.91789300	2.14646200
H	-3.90199000	4.31225100	-1.20094400
H	-3.67934700	6.01638300	0.58388500
C	-2.78844500	-2.77549300	0.30783700
C	-3.69764500	-3.70889200	0.79801100
C	-2.91679400	-1.43461900	0.67665100
C	-4.72389300	-3.31487900	1.65246700
H	-3.60592800	-4.75039300	0.50711500
C	-3.94186100	-1.04205600	1.52881600
H	-2.21912700	-0.69618600	0.29137000
C	-4.84744100	-1.97998800	2.01917900
H	-5.42787700	-4.04953000	2.02527800

H	-4.03626300	0.00117800	1.80731300
H	-5.64724500	-1.66975800	2.68114200
C	2.90846800	-0.07679500	0.50865700
C	3.55259500	-1.29717700	1.16676800
O	2.76612900	0.99604900	1.38557500
C	3.97910800	1.53404800	1.91145600
H	3.73485400	2.52268800	2.29432900
H	4.73650000	1.61589300	1.13046700
H	4.35575300	0.91371600	2.72794000
F	3.38359400	-2.37876900	0.39975400
F	4.86695000	-1.14658700	1.36579400
F	2.98933100	-1.54460200	2.35339800
O	3.68747900	0.21121300	-0.60446400
H	3.12312000	0.67360500	-1.23973300
H	1.88970300	-0.38018100	0.25162200

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C	1.04614500	2.54350700	-0.01725500
C	0.39919500	1.74160400	1.08147100
O	-0.89268300	2.09794900	1.36916200
C	-0.20313300	0.19553800	2.51782000
C	-1.22941900	1.34517900	2.55572200
H	0.15036000	-0.05104600	3.51996100
H	-1.08788600	1.99883900	3.41816000
C	2.39764700	1.92223700	-0.27376000
O	3.35495500	2.21886800	0.63393900
C	4.07238900	0.70170900	-1.02228200
C	4.54666700	1.54376700	0.19201100
H	4.66123200	0.92657900	-1.91352100
H	5.28407500	2.29940400	-0.08000500
N	0.88976400	0.76669300	1.71742200
N	2.68266000	1.15253100	-1.23602400
C	0.16937200	2.43317300	-1.27437200
H	-0.01850500	1.39000500	-1.53041300
H	-0.78477200	2.93651900	-1.10714500
H	0.67871300	2.91248800	-2.11087000
C	1.19297500	4.00898800	0.42359400
H	1.81332800	4.08821300	1.31586400
H	1.65864100	4.58596100	-0.37773200
H	0.20819100	4.42938500	0.62980000
H	-2.26929600	1.03117400	2.47863000
H	4.92116100	0.93566000	1.01421200
C	-0.76720500	-1.04666900	1.84393400
C	-1.85006700	-1.69743900	2.44328100
C	-0.29781900	-1.50122300	0.61319100
C	-2.47657000	-2.76019600	1.80678600
H	-2.21865900	-1.35389700	3.40540500
C	-0.92106300	-2.57551100	-0.01993000
H	0.53546700	-1.00460900	0.13085400
C	-2.01560700	-3.19776100	0.56554800
H	-3.32843200	-3.24180800	2.27159600
H	-0.55927100	-2.90391500	-0.98641700
H	-2.51315500	-4.01596500	0.05947500
C	4.10503000	-0.79097900	-0.77380300
C	4.85630900	-1.63881100	-1.58106600
C	3.36398300	-1.32905800	0.28107700
C	4.87063100	-3.01132600	-1.34283500
H	5.42915700	-1.22627700	-2.40505900
C	3.37116200	-2.69823400	0.51456200
H	2.76757500	-0.67136700	0.90917200
C	4.12628300	-3.54305200	-0.29693400
H	5.45829000	-3.66301700	-1.97860300

H	2.78179900	-3.10790300	1.32686500
H	4.13074100	-4.61109700	-0.11453600
C	-2.99203800	0.21808300	-0.61241300
C	-4.39489800	-0.32924700	-0.87619400
O	-2.13497200	0.02845500	-1.68894800
C	-2.48934600	0.70713800	-2.89154400
H	-1.59286700	0.72245000	-3.50825600
H	-2.81091300	1.72885300	-2.68174400
H	-3.28300500	0.17241500	-3.41950400
F	-5.06426300	-0.46017000	0.27551100
F	-5.12095100	0.46049100	-1.67560700
F	-4.33275000	-1.53475700	-1.45047000
O	-3.16570600	1.54935000	-0.25262400
H	-2.35849400	1.84888800	0.19056500
H	-2.57524500	-0.38607200	0.19667200

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C	0.28804800	-1.92735200	0.32455100
C	-1.12168600	-2.17957200	-0.15675900
O	-1.65952700	-3.35697700	0.22940400
C	-3.15027400	-1.99744700	-0.99674900
C	-2.98424300	-3.39687600	-0.33838000
H	-3.38675700	-2.09585100	-2.05828900
H	-3.01831000	-4.21117100	-1.06181900
C	0.57829500	-0.48882300	-0.02344500
O	1.00910300	-0.25785700	-1.30014700
C	0.70488800	1.71716700	-0.04842400
C	0.95681300	1.17679100	-1.47833400
H	1.60389600	2.19532000	0.35043000
H	1.90581800	1.50481500	-1.89879400
N	-1.82234300	-1.38724100	-0.85243900
N	0.42682600	0.50172100	0.74227100
C	0.34986600	-2.12288700	1.84528600
H	-0.32332800	-1.43368800	2.35429700
H	0.07622000	-3.14828400	2.09237800
H	1.36631100	-1.93129200	2.19431200
C	1.25341900	-2.89219300	-0.38294100
H	1.20048600	-2.77773500	-1.46631000
H	2.27920100	-2.70338400	-0.05836400
H	0.99029000	-3.91807000	-0.12365700
H	-3.69534000	-3.57939000	0.46597800
H	0.13264500	1.39554700	-2.15758300
C	-4.21874500	-1.14563500	-0.34091000
C	-5.52005600	-1.15824800	-0.84162800
C	-3.93088100	-0.37049300	0.78245100
C	-6.52188800	-0.41408400	-0.22801300
H	-5.74872400	-1.74926100	-1.72286700
C	-4.93098000	0.37853000	1.39395400
H	-2.91646500	-0.33164500	1.16494000
C	-6.22855800	0.35752500	0.89208200
H	-7.52833000	-0.42990400	-0.62920000
H	-4.69139600	0.98705800	2.25803800
H	-7.00585500	0.94355400	1.36769900
C	-0.46280800	2.67469400	0.02453900
C	-0.28247300	4.01008300	0.36922700
C	-1.74730500	2.20735100	-0.26473600
C	-1.37282200	4.87585700	0.42305100
H	0.71251900	4.37465900	0.60214800
C	-2.83572800	3.06744100	-0.20259000
H	-1.89019000	1.16259100	-0.52868900
C	-2.64962100	4.40588700	0.13960800
H	-1.22331000	5.91472800	0.69255100

H	-3.82937800	2.68865500	-0.41536100
H	-3.49830000	5.07795500	0.18727000
C	3.89381300	0.00610000	-0.11318400
C	5.08990200	-0.53413900	0.67341400
O	4.02240500	1.35393300	-0.43190500
C	5.13226300	1.68647900	-1.26646400
H	4.92872500	2.67771900	-1.66484100
H	5.22891000	0.97055400	-2.08393500
H	6.05740300	1.71264200	-0.68586200
F	4.76331300	-1.69418000	1.25688000
F	6.15871400	-0.75642800	-0.09629900
F	5.45178300	0.31954800	1.63466700
O	3.76193000	-0.82656400	-1.21440400
H	2.83714300	-0.79064100	-1.50037400
H	3.03371400	-0.04449200	0.56261200

COM3-(*S*)-1

C	4.56825400	1.89471900	-0.52888300
C	3.37988900	2.80467000	-0.32908100
O	3.21085900	3.74313400	-1.28603800
C	1.45700200	3.67726100	0.27522100
C	2.08052100	4.53029000	-0.85949600
H	1.22695000	4.29538100	1.14464800
H	2.45521100	5.49010000	-0.50005900
C	4.46151500	0.84740000	0.55123900
O	4.94252200	1.19266600	1.75423700
C	3.90687500	-0.92773700	1.76201600
C	4.55022600	0.15031100	2.66973900
H	4.51323300	-1.83540500	1.72242400
H	5.43899200	-0.19644300	3.19294100
N	2.52772800	2.72649400	0.60433000
N	3.91588900	-0.29254800	0.42765900
C	4.46303800	1.25095000	-1.91955700
H	3.50740800	0.74322700	-2.05667800
H	4.55771200	2.02437000	-2.68138700
H	5.26413400	0.52158300	-2.04712700
C	5.87141400	2.69804400	-0.39786900
H	5.94872600	3.16096000	0.58539300
H	6.72911400	2.03863800	-0.54346800
H	5.89246000	3.47416400	-1.16323000
H	1.42042300	4.67488400	-1.71213300
H	3.83848600	0.57717800	3.37673600
C	0.20067000	2.94654300	-0.16337500
C	-1.02885800	3.60449600	-0.10254900
C	0.25420600	1.65564000	-0.68712900
C	-2.18241100	2.99192300	-0.57796800
H	-1.08109500	4.60501700	0.31637500
C	-0.90103100	1.03964700	-1.16062200
H	1.19205100	1.11329800	-0.72114300
C	-2.12003100	1.70859000	-1.11501500
H	-3.13098700	3.51383200	-0.52978200
H	-0.84339800	0.03582400	-1.56634100
H	-3.01507400	1.23679500	-1.50226900
C	2.49007400	-1.29476900	2.14202800
C	2.16284900	-2.59232800	2.52424900
C	1.48015500	-0.33410200	2.02612600
C	0.83586700	-2.93813800	2.77294200
H	2.94152000	-3.34441600	2.59405400
C	0.15536400	-0.68373200	2.25723000
H	1.73107700	0.67510200	1.70888900
C	-0.16922200	-1.98832200	2.62886600
H	0.58742100	-3.95507400	3.05178400

H	-0.62709800	0.05400400	2.11904000
H	-1.20499600	-2.26551800	2.77881100
C	1.28510400	-2.19856000	-0.87678100
C	2.08338200	-3.50173300	-0.95921200
O	0.05974200	-2.33777200	-1.53363100
C	0.04323200	-2.26295800	-2.96672700
H	-0.99077600	-2.04547600	-3.22525000
H	0.69520300	-1.45885200	-3.30442000
H	0.35411000	-3.21241500	-3.40256300
F	3.24775300	-3.36619700	-0.30298800
F	2.37472100	-3.85440600	-2.21562100
F	1.41636200	-4.51326900	-0.39581500
O	2.02423600	-1.16042700	-1.40454300
H	2.72815200	-0.88501900	-0.76409400
H	1.03138700	-2.05378000	0.17636700
C	-7.46022800	1.00273300	2.22911300
C	-6.33946600	0.50212800	1.58165500
C	-6.38944600	0.20642900	0.21660600
C	-7.57077000	0.43754200	-0.49249500
C	-8.69164200	0.93450200	0.16008500
C	-8.63997200	1.21583200	1.52122700
H	-7.41081100	1.23564500	3.28573800
H	-5.41777200	0.36584300	2.13367400
H	-7.60134400	0.21950900	-1.55197500
H	-9.60614400	1.10309900	-0.39537600
H	-9.51361000	1.60668000	2.02887100
C	-5.21526900	-0.34022900	-0.49588800
O	-5.25352400	-0.15182200	-1.81398500
C	-4.18839000	-0.98315100	0.12022800
H	-4.44818300	-0.58434300	-2.19031000
H	-4.19073100	-1.15460800	1.18441800
C	-3.05997700	-1.45533500	-0.65646500
O	-2.98016700	-1.34789200	-1.88276900
O	-2.09375000	-2.00999700	0.05600800
H	-1.34347600	-2.22101100	-0.54763000

COM3-(*S*)-2

C	2.91903100	2.60726800	-1.53622800
C	1.97821300	2.86389000	-0.37852600
O	0.76247300	3.34220500	-0.72390200
C	0.97818600	2.91516000	1.58554000
C	0.05208800	3.55292500	0.51444400
H	1.17773500	3.61031600	2.40253700
H	-0.07409300	4.62693600	0.65331800
C	3.97354900	1.66267500	-1.01261300
O	4.95375600	2.20126100	-0.27493100
C	5.04947500	-0.15364800	-0.32379300
C	5.80515200	1.11228200	0.14065700
H	5.68759500	-0.80502000	-0.92299300
H	6.76839200	1.23285000	-0.35448500
N	2.22337300	2.65017700	0.84466400
N	3.97600200	0.40258300	-1.17644600
C	2.14587200	1.94664600	-2.68566600
H	1.63696000	1.04114900	-2.35094900
H	1.40103200	2.64341000	-3.06858400
H	2.83753700	1.68167700	-3.48682600
C	3.54341600	3.93849200	-1.98489000
H	4.10348400	4.39787700	-1.17107600
H	4.21832800	3.76699200	-2.82581000
H	2.75206700	4.61717800	-2.30585300
H	-0.91615100	3.06142600	0.43380800
H	5.92715100	1.17044400	1.22063400
C	0.42801500	1.62098600	2.14834500
C	0.05859200	1.50147600	3.48436600
C	0.24846100	0.53327700	1.29491400
C	-0.49950600	0.31365600	3.95530300
H	0.20192700	2.33918300	4.15905600
C	-0.32772300	-0.64450100	1.75068300
H	0.57234200	0.61696900	0.26096900
C	-0.70211300	-0.75470600	3.08877300
H	-0.78321700	0.22885000	4.99774800
H	-0.49476100	-1.46958900	1.06615800
H	-1.14950900	-1.67236000	3.45137600
C	4.40395900	-0.95744600	0.78532400
C	4.50651400	-2.34448300	0.81582900
C	3.61311900	-0.30408400	1.73449800
C	3.83195300	-3.07625500	1.79033800
H	5.09582100	-2.85734500	0.06319500
C	2.93457600	-1.03457100	2.70113500
H	3.48914300	0.77480200	1.68881300
C	3.04419200	-2.42357400	2.73103800
H	3.90560800	-4.15700900	1.79819900

H	2.29828900	-0.52041300	3.41382000
H	2.50535000	-2.99385900	3.47856000
C	1.43869300	-1.73447100	-1.21357600
C	1.05350500	-3.21179200	-1.11083000
O	0.31965500	-0.95207200	-1.58150600
C	-0.21581600	-1.20370100	-2.88867700
H	-0.71888400	-0.28821400	-3.19662100
H	0.58853000	-1.43676000	-3.58513200
H	-0.93644200	-2.02214500	-2.84491100
F	2.02838500	-3.91519100	-0.52925000
F	0.82631400	-3.76245600	-2.30980300
F	-0.05569600	-3.36923500	-0.38056500
O	2.47205900	-1.64783800	-2.10837100
H	3.00717400	-0.84829700	-1.87432700
H	1.71152400	-1.39385400	-0.20583400
C	-8.32221400	1.80286500	-0.59751300
C	-7.03188300	1.31108000	-0.73564500
C	-6.68457400	0.07897500	-0.17499800
C	-7.65266200	-0.65938000	0.50996200
C	-8.94187400	-0.16171800	0.65029800
C	-9.27909800	1.06994500	0.09930200
H	-8.58456600	2.75514500	-1.04197100
H	-6.30170900	1.87579100	-1.30200900
H	-7.38305100	-1.61866700	0.93187200
H	-9.68447600	-0.73740500	1.18922300
H	-10.28595000	1.45552400	0.20556900
C	-5.31406600	-0.46411800	-0.29541200
O	-5.24104800	-1.77724500	-0.10435200
C	-4.22027400	0.30295200	-0.55090700
H	-4.28993000	-2.02954100	-0.18351900
H	-4.29574000	1.37279400	-0.65699000
C	-2.91438100	-0.31518600	-0.64732100
O	-2.70463000	-1.51730300	-0.50595000
O	-1.92319300	0.53419000	-0.91069100
H	-1.08899700	0.02270100	-0.92522900

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C	4.75061700	-1.50052200	1.10650700
C	3.58186700	-2.12220900	0.37944500
O	3.58135600	-3.46507800	0.34646400
C	1.70005800	-2.52043800	-0.73092200
C	2.39868500	-3.86353200	-0.37981400
H	1.63709000	-2.37492200	-1.81232000
H	2.71547900	-4.42532600	-1.25711800
C	4.52739600	-0.00822700	1.13163200
O	4.66113500	0.61775200	-0.06025100
C	3.93074800	2.03950100	1.66555300
C	4.44053700	2.01985000	0.19975100
H	4.49280600	2.75614000	2.26713900
H	5.39339700	2.53701300	0.08050400
N	2.61809600	-1.51146500	-0.17972400
N	4.20083100	0.67270300	2.14582800
C	4.79157300	-2.05426400	2.53658500
H	3.86764900	-1.82475300	3.06796900
H	4.93722900	-3.13392600	2.50775900
H	5.61644900	-1.59134100	3.07876000
C	6.04802700	-1.83845700	0.35065200
H	6.01699600	-1.45378500	-0.66862900
H	6.89604000	-1.38679900	0.86877600
H	6.18736100	-2.91950800	0.32522800
H	1.79700100	-4.49405400	0.27329100
H	3.71000100	2.38127800	-0.52092000
C	0.30485400	-2.40882000	-0.15489300
C	-0.78935800	-2.78344500	-0.93271500
C	0.09636700	-2.01361600	1.16628200
C	-2.07084700	-2.78829000	-0.39305900
H	-0.63690000	-3.06913400	-1.96869400
C	-1.18885500	-1.99464900	1.69954500
H	0.94076900	-1.71867300	1.78045000
C	-2.27445000	-2.38640800	0.92301700
H	-2.91444400	-3.07707400	-1.00936900
H	-1.34205500	-1.67018000	2.72232800
H	-3.27578000	-2.36438100	1.33732400
C	2.45219200	2.35968900	1.77225100
C	2.02770000	3.66674700	2.00027200
C	1.49701400	1.35922600	1.60026700
C	0.66999500	3.96927400	2.05359400
H	2.76264100	4.45320400	2.14083400
C	0.14122500	1.65631100	1.66587700
H	1.81750700	0.34070200	1.41669300
C	-0.27693700	2.96413000	1.88936800
H	0.35309600	4.99062800	2.22924600

H	-0.58199900	0.86219700	1.52016600
H	-1.33441100	3.19760500	1.93018900
C	0.97414600	0.77289600	-1.79691500
C	0.57082600	2.19673300	-2.18666900
O	0.45211300	-0.15861600	-2.73048500
C	0.98236100	-0.07559900	-4.05657700
H	0.74428200	-1.01974100	-4.54267900
H	2.06248400	0.06306200	-4.01852300
H	0.52140700	0.74725800	-4.60777500
F	0.71542100	3.03024800	-1.15731100
F	1.32111900	2.67175400	-3.19365100
F	-0.70361400	2.24717200	-2.59320300
O	2.34327500	0.76024100	-1.72380900
H	2.60900400	0.05568200	-1.09247600
H	0.47739500	0.52561300	-0.85567900
C	-8.12439700	-1.00673400	0.26067900
C	-6.80349400	-0.86358700	-0.14031400
C	-5.93407000	-0.04008500	0.58051400
C	-6.40356500	0.62197000	1.71773100
C	-7.72730700	0.47945300	2.11369100
C	-8.59067100	-0.33261000	1.38602700
H	-8.78935600	-1.65152800	-0.30082000
H	-6.44426400	-1.41101400	-1.00295700
H	-5.72451300	1.24936400	2.28005400
H	-8.08466900	1.00287900	2.99212400
H	-9.62217700	-0.44581300	1.69724100
C	-4.52386700	0.13931600	0.17203500
O	-3.73545100	0.58064800	1.14910400
C	-4.05972800	-0.11704400	-1.07993100
H	-2.83152300	0.67954400	0.75623100
H	-4.71568200	-0.44722000	-1.86923400
C	-2.64830900	0.04266200	-1.36909800
O	-1.83405200	0.48897500	-0.55969700
O	-2.28157200	-0.34795700	-2.57982600
H	-1.30355200	-0.25728300	-2.64457300

COM3-(*R*)-2

C	-4.77286200	2.33223200	-0.30854200
C	-3.27945900	2.56059000	-0.31817000
O	-2.88520100	3.82331400	-0.07972100
C	-1.07062400	2.34053900	-0.32066800
C	-1.44908100	3.83885900	-0.24092800
H	-0.43265000	2.13138500	-1.18127900
H	-1.22161200	4.37836600	-1.16039400
C	-4.98389600	0.83927400	-0.22530000
O	-4.75718400	0.15347000	-1.36775200
C	-5.22523500	-1.22907800	0.47973100
C	-5.01930000	-1.23156600	-1.06040500
H	-6.16321400	-1.71767900	0.75055500
H	-5.91549900	-1.53212800	-1.60415600
N	-2.37963100	1.68419000	-0.51243100
N	-5.30065100	0.20069100	0.81953500
C	-5.38159200	3.01818900	0.92055000
H	-4.94783700	2.62537100	1.84013500
H	-5.20850800	4.09253400	0.86655600
H	-6.45442000	2.82501100	0.94412000
C	-5.36983500	2.90405300	-1.60634100
H	-4.94071200	2.41662500	-2.48132000
H	-6.44971800	2.74461200	-1.61107900
H	-5.17481900	3.97609700	-1.65651600
H	-1.01694100	4.35170400	0.61569800
H	-4.15851500	-1.81412200	-1.38264500
C	-0.39973400	1.80505600	0.92733000
C	0.89574200	1.29975800	0.86750800
C	-1.07223400	1.82467800	2.15140600
C	1.51461900	0.81290700	2.01736800
H	1.41858300	1.29191800	-0.08294200
C	-0.45401400	1.34700500	3.29970600
H	-2.08693000	2.20988400	2.20646200
C	0.84212900	0.83780700	3.23351100
H	2.51928300	0.41024500	1.95705200
H	-0.98483500	1.36177600	4.24411400
H	1.32153000	0.45879200	4.12816700
C	-4.08692900	-1.91039900	1.21422900
C	-4.15319900	-3.27687000	1.48244400
C	-2.93669900	-1.20676300	1.56551900
C	-3.08006700	-3.93434700	2.07371400
H	-5.04961800	-3.83138300	1.22252900
C	-1.86093000	-1.86290900	2.15705000
H	-2.87843300	-0.14161900	1.37186700
C	-1.92758300	-3.22964400	2.40707000
H	-3.14307700	-4.99771700	2.27252100

H	-0.97012300	-1.29935500	2.41778200
H	-1.08772700	-3.74204700	2.86067000
C	-0.92189200	-1.06751200	-1.23055600
C	-0.86924500	-2.58890100	-1.34117700
O	0.30284000	-0.50392300	-1.65858900
C	0.55793700	-0.48073100	-3.07002700
H	1.34905000	0.25224100	-3.20825300
H	-0.34339100	-0.18524700	-3.60504000
H	0.89441500	-1.45853000	-3.41904900
F	-1.95996100	-3.14478500	-0.81200100
F	-0.78516300	-3.00384100	-2.61264500
F	0.19748100	-3.06829800	-0.68944600
O	-2.01135400	-0.64209700	-1.94216300
H	-2.36405200	0.16150800	-1.49714400
H	-0.98116900	-0.81741400	-0.16709300
C	9.02869000	-1.06623100	0.91697600
C	7.73342600	-0.97122100	0.42827100
C	7.25175300	0.24826300	-0.05580400
C	8.09182400	1.36461100	-0.05841700
C	9.38612800	1.26663300	0.43588900
C	9.85663800	0.05305600	0.92610600
H	9.39599300	-2.01701900	1.28333500
H	7.10637300	-1.85365200	0.40127400
H	7.71949400	2.30402200	-0.44547800
H	10.02849900	2.13877600	0.43677300
H	10.86763700	-0.02357900	1.30780700
C	5.87200100	0.38256100	-0.57073600
O	5.69453000	1.44121200	-1.35428100
C	4.86366000	-0.47592900	-0.25754400
H	4.74528100	1.44484000	-1.62390100
H	5.01899300	-1.30651300	0.41166400
C	3.53769100	-0.26824300	-0.80145800
O	3.24021700	0.66666800	-1.55002100
O	2.64158900	-1.16330300	-0.41648300
H	1.76895100	-0.93664700	-0.81344200

TS1-1

C	0.78341200	3.19524600	-1.08906200
C	-0.02620700	2.77657800	0.11648000
O	-1.36177000	2.86054000	0.01979700
C	-0.60724900	2.03485300	2.10938400
C	-1.87360200	2.27110000	1.24003300
H	-0.58972200	2.69763500	2.97804900
H	-2.58709500	2.96587700	1.67747700
C	2.15345600	2.58420000	-0.88366700
O	3.12449800	3.38656000	-0.52623200
C	3.91421700	1.15271800	-0.62784100
C	4.35696600	2.62036200	-0.44672100
H	4.43292100	0.65773700	-1.44624300
H	5.00376600	2.97546200	-1.24674600
N	0.49414700	2.40002300	1.20569900
N	2.49647100	1.34756800	-1.02500900
C	0.16855800	2.66697800	-2.39040800
H	0.01336200	1.59161600	-2.34335400
H	-0.80669700	3.13318500	-2.53094800
H	0.81126500	2.92821200	-3.23352700
C	0.86861800	4.72998700	-1.11060500
H	1.31641800	5.11379100	-0.19471600
H	1.46071700	5.06406900	-1.96370700
H	-0.14224800	5.12680500	-1.20822700
H	-2.36804200	1.33647600	0.97622200
H	4.80164700	2.81629500	0.52541400
C	-0.43993200	0.60276400	2.57124100
C	-0.57777400	0.25461900	3.91162700
C	-0.13827300	-0.38928300	1.63614900
C	-0.42259000	-1.07095000	4.31324200
H	-0.80437300	1.02109600	4.64569600
C	0.00798100	-1.71227600	2.03078800
H	0.00489200	-0.11587900	0.59515900
C	-0.13182800	-2.05434900	3.37448900
H	-0.52933600	-1.33233700	5.35951400
H	0.23338200	-2.46840600	1.28804300
H	-0.01181600	-3.08479400	3.68710900
C	4.04107700	0.30819300	0.62060400
C	5.03866900	-0.66191300	0.69477700
C	3.15815900	0.48026300	1.68532100
C	5.14147200	-1.46499600	1.82459100
H	5.69415400	-0.82315700	-0.15250800
C	3.25023200	-0.33904700	2.80586900
H	2.36911800	1.22278300	1.62721600
C	4.24136100	-1.31205400	2.87655200
H	5.90825400	-2.22877100	1.87282600

H	2.52808300	-0.22784000	3.60793900
H	4.30773600	-1.95834500	3.74377200
C	2.74009100	-1.87969200	-1.23063000
C	2.14301200	-3.26749500	-1.49139700
O	1.30093800	-0.86070800	-1.78629100
C	1.31174500	-0.75502000	-3.20207400
H	2.28893800	-1.06525700	-3.58574900
H	0.53714500	-1.39038700	-3.64056900
H	1.13437500	0.27841100	-3.51281600
F	1.87233900	-3.49387200	-2.77919100
F	1.01658200	-3.48103500	-0.79447100
F	3.02319000	-4.20235100	-1.09843000
O	3.74070300	-1.56616600	-1.87481900
H	1.87880600	0.48275100	-1.29981200
H	2.58088600	-1.58531900	-0.17782800
C	-7.31711200	-1.80518100	0.66670500
C	-5.98445300	-1.57042200	0.35867100
C	-5.61800500	-0.42582500	-0.35489100
C	-6.60404400	0.48657600	-0.73822700
C	-7.93748500	0.24604600	-0.43189600
C	-8.29746200	-0.90012900	0.26883800
H	-7.59077400	-2.69197500	1.22522800
H	-5.22644500	-2.26720400	0.69438000
H	-6.31503300	1.37736800	-1.28035700
H	-8.69618400	0.95506200	-0.74035900
H	-9.33716500	-1.08599700	0.51017800
C	-4.20695100	-0.15590300	-0.70861800
O	-3.96286900	1.12417600	-0.99306000
C	-3.24641700	-1.11635700	-0.76083000
H	-3.00176500	1.18485500	-1.23445600
H	-3.47584700	-2.15201200	-0.56846500
C	-1.88490100	-0.76520100	-1.12479400
O	-1.54725500	0.40121700	-1.37278500
O	-1.03108500	-1.75541700	-1.16284700
H	-0.10038400	-1.39760800	-1.38215100

Value of Imaginary Frequency= -134.4 cm^{-1}

TS1-2

C	2.73000800	2.90994100	-0.99708500
C	1.32624600	2.88811800	-0.43200200
O	0.39116900	3.44715200	-1.20560400
C	-0.45445600	2.56428300	0.81679800
C	-0.87489400	3.09555500	-0.57907100
H	-0.62854600	3.31462000	1.59429000
H	-1.49106700	3.99090600	-0.54263700
C	3.54491100	2.14508000	0.00719100
O	4.01685100	2.75831100	1.05238200
C	4.50303800	0.42846900	1.20220200
C	4.69206500	1.79130200	1.90947900
H	5.45879800	-0.01945300	0.93154400
H	5.73204700	2.09918200	1.97923600
N	1.00437900	2.38132100	0.68203900
N	3.83050100	0.88440400	-0.03341500
C	2.73743000	2.20245500	-2.35978000
H	2.28678400	1.20929800	-2.28883300
H	2.13782400	2.78900800	-3.05474500
H	3.75666000	2.13136700	-2.74468500
C	3.23221400	4.35796700	-1.10542200
H	3.22288700	4.85443100	-0.13548500
H	4.24625700	4.37625400	-1.50797900
H	2.57498500	4.89699800	-1.78690500
H	-1.31783100	2.31229600	-1.19460900
H	4.20970500	1.83327700	2.88286900
C	-1.16491300	1.28719400	1.20104400
C	-2.33166700	1.33840300	1.96182900
C	-0.70501100	0.05519400	0.74041800
C	-3.03277200	0.17258700	2.25403400
H	-2.69958600	2.29555800	2.31865000
C	-1.39833500	-1.11240500	1.03745300
H	0.18457600	0.02176300	0.12089700
C	-2.56388800	-1.05424400	1.79562400
H	-3.95392100	0.22382900	2.82331600
H	-1.04988300	-2.05852800	0.64113900
H	-3.12211100	-1.95991800	2.00104500
C	3.64556100	-0.57390300	1.93720700
C	4.08033500	-1.88926100	2.07692900
C	2.38089100	-0.20310800	2.39697300
C	3.24919000	-2.83753200	2.66320200
H	5.05327900	-2.18023200	1.69619300
C	1.55394600	-1.15215200	2.98833000
H	2.01289600	0.80808000	2.24315300
C	1.98556200	-2.46961500	3.11630500
H	3.58172600	-3.86420300	2.75231000

H	0.56251400	-0.86623000	3.31830500
H	1.33314900	-3.21120800	3.56095700
C	2.37509100	-1.99072200	-0.68138500
C	1.73582300	-3.31415000	-1.10821100
O	1.19784800	-0.70356500	-2.12956900
C	1.51900600	-1.01948700	-3.47179600
H	1.49125000	-0.12338900	-4.10189700
H	2.52893300	-1.43661200	-3.49749100
H	0.81777600	-1.75496000	-3.87663100
F	2.14719700	-4.25644000	-0.23762200
F	2.12000400	-3.69022100	-2.32224100
F	0.41390000	-3.27141000	-1.05943700
O	3.48856000	-1.70616900	-1.04552500
H	3.53430100	0.20750700	-0.74350700
H	1.82123700	-1.46330200	0.10842500
C	-6.95480000	1.63409400	0.35828900
C	-5.85885400	1.19508800	-0.37220200
C	-5.39381000	-0.11573700	-0.23565700
C	-6.06455700	-0.98255300	0.63030300
C	-7.16016200	-0.54133100	1.36382300
C	-7.60672200	0.76941300	1.23433600
H	-7.30766700	2.65169600	0.23821400
H	-5.37226400	1.87100100	-1.06470600
H	-5.71105600	-2.00150400	0.72050000
H	-7.66763000	-1.22371800	2.03574600
H	-8.46238500	1.11376000	1.80307300
C	-4.19131900	-0.60421300	-0.95398400
O	-4.05301300	-1.92828500	-0.95491300
C	-3.25374300	0.21027800	-1.49758300
H	-3.14796700	-2.06629700	-1.42693300
H	-3.35031500	1.28394800	-1.44542100
C	-1.99420900	-0.36267800	-2.01829500
O	-1.89061600	-1.62067500	-2.07855200
O	-1.05270300	0.43080900	-2.31838100
H	0.25257000	-0.30726000	-2.15852200

Value of Imaginary Frequency= -44.5 cm^{-1}

TS1-3

C	-4.94208900	-1.51684400	-0.12575800
C	-3.75481100	-1.76046300	0.76658700
O	-3.73335400	-2.86768900	1.46832300
C	-1.68388100	-1.71184600	1.72934300
C	-2.55530100	-2.83027800	2.33252600
H	-1.30383100	-1.01502500	2.47589300
H	-2.90896600	-2.60281100	3.33698200
C	-4.57473300	-0.35589500	-1.01953700
O	-4.68488300	0.85949400	-0.44957100
C	-3.63656800	0.89657700	-2.55072200
C	-4.28660600	1.80155100	-1.47163200
H	-4.00891400	1.14857800	-3.54545400
H	-5.18928800	2.29770300	-1.83034000
N	-2.70923800	-1.02174800	0.91366500
N	-4.09014900	-0.45566500	-2.18161900
C	-5.17820000	-2.78288800	-0.96349900
H	-4.30728800	-3.01401200	-1.57650800
H	-5.40610600	-3.62448400	-0.31033100
H	-6.02228400	-2.60413300	-1.62943100
C	-6.16246400	-1.19786000	0.75615800
H	-5.99272900	-0.30476600	1.35621000
H	-7.02442600	-1.02416700	0.11055500
H	-6.37828600	-2.04428200	1.40882800
H	-2.09016600	-3.81087300	2.29391700
H	-3.60076900	2.51311000	-1.01892000
C	-0.55175100	-2.20476700	0.85648600
C	0.75295500	-1.81838300	1.13368000
C	-0.80916700	-3.07192100	-0.21089400
C	1.80317700	-2.30192100	0.35393100
H	0.95013300	-1.12409500	1.94304400
C	0.23517900	-3.54835600	-0.98874900
H	-1.82742500	-3.37805300	-0.43876100
C	1.54670300	-3.16568900	-0.70097400
H	2.81782900	-1.99075900	0.57335000
H	0.03161200	-4.21461900	-1.81823900
H	2.36370600	-3.53051100	-1.31174100
C	-2.11719300	0.97570800	-2.55416800
C	-1.51317800	2.19427400	-2.86134800
C	-1.31195400	-0.11266800	-2.22038900
C	-0.12966000	2.32649600	-2.82914100
H	-2.12854000	3.05230200	-3.11600300
C	0.07392400	0.02065000	-2.17894100
H	-1.76775500	-1.06712800	-1.98822400
C	0.66867900	1.24010300	-2.48569700
H	0.32448000	3.28331600	-3.05673500

H	0.68816300	-0.82307100	-1.88319100
H	1.74501100	1.34937600	-2.43768300
C	-0.91491100	1.78894600	0.61440700
C	-0.54974100	3.24918000	0.90777800
O	-0.23184900	1.09397600	2.47901600
C	-0.75411900	1.66551900	3.66168300
H	-0.61740600	0.98929600	4.51185100
H	-1.82311800	1.83915600	3.51469300
H	-0.27497500	2.62217900	3.89040100
F	-0.66384000	3.95334100	-0.23210900
F	-1.39394500	3.79378200	1.78919100
F	0.68714200	3.41076900	1.35972200
O	-2.10628700	1.51934800	0.57174600
H	-2.54297200	-0.04043900	0.55139900
H	-0.10547200	1.17663800	0.20427900
C	8.18045600	-1.09194500	0.46712900
C	6.87090000	-0.72882600	0.74956000
C	6.00670400	-0.33868800	-0.27780500
C	6.47620600	-0.33697700	-1.59344200
C	7.78835000	-0.69927900	-1.87407700
C	8.64507700	-1.07571800	-0.84558600
H	8.83891500	-1.39551200	1.27225400
H	6.51534700	-0.76493000	1.77183000
H	5.80116800	-0.04575100	-2.38741500
H	8.14196700	-0.68747400	-2.89827600
H	9.66753300	-1.36014500	-1.06405400
C	4.60498900	0.06665800	-0.01115200
O	3.82275400	0.07477100	-1.09152500
C	4.12818900	0.40766800	1.21332100
H	2.92076400	0.40578100	-0.72105200
H	4.75975200	0.41940100	2.08794300
C	2.70655600	0.76729900	1.38112500
O	1.98861000	0.84685000	0.33511400
O	2.25812700	0.93763000	2.54755200
H	0.81057200	1.07952800	2.50690600

Value of Imaginary Frequency= -100.3 cm^{-1}

TS1-4

C	-4.86258300	-1.85218800	-0.25710500
C	-3.68181500	-1.99785900	0.66507900
O	-3.56180300	-3.10538000	1.35399500
C	-1.65478200	-1.74145900	1.68643800
C	-2.42739300	-2.94443800	2.26492300
H	-1.36150900	-1.01486500	2.44432400
H	-2.84358000	-2.75290900	3.25279100
C	-4.57343200	-0.65048600	-1.12892900
O	-4.88298900	0.54134600	-0.58473900
C	-3.66557700	0.71081700	-2.58639200
C	-4.51332200	1.52644800	-1.57583200
H	-3.98174100	0.91445000	-3.61124800
H	-5.43375400	1.90983700	-2.01756000
N	-2.72367600	-1.15605800	0.85004600
N	-3.97862400	-0.68788000	-2.24300800
C	-4.96336200	-3.12279300	-1.11534700
H	-4.06695500	-3.25855900	-1.71974200
H	-5.11604200	-3.99245300	-0.47708300
H	-5.81414200	-3.01779300	-1.78868000
C	-6.12844800	-1.65628500	0.59565200
H	-6.05480800	-0.76124700	1.21204100
H	-6.98593300	-1.54998000	-0.06993000
H	-6.28336100	-2.52884800	1.23086200
H	-1.86166100	-3.87092200	2.24853000
H	-3.96629800	2.31912300	-1.07090100
C	-0.45711100	-2.13482100	0.85024800
C	0.81591200	-1.74541400	1.24964500
C	-0.61429900	-2.94963700	-0.27480500
C	1.93326000	-2.19028500	0.54432200
H	0.95258700	-1.08600300	2.09943200
C	0.49724000	-3.37181100	-0.99044800
H	-1.60439600	-3.25876200	-0.60037900
C	1.77527500	-2.99831900	-0.57380800
H	2.92067100	-1.89698600	0.87958700
H	0.36991800	-3.99499200	-1.86736800
H	2.64470500	-3.33426700	-1.12606400
C	-2.16980700	0.97198600	-2.47051700
C	-1.69032800	2.26773000	-2.66919300
C	-1.26455800	-0.03931900	-2.15088000
C	-0.33281800	2.54707600	-2.54565000
H	-2.38194500	3.06859500	-2.91354500
C	0.09391900	0.24100500	-2.01350100
H	-1.62377700	-1.04934200	-2.00270800
C	0.56406400	1.53438100	-2.21517200
H	0.02166700	3.56087000	-2.68936200

H	0.77851600	-0.54810500	-1.71975900
H	1.61150600	1.75842700	-2.06453300
C	-1.41466200	1.94930200	0.60893900
C	-1.26289800	3.42597400	0.97146300
O	-0.20635100	1.27416700	2.20920200
C	0.08626000	1.86897400	3.46386400
H	0.92274500	1.34002200	3.92883300
H	-0.79638700	1.80046600	4.10118700
H	0.35886900	2.92301000	3.35229800
F	-1.89119700	4.15893400	0.03241700
F	-1.83164500	3.71071300	2.14176600
F	0.00528400	3.81802700	1.00393100
O	-2.52358000	1.45766200	0.72229200
H	-2.68529900	-0.14828400	0.54148500
H	-0.60447300	1.52023800	0.01284500
C	8.24220600	-1.54554900	-0.71541400
C	7.12562800	-1.30557800	0.07711200
C	6.24067900	-0.27243000	-0.24018100
C	6.50739700	0.52985500	-1.35363200
C	7.62390500	0.29017600	-2.14242400
C	8.49364400	-0.75126400	-1.82864700
H	8.91856300	-2.35287600	-0.46052500
H	6.92692400	-1.91304200	0.95033400
H	5.85211200	1.35813400	-1.59306900
H	7.82186400	0.92306900	-2.99929300
H	9.36593000	-0.93554600	-2.44443000
C	5.04975000	-0.04963400	0.61514700
O	5.09946000	-0.66939900	1.79577500
C	3.96551600	0.67392100	0.24199400
H	4.22327900	-0.38914000	2.24968400
H	3.90251200	1.13494600	-0.73142500
C	2.80662500	0.80380400	1.14785100
O	2.88261800	0.27854300	2.30188300
O	1.78204000	1.40136900	0.72067900
H	0.66815500	1.28449300	1.64958000

Value of Imaginary Frequency= -96.3 cm^{-1}

IM1-1

C	0.48462200	3.30667500	-1.00607000
C	-0.25334900	2.75707700	0.19221300
O	-1.60182200	2.77551700	0.12948000
C	-0.76742600	1.95061200	2.18056700
C	-2.05621100	2.11774400	1.33209500
H	-0.76427600	2.63111000	3.03656400
H	-2.81646300	2.74194800	1.79677100
C	1.91997600	2.83708900	-0.87547600
O	2.80728600	3.74489400	-0.44316200
C	3.77706000	1.62287600	-0.78950800
C	4.09615200	3.09974500	-0.43862100
H	4.34296500	1.29446000	-1.66427100
H	4.71840100	3.58920200	-1.18749500
N	0.30098600	2.35434700	1.25615900
N	2.34284200	1.66572800	-1.13269800
C	-0.11032500	2.77418800	-2.31586700
H	-0.08382500	1.68755400	-2.33797400
H	-1.14977600	3.09362800	-2.39966500
H	0.45402200	3.17779800	-3.15901700
C	0.38806100	4.84076900	-0.95794900
H	0.81082200	5.23117300	-0.03274400
H	0.92817800	5.27592500	-1.80028700
H	-0.66114200	5.13138100	-1.02483700
H	-2.48151600	1.15335600	1.05223500
H	4.53267800	3.21963900	0.55121000
C	-0.55545000	0.53695800	2.67569700
C	-0.74663900	0.20566000	4.01420200
C	-0.18458300	-0.46178300	1.77365100
C	-0.57922100	-1.10818900	4.44601500
H	-1.02481800	0.97805500	4.72386800
C	-0.02494100	-1.77442100	2.19850100
H	-0.00344400	-0.19433300	0.73769800
C	-0.22238700	-2.09981900	3.53895000
H	-0.72834800	-1.35492000	5.49063100
H	0.25384300	-2.53782600	1.48251500
H	-0.09547300	-3.12238100	3.87416600
C	4.05243700	0.66451900	0.35053700
C	5.25498400	-0.03996400	0.39585400
C	3.11548000	0.49051600	1.37000600
C	5.51307700	-0.92088300	1.44106700
H	5.97650800	0.07488500	-0.40566800
C	3.36979500	-0.39914700	2.41054000
H	2.18328400	1.04547600	1.34690500
C	4.56718400	-1.10819600	2.44675400
H	6.44481800	-1.47370600	1.46180500

H	2.62122100	-0.54107400	3.18302000
H	4.76382100	-1.80533100	3.25267300
C	3.39942700	-2.26046100	-1.00755200
C	2.48860300	-3.47294700	-1.24843000
O	1.38118700	-0.88157100	-1.68963300
C	1.46193900	-0.79560100	-3.11276500
H	2.46416400	-1.07301100	-3.45074500
H	0.73811000	-1.49054900	-3.53861300
H	1.23231200	0.21769100	-3.44632100
F	2.09486600	-3.56440300	-2.51437300
F	1.40549000	-3.43380700	-0.46769000
F	3.16083600	-4.59167100	-0.94348000
O	4.18854400	-1.92655100	-1.84010600
H	1.62057100	0.01180100	-1.34503300
H	3.30704900	-1.81180800	-0.00702300
C	-7.36290700	-1.92447700	0.42822200
C	-6.01366300	-1.69190900	0.20166700
C	-5.60325800	-0.55087800	-0.49340500
C	-6.56290400	0.36022700	-0.94150200
C	-7.91275400	0.12135500	-0.71720900
C	-8.31599700	-1.02110900	-0.03422500
H	-7.67104700	-2.80794900	0.97384100
H	-5.27867500	-2.38708400	0.58802100
H	-6.24087400	1.24892600	-1.46818000
H	-8.65045500	0.82923300	-1.07509200
H	-9.36871500	-1.20505500	0.14374800
C	-4.17275400	-0.28229600	-0.75892200
O	-3.91435200	0.99598400	-1.03022700
C	-3.21351400	-1.24697300	-0.74824800
H	-2.94325500	1.07619300	-1.20047200
H	-3.46015600	-2.28095500	-0.56928900
C	-1.83565200	-0.90367300	-1.03608000
O	-1.46328700	0.25155000	-1.26069700
O	-0.98719800	-1.91479800	-1.03754200
H	-0.08007900	-1.55494400	-1.23044000

IM1-2

C	2.29656000	3.16916600	-0.95632800
C	1.04257800	2.99607000	-0.13480400
O	0.02515800	3.79989200	-0.51552500
C	-0.49607200	2.45803900	1.33761800
C	-1.11539300	3.36968500	0.24993400
H	-0.40113100	3.00733900	2.28142500
H	-1.61986000	4.25098900	0.64059500
C	3.36118900	2.26557200	-0.37772600
O	4.17251100	2.82715800	0.53339300
C	4.64727900	0.54792200	0.18571200
C	5.16968400	1.84040000	0.86120100
H	5.41409800	0.09177300	-0.44207500
H	6.12110700	2.17670900	0.44845800
N	0.86561900	2.20899200	0.84000600
N	3.55273600	1.04415600	-0.67313100
C	1.98787100	2.77530100	-2.40904100
H	1.60150500	1.76001400	-2.46414200
H	1.23499900	3.45215300	-2.81216500
H	2.89432300	2.84305600	-3.01279100
C	2.74237200	4.64015700	-0.89309200
H	2.93054900	4.95201100	0.13366500
H	3.65982200	4.77191300	-1.46934700
H	1.96211800	5.26843100	-1.32126900
H	-1.77133800	2.81000000	-0.41566900
H	5.23368100	1.76523600	1.94474900
C	-1.31298300	1.21360200	1.60177500
C	-2.61691500	1.37136400	2.07948900
C	-0.82724700	-0.06980800	1.36567900
C	-3.42891500	0.26775100	2.30626300
H	-3.00164300	2.36941900	2.27054700
C	-1.63883800	-1.17803000	1.60279200
H	0.17579000	-0.20106500	0.97317700
C	-2.93763100	-1.01298700	2.06957600
H	-4.44747100	0.40509600	2.65231700
H	-1.25837000	-2.17074200	1.40005400
H	-3.57083300	-1.87705900	2.23464000
C	4.15088900	-0.47877400	1.18014800
C	4.87166000	-1.64994700	1.39976000
C	2.97252000	-0.24959900	1.89606700
C	4.41889200	-2.59266200	2.31904000
H	5.77585900	-1.83872600	0.83147500
C	2.51959800	-1.19398400	2.81210900
H	2.39201600	0.65110000	1.71342700
C	3.24033500	-2.36791000	3.02372900
H	4.97928600	-3.50687000	2.47387800

H	1.59479200	-1.01743000	3.34948600
H	2.88190500	-3.10585500	3.73137400
C	2.53972500	-2.78339500	-0.58408300
C	1.22997100	-3.52598500	-0.87969500
O	1.55508800	-0.60344100	-1.69784300
C	1.78076800	-0.91078900	-3.07389800
H	2.08063900	-0.01984000	-3.63240100
H	2.55255600	-1.67677700	-3.17620100
H	0.84201400	-1.29463100	-3.47115600
F	1.35723300	-4.80235100	-0.48016700
F	0.92264700	-3.53417300	-2.16957300
F	0.22555500	-2.98966900	-0.18937300
O	3.49230100	-2.90725400	-1.29459000
H	2.30870800	-0.06449300	-1.35696200
H	2.52147200	-2.20753200	0.35014200
C	-7.03358600	1.40245300	0.01752400
C	-5.82304400	1.05116200	-0.56373900
C	-5.33448700	-0.25192100	-0.44129100
C	-6.08763600	-1.20155900	0.25277100
C	-7.29680700	-0.84602100	0.83788100
C	-7.77066900	0.45697500	0.72609700
H	-7.40703100	2.41384300	-0.08826500
H	-5.26729900	1.78864200	-1.12979000
H	-5.71019000	-2.21253200	0.33495900
H	-7.86990900	-1.58781600	1.38098300
H	-8.71436500	0.73386300	1.18060500
C	-4.01654400	-0.64124500	-0.98868700
O	-3.85163100	-1.95498000	-1.11284500
C	-3.03127600	0.25207800	-1.26419100
H	-2.92195500	-2.09429500	-1.42276400
H	-3.17397800	1.30256900	-1.07546400
C	-1.71027500	-0.22802000	-1.62092300
O	-1.45586800	-1.40834900	-1.85309200
O	-0.75968100	0.70063600	-1.63800900
H	0.11626800	0.22553200	-1.64951900

IM1-3

C	-4.96004800	-1.53912300	-0.08372800
C	-3.78266200	-1.69809800	0.83923300
O	-3.76508900	-2.72435800	1.65044700
C	-1.70721200	-1.55444200	1.79582200
C	-2.58331800	-2.60493700	2.50652800
H	-1.32695400	-0.78421100	2.46962200
H	-2.93655500	-2.27742300	3.48283600
C	-4.60384500	-0.42920900	-1.04408900
O	-4.69832000	0.81500300	-0.53172000
C	-3.68915900	0.74802100	-2.64653300
C	-4.34869200	1.70193800	-1.61870400
H	-4.05360900	0.94666900	-3.65571100
H	-5.27332300	2.14421400	-1.99255800
N	-2.73343600	-0.95241400	0.91502600
N	-4.13951400	-0.58565500	-2.20814200
C	-5.15454600	-2.86202800	-0.84022300
H	-4.27334400	-3.10690700	-1.43293900
H	-5.36467100	-3.66632600	-0.13589400
H	-5.99838000	-2.74929000	-1.52084800
C	-6.20149100	-1.18983800	0.75629300
H	-6.05763400	-0.25992300	1.30502800
H	-7.05339400	-1.07028400	0.08566000
H	-6.41527200	-1.99947800	1.45442100
H	-2.12264200	-3.58659700	2.56394600
H	-3.67981200	2.46323500	-1.22588400
C	-0.57866100	-2.13214600	0.97211100
C	0.73015800	-1.75762200	1.24497700
C	-0.84128100	-3.05726100	-0.04438100
C	1.77935600	-2.30363400	0.50593100
H	0.93416800	-1.02566600	2.01899300
C	0.20218700	-3.59667000	-0.78089900
H	-1.86180300	-3.35935600	-0.26701700
C	1.51746000	-3.21975100	-0.50212000
H	2.79726400	-1.99798000	0.71859700
H	-0.00481800	-4.30655700	-1.57248600
H	2.33345700	-3.63164300	-1.08352100
C	-2.17019400	0.83924100	-2.62991900
C	-1.57451800	2.05254300	-2.97283800
C	-1.36053400	-0.22095000	-2.22352600
C	-0.19614300	2.21139400	-2.89273700
H	-2.19373700	2.88714400	-3.28860100
C	0.02023700	-0.06092500	-2.13365000
H	-1.80861900	-1.17325100	-1.96734700
C	0.60573900	1.15649100	-2.46666500
H	0.25165400	3.16445900	-3.14690300

H	0.63768600	-0.88003400	-1.77964400
H	1.67677700	1.28860700	-2.37748900
C	-0.85632400	1.84959400	0.47264400
C	-0.48275400	3.30637500	0.77947000
O	-0.23623400	1.22607600	2.67999500
C	-0.48245100	2.00374500	3.83580900
H	-0.17570800	1.47372600	4.74390400
H	-1.55268400	2.21043500	3.89290800
H	0.05111400	2.95859300	3.79284100
F	-0.54263600	4.01771400	-0.35956300
F	-1.35117400	3.85522100	1.63253100
F	0.73901700	3.43988000	1.27713800
O	-2.03330300	1.59416700	0.35406600
H	-2.56683300	-0.04456000	0.43398700
H	-0.01836200	1.17049600	0.27461300
C	8.19164300	-1.12418700	0.37971300
C	6.88764400	-0.75608200	0.68091100
C	6.00179200	-0.38926700	-0.33664900
C	6.44439300	-0.41654800	-1.66123300
C	7.75099400	-0.78396100	-1.96087500
C	8.62935300	-1.13670500	-0.94226400
H	8.86692000	-1.40909800	1.17774200
H	6.55314100	-0.76969600	1.71081100
H	5.75249200	-0.14344700	-2.44711900
H	8.08331200	-0.79458200	-2.99222100
H	9.64753200	-1.42493400	-1.17529900
C	4.60579900	0.02278700	-0.05014500
O	3.79943100	0.00380800	-1.11336400
C	4.15668700	0.39680300	1.17445200
H	2.90736700	0.34889000	-0.72740900
H	4.80786100	0.42856400	2.03418800
C	2.73700900	0.76158600	1.37035200
O	2.00147400	0.82399900	0.32932900
O	2.31371000	0.94756200	2.53678600
H	0.76814600	1.13450400	2.58692200

IM1-4

C	-4.77408100	-1.91972500	-0.26504100
C	-3.64606400	-1.93643900	0.73078700
O	-3.55771700	-2.94114800	1.56245800
C	-1.65808500	-1.54240700	1.79462700
C	-2.46016000	-2.65945000	2.49243800
H	-1.38708400	-0.72323100	2.46288300
H	-2.91816500	-2.33877700	3.42672600
C	-4.47729600	-0.78761300	-1.22250800
O	-4.81391200	0.43909900	-0.77733800
C	-3.55383100	0.47522900	-2.75640400
C	-4.45460600	1.34613300	-1.84407000
H	-3.83201700	0.59291600	-3.80520300
H	-5.37665200	1.65309400	-2.33933500
N	-2.69518300	-1.07328600	0.85114600
N	-3.85432500	-0.89962900	-2.31587700
C	-4.77187800	-3.26513000	-1.00820300
H	-3.83776600	-3.41144900	-1.54990700
H	-4.92431700	-4.08075300	-0.30203800
H	-5.58600200	-3.26043800	-1.73300800
C	-6.09682000	-1.70250700	0.49048700
H	-6.09171700	-0.75699400	1.03121300
H	-6.91350800	-1.68497700	-0.23219300
H	-6.26268100	-2.52393500	1.18784800
H	-1.89924600	-3.57977200	2.62219100
H	-3.94907300	2.20057900	-1.40068500
C	-0.43610400	-2.03830400	1.05337500
C	0.82630100	-1.64632500	1.48367700
C	-0.56099800	-2.93700500	-0.01011900
C	1.96382300	-2.16483800	0.86644700
H	0.93753800	-0.92470900	2.28547600
C	0.57195400	-3.43400700	-0.63895000
H	-1.54145500	-3.25176400	-0.35809900
C	1.83776300	-3.05172000	-0.19465300
H	2.94171600	-1.86163200	1.22023300
H	0.47027400	-4.12087900	-1.47047400
H	2.72338500	-3.44235300	-0.68138000
C	-2.07059500	0.78136200	-2.59632600
C	-1.61543700	2.07117800	-2.87153900
C	-1.15891400	-0.17417900	-2.14785200
C	-0.27617200	2.40196700	-2.69158200
H	-2.31292600	2.82829500	-3.21763700
C	0.18092200	0.15773300	-1.95510400
H	-1.49788700	-1.18164600	-1.94346800
C	0.62559900	1.44661100	-2.22992600
H	0.05983100	3.41157700	-2.89613300

H	0.86860400	-0.58428400	-1.56088600
H	1.65539100	1.71605900	-2.03781100
C	-1.34698500	2.05496700	0.44747500
C	-1.21142800	3.52997900	0.83721800
O	-0.27164900	1.38756700	2.46579700
C	0.07055900	2.07596200	3.65600500
H	0.97215900	1.64411000	4.09975800
H	-0.75915600	1.98884500	4.35923200
H	0.25163300	3.13879800	3.46373200
F	-1.69321900	4.27906100	-0.17191000
F	-1.92482300	3.81686300	1.92374000
F	0.04815200	3.88943800	1.04342400
O	-2.45682200	1.57912500	0.43258200
H	-2.63467700	-0.14924300	0.38359400
H	-0.43898000	1.55673500	0.09253300
C	8.03227300	-1.62663000	-0.81448900
C	6.97203000	-1.31026300	0.02712800
C	6.06603900	-0.30580300	-0.32165700
C	6.25573700	0.39127700	-1.51856100
C	7.31630700	0.07582900	-2.35636600
C	8.20668400	-0.93731700	-2.00942200
H	8.72562800	-2.41072000	-0.53389700
H	6.83408400	-1.83445200	0.96382100
H	5.58459200	1.19783900	-1.78665900
H	7.45493000	0.62800100	-3.27827800
H	9.03557000	-1.18044200	-2.66356400
C	4.93534000	-0.00188400	0.58899800
O	5.06905400	-0.50386700	1.81735700
C	3.82170900	0.67957700	0.22265400
H	4.21416700	-0.18097300	2.29725900
H	3.69098700	1.04260700	-0.78503800
C	2.72170200	0.88702000	1.18855000
O	2.88712600	0.46569900	2.37836100
O	1.66263200	1.43158800	0.78601700
H	0.55696900	1.36191800	1.89056600

TSa

C	3.07964500	0.68912200	-0.58123500
C	2.70159200	0.11890300	0.75645900
O	3.09035500	0.71295700	1.85403300
C	1.63812600	-1.09506800	2.37780600
C	2.58176700	-0.03892600	2.99377200
H	1.89618800	-2.10244700	2.70330600
H	3.44295100	-0.47692000	3.49371000
C	1.88717200	1.52887100	-0.98951300
O	1.75685200	1.73883600	-2.30669600
C	0.13422100	2.84959700	-1.01920600
C	0.46438300	2.36754500	-2.45106000
H	0.37982300	3.91014900	-0.89924700
H	0.55341000	3.17188500	-3.17751100
N	1.99485400	-0.94110600	0.95452700
N	1.08382800	2.08033300	-0.18324700
C	4.30860500	1.60259500	-0.44952800
H	4.13954200	2.38626300	0.28814600
H	5.18558700	1.02000100	-0.16143000
H	4.49976100	2.06183300	-1.41973000
C	3.32285000	-0.44053200	-1.59290100
H	2.38674800	-0.96359100	-1.79757600
H	3.67734800	0.00224100	-2.52323100
H	4.08676700	-1.12368200	-1.21549300
H	2.07182000	0.66385100	3.64732000
H	-0.22553900	1.59889100	-2.79849900
C	0.16138600	-0.84221800	2.56570300
C	-0.69089900	-1.88848800	2.90264000
C	-0.35721800	0.42942000	2.31650700
C	-2.06078900	-1.66444900	2.99909700
H	-0.28865500	-2.88253800	3.06305200
C	-1.72381700	0.65114200	2.41404200
H	0.29158000	1.23626300	1.98760600
C	-2.57615000	-0.39597300	2.75518800
H	-2.72394300	-2.48316900	3.25024400
H	-2.12490300	1.63389300	2.19310900
H	-3.64449100	-0.22373100	2.81468500
C	-1.30733700	2.64479600	-0.60900900
C	-2.01769000	3.67250200	0.00901400
C	-1.93955500	1.42290300	-0.84441100
C	-3.34885100	3.49024700	0.37727600
H	-1.53052000	4.62395500	0.19733800
C	-3.27047500	1.24352500	-0.48566900
H	-1.37205400	0.61443600	-1.29631200
C	-3.97938100	2.27622400	0.12335500
H	-3.89313200	4.29849500	0.85183000

H	-3.74651900	0.28944100	-0.67856100
H	-5.01826100	2.13601700	0.39917600
C	-0.47885900	-1.67453100	-0.85313600
C	-1.57780600	-2.38128600	-1.66967200
O	0.33786500	-2.74080800	-0.21091200
C	1.01879000	-3.58788000	-1.12629300
H	1.90177900	-3.98429700	-0.62063500
H	1.32280500	-3.02820900	-2.01434500
H	0.37972700	-4.42265300	-1.42788800
F	-2.56000400	-1.50514400	-1.96671400
F	-1.14338800	-2.87800500	-2.83661900
F	-2.16186500	-3.39698300	-1.00646100
O	0.22843500	-0.83881000	-1.55584700
H	1.47596600	-1.48514000	0.23345200
H	-1.01354200	-1.27029900	0.03668400

Value of Imaginary Frequency = -92.5 cm^{-1}

TSb

C	2.78519000	-1.71930900	-0.31717000
C	2.95449200	-0.24126800	-0.59301400
O	3.33037300	0.07762200	-1.84501700
C	2.83899000	1.95159500	-0.49920100
C	3.46056300	1.51823400	-1.85244400
H	3.50051800	2.63433200	0.03527000
H	4.52194700	1.75740200	-1.92219200
C	1.83171300	-1.78278100	0.84937400
O	2.30547500	-1.84005900	2.06367900
C	-0.07516100	-1.67247200	2.11899700
C	1.17968700	-1.89733800	2.99384500
H	-0.80649500	-2.47153900	2.20166700
H	1.20802800	-2.88068800	3.45841900
N	2.73165600	0.68038000	0.24245500
N	0.54568100	-1.76481800	0.77725700
C	2.16113400	-2.40005600	-1.54331100
H	1.27040600	-1.86507300	-1.87514600
H	2.88547500	-2.39491000	-2.35632800
H	1.89635900	-3.43203200	-1.30687700
C	4.14060100	-2.34194600	0.04622300
H	4.56401400	-1.86933700	0.93160600
H	4.02716400	-3.41144500	0.23082100
H	4.82183800	-2.20403500	-0.79392500
H	2.92590300	1.90108100	-2.71899600
H	1.33347600	-1.11538000	3.73255000
C	1.46600100	2.58009000	-0.62741900
C	1.26372100	3.91234500	-0.27825800
C	0.38988600	1.82908500	-1.10737900
C	0.00356100	4.49252600	-0.40679100
H	2.09425100	4.49975400	0.09999100
C	-0.86519700	2.40735300	-1.24270700
H	0.51046100	0.78053300	-1.36996100
C	-1.06109000	3.74062900	-0.88881900
H	-0.14319600	5.52950600	-0.12813100
H	-1.68872600	1.81115700	-1.61710000
H	-2.04305500	4.18782600	-0.98671200
C	-0.75091800	-0.33489100	2.31555400
C	-2.12035600	-0.27814800	2.55934600
C	-0.01146300	0.84278700	2.20605000
C	-2.74801800	0.95575200	2.68801100
H	-2.69544500	-1.19489100	2.56366500
C	-0.64371300	2.07491700	2.32608900
H	1.05035200	0.80491900	1.97864200
C	-2.01252100	2.13136800	2.56788200
H	-3.81741600	0.99815900	2.85543100

H	-0.07162400	2.98697200	2.20191500
H	-2.50879500	3.09169600	2.64665700
C	-2.09319600	-1.11867700	-0.53727500
C	-3.39431900	-0.76368700	-1.28346600
O	-1.03037200	-1.34145400	-1.58565900
C	-1.29965900	-2.48124300	-2.38981100
H	-0.36423000	-2.82183100	-2.83634000
H	-1.72653500	-3.27568700	-1.77271500
H	-1.99621600	-2.22986700	-3.19486600
F	-4.24527100	-0.14793000	-0.44384400
F	-4.03886100	-1.83030800	-1.77580100
F	-3.20467800	0.08393400	-2.32045000
O	-2.22218300	-2.11215300	0.27389400
H	-0.01826800	-1.73196000	-0.09426800
H	-1.73814800	-0.14568700	-0.12122500

Value of Imaginary Frequency = -44.3 cm^{-1}

(*R*)-TMH•*β*-CA$_1$

C	-6.10494400	1.09887400	0.53992300
C	-4.72062100	1.00461100	0.54289700
C	-4.09342700	-0.14555700	0.05568100
C	-4.87264200	-1.20413900	-0.41819200
C	-6.25776200	-1.10345000	-0.42428900
C	-6.87633500	0.04741900	0.05231000
H	-6.58326400	1.99051200	0.92610700
H	-4.13100200	1.81745800	0.94807000
H	-4.38413300	-2.09765200	-0.78398600
H	-6.85455700	-1.92525000	-0.80052000
H	-7.95697100	0.12375300	0.05062400
C	-2.62069800	-0.26949800	0.03307600
O	-2.19399800	-1.52348900	-0.05774200
C	-1.77669300	0.79876100	0.07629300
H	-1.21223800	-1.50198900	-0.08483900
H	-2.15385300	1.80764500	0.10941700
C	-0.34702100	0.61137700	0.04407200
O	0.19646200	-0.50169800	-0.03475200
O	0.35633600	1.72548000	0.10938000
H	1.32063300	1.51768200	0.08336700
C	3.23692900	-0.20094300	0.20819800
C	4.73244900	-0.46173300	0.38327600
O	2.98468100	1.15269500	-0.09309700
C	3.52422300	1.63335300	-1.33212200
H	2.96522000	2.53334200	-1.57917600
H	3.39738700	0.88658900	-2.11544000
H	4.57993100	1.87912500	-1.21052900
F	4.92746600	-1.63174700	0.99411900
F	5.38209200	-0.49824500	-0.78377600
F	5.29423500	0.49315400	1.13002300
O	2.78875600	-1.06778100	-0.75846900
H	1.82000800	-1.07534500	-0.67563300
H	2.76004100	-0.36042100	1.17993100

TSc

C	-5.91832500	1.21454900	0.77946500
C	-4.54963200	0.99625500	0.70953400
C	-4.05011700	-0.13585700	0.05970600
C	-4.94214300	-1.05336100	-0.50150200
C	-6.31096200	-0.82818000	-0.43424900
C	-6.80194200	0.30585900	0.20386700
H	-6.29657000	2.09039700	1.29215600
H	-3.87210100	1.69454800	1.18486400
H	-4.55373600	-1.93586900	-0.99256900
H	-6.99490600	-1.54026200	-0.87959700
H	-7.86997500	0.47846300	0.25975100
C	-2.59542600	-0.38918300	-0.04244100
O	-2.30801700	-1.67324200	-0.24609300
C	-1.67027500	0.60369100	0.03846300
H	-1.34189600	-1.76594900	-0.33234900
H	-1.98874300	1.62688900	0.15688400
C	-0.23721000	0.40695900	-0.04991900
O	0.16481900	-0.83813500	-0.23014500
O	0.54766200	1.35610000	0.04453700
H	2.06617700	1.47564100	-0.06659100
C	3.18270300	-0.28139900	0.35747500
C	4.70401400	-0.37903700	0.46168400
O	3.06480200	1.40098500	-0.21656300
C	3.27266800	1.54170000	-1.63295500
H	2.62075100	2.33513800	-1.99466900
H	3.03232100	0.60036200	-2.13123100
H	4.31455900	1.80326800	-1.79414900
F	5.02305200	-1.54988200	1.02075400
F	5.28385400	-0.32358000	-0.73787500
F	5.21777400	0.58879700	1.21966400
O	2.62270800	-1.03663500	-0.46511200
H	1.20620800	-0.94257700	-0.33902800
H	2.71989500	-0.04264600	1.32588900

Value of Imaginary Frequency= -189.1 cm^{-1}

(*S*)-TMH•*β*-CA$_1$

C	-6.10494400	1.09887400	-0.53992300
C	-4.72062100	1.00461100	-0.54289700
C	-4.09342700	-0.14555700	-0.05568100
C	-4.87264200	-1.20413900	0.41819200
C	-6.25776200	-1.10345000	0.42428900
C	-6.87633500	0.04741900	-0.05231000
H	-6.58326400	1.99051200	-0.92610700
H	-4.13100200	1.81745800	-0.94807000
H	-4.38413300	-2.09765200	0.78398600
H	-6.85455700	-1.92525000	0.80052000
H	-7.95697100	0.12375300	-0.05062400
C	-2.62069800	-0.26949800	-0.03307600
O	-2.19399800	-1.52348900	0.05774200
C	-1.77669300	0.79876100	-0.07629300
H	-1.21223800	-1.50198900	0.08483900
H	-2.15385300	1.80764500	-0.10941700
C	-0.34702100	0.61137700	-0.04407200
O	0.19646200	-0.50169800	0.03475200
O	0.35633600	1.72548000	-0.10938000
H	1.32063300	1.51768200	-0.08336700
C	3.23692900	-0.20094300	-0.20819800
C	4.73244900	-0.46173300	-0.38327600
O	2.98468100	1.15269500	0.09309700
C	3.52422300	1.63335300	1.33212200
H	2.96522000	2.53334200	1.57917600
H	3.39738700	0.88658900	2.11544000
H	4.57993100	1.87912500	1.21052900
F	4.92746600	-1.63174700	-0.99411900
F	5.38209200	-0.49824500	0.78377600
F	5.29423500	0.49315400	-1.13002300
O	2.78875600	-1.06778100	0.75846900
H	1.82000800	-1.07534500	0.67563300
H	2.76004100	-0.36042100	-1.17993100

TSd

C	-5.91832500	1.21454900	-0.77946500
C	-4.54963200	0.99625500	-0.70953400
C	-4.05011700	-0.13585700	-0.05970600
C	-4.94214300	-1.05336100	0.50150200
C	-6.31096200	-0.82818000	0.43424900
C	-6.80194200	0.30585900	-0.20386700
H	-6.29657000	2.09039700	-1.29215600
H	-3.87210100	1.69454800	-1.18486400
H	-4.55373600	-1.93586900	0.99256900
H	-6.99490600	-1.54026200	0.87959700
H	-7.86997500	0.47846300	-0.25975100
C	-2.59542600	-0.38918300	0.04244100
O	-2.30801700	-1.67324200	0.24609300
C	-1.67027500	0.60369100	-0.03846300
H	-1.34189600	-1.76594900	0.33234900
H	-1.98874300	1.62688900	-0.15688400
C	-0.23721000	0.40695900	0.04991900
O	0.16481900	-0.83813500	0.23014500
O	0.54766200	1.35610000	-0.04453700
H	2.06617700	1.47564100	0.06659100
C	3.18270300	-0.28139900	-0.35747500
C	4.70401400	-0.37903700	-0.46168400
O	3.06480200	1.40098500	0.21656300
C	3.27266800	1.54170000	1.63295500
H	2.62075100	2.33513800	1.99466900
H	3.03232100	0.60036200	2.13123100
H	4.31455900	1.80326800	1.79414900
F	5.02305200	-1.54988200	-1.02075400
F	5.28385400	-0.32358000	0.73787500
F	5.21777400	0.58879700	-1.21966400
O	2.62270800	-1.03663500	0.46511200
H	1.20620800	-0.94257700	0.33902800
H	2.71989500	-0.04264600	-1.32588900

Value of Imaginary Frequency= -189.1 cm^{-1}

TS2a'

C	1.14985800	3.72433000	1.05607300
C	2.02504100	3.08496400	0.00422500
O	3.34670000	3.30192500	0.16990300
C	2.83889000	2.03992100	-1.75291000
C	3.99525000	2.72936200	-0.98160500
H	2.76039700	2.45776200	-2.76128500
H	4.44994100	3.54436900	-1.54569400
C	-0.29299200	3.51004900	0.64984000
O	-0.85323400	4.52094200	-0.04459300
C	-2.32356000	2.71476500	0.26169800
C	-2.24765600	4.19752800	-0.17951900
H	-3.11202600	2.55730100	0.99914400
H	-2.81081200	4.86052900	0.47935700
N	1.63627900	2.42946100	-1.00627300
N	-1.01468900	2.49526200	0.90340300
C	1.42756300	3.08037600	2.42319200
H	1.25931400	2.00687200	2.39528300
H	2.47016200	3.25398000	2.69114600
H	0.78293000	3.54131000	3.17491700
C	1.47133600	5.22866600	1.11363600
H	1.33063600	5.70392200	0.14307300
H	0.81552000	5.71756000	1.83614600
H	2.50572200	5.35860700	1.42954400
H	4.76222500	2.03587300	-0.64384100
H	-2.54033600	4.35818000	-1.21511700
C	2.99052300	0.53736000	-1.90064900
C	4.15916500	0.03134600	-2.47604500
C	1.98350800	-0.34901600	-1.52893100
C	4.31232100	-1.33241300	-2.69026600
H	4.95631800	0.71083000	-2.76400400
C	2.13511800	-1.71742300	-1.74354800
H	1.09048500	0.02716600	-1.04438500
C	3.29358900	-2.21142700	-2.33102500
H	5.22855500	-1.70914200	-3.13039800
H	1.34726900	-2.39182800	-1.43032700
H	3.40902100	-3.27640600	-2.49861200
C	-2.56946100	1.78247200	-0.90604000
C	-3.88106300	1.48604300	-1.28207300
C	-1.51178600	1.24707300	-1.63691500
C	-4.13467300	0.66334900	-2.37583200
H	-4.70926100	1.89018500	-0.70665100
C	-1.76543900	0.40658200	-2.71945600
H	-0.49172700	1.49547600	-1.36214600
C	-3.07347600	0.11406700	-3.09359800
H	-5.15808200	0.43952400	-2.65883900

H	-0.93259000	-0.01757900	-3.26929900
H	-3.26802800	-0.53668600	-3.93793100
C	-2.77461900	-1.04263700	0.52022800
C	-1.64599400	-2.07843400	0.60629300
O	-0.06988100	0.15395500	2.17333900
C	-0.59037300	0.09444800	3.48960400
H	-1.62601700	-0.24981000	3.47787700
H	0.02047900	-0.61465700	4.05008500
H	-0.52712200	1.07207600	3.97862600
F	-1.31612300	-2.38806900	1.85501400
F	-0.56784600	-1.57228400	-0.00582100
F	-1.95132600	-3.21461800	-0.03977500
O	-2.79706100	-0.12269000	1.37800000
H	-0.49497200	0.88406900	1.67436000
H	-3.01871700	-0.85040200	-0.53404900
C	7.59824800	-3.48682800	-0.87706500
C	6.46242300	-2.83246400	-0.42137100
C	6.56553000	-1.57039200	0.17154200
C	7.82161600	-0.97000200	0.28335000
C	8.95736100	-1.62850600	-0.17258800
C	8.84946900	-2.88801700	-0.75172700
H	7.50738800	-4.46267100	-1.33879300
H	5.48972600	-3.29113500	-0.54995700
H	7.89688300	0.01127700	0.73338100
H	9.92768700	-1.15666300	-0.07498000
H	9.73470600	-3.40037200	-1.10917700
C	5.37135700	-0.85204800	0.66670300
O	5.56665800	0.45776500	0.84558600
C	4.18500300	-1.44874500	0.93714200
H	4.69925200	0.82039000	1.17270200
H	4.04738400	-2.51179000	0.82462100
C	3.04334700	-0.64405400	1.34264000
O	3.10541800	0.58342100	1.47768800
O	1.93777100	-1.32372100	1.54259800
H	1.17607300	-0.70298300	1.75359200
C	-7.23361600	-1.95359100	-2.42429600
C	-6.36567200	-2.09321500	-1.35062100
C	-6.26369300	-1.07455800	-0.39734500
C	-7.06303500	0.06922000	-0.51856600
C	-7.93906700	0.19706800	-1.58489100
C	-8.01870900	-0.81028100	-2.54404400
H	-7.30068900	-2.73926800	-3.16613800
H	-5.76872100	-2.99178500	-1.27035800
H	-6.98276200	0.84990200	0.22654900
H	-8.55596500	1.08247800	-1.67361400
H	-8.69714300	-0.70670600	-3.38224200

C	-5.30340800	-1.14195800	0.71429900
O	-5.23130600	-0.10474400	1.47545800
C	-4.38554800	-2.19848500	0.91067600
H	-4.23079000	-0.00573500	1.75364800
H	-4.40693500	-3.02613900	0.21804400
C	-4.06682800	-2.57975300	2.30894800
O	-4.09327000	-1.85088500	3.26449100
O	-3.72589200	-3.87687100	2.37787700
H	-3.47118700	-4.05745400	3.29332200

Value of Imaginary Frequency= -536.0 cm^{-1}

TS2b'

C	1.29031700	-3.57453000	-1.88840900
C	2.26976900	-3.02535400	-0.87877500
O	3.54194300	-2.95438400	-1.32481500
C	3.29015100	-2.24130600	0.90681900
C	4.32806300	-2.45333300	-0.22769400
H	3.50750500	-2.90976700	1.74610500
H	5.08011300	-3.20394500	0.01487300
C	-0.05180300	-3.73439400	-1.20563000
O	-0.31282700	-4.96388700	-0.71937000
C	-2.04960400	-3.44252400	-0.29196700
C	-1.68901600	-4.94756400	-0.29884500
H	-2.99160400	-3.25034800	-0.80655700
H	-2.26827000	-5.51306100	-1.03085000
N	2.01927600	-2.67168100	0.30997000
N	-0.94541200	-2.84195500	-1.06306800
C	1.18169900	-2.59474000	-3.06799500
H	0.89433000	-1.60185400	-2.73015800
H	2.15415900	-2.51874000	-3.55519600
H	0.44967300	-2.97217400	-3.78538700
C	1.80233100	-4.93771700	-2.38624900
H	1.93441800	-5.63884100	-1.56251700
H	1.08653600	-5.36409900	-3.09117400
H	2.75645700	-4.79592600	-2.89227200
H	4.81002200	-1.52804000	-0.53712400
H	-1.75624100	-5.41731400	0.68007100
C	3.24934500	-0.82802100	1.45479800
C	4.43388400	-0.24731700	1.91627700
C	2.06212300	-0.10776300	1.55340600
C	4.43040100	1.02310800	2.47859500
H	5.36982600	-0.79360900	1.83564700
C	2.05624900	1.16452300	2.12136700
H	1.14536100	-0.52983400	1.16040600
C	3.23589800	1.72975000	2.59147600
H	5.36119300	1.46682600	2.81475900
H	1.12433500	1.71514400	2.17278000
H	3.23119100	2.72219800	3.02737100
C	-2.15583900	-2.88613800	1.11227400
C	-3.37765500	-2.96711900	1.78411100
C	-1.05443200	-2.33429600	1.75904400
C	-3.49306800	-2.50413000	3.09006300
H	-4.24495600	-3.37372200	1.27349100
C	-1.17826100	-1.84696200	3.05962900
H	-0.09874400	-2.29347200	1.24728800
C	-2.39345400	-1.93254800	3.72993800
H	-4.43994400	-2.58271000	3.61177600

H	-0.31635400	-1.40281500	3.54532500
H	-2.48739000	-1.55890300	4.74258800
C	-3.12007200	0.09683400	0.59168300
C	-2.14664400	1.28296100	0.56545500
O	-0.64784800	-0.16752300	-1.80415700
C	-1.42942600	0.06282700	-2.95813700
H	-1.28882500	-0.73332600	-3.69654800
H	-2.48748300	0.13847800	-2.69819200
H	-1.10189100	1.00679700	-3.39612900
F	-2.15040900	1.91284200	-0.60886100
F	-0.90984600	0.83927400	0.80908000
F	-2.42416700	2.18982500	1.51701100
O	-3.20322900	-0.62047600	-0.43799300
H	-0.82385200	-1.06910800	-1.45146500
H	-3.15912000	-0.35047900	1.59606000
C	6.68266600	4.33953700	0.88929400
C	5.65500400	3.68910500	0.22113600
C	5.83568000	2.38778000	-0.25568900
C	7.06864900	1.75899500	-0.06881400
C	8.09501600	2.41121400	0.60438700
C	7.90417000	3.70074000	1.08871800
H	6.53299000	5.34957300	1.25127900
H	4.71451900	4.20131600	0.06089000
H	7.20925300	0.75492200	-0.44742600
H	9.04513900	1.91132600	0.75004300
H	8.70427300	4.21002300	1.61245200
C	4.73698300	1.64007700	-0.90412400
O	5.13750300	0.54704000	-1.56074100
C	3.43062000	1.98229500	-0.80192200
H	4.30812500	0.10223000	-1.87986600
H	3.11505300	2.84087500	-0.23302200
C	2.40096900	1.09350100	-1.31676200
O	2.65797600	0.02543500	-1.88399600
O	1.17353100	1.50882700	-1.10314100
H	0.50572700	0.81188800	-1.37975900
C	-5.42309000	5.25271200	-0.26720000
C	-5.42112600	3.90753400	0.07274800
C	-5.00954000	2.95327100	-0.86264800
C	-4.60651300	3.35609000	-2.14098100
C	-4.60580000	4.70125100	-2.47270600
C	-5.01300300	5.64940700	-1.53648800
H	-5.74766000	5.99088200	0.45519100
H	-5.76335800	3.60080800	1.05314900
H	-4.28294700	2.60701500	-2.85223500
H	-4.28304400	5.01443900	-3.45758500
H	-5.01185200	6.70069000	-1.79819800

C	-4.98973000	1.52478700	-0.52920100
O	-4.95000700	0.69191100	-1.51142700
C	-4.88817700	1.03680500	0.79287700
H	-4.38619300	-0.12012500	-1.19989100
H	-4.80903800	1.76146900	1.59017200
C	-5.62567000	-0.19612500	1.15469300
O	-5.95409700	-1.07915700	0.40836500
O	-5.87212300	-0.22160000	2.47714600
H	-6.32361100	-1.05552500	2.66617300

Value of Imaginary Frequency= -524.0 cm^{-1}

TS2c'

C	1.72644700	-3.90701900	-1.09560700
C	2.48754200	-3.09212000	-0.07710600
O	3.81064200	-2.98216000	-0.32442200
C	3.14052000	-1.91566000	1.66368200
C	4.37864500	-2.32958500	0.82725200
H	3.21370800	-2.33255900	2.67240000
H	5.00668300	-3.05666500	1.34377800
C	0.28938600	-4.01255500	-0.62889900
O	-0.01155100	-5.12971900	0.06205400
C	-1.84894200	-3.68299100	-0.15366000
C	-1.43696800	-5.11974500	0.25167500
H	-2.67943000	-3.69318700	-0.86137600
H	-1.86731900	-5.88004200	-0.40211000
N	2.01989200	-2.57259900	0.97820700
N	-0.64376200	-3.17416700	-0.83483200
C	1.79581100	-3.22701800	-2.47140500
H	1.39519100	-2.21739400	-2.43364100
H	2.83806400	-3.16759800	-2.78650500
H	1.23741200	-3.82528400	-3.19496000
C	2.36771300	-5.30468700	-1.17365200
H	2.37508700	-5.79402500	-0.19995100
H	1.80578700	-5.92946200	-1.86999600
H	3.39133000	-5.20552400	-1.53307600
H	4.97881700	-1.48675100	0.49203900
H	-1.64857900	-5.35479500	1.29269700
C	2.94956200	-0.41675900	1.80862400
C	3.98968900	0.35047800	2.33936700
C	1.75007100	0.20837400	1.48030100
C	3.82795200	1.71341000	2.55381400
H	4.93383500	-0.12288500	2.59346000
C	1.58453300	1.57455600	1.69760400
H	0.95342100	-0.37124700	1.03080100
C	2.61789100	2.32804200	2.24157400
H	4.64745200	2.29596800	2.95901800
H	0.64717600	2.04398400	1.42400800
H	2.48725100	3.39076300	2.41230000
C	-2.25131400	-2.84516100	1.04162400
C	-3.58287000	-2.85141700	1.46144800
C	-1.31270800	-2.10165500	1.75274800
C	-3.97597400	-2.11414900	2.57427100
H	-4.32388100	-3.41170800	0.90023600
C	-1.70901900	-1.35240500	2.85932900
H	-0.27255600	-2.11656100	1.44357900
C	-3.03767400	-1.35581700	3.27341500
H	-5.01580500	-2.11659500	2.87903000

H	-0.97181100	-0.76506200	3.39534800
H	-3.34264400	-0.77193200	4.13382300
C	-3.16508900	-0.08012000	-0.24932400
C	-2.18976500	1.09156700	-0.31274600
O	-0.34162500	-0.71242800	-2.20126500
C	-0.93900500	-0.88514000	-3.47049900
H	-2.02654000	-0.90902100	-3.37845900
H	-0.64820200	-0.03616300	-4.09024200
H	-0.58803900	-1.80454300	-3.95121500
F	-2.09139500	1.61548800	-1.53342600
F	-0.98216400	0.66867900	0.06778400
F	-2.53257600	2.07327700	0.53820200
O	-3.05879000	-0.95593500	-1.16133100
H	-0.53533800	-1.49272000	-1.63829500
H	-3.31621300	-0.37539800	0.79936800
C	6.45192500	4.52448000	0.63770600
C	5.46706800	3.64381700	0.21333400
C	5.81666600	2.42426400	-0.37457600
C	7.16725200	2.09671400	-0.51340000
C	8.15138600	2.98148000	-0.08871200
C	7.79723000	4.19716700	0.48567800
H	6.17058400	5.46492200	1.09612000
H	4.42354500	3.89193200	0.36336000
H	7.43483000	1.14798200	-0.95989900
H	9.19615800	2.72037800	-0.20685600
H	8.56443800	4.88583100	0.81887400
C	4.78699300	1.46831700	-0.83664500
O	5.24849200	0.22869400	-1.02357400
C	3.49418700	1.80130600	-1.07197700
H	4.46873100	-0.31210600	-1.32448600
H	3.13906900	2.81179000	-0.95229300
C	2.53848100	0.77317800	-1.44960800
O	2.85492000	-0.41230300	-1.59566000
O	1.30647200	1.20130400	-1.61449700
H	0.69725100	0.43331700	-1.82242600
C	-4.25114000	4.84003900	-1.85563300
C	-4.46860700	3.52197100	-1.48624800
C	-5.03093900	3.23070700	-0.23786800
C	-5.37161900	4.27459000	0.63189100
C	-5.14753300	5.58954000	0.25813800
C	-4.58845000	5.87295200	-0.98540900
H	-3.81507800	5.06189200	-2.82115600
H	-4.18788300	2.73184400	-2.16877600
H	-5.80678600	4.04139600	1.59455900
H	-5.40789400	6.39426100	0.93388600
H	-4.41410700	6.90158900	-1.27725400

C	-5.29390700	1.85424100	0.18676400
O	-5.89709100	1.70292200	1.31004200
C	-4.92041700	0.69142700	-0.56280700
H	-4.40315500	-1.50896500	-1.21304300
H	-4.76953100	0.83703200	-1.62410300
C	-5.65958700	-0.55718300	-0.20048400
O	-5.40052700	-1.61116100	-0.91048100
O	-6.42274400	-0.59119700	0.76976200
H	-6.22087500	0.70096800	1.32589100

Value of Imaginary Frequency= -474.5 cm^{-1}

TS2d'

C	1.85145800	3.96309000	0.43263900
C	2.54887700	2.95703400	-0.45242900
O	3.88513600	2.88565200	-0.26947200
C	3.10026100	1.46710900	-1.97510900
C	4.38500800	2.03054500	-1.31536700
H	3.10424400	1.68500300	-3.04707100
H	4.96779600	2.64954500	-1.99885800
C	0.38872900	3.99215000	0.04451100
O	0.03279000	4.96204600	-0.81803700
C	-1.77722800	3.59148900	-0.20613800
C	-1.40166800	4.91706500	-0.91633100
H	-2.54935300	3.74774000	0.54921300
H	-1.79946600	5.79543100	-0.40610100
N	2.01857700	2.24734100	-1.35661300
N	-0.52257000	3.21237100	0.46566900
C	2.00175400	3.56303400	1.90877400
H	1.60379400	2.56836100	2.09186100
H	3.06055700	3.55534200	2.16908800
H	1.48474300	4.29501700	2.53321700
C	2.49527400	5.34173400	0.19813800
H	2.44031300	5.63312100	-0.85064900
H	1.97875700	6.09595700	0.79417800
H	3.53975300	5.30189600	0.50478600
H	5.01617100	1.26603700	-0.86793700
H	-1.67532300	4.93700500	-1.96923600
C	2.91601200	-0.03171300	-1.82029300
C	3.93774000	-0.88912700	-2.23549500
C	1.73470800	-0.58036300	-1.32953800
C	3.77694300	-2.26806300	-2.17352500
H	4.86981400	-0.47685900	-2.61226100
C	1.56805200	-1.96205300	-1.27354800
H	0.95527600	0.07597400	-0.96493500
C	2.58417100	-2.80883100	-1.70132900
H	4.58787400	-2.91913900	-2.48129200
H	0.64554800	-2.36779600	-0.87511000
H	2.45707800	-3.88407300	-1.65121800
C	-2.27202300	2.54107400	-1.17740900
C	-3.62645200	2.51691400	-1.51736200
C	-1.40245200	1.63210600	-1.77116000
C	-4.10563900	1.58991700	-2.43486000
H	-4.30840800	3.22236100	-1.05254500
C	-1.88848400	0.68450100	-2.67190800
H	-0.34530100	1.67101200	-1.53020100
C	-3.23786200	0.65872900	-3.00615700
H	-5.15748000	1.58769800	-2.69926600

H	-1.20394600	-0.03307800	-3.11005500
H	-3.61592400	-0.08079300	-3.70245700
C	-3.11213000	0.07152600	0.68575400
C	-2.05077000	-1.02711200	0.83994900
O	-0.23058000	1.06634400	2.21366700
C	-0.74183800	1.54648900	3.44114800
H	-1.61922900	2.17413400	3.26745200
H	-1.04100900	0.68890600	4.04508300
H	0.01059000	2.12517500	3.98751100
F	-1.77175600	-1.29557100	2.11423400
F	-0.92773100	-0.65408400	0.22280800
F	-2.44877100	-2.16739900	0.25407000
O	-3.03549300	1.10897800	1.37449000
H	-0.33123000	1.76486000	1.52870000
H	-3.51855700	0.08704700	-0.33449500
C	6.43572800	-4.69616700	0.19345100
C	5.55630300	-3.75796300	0.71542700
C	5.77316300	-2.39354700	0.50506300
C	6.89666000	-1.98663700	-0.21815200
C	7.77412000	-2.92812900	-0.74266100
C	7.54424300	-4.28500800	-0.54261400
H	6.25924100	-5.75108700	0.36543100
H	4.70543700	-4.09059200	1.29664800
H	7.06823800	-0.92908100	-0.37141300
H	8.63868700	-2.60130500	-1.30797300
H	8.22821000	-5.01946200	-0.95079000
C	4.81510900	-1.37172500	0.98080600
O	5.29424000	-0.12532400	0.95045300
C	3.54368300	-1.64839700	1.35999600
H	4.53914600	0.46693900	1.21356800
H	3.15227500	-2.65189100	1.33851100
C	2.62175400	-0.56309400	1.65004000
O	2.95296300	0.62689400	1.60506100
O	1.39728700	-0.94426700	1.93762200
H	0.80369300	-0.14523800	2.05061900
C	-6.35974800	-1.33399600	-2.55777700
C	-5.90206500	-1.18644600	-1.25413700
C	-5.61077500	-2.31394800	-0.48311300
C	-5.78019000	-3.58822200	-1.03235200
C	-6.23303400	-3.73232300	-2.33453900
C	-6.52418600	-2.60452600	-3.09881000
H	-6.58848700	-0.45738000	-3.15191800
H	-5.77824600	-0.18764700	-0.85407600
H	-5.54632300	-4.45107400	-0.42203200
H	-6.35894300	-4.72158400	-2.75667600
H	-6.87906800	-2.71669200	-4.11628400

C	-5.10967300	-2.22175600	0.91376400
O	-4.93439400	-3.25928800	1.56617600
C	-4.78346600	-0.92079800	1.48919900
H	-3.67015600	0.81162600	2.71052700
H	-5.34056200	-0.05631400	1.16043500
C	-4.39736200	-0.89793500	2.86731100
O	-4.07229800	0.20953300	3.43964400
O	-4.28798100	-1.96773900	3.56939800
H	-4.53752900	-2.73201300	2.93949100

Value of Imaginary Frequency= -375.2 cm^{-1}

IM2a'

C	1.53266600	3.71572900	0.91159500
C	2.31732900	2.95076200	-0.12641500
O	3.65192500	2.89570000	0.10572800
C	3.02962900	1.89170300	-1.91551700
C	4.23667200	2.46320600	-1.13896400
H	3.02924100	2.27006200	-2.94089600
H	4.65648200	3.34356600	-1.63001100
C	0.05512300	3.57383700	0.60925400
O	-0.52019200	4.63759100	0.01806000
C	-2.04061700	2.88946200	0.38826900
C	-1.93793700	4.39314500	0.04093300
H	-2.76469900	2.71051300	1.18340000
H	-2.37365500	5.03267600	0.81081300
N	1.87276600	2.46195300	-1.20584700
N	-0.68530800	2.57893100	0.89233100
C	1.81901900	3.17896100	2.32026600
H	1.55217700	2.12925300	2.38916500
H	2.88369200	3.27550700	2.53633000
H	1.25294500	3.76032200	3.05113700
C	1.97045300	5.18961200	0.81685900
H	1.79607800	5.59013600	-0.18159600
H	1.40867200	5.79037100	1.53353900
H	3.03245300	5.25766000	1.05257700
H	5.01415500	1.73685000	-0.91897000
H	-2.34741900	4.64424400	-0.93493800
C	2.98309900	0.37456300	-1.98343700
C	4.07117200	-0.31537100	-2.52310200
C	1.86208800	-0.34394500	-1.57814300
C	4.03324600	-1.69641100	-2.66876700
H	4.95490900	0.23127300	-2.83939200
C	1.81974000	-1.72827800	-1.72871300
H	1.03136400	0.18131500	-1.12528700
C	2.90075100	-2.40672700	-2.27901000
H	4.88927800	-2.21732500	-3.08218600
H	0.94105400	-2.27135600	-1.40198400
H	2.86645600	-3.48394400	-2.39637700
C	-2.44375400	2.05893100	-0.81159500
C	-3.80245300	1.84930200	-1.06031200
C	-1.50071800	1.54966000	-1.69776100
C	-4.21437400	1.12930400	-2.17475800
H	-4.54042000	2.23061000	-0.36073900
C	-1.91241000	0.80445400	-2.80228500
H	-0.44527200	1.73158500	-1.52193100
C	-3.26531900	0.59179100	-3.04381400
H	-5.27164600	0.96369200	-2.35206100

H	-1.16737100	0.39087200	-3.47268400
H	-3.58439900	0.01142900	-3.90204300
C	-3.02006400	-1.00462600	0.53666300
C	-1.71036300	-1.73709700	0.27653000
O	-0.38563400	0.20097200	2.41979800
C	-0.05041300	0.56137900	3.75468700
H	-0.48686500	-0.18470600	4.41805200
H	1.03540000	0.57767300	3.89119000
H	-0.45795800	1.54406800	4.00441000
F	-1.26023800	-2.41202300	1.34044400
F	-0.74754300	-0.90445500	-0.11322300
F	-1.88799700	-2.64061700	-0.70941500
O	-2.86694100	0.13730800	1.30837100
H	-0.37770300	0.99843700	1.83970900
H	-3.35009200	-0.67434500	-0.45333200
C	7.15803900	-3.74378000	-0.68498900
C	6.01328700	-3.08393600	-0.26142900
C	6.09706600	-1.78956600	0.26074300
C	7.34395200	-1.16472000	0.33621300
C	8.48912500	-1.82879100	-0.08763200
C	8.39999600	-3.11917900	-0.59725200
H	7.08145500	-4.74480900	-1.09207700
H	5.04848100	-3.56522200	-0.36329800
H	7.40632300	-0.16050500	0.73462800
H	9.45198300	-1.33711700	-0.01835200
H	9.29230600	-3.63619800	-0.92942200
C	4.89305800	-1.06364400	0.72208900
O	5.07812100	0.25306700	0.84014900
C	3.71568200	-1.66737100	1.01917000
H	4.21913100	0.64676000	1.13645700
H	3.59496000	-2.73575300	0.94481500
C	2.56876900	-0.87209700	1.41552700
O	2.60735000	0.35550500	1.53732200
O	1.46699200	-1.56087600	1.63908000
H	0.73314000	-0.93072700	1.87247100
C	-6.10149100	-1.85166300	-2.75636400
C	-5.49717000	-1.95222800	-1.50843100
C	-6.03842400	-1.27679500	-0.41240700
C	-7.18546000	-0.49643700	-0.58060900
C	-7.78242200	-0.39077600	-1.82803700
C	-7.24135900	-1.07140000	-2.91758700
H	-5.67858600	-2.37972300	-3.60205100
H	-4.59945600	-2.55160900	-1.41112900
H	-7.59224500	0.01756100	0.28155100
H	-8.66954300	0.21775100	-1.95383200
H	-7.70879800	-0.99186800	-3.89182100

C	-5.44899500	-1.34861100	0.96195400
O	-6.01737700	-0.88939200	1.92071100
C	-4.06393400	-1.98525000	1.11603000
H	-2.34916600	-0.08339300	2.09974000
H	-4.03798400	-2.93154700	0.57045600
C	-3.84079900	-2.29468500	2.58575400
O	-3.13498000	-1.69026200	3.34400500
O	-4.56084900	-3.36149900	2.94591200
H	-4.43526700	-3.49578600	3.89599400

IM2b'

C	-2.10322100	3.16625900	-2.14102600
C	-3.02049500	2.48833600	-1.15253300
O	-4.05868900	1.81116200	-1.69691100
C	-4.05696100	1.76958200	0.64639600
C	-4.94560900	1.52826900	-0.59453600
H	-4.59648100	2.36775100	1.38489600
H	-5.77315900	2.23867800	-0.64643100
C	-0.86926600	3.62345800	-1.39048700
O	-0.84118700	4.92002900	-1.03590800
C	1.06093300	3.75185000	-0.29859600
C	0.47811800	5.16838300	-0.51195800
H	2.06479800	3.65947200	-0.71403700
H	1.02957900	5.74206700	-1.25870200
N	-2.94616900	2.56715900	0.10834100
N	0.13305300	2.90374800	-1.08265300
C	-1.69991700	2.19346100	-3.25616600
H	-1.22791500	1.30824100	-2.83942400
H	-2.59052500	1.87901700	-3.80123200
H	-1.01768300	2.69350600	-3.94654700
C	-2.86369900	4.36602200	-2.73379800
H	-3.16406900	5.06585900	-1.95458200
H	-2.22899500	4.89224800	-3.44873700
H	-3.75042000	4.00041300	-3.25255800
H	-5.30565900	0.50826600	-0.69764100
H	0.37935700	5.74037600	0.40781100
C	-3.57102700	0.50601000	1.33849300
C	-4.51433500	-0.39481300	1.83831000
C	-2.21684400	0.24656900	1.54046700
C	-4.11549600	-1.52606600	2.53947200
H	-5.57355500	-0.20990700	1.68108200
C	-1.81613200	-0.87901100	2.25714400
H	-1.47183400	0.91821300	1.13055500
C	-2.76191300	-1.76383300	2.76240800
H	-4.86137700	-2.22348600	2.90462200
H	-0.75799300	-1.06432200	2.39999200
H	-2.44752800	-2.64218200	3.31422000
C	1.10316700	3.35492800	1.16169700
C	2.32054200	3.29611600	1.83593100
C	-0.07615700	3.08942200	1.85522300
C	2.36414900	2.94877000	3.18273600
H	3.24011700	3.48769700	1.29206000
C	-0.03155100	2.72947500	3.19830200
H	-1.03047800	3.13518000	1.33811800
C	1.18744400	2.65300300	3.86444700
H	3.31811200	2.89624600	3.69593700

H	-0.95271100	2.49572500	3.71989700
H	1.22161900	2.36429300	4.90824600
C	3.54168800	0.48228800	0.78178400
C	2.36704900	-0.35648000	1.29078200
O	1.08070100	0.35615200	-1.61181400
C	1.13200900	0.11064500	-3.01625000
H	1.31577400	1.04013100	-3.56080600
H	1.95436200	-0.57944100	-3.19414200
H	0.19254400	-0.33059500	-3.36071100
F	2.16246100	-1.47817200	0.58528800
F	1.22604700	0.32895100	1.29122800
F	2.61326000	-0.74478500	2.55606700
O	3.21407100	1.33390100	-0.26391000
H	0.61056200	1.20916100	-1.43093600
H	3.80948200	1.10814900	1.63468200
C	-5.59880200	-5.22576500	0.83689100
C	-4.59882000	-4.44463000	0.27473400
C	-4.90804100	-3.21022300	-0.30266200
C	-6.23813500	-2.78454700	-0.32675000
C	-7.23712800	-3.56633700	0.24045300
C	-6.92022800	-4.78659800	0.82757900
H	-5.34787900	-6.18257600	1.27854700
H	-3.57767900	-4.80475300	0.27525700
H	-6.47915200	-1.83521600	-0.78747100
H	-8.26444100	-3.22273900	0.22236700
H	-7.69887500	-5.39732900	1.26857300
C	-3.85644500	-2.32335100	-0.84713800
O	-4.32730800	-1.34484600	-1.62335900
C	-2.54045900	-2.45067700	-0.54873700
H	-3.55937400	-0.76682400	-1.86291200
H	-2.18655000	-3.21351600	0.12461500
C	-1.58911000	-1.45886100	-1.01206500
O	-1.90338200	-0.49887500	-1.72272700
O	-0.35306800	-1.64856600	-0.59807500
H	0.21829500	-0.89727900	-0.91173900
C	7.06262800	-4.11519500	-0.03397300
C	6.38496600	-2.90672600	0.07210100
C	5.32634800	-2.61947900	-0.79129300
C	4.95603000	-3.55288000	-1.76261400
C	5.62587200	-4.76286000	-1.86026400
C	6.68109900	-5.04452400	-0.99571600
H	7.88882300	-4.32989100	0.63235200
H	6.70481200	-2.19045100	0.81895100
H	4.13610700	-3.31145700	-2.42729100
H	5.32882600	-5.48705000	-2.60881200
H	7.20713400	-5.98858100	-1.07304300

C	4.56897600	-1.33354200	-0.74216600
O	3.81685000	-1.01648600	-1.63149200
C	4.75523600	-0.41857500	0.47836000
H	2.69632300	0.84033800	-0.92851000
H	4.96258000	-1.01567600	1.37273800
C	5.97646700	0.45208700	0.23058100
O	6.73944200	0.31324800	-0.68253000
O	6.11960000	1.39207400	1.17417300
H	6.90720700	1.90983300	0.95474700

IM2c'

C	1.79584300	-3.86546400	-1.16421500
C	2.53831900	-3.05019500	-0.13209800
O	3.85457900	-2.88452400	-0.38614600
C	3.16704100	-1.90718000	1.63937400
C	4.41257000	-2.28143700	0.79766700
H	3.25256600	-2.33223100	2.64344400
H	5.03433500	-3.03144400	1.28892600
C	0.36278200	-4.01218900	-0.69563600
O	0.09605700	-5.14152700	-0.01109900
C	-1.78319700	-3.74778400	-0.21493000
C	-1.32574500	-5.17055700	0.19499300
H	-2.60955800	-3.79738100	-0.92718600
H	-1.74295200	-5.94773000	-0.44708800
N	2.06349400	-2.58520900	0.94549100
N	-0.59451600	-3.19861100	-0.89363300
C	1.84645800	-3.17109000	-2.53303100
H	1.41323300	-2.17546200	-2.48905000
H	2.88706300	-3.07635600	-2.84507200
H	1.31031600	-3.78202100	-3.26294700
C	2.47170300	-5.24634200	-1.25808700
H	2.49450300	-5.74522600	-0.28950100
H	1.92420400	-5.87802900	-1.95965100
H	3.49137000	-5.11703800	-1.61930600
H	5.01562200	-1.42580100	0.50353800
H	-1.51885400	-5.40242200	1.24036000
C	2.93465200	-0.41508800	1.79801800
C	3.95140100	0.37769200	2.33581700
C	1.71625700	0.17663000	1.47755800
C	3.74772300	1.73268400	2.56512900
H	4.90994100	-0.06885400	2.58436600
C	1.50885900	1.53461100	1.70870400
H	0.93758600	-0.42388900	1.02483600
C	2.51939500	2.31353700	2.25998800
H	4.54936200	2.33553300	2.97629500
H	0.55721400	1.97844000	1.44127700
H	2.35662700	3.36989600	2.44188600
C	-2.21827700	-2.92768600	0.98173200
C	-3.55726800	-2.94671000	1.37743900
C	-1.29246900	-2.20575100	1.73153400
C	-3.96715800	-2.25489000	2.51424400
H	-4.28847100	-3.49634500	0.79143200
C	-1.70718000	-1.49688800	2.85709900
H	-0.24749300	-2.20766500	1.43765500
C	-3.04143300	-1.52125000	3.25381600
H	-5.00955900	-2.27637900	2.80771100

H	-0.98024700	-0.92591400	3.42376900
H	-3.35975100	-0.97181200	4.13175100
C	-3.28772900	0.03186900	-0.14690200
C	-2.16536400	1.05103700	-0.25324900
O	-0.35790000	-0.72472000	-2.28722800
C	-0.99008700	-0.92891300	-3.53334500
H	-2.07689700	-0.91354500	-3.42228400
H	-0.68801700	-0.11684600	-4.19527300
H	-0.68011800	-1.87846600	-3.98236800
F	-2.06640800	1.57427700	-1.47653400
F	-1.00112100	0.49109100	0.06413300
F	-2.35686000	2.06454300	0.60954200
O	-3.00908700	-0.93609700	-1.11282900
H	-0.53536100	-1.48891000	-1.69999100
H	-3.23112600	-0.36500100	0.87393000
C	6.31402700	4.59254000	0.68956400
C	5.33921700	3.70911200	0.24829300
C	5.70226700	2.49394900	-0.34060900
C	7.05619500	2.17413700	-0.46398400
C	8.03039700	3.06165000	-0.02225900
C	7.66286500	4.27260900	0.55357200
H	6.02197300	5.52937400	1.14864700
H	4.29279500	3.95186500	0.38625400
H	7.33446600	1.22925800	-0.91208900
H	9.07788500	2.80631500	-0.12837400
H	8.42223800	4.96338700	0.90007000
C	4.68347000	1.53417100	-0.81896600
O	5.15614700	0.29994600	-1.01263500
C	3.38980400	1.85956700	-1.06117500
H	4.38340000	-0.24662700	-1.32084600
H	3.02568900	2.86604800	-0.93511900
C	2.44646000	0.82832500	-1.45908900
O	2.77307200	-0.35254700	-1.61572800
O	1.21135400	1.24739100	-1.63253000
H	0.62105700	0.47598600	-1.87052900
C	-4.49491200	4.71060900	-2.06726600
C	-4.54195800	3.42614000	-1.54010400
C	-4.91961500	3.23248100	-0.20861200
C	-5.24610500	4.33742300	0.58622100
C	-5.20124900	5.61564100	0.05551300
C	-4.82630000	5.80279900	-1.27361000
H	-4.19638600	4.85672800	-3.09756600
H	-4.26117600	2.59475500	-2.17217300
H	-5.53152000	4.17055000	1.61695100
H	-5.45593800	6.46735200	0.67376100
H	-4.78974100	6.80260300	-1.68934000

C	-4.99572000	1.89420600	0.42911600
O	-5.30737000	1.78131000	1.60316000
C	-4.71073500	0.63320300	-0.38029300
H	-3.77540200	-1.52408900	-1.17522800
H	-4.80462400	0.81120600	-1.44974700
C	-5.65736900	-0.54198300	-0.06604600
O	-5.73674400	-1.46145100	-0.84264000
O	-6.30042500	-0.54685900	1.08299100
H	-6.03809200	0.24499300	1.60274500

IM2d'

C	2.06812600	3.74871900	0.99832300
C	2.83977500	2.88330500	0.03219100
O	4.08223500	2.53132100	0.43749800
C	3.54542300	1.72721700	-1.69767500
C	4.72584300	1.99409800	-0.73675800
H	3.77947700	2.10587600	-2.69575000
H	5.40008600	2.76098600	-1.12322200
C	0.63730400	3.82377400	0.50754300
O	0.31346500	4.92201200	-0.19663200
C	-1.48436900	3.41826500	-0.00969300
C	-1.11104400	4.86661800	-0.40406700
H	-2.33359000	3.39229500	0.67370200
H	-1.57122200	5.61162800	0.24690400
N	2.46109400	2.53719500	-1.12476200
N	-0.27298200	2.95871400	0.70955100
C	2.10279200	3.14663600	2.40847000
H	1.70904800	2.13422300	2.40410200
H	3.13455500	3.10652400	2.75920300
H	1.52013500	3.77391300	3.08609200
C	2.72267800	5.14182300	1.00156400
H	2.71574400	5.58265100	0.00518600
H	2.18254600	5.80471600	1.67957800
H	3.75231000	5.04719500	1.34765500
H	5.27864800	1.10437900	-0.44780200
H	-1.31459500	5.09840100	-1.44710000
C	3.15475100	0.26462600	-1.83596100
C	4.10794300	-0.64859800	-2.29257900
C	1.86112300	-0.18313200	-1.57567000
C	3.77374000	-1.98106400	-2.50041200
H	5.12311900	-0.31541800	-2.49061500
C	1.52052200	-1.51552700	-1.79911200
H	1.12007800	0.50644100	-1.18870100
C	2.47181600	-2.41524800	-2.26618500
H	4.53165700	-2.67967000	-2.83740700
H	0.51030200	-1.84524500	-1.58678000
H	2.20605900	-3.45276700	-2.43265900
C	-1.80205600	2.55132200	-1.20951800
C	-3.11554400	2.16470700	-1.46608900
C	-0.79257800	2.16553400	-2.08927000
C	-3.41650800	1.37121500	-2.56896700
H	-3.89949100	2.46031700	-0.77582900
C	-1.09112300	1.36528500	-3.18775300
H	0.23436000	2.46581800	-1.89969100
C	-2.40027600	0.95964800	-3.42653400
H	-4.44076200	1.06253300	-2.75067500

H	-0.29352500	1.04648500	-3.84911300
H	-2.62877100	0.32635700	-4.27543800
C	-3.50641300	-0.22684000	0.67363900
C	-2.37175100	-1.08462200	0.10585700
O	-0.58350800	0.62843700	2.19856800
C	-0.26919900	0.80833000	3.58149200
H	-0.49836000	1.82949900	3.89501300
H	-0.88768100	0.11198400	4.14447700
H	0.78946400	0.60126300	3.75842400
F	-1.79210600	-1.85378600	1.04020200
F	-1.41743200	-0.35102900	-0.45638600
F	-2.86079100	-1.91664200	-0.83089400
O	-3.06582900	0.93995800	1.26488700
H	-0.32069300	1.42644200	1.67413300
H	-4.09871900	0.05393100	-0.19919500
C	6.26882100	-4.74342600	-0.30352900
C	5.29926300	-3.93153500	0.26825700
C	5.50178600	-2.55235800	0.36605000
C	6.70069900	-2.00589000	-0.09766400
C	7.66808900	-2.82013400	-0.67393300
C	7.45340600	-4.18991000	-0.78265700
H	6.10286000	-5.81181600	-0.37031500
H	4.38927400	-4.37659500	0.65070600
H	6.86348000	-0.93961100	-0.00742200
H	8.59129400	-2.38449900	-1.03679000
H	8.20794300	-4.82559100	-1.23024000
C	4.45936600	-1.65199100	0.90556400
O	4.90893400	-0.43410100	1.21547500
C	3.15554300	-2.00287600	1.02568800
H	4.12508700	0.10698000	1.48598900
H	2.80244300	-2.97295500	0.71797100
C	2.17139200	-1.01849200	1.43023200
O	2.45806200	0.14379200	1.73306300
O	0.92707900	-1.45413200	1.43088200
H	0.31929800	-0.70548400	1.66222200
C	-7.56716400	-0.13878300	-1.28210700
C	-6.65683300	-0.45806900	-0.28276700
C	-6.11593600	-1.74571500	-0.21471300
C	-6.49475900	-2.70549800	-1.15740900
C	-7.39589800	-2.38048300	-2.15972500
C	-7.93324500	-1.09719100	-2.22214200
H	-7.99070000	0.85678900	-1.32589300
H	-6.38758600	0.30121600	0.44203900
H	-6.06533300	-3.69715000	-1.09080400
H	-7.67998500	-3.12478800	-2.89309000
H	-8.63906500	-0.84374600	-3.00397100

C	-5.13914400	-2.15988600	0.83275400
O	-4.90386300	-3.33966800	1.01596600
C	-4.41564000	-1.07465100	1.62068500
H	-2.30638400	0.75237800	1.85358700
H	-5.15229500	-0.35298500	1.98016900
C	-3.64502300	-1.50377000	2.88361700
O	-3.18470500	-0.66421900	3.60954600
O	-3.52109100	-2.79375000	3.14234800
H	-3.92478800	-3.31097500	2.41449500

IM2a

C	3.01207000	-2.73611200	-0.19441600
C	3.66398100	-1.43320900	-0.60113500
O	3.99735800	-1.34095000	-1.90584700
C	4.54241200	0.57525300	-0.66585800
C	4.42314000	0.01618600	-2.10665300
H	5.59624000	0.66647500	-0.37767300
H	5.36283300	0.00403700	-2.65605300
C	2.16619400	-2.39897300	1.00834600
O	2.77946000	-2.44197500	2.20615200
C	0.53836100	-1.76023100	2.35840000
C	1.87830700	-1.80755500	3.13058100
H	-0.13961100	-2.55129200	2.69353900
H	1.84511200	-2.39584400	4.04475500
N	3.92821000	-0.46523600	0.16831000
N	0.94697000	-2.04948800	0.97268600
C	2.13406800	-3.27196500	-1.33092200
H	1.43354400	-2.51304200	-1.67481400
H	2.76588000	-3.56363900	-2.16965400
H	1.57679400	-4.14278800	-0.98216900
C	4.11355200	-3.74675500	0.16782100
H	4.72948800	-3.37343900	0.98483100
H	3.66477800	-4.69615700	0.46686000
H	4.74193200	-3.91980900	-0.70728300
H	3.64980900	0.52526700	-2.68416700
H	2.26085400	-0.80539900	3.33776000
C	3.89312600	1.92788600	-0.46709700
C	3.17170800	2.21307800	0.69266600
C	4.03596000	2.92555000	-1.43566400
C	2.59223800	3.46527600	0.87284300
H	3.06146800	1.43993100	1.44225600
C	3.45353500	4.17811300	-1.25630800
H	4.60289400	2.72621900	-2.33966500
C	2.72590700	4.44978800	-0.10172700
H	2.02795600	3.66729000	1.77591200
H	3.56494800	4.93725500	-2.02110000
H	2.26595600	5.42063500	0.03557400
C	-0.16931800	-0.43062100	2.47376400
C	-1.14478300	-0.21982300	3.44628800
C	0.16249100	0.60769100	1.60141900
C	-1.79573900	1.00851500	3.53250200
H	-1.41884400	-1.02543900	4.11941400
C	-0.50663800	1.82534000	1.66701200
H	0.93783900	0.44198700	0.86130000
C	-1.49014300	2.02728100	2.63348500
H	-2.56565700	1.15896400	4.28017900

H	-0.26627900	2.60459600	0.95182300
H	-2.02284600	2.96953200	2.68061000
C	-3.43776300	-0.13574100	1.20965900
C	-4.17332200	1.11177400	0.68311900
F	-4.55544700	1.88688600	1.70443700
F	-5.26218100	0.77281000	-0.00224900
F	-3.38442900	1.83960300	-0.11112300
O	-4.03250700	-0.93201300	1.86974700
H	-0.14884600	-1.51866600	-0.56853600
H	-2.37087300	-0.20354600	0.94199200
C	-5.03389500	-0.22154900	-3.05978500
C	-3.69111800	-0.00230500	-2.79233000
C	-3.00739500	-0.82085600	-1.88633000
C	-3.69181900	-1.87547300	-1.27451300
C	-5.03961200	-2.08697100	-1.53887000
C	-5.71353200	-1.26112900	-2.43001900
H	-5.55129000	0.41747500	-3.76478000
H	-3.16771000	0.79309800	-3.30748500
H	-3.16162500	-2.51764700	-0.58315900
H	-5.56182800	-2.89634600	-1.04380700
H	-6.76399900	-1.42641600	-2.63687200
C	-1.57277600	-0.60163900	-1.56903200
O	-1.00867800	-1.67360400	-1.02143200
C	-0.97099400	0.59470900	-1.78178500
H	1.72447400	2.21407800	-1.57013000
H	-1.56463200	1.43937600	-2.09350700
C	0.45359200	0.81918300	-1.62020200
O	0.76631900	2.12461000	-1.69811500
O	1.30464000	-0.03302800	-1.44226400

IM2b

C	-1.81800600	1.67608000	-2.60796500
C	-1.89482300	2.30437200	-1.23061000
O	-3.13450400	2.61028800	-0.79116900
C	-1.48937100	2.96607300	0.83816700
C	-2.95141000	3.28627500	0.46698800
H	-0.95046400	3.84401900	1.19079100
H	-3.11353400	4.35300100	0.30209500
C	-1.74731000	0.17586600	-2.37601400
O	-0.70787800	-0.47939400	-2.93756400
C	-2.21383500	-1.90784300	-1.84050400
C	-0.82860900	-1.85722500	-2.52480100
H	-2.93217700	-2.39400200	-2.51096100
H	-0.77010200	-2.48157900	-3.41451000
N	-0.91590200	2.52554400	-0.45267800
N	-2.61614500	-0.49203100	-1.74446700
C	-3.09526600	1.97053000	-3.41079900
H	-3.97381300	1.59585000	-2.88991800
H	-3.20092300	3.04637200	-3.56277100
H	-3.02361100	1.48585300	-4.38646400
C	-0.58800900	2.19179200	-3.35983700
H	0.33287200	1.95576500	-2.83303700
H	-0.55176900	1.73638600	-4.35040300
H	-0.66421100	3.27460100	-3.47447900
H	-3.68091000	2.89799900	1.17464200
H	0.00506900	-2.06625600	-1.85723600
C	-1.36883900	1.85555900	1.86280500
C	-0.63316200	2.03990000	3.03217000
C	-2.00158600	0.62822600	1.64316100
C	-0.51699000	1.01413300	3.96913600
H	-0.14404300	2.99258500	3.20190200
C	-1.88697500	-0.39638100	2.57564300
H	-2.55623600	0.45387900	0.72372000
C	-1.14139900	-0.20733500	3.73903900
H	0.06671800	1.16879200	4.86894000
H	-2.36222700	-1.35066100	2.38192100
H	-1.04508900	-1.01285700	4.45744900
C	-2.33499400	-2.61349200	-0.50210300
C	-1.30552100	-3.33167600	0.09835300
C	-3.58633800	-2.58452200	0.12305100
C	-1.52202400	-4.01375300	1.29593100
H	-0.32579700	-3.38311100	-0.36021500
C	-3.80700000	-3.26997000	1.30939900
H	-4.38694700	-2.01554800	-0.33684400
C	-2.77126800	-3.99189700	1.90111300
H	-0.70571400	-4.56177800	1.75081200

H	-4.78513000	-3.24059400	1.77517500
H	-2.93914400	-4.52933200	2.82682600
C	0.77779400	-0.58625600	0.93041900
C	1.69513400	-1.77074500	1.27671500
F	1.09934700	-2.52543700	2.21075900
F	1.94380800	-2.53604000	0.21963300
F	2.85884200	-1.35553900	1.78387700
O	0.23559000	-0.52872800	-0.13126600
H	1.04346600	2.36132100	-0.60993900
H	0.65474900	0.14639000	1.73985700
C	5.15963800	-1.38598900	-1.30747400
C	4.59368300	-0.28552600	-0.67970500
C	3.33010100	0.17023200	-1.06494700
C	2.64825000	-0.47919400	-2.09914700
C	3.21965000	-1.58103500	-2.72311000
C	4.47186000	-2.03883800	-2.32723800
H	6.14096600	-1.73137300	-1.00606900
H	5.14231800	0.22962000	0.09942100
H	1.66231400	-0.13234400	-2.38595700
H	2.68191100	-2.08555400	-3.51735200
H	4.91551200	-2.89889900	-2.81461600
C	2.66170300	1.29749200	-0.37301500
O	1.73050500	1.86815000	-1.11594900
C	2.94907800	1.63037100	0.91453800
H	2.34893100	3.70867400	3.19469800
H	3.67742600	1.06168700	1.47031800
C	2.32282700	2.75602700	1.58040600
O	2.77904400	2.91973700	2.83994900
O	1.48274700	3.50021500	1.11415000

IM2c

C	1.61770900	-3.33468200	-0.41826300
C	2.58501600	-2.18181500	-0.59164500
O	3.13314200	-2.07674600	-1.81795600
C	4.07300700	-0.61483700	-0.25885600
C	3.91843800	-0.86873000	-1.77352800
H	5.01362400	-1.06088600	0.09039300
H	4.85439700	-1.05138300	-2.29627600
C	0.71796500	-2.94201600	0.72137800
O	1.12605300	-3.16690100	1.94814500
C	-0.95615700	-2.04035400	1.96294500
C	0.06303500	-2.78325700	2.85769900
H	-1.96332400	-2.44001100	2.07389100
H	-0.33571000	-3.70019600	3.28939200
N	2.98477000	-1.41304000	0.32970600
N	-0.44439800	-2.39767000	0.63052500
C	0.81379800	-3.60188500	-1.69494800
H	0.30394400	-2.70139600	-2.03012900
H	1.50168700	-3.93625400	-2.47079300
H	0.07907600	-4.38832600	-1.51112900
C	2.44435300	-4.57502400	-0.02472700
H	3.01018200	-4.39784800	0.88878500
H	1.78517500	-5.43317800	0.11879300
H	3.13526200	-4.80109700	-0.83756900
H	3.35262700	-0.07988100	-2.27319500
H	0.49698400	-2.15039600	3.62707200
C	4.08387700	0.83469700	0.16460300
C	3.33625400	1.27521800	1.25423000
C	4.92064700	1.73832300	-0.49424900
C	3.43085000	2.59590800	1.68389500
H	2.68760400	0.57453400	1.76479100
C	5.02175900	3.05538000	-0.05932000
H	5.51343300	1.40837400	-1.34218000
C	4.27856500	3.48720700	1.03588500
H	2.84076600	2.92473400	2.53191400
H	5.68158900	3.74331700	-0.57499400
H	4.35655600	4.51287700	1.37627300
C	-0.98471100	-0.54474600	2.20073400
C	-1.89241500	-0.04171400	3.13491000
C	-0.12011600	0.32502100	1.54068400
C	-1.94564600	1.32061000	3.39841600
H	-2.58072400	-0.71705800	3.63296000
C	-0.18286400	1.69523100	1.79964500
H	0.57603500	-0.04736800	0.79495400
C	-1.09320700	2.19378200	2.72369900
H	-2.66217900	1.70361200	4.11523200

H	0.47339800	2.36752000	1.25609600
H	-1.14664500	3.25938800	2.91259300
C	-3.54382400	0.16231100	0.39508900
C	-4.77994300	0.84630000	-0.21105600
F	-5.30042000	1.64661700	0.73615900
F	-5.70906800	-0.02402600	-0.57117800
F	-4.48515400	1.62127600	-1.25753700
O	-3.60296700	-0.98722600	0.72428200
H	-0.98728100	-2.21104000	-0.29112400
H	-2.69312900	0.83250800	0.59481000
C	-0.74636400	4.09778200	-1.13274700
C	-1.15713700	2.79023600	-1.37031100
C	-0.21510500	1.77459800	-1.55224400
C	1.13994500	2.09643000	-1.49526000
C	1.55535000	3.40291700	-1.27281600
C	0.60997900	4.40800400	-1.08465900
H	-1.48673300	4.87460800	-0.98091000
H	-2.21561800	2.56100000	-1.38735400
H	1.85983400	1.29609600	-1.60026000
H	2.61361700	3.63016100	-1.23227500
H	0.92822700	5.42767200	-0.90035700
C	-0.59372400	0.31697300	-1.69772400
O	0.28660000	-0.52625900	-1.45083400
C	-1.93295000	0.02928400	-2.06532500
H	-4.06241200	-2.23248500	-2.21819600
H	-2.55462800	0.79484500	-2.50096500
C	-2.48852500	-1.25583800	-1.96450500
O	-3.74690800	-1.35330500	-2.46169200
O	-2.01762100	-2.27083100	-1.41427400

IM2d

C	-3.61468500	-0.14839700	0.19225900
C	-3.08281500	1.03711000	-0.57067500
O	-3.82917300	2.11633400	-0.64649000
C	-1.76390700	2.45736900	-1.76830900
C	-3.15044900	3.08643300	-1.48964500
H	-1.58354300	2.35151200	-2.83831800
H	-3.75373500	3.20785500	-2.38708100
C	-2.71990300	-0.34655300	1.39203300
O	-2.86255500	-1.53284800	2.01060300
C	-1.38197000	-0.07369100	3.10980700
C	-1.85365300	-1.54949400	3.03993800
H	-1.84150100	0.43209200	3.96571100
H	-2.30617400	-1.91251900	3.96029200
N	-1.96571500	1.11666400	-1.19810200
N	-1.94484300	0.52091900	1.88778400
C	-5.03481500	0.13587000	0.71127900
H	-5.05441600	1.02206600	1.34572300
H	-5.71956600	0.28313800	-0.12458300
H	-5.36615000	-0.72596200	1.29055600
C	-3.61191700	-1.38599800	-0.72224800
H	-2.61063500	-1.62393000	-1.07524500
H	-4.00677600	-2.22992400	-0.15709300
H	-4.25773600	-1.20116300	-1.58315800
H	-3.09180200	4.01921500	-0.93465200
H	-1.05536800	-2.21901100	2.71717500
C	-0.60989100	3.20098200	-1.13044800
C	0.15704300	4.05999300	-1.91211100
C	-0.32577100	3.05847400	0.22730300
C	1.19831500	4.78698500	-1.34044200
H	-0.04784700	4.15266100	-2.97369000
C	0.72432300	3.77262900	0.79183200
H	-0.89570300	2.36194200	0.83549000
C	1.48340400	4.64326400	0.01287500
H	1.79284000	5.45123000	-1.95618400
H	0.95741200	3.63612300	1.84146400
H	2.30149600	5.19765500	0.45746600
C	0.11788300	0.05846500	3.23171900
C	0.69419700	-0.05133000	4.49820500
C	0.93933300	0.23364000	2.11717400
C	2.07434900	-0.00294600	4.65669900
H	0.05511200	-0.17202500	5.36790500
C	2.32336400	0.28757200	2.27997100
H	0.50360400	0.33184700	1.12578300
C	2.89205800	0.16538400	3.54403400
H	2.50828500	-0.09009600	5.64590200

H	2.95923700	0.42903600	1.41384700
H	3.96875700	0.20743700	3.65979700
C	0.47453700	-2.35164500	0.06002400
C	0.60416000	-3.80783200	-0.40095700
F	0.51502200	-4.59278100	0.68891300
F	-0.36577200	-4.16219200	-1.23358100
F	1.78364600	-4.06382900	-0.96946200
O	-0.61304800	-1.87231500	0.21635400
H	-0.95423800	-3.05530200	-4.10868200
H	1.41484600	-1.87890100	0.38537300
C	5.00951600	-0.41749000	-0.59611400
C	3.76754500	-0.84194400	-1.06009700
C	2.74710000	0.08427800	-1.27957500
C	2.98482700	1.43871500	-1.03324100
C	4.23126300	1.86401100	-0.59306000
C	5.24542100	0.93517700	-0.36720600
H	5.79177300	-1.14376000	-0.40956900
H	3.58378500	-1.89875900	-1.22241500
H	2.17060300	2.14050400	-1.17527400
H	4.40702300	2.91832300	-0.41128100
H	6.21459600	1.26319900	-0.00998300
C	1.35698200	-0.31199900	-1.69912100
O	0.44072900	0.44232700	-1.28761200
C	1.18044400	-1.47155700	-2.45888800
H	-1.13791700	0.43961200	-1.25444100
H	2.03392900	-2.02332900	-2.82245600
C	-0.10359800	-1.81927500	-2.99038700
O	-1.18289300	-1.29356200	-2.75598500
O	-0.04287300	-2.87516400	-3.84746200

IM2e

C	2.11148600	-3.12035500	-1.18880400
C	2.23119200	-1.65528000	-1.56150700
O	1.09578000	-1.07588300	-2.00958100
C	2.89276300	0.42301400	-1.83693300
C	1.36190300	0.33961700	-2.03172600
H	3.39745800	0.63155700	-2.78689200
H	0.99399400	0.74508100	-2.97254000
C	1.45387200	-3.07987200	0.17906400
O	2.21655100	-3.42952400	1.22349700
C	0.16160300	-2.53501500	1.89593900
C	1.35412600	-3.38244300	2.38179100
H	-0.79229300	-2.93744900	2.23199300
H	1.06507100	-4.40667200	2.62215900
N	3.26645400	-0.94095700	-1.42174800
N	0.27689100	-2.65659100	0.42925600
C	1.21229700	-3.86430100	-2.18790800
H	0.22473700	-3.41424700	-2.25799700
H	1.67839600	-3.84225700	-3.17465900
H	1.10928400	-4.90553500	-1.87780100
C	3.49666800	-3.76322400	-1.11791900
H	4.14771500	-3.22521400	-0.43243200
H	3.40668700	-4.79866700	-0.78713800
H	3.94664600	-3.74586100	-2.11111900
H	0.82967000	0.79993400	-1.19725400
H	1.91037200	-2.93712200	3.20280400
C	3.32165200	1.47242300	-0.83172000
C	4.38498800	1.23402600	0.03964100
C	2.67355100	2.70847700	-0.78895000
C	4.79813000	2.21829600	0.93223000
H	4.87812800	0.27041900	0.01494700
C	3.09027500	3.69339900	0.10123300
H	1.83140800	2.91266300	-1.44528800
C	4.15573900	3.45265300	0.96309300
H	5.62313300	2.01903900	1.60599700
H	2.57489600	4.64649400	0.12126700
H	4.48021700	4.21931500	1.65652800
C	0.27876300	-1.08357200	2.32282400
C	-0.55543800	-0.58420300	3.32151700
C	1.28056600	-0.25933500	1.79892900
C	-0.38188000	0.70996000	3.80749000
H	-1.34329100	-1.21562400	3.71914700
C	1.45946600	1.03081600	2.28697800
H	1.94761400	-0.62301600	1.02169700
C	0.63298600	1.51355900	3.29929400
H	-1.03377700	1.08425300	4.58803100

H	2.24366600	1.65573300	1.87404300
H	0.78012700	2.51346900	3.69070800
C	-3.16719900	-0.64754000	1.35571800
C	-4.46533100	-0.21950200	0.65345100
F	-5.47427500	-0.29786100	1.53161400
F	-4.75622600	-0.99668300	-0.38045300
F	-4.38839500	1.04586600	0.24013200
O	-2.91571700	-1.80389600	1.52496500
H	-0.99358600	-2.46418900	-0.60120000
H	-2.56646600	0.18447100	1.75749200
C	-0.37355700	3.67782200	0.66868400
C	-0.90773700	2.47228500	0.22974000
C	-1.52109400	2.39249900	-1.02234700
C	-1.59611300	3.53237100	-1.82505700
C	-1.05217100	4.73369600	-1.38928600
C	-0.44215700	4.80843100	-0.13981900
H	0.10324900	3.73012000	1.63983500
H	-0.84029700	1.60079900	0.87228300
H	-2.08684900	3.45398800	-2.78701400
H	-1.10819500	5.61278500	-2.01994700
H	-0.02408500	5.74737900	0.20461500
C	-2.09553000	1.11908600	-1.55572900
O	-2.89416200	1.18954800	-2.51949000
C	-1.69889100	-0.12335500	-0.99617100
H	-3.12274600	-0.26386100	-2.79408800
H	-0.93146000	-0.20548400	-0.24048900
C	-2.11911300	-1.29482200	-1.63873300
O	-2.94339600	-1.26335400	-2.63757700
O	-1.73626400	-2.48426700	-1.28955500

IM2f

C	3.92884200	-0.33532200	0.37311200
C	3.29357100	1.03240100	0.49569100
O	3.99195400	2.06445400	0.00311900
C	1.96416900	2.75232400	0.96605700
C	3.33794100	3.26203100	0.46896700
H	1.72799800	3.15179000	1.95404700
H	3.94630700	3.68045300	1.27186300
C	3.20270200	-1.12284200	-0.69046100
O	3.40940300	-2.45341600	-0.62166300
C	2.01169200	-1.82980500	-2.40490900
C	2.54419100	-3.04341200	-1.60601000
H	2.47357900	-1.78831000	-3.39698400
H	3.12780500	-3.73959500	-2.20499600
N	2.18807000	1.29763800	1.07292300
N	2.49129700	-0.66256200	-1.62921600
C	5.40356300	-0.22328200	-0.05158300
H	5.49966300	0.30027700	-1.00237500
H	5.97206100	0.31836100	0.70573100
H	5.81722000	-1.22741000	-0.15073700
C	3.82213700	-1.05228800	1.73107700
H	2.78425600	-1.23168000	2.00549900
H	4.33468500	-2.01154500	1.67020200
H	4.29855100	-0.44374200	2.50202700
H	3.26888000	3.96101400	-0.36094000
H	1.76337700	-3.57721000	-1.06433900
C	0.85475600	3.11191100	0.00085700
C	-0.01172900	4.16212500	0.29948800
C	0.77520600	2.48535500	-1.24426700
C	-0.92307100	4.61620000	-0.64957500
H	0.03466900	4.63474900	1.27497100
C	-0.13105600	2.94718900	-2.19438600
H	1.43156200	1.64743700	-1.46642400
C	-0.96917100	4.02135200	-1.90577900
H	-1.59018900	5.43524500	-0.40962000
H	-0.17458500	2.48017500	-3.17208600
H	-1.66010500	4.38906800	-2.65537800
C	0.50335800	-1.75775800	-2.56818400
C	-0.34244200	-2.84975200	-2.37912000
C	-0.06517400	-0.51761800	-2.86464100
C	-1.72785700	-2.68493100	-2.39952500
H	0.05951000	-3.83647900	-2.18163800
C	-1.44330100	-0.35051000	-2.88474100
H	0.59221400	0.32455600	-3.03781500
C	-2.28337000	-1.43101400	-2.62352500
H	-2.36858200	-3.53815200	-2.21107100

H	-1.86661700	0.62816300	-3.07598300
H	-3.35763500	-1.28992400	-2.59238100
C	-0.28993200	-1.71216100	0.43065400
C	-1.37876100	-2.63723100	1.00707000
F	-1.18165400	-3.88841900	0.56920700
F	-1.34068100	-2.66261900	2.33675400
F	-2.59888900	-2.25872800	0.62516100
O	0.84707300	-1.88917200	0.76432600
H	1.35346900	0.51496200	2.25826600
H	-0.62983500	-0.96951900	-0.30465400
C	-3.68159000	1.86605200	-1.33261900
C	-2.87430400	1.57458000	-0.23737300
C	-3.32821500	0.69744900	0.74739400
C	-4.58963400	0.11060600	0.62141700
C	-5.38310700	0.38601700	-0.48253600
C	-4.93029300	1.26811600	-1.46209200
H	-3.33102300	2.56377300	-2.08392900
H	-1.90501400	2.05263400	-0.14876600
H	-4.92304000	-0.56561000	1.39843700
H	-6.35616900	-0.08045600	-0.57936300
H	-5.55328100	1.49290800	-2.32001400
C	-2.50887600	0.34580100	1.94670400
O	-3.09215300	-0.16264700	2.93445400
C	-1.10010800	0.52278200	1.92064200
H	-1.94485500	-0.39809100	3.84252000
H	-0.58192700	0.96119900	1.08147700
C	-0.36364700	0.10934600	3.03733500
O	-0.94174100	-0.38091000	4.08658400
O	0.93465900	0.15432500	3.10537800

IM2g

C	3.77639300	-2.56924300	-0.32112000
C	3.52958000	-1.46404800	-1.32856300
O	2.27634400	-1.41814200	-1.82679500
C	3.62732600	0.37693600	-2.52258700
C	2.24706800	-0.30277000	-2.73776400
H	4.15851200	0.47852600	-3.47229800
H	2.12346700	-0.69859700	-3.74621500
C	3.17319500	-2.01806500	0.95649800
O	4.02595500	-1.53553400	1.87446800
C	1.77705300	-1.14727200	2.43518000
C	3.21690800	-1.13778200	3.00210300
H	1.08803800	-1.66584300	3.10399000
H	3.36010900	-1.87748100	3.79064900
N	4.35785500	-0.56825500	-1.66547500
N	1.92839100	-1.91294500	1.18816400
C	3.02964100	-3.84636500	-0.73088200
H	1.96000700	-3.66676000	-0.82077700
H	3.40968200	-4.19723600	-1.69214700
H	3.19898700	-4.62354100	0.01616100
C	5.27526700	-2.82438100	-0.16763300
H	5.80529800	-1.90857900	0.08457500
H	5.44626500	-3.56469800	0.61539100
H	5.67084100	-3.20727200	-1.10923600
H	1.39642400	0.32039300	-2.46985600
H	3.55123000	-0.15743800	3.33443400
C	3.52488500	1.75424700	-1.88925900
C	4.09134400	2.04659400	-0.65158600
C	2.83684500	2.75948500	-2.57433100
C	3.96901900	3.32246100	-0.10656800
H	4.62028800	1.26860600	-0.11464000
C	2.71538500	4.03251800	-2.03167500
H	2.39633700	2.54362700	-3.54344900
C	3.28358300	4.31762400	-0.79192100
H	4.40754800	3.53486800	0.86138400
H	2.18042400	4.80209100	-2.57571100
H	3.18958700	5.30900600	-0.36509500
C	1.23532800	0.24289300	2.16099800
C	0.65375100	0.96870900	3.20452300
C	1.31495800	0.81857500	0.89660900
C	0.14718100	2.24224600	2.98031800
H	0.56896800	0.51828300	4.18857700
C	0.81525100	2.10023900	0.67054800
H	1.72857400	0.25729600	0.06776400
C	0.22658000	2.81173500	1.70804400
H	-0.31842800	2.78857600	3.79206400

H	0.89168800	2.53128200	-0.32189900
H	-0.17179300	3.80376500	1.53178000
C	-2.02051800	0.00452000	1.86140200
C	-3.36734100	0.74278900	1.78722200
F	-3.49443400	1.54633700	2.85042000
F	-4.39603300	-0.09737700	1.77712500
F	-3.42715900	1.50797900	0.69311600
O	-1.88338100	-0.92138900	2.60183300
H	0.45479300	-2.05775400	0.19290300
H	-1.22784300	0.43189800	1.22665600
C	-6.87578300	-1.68492400	-1.21859700
C	-5.48801400	-1.70079900	-1.22095700
C	-4.77330400	-0.51639700	-1.41458800
C	-5.46457800	0.68012800	-1.61701200
C	-6.85318300	0.69266800	-1.60844100
C	-7.56102500	-0.48809600	-1.40822400
H	-7.42371200	-2.60809600	-1.07496500
H	-4.96050000	-2.63822900	-1.09443700
H	-4.90353400	1.59332000	-1.76635500
H	-7.38361300	1.62546000	-1.75634600
H	-8.64438900	-0.47768700	-1.40397200
C	-3.29633800	-0.49833700	-1.39146900
O	-2.75828700	0.53332500	-2.03043800
C	-2.54763800	-1.42399600	-0.72889300
H	-1.78087100	0.46866300	-1.89949400
H	-3.01197400	-2.22438400	-0.17447800
C	-1.09793700	-1.31123700	-0.70135200
O	-0.48751500	-0.38800900	-1.24567700
O	-0.50446400	-2.24900700	0.00787600

IM2h

C	-3.41872000	-0.91746800	-1.82317500
C	-3.45823200	0.56864000	-1.55782500
O	-4.62878500	1.06741900	-1.14487300
C	-2.93870200	2.71141900	-1.22595300
C	-4.45043900	2.48984400	-0.98676900
H	-2.76661300	3.43468700	-2.02501400
H	-5.07464500	2.98806700	-1.72775400
C	-3.09114800	-1.58426300	-0.50895700
O	-2.81954300	-2.90340200	-0.60037700
C	-2.75418100	-2.08102800	1.60522700
C	-2.42223100	-3.31430800	0.72072900
H	-3.64396500	-2.27481400	2.21297600
H	-2.98475800	-4.20743400	0.98657400
N	-2.48474700	1.37904500	-1.68422500
N	-3.08798400	-1.03432200	0.62986600
C	-4.79483000	-1.42016700	-2.29553200
H	-5.56744700	-1.19804400	-1.56035300
H	-5.06092300	-0.94230400	-3.24028100
H	-4.74410000	-2.49814500	-2.45010800
C	-2.34436300	-1.25349500	-2.86663000
H	-1.34820300	-0.98488000	-2.52162300
H	-2.35925900	-2.32603600	-3.05851200
H	-2.55786400	-0.72086400	-3.79500100
H	-4.76913900	2.76269400	0.01745000
H	-1.35404400	-3.53265000	0.70055900
C	-2.16330300	3.12946700	0.00271900
C	-1.28860200	4.20930200	-0.04495400
C	-2.27599400	2.38368800	1.17625000
C	-0.52140400	4.54181600	1.06804300
H	-1.19344300	4.78367300	-0.96077500
C	-1.51407300	2.71671100	2.28790200
H	-2.92024400	1.50770300	1.20334900
C	-0.63220000	3.79433500	2.23454600
H	0.16491900	5.37892700	1.02101700
H	-1.59265500	2.12201700	3.19054900
H	-0.03158000	4.04712900	3.10038800
C	-1.62177700	-1.69364700	2.52900300
C	-1.40742000	-2.42761800	3.69646500
C	-0.76473300	-0.64080500	2.21878800
C	-0.34123900	-2.12401300	4.53551900
H	-2.08179000	-3.23958100	3.95227400
C	0.30146600	-0.33298900	3.06130500
H	-0.93107100	-0.06822700	1.31379000
C	0.51763900	-1.07514900	4.21836200
H	-0.18399100	-2.70135300	5.43899300

H	0.96662600	0.48678400	2.80889300
H	1.34842800	-0.83620600	4.87152500
C	1.05591400	-1.66960800	-0.25025200
C	2.13250900	-2.45868000	-1.01133000
F	1.96629500	-3.76696800	-0.78969500
F	2.05593000	-2.25211700	-2.32362200
F	3.35490500	-2.12375000	-0.59748600
O	-0.08380400	-1.74220000	-0.60487500
H	-0.93639400	1.15742900	-1.97985800
H	1.39870500	-1.11416900	0.63836400
C	6.52490300	0.07331800	-1.54324700
C	5.14236500	0.18541700	-1.47761100
C	4.53974200	0.80436800	-0.38017800
C	5.33801500	1.29929700	0.65244200
C	6.72073200	1.19458900	0.58119800
C	7.31634800	0.58243200	-0.51752100
H	6.98533600	-0.41640100	-2.39263500
H	4.53531000	-0.23851000	-2.26786700
H	4.85539500	1.76557800	1.50193000
H	7.33437300	1.58832500	1.38243300
H	8.39508900	0.49669200	-0.57268800
C	3.06082400	0.95775600	-0.26262500
O	2.58351600	1.22822800	0.87799500
C	2.22823800	0.81899800	-1.39584900
H	1.19567100	1.40348700	0.56002600
H	2.60636100	0.63817700	-2.38794400
C	0.86008000	1.08068600	-1.24045900
O	0.36409300	1.37112900	-0.07735000
O	0.04949100	1.01853000	-2.24811000

TS2a

C	-1.48096000	3.11422500	1.00965100
C	-2.22321100	2.55055600	-0.18806300
O	-1.85885700	3.04399400	-1.38333400
C	-3.59839900	1.49168500	-1.52362600
C	-2.51441400	2.20444400	-2.35409500
H	-4.55718900	2.01175900	-1.63914900
H	-2.90739200	2.83652200	-3.14692500
C	-1.29008700	1.94862000	1.94657400
O	-2.18296500	1.75134000	2.88327800
C	-0.58517000	0.00098400	2.90731500
C	-1.74543900	0.63316700	3.70483500
H	0.30615600	-0.14412700	3.51208500
H	-1.43026100	1.04886600	4.66076500
N	-3.15880700	1.70244700	-0.12786400
N	-0.32829700	1.08818000	1.94119200
C	-0.12713700	3.69777200	0.59397100
H	0.45578400	2.97496700	0.02785600
H	-0.30332300	4.57480200	-0.02779600
H	0.43599500	3.99900700	1.47921800
C	-2.36676600	4.18278800	1.67251600
H	-3.32576400	3.76487600	1.97420700
H	-1.86336900	4.60160800	2.54576500
H	-2.53643600	4.98411800	0.95218200
H	-1.75703000	1.52253700	-2.73896100
H	-2.59431000	-0.03254100	3.83193200
C	-3.85550100	0.02861000	-1.82198400
C	-4.76036900	-0.65356600	-1.00320400
C	-3.29920600	-0.64317900	-2.90921500
C	-5.11303100	-1.96838800	-1.27340500
H	-5.18557800	-0.13680500	-0.14988500
C	-3.64098900	-1.97104000	-3.17359400
H	-2.61472900	-0.13857300	-3.58159900
C	-4.55285500	-2.63379400	-2.36266500
H	-5.81941700	-2.47926100	-0.62991600
H	-3.19932400	-2.47723900	-4.02375700
H	-4.82484600	-3.66072200	-2.57433500
C	-0.94792400	-1.29925300	2.22596600
C	-0.43509200	-2.49293700	2.72940300
C	-1.78319200	-1.32040300	1.11122100
C	-0.73932100	-3.70107300	2.11527500
H	0.24544600	-2.46902800	3.57304700
C	-2.07129800	-2.53155400	0.48576300
H	-2.18594100	-0.39849900	0.70117500
C	-1.55187100	-3.72083800	0.98429500
H	-0.32010200	-4.62204800	2.50211100

H	-2.69947700	-2.53899300	-0.39703500
H	-1.77014100	-4.65913500	0.48848100
C	1.76427300	-1.51631100	0.64155800
C	2.99721500	-2.38484500	0.38537700
F	3.09102000	-3.31020800	1.35905800
F	4.13896900	-1.69245700	0.39048200
F	2.93622700	-3.06293000	-0.77470400
O	1.79149200	-0.80742000	1.66540200
H	0.47293200	1.07150000	1.27374500
H	0.85602500	-2.07233800	0.34322600
C	5.81856500	0.79778300	-2.42111100
C	4.48837600	0.54212100	-2.10659200
C	3.95444700	0.98779300	-0.89757500
C	4.76740400	1.68988600	-0.00651900
C	6.09823400	1.93398200	-0.31448400
C	6.62604400	1.48915100	-1.52434300
H	6.22447300	0.45600500	-3.36568800
H	3.86437500	0.01082900	-2.81497200
H	4.33559300	2.02333800	0.92872900
H	6.72752900	2.46772400	0.38779900
H	7.66471600	1.68086400	-1.76675700
C	2.52413800	0.75525700	-0.51137800
O	2.01318600	1.49044800	0.33347300
C	1.82418000	-0.39715700	-1.03539700
H	-1.05122400	-1.24260200	-1.99823600
H	2.32604200	-1.01592700	-1.76687700
C	0.39188300	-0.28177400	-1.27160400
O	-0.08531100	-1.32504500	-1.98848700
O	-0.36387000	0.58646000	-0.87488900

Value of Imaginary Frequency= -168.9 cm^{-1}

TS2b

C	-1.03566800	3.43379100	-0.28747100
C	-1.58731500	2.67441300	0.89341100
O	-2.83024700	2.88251600	1.24935600
C	-1.88007600	1.14749800	2.56734200
C	-3.12015900	2.05756200	2.41159700
H	-1.44326400	1.22372500	3.55996000
H	-3.26257500	2.73311900	3.25295800
C	-0.86552900	2.37515500	-1.36695400
O	0.37260700	2.16269300	-1.83414200
C	-1.25480800	0.85093200	-2.89164600
C	0.26719700	0.98293600	-2.67447300
H	-1.53318000	1.29903000	-3.85415900
H	0.82769400	1.17170100	-3.58750200
N	-0.96872700	1.79515900	1.60346300
N	-1.83392900	1.71771300	-1.84451400
C	-2.06082200	4.46921000	-0.77089000
H	-2.99957400	3.98991500	-1.04084300
H	-2.24178900	5.21444200	0.00513600
H	-1.65488100	4.97093700	-1.65018400
C	0.28918000	4.11335400	0.08452500
H	1.04305200	3.39252600	0.39370500
H	0.65786900	4.65111100	-0.78973300
H	0.11509500	4.83375200	0.88591100
H	-4.03188000	1.50542800	2.19981100
H	0.68491600	0.16021500	-2.09745300
C	-2.13496000	-0.30295600	2.22794800
C	-2.04133600	-1.27003700	3.22669200
C	-2.48975800	-0.67577000	0.93205700
C	-2.29901900	-2.60610000	2.93581900
H	-1.75381000	-0.97243900	4.22982900
C	-2.72748800	-2.01240700	0.63682500
H	-2.52390000	0.05958000	0.13277900
C	-2.63307200	-2.97720400	1.63703000
H	-2.22040200	-3.35496800	3.71478800
H	-2.95941300	-2.29736800	-0.38263200
H	-2.81078200	-4.01960700	1.40035700
C	-1.85234300	-0.53973800	-2.86824600
C	-1.08213000	-1.69469400	-2.93320600
C	-3.24613700	-0.65558700	-2.85402700
C	-1.69192500	-2.94649800	-2.99986700
H	-0.00067700	-1.63784200	-2.92185000
C	-3.85537900	-1.90070200	-2.92549700
H	-3.84606800	0.24511600	-2.78532200
C	-3.07612000	-3.05427400	-3.00604500
H	-1.07503000	-3.83620300	-3.03632500

H	-4.93674300	-1.97390100	-2.91685100
H	-3.54765600	-4.02834500	-3.06246700
C	0.63205100	-1.34110800	0.59140800
C	1.36345100	-2.40771900	-0.23312800
F	0.46073300	-3.15855300	-0.89328200
F	2.17515200	-1.87351200	-1.15563800
F	2.09139000	-3.26915700	0.49780300
O	0.11784100	-0.39703800	-0.05401800
H	0.01438900	1.47704800	1.43789200
H	0.05803100	-1.85316700	1.38810700
C	5.81975200	-0.27197900	-0.57263400
C	4.75359000	-0.31626900	0.31838800
C	3.63810900	0.49656700	0.11637600
C	3.59676700	1.35052700	-0.98832800
C	4.65547800	1.38113900	-1.88579100
C	5.76958200	0.57142900	-1.67778800
H	6.68825900	-0.89761100	-0.40575100
H	4.80369200	-0.97230400	1.17898000
H	2.71478300	1.96480700	-1.13186200
H	4.61454400	2.03446500	-2.74943500
H	6.59746800	0.59742400	-2.37658000
C	2.45206800	0.49093600	1.02976000
O	1.72101600	1.47837200	1.05067200
C	2.10473000	-0.73211800	1.72492900
H	0.92932000	-1.65347500	4.49134700
H	2.84113400	-1.52315900	1.73233800
C	1.38418400	-0.62646100	2.99175600
O	1.48372300	-1.76907100	3.70882400
O	0.70655000	0.29677600	3.39096300

Value of Imaginary Frequency= -203.6 cm^{-1}

TS2c

C	-1.23880500	3.39413400	-0.31502500
C	-2.27345000	2.32438900	-0.60513000
O	-2.72455000	2.30315200	-1.87538700
C	-3.92299800	0.89698100	-0.45139600
C	-3.61544100	1.17068100	-1.93744500
H	-4.83642600	1.43535600	-0.16555500
H	-4.48087100	1.45133800	-2.53292100
C	-0.45276300	2.90375700	0.87135200
O	-0.94173100	3.11603100	2.06616000
C	1.04064100	1.82600200	2.21968800
C	0.01172800	2.62597800	3.04769500
H	2.06363100	2.12762900	2.42857600
H	0.44189500	3.49979400	3.53485400
N	-2.81172800	1.56374000	0.25054600
N	0.67892600	2.28414900	0.86432100
C	-0.33583500	3.65626500	-1.52313500
H	0.13156100	2.74013500	-1.87320000
H	-0.94504200	4.07990300	-2.32074400
H	0.44369500	4.37203100	-1.25559200
C	-2.00685600	4.67440000	0.07392000
H	-2.64661800	4.50366900	0.93827700
H	-1.30301500	5.47824500	0.29711200
H	-2.62108300	4.97729700	-0.77462700
H	-3.08193100	0.34331800	-2.41169200
H	-0.53510300	2.01474200	3.76004200
C	-4.12758100	-0.55147600	-0.07714600
C	-3.59040200	-1.07644500	1.09643400
C	-4.94396200	-1.36022800	-0.87091100
C	-3.87307800	-2.38593300	1.47455500
H	-2.95879500	-0.44991100	1.71395300
C	-5.23393700	-2.66562700	-0.48799900
H	-5.37357100	-0.96473400	-1.78623200
C	-4.70139700	-3.18131900	0.69016100
H	-3.44668700	-2.78119300	2.38951900
H	-5.87556300	-3.27877600	-1.10982100
H	-4.92673900	-4.19755400	0.99053000
C	0.91815700	0.32662000	2.38327100
C	1.83630400	-0.33013800	3.20199000
C	-0.08959900	-0.40062300	1.75469100
C	1.75253800	-1.70331100	3.38978400
H	2.64306300	0.23173000	3.65982400
C	-0.16818400	-1.78095200	1.93991600
H	-0.78759400	0.08971300	1.08172500
C	0.74925800	-2.43273500	2.75493100
H	2.48167400	-2.20668700	4.01328900

H	-0.93394700	-2.34456000	1.41808500
H	0.69388400	-3.50729000	2.88262800
C	3.08438500	-0.31620600	0.18696300
C	4.43226900	-0.94394600	-0.17999400
F	5.08176100	-1.25607500	0.95759700
F	5.21760800	-0.11914400	-0.86940300
F	4.32912300	-2.09135100	-0.87681200
O	3.12953300	0.81313900	0.68477200
H	1.21910200	2.03023000	0.01314800
H	2.35897300	-1.08121200	0.51626800
C	0.57724800	-4.17825700	-1.14247100
C	1.14598500	-2.91707300	-1.29256100
C	0.33062600	-1.79031900	-1.40733000
C	-1.05543100	-1.94812300	-1.38068500
C	-1.62549500	-3.20634200	-1.25284600
C	-0.80617600	-4.32614700	-1.12575800
H	1.21752200	-5.04615200	-1.03832200
H	2.22383400	-2.81808100	-1.29492500
H	-1.67378400	-1.06154300	-1.43453400
H	-2.70386300	-3.30860700	-1.23734400
H	-1.24489000	-5.31096400	-1.01372900
C	0.86629900	-0.38391100	-1.48093300
O	0.08335000	0.53757100	-1.24251400
C	2.27304500	-0.20178400	-1.77768900
H	4.03136400	2.10776600	-2.99328600
H	2.75385800	-0.98388600	-2.35068800
C	2.72660400	1.13950700	-2.06992700
O	3.72979100	1.19034800	-2.97174000
O	2.32891600	2.16166800	-1.53540800

Value of Imaginary Frequency= -147.6 cm^{-1}

TS2d

C	3.61105800	-0.36998900	0.18317800
C	2.88927000	-1.44277900	-0.58974400
O	3.43221200	-2.63341000	-0.67283900
C	1.34654100	-2.60348900	-1.81088300
C	2.61781100	-3.44977700	-1.56065000
H	1.17073100	-2.44934500	-2.87525300
H	3.20429200	-3.61951400	-2.46170400
C	2.75703400	-0.04729500	1.38620900
O	3.02366300	1.13057000	1.97662100
C	1.39502000	-0.13903000	3.10368500
C	2.01531300	1.27868200	2.99702000
H	1.79543500	-0.66487200	3.97685000
H	2.49714900	1.61980200	3.91076700
N	1.77747600	-1.32438200	-1.22530200
N	1.89908000	-0.82020400	1.90099400
C	4.96413500	-0.89230500	0.69564200
H	4.83548500	-1.77811900	1.31748900
H	5.61705900	-1.13735800	-0.14282900
H	5.43216800	-0.10527700	1.28734400
C	3.81335700	0.85906200	-0.72093700
H	2.86493500	1.26392700	-1.06824500
H	4.34045800	1.62110000	-0.14736100
H	4.42321500	0.57806600	-1.58196500
H	2.41352500	-4.38620800	-1.04891200
H	1.29225100	2.01709600	2.64794100
C	0.10125500	-3.17100200	-1.16561800
C	-0.80105100	-3.88021700	-1.95244700
C	-0.13487600	-3.02227600	0.19941700
C	-1.93565500	-4.44779700	-1.37898000
H	-0.62865600	-3.97528400	-3.01952100
C	-1.27916900	-3.57191600	0.76599400
H	0.55100400	-2.44773200	0.81527700
C	-2.17800400	-4.29057500	-0.01854900
H	-2.63560800	-4.99583400	-1.99846700
H	-1.47270500	-3.42560900	1.82237600
H	-3.06841000	-4.71744800	0.42773200
C	-0.11163600	-0.11628700	3.21585500
C	-0.68401800	0.03304100	4.47988100
C	-0.93951900	-0.18843600	2.09420800
C	-2.06321500	0.12434900	4.62901800
H	-0.04254800	0.07408300	5.35510300
C	-2.32241600	-0.10347400	2.24670800
H	-0.50809600	-0.31334700	1.10463500
C	-2.88545200	0.05702400	3.50909100
H	-2.49337700	0.24128000	5.61679500

H	-2.96148100	-0.16629800	1.37376700
H	-3.96168800	0.12427100	3.61725200
C	-0.10348500	2.23481800	-0.00444800
C	0.10410300	3.72444200	-0.28625800
F	0.35862700	4.33028100	0.89138800
F	1.14092600	3.95381600	-1.08369000
F	-0.97738000	4.31672600	-0.79719600
O	0.85907400	1.51572100	0.11067900
H	1.40561800	2.98479000	-3.99544800
H	-1.11222400	1.97738500	0.35418600
C	-4.89441400	1.28147500	-0.48601200
C	-3.61045700	1.48694400	-0.98284700
C	-2.79966400	0.39736100	-1.30437900
C	-3.29042900	-0.89808900	-1.12564300
C	-4.57972500	-1.10254400	-0.65209600
C	-5.38337000	-0.01182100	-0.32558300
H	-5.51163600	2.13174800	-0.22118600
H	-3.23203300	2.49784900	-1.09038500
H	-2.63231000	-1.73219000	-1.34251000
H	-4.95260000	-2.11225000	-0.52209700
H	-6.38515700	-0.16860900	0.05699500
C	-1.36851800	0.53828500	-1.75768600
O	-0.62214700	-0.42959700	-1.52289300
C	-0.95152200	1.75104100	-2.34745200
H	1.15095700	-0.49333200	-1.31397100
H	-1.67672100	2.50032900	-2.62716500
C	0.35535100	1.86454500	-2.92575800
O	1.31662900	1.12550800	-2.76067900
O	0.48101900	2.96243000	-3.71982200

Value of Imaginary Frequency= -37.4 cm^{-1}

TS2e

C	2.09300900	-3.10487400	-1.15873600
C	2.16970300	-1.63913000	-1.55300400
O	0.98910400	-1.07167100	-1.88015900
C	2.79447900	0.43204800	-1.93662100
C	1.25008500	0.34153600	-1.99720200
H	3.21256700	0.62751400	-2.92974200
H	0.80812400	0.69548700	-2.92669700
C	1.49295000	-3.05307800	0.22823700
O	2.26801200	-3.32784800	1.25396900
C	0.22896100	-2.41989200	1.99580200
C	1.44281800	-3.24434200	2.45374900
H	-0.71776300	-2.79303400	2.37395400
H	1.18104000	-4.26562600	2.72957900
N	3.21176000	-0.92487600	-1.53751900
N	0.30651300	-2.65848200	0.54008400
C	1.17280200	-3.87926000	-2.11831600
H	0.16847600	-3.46188000	-2.15169000
H	1.60673800	-3.84157400	-3.11863600
H	1.12014000	-4.92303300	-1.80480200
C	3.49134400	-3.72066700	-1.11859000
H	4.15646500	-3.15921900	-0.46595200
H	3.43035700	-4.75256900	-0.77095100
H	3.90483400	-3.71037600	-2.12693500
H	0.78444400	0.84491400	-1.14743000
H	2.03550300	-2.76777800	3.22879800
C	3.30208100	1.49689700	-0.98605800
C	4.42415400	1.27451500	-0.18829100
C	2.65880900	2.73437800	-0.92462100
C	4.89568600	2.27602500	0.65561600
H	4.91915000	0.31243200	-0.23086200
C	3.13132000	3.73484200	-0.08183700
H	1.77743700	2.92660300	-1.52999500
C	4.25297500	3.50924800	0.71044200
H	5.76667200	2.09064400	1.27301400
H	2.61823900	4.68896800	-0.04516500
H	4.62224200	4.28784900	1.36703300
C	0.37418500	-0.94468400	2.31531600
C	-0.49980600	-0.35455000	3.22584100
C	1.43321000	-0.19322800	1.79551700
C	-0.29211900	0.95462700	3.65012400
H	-1.35205100	-0.92348400	3.57891300
C	1.63932000	1.11692000	2.21735100
H	2.12885000	-0.62263400	1.07784600
C	0.78634600	1.68424800	3.16056300
H	-0.97434700	1.40266800	4.36249200

H	2.46771700	1.68688600	1.81197000
H	0.95647300	2.69729500	3.50626700
C	-2.78896300	-0.57412100	0.96912400
C	-4.27482400	-0.33844200	0.67692400
F	-5.00131000	-0.60534700	1.77290800
F	-4.75194800	-1.10421900	-0.30935600
F	-4.52298300	0.94372200	0.35311900
O	-2.46813900	-1.71771700	1.36775700
H	-0.52507000	-2.48867300	-0.16032300
H	-2.39224900	0.33092600	1.47167500
C	-0.37881800	3.64915200	0.53100300
C	-0.93241700	2.41998800	0.18913400
C	-1.77907000	2.31792200	-0.91782200
C	-2.06758100	3.46052200	-1.66931400
C	-1.50850000	4.68405700	-1.33019800
C	-0.66136800	4.77960700	-0.22829500
H	0.28221500	3.71734100	1.38591500
H	-0.69465200	1.55253900	0.79543300
H	-2.73450500	3.36414400	-2.51669100
H	-1.73378100	5.56387900	-1.92065300
H	-0.22566700	5.73519600	0.03997800
C	-2.38770600	1.02410700	-1.36123500
O	-3.24504000	1.04489800	-2.24898900
C	-1.96324400	-0.22342000	-0.72799400
H	-3.38414200	-0.56785400	-2.58364100
H	-0.96559000	-0.20654700	-0.30192600
C	-2.16694100	-1.46652000	-1.49057700
O	-3.02469500	-1.48630700	-2.48677100
O	-1.56760400	-2.50029100	-1.20017600

Value of Imaginary Frequency= -185.2 cm^{-1}

TS2f

C	4.09565500	-0.59030200	0.28058400
C	3.60778400	0.83138900	0.26871400
O	4.35625000	1.77214500	-0.25040200
C	2.36950000	2.71334100	0.66879100
C	3.72755800	3.06166200	0.01111700
H	2.27281600	3.13707000	1.66779900
H	4.39560400	3.61089900	0.67034800
C	3.21829000	-1.39254800	-0.65173700
O	3.19520500	-2.70695200	-0.37410100
C	1.85877400	-2.11466000	-2.21727800
C	2.18775500	-3.26774200	-1.23489100
H	2.28529400	-2.31398300	-3.20614800
H	2.59949300	-4.15422000	-1.71305600
N	2.52111900	1.26035600	0.80534800
N	2.57021200	-0.95024100	-1.64125900
C	5.54737000	-0.67236600	-0.21542300
H	5.64191500	-0.26426300	-1.22152100
H	6.20993800	-0.12447500	0.45590000
H	5.84749000	-1.72039400	-0.22636100
C	3.97344800	-1.11844000	1.72456400
H	2.93280100	-1.14395500	2.04873400
H	4.37206800	-2.13092100	1.76001700
H	4.55326000	-0.48477000	2.39788400
H	3.62270700	3.57277800	-0.94238400
H	1.34122300	-3.53233600	-0.60132800
C	1.16441200	3.07377200	-0.16542200
C	0.17791700	3.90906800	0.34886800
C	1.05551400	2.58732900	-1.46783400
C	-0.89875700	4.28713400	-0.44787800
H	0.24960500	4.25760400	1.37310300
C	-0.01993800	2.96431600	-2.26257600
H	1.80962400	1.90589800	-1.85495800
C	-0.99266000	3.82322500	-1.75603700
H	-1.66574600	4.93711800	-0.04474900
H	-0.09683400	2.59399500	-3.27854200
H	-1.82851800	4.12242200	-2.37781200
C	0.37436100	-1.84148800	-2.36974800
C	-0.57251900	-2.84720100	-2.17660800
C	-0.06773300	-0.55495300	-2.67852200
C	-1.93450700	-2.55957300	-2.22676100
H	-0.26173900	-3.86233200	-1.95710700
C	-1.42648300	-0.26603400	-2.72644000
H	0.66574400	0.22457400	-2.83453400
C	-2.36706000	-1.26384300	-2.48124000
H	-2.65521000	-3.34634000	-2.03919600

H	-1.75742300	0.74754500	-2.92241600
H	-3.42430100	-1.02528700	-2.47387800
C	-0.34857200	-1.22211900	0.66662700
C	-1.13818500	-2.29961100	1.41681500
F	-0.64510000	-3.50960700	1.07329600
F	-1.04045600	-2.19830100	2.73786000
F	-2.43080200	-2.30384100	1.07961600
O	0.84724900	-1.12882600	0.89444200
H	1.79097800	0.72383300	1.31498200
H	-0.83858100	-0.86512400	-0.24345500
C	-4.28854900	1.55261500	-1.51797600
C	-3.39781900	1.43452900	-0.45542600
C	-3.63647100	0.51472700	0.56509700
C	-4.77165200	-0.29517500	0.50306800
C	-5.64853900	-0.19515700	-0.56903300
C	-5.41282400	0.73542300	-1.57979600
H	-4.10516300	2.28501000	-2.29669700
H	-2.52794100	2.07829200	-0.41201800
H	-4.94496900	-0.99679000	1.30959600
H	-6.52274000	-0.83394500	-0.61416600
H	-6.10519400	0.82445300	-2.40894700
C	-2.73520500	0.38606600	1.76076000
O	-3.23331100	-0.03641500	2.82434100
C	-1.35267400	0.68325700	1.61236800
H	-1.90910000	0.14177800	3.79434700
H	-0.99267000	1.18112700	0.72246600
C	-0.47660300	0.76692600	2.75881000
O	-0.96601900	0.41828000	3.94424100
O	0.70362000	1.11280000	2.67087800

Value of Imaginary Frequency= -84.7 cm^{-1}

TS2g

C	3.12551000	-2.87857900	-0.10034800
C	3.32509500	-1.81326400	-1.16967600
O	2.21343300	-1.47686900	-1.84576600
C	4.03869100	-0.06777200	-2.28160500
C	2.61568800	-0.44835400	-2.77141700
H	4.74335100	-0.04013300	-3.11501200
H	2.61673900	-0.88310400	-3.77143600
C	2.65138800	-2.03828500	1.06193600
O	3.55438300	-1.55075700	1.87288700
C	1.44248300	-0.60071200	2.35206600
C	2.87783300	-0.75855000	2.89133200
H	0.68965700	-0.83875200	3.09893300
H	2.92716200	-1.32909100	3.81732600
N	4.39388900	-1.16698100	-1.36741500
N	1.44518000	-1.65195800	1.31926100
C	2.06379500	-3.90328200	-0.51373800
H	1.12530200	-3.42536800	-0.78905200
H	2.43808700	-4.45765200	-1.37553500
H	1.89666100	-4.60830000	0.30246300
C	4.45996800	-3.54509700	0.24301500
H	5.22154700	-2.80670600	0.48221500
H	4.32919500	-4.22393700	1.08709900
H	4.79045700	-4.12076200	-0.62161700
H	1.88474900	0.35667900	-2.71132700
H	3.41324400	0.18307600	2.98350700
C	4.07536400	1.26981300	-1.55810200
C	4.39487200	1.37477500	-0.20650100
C	3.74833800	2.42649800	-2.26862500
C	4.36877100	2.61424100	0.42786800
H	4.66141200	0.48243900	0.34737500
C	3.72431900	3.66310800	-1.63670400
H	3.50649100	2.35787500	-3.32539300
C	4.03049300	3.75910700	-0.28165700
H	4.60878800	2.68254400	1.48284200
H	3.46462400	4.55156200	-2.20024000
H	4.00234900	4.72106700	0.21588400
C	1.15143400	0.76168300	1.75953100
C	0.87012100	1.81140800	2.63414700
C	1.14655900	0.99018700	0.38821800
C	0.60131300	3.08124800	2.13979900
H	0.83874800	1.62953800	3.70396300
C	0.86382200	2.26076800	-0.10589400
H	1.31475000	0.18023000	-0.31211600
C	0.59919000	3.30871900	0.76532200
H	0.37669400	3.88912200	2.82579500

H	0.85051600	2.42279000	-1.17728600
H	0.37992900	4.29648600	0.37814300
C	-1.95756100	-0.03980700	1.22379200
C	-3.31249600	0.23369600	1.88205700
F	-3.10855600	0.71256100	3.12163100
F	-4.06863800	-0.86287000	2.00894300
F	-4.03230800	1.15818800	1.22896700
O	-1.22505500	-0.85660600	1.80900200
H	0.60102000	-1.84855100	0.74204500
H	-1.55535700	0.88292300	0.76146700
C	-6.94249500	-1.24625400	-0.73812300
C	-5.55366800	-1.18407300	-0.72548800
C	-4.89722000	-0.05559800	-1.21849300
C	-5.65016800	1.00713000	-1.72348900
C	-7.03576700	0.94673300	-1.73101600
C	-7.68525300	-0.18239200	-1.23805100
H	-7.44394600	-2.12717400	-0.35613000
H	-4.99311300	-2.02158800	-0.33264300
H	-5.12457800	1.87415800	-2.10273000
H	-7.61166400	1.77813200	-2.11948700
H	-8.76775100	-0.23228400	-1.24359200
C	-3.40577200	0.07266600	-1.25092400
O	-2.90895100	1.01798400	-1.88629800
C	-2.56823200	-0.85751400	-0.52342700
H	-1.37174200	0.50790000	-1.97651800
H	-3.01338800	-1.75071800	-0.11055000
C	-1.20476200	-1.08961500	-1.00204800
O	-0.66553900	-0.17320900	-1.80540600
O	-0.53799600	-2.04261000	-0.62313500

Value of Imaginary Frequency= -187.9 cm^{-1}

TS2h

C	-2.96385700	-1.80693900	-1.74692900
C	-3.28617100	-0.34093700	-1.85137400
O	-4.53546000	0.03804700	-1.76260300
C	-3.11553200	1.93571900	-1.96833300
C	-4.58994700	1.48854700	-1.82290900
H	-2.94532800	2.44394400	-2.91811800
H	-5.20905800	1.75370000	-2.67635800
C	-2.67067300	-2.03169500	-0.28077700
O	-2.14425600	-3.22516300	0.02367000
C	-2.53064400	-1.86339200	1.90193800
C	-1.75974400	-3.11639300	1.41332500
H	-3.43954100	-2.15218800	2.44067000
H	-2.04448800	-4.03597300	1.91976400
N	-2.44567900	0.62185900	-2.01468900
N	-2.93682200	-1.20986700	0.64432500
C	-4.18582000	-2.65320300	-2.14290000
H	-5.05529500	-2.40491400	-1.53495700
H	-4.42836500	-2.49492800	-3.19521400
H	-3.93575400	-3.70372700	-1.99618700
C	-1.74665300	-2.16202200	-2.61287200
H	-0.84979900	-1.64641400	-2.27222500
H	-1.56704700	-3.23292800	-2.52264900
H	-1.95726300	-1.92390800	-3.65754600
H	-5.04281500	1.83469200	-0.89655800
H	-0.68102400	-2.96401200	1.43721700
C	-2.60145800	2.78408100	-0.83067900
C	-2.05783900	4.03787300	-1.08650700
C	-2.65510700	2.29787800	0.47551400
C	-1.56950900	4.81187200	-0.03882800
H	-2.00331300	4.40553800	-2.10566100
C	-2.16660000	3.07179400	1.51957700
H	-3.03874600	1.29930800	0.67339500
C	-1.62377900	4.32880200	1.26342300
H	-1.14127700	5.78605500	-0.24131200
H	-2.19320300	2.68378300	2.53081800
H	-1.23864900	4.92839700	2.07966200
C	-1.70597900	-0.96542900	2.79305200
C	-1.77566100	-1.09879500	4.17911400
C	-0.83682900	-0.02629000	2.23938400
C	-0.97598800	-0.31455700	5.00468600
H	-2.46035000	-1.81949900	4.61548800
C	-0.03571000	0.75654200	3.06461700
H	-0.79011800	0.07486500	1.16058100
C	-0.10138900	0.61350000	4.44798100
H	-1.03700300	-0.42723000	6.08076300

H	0.64478000	1.47812000	2.62430200
H	0.52552800	1.22222900	5.08874100
C	1.32334300	-1.14538000	0.07463500
C	2.39359800	-2.23670000	0.00722100
F	2.00145100	-3.30238100	0.72302900
F	2.63180400	-2.67160900	-1.23872800
F	3.56672900	-1.83366500	0.52363100
O	0.18283300	-1.48317900	-0.32196200
H	-1.38429300	0.54776100	-2.10018000
H	1.44413800	-0.55970400	1.00719800
C	6.47137300	-0.28692200	-1.56068700
C	5.09790500	-0.19041900	-1.37894600
C	4.57209600	0.75843100	-0.49866200
C	5.44022500	1.60202300	0.19811400
C	6.81195700	1.50898400	0.01034500
C	7.32954400	0.56439500	-0.87135100
H	6.87246900	-1.03059300	-2.23831200
H	4.44759900	-0.87676100	-1.90584100
H	5.01689600	2.32622900	0.88241800
H	7.47804800	2.17039700	0.55102900
H	8.40045700	0.48844200	-1.01832400
C	3.10534500	0.93152400	-0.27068000
O	2.72454500	1.69614600	0.62674700
C	2.13165300	0.20334700	-1.07731800
H	1.12800200	1.89720300	0.19439300
H	2.48798800	-0.32182900	-1.95278700
C	0.85879800	0.87056400	-1.35129000
O	0.40575800	1.74418000	-0.46767900
O	0.16517900	0.56473000	-2.31621700

Value of Imaginary Frequency= -215.3 cm^{-1}

IM3a

C	-2.66559100	0.39700800	2.43792100
C	-2.73821600	1.51149100	1.42373000
O	-2.68329200	2.74783000	1.94145800
C	-2.92334200	2.77838800	-0.37945300
C	-2.50054100	3.64025500	0.81889900
H	-3.97664400	2.96150000	-0.61841100
H	-3.12630200	4.51532300	0.97371900
C	-2.80736100	-0.91919000	1.71272700
O	-4.05451200	-1.25422500	1.33534700
C	-2.45870100	-2.89353800	0.75616100
C	-3.96589100	-2.54622700	0.70216700
H	-2.28182600	-3.78535100	1.36094600
H	-4.58046500	-3.24225200	1.27071800
N	-2.84663600	1.39615200	0.16160600
N	-1.87003900	-1.73724300	1.46483200
C	-1.32674200	0.45984400	3.18961900
H	-0.46842100	0.30351700	2.53834700
H	-1.22550500	1.43809700	3.65953000
H	-1.31677700	-0.31048200	3.96235300
C	-3.83478200	0.56749700	3.42861000
H	-4.79439300	0.56776900	2.91222700
H	-3.82371400	-0.25419000	4.14686400
H	-3.71432600	1.50692300	3.96748400
H	-1.44749800	3.91538500	0.80323400
H	-4.35265100	-2.45785100	-0.31216400
C	-2.13459000	2.89563400	-1.66870300
C	-2.67890900	2.28498900	-2.80206100
C	-0.89076600	3.51299600	-1.77153100
C	-1.99358800	2.27929800	-4.00909800
H	-3.64803500	1.80177600	-2.72649600
C	-0.20536300	3.51610800	-2.98431400
H	-0.42803800	3.97612800	-0.91066600
C	-0.74975800	2.89800700	-4.10268900
H	-2.43020700	1.79876800	-4.87660300
H	0.76136400	4.00117900	-3.04882600
H	-0.21106100	2.89974000	-5.04264100
C	-1.78126700	-3.07447200	-0.58422400
C	-0.84619600	-4.09131100	-0.76394700
C	-2.01293300	-2.16987900	-1.62008500
C	-0.15073800	-4.20596000	-1.96412800
H	-0.64414200	-4.78243400	0.04727100
C	-1.31891300	-2.27968800	-2.81807800
H	-2.71019900	-1.34900400	-1.47468800
C	-0.38585600	-3.29924900	-2.99213700
H	0.58413000	-4.99198700	-2.08782000

H	-1.49126700	-1.55793700	-3.60752700
H	0.16128300	-3.38109500	-3.92367800
C	1.36494200	-1.49691800	0.12147900
C	2.60200300	-2.32498000	-0.16411800
F	2.34579500	-3.63289700	-0.10894000
F	3.59703200	-2.07506500	0.69671700
F	3.07378400	-2.06416100	-1.40079600
O	0.91526200	-1.87040600	1.38046600
H	-0.05852400	-1.76118000	1.43558900
H	0.65218200	-1.74808700	-0.67207800
C	5.91898100	1.15967000	-0.61635300
C	4.62326600	0.70543000	-0.39569300
C	3.97267500	0.99869800	0.80380600
C	4.63666500	1.74806300	1.77877900
C	5.92422100	2.21026500	1.55289300
C	6.56762200	1.91645500	0.35272700
H	6.42184200	0.91884600	-1.54492800
H	4.14626200	0.09931800	-1.15532600
H	4.12060200	1.95823700	2.70723400
H	6.42904800	2.79759100	2.31027900
H	7.57499700	2.27420100	0.17568700
C	2.58156500	0.53772300	1.12272800
O	2.15357400	0.60246300	2.24760000
C	1.67865500	0.01965900	0.00058300
H	-1.42033000	0.61742300	-0.61132100
H	2.11494600	0.19234700	-0.98662800
C	0.36870600	0.80478300	0.00022300
O	-0.53423000	0.20899600	-0.76527500
O	0.18261800	1.83652300	0.59312900

IM3b

C	0.84158400	3.34268900	0.95695000
C	-0.41778900	2.60308400	1.33144800
O	-1.13909100	3.18482000	2.31157600
C	-2.04527800	1.13657700	1.62419500
C	-2.36144100	2.42678900	2.40710700
H	-1.76169300	0.33388500	2.31257900
H	-2.58476000	2.25983100	3.45780500
C	1.43121200	2.65550800	-0.24902800
O	2.13617600	1.53125700	0.00931900
C	1.91041600	1.97094400	-2.27525400
C	2.72516500	1.15011500	-1.24810400
H	2.56375400	2.41908500	-3.02670800
H	3.77958500	1.43510900	-1.22375000
N	-0.83814100	1.50534900	0.85194900
N	1.30031800	3.02810300	-1.45242300
C	0.50328700	4.80001000	0.62049300
H	-0.18057900	4.85381800	-0.22650500
H	0.04930300	5.28050200	1.48670900
H	1.41752600	5.33095800	0.35202800
C	1.80846600	3.25890900	2.15314600
H	1.99586000	2.21807400	2.42011400
H	2.75476000	3.73679400	1.89184900
H	1.37492400	3.77916700	3.00782100
H	-3.15889500	3.00759000	1.93804800
H	2.61831500	0.07441500	-1.36104000
C	-3.17291100	0.65505600	0.74253800
C	-3.86863000	-0.50837800	1.06745000
C	-3.52686300	1.36657900	-0.40406400
C	-4.90841000	-0.95472300	0.25697900
H	-3.57285800	-1.07703500	1.94310000
C	-4.56927100	0.92423300	-1.20952900
H	-2.97482000	2.26280200	-0.66968500
C	-5.26095200	-0.23925200	-0.88115400
H	-5.43496000	-1.86679100	0.51099200
H	-4.83823100	1.48256500	-2.09892200
H	-6.06730500	-0.58802400	-1.51508300
C	0.85842000	1.11993700	-2.96820600
C	1.28401500	0.05885800	-3.76928900
C	-0.50503900	1.31198300	-2.76912500
C	0.36544300	-0.81037600	-4.34116700
H	2.34698900	-0.09807800	-3.93047900
C	-1.42724500	0.43904000	-3.34019900
H	-0.84004600	2.12662800	-2.13874800
C	-0.99694000	-0.62434500	-4.12230300
H	0.71076500	-1.63777000	-4.95001700

H	-2.48482600	0.57812900	-3.15013900
H	-1.71619400	-1.31249300	-4.54993300
C	-0.49277400	-1.60483800	0.25863800
C	-1.11720000	-2.67023000	-0.61717300
F	-2.02245200	-2.15976300	-1.44873400
F	-0.19747200	-3.31129900	-1.35689800
F	-1.73347500	-3.60103600	0.13512400
O	0.22461500	-0.73957000	-0.56589800
H	-0.02279900	0.16862500	-0.30056400
H	-1.32624500	-1.10206500	0.74884100
C	4.22099400	-2.22488300	-0.74162700
C	2.98823200	-2.18701000	-0.09949100
C	2.80498900	-1.35803500	1.00864700
C	3.86087700	-0.56556100	1.46426500
C	5.09145900	-0.61000000	0.82678400
C	5.27225800	-1.44073700	-0.27778100
H	4.35681500	-2.86129300	-1.60739700
H	2.16699000	-2.76766900	-0.50104000
H	3.69323500	0.08362300	2.31466700
H	5.90965600	0.00299400	1.18491100
H	6.23321200	-1.47475400	-0.77757600
C	1.49680600	-1.24498200	1.71248700
O	1.28098200	-0.39811600	2.54593900
C	0.38366900	-2.24722800	1.35497700
H	-0.26249100	-3.44172400	4.24127700
H	0.82248100	-3.19119900	1.02886600
C	-0.41107500	-2.52066300	2.61439900
O	0.26080100	-3.33327900	3.43442900
O	-1.49035100	-2.06453600	2.87761400

IM3c

C	-0.44216500	3.51369000	-0.56977800
C	-1.65527800	2.62775600	-0.75745800
O	-2.04108800	2.48354700	-2.04663100
C	-3.49670400	1.46499700	-0.54638300
C	-3.05746300	1.46712200	-2.02289900
H	-4.35217500	2.14074000	-0.41285100
H	-3.83763300	1.74411600	-2.72839600
C	0.17474400	3.15280800	0.75673100
O	-0.46794700	3.57848300	1.85421400
C	1.37856600	2.20716100	2.36363100
C	0.27738600	3.09682000	2.98861400
H	2.37405400	2.50906700	2.69287900
H	0.68097500	3.95923000	3.51859800
N	-2.35305800	2.08108100	0.14639500
N	1.23474900	2.46880500	0.91694500
C	0.55563500	3.27444700	-1.70687300
H	0.77664200	2.21361500	-1.81387900
H	0.12467700	3.62658100	-2.64327900
H	1.47994900	3.81998900	-1.50855700
C	-0.91928600	4.97840600	-0.55076500
H	-1.61570600	5.14965800	0.26945000
H	-0.06167600	5.64458800	-0.43558100
H	-1.41227000	5.20714500	-1.49663600
H	-2.59300500	0.51991500	-2.30800500
H	-0.40461600	2.54499100	3.63357900
C	-3.89681800	0.11513100	-0.00576300
C	-3.49801900	-0.30818500	1.25995100
C	-4.73545000	-0.70720400	-0.76158100
C	-3.92538900	-1.53524600	1.75962100
H	-2.86142300	0.33591900	1.85286900
C	-5.16771300	-1.93020300	-0.26083600
H	-5.06179300	-0.38759000	-1.74664300
C	-4.76381500	-2.34724000	1.00447700
H	-3.60504400	-1.85281600	2.74545800
H	-5.82173100	-2.55568800	-0.85752700
H	-5.09826000	-3.30059900	1.39649900
C	1.19828800	0.72305900	2.60067800
C	2.20774500	-0.04216700	3.17445000
C	0.03918400	0.09604400	2.13287400
C	2.07285800	-1.42648700	3.26883600
H	3.11867900	0.43789500	3.51540300
C	-0.10014500	-1.28201100	2.23438600
H	-0.72611900	0.68282200	1.63013900
C	0.92245500	-2.04686600	2.79688300
H	2.87485500	-2.01751300	3.69458900

H	-0.99127000	-1.76352100	1.84497200
H	0.82247200	-3.12457800	2.85195900
C	2.59399000	-0.21580500	-0.46637300
C	3.90057500	-0.89638000	-0.09481000
F	4.47170300	-0.28220300	0.94731900
F	4.79551100	-0.92413100	-1.08086800
F	3.67722400	-2.17669800	0.27376400
O	2.86130400	1.10369600	-0.80879400
H	2.29770600	1.68242200	-0.23995100
H	1.98739700	-0.27966100	0.44352300
C	0.06993100	-4.72004000	-0.13002600
C	0.63353200	-3.50001900	-0.48532800
C	-0.18410300	-2.44283700	-0.89390500
C	-1.56975500	-2.61860200	-0.93811900
C	-2.12537600	-3.84894200	-0.61661200
C	-1.30680200	-4.89933200	-0.20788500
H	0.70750400	-5.53026500	0.20212800
H	1.70531700	-3.37362000	-0.39938000
H	-2.20002900	-1.78402400	-1.22307100
H	-3.19746400	-3.98459300	-0.67635700
H	-1.74328700	-5.85661200	0.05168100
C	0.36897700	-1.09189800	-1.21826700
O	-0.31449400	-0.09740100	-1.14327000
C	1.84474200	-0.98448500	-1.59818100
H	3.35096200	0.13300300	-4.17480700
H	2.28859900	-1.96969900	-1.73895700
C	2.01754700	-0.24761800	-2.91900600
O	3.27115400	-0.38924300	-3.36451100
O	1.17240700	0.35490800	-3.51436500

IM3d

C	-3.59913400	0.79014700	0.41748400
C	-2.60588900	1.80998600	-0.08816200
O	-3.04466700	3.07910300	-0.16140400
C	-0.83899200	2.81730200	-0.96399700
C	-2.00040500	3.83611900	-0.80561600
H	-0.54571900	2.71212500	-2.00917200
H	-2.38494600	4.19042100	-1.76167600
C	-2.89341900	-0.13470100	1.38134200
O	-3.33053200	-1.41128000	1.38263400
C	-1.67596600	-0.99667500	2.99293300
C	-2.41366000	-2.12539900	2.23154600
H	-2.08833100	-0.87325300	4.00045900
H	-2.98306900	-2.79515400	2.87282800
N	-1.43893300	1.55547100	-0.51636900
N	-2.00190000	0.20651700	2.21288500
C	-4.75471800	1.46031400	1.17813900
H	-4.37668500	2.05335700	2.01128300
H	-5.31924300	2.10942400	0.50858300
H	-5.41986500	0.68617800	1.56507300
C	-4.12975700	0.02199800	-0.80701200
H	-3.32200300	-0.51082400	-1.30926700
H	-4.88836500	-0.69328200	-0.48887500
H	-4.58003800	0.73037800	-1.50581800
H	-1.74753200	4.68023300	-0.16589900
H	-1.73534000	-2.68677600	1.58842500
C	0.38468600	3.18049000	-0.14990700
C	1.32054000	4.07046800	-0.67964300
C	0.57469400	2.67311000	1.13454600
C	2.43363100	4.44898800	0.06253800
H	1.18406100	4.45331500	-1.68619300
C	1.70269700	3.03439400	1.86874200
H	-0.15935500	1.99482800	1.55852900
C	2.63124800	3.92378500	1.33832100
H	3.15395500	5.14037100	-0.35911100
H	1.85004400	2.61766100	2.85858500
H	3.50419100	4.20853000	1.91411700
C	-0.19107700	-1.24320300	3.11218100
C	0.30130700	-2.01886400	4.16144500
C	0.70068400	-0.73343500	2.16931000
C	1.66207800	-2.28947500	4.26548100
H	-0.38537500	-2.40800500	4.90704800
C	2.06359700	-0.98754200	2.28262700
H	0.31938000	-0.12770200	1.35522100
C	2.54774900	-1.77071700	3.32651400
H	2.03033900	-2.89466500	5.08559900

H	2.74816200	-0.56188400	1.55942100
H	3.61030200	-1.96784000	3.41022700
C	0.06463600	-1.78575400	-1.09786400
C	-0.36407700	-3.20566100	-1.42978000
F	-0.88397700	-3.82613100	-0.36997200
F	-1.27343300	-3.24518600	-2.41055100
F	0.69379400	-3.93209600	-1.83807400
O	-1.03768200	-1.15710300	-0.54459800
H	-0.72514800	-0.79270900	-5.23346900
H	0.87525300	-1.88985400	-0.36194600
C	4.54987300	-1.49211200	-0.37261100
C	3.36403600	-1.37650600	-1.08871000
C	2.75133600	-0.12735500	-1.22758100
C	3.32870500	0.99762600	-0.63282400
C	4.50488100	0.87550000	0.09363500
C	5.12041900	-0.36811100	0.21810200
H	5.02603800	-2.45971100	-0.27486900
H	2.93441900	-2.26475000	-1.53740500
H	2.84089800	1.95799500	-0.74614600
H	4.93795300	1.75102100	0.56246600
H	6.04253100	-0.46311600	0.77920500
C	1.51567500	0.08835900	-2.04400800
O	1.22137800	1.18346000	-2.45593400
C	0.64793200	-1.13305000	-2.37349800
H	-1.01731100	-0.17139000	-0.64540600
H	1.30308400	-1.86411600	-2.85347900
C	-0.40814400	-0.72534300	-3.38649700
O	-1.41373000	-0.12095500	-3.15382800
O	-0.04412900	-1.10473400	-4.62057300

IM3e

C	1.64356700	-3.05043600	-0.66358700
C	2.28811200	-1.84295500	-1.30627900
O	1.42686200	-0.89731700	-1.77675300
C	3.65643700	-0.25052500	-1.93233400
C	2.25611800	0.01863000	-2.51945500
H	4.42269400	-0.21824400	-2.70787900
H	2.19426500	-0.25555000	-3.57444500
C	1.25481900	-2.61985900	0.73484100
O	2.27530500	-2.49308000	1.60563400
C	0.18398600	-2.04948800	2.59760900
C	1.70633000	-2.08280900	2.86495900
H	-0.32466200	-2.83812600	3.15633400
H	1.98959500	-2.81571200	3.61748000
N	3.52882600	-1.61650700	-1.40166900
N	0.08140200	-2.38767800	1.15966400
C	0.40598200	-3.48798100	-1.45068000
H	-0.35721500	-2.71502500	-1.50551700
H	0.69802600	-3.74468500	-2.47068200
H	-0.02895900	-4.37159400	-0.98070100
C	2.66777900	-4.18960300	-0.56752300
H	3.57233600	-3.86463200	-0.05890100
H	2.22753000	-5.02990500	-0.02731500
H	2.92953400	-4.51842200	-1.57381600
H	1.88816200	1.03105200	-2.36442700
H	2.12245600	-1.11012100	3.12795500
C	4.01605800	0.73514100	-0.83178800
C	3.93339100	0.40103100	0.51957400
C	4.39884400	2.03005700	-1.18852700
C	4.22112800	1.35438700	1.49600800
H	3.66371000	-0.60864000	0.80816300
C	4.68434900	2.97970800	-0.21555500
H	4.47236700	2.29612800	-2.23869300
C	4.59428500	2.64392000	1.13374800
H	4.16120700	1.08333300	2.54400900
H	4.98225100	3.97942100	-0.50868100
H	4.82175800	3.38044700	1.89497300
C	-0.51254100	-0.73826600	2.88313700
C	-1.79780200	-0.75237400	3.42180500
C	0.05982200	0.48223400	2.52162200
C	-2.50399000	0.43256100	3.59906500
H	-2.25801200	-1.69982800	3.68050500
C	-0.64367600	1.66897900	2.70282100
H	1.04931800	0.51314200	2.07129300
C	-1.92733200	1.64539500	3.23949600
H	-3.50956800	0.40523200	4.00023400

H	-0.19715600	2.61043700	2.40624800
H	-2.47919100	2.56882100	3.36510300
C	-2.44936200	-0.56418700	-0.05530400
C	-3.85551000	-0.09204900	0.29913400
F	-4.30640500	-0.67784300	1.40693900
F	-4.74005900	-0.34421900	-0.67446100
F	-3.86974500	1.23544300	0.51406100
O	-2.43403700	-1.94412600	0.05292400
H	-1.55346200	-2.21720100	0.38949700
H	-1.78845300	-0.07939800	0.67498300
C	1.07149400	2.70868600	-0.04935200
C	0.11221000	1.82197700	-0.52812500
C	-1.09769600	2.30600900	-1.02984300
C	-1.35122600	3.68250000	-1.01454300
C	-0.40127600	4.56196800	-0.52047600
C	0.81746900	4.07508100	-0.04778200
H	2.01318100	2.33003700	0.32971200
H	0.32839900	0.75957900	-0.50717400
H	-2.29857600	4.03891200	-1.39895500
H	-0.60320300	5.62597100	-0.50990400
H	1.56929400	4.76060300	0.32642600
C	-2.14234000	1.41971100	-1.61583400
O	-3.11390000	1.89987800	-2.16985700
C	-1.99756700	-0.08965000	-1.47970400
H	-3.88686800	0.47231800	-2.89330500
H	-0.94285500	-0.36698200	-1.53072400
C	-2.64309700	-0.92048900	-2.60369500
O	-3.70454600	-0.42523400	-3.22969600
O	-2.17421100	-1.97966200	-2.91065300

IM3f

C	4.43362500	-0.02812600	-0.23036800
C	3.48378800	0.98319900	0.36468700
O	4.06898600	2.12876900	0.75676600
C	1.73660000	2.12165700	1.11220300
C	3.02984400	2.95671000	1.31717500
H	1.26513400	1.88285500	2.06608900
H	3.26205400	3.12607100	2.36748200
C	3.61563100	-1.23508800	-0.60426000
O	3.15644200	-1.96233400	0.43523900
C	2.33076600	-2.67764600	-1.63319100
C	2.47308100	-3.08816900	-0.14753300
H	2.59740900	-3.50448400	-2.29472200
H	3.10871400	-3.96668200	-0.02281600
N	2.22643700	0.86964600	0.50997200
N	3.30142000	-1.58325500	-1.78012400
C	5.08400000	0.58560900	-1.47689100
H	4.32867100	0.86088000	-2.21369700
H	5.65477700	1.46984300	-1.19345800
H	5.75197500	-0.14478200	-1.93443900
C	5.49794300	-0.40214500	0.81591500
H	5.03493200	-0.81638600	1.71126600
H	6.17289200	-1.14904400	0.39358500
H	6.07542100	0.48219200	1.08502400
H	3.02008100	3.90249200	0.77675200
H	1.52947300	-3.21465900	0.37664800
C	0.72278100	2.82560000	0.23716400
C	-0.25988500	3.61780300	0.83519700
C	0.79499500	2.76681600	-1.15478900
C	-1.13559400	4.36632400	0.05447200
H	-0.33487500	3.64026000	1.91801200
C	-0.08318000	3.51300800	-1.93640000
H	1.54598600	2.14023500	-1.62342400
C	-1.04278400	4.32197600	-1.33373900
H	-1.89171800	4.98000000	0.52921800
H	-0.01187200	3.46802800	-3.01745000
H	-1.72208700	4.90719000	-1.94230700
C	0.93151600	-2.20071900	-1.99118700
C	-0.13044000	-3.10604200	-1.94757400
C	0.67655100	-0.88105800	-2.36041500
C	-1.42410000	-2.69992700	-2.25486200
H	0.05453000	-4.13621600	-1.65884700
C	-0.61758200	-0.47467600	-2.67547500
H	1.49713700	-0.17683200	-2.39896000
C	-1.67324900	-1.37906700	-2.61977600
H	-2.23912800	-3.41167000	-2.20099400

H	-0.80077900	0.55697100	-2.95472200
H	-2.68297200	-1.05458100	-2.84646900
C	-0.77684300	-1.09120000	0.99073100
C	-1.46241700	-2.41077000	1.33337000
F	-0.69942400	-3.46069400	1.02216700
F	-1.75800200	-2.51045800	2.63553400
F	-2.61224600	-2.54478900	0.65179200
O	0.50886500	-1.17186800	1.50173500
H	1.11509300	-0.56339000	1.02840200
H	-0.79526600	-1.01909200	-0.10294700
C	-3.30754500	1.72298500	-2.18982600
C	-2.79191200	1.35339500	-0.95170600
C	-3.49802500	0.45910400	-0.14664000
C	-4.70843900	-0.07965300	-0.59810000
C	-5.20310800	0.26880700	-1.84425600
C	-4.50520100	1.17910100	-2.63854200
H	-2.76501200	2.43289900	-2.80276500
H	-1.84999200	1.78120900	-0.62945900
H	-5.23898300	-0.77323000	0.04231400
H	-6.13311800	-0.15940800	-2.19719100
H	-4.89761600	1.46154600	-3.60829600
C	-3.03903900	0.06178900	1.21089900
O	-3.82892600	-0.38572000	2.02093900
C	-1.55722600	0.15062200	1.55348400
H	-2.82739700	-0.52638300	3.50341400
H	-1.10374900	0.99866900	1.04044800
C	-1.25681800	0.41034600	3.03805600
O	-2.06501500	-0.11010800	3.94878400
O	-0.31711300	1.08886400	3.35441200

IM3g

C	3.11289000	-2.38069000	-1.14412400
C	3.14199400	-0.93464200	-1.60186200
O	1.92819400	-0.38191500	-1.81810100
C	3.67967000	1.14019000	-2.05150900
C	2.19779300	0.90185200	-2.41544700
H	4.23083100	1.55069300	-2.89987300
H	2.04315600	0.80497000	-3.49159400
C	2.64345000	-2.30171600	0.29296500
O	3.60000000	-2.04569400	1.20707700
C	1.44303800	-1.98670900	2.12778800
C	2.94255000	-2.05165700	2.49051400
H	0.85389400	-2.70195300	2.70196000
H	3.20979000	-2.97808100	3.00034000
N	4.17440800	-0.21454000	-1.74807400
N	1.44049000	-2.36281800	0.69665400
C	2.11181400	-3.17490400	-1.99245100
H	1.12662100	-2.71292300	-1.98869300
H	2.47107600	-3.21196800	-3.02274000
H	2.03477200	-4.19470800	-1.61236900
C	4.51467900	-2.98954700	-1.21923500
H	5.23051700	-2.40060600	-0.65027300
H	4.49373700	-4.00849100	-0.82753400
H	4.83786200	-3.01857900	-2.26023000
H	1.50178100	1.62480600	-1.99935700
H	3.29266100	-1.19125900	3.05723600
C	3.84572900	2.07460300	-0.86227300
C	4.41784900	1.66059200	0.33805300
C	3.39193900	3.39195600	-0.97579300
C	4.51725100	2.54328100	1.41203100
H	4.77438500	0.64142400	0.43228500
C	3.49770600	4.27440900	0.09141200
H	2.95059200	3.72759100	-1.90955600
C	4.05866600	3.84920400	1.29391700
H	4.95610300	2.20516000	2.34356400
H	3.14142500	5.29248400	-0.01316400
H	4.13726900	4.53341800	2.13020600
C	0.84957300	-0.60045400	2.26569100
C	-0.24901800	-0.35255000	3.08475400
C	1.39114200	0.44393100	1.51418500
C	-0.81341800	0.92005900	3.13282600
H	-0.68531600	-1.16240300	3.65944800
C	0.84646700	1.71996000	1.57666300
H	2.23931700	0.26411300	0.86309700
C	-0.26923600	1.95597700	2.37920500
H	-1.68590200	1.09919700	3.74929800

H	1.29051200	2.51744000	0.98898100
H	-0.71704600	2.94191000	2.41393100
C	-1.59422700	-0.87047400	-0.10675900
C	-2.52902100	-1.70308000	0.76027100
F	-1.82674300	-2.55550000	1.51813500
F	-3.38249900	-2.43078600	0.02801300
F	-3.26285700	-0.94325000	1.58923900
O	-0.78574900	-1.72786500	-0.83833600
H	-0.00676800	-1.99430400	-0.29661700
H	-1.03246100	-0.22289000	0.57554100
C	-6.78520000	-0.36007300	-1.18445000
C	-5.39908900	-0.27416500	-1.12885000
C	-4.79360800	0.80535900	-0.48096200
C	-5.58984900	1.79303000	0.11018900
C	-6.97053400	1.70768400	0.04550500
C	-7.56967600	0.62935600	-0.60337200
H	-7.25065900	-1.20118800	-1.68258000
H	-4.80863400	-1.06309300	-1.57402600
H	-5.10347200	2.61966300	0.61231500
H	-7.58251700	2.47758000	0.49879600
H	-8.64979800	0.56078100	-0.65356400
C	-3.31976500	0.96370700	-0.37011600
O	-2.83571500	1.85362200	0.30495300
C	-2.37340700	0.01317400	-1.10321200
H	-1.10692400	1.91126700	-0.38229400
H	-2.87871200	-0.63307200	-1.81533700
C	-1.31731300	0.78555400	-1.90783700
O	-0.66656800	1.74209900	-1.23649800
O	-1.05872700	0.53113600	-3.04560000

IM3h

C	2.91132500	-2.38268500	-1.33545200
C	2.30726100	-2.54982200	0.03554900
O	3.10784600	-3.04661900	0.99136700
C	0.98818300	-2.42761300	1.81351500
C	2.41455300	-2.84598300	2.24108300
H	0.26561000	-3.23185100	1.96630500
H	2.44715700	-3.77609200	2.80366200
C	3.59501300	-1.03706500	-1.30732600
O	4.16195500	-0.65496500	-2.47469800
C	4.51651900	0.87391300	-0.73253800
C	4.56011800	0.71585200	-2.26945400
H	5.51583400	0.73677300	-0.30600200
H	5.54549200	0.86151900	-2.70584100
N	1.13138500	-2.20373200	0.36204600
N	3.69318000	-0.26862200	-0.30494100
C	3.95826500	-3.47383200	-1.61464400
H	4.73778500	-3.47466100	-0.85324400
H	3.47495700	-4.45243800	-1.62278000
H	4.40932200	-3.29707100	-2.59113600
C	1.82197700	-2.39034600	-2.41788500
H	1.10520900	-1.58096500	-2.28076900
H	2.29126500	-2.28386600	-3.39613200
H	1.27440900	-3.33285500	-2.38005100
H	2.93311400	-2.05544300	2.78583500
H	3.82781400	1.36074600	-2.76080200
C	0.47392400	-1.16482800	2.46575700
C	-0.68805100	-1.17501700	3.23350500
C	1.12352300	0.04816800	2.21699500
C	-1.21489300	0.01523200	3.73145700
H	-1.19324000	-2.11593700	3.42917300
C	0.59875300	1.23451300	2.71403800
H	2.01758300	0.06372100	1.59736300
C	-0.57656500	1.22134600	3.46447500
H	-2.13025500	-0.00099500	4.31050600
H	1.09800700	2.17170100	2.49593900
H	-0.99379100	2.14959200	3.83601400
C	3.98510400	2.21222900	-0.28167900
C	4.88235600	3.23472800	0.02344100
C	2.61305200	2.46036200	-0.20816400
C	4.42427500	4.49521000	0.39100100
H	5.94911900	3.03934800	-0.02164500
C	2.15647000	3.72229200	0.16213800
H	1.90116200	1.66958800	-0.43093100
C	3.05770000	4.74032600	0.46088400
H	5.13267800	5.28022200	0.62768400

H	1.09178300	3.90965800	0.21698500
H	2.69433900	5.71947100	0.74942500
C	-1.32139800	0.17673200	-0.15432700
C	-1.65068800	1.63850800	-0.39289600
F	-0.67660800	2.43561900	0.04956100
F	-1.83100400	1.90731900	-1.69322600
F	-2.77795000	1.99140700	0.24591200
O	-0.11985400	-0.06421300	-0.80393300
H	0.32217900	-0.85212100	-0.39542700
H	-1.25391900	0.04938400	0.93274900
C	-6.11630700	1.21003100	-2.27577000
C	-4.94291500	0.67960800	-1.75431900
C	-4.96159000	0.03264800	-0.51640400
C	-6.16190400	-0.07343400	0.19373600
C	-7.33229700	0.44595100	-0.33575400
C	-7.30960800	1.08823600	-1.57206600
H	-6.09746700	1.71874900	-3.23134900
H	-4.02048400	0.80073400	-2.30699000
H	-6.15502400	-0.57013100	1.15578600
H	-8.26203200	0.35364200	0.21177700
H	-8.22383100	1.49693900	-1.98565400
C	-3.74270500	-0.54241000	0.10820800
O	-3.74268400	-0.89589900	1.27448500
C	-2.46283700	-0.72850700	-0.70229200
H	-2.37453400	-2.10831700	1.23634100
H	-2.59120200	-0.52863300	-1.76261100
C	-1.95607900	-2.17655500	-0.61267100
O	-1.89782400	-2.69430700	0.61700900
O	-1.58995500	-2.78021800	-1.57635300

TS3e'

C	-0.69138000	2.95227900	-1.36791700
C	-1.44047000	1.71712200	-1.81566200
O	-0.75032000	0.55006000	-1.73669800
C	-2.93584900	0.25549700	-2.45840700
C	-1.53366800	-0.38415000	-2.50300700
H	-3.46393800	0.11948600	-3.40295200
H	-1.12712500	-0.40360700	-3.51663600
C	-0.57208500	2.87238000	0.13969700
O	-1.60727100	3.37849700	0.84388900
C	0.04116900	2.48168400	2.23628700
C	-1.15304200	3.44769200	2.21067700
H	0.88518800	2.90868500	2.77947900
H	-0.84651100	4.47631800	2.40559600
N	-2.62993100	1.68036000	-2.24903400
N	0.39936400	2.38593000	0.80004600
C	0.70537700	2.95891800	-2.00443500
H	1.27949900	2.06809900	-1.76202600
H	0.60032500	3.00197400	-3.09020900
H	1.25400800	3.84140000	-1.67030900
C	-1.47733100	4.20731700	-1.76130900
H	-2.48819500	4.18640200	-1.36048600
H	-0.95997100	5.09328500	-1.38826800
H	-1.53468600	4.26425900	-2.84844900
H	-1.46533000	-1.36651100	-2.04226900
H	-1.97457600	3.17559400	2.86813900
C	-3.78471400	-0.29737600	-1.32502200
C	-3.93594800	0.37802800	-0.11550200
C	-4.39072100	-1.54549300	-1.48272100
C	-4.67090600	-0.19302600	0.92231300
H	-3.49125900	1.35879400	0.01002800
C	-5.12197700	-2.11658600	-0.44890400
H	-4.28308800	-2.07581800	-2.42425200
C	-5.26201600	-1.44134200	0.76219600
H	-4.79104000	0.34615600	1.85592200
H	-5.58979800	-3.08422800	-0.58881500
H	-5.83837800	-1.88038400	1.56779700
C	-0.25362900	1.10088400	2.78442000
C	0.77995600	0.34703300	3.33858400
C	-1.53341800	0.54739300	2.71504000
C	0.54255200	-0.93863500	3.81637600
H	1.77269100	0.78022400	3.41422500
C	-1.77801100	-0.72601300	3.21660700
H	-2.34788300	1.10763500	2.26766800
C	-0.73994100	-1.47408800	3.76316100
H	1.35492200	-1.51397600	4.24399700

H	-2.77983200	-1.13813800	3.16707300
H	-0.92954500	-2.47032100	4.14372900
C	3.11806200	0.25893200	0.40346200
C	4.62626400	0.03545900	0.36545400
F	5.18407000	0.65052400	1.41909700
F	5.20552400	0.52043000	-0.72481800
F	4.95145100	-1.26621200	0.47006300
O	2.97058200	1.61119100	0.11471900
H	2.05249300	1.88679900	0.33030400
H	2.83619800	0.03217600	1.44141600
C	-1.68297500	-2.43705600	0.40798100
C	-0.42509600	-1.85310800	0.33657300
C	0.63767000	-2.57077800	-0.22210600
C	0.43793900	-3.87832400	-0.68800100
C	-0.82296200	-4.44805600	-0.62426000
C	-1.88327500	-3.72503100	-0.07893900
H	-2.51172200	-1.88232200	0.82985200
H	-0.26991500	-0.84904300	0.71798200
H	1.27284800	-4.42215300	-1.11076400
H	-0.98288200	-5.45093900	-1.00011600
H	-2.87318800	-4.16419100	-0.03257500
C	1.97197600	-1.97707900	-0.31646400
O	2.95101900	-2.83271600	-0.35745500
C	2.19282800	-0.59156800	-0.50209100
H	3.70528200	-2.39870500	-0.83527700
H	1.25645500	-0.04748200	-0.60252100
C	2.93830300	-0.57350700	-2.18615500
O	3.86699200	-1.36278500	-2.22174700
O	2.36992600	0.22543000	-2.86908000

Value of Imaginary Frequency= -390.5 cm^{-1}

TS3f'

C	4.51993900	0.23290600	0.37083000
C	3.39897800	1.05623200	0.95977400
O	3.79264800	2.20261200	1.54946800
C	1.45684600	1.95033800	1.52715800
C	2.60977800	2.76498600	2.15623900
H	0.75646100	1.60000100	2.28247100
H	2.68168900	2.61570700	3.23406300
C	3.86101000	-0.83262000	-0.46565800
O	3.34248300	-1.87172500	0.22144400
C	2.80381700	-1.90679100	-2.05259100
C	2.84289400	-2.78075500	-0.77641000
H	3.18513100	-2.45589400	-2.91559000
H	3.55376900	-3.60458400	-0.86658600
N	2.15658400	0.79131000	0.93141300
N	3.70317700	-0.79208000	-1.72190800
C	5.39344000	1.13256500	-0.51301300
H	4.80557500	1.57965700	-1.31493500
H	5.84068300	1.92002000	0.09269800
H	6.18347600	0.53318200	-0.96700800
C	5.34654400	-0.38147300	1.51253000
H	4.72677600	-1.01679200	2.14442900
H	6.15502000	-0.98460700	1.09486200
H	5.78061300	0.41581700	2.11688400
H	2.57801500	3.82705700	1.92188900
H	1.87506800	-3.14495800	-0.44547500
C	0.69677500	2.71204400	0.45997000
C	-0.64593700	3.03379900	0.64578000
C	1.34565900	3.14360400	-0.70014700
C	-1.33166200	3.77802300	-0.31420900
H	-1.15016600	2.69628200	1.54628300
C	0.66288100	3.87913500	-1.65987000
H	2.39415800	2.90262400	-0.85191600
C	-0.68155000	4.19802100	-1.46859300
H	-2.37443300	4.02733000	-0.15425700
H	1.17609300	4.20534500	-2.55672800
H	-1.21309800	4.77755700	-2.21428800
C	1.40558900	-1.39856100	-2.37190400
C	0.43680000	-2.30796900	-2.80460600
C	1.04911000	-0.06111200	-2.20663300
C	-0.86522300	-1.89263900	-3.05608200
H	0.70181700	-3.35310400	-2.93348500
C	-0.25665200	0.35803800	-2.45731600
H	1.78867000	0.64980100	-1.86468200
C	-1.21722200	-0.55514500	-2.88135400
H	-1.60758200	-2.61165300	-3.38052400

H	-0.51015600	1.40547900	-2.31828200
H	-2.23392000	-0.23273500	-3.07602200
C	-0.64518500	-1.54015400	0.57343200
C	-1.15093800	-2.97293500	0.46943300
F	-0.18133200	-3.78287900	0.02453800
F	-1.58050400	-3.48937700	1.62580600
F	-2.15975200	-3.05973400	-0.41218100
O	0.46136900	-1.54824000	1.42187500
H	1.10502300	-0.87357700	1.12876300
H	-0.34901700	-1.29946100	-0.45121600
C	-4.38874600	2.07661700	-1.40946200
C	-3.51422000	1.20646500	-0.77475000
C	-4.00336400	0.26221700	0.13525800
C	-5.37911800	0.19602400	0.39629100
C	-6.24682600	1.06894800	-0.23986100
C	-5.75312500	2.00900800	-1.14245200
H	-4.00439800	2.80295500	-2.11557500
H	-2.45678300	1.25290400	-0.99933300
H	-5.74938400	-0.53604800	1.10181900
H	-7.30837000	1.02073000	-0.03258200
H	-6.43475000	2.68868100	-1.63968700
C	-3.09908800	-0.67607900	0.80320300
O	-3.67954700	-1.68160700	1.39289600
C	-1.70494800	-0.47429700	0.93983900
H	-3.08326100	-1.98384200	2.13319800
H	-1.37378800	0.48310800	0.55014100
C	-1.57618700	-0.32506600	2.77903400
O	-2.04104800	-1.31895500	3.29745900
O	-1.04882900	0.71367500	3.05904600

Value of Imaginary Frequency= -406.4 cm^{-1}

TS3h'

C	2.70787800	-2.60086900	-1.22093600
C	2.09728200	-2.63945400	0.15695400
O	2.85404700	-3.15557700	1.13886500
C	0.79857600	-2.30626500	1.92311200
C	2.17983800	-2.83786700	2.37481600
H	-0.00084500	-3.02370100	2.11537800
H	2.12409700	-3.74260800	2.97597200
C	3.51148600	-1.32391100	-1.26660500
O	4.10574100	-1.06075300	-2.45358400
C	4.60387700	0.52535800	-0.80054900
C	4.62500700	0.27831100	-2.32620400
H	5.58910000	0.32279600	-0.36717900
H	5.61689800	0.31110000	-2.77092900
N	0.95837100	-2.17357100	0.46240900
N	3.68315300	-0.51214300	-0.30939200
C	3.64846500	-3.79684500	-1.44279400
H	4.42880300	-3.82976300	-0.68289300
H	3.07699400	-4.72578100	-1.39890700
H	4.10866800	-3.71407600	-2.42750500
C	1.61669200	-2.56470500	-2.30121900
H	0.98134200	-1.68411100	-2.20838300
H	2.08847400	-2.55736700	-3.28405700
H	0.98128500	-3.44668300	-2.21142200
H	2.76954000	-2.07781700	2.88960200
H	3.94985000	0.95739500	-2.85223000
C	0.41182700	-0.96888400	2.51137200
C	-0.73920500	-0.83402000	3.28496400
C	1.16926200	0.16371700	2.20203900
C	-1.14599300	0.42224600	3.72950400
H	-1.33134000	-1.71406100	3.51489400
C	0.76194000	1.41738400	2.64327000
H	2.05553800	0.06611300	1.57865600
C	-0.40079700	1.55041400	3.39977100
H	-2.05019400	0.52068700	4.31871700
H	1.34335300	2.29225200	2.37549500
H	-0.72590600	2.53023900	3.72848700
C	4.19844300	1.92975800	-0.42660100
C	5.18724800	2.88577400	-0.19796300
C	2.85490800	2.30197100	-0.35027700
C	4.84812000	4.20195900	0.09575500
H	6.23189700	2.59441100	-0.24422100
C	2.51755700	3.61986500	-0.05377600
H	2.07229300	1.56514500	-0.51306800
C	3.50966600	4.57066200	0.16812600
H	5.62673600	4.93434500	0.27323100

H	1.47448100	3.90317000	0.00341000
H	3.23884200	5.59402300	0.39929300
C	-1.28617700	0.38174800	-0.16438800
C	-1.45894700	1.87129700	-0.42498000
F	-0.40270700	2.57390600	-0.00758600
F	-1.63091000	2.14105200	-1.72602000
F	-2.53625300	2.34753400	0.22316400
O	-0.12396700	-0.00104700	-0.81978000
H	0.24450600	-0.80634400	-0.37735200
H	-1.20922800	0.27418400	0.92348400
C	-6.36371700	1.09104100	-2.28045500
C	-5.11937500	0.79678800	-1.74355800
C	-5.03200800	0.10034900	-0.53229800
C	-6.19791000	-0.28217200	0.14298000
C	-7.43723700	0.00717500	-0.40479500
C	-7.51988500	0.69126900	-1.61591600
H	-6.43302300	1.63747700	-3.21237000
H	-4.21930200	1.13521800	-2.24211100
H	-6.11589900	-0.81325100	1.08247300
H	-8.33993500	-0.29909500	0.10860300
H	-8.49037900	0.91904600	-2.04026200
C	-3.72696200	-0.20098700	0.05101100
O	-3.72002000	-0.42213800	1.33845400
C	-2.53527800	-0.33860400	-0.68920500
H	-2.92633800	-0.98527100	1.53939000
H	-2.64467200	-0.24454800	-1.76350700
C	-2.06477300	-2.11178400	-0.37835900
O	-2.04009500	-2.29149000	0.82774800
O	-1.85024700	-2.65147700	-1.41727800

Value of Imaginary Frequency= -377.7 cm^{-1}

IM4dh

C	0.12997600	2.81635100	-1.84245400
C	-0.49658600	2.53660600	-0.50816200
O	-0.61346400	3.50685200	0.34510800
C	-1.59966000	1.52838200	1.23192700
C	-1.12716100	2.95515400	1.59641400
H	-1.09125400	0.80836600	1.87348300
H	-0.28597200	2.91645000	2.28653900
C	0.45893400	1.48783700	-2.49635100
O	1.75479700	1.18508000	-2.62455900
C	0.32718200	-0.45746100	-3.50981000
C	1.79839600	-0.17447600	-3.12417100
H	0.20622100	-0.37855300	-4.59705400
H	2.48288000	-0.19355500	-3.96942900
N	-1.04891400	1.42892400	-0.13161400
N	-0.41516500	0.67458700	-2.92072400
C	-0.94829300	3.54036200	-2.68070100
H	-1.81799800	2.90025400	-2.82569500
H	-1.24227000	4.46668700	-2.18510200
H	-0.52559000	3.78262300	-3.65650600
C	1.36851200	3.70247100	-1.66305000
H	2.08624700	3.23584200	-0.99191800
H	1.82844900	3.86229900	-2.63832200
H	1.06853000	4.66463300	-1.24820700
H	-1.92562500	3.60837800	1.93824100
H	2.16594600	-0.79126400	-2.30797500
C	-3.08636700	1.27337200	1.23386700
C	-3.58121000	0.12770900	1.84849300
C	-3.96315900	2.15090100	0.59460700
C	-4.94716400	-0.13950200	1.83161900
H	-2.89519100	-0.55696400	2.33697400
C	-5.32575400	1.88531500	0.57905300
H	-3.58083900	3.04263800	0.10524800
C	-5.81889200	0.73884400	1.19928400
H	-5.32601100	-1.03347400	2.31248800
H	-6.00442200	2.56946300	0.08447300
H	-6.88246200	0.53338100	1.18679100
C	-0.25109400	-1.79658600	-3.09937600
C	0.55520000	-2.91438000	-2.89621500
C	-1.63561900	-1.93488700	-2.98765400
C	-0.01005900	-4.14693800	-2.58046000
H	1.63327500	-2.83253200	-2.97884400
C	-2.20228300	-3.16697700	-2.67836700
H	-2.26507600	-1.06619500	-3.13968200
C	-1.39051600	-4.27901600	-2.47277000
H	0.63145600	-5.00513100	-2.41889500

H	-3.27931900	-3.25708600	-2.59553100
H	-1.82899900	-5.23934900	-2.22888300
C	-1.31760300	-2.47031500	3.53478900
C	-0.30622500	-1.75690100	2.89928200
C	-0.20159800	-1.79998400	1.50565000
C	-1.11726900	-2.54640100	0.75868900
C	-2.11535800	-3.26770300	1.39902100
C	-2.21343300	-3.23280100	2.78872500
H	-1.40562200	-2.43083800	4.61364200
H	0.36687200	-1.13420800	3.47730900
H	-1.02073600	-2.56098500	-0.32115400
H	-2.81251300	-3.85741200	0.81531500
H	-2.98999800	-3.79727500	3.29174400
C	0.85077400	-1.05216600	0.74463000
O	0.69839000	-0.84532900	-0.44465900
C	2.04427900	-0.49720900	1.47922200
H	2.80356100	0.93649300	-0.31159600
H	2.18409000	-1.00615800	2.42999000
C	1.60660300	0.99147600	1.77422500
O	1.11649500	1.20100700	2.88649100
O	1.70638300	1.77502500	0.79686200
H	-1.00186600	0.57732500	-0.69028900
C	3.33432900	-0.62802600	0.65059000
C	4.53166900	-0.33417600	1.54563100
F	4.58599500	-1.18694700	2.58644500
F	4.49557000	0.90508700	2.04893900
F	5.68138700	-0.46102200	0.87538900
O	3.40593400	0.18207100	-0.47866400
H	3.45461900	-1.67339800	0.34055300

IM4e

C	-0.33188500	3.24352000	0.07923800
C	0.52712900	2.42573900	-0.84910500
O	0.86971200	2.94373800	-1.98994000
C	1.73682300	0.72824100	-1.80678400
C	1.61425200	1.94674400	-2.75421200
H	1.16589400	-0.10525600	-2.21241800
H	1.00931900	1.71594700	-3.62461600
C	-0.35780500	2.52855400	1.41508300
O	-1.54466900	2.11703800	1.88954800
C	0.29619500	1.39516900	3.18463100
C	-1.25115700	1.31851200	3.06056100
H	0.58360100	1.87506500	4.12466600
H	-1.77630300	1.76113400	3.90454900
N	1.00783000	1.24538000	-0.64391800
N	0.69221800	2.26120100	2.06702000
C	0.33404500	4.62247800	0.25414600
H	1.33310800	4.51876400	0.67793100
H	0.38993500	5.13212700	-0.70746600
H	-0.27505500	5.21820200	0.93487400
C	-1.72545800	3.38315200	-0.55390700
H	-2.23432900	2.42687800	-0.64896000
H	-2.33056800	4.03030200	0.08235500
H	-1.63508000	3.83046100	-1.54353300
H	2.57119800	2.39393000	-3.01545800
H	-1.61547300	0.30959900	2.86651700
C	3.12553600	0.29388300	-1.40798000
C	3.54260900	-1.00214700	-1.69147200
C	3.97509300	1.15699500	-0.71360600
C	4.80411400	-1.43566300	-1.29235000
H	2.87111000	-1.67535100	-2.21356500
C	5.23173600	0.72442700	-0.31043700
H	3.64665300	2.16420900	-0.47169900
C	5.64821400	-0.57381500	-0.60188000
H	5.12161100	-2.44732700	-1.51538400
H	5.88581500	1.39569000	0.23259100
H	6.62866900	-0.91012400	-0.28670300
C	1.02509200	0.06298200	3.09042700
C	0.55576800	-1.05551300	3.77929900
C	2.20477500	-0.04770200	2.35049500
C	1.25381000	-2.25845600	3.73269000
H	-0.35665500	-0.99212500	4.36346400
C	2.89782600	-1.25357100	2.29291000
H	2.58537700	0.81839300	1.82300200
C	2.42843700	-2.36081300	2.99190400
H	0.87780300	-3.11742200	4.27555800

H	3.80274600	-1.31791900	1.69718100
H	2.96986900	-3.29911100	2.95991900
C	0.61473300	-3.46038100	-2.53551900
C	-0.29642500	-2.45809100	-2.22718600
C	-0.35487000	-1.94684400	-0.92715000
C	0.51590800	-2.43233500	0.05075900
C	1.41745600	-3.44361900	-0.25870100
C	1.46175000	-3.96312900	-1.54879800
H	0.66168100	-3.85358900	-3.54376000
H	-0.93746100	-2.05178100	-2.99985900
H	0.45887200	-2.02551300	1.05446200
H	2.07979300	-3.82504000	0.50909300
H	2.15954800	-4.75666800	-1.79017500
C	-1.33107500	-0.89087400	-0.52563200
O	-1.11128600	-0.22546400	0.48001100
C	-2.55405800	-0.64436500	-1.36192100
H	-2.79619700	0.74311800	0.72991800
H	-2.78411900	-1.52378900	-1.96705800
C	-2.21072200	0.52388600	-2.39749200
O	-3.17571400	1.09384500	-2.89039300
O	-0.98167300	0.70121500	-2.57657900
H	0.78205100	0.68061900	0.17261000
C	-3.80684000	-0.29218200	-0.56076800
C	-4.32390100	-1.49356400	0.21369100
F	-5.46387400	-1.21867900	0.85368600
F	-3.44461200	-1.91560100	1.14314000
F	-4.56415400	-2.53723400	-0.59820100
O	-3.67091900	0.79044800	0.31826800
H	-4.57623000	-0.02974800	-1.2903110

IM4f

C	0.51283500	-3.66920200	0.06730400
C	1.42099500	-2.86769900	-0.84391500
O	1.21747000	-3.01044000	-2.16113500
C	3.05485300	-1.64839400	-1.65526800
C	2.03683300	-1.98219400	-2.76704800
H	3.97368400	-2.23136300	-1.78253900
H	2.48428600	-2.38941800	-3.67040500
C	0.26259300	-2.82213200	1.28801400
O	0.55658100	-3.29456400	2.47525700
C	-0.33332700	-1.09217300	2.63251700
C	0.14538900	-2.31159300	3.46486400
H	-1.36635400	-0.83725700	2.87046700
H	-0.64855500	-2.76442200	4.05506900
N	2.37970700	-2.14884900	-0.43527700
N	-0.27288900	-1.65234000	1.27777000
C	-0.84551900	-3.96781500	-0.59157300
H	-1.35658800	-3.04676000	-0.86830300
H	-0.67644900	-4.56679100	-1.48577200
H	-1.47192300	-4.53251100	0.10190800
C	1.23857400	-4.96909400	0.44466100
H	2.18102400	-4.75498300	0.94804200
H	0.61311200	-5.57971600	1.09698400
H	1.44341700	-5.52835900	-0.46928100
H	1.37711500	-1.14172700	-2.99474300
H	1.00997300	-2.09068800	4.08595900
C	3.42757700	-0.18812300	-1.56255200
C	4.75329800	0.21375600	-1.70987800
C	2.44816300	0.77589800	-1.31479800
C	5.10129400	1.55882600	-1.61476300
H	5.52028300	-0.53060400	-1.89748400
C	2.79481400	2.11687800	-1.21008300
H	1.41747600	0.46280100	-1.18447500
C	4.12185900	2.51288100	-1.36302000
H	6.13605700	1.85807500	-1.73387900
H	2.02611600	2.85075200	-0.99860700
H	4.38989700	3.56020400	-1.28432300
C	0.53262500	0.13647700	2.79679500
C	0.23926400	1.02879900	3.82824200
C	1.63571300	0.36149900	1.97721500
C	1.05137300	2.13509500	4.04733100
H	-0.63380400	0.86503800	4.45199100
C	2.44003100	1.47871700	2.19144500
H	1.87581900	-0.32911100	1.17387000
C	2.15399900	2.36184600	3.22625900
H	0.81828700	2.82448900	4.85022400

H	3.28771000	1.65237500	1.53858200
H	2.78439500	3.22757900	3.39172800
C	-0.15429400	4.33556700	-1.61242600
C	-0.85059400	3.13901500	-1.48475300
C	-1.02468700	2.56709600	-0.21962600
C	-0.45652800	3.17842800	0.90180900
C	0.24671500	4.36614500	0.76779600
C	0.38345700	4.95478700	-0.48797400
H	-0.02499400	4.77863200	-2.59199100
H	-1.23093500	2.65148300	-2.37387200
H	-0.57763100	2.70690700	1.86954500
H	0.68620200	4.83268900	1.64139700
H	0.92233400	5.88928700	-0.59261500
C	-1.81446200	1.31848500	-0.00546400
O	-1.95956300	0.86431600	1.11770800
C	-2.33754100	0.59351300	-1.22673500
H	-2.82611400	-0.78217000	0.83959200
H	-2.73465200	1.29739100	-1.95584800
C	-1.09672900	-0.09718500	-1.87828100
O	-0.88834600	0.07994700	-3.06653600
O	-0.39807200	-0.79077900	-1.07028800
H	-0.47131700	-1.13890300	0.30809300
C	-3.41795000	-0.46475400	-0.94485800
C	-4.77234100	0.19249300	-0.70956700
F	-4.76927700	0.98395800	0.37343900
F	-5.72946400	-0.72110600	-0.53061400
F	-5.13187000	0.95153200	-1.75634900
O	-3.13367900	-1.34092700	0.11033000
H	-3.54490500	-1.06951500	-1.84777100

TS3dh

C	0.66226600	2.31943500	2.26913000
C	-0.00595600	0.98253300	2.41875800
O	-0.10230200	0.46730100	3.61595500
C	-0.99107400	-1.02631200	1.98816800
C	-0.64166900	-0.88060800	3.49212600
H	-0.40887600	-1.83228500	1.53777300
H	0.14244900	-1.56393200	3.80826600
C	0.36026800	2.83393400	0.87505200
O	1.41291000	3.05322400	0.06899200
C	-0.66281300	3.47720500	-0.96326700
C	0.86034800	3.36808800	-1.22893700
H	-0.98556400	4.52213900	-1.02603300
H	1.31345800	4.29632300	-1.56994200
N	-0.49474000	0.25241900	1.47914400
N	-0.80682100	3.04868200	0.44058000
C	0.06306900	3.28920500	3.30502200
H	-1.00756400	3.41480200	3.14372100
H	0.24360800	2.91774700	4.31361000
H	0.54934100	4.25913100	3.19363400
C	2.17132200	2.12328400	2.50820500
H	2.60646400	1.41944600	1.79954400
H	2.66597700	3.08895100	2.40204200
H	2.32784200	1.75049300	3.52106100
H	-1.51105200	-0.94592300	4.14180200
H	1.11836000	2.54187600	-1.88933100
C	-2.45582400	-1.22847600	1.67468200
C	-2.97464000	-2.52091400	1.69644300
C	-3.28449400	-0.15521900	1.35414300
C	-4.31557200	-2.73998400	1.40513300
H	-2.32229200	-3.36038100	1.91496300
C	-4.62385900	-0.37798400	1.05248300
H	-2.87809400	0.84990500	1.31227800
C	-5.14179800	-1.66898500	1.07850900
H	-4.71148000	-3.74840800	1.41711000
H	-5.26234000	0.45964100	0.79644600
H	-6.18505500	-1.84091700	0.84227600
C	-1.56250200	2.65914000	-1.87182500
C	-1.18194800	2.30624800	-3.16495900
C	-2.82941600	2.28500700	-1.41795700
C	-2.04127400	1.57729900	-3.98249400
H	-0.20900200	2.59120200	-3.54821200
C	-3.68928100	1.55854300	-2.23399600
H	-3.13100000	2.56333200	-0.41545000
C	-3.29582000	1.19798500	-3.51957600
H	-1.72446300	1.30092000	-4.98093900

H	-4.66584700	1.26847200	-1.86313000
H	-3.95999500	0.62357800	-4.15423700
C	-1.25785400	-3.90931600	-1.31670000
C	-0.12509900	-3.12162300	-1.15200400
C	-0.21636800	-1.72981100	-1.27295500
C	-1.45474800	-1.14999400	-1.56279500
C	-2.58275900	-1.94254200	-1.73939800
C	-2.48669100	-3.32347500	-1.61557800
H	-1.18101900	-4.98510200	-1.21158600
H	0.82059700	-3.58694300	-0.90178100
H	-1.52017500	-0.07216600	-1.65554700
H	-3.53542200	-1.47423100	-1.96001800
H	-3.36653700	-3.94376100	-1.74196700
C	0.95662800	-0.81144500	-1.08959600
O	0.69588900	0.41059000	-0.84843200
C	2.26781200	-1.31192600	-1.08156300
H	2.41242700	1.07494700	-0.44261100
H	2.43515700	-2.28112000	-1.53396800
C	2.23868500	-1.89524700	0.93010700
O	2.40728800	-3.06961000	0.90274700
O	2.04540000	-0.91719400	1.58569500
H	-0.28215300	0.43262500	0.46138800
C	3.41093000	-0.33258900	-1.27441000
C	4.74357500	-0.98106100	-0.94986200
F	4.92435800	-2.09663500	-1.67723900
F	4.85466400	-1.32278500	0.33841600
F	5.76366000	-0.15927800	-1.22870600
O	3.35029500	0.83210700	-0.49470700
H	3.48256800	-0.07351400	-2.34398800

Value of Imaginary Frequency= -364.5 cm^{-1}

TS3e

C	-0.24681200	3.17098600	1.14437500
C	0.79439900	2.73097200	0.15804300
O	1.55726600	3.63522500	-0.40672300
C	2.02120600	1.47375100	-1.28507200
C	2.28282600	2.98687600	-1.49301000
H	1.59502300	1.02673700	-2.18474400
H	1.85517700	3.35930500	-2.42153200
C	-0.60831100	1.97551400	2.00460800
O	-1.91733100	1.68821700	2.10460600
C	-0.53605500	0.18922600	3.28818900
C	-1.99549700	0.44467800	2.83949200
H	-0.43940900	0.34641900	4.36780600
H	-2.68597800	0.58812700	3.66771800
N	0.97728200	1.53337300	-0.26369000
N	0.23256000	1.25690900	2.61492700
C	0.31023600	4.29045200	2.03799100
H	1.17549900	3.94060700	2.60138400
H	0.59290900	5.15092200	1.43152500
H	-0.46685700	4.59445300	2.74059300
C	-1.44588600	3.66388500	0.31048200
H	-1.82413000	2.87659800	-0.34244400
H	-2.24274300	3.97420400	0.98581700
H	-1.13704300	4.51511800	-0.29779100
H	3.33010600	3.26162700	-1.40082900
H	-2.37491300	-0.30412200	2.14764500
C	3.21865400	0.67869500	-0.81296900
C	4.13452200	0.22264900	-1.75885400
C	3.41344100	0.38731700	0.53534400
C	5.24064600	-0.51779700	-1.36129900
H	3.96725800	0.42546000	-2.81204300
C	4.51887600	-0.36008000	0.93023500
H	2.68863700	0.71389300	1.27488000
C	5.43344600	-0.81307600	-0.01442400
H	5.94534600	-0.87492500	-2.10271400
H	4.66280900	-0.58883400	1.97997500
H	6.29231100	-1.39616100	0.29566700
C	0.05162700	-1.17519800	2.97025100
C	-0.72810700	-2.27639700	2.62400900
C	1.43678600	-1.33565900	3.06491700
C	-0.13443000	-3.51028600	2.36761500
H	-1.80379100	-2.19018200	2.53632600
C	2.03041500	-2.56550600	2.80653800
H	2.04682000	-0.48125800	3.33663400
C	1.24422900	-3.65952200	2.45452000
H	-0.75575700	-4.35261300	2.08821300

H	3.10699800	-2.67067500	2.87813400
H	1.70335200	-4.61838200	2.24571000
C	1.53797600	-2.29295700	-3.31799700
C	0.37637700	-1.64742000	-2.91310900
C	0.12486800	-1.44595200	-1.55190600
C	1.05600700	-1.89153500	-0.61084700
C	2.20723900	-2.55573200	-1.01731700
C	2.45129200	-2.75471600	-2.37096200
H	1.73262500	-2.43590400	-4.37429200
H	-0.32537700	-1.28522300	-3.65619100
H	0.86334500	-1.71680200	0.44121800
H	2.92024500	-2.89343600	-0.27316900
H	3.35615900	-3.25772600	-2.69191000
C	-1.09447000	-0.74013000	-1.04780600
O	-0.98909700	-0.13506900	0.06045000
C	-2.23738300	-0.64163700	-1.85979000
H	-2.65408900	0.83291200	0.10612300
H	-2.33912900	-1.36144800	-2.66284200
C	-1.76014500	1.05095900	-2.92456200
O	-2.55503400	1.03794400	-3.80643800
O	-0.84200700	1.62119800	-2.40863100
H	0.31541600	0.73582900	-0.01127700
C	-3.54696300	-0.18769500	-1.25930500
C	-4.21667400	-1.30976900	-0.47629000
F	-5.41581000	-0.94531300	-0.00652600
F	-3.48628900	-1.69850100	0.58888200
F	-4.40324100	-2.39665000	-1.24024800
O	-3.45217400	0.94690800	-0.43416900
H	-4.24064100	0.05292700	-2.07052900

Value of Imaginary Frequency= -372.6 cm^{-1}

TS3f

C	0.78356300	-3.59873700	-0.06908700
C	1.58658600	-2.70494500	-0.98586700
O	1.44486700	-2.93549300	-2.30067800
C	3.05861800	-1.29747700	-1.80389400
C	2.18783100	-1.87714900	-2.94661600
H	4.07590100	-1.69938000	-1.85471000
H	2.75862000	-2.30834900	-3.76550700
C	0.65280800	-2.86519600	1.23875800
O	1.12627200	-3.40863200	2.32657700
C	0.12841200	-1.30313900	2.83334400
C	0.82427400	-2.53887600	3.45801700
H	-0.89089000	-1.18295700	3.20029600
H	0.18280400	-3.10364100	4.12990500
N	2.42230800	-1.84132600	-0.59130000
N	0.06617000	-1.73222100	1.42889200
C	-0.62587200	-3.89696000	-0.61432500
H	-1.23278000	-2.99774900	-0.71158500
H	-0.52164600	-4.36506400	-1.59274700
H	-1.12994400	-4.59518400	0.05662400
C	1.57451500	-4.90399900	0.12045000
H	2.56565800	-4.70666700	0.52873700
H	1.03895800	-5.57708100	0.79052900
H	1.67862400	-5.38504500	-0.85246000
H	1.47171000	-1.14404500	-3.32317900
H	1.76923100	-2.29563100	3.93727100
C	3.13793700	0.21004400	-1.81652600
C	4.16319600	0.83658100	-2.52473300
C	2.18503200	0.99197400	-1.16396300
C	4.23347800	2.22413200	-2.58833700
H	4.91464000	0.23353400	-3.02499300
C	2.26195600	2.37962900	-1.21581000
H	1.38941300	0.51900100	-0.59797300
C	3.28262100	2.99817700	-1.93105900
H	5.03442300	2.69860500	-3.14304000
H	1.52463300	2.97356700	-0.69075700
H	3.33660000	4.07980100	-1.97208100
C	0.88719300	-0.00963900	3.01099200
C	0.51282200	0.86254300	4.03013100
C	1.96698700	0.30334200	2.18781600
C	1.21426800	2.04785100	4.22557800
H	-0.34056800	0.62713000	4.65743500
C	2.65099200	1.50061300	2.37060300
H	2.26204400	-0.37058800	1.38842000
C	2.28005300	2.37075600	3.39099000
H	0.91599100	2.72578900	5.01632100

H	3.46765700	1.75396000	1.70474000
H	2.81503200	3.30267300	3.53032300
C	-0.66670400	4.57384500	-1.07875900
C	-1.23572400	3.30718400	-1.13511500
C	-1.19277500	2.46140700	-0.02141100
C	-0.54023600	2.89905700	1.13326000
C	0.02251900	4.16942400	1.19140300
C	-0.04592800	5.01463600	0.08795600
H	-0.70336000	5.21668100	-1.95026100
H	-1.69011300	2.97330300	-2.05948600
H	-0.49028100	2.22788400	1.98140000
H	0.51678100	4.49443100	2.09995400
H	0.38967300	6.00613500	0.13054700
C	-1.82573100	1.09610800	0.00697200
O	-1.49129100	0.32704900	0.97232800
C	-2.65754000	0.69701400	-1.03186600
H	-2.52420400	-1.00544200	0.61780900
H	-3.00746500	1.43038800	-1.74377500
C	-0.86348400	-0.06445600	-2.17376200
O	-0.88628600	0.58112800	-3.15276600
O	-0.45190700	-0.91420400	-1.46117900
H	-0.37930600	-1.11219800	0.72979000
C	-3.51224000	-0.54742500	-0.93782800
C	-4.92906800	-0.17227700	-0.51426500
F	-4.96419800	0.36197900	0.71295900
F	-5.73971600	-1.24108400	-0.50180000
F	-5.47364300	0.72130800	-1.35834700
O	-3.04054400	-1.51830400	-0.03814300
H	-3.63019000	-1.01545000	-1.92338600

Value of Imaginary Frequency= -277.5 cm^{-1}

IM5dh

C	1.20598200	-2.75081300	-1.72594900
C	0.70625100	-1.36423900	-2.05256700
O	0.88969300	-0.98306100	-3.32615500
C	-0.20404600	0.65569800	-2.02184900
C	0.36673100	0.35756900	-3.43591100
H	0.31739200	1.50302700	-1.56880500
H	1.18863000	1.01677800	-3.71001300
C	0.87430100	-2.99539900	-0.27690300
O	1.68390100	-2.36880000	0.61580800
C	-0.13527600	-3.44860700	1.61994600
C	1.22523700	-2.77580000	1.92217700
H	-0.20867700	-4.41172900	2.13025900
H	1.95578000	-3.47759900	2.32619300
N	0.13049300	-0.55739100	-1.25843000
N	-0.09764400	-3.66929500	0.16598900
C	0.47103000	-3.76183300	-2.61593200
H	-0.60551700	-3.71431000	-2.45059100
H	0.68761300	-3.54986700	-3.66274800
H	0.80937600	-4.77033300	-2.37528100
C	2.72538200	-2.80980100	-1.96400700
H	3.25136500	-2.05298600	-1.38106900
H	3.09903200	-3.79586500	-1.68168500
H	2.93106800	-2.64561900	-3.02181300
H	-0.39748100	0.36117200	-4.21190400
H	1.15303500	-1.88515800	2.54187500
C	-1.69098300	0.93614300	-2.02183400
C	-2.14277700	2.24163000	-2.20257900
C	-2.62030300	-0.09431800	-1.88935900
C	-3.50445600	2.51507700	-2.25882000
H	-1.42401100	3.05122300	-2.27934000
C	-3.98307000	0.17941700	-1.93961200
H	-2.27200400	-1.10883500	-1.73322200
C	-4.42887300	1.48430300	-2.12622100
H	-3.84324300	3.53626900	-2.38935800
H	-4.69847800	-0.62864700	-1.83620100
H	-5.49068200	1.69686900	-2.16419500
C	-1.34245000	-2.60783600	2.01266400
C	-1.46146400	-2.15312700	3.32796400
C	-2.35467000	-2.30912200	1.10339900
C	-2.57302500	-1.42294600	3.72855200
H	-0.68061000	-2.37580800	4.04868900
C	-3.47217800	-1.57946100	1.50446900
H	-2.26533300	-2.66064200	0.08382300
C	-3.58775100	-1.13921900	2.81730700
H	-2.64912800	-1.07588000	4.75204600

H	-4.24784200	-1.34909800	0.78297500
H	-4.45641000	-0.57204700	3.13051100
C	-1.86373300	4.20073300	0.68987900
C	-0.63567200	3.55798600	0.74824400
C	-0.56060800	2.20253900	1.09042300
C	-1.74319300	1.50608000	1.35116100
C	-2.97385600	2.14784700	1.27243400
C	-3.03832900	3.49752900	0.95035400
H	-1.90676300	5.25198800	0.42992300
H	0.26544700	4.11479000	0.51990200
H	-1.69685900	0.45796200	1.61965600
H	-3.88047100	1.58477600	1.46315500
H	-3.99685500	3.99941400	0.88890200
C	0.72861000	1.47525200	1.15928100
O	0.64224600	0.12455100	1.37536200
C	1.94460300	2.01469900	1.04096600
H	2.46096500	-0.53832000	0.30698500
H	2.07474600	3.08543000	0.95973400
H	0.22786000	-0.28872900	0.58298600
C	3.16352400	1.12504200	0.99830800
C	4.39080600	1.94735700	0.66718000
F	4.55544100	2.93564600	1.56279400
F	4.30045600	2.51970900	-0.53995800
F	5.50446500	1.21059300	0.67877300
O	3.10380100	0.12145100	0.01059200
H	3.35327600	0.68764000	1.98738100

IM5e

C	0.31230100	3.38349400	-0.20155700
C	1.43635200	2.57799000	-0.81130400
O	2.53771400	3.25799500	-1.16507300
C	2.69927600	0.95736700	-1.63932000
C	3.35351500	2.33480400	-1.91820700
H	2.54810400	0.39997300	-2.56574700
H	3.29412200	2.62125900	-2.96896100
C	-0.33925100	2.54879100	0.88069000
O	-1.68802500	2.57451900	0.90887500
C	-0.74631600	1.19461300	2.57292900
C	-2.08534300	1.66315600	1.95552800
H	-0.65223100	1.57221100	3.59593400
H	-2.70977500	2.21041800	2.65917000
N	1.39672800	1.33530900	-1.07507800
N	0.27786000	1.86996000	1.74913600
C	0.83965800	4.67624100	0.43995900
H	1.58069400	4.45047500	1.20701300
H	1.29395300	5.31465800	-0.31778200
H	0.00591500	5.20997300	0.89957000
C	-0.68133000	3.70421000	-1.33278700
H	-1.10558900	2.79033500	-1.75144200
H	-1.49517400	4.31830300	-0.94749700
H	-0.16412100	4.25318500	-2.12210200
H	4.37733300	2.41222100	-1.55948800
H	-2.66712300	0.87326100	1.48651200
C	3.50823700	0.10573500	-0.68071400
C	4.52271800	-0.70570500	-1.18919300
C	3.28329300	0.14246000	0.69387600
C	5.31069600	-1.46957500	-0.33698600
H	4.68627800	-0.75075200	-2.26155700
C	4.07213000	-0.62686400	1.54606600
H	2.47540200	0.74765900	1.09584700
C	5.08639900	-1.43114000	1.03690000
H	6.09285100	-2.09983100	-0.74348000
H	3.89114400	-0.59657800	2.61454100
H	5.69664100	-2.02776600	1.70453200
C	-0.46830100	-0.30083800	2.61251400
C	-1.38121200	-1.27743800	2.22324200
C	0.79032200	-0.70467500	3.06752500
C	-1.04050500	-2.62737200	2.28097700
H	-2.36271500	-1.01193100	1.85510300
C	1.13286100	-2.04953800	3.12300900
H	1.50696700	0.05390400	3.36616700
C	0.21447800	-3.01880600	2.72778100
H	-1.76090700	-3.37062400	1.96015600

H	2.11709900	-2.34277200	3.47008600
H	0.48009900	-4.06862000	2.76009200
C	0.80376100	-3.69181600	-2.61562000
C	-0.23694800	-2.78478600	-2.46934700
C	-0.25007400	-1.89379300	-1.39117500
C	0.80557800	-1.91660600	-0.47710700
C	1.84922100	-2.82217000	-0.62813000
C	1.85036000	-3.71306200	-1.69526400
H	0.80708700	-4.37412300	-3.45740300
H	-1.03113500	-2.74780700	-3.20585900
H	0.80855700	-1.23032700	0.36268400
H	2.66309600	-2.81610900	0.08956400
H	2.66612200	-4.41601600	-1.81716900
C	-1.34948300	-0.91462900	-1.20597200
O	-1.01279900	0.23576100	-0.56795400
C	-2.61268800	-1.13935800	-1.58952000
H	-2.58164000	1.20153000	-0.76885700
H	-2.85739600	-2.11048100	-1.99919600
H	-0.06298200	0.49578000	-0.74065800
C	-3.75354500	-0.15842400	-1.51972800
C	-4.80311100	-0.63984900	-0.52323600
F	-5.89085900	0.13594100	-0.53970400
F	-4.34460800	-0.64212300	0.74194700
F	-5.19977200	-1.89122400	-0.80142100
O	-3.43795400	1.17313400	-1.22031500
H	-4.27541800	-0.16739500	-2.48481100

IM5f

C	0.14917800	-2.42331000	1.22671400
C	1.51080600	-2.53729200	0.58575300
O	1.69149700	-3.64037600	-0.17611300
C	3.55747900	-2.20642700	-0.15165900
C	2.93526300	-3.42970400	-0.87430600
H	4.35697500	-2.52315900	0.52526600
H	3.53079400	-4.33707200	-0.80156000
C	0.18103400	-1.18830700	2.09301100
O	0.91904800	-1.28126100	3.20814800
C	0.02494300	0.87487100	2.89790400
C	0.76460400	-0.03296300	3.91197500
H	-0.85569100	1.33560500	3.34939800
H	0.17946500	-0.22521400	4.81168300
N	2.44920100	-1.69299800	0.66191900
N	-0.40375100	-0.08314400	1.85797300
C	-0.88171900	-2.28454900	0.09883400
H	-0.65763100	-1.41402100	-0.52081000
H	-0.84764400	-3.17747400	-0.52547500
H	-1.89038100	-2.18008300	0.50044500
C	-0.13886800	-3.66682500	2.08424100
H	0.60485200	-3.78114900	2.87253400
H	-1.12620700	-3.57445700	2.54056800
H	-0.12873900	-4.55319800	1.45022400
H	2.70614400	-3.21187600	-1.91936500
H	1.75429400	0.33467600	4.17451200
C	4.11481400	-1.17293800	-1.10257600
C	5.42146200	-1.31096900	-1.57067900
C	3.33737500	-0.10588400	-1.55383200
C	5.94764500	-0.40327600	-2.48264700
H	6.03377900	-2.13230700	-1.21152000
C	3.86845400	0.80617100	-2.46129700
H	2.32374300	0.02383300	-1.18573700
C	5.17045200	0.66051100	-2.92932500
H	6.96482600	-0.52132800	-2.83676000
H	3.26004700	1.63658800	-2.79812000
H	5.57899100	1.37451000	-3.63438300
C	0.91123300	1.95671000	2.31372100
C	0.67199800	3.29818200	2.59964600
C	2.00819200	1.60817000	1.52263800
C	1.52715800	4.28607800	2.11501100
H	-0.18322100	3.57403400	3.20839100
C	2.85593000	2.59414100	1.03283600
H	2.19933200	0.56451500	1.28647100
C	2.62180500	3.93479600	1.33297500
H	1.33490500	5.32691800	2.34774400

H	3.70033200	2.31160300	0.41368900
H	3.28739800	4.70195900	0.95491800
C	0.27040200	1.57577300	-2.92592600
C	-0.80392800	0.82131600	-2.46929500
C	-1.45547300	1.16999900	-1.28326300
C	-0.99540200	2.26537800	-0.54867600
C	0.07511000	3.02020800	-1.00721700
C	0.70664900	2.68083100	-2.19910300
H	0.77301300	1.29422200	-3.84421800
H	-1.13038600	-0.05298400	-3.02113600
H	-1.48738700	2.53076900	0.37995700
H	0.42097400	3.86654500	-0.42660300
H	1.53954300	3.27564900	-2.55631300
C	-2.62014500	0.40129200	-0.78188700
O	-2.74160400	0.33106200	0.57211000
C	-3.53416500	-0.16149500	-1.58110900
H	-3.99638500	-1.05946600	0.69802400
H	-3.46761100	0.00889100	-2.64723700
H	-1.83961400	0.23423100	0.98934400
C	-4.69649000	-0.98155700	-1.08286900
C	-5.93061300	-0.10118400	-0.92007500
F	-5.75979600	0.81800400	0.03875900
F	-7.01079500	-0.82020000	-0.59131900
F	-6.21789300	0.54861200	-2.05909500
O	-4.47454900	-1.67142800	0.11978600
H	-4.96653100	-1.72597600	-1.83684000

(*S*)-enol-P

C	-1.96935700	0.15295300	-0.92800700
C	-2.73335200	-0.49817200	0.21850800
F	-4.03779500	-0.16081100	0.15845500
F	-2.28462400	-0.10630400	1.41217100
F	-2.65949200	-1.82912200	0.15984900
O	-2.16646700	1.55613600	-0.84798000
H	-3.11028800	1.74788200	-0.86567000
H	-2.40437400	-0.24804600	-1.84931900
C	3.57750400	-1.52572300	-0.14445000
C	2.23014100	-1.19667100	-0.20537700
C	1.81998400	0.13064800	-0.05661400
C	2.77902600	1.11738400	0.18139700
C	4.12710800	0.78527200	0.24116900
C	4.53058900	-0.53512900	0.07486900
H	3.88355200	-2.55905700	-0.25469200
H	1.49144200	-1.97751300	-0.34097800
H	2.45799100	2.14217700	0.31539800
H	4.86337800	1.55975800	0.41952900
H	5.58137900	-0.79392900	0.12572100
C	0.38926100	0.51048200	-0.13741500
O	0.11433200	1.63384400	0.55817100
C	-0.50965000	-0.17858800	-0.86035900
H	-0.77968100	1.92933500	0.32776600
H	-0.17663600	-1.02905400	-1.43588900

(*R*)-enol-P

C	-1.96935700	0.15295300	0.92800700
C	-2.73335200	-0.49817200	-0.21850800
F	-4.03779500	-0.16081100	-0.15845500
F	-2.28462400	-0.10630400	-1.41217100
F	-2.65949200	-1.82912200	-0.15984900
O	-2.16646700	1.55613600	0.84798000
H	-3.11028800	1.74788200	0.86567000
H	-2.40437400	-0.24804600	1.84931900
C	3.57750400	-1.52572300	0.14445000
C	2.23014100	-1.19667100	0.20537700
C	1.81998400	0.13064800	0.05661400
C	2.77902600	1.11738400	-0.18139700
C	4.12710800	0.78527200	-0.24116900
C	4.53058900	-0.53512900	-0.07486900
H	3.88355200	-2.55905700	0.25469200
H	1.49144200	-1.97751300	0.34097800
H	2.45799100	2.14217700	-0.31539800
H	4.86337800	1.55975800	-0.41952900
H	5.58137900	-0.79392900	-0.12572100
C	0.38926100	0.51048200	0.13741500
O	0.11433200	1.63384400	-0.55817100
C	-0.50965000	-0.17858800	0.86035900
H	-0.77968100	1.92933500	-0.32776600
H	-0.17663600	-1.02905400	1.43588900

TS_T-*S*

C	-7.00689700	0.44526200	1.23996800
C	-5.63202800	0.41496000	1.05311000
C	-5.08085700	-0.30995300	-0.00712800
C	-5.92962000	-0.98759100	-0.88587400
C	-7.30504100	-0.95870400	-0.69318700
C	-7.84680300	-0.24483800	0.37024400
H	-7.42452300	1.01540200	2.06082100
H	-4.98953100	0.97623000	1.72003800
H	-5.50118400	-1.53728100	-1.71360100
H	-7.95446000	-1.49349900	-1.37557500
H	-8.91977800	-0.21951800	0.51794700
C	-3.61772300	-0.37290200	-0.22474500
O	-3.28453500	-0.71579200	-1.46751700
C	-2.70721900	-0.13039200	0.75378100
H	-2.30318400	-0.75434500	-1.50219600
H	-3.02659300	0.10061500	1.75721000
C	-1.27231200	-0.20050300	0.52174500
O	-0.84992800	-0.52650400	-0.63543200
O	-0.50514000	0.05862500	1.50138300
H	0.70921800	0.17463400	1.20993600
C	1.62837400	1.91189300	0.23737200
C	2.90641400	2.59696400	-0.23238300
F	2.63534700	3.80168500	-0.75976200
F	3.54719900	1.88770300	-1.16588700
F	3.75998500	2.78678100	0.78553200
O	0.74445400	1.81942000	-0.84567600
H	0.43219400	2.69970900	-1.07565500
H	1.22488500	2.53371700	1.04593700
C	5.73444200	-1.68077500	0.84653700
C	4.61736300	-0.87023400	0.69730800
C	3.46469600	-1.37687600	0.09029100
C	3.44433900	-2.69485700	-0.37688200
C	4.55779300	-3.50469500	-0.21333200
C	5.70199100	-2.99809100	0.39893700
H	6.63120700	-1.28415400	1.30578600
H	4.65163000	0.16341400	1.02029300
H	2.54816900	-3.06876300	-0.85537800
H	4.53738400	-4.52943600	-0.56280800
H	6.57303200	-3.63063400	0.52197100
C	2.27694500	-0.52177400	-0.10536800
O	1.50746900	-0.86023300	-1.06670700
C	1.95448200	0.53636100	0.79204600
H	0.47251600	-0.56385800	-0.91709400
H	2.62765800	0.60857100	1.64036400

Value of Imaginary Frequency= -1384.3 cm^{-1}

TS_T-*R*

C	-7.00689700	0.44526200	-1.23996800
C	-5.63202800	0.41496000	-1.05311000
C	-5.08085700	-0.30995300	0.00712800
C	-5.92962000	-0.98759100	0.88587400
C	-7.30504100	-0.95870400	0.69318700
C	-7.84680300	-0.24483800	-0.37024400
H	-7.42452300	1.01540200	-2.06082100
H	-4.98953100	0.97623000	-1.72003800
H	-5.50118400	-1.53728100	1.71360100
H	-7.95446000	-1.49349900	1.37557500
H	-8.91977800	-0.21951800	-0.51794700
C	-3.61772300	-0.37290200	0.22474500
O	-3.28453500	-0.71579200	1.46751700
C	-2.70721900	-0.13039200	-0.75378100
H	-2.30318400	-0.75434500	1.50219600
H	-3.02659300	0.10061500	-1.75721000
C	-1.27231200	-0.20050300	-0.52174500
O	-0.84992800	-0.52650400	0.63543200
O	-0.50514000	0.05862500	-1.50138300
H	0.70921800	0.17463400	-1.20993600
C	1.62837400	1.91189300	-0.23737200
C	2.90641400	2.59696400	0.23238300
F	2.63534700	3.80168500	0.75976200
F	3.54719900	1.88770300	1.16588700
F	3.75998500	2.78678100	-0.78553200
O	0.74445400	1.81942000	0.84567600
H	0.43219400	2.69970900	1.07565500
H	1.22488500	2.53371700	-1.04593700
C	5.73444200	-1.68077500	-0.84653700
C	4.61736300	-0.87023400	-0.69730800
C	3.46469600	-1.37687600	-0.09029100
C	3.44433900	-2.69485700	0.37688200
C	4.55779300	-3.50469500	0.21333200
C	5.70199100	-2.99809100	-0.39893700
H	6.63120700	-1.28415400	-1.30578600
H	4.65163000	0.16341400	-1.02029300
H	2.54816900	-3.06876300	0.85537800
H	4.53738400	-4.52943600	0.56280800
H	6.57303200	-3.63063400	-0.52197100
C	2.27694500	-0.52177400	0.10536800
O	1.50746900	-0.86023300	1.06670700
C	1.95448200	0.53636100	-0.79204600
H	0.47251600	-0.56385800	0.91709400
H	2.62765800	0.60857100	-1.64036400

Value of Imaginary Frequency= -1384.3 cm^{-1}

TS_T-*S'*

C	2.16137600	0.56471100	0.47814600
C	2.06040700	-0.81725900	-0.15655600
F	3.20493300	-1.14032100	-0.79046600
F	1.07901500	-0.89430400	-1.06121500
F	1.83781500	-1.76884200	0.76321500
O	2.44100400	1.48649900	-0.55030600
H	3.26876000	1.23743400	-0.97338400
H	2.98358700	0.49931500	1.20094100
C	-2.68355200	-1.63310700	0.35581700
C	-1.52992700	-0.89560800	0.58002900
C	-1.48591800	0.45280600	0.21314200
C	-2.59986900	1.05845500	-0.37932500
C	-3.74590900	0.31441700	-0.61148500
C	-3.78701900	-1.02865600	-0.24088800
H	-2.72223100	-2.67792100	0.63695300
H	-0.65661000	-1.35989600	1.02255800
H	-2.54802900	2.10698000	-0.64524100
H	-4.60952900	0.77708000	-1.07252000
H	-4.68578700	-1.60746400	-0.41800000
C	-0.27599800	1.23706900	0.44741100
O	-0.16777400	2.42695800	0.00216700
C	0.90741600	0.95135800	1.23620600
H	0.78642800	2.38575900	0.77098900
H	0.77566300	0.33716100	2.12403100

Value of Imaginary Frequency= -2061.7 cm^{-1}

TS_T-*R'*

C	2.16137600	0.56471100	-0.47814600
C	2.06040700	-0.81725900	0.15655600
F	3.20493300	-1.14032100	0.79046600
F	1.07901500	-0.89430400	1.06121500
F	1.83781500	-1.76884200	-0.76321500
O	2.44100400	1.48649900	0.55030600
H	3.26876000	1.23743400	0.97338400
H	2.98358700	0.49931500	-1.20094100
C	-2.68355200	-1.63310700	-0.35581700
C	-1.52992700	-0.89560800	-0.58002900
C	-1.48591800	0.45280600	-0.21314200
C	-2.59986900	1.05845500	0.37932500
C	-3.74590900	0.31441700	0.61148500
C	-3.78701900	-1.02865600	0.24088800
H	-2.72223100	-2.67792100	-0.63695300
H	-0.65661000	-1.35989600	-1.02255800
H	-2.54802900	2.10698000	0.64524100
H	-4.60952900	0.77708000	1.07252000
H	-4.68578700	-1.60746400	0.41800000
C	-0.27599800	1.23706900	-0.44741100
O	-0.16777400	2.42695800	-0.00216700
C	0.90741600	0.95135800	-1.23620600
H	0.78642800	2.38575900	-0.77098900
H	0.77566300	0.33716100	-2.12403100

Value of Imaginary Frequency= -2061.7 cm^{-1}

(*S*)-P

C	2.06495900	0.15909100	-0.93332700
C	2.64962500	0.36873700	0.45796500
F	2.46219200	1.63838300	0.86242700
F	2.09667100	-0.42588000	1.38265300
F	3.96401700	0.13705000	0.46773800
O	2.36675800	-1.12182500	-1.40295700
H	2.60400400	0.86912000	-1.56606700
C	-3.65829900	1.34612600	-0.33336400
C	-2.31588900	1.06244400	-0.55585900
C	-1.78170500	-0.16028300	-0.14385400
C	-2.60388100	-1.09388200	0.49271100
C	-3.94045400	-0.80547700	0.72106900
C	-4.46877700	0.41533000	0.30722400
H	-4.06978100	2.29341900	-0.65931800
H	-1.69868400	1.79688900	-1.05848700
H	-2.17350500	-2.03838600	0.80177600
H	-4.57277800	-1.52951900	1.21996400
H	-5.51392700	0.63995100	0.48420200
C	-0.35297500	-0.53170100	-0.37463800
O	0.03888600	-1.65053000	-0.11389900
C	0.57456900	0.51124500	-0.97800500
H	1.78004300	-1.73107200	-0.93283700
H	0.28142400	0.62267000	-2.02736300
H	0.40909100	1.48000500	-0.50191800

(*R*)-P

C	2.06495900	0.15909100	0.93332700
C	2.64962500	0.36873700	-0.45796500
F	2.46219200	1.63838300	-0.86242700
F	2.09667100	-0.42588000	-1.38265300
F	3.96401700	0.13705000	-0.46773800
O	2.36675800	-1.12182500	1.40295700
H	2.60400400	0.86912000	1.56606700
C	-3.65829900	1.34612600	0.33336400
C	-2.31588900	1.06244400	0.55585900
C	-1.78170500	-0.16028300	0.14385400
C	-2.60388100	-1.09388200	-0.49271100
C	-3.94045400	-0.80547700	-0.72106900
C	-4.46877700	0.41533000	-0.30722400
H	-4.06978100	2.29341900	0.65931800
H	-1.69868400	1.79688900	1.05848700
H	-2.17350500	-2.03838600	-0.80177600
H	-4.57277800	-1.52951900	-1.21996400
H	-5.51392700	0.63995100	-0.48420200
C	-0.35297500	-0.53170100	0.37463800
O	0.03888600	-1.65053000	0.11389900
C	0.57456900	0.51124500	0.97800500
H	1.78004300	-1.73107200	0.93283700
H	0.28142400	0.62267000	2.02736300
H	0.40909100	1.48000500	0.50191800

17. Cartesian coordinates of all the optimized structures of the reactant, intermediates, transition states and products in the reaction between *β*-CA_1 and CF_3CHO catalyzed by Box in Scheme 1d.

CF_3CHO

C	-1.06110300	-0.58379300	-0.00065700
C	0.35783200	0.00155600	-0.00014700
F	1.01905700	-0.42695200	1.07979000
F	0.34914900	1.32406200	0.00060400
F	1.02006000	-0.42578000	-1.07963900
O	-2.02291900	0.11715800	-0.00005900
H	-1.09140800	-1.68580700	-0.00149700

Box(Closed-1)

C	-0.00004600	2.49557700	0.00001200
C	1.02528300	1.59334800	0.64034600
O	0.50840300	0.67655800	1.50015300
C	2.83837200	0.49945900	1.23830700
C	1.63801700	0.01033400	2.09205800
H	3.64258600	0.87451900	1.87340500
H	1.70998800	0.32454200	3.13426400
C	-1.02538200	1.59340700	-0.64038700
O	-0.50850200	0.67667600	-1.50024200
C	-2.83845400	0.49948600	-1.23829800
C	-1.63811200	0.01041000	-2.09211000
H	-3.64271600	0.87451100	-1.87335600
H	-1.71013200	0.32461900	-3.13431100
N	2.27481200	1.61285300	0.45411700
N	-2.27490400	1.61287400	-0.45410900
C	-0.66069300	3.35866900	1.08049100
H	-1.13504300	2.73527800	1.83752700
H	0.09463200	3.99142200	1.55052400
H	-1.42548000	3.99019500	0.62801500
C	0.66062000	3.35875200	-1.08039000
H	1.13492800	2.73541800	-1.83749900
H	-0.09468600	3.99158900	-1.55034300
H	1.42544100	3.99019000	-0.62785300
H	1.47543900	-1.06450600	2.03375400
H	-1.47549600	-1.06442300	-2.03380700
C	3.39046500	-0.57830500	0.32891200
C	4.59873900	-1.20192600	0.62840600
C	2.66833400	-0.99101300	-0.79232900
C	5.08264800	-2.23038000	-0.17529900
H	5.16795300	-0.87831100	1.49377600
C	3.15108500	-2.01777100	-1.59473400
H	1.73272700	-0.49915500	-1.04109000
C	4.35859300	-2.64060600	-1.28843800
H	6.02635500	-2.70529800	0.06558700
H	2.58672200	-2.33042700	-2.46549900
H	4.73427800	-3.43825700	-1.91812200
C	-3.39045000	-0.57833300	-0.32890200
C	-4.59863400	-1.20211900	-0.62844900
C	-2.66833100	-0.99091500	0.79238700
C	-5.08244600	-2.23061700	0.17524400
H	-5.16783800	-0.87858800	-1.49385800
C	-3.15099400	-2.01772700	1.59478800
H	-1.73280300	-0.49892700	1.04119900
C	-4.35839400	-2.64072800	1.28843600
H	-6.02607800	-2.70566900	-0.06567400

H	-2.58663100	-2.33028500	2.46558900
H	-4.73402100	-3.43841600	1.91810900

Box(Closed-3)

C	1.19575400	-2.52640800	0.46094500
C	-0.19520900	-2.25666600	-0.06199500
O	-1.14327900	-3.12667300	0.35665600
C	-1.99789300	-1.37750300	-0.97525900
C	-2.37296500	-2.71009900	-0.26783700
H	-2.24496800	-1.42158800	-2.03793700
H	-2.67801300	-3.48721700	-0.96881900
C	2.02634900	-1.31318100	0.11500900
O	2.49527400	-1.26462700	-1.15149100
C	2.99088100	0.66887800	0.10745000
C	3.20860600	-0.02041500	-1.26726100
H	3.94350500	0.89320000	0.59193300
H	4.25607900	-0.24577200	-1.46830200
N	-0.54035300	-1.30226800	-0.81820500
N	2.27540100	-0.35072200	0.89766500
C	1.13534800	-2.70614800	1.98362600
H	0.72807200	-1.81705500	2.46460900
H	0.51245100	-3.56675800	2.22627900
H	2.14264800	-2.86964100	2.36886300
C	1.75205400	-3.79123500	-0.21328500
H	1.79494500	-3.66872100	-1.29508400
H	2.75972400	-3.99209700	0.15583900
H	1.11439500	-4.64237300	0.02885200
H	-3.12703600	-2.58771000	0.50823700
H	2.78171700	0.54223700	-2.09658100
C	-2.67409400	-0.16226700	-0.37152600
C	-3.87510000	0.30294500	-0.90638200
C	-2.12942900	0.48464700	0.73750200
C	-4.52813900	1.39187600	-0.33886700
H	-4.29792500	-0.18678600	-1.77797400
C	-2.77960800	1.57625000	1.30362200
H	-1.17831900	0.15443700	1.14106000
C	-3.98060500	2.03147100	0.76907400
H	-5.45880900	1.74562100	-0.76660500
H	-2.33802100	2.07902300	2.15594100
H	-4.48389500	2.88444300	1.20842300
C	2.17331100	1.94048200	0.01948800
C	2.71710800	3.17189800	0.37202300
C	0.85129000	1.87907400	-0.42743900
C	1.95353600	4.33341900	0.27877400
H	3.74126800	3.22447500	0.72696100
C	0.08659200	3.03568800	-0.51350400
H	0.41836300	0.91875300	-0.69592300
C	0.63711900	4.26683300	-0.16226700
H	2.38645600	5.28721700	0.55687100

H	-0.94369500	2.97152100	-0.84633900
H	0.04032600	5.16887400	-0.22920400

***β*-CA$_1$**

C	2.83152000	-1.43088500	-0.17563400
C	1.46390000	-1.20272600	-0.22958300
C	0.95775400	0.08590300	-0.03746900
C	1.84201800	1.14265100	0.19315300
C	3.20993500	0.90926900	0.25121300
C	3.70737100	-0.37665200	0.06908800
H	3.21562700	-2.43129400	-0.33281200
H	0.79345000	-2.02524400	-0.44546900
H	1.44751800	2.14082400	0.33025000
H	3.88802200	1.73304600	0.43769900
H	4.77472700	-0.55737700	0.11089700
C	-0.49509400	0.35785400	-0.07579700
O	-0.79281300	1.63653400	-0.27840300
C	-1.44581900	-0.59942500	0.10378700
H	-1.77390100	1.71864500	-0.26456800
H	-1.18277200	-1.62362500	0.31067500
C	-2.84431700	-0.23885800	0.05808300
O	-3.27390200	0.89372900	-0.12705000
O	-3.67682600	-1.26976400	0.24429200
H	-4.57795200	-0.92175200	0.20158300

H_2O

O	0.00000000	0.00000000	0.11829200
H	0.00000000	0.75558100	-0.47316900
H	0.00000000	-0.75558100	-0.47316900

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15437300
O	0.00000000	0.00000000	-1.15437300

MeOH

C	0.66209000	-0.01966700	0.00000300
H	1.08506700	0.98450000	-0.00102600
H	1.02394100	-0.54346100	0.89134500
H	1.02378600	-0.54520100	-0.89037200
O	-0.74684600	0.12238500	0.00000300
H	-1.13056400	-0.75691700	0.00001600

COM2-1

C	7.22025300	-0.86054400	0.71220700
C	5.99626900	-0.30803500	0.36014100
C	5.23974800	-0.87341300	-0.67030500
C	5.71621200	-2.01102800	-1.32568200
C	6.94357300	-2.55851500	-0.97376700
C	7.69884300	-1.98401400	0.04325800
H	7.79806600	-0.42007700	1.51574200
H	5.61288100	0.54706100	0.90367700
H	5.11898500	-2.45442500	-2.11191100
H	7.31030300	-3.43543300	-1.49341200
H	8.65414500	-2.41377900	0.31989000
C	3.93279500	-0.30432100	-1.06210800
O	3.12412100	-1.18060800	-1.65507300
C	3.57524400	0.98482200	-0.83102800
H	2.28122800	-0.69746700	-1.84509300
H	4.25051300	1.67931400	-0.35807100
C	2.22400800	1.41973400	-1.12584700
O	1.39107300	0.71122900	-1.69318400
O	1.93442700	2.64310000	-0.70528900
H	0.95123500	2.70518900	-0.59440400
C	-2.48422800	2.08214300	-1.09707400
C	-3.02366800	0.68812300	-1.30464500
O	-2.09613500	-0.29573700	-1.19347600
C	-4.26281400	-1.10171000	-1.61319200
C	-2.76677200	-1.51084600	-1.57369600
H	-4.73150800	-1.42240500	-2.54475400
H	-2.38975800	-1.81354100	-2.55152500
C	-1.71814000	2.05532200	0.20012000
O	-2.40106000	1.57508000	1.25928600
C	-0.17486500	2.13490200	1.79163800
C	-1.53727700	1.72373800	2.40468300
H	0.21378900	3.03756100	2.26544100
H	-1.96037500	2.49703100	3.04603600
N	-4.21845800	0.37180600	-1.56778800
N	-0.52377500	2.43532600	0.38658100
C	-1.54532900	2.43596500	-2.25709100
H	-0.71070800	1.73588900	-2.30970000
H	-2.10743100	2.41126900	-3.19243400
H	-1.15037000	3.44355500	-2.11432400
C	-3.63975800	3.08254300	-0.97744500
H	-4.30354100	2.81394800	-0.15608500
H	-3.23817800	4.08374900	-0.80991400
H	-4.21867800	3.07894200	-1.90086300
H	-2.54509900	-2.27542900	-0.83139500
H	-1.50201000	0.77258500	2.93225500

C	-5.05491100	-1.65345500	-0.44602500
C	-5.94682300	-2.70601300	-0.63339700
C	-4.86230100	-1.14331200	0.83924500
C	-6.63684300	-3.24991900	0.44639300
H	-6.10670800	-3.10060100	-1.63154400
C	-5.55034200	-1.68613000	1.91744000
H	-4.17910100	-0.31345400	0.99261200
C	-6.43911600	-2.74089700	1.72440400
H	-7.33150800	-4.06612000	0.28702600
H	-5.39747900	-1.28255400	2.91154400
H	-6.97741100	-3.15969300	2.56623600
C	0.87605400	1.04470100	1.86322400
C	2.04523700	1.23005900	2.59637700
C	0.66825200	-0.16765200	1.20227000
C	2.99492000	0.21510100	2.67901300
H	2.21616200	2.17579000	3.10000500
C	1.61936100	-1.17790800	1.27794000
H	-0.22476800	-0.30724300	0.59898600
C	2.78387200	-0.98979500	2.01872800
H	3.90216100	0.36935900	3.25186000
H	1.46204700	-2.10716700	0.74379700
H	3.53061900	-1.77417100	2.06597100

COM2-2

C	6.83527700	-1.66519200	-2.07827200
C	5.91807400	-0.67989000	-1.74063500
C	5.69168200	-0.35778400	-0.39977100
C	6.41066600	-1.02635400	0.59429300
C	7.32449300	-2.01592500	0.25319600
C	7.53729800	-2.33948400	-1.08251300
H	7.00859300	-1.90287700	-3.12078000
H	5.39277300	-0.14691300	-2.52340900
H	6.24394000	-0.76317800	1.63072700
H	7.87283300	-2.53292600	1.03141800
H	8.25248600	-3.10847600	-1.34878600
C	4.69446900	0.66074200	-0.00551600
O	4.84263700	1.10528100	1.23975200
C	3.67517900	1.06455900	-0.80850200
H	4.08192100	1.71751300	1.40808100
H	3.52607400	0.63693400	-1.78642400
C	2.64800600	1.93773800	-0.27854100
O	2.68584200	2.43122400	0.85102100
O	1.61536500	2.13171000	-1.08739300
H	0.83762800	2.36976200	-0.52164700
C	-2.63202100	2.32212300	-0.44825300
C	-3.37922300	1.14657600	-1.02934300
O	-2.57962000	0.15266200	-1.49579700
C	-4.87365300	-0.33216200	-1.67481700
C	-3.46086200	-0.80591900	-2.10990500
H	-5.54008500	-0.24917400	-2.53469500
H	-3.31622300	-0.75637500	-3.18991300
C	-1.70495200	1.75457000	0.59689100
O	-2.29927000	0.99419300	1.53848000
C	0.04277600	1.08635300	1.78365400
C	-1.26587800	0.63223700	2.47898200
H	0.65329300	1.70734900	2.43915500
H	-1.45571700	1.17023800	3.40802000
N	-4.63180700	1.00919500	-1.11203200
N	-0.44996200	1.91297700	0.66397100
C	-1.82189300	3.00440100	-1.55706800
H	-1.12578800	2.30470300	-2.02082600
H	-2.50348000	3.38741700	-2.31845300
H	-1.25533300	3.83917900	-1.14167300
C	-3.61031600	3.29688700	0.21598200
H	-4.18091000	2.79938100	0.99931700
H	-3.05533200	4.13350000	0.64444300
H	-4.30951000	3.67508700	-0.52981200
H	-3.20407700	-1.79705000	-1.74037100
H	-1.31705700	-0.44183000	2.64593000

C	-5.50713500	-1.24391100	-0.64469800
C	-6.53367700	-2.11169000	-1.00767100
C	-5.03296800	-1.25850400	0.66821200
C	-7.08023000	-2.98977300	-0.07597800
H	-6.91194300	-2.09818500	-2.02468500
C	-5.57858300	-2.13462600	1.59854500
H	-4.24323100	-0.57447000	0.96350300
C	-6.60287700	-3.00289700	1.22925600
H	-7.88146500	-3.65771700	-0.36919400
H	-5.20773700	-2.13722300	2.61683500
H	-7.02915600	-3.68236800	1.95756400
C	0.88935900	-0.06731700	1.27991700
C	2.02114000	-0.46084000	1.99181000
C	0.54349300	-0.75329500	0.11542500
C	2.79842700	-1.52645700	1.55143200
H	2.31020800	0.08836300	2.88196500
C	1.32279800	-1.81810700	-0.32604600
H	-0.32301300	-0.44093300	-0.45927600
C	2.45187600	-2.20650800	0.38847300
H	3.68708200	-1.81032800	2.10330800
H	1.05300100	-2.33817400	-1.23776100
H	3.06849300	-3.02430400	0.03413600

COM2-3

C	1.31064000	0.22220800	2.15372600
C	0.99548100	-0.74591000	1.04303000
O	0.92199300	-0.17713400	-0.20719800
C	0.48365700	-2.49294300	-0.19957300
C	0.73284100	-1.27645000	-1.12570200
H	-0.57236500	-2.77096000	-0.21373800
H	-0.11413400	-1.04649000	-1.77057500
C	2.58560100	0.92864500	1.76578900
O	3.62056900	0.09827100	1.47535500
C	4.14520200	2.37203500	1.19663900
C	4.76240400	0.95132100	1.27753700
H	4.66956700	3.06528300	1.85600000
H	5.42682500	0.83358200	2.13496900
N	0.79531000	-1.98314900	1.14410000
N	2.76740900	2.17686300	1.68571500
C	0.16313200	1.22898400	2.29642000
H	0.06402500	1.85128200	1.40763700
H	-0.77038500	0.69030800	2.46990600
H	0.36298900	1.88896400	3.14091800
C	1.53428000	-0.54658400	3.46131400
H	2.33330100	-1.27821700	3.34926400
H	1.79410400	0.15781100	4.25373700
H	0.62073200	-1.07395900	3.73610000
H	1.64478900	-1.38098500	-1.71526900
H	5.26932600	0.64547900	0.36426500
C	1.33173100	-3.68822200	-0.56585000
C	0.77819500	-4.76356200	-1.25506900
C	2.69189900	-3.70494100	-0.25330800
C	1.57158700	-5.84254500	-1.63535600
H	-0.28098200	-4.75955100	-1.49078500
C	3.48390900	-4.78249600	-0.62881600
H	3.12158300	-2.87332400	0.29635300
C	2.92568700	-5.85364900	-1.32259600
H	1.12977600	-6.67548100	-2.16928300
H	4.53769800	-4.79082200	-0.37641300
H	3.54405900	-6.69456300	-1.61296800
C	4.14413300	2.93325300	-0.20998300
C	5.01213200	3.96319600	-0.56150000
C	3.30258200	2.38917500	-1.18218700
C	5.04716100	4.44449000	-1.86749200
H	5.66241600	4.39553300	0.19196000
C	3.33690900	2.86864600	-2.48566800
H	2.61318700	1.59471500	-0.91261500
C	4.20964100	3.89746100	-2.83207300
H	5.72420000	5.24943800	-2.12787000

H	2.67753300	2.44361600	-3.23339700
H	4.23188400	4.27280200	-3.84815800
C	-7.84435400	1.94701600	-1.16028900
C	-6.50937400	1.57748400	-1.07822400
C	-6.10449100	0.60350500	-0.16116800
C	-7.05785900	-0.00500600	0.65895500
C	-8.39237900	0.37099700	0.57696300
C	-8.78812400	1.34806800	-0.33030900
H	-8.15051600	2.69786800	-1.87828900
H	-5.78732500	2.03142400	-1.74551600
H	-6.74209900	-0.76645700	1.35993000
H	-9.12391900	-0.10021700	1.22193600
H	-9.82971200	1.63864400	-0.39608800
C	-4.68735900	0.19950400	-0.04102000
O	-4.51655200	-0.97860600	0.54865500
C	-3.64655800	0.96723400	-0.46614200
H	-3.54610800	-1.14016700	0.60633000
H	-3.80540000	1.94202500	-0.89730400
C	-2.28956400	0.49855500	-0.30309000
O	-1.98261600	-0.57724500	0.21343300
O	-1.35981700	1.33399800	-0.76025700
H	-0.48516400	0.94533700	-0.55938500

COM2-4

C	3.64835200	-1.89168700	-0.68071000
C	3.46221000	-0.44525200	-1.08619600
O	2.38258800	-0.19134100	-1.88521100
C	3.47159700	1.74949000	-1.19289200
C	2.49245600	1.20387500	-2.25144500
H	4.19786500	2.42584900	-1.64775400
H	2.91156000	1.24566500	-3.25858600
C	2.65499300	-2.09401900	0.44670500
O	3.04941100	-1.62552900	1.65818800
C	0.83756100	-2.40543400	1.64468000
C	2.01445700	-2.02354200	2.57668000
H	0.36979300	-3.34037400	1.95538000
H	2.38313600	-2.87403400	3.15345200
N	4.15870300	0.53956600	-0.71155200
N	1.49555800	-2.58706300	0.33615400
C	3.31600400	-2.82983100	-1.84519300
H	2.26691800	-2.76175000	-2.12630000
H	3.94046300	-2.58478300	-2.70637700
H	3.51996400	-3.85888200	-1.54568500
C	5.07995500	-2.10868500	-0.18223900
H	5.33102900	-1.40110100	0.60444200
H	5.18144500	-3.12546900	0.20183500
H	5.77717100	-1.97418700	-1.01062200
H	1.49398000	1.63221100	-2.22489800
H	1.79588300	-1.18467500	3.23455300
C	2.77104900	2.47525800	-0.05300700
C	2.02058200	3.61739900	-0.34441500
C	2.85104500	2.03736800	1.26679000
C	1.36131900	4.30922600	0.66337700
H	1.95410200	3.96977500	-1.36947100
C	2.18683300	2.72996000	2.27705700
H	3.42243200	1.14664100	1.49984700
C	1.44339100	3.86523200	1.98122600
H	0.78316300	5.19319000	0.42137400
H	2.24913400	2.37395900	3.29876700
H	0.92608400	4.39986900	2.76879500
C	-0.20948700	-1.31108500	1.58717000
C	-1.46549500	-1.49008200	2.16258400
C	0.11421600	-0.06839600	1.04232400
C	-2.37764000	-0.43827500	2.20732300
H	-1.72893800	-2.45511200	2.58380900
C	-0.78617500	0.98779700	1.09919900
H	1.07887700	0.08279700	0.56805700
C	-2.03687800	0.80407000	1.68317700
H	-3.35722500	-0.59067200	2.64598400

H	-0.50886700	1.94466200	0.67019400
H	-2.75141500	1.61862100	1.70631200
C	-6.21838400	-1.53779300	0.40490200
C	-4.93615800	-1.27372600	-0.05617400
C	-4.65177100	-0.05864300	-0.68609500
C	-5.66366000	0.89367500	-0.82727500
C	-6.94691600	0.62437300	-0.36755600
C	-7.22774200	-0.59146400	0.24660600
H	-6.42939000	-2.47964600	0.89672700
H	-4.14638500	-1.99847600	0.10051600
H	-5.43518600	1.83857100	-1.30303200
H	-7.72802500	1.36510200	-0.48849000
H	-8.22768400	-0.79965000	0.60800600
C	-3.29483600	0.24475500	-1.18771000
O	-3.05183200	1.54773900	-1.31733700
C	-2.37321000	-0.70748700	-1.48382600
H	-2.12157000	1.63223300	-1.63639400
H	-2.59550700	-1.75759100	-1.38620500
C	-1.03226000	-0.31940100	-1.86453200
O	-0.67256400	0.84807100	-2.03126500
O	-0.19293100	-1.33515000	-2.00191100
H	0.71753600	-0.98661500	-2.04935700

COM2-5

C	3.52215400	-1.73386300	-1.29040700
C	3.63843100	-0.23094800	-1.43529400
O	3.49629300	0.25786100	-2.68826900
C	3.69205700	1.93488600	-1.05361800
C	3.74030300	1.67527400	-2.57867600
H	4.52401200	2.56295000	-0.73263300
H	4.72364200	1.88169200	-3.00443100
C	2.84005200	-1.95981500	0.04225600
O	3.61474200	-2.26642600	1.09075700
C	1.35224400	-1.97559300	1.69688800
C	2.72092200	-2.47907000	2.20807200
H	0.55957300	-2.70590000	1.85694000
H	2.71861000	-3.54633600	2.43006100
N	3.82977400	0.58033200	-0.48329100
N	1.59105200	-1.84473300	0.24334100
C	2.65240100	-2.31924800	-2.41166400
H	1.66338400	-1.86066300	-2.43098600
H	3.13254800	-2.14757300	-3.37448900
H	2.53583700	-3.39295400	-2.25702400
C	4.93028400	-2.34542600	-1.31519400
H	5.54242200	-1.93833500	-0.51160500
H	4.87043600	-3.42907200	-1.19932500
H	5.40073400	-2.12216200	-2.27437000
H	2.96723200	2.19902600	-3.13701500
H	3.10245300	-1.91711200	3.05782600
C	2.38651900	2.54695800	-0.58430700
C	2.35020500	3.81227600	-0.00748800
C	1.19556700	1.83160700	-0.72960300
C	1.14086300	4.35823100	0.42031700
H	3.27138100	4.37316400	0.11475700
C	-0.00861700	2.36848700	-0.29954900
H	1.20465800	0.83620900	-1.16059400
C	-0.03792400	3.63653700	0.27756500
H	1.12459600	5.34350400	0.87170000
H	-0.91647500	1.78377800	-0.39656900
H	-0.97616100	4.05388700	0.62394400
C	0.92541300	-0.63855800	2.26784800
C	-0.35952700	-0.45630200	2.77231500
C	1.82191300	0.43282700	2.26861800
C	-0.74478900	0.78198600	3.28122400
H	-1.06337900	-1.28023900	2.74705700
C	1.43869500	1.66523600	2.77970500
H	2.80935500	0.31291500	1.83136400
C	0.15461000	1.84153700	3.28872500
H	-1.74829100	0.91647200	3.66771100

H	2.13369800	2.49641200	2.75786700
H	-0.14633400	2.80792700	3.67655900
C	-6.75672400	0.81979000	-2.08219600
C	-5.52956300	0.23774800	-1.79716300
C	-5.33609500	-0.44370600	-0.59233700
C	-6.39525900	-0.54700900	0.31253500
C	-7.62107100	0.04041200	0.02589300
C	-7.80433000	0.72645900	-1.16988200
H	-6.89888400	1.34006900	-3.02154000
H	-4.72915400	0.29464100	-2.52440900
H	-6.24580700	-1.08658700	1.23848000
H	-8.43447600	-0.03923000	0.73686200
H	-8.76156700	1.18133900	-1.39470300
C	-4.03513200	-1.06222700	-0.25414700
O	-4.11228000	-1.98652500	0.69961600
C	-2.85704400	-0.70977500	-0.83379100
H	-3.18910000	-2.31683600	0.84326500
H	-2.80551300	0.06973000	-1.57688300
C	-1.62273900	-1.35547000	-0.42205000
O	-1.57960100	-2.24158500	0.43847900
O	-0.53909000	-0.91458000	-1.02657000
H	0.28135200	-1.32930300	-0.59784900

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C	3.74433700	-1.10513700	-0.97591100
C	3.58031400	0.34682600	-0.59506300
O	4.21450900	1.21820400	-1.41709000
C	3.12315000	2.26554300	0.37225300
C	3.74279300	2.52103100	-1.02037500
H	3.84222200	2.51129500	1.16129600
H	4.58415100	3.21019400	-1.01663000
C	2.96044000	-1.90985000	0.02703700
O	3.46830400	-1.97667500	1.26639800
C	1.35456400	-3.01591900	1.08978800
C	2.53045200	-2.73215200	2.05939400
H	1.16113700	-4.08655400	1.00105000
H	3.02978300	-3.63915100	2.39861900
N	2.93022000	0.80731600	0.38773700
N	1.86276000	-2.50488400	-0.19955200
C	3.18184000	-1.31274700	-2.38839100
H	2.14260800	-0.98393800	-2.43958000
H	3.77442600	-0.73597900	-3.09843000
H	3.23581400	-2.36975200	-2.65436900
C	5.23495500	-1.48191800	-0.91248400
H	5.63454600	-1.32861500	0.08996800
H	5.35907800	-2.53206600	-1.18416500
H	5.79389700	-0.86843700	-1.61914000
H	2.98855200	2.84544500	-1.74127300
H	2.23947200	-2.12087800	2.91212600
C	1.85841900	3.05097300	0.61705900
C	1.94638300	4.34137500	1.13846000
C	0.60637300	2.52760400	0.29523200
C	0.80128800	5.10609800	1.33123600
H	2.91834000	4.74658000	1.40272500
C	-0.54139100	3.29055300	0.49621900
H	0.53563800	1.51824600	-0.10035600
C	-0.44587100	4.57980400	1.01141100
H	0.88243000	6.10692700	1.73870200
H	-1.50892700	2.87013400	0.24756700
H	-1.34102700	5.17006300	1.16731300
C	0.06447400	-2.30736800	1.45660600
C	-1.10488400	-3.02648900	1.68748600
C	0.04134300	-0.91331800	1.54863400
C	-2.28582700	-2.36613200	2.01778900
H	-1.09376900	-4.10815900	1.60248200
C	-1.13980600	-0.25383000	1.86885400
H	0.94620100	-0.34238100	1.35006200
C	-2.30539200	-0.97900300	2.10720300
H	-3.19004100	-2.93612500	2.19927800

H	-1.14824300	0.82867200	1.92932000
H	-3.22732800	-0.46256300	2.34940100
C	-6.36931100	-0.84477300	-0.00342800
C	-5.02107500	-0.99786000	-0.29685900
C	-4.29670300	0.06284700	-0.84819600
C	-4.93628300	1.28255800	-1.08135700
C	-6.28669400	1.43051800	-0.79045100
C	-7.00602100	0.36800600	-0.25322800
H	-6.92276800	-1.66946000	0.42908400
H	-4.52070400	-1.93223500	-0.07236700
H	-4.36825200	2.10450600	-1.49796900
H	-6.77787700	2.37665000	-0.98295400
H	-8.05819500	0.48541100	-0.02315500
C	-2.86145500	-0.07895800	-1.16916500
O	-2.19958500	1.07852600	-1.19298700
C	-2.25976100	-1.26893800	-1.41796800
H	-1.25887700	0.85880100	-1.41357900
H	-2.81696500	-2.19185200	-1.41298200
C	-0.82149700	-1.32789900	-1.59310000
O	-0.10084900	-0.32548600	-1.62549800
O	-0.32604600	-2.54869300	-1.69475600
H	0.62822500	-2.51748400	-1.39999400

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C	-3.91985000	-1.68158000	-0.06450400
C	-3.63898400	-0.31614300	-0.64850000
O	-4.70474800	0.49633300	-0.77023400
C	-2.69260700	1.56419100	-1.34861800
C	-4.22901300	1.67187700	-1.46534900
H	-2.19238500	1.77921000	-2.29225000
H	-4.57437900	1.61018500	-2.49836800
C	-2.58630100	-2.25213400	0.36487500
O	-1.87392900	-2.87223800	-0.59984600
C	-0.71350500	-2.67121300	1.43665100
C	-0.67905300	-3.35715400	0.04499600
H	-0.55768200	-3.40543200	2.23002100
H	-0.75800800	-4.44307700	0.11689300
N	-2.50707700	0.13821500	-1.00614000
N	-2.08511600	-2.14413600	1.52177300
C	-4.83471500	-1.52673900	1.15831000
H	-4.36186900	-0.90774700	1.92045300
H	-5.78075600	-1.07752800	0.85798400
H	-5.02360400	-2.51040400	1.58995500
C	-4.58969200	-2.55461600	-1.13813200
H	-3.94414900	-2.66777800	-2.00838600
H	-4.79787700	-3.54435200	-0.72749300
H	-5.53208500	-2.09719000	-1.44277700
H	-4.64728700	2.54789400	-0.97522100
H	0.17216900	-3.06783300	-0.56550800
C	-2.10861200	2.45014100	-0.26489900
C	-1.18881100	3.44549200	-0.58257400
C	-2.51026400	2.29649400	1.06290100
C	-0.68118300	4.28102100	0.40806700
H	-0.85285600	3.54893200	-1.60766700
C	-1.99955000	3.12361000	2.05618600
H	-3.21984200	1.51753200	1.32838100
C	-1.08468600	4.12114400	1.72943200
H	0.03689500	5.04981900	0.14814000
H	-2.31128300	2.98649600	3.08458900
H	-0.68418400	4.76513600	2.50322900
C	0.31668800	-1.56503900	1.59893300
C	1.63656400	-1.89111200	1.91861900
C	-0.02093700	-0.22665200	1.41434600
C	2.59812000	-0.89541300	2.05383000
H	1.91184900	-2.93113500	2.06903700
C	0.93787400	0.77298500	1.55267900
H	-1.03756500	0.03780900	1.15614700
C	2.24803600	0.44105700	1.87836900
H	3.62264800	-1.15959700	2.29210300

H	0.65093000	1.80679000	1.38776800
H	2.99987800	1.21563000	1.97811700
C	6.29389200	-1.53851100	-0.72510900
C	5.01302100	-1.19006800	-1.13036100
C	4.48633300	0.06214500	-0.80307000
C	5.27081000	0.96552900	-0.08208600
C	6.55091800	0.61196400	0.32688100
C	7.06425200	-0.64116300	0.01001600
H	6.69527100	-2.50953800	-0.98871000
H	4.42966600	-1.88718400	-1.71910800
H	4.86451700	1.93982700	0.15668600
H	7.14847800	1.31674000	0.89241800
H	8.06322900	-0.91595000	0.32675600
C	3.10609900	0.44240900	-1.17380600
O	2.87312800	1.75179700	-1.11437100
C	2.13623100	-0.45957700	-1.47066000
H	1.91015900	1.87378100	-1.30782500
H	2.32651600	-1.51957800	-1.42199000
C	0.76892700	-0.01242200	-1.65397400
O	0.43736700	1.17426100	-1.70020700
O	-0.11765200	-0.98920800	-1.73178300
H	-1.02440100	-0.62069200	-1.54196900

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C	-4.36362800	-0.92722200	-0.56636500
C	-3.70010500	0.37338700	-0.95033100
O	-4.54162600	1.40539300	-1.16906400
C	-2.27713000	2.02687900	-1.33970800
C	-3.72196500	2.50596000	-1.61530100
H	-1.64136000	2.14935100	-2.21756500
H	-3.91519900	2.66002100	-2.67720500
C	-3.28534700	-1.82715700	-0.00972200
O	-2.50669100	-2.45217100	-0.91982500
C	-1.81403300	-2.80628200	1.28611300
C	-1.67487900	-3.35003300	-0.15585500
H	-1.93486800	-3.62012100	2.00343400
H	-2.09084500	-4.35512600	-0.25668400
N	-2.45522300	0.58523900	-1.06754500
N	-3.04688000	-2.00513000	1.22143500
C	-5.42049600	-0.65451300	0.51201800
H	-4.96563800	-0.20620000	1.39522400
H	-6.18637800	0.01260900	0.11780500
H	-5.88046000	-1.59707600	0.81076600
C	-5.00898300	-1.54323100	-1.81922800
H	-4.26054200	-1.73753600	-2.58676200
H	-5.49185700	-2.48614200	-1.55543200
H	-5.76436300	-0.86189000	-2.21323100
H	-4.00290900	3.39177500	-1.04898800
H	-0.66452000	-3.29422900	-0.55043600
C	-1.61580500	2.69777500	-0.15308900
C	-0.39451200	3.35038100	-0.29050500
C	-2.23170200	2.66295900	1.09929300
C	0.19959300	3.97432300	0.80371000
H	0.09745500	3.35968800	-1.25682400
C	-1.63889200	3.27829900	2.19449200
H	-3.17924800	2.14390200	1.21978300
C	-0.42176100	3.94040600	2.04691300
H	1.14965100	4.48186200	0.68501500
H	-2.12236100	3.23901300	3.16311600
H	0.04134300	4.42061600	2.90053400
C	-0.61762400	-1.95932700	1.68388400
C	0.57665600	-2.59648400	2.02334300
C	-0.64941200	-0.56932100	1.62371400
C	1.72998900	-1.85902100	2.25725900
H	0.60878100	-3.68084600	2.07897600
C	0.50390500	0.17405500	1.86190200
H	-1.56993900	-0.06285700	1.36526000
C	1.69826500	-0.46868200	2.16734000
H	2.65732100	-2.36528200	2.49774100

H	0.46313100	1.25587100	1.78432300
H	2.60246700	0.10633900	2.33245100
C	6.51507300	1.64767500	-0.39110500
C	5.21277200	1.17683900	-0.48596600
C	4.96808000	-0.18751900	-0.66481800
C	6.04655000	-1.07333800	-0.72620900
C	7.34874200	-0.59817300	-0.63528200
C	7.58643700	0.76228700	-0.47016200
H	6.69464000	2.70598100	-0.24578400
H	4.38437800	1.86885200	-0.39572800
H	5.85287500	-2.13083700	-0.85016300
H	8.17902700	-1.29162500	-0.69207200
H	8.60215800	1.13169500	-0.39553100
C	3.59054300	-0.71455600	-0.78026100
O	3.48765500	-2.00809700	-0.48160300
C	2.52693400	0.03977400	-1.15654800
H	2.53569200	-2.24980500	-0.58235800
H	2.63880900	1.08244700	-1.40675800
C	1.19683900	-0.54351800	-1.19007200
O	0.96917100	-1.73480500	-0.99912800
O	0.23533900	0.33007400	-1.45114800
H	-0.65792700	-0.05008600	-1.29071900

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C	-3.10712400	-1.84500100	-1.28969300
C	-2.32888200	-2.02765400	-0.00966400
O	-1.39547900	-3.03095600	-0.02752600
C	-1.39457600	-1.82326400	1.96754900
C	-0.98995900	-3.18047000	1.35608500
H	-1.80022800	-1.95109700	2.97203200
H	-1.56276100	-4.00814300	1.77844800
C	-3.79668600	-0.50473300	-1.18128400
O	-4.95812400	-0.49337600	-0.49176400
C	-4.26794200	1.64872100	-1.20287400
C	-5.40307900	0.87541500	-0.47844800
H	-4.64809600	2.18205500	-2.07664900
H	-6.35640200	0.92837200	-1.00409500
N	-2.44692400	-1.35584100	1.05373500
N	-3.35193400	0.58227400	-1.65178300
C	-2.14655400	-1.84225100	-2.48605100
H	-1.39451500	-1.06005200	-2.38822900
H	-1.65228800	-2.81150100	-2.56692500
H	-2.71334900	-1.65990700	-3.39979900
C	-4.12680100	-2.98933800	-1.41589100
H	-4.81589400	-2.99168400	-0.57210800
H	-4.70100300	-2.87021900	-2.33673100
H	-3.59872300	-3.94314900	-1.45454900
H	0.07892100	-3.37885300	1.37805700
H	-5.53134900	1.18245400	0.55886300
C	-0.23173000	-0.84715000	2.00784600
C	0.71928000	-0.98066000	3.02132100
C	-0.04051600	0.11417200	1.01846300
C	1.86061500	-0.19136700	3.02827300
H	0.57250800	-1.72543200	3.79781800
C	1.10016500	0.91503400	1.03279500
H	-0.77630800	0.24626800	0.23307600
C	2.05716200	0.75742700	2.02703300
H	2.60139400	-0.31705600	3.80908200
H	1.24076600	1.65683300	0.25500300
H	2.95449800	1.36531500	2.02301500
C	-3.53550900	2.62743200	-0.31027400
C	-3.49812600	3.98581300	-0.60888100
C	-2.87598700	2.15853100	0.82810500
C	-2.80996100	4.87130100	0.21741700
H	-4.00360300	4.35385600	-1.49571700
C	-2.18022700	3.03873200	1.64683600
H	-2.89392300	1.09653100	1.06050300
C	-2.14744300	4.39865700	1.34400300
H	-2.78606700	5.92735200	-0.02460200

H	-1.65479900	2.66030200	2.51631300
H	-1.60413900	5.08474700	1.98293300
C	5.87807500	2.20043700	-1.96850200
C	4.86798700	1.31356900	-1.62197800
C	5.12112400	0.27784000	-0.71842600
C	6.39303500	0.15611000	-0.15330100
C	7.40243400	1.04220000	-0.50668500
C	7.14829900	2.06416400	-1.41564300
H	5.67127700	3.00483100	-2.66374500
H	3.87531300	1.44276300	-2.03567900
H	6.58076000	-0.63890100	0.55659900
H	8.38832400	0.93557200	-0.07077600
H	7.93499600	2.75766700	-1.68744300
C	4.06450400	-0.68254100	-0.33498500
O	4.28159500	-1.26986500	0.83855100
C	2.97321400	-0.94229500	-1.10136100
H	3.52042600	-1.87087400	1.01090100
H	2.83278100	-0.46679900	-2.05853600
C	1.94985200	-1.84518400	-0.61897700
O	2.02957300	-2.49401200	0.42029200
O	0.87970800	-1.92314600	-1.40992600
H	0.20742900	-2.48731400	-0.98458600

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C	-3.21760100	-1.79271500	-0.83050100
C	-2.17188500	-1.97517900	0.24217600
O	-1.50585400	-3.17008400	0.19872500
C	-0.85683300	-1.81760400	2.00417100
C	-0.80013400	-3.26233100	1.45638700
H	-1.19052600	-1.82886900	3.04492000
H	-1.34328400	-3.96578400	2.08865200
C	-3.75436600	-0.38559200	-0.70699100
O	-4.68817900	-0.19851900	0.25754700
C	-4.12172700	1.77968600	-0.88310200
C	-5.12414900	1.16539100	0.12662200
H	-4.64070100	2.28428900	-1.69987300
H	-6.14792500	1.15996700	-0.25063200
N	-1.90448300	-1.18591800	1.19085200
N	-3.40757000	0.60217200	-1.41672400
C	-2.61398500	-2.00745000	-2.22372100
H	-1.81681600	-1.29501900	-2.41755600
H	-2.21769300	-3.02208500	-2.29804700
H	-3.39796000	-1.88407800	-2.97250800
C	-4.33963100	-2.81705300	-0.57316500
H	-4.76548500	-2.69086900	0.42180600
H	-5.13314900	-2.68172900	-1.31064500
H	-3.93906500	-3.82653600	-0.67063200
H	0.20727100	-3.62399300	1.26198700
H	-5.09049800	1.63438400	1.10857600
C	0.45973600	-1.06023400	1.95452800
C	1.57280200	-1.59313600	2.60909900
C	0.57116700	0.18264500	1.33590800
C	2.77219400	-0.89274200	2.65552000
H	1.49789300	-2.55917700	3.10014000
C	1.76670600	0.89398300	1.40124700
H	-0.27559100	0.58682900	0.79546800
C	2.86962800	0.36098300	2.05832800
H	3.62781200	-1.32133500	3.16409900
H	1.83659300	1.86001700	0.91382100
H	3.80345100	0.91091400	2.09103700
C	-3.14493500	2.74484800	-0.24610600
C	-3.02159200	4.05316200	-0.70229100
C	-2.35527300	2.31572200	0.82302000
C	-2.12095000	4.92921700	-0.10028600
H	-3.62882500	4.38938300	-1.53626000
C	-1.45406800	3.18715400	1.42190300
H	-2.43730300	1.28871700	1.17248300
C	-1.33601400	4.49760100	0.96192300
H	-2.03144200	5.94574400	-0.46492600

H	-0.83824200	2.84116800	2.24463500
H	-0.63323600	5.17674200	1.42995200
C	6.71522700	0.00343300	-0.55209600
C	5.46322400	-0.51962600	-0.84317700
C	4.36657900	0.32995900	-1.01142100
C	4.54898300	1.71106800	-0.90225000
C	5.80308900	2.23126200	-0.60767700
C	6.88785100	1.37954600	-0.42811100
H	7.55983200	-0.66322100	-0.42762800
H	5.34691600	-1.59023000	-0.95491300
H	3.70024700	2.36720200	-1.04455300
H	5.93307400	3.30305600	-0.51931600
H	7.86616900	1.78519500	-0.19986200
C	3.00783300	-0.19542900	-1.26650700
O	2.15057500	0.72859200	-1.68423800
C	2.64755300	-1.48914900	-1.04767500
H	1.26076100	0.30730300	-1.73625600
H	3.34674600	-2.21466700	-0.66636900
C	1.27457500	-1.88920700	-1.23607700
O	0.36428800	-1.13514700	-1.56743200
O	1.03987900	-3.18535200	-1.00287800
H	0.07564200	-3.31228900	-1.03834100

COM4-1

C	0.61381500	-1.90610900	1.19008300
C	1.60280600	-1.58575300	0.09657000
O	1.08140800	-0.87624300	-0.93801500
C	3.38249900	-1.30341600	-1.16473800
C	2.12925800	-0.78635100	-1.92084200
H	3.89796800	-2.07213700	-1.74256900
H	1.85768000	-1.42139000	-2.76514200
C	0.01362500	-0.59234500	1.62450300
O	0.91149300	0.38785800	1.88145500
C	-1.32023400	1.10092400	2.09576000
C	0.15050900	1.51278900	2.36300500
H	-1.93155100	1.22541300	2.99091800
H	0.36489000	1.63620400	3.42500200
N	2.82433500	-1.90486400	0.06021200
N	-1.21670900	-0.33195300	1.76268300
C	-0.48002700	-2.82081300	0.62588200
H	-0.95521500	-2.35895700	-0.24088500
H	-0.03849000	-3.77200900	0.32365100
H	-1.23995700	-3.00736700	1.38593800
C	1.33077900	-2.55054300	2.38148300
H	2.09879900	-1.88540900	2.77533600
H	0.60400400	-2.77327300	3.16478800
H	1.81072100	-3.47576100	2.06237100
H	2.21456600	0.25031400	-2.24152500
H	0.45900900	2.39810200	1.80994900
C	4.36225400	-0.19833400	-0.82879500
C	5.54057100	-0.05595400	-1.55716200
C	4.06817800	0.71990800	0.18054100
C	6.41573400	0.99270300	-1.28857200
H	5.77815600	-0.77235500	-2.33691900
C	4.94207100	1.76651900	0.44908300
H	3.15839000	0.60778000	0.76199800
C	6.11734100	1.90647500	-0.28466300
H	7.33161400	1.09077400	-1.85924500
H	4.70887600	2.47329300	1.23687200
H	6.79864100	2.72129800	-0.07078600
C	-1.95942600	1.85203700	0.94589800
C	-3.00974800	2.73791100	1.16883800
C	-1.47912200	1.67350300	-0.35341100
C	-3.57099200	3.44738500	0.11064400
H	-3.39245800	2.87287400	2.17517700
C	-2.03759600	2.38328300	-1.40850800
H	-0.67529800	0.96694400	-0.54163700
C	-3.08350500	3.27296700	-1.17881400
H	-4.39124200	4.13103000	0.29450400

H	-1.66536000	2.23141400	-2.41471600
H	-3.52283600	3.81985400	-2.00440700
C	-3.73698600	-1.64627300	0.11246500
C	-3.98870900	-0.87256900	-1.18949400
F	-4.43942600	0.35374400	-0.91421800
F	-4.86815800	-1.48064300	-1.97512900
F	-2.83712900	-0.74787500	-1.86443700
O	-4.26983000	-2.69732900	0.30871300
H	-3.02501200	-1.15790300	0.79935500

COM4-2

C	-0.37336300	0.06674000	2.58211800
C	-1.23169400	0.65263700	1.48842600
O	-0.53393500	1.12357900	0.41439800
C	-2.87531800	1.25644700	0.14954200
C	-1.51801300	1.59845100	-0.52566500
H	-3.47807500	2.15492100	0.29564200
H	-1.37469600	2.67132300	-0.66679600
C	0.35840500	-1.09729000	1.95646300
O	-0.45222800	-2.01279000	1.36221700
C	1.83346300	-2.51911500	1.15197800
C	0.40647800	-3.09626500	0.96252900
H	2.45915100	-3.20199800	1.72858000
H	0.20786500	-3.94575300	1.61765800
N	-2.49147200	0.71495200	1.46318000
N	1.60673000	-1.28792400	1.93474200
C	0.62996600	1.11047600	3.08178200
H	1.31285100	1.40371700	2.28596900
H	0.09370500	1.98574700	3.45542900
H	1.22366400	0.68721300	3.89234000
C	-1.26039800	-0.44810000	3.72145300
H	-1.97706200	-1.18087200	3.35372400
H	-0.63274800	-0.90472700	4.48898700
H	-1.81294400	0.38305300	4.16079900
H	-1.36657300	1.07978900	-1.47111700
H	0.17799800	-3.35558400	-0.06974200
C	-3.68000600	0.24869900	-0.64347500
C	-4.75515700	0.66462000	-1.42421800
C	-3.31734800	-1.09920100	-0.63999500
C	-5.46010100	-0.25066500	-2.20071100
H	-5.04622500	1.71003700	-1.42251000
C	-4.02241000	-2.01295500	-1.41399600
H	-2.49096200	-1.43156200	-0.01907800
C	-5.09411000	-1.59149600	-2.19712400
H	-6.29709900	0.08359000	-2.80217900
H	-3.73887100	-3.05887200	-1.40303300
H	-5.64349700	-2.30687500	-2.79731000
C	2.52190700	-2.20559600	-0.15960200
C	3.61598200	-2.95442000	-0.58372400
C	2.03850800	-1.18126100	-0.97555100
C	4.22208300	-2.68993700	-1.80902400
H	4.00066300	-3.74643400	0.05048400
C	2.64485500	-0.91334000	-2.19635800
H	1.19980600	-0.57630200	-0.64284400
C	3.73704300	-1.66868900	-2.61703300
H	5.07568800	-3.27686800	-2.12679300

H	2.27063000	-0.10700100	-2.81571800
H	4.21044800	-1.45616200	-3.56813700
C	1.32948700	3.61320100	0.05331100
C	2.07497300	2.50303700	-0.70594000
F	2.50602200	1.57783800	0.14901100
F	3.10992900	2.98099400	-1.38079000
F	1.24504000	1.91385900	-1.58058300
O	1.55129900	4.76275700	-0.16645400
H	0.59806900	3.24197300	0.78904900

COM4-3

C	-1.34364200	-2.14600100	-1.35503300
C	-0.18943000	-2.14205200	-0.38092500
O	0.44894300	-3.32806700	-0.25483000
C	1.41175500	-1.61348600	1.04557000
C	1.45345500	-3.13662800	0.76032100
H	1.26179500	-1.42109000	2.10749800
H	1.17405300	-3.73227300	1.62931800
C	-1.70721300	-0.70401200	-1.61879600
O	-2.59530800	-0.13124700	-0.76322100
C	-1.71263800	1.37832600	-2.29018200
C	-2.92852200	1.12879600	-1.38268600
H	-2.00595600	1.86089700	-3.22404100
H	-3.84323600	0.98323000	-1.96250000
N	0.22276600	-1.15720100	0.30057700
N	-1.23261300	0.00994800	-2.55049200
C	-0.89458200	-2.80822600	-2.66603600
H	-0.05330500	-2.27121000	-3.10402600
H	-0.60599700	-3.84110900	-2.47406900
H	-1.71875200	-2.79152500	-3.38045700
C	-2.51898800	-2.91681000	-0.73260800
H	-2.84029600	-2.45162700	0.19812600
H	-3.36067300	-2.92791700	-1.42785100
H	-2.21348300	-3.94541800	-0.53665300
H	2.40897700	-3.47794700	0.36490400
H	-3.08108200	1.87028800	-0.60306100
C	2.63895300	-0.86082100	0.57845900
C	3.38619900	-0.09277300	1.46561800
C	3.03291000	-0.92983000	-0.75958200
C	4.52016400	0.58982600	1.02960200
H	3.07799600	-0.02552800	2.50368400
C	4.16001800	-0.24840800	-1.19918800
H	2.44779600	-1.51819500	-1.46164000
C	4.90962000	0.51163500	-0.30204200
H	5.09518700	1.18321200	1.73050900
H	4.45472500	-0.30609800	-2.24018500
H	5.78983500	1.04261900	-0.64410000
C	-0.63263800	2.20326300	-1.59949500
C	-0.94620100	3.47762900	-1.12255000
C	0.65161300	1.70271600	-1.39207600
C	-0.00223600	4.22866100	-0.43393700
H	-1.94260600	3.88084300	-1.27515000
C	1.59814200	2.45157600	-0.69759400
H	0.90233500	0.71196500	-1.74615300
C	1.27292900	3.71349700	-0.21367900
H	-0.26510600	5.21103300	-0.05995900

H	2.58567900	2.03587600	-0.52955400
H	2.00674700	4.29404700	0.33299300
C	-1.52174000	1.18558000	1.56924900
C	-1.61903800	0.08592300	2.64230400
F	-2.07946700	-1.06069600	2.13694100
F	-2.42317700	0.44739800	3.63566800
F	-0.40365700	-0.15266000	3.15933600
O	-2.28395600	2.10540100	1.60114600
H	-0.71977100	1.04134200	0.83122500

COM4-4

C	1.69477700	-2.61812600	0.14478100
C	0.23885800	-2.57358600	-0.25291400
O	-0.50920400	-3.56299300	0.28304900
C	-1.73734900	-2.15239800	-1.12520300
C	-1.87259300	-3.24001900	-0.03703400
H	-1.89694600	-2.58343900	-2.12068600
H	-2.37250000	-4.14698600	-0.37083400
C	2.31991600	-1.27095700	-0.14599900
O	3.11209800	-1.18949600	-1.23787000
C	2.93560000	0.85008500	-0.07057000
C	3.71238900	0.11959300	-1.19568400
H	3.61645200	1.28850500	0.66092000
H	4.77025500	-0.00408600	-0.96129300
N	-0.31733700	-1.75024200	-1.03794300
N	2.17900600	-0.23921000	0.57598600
C	1.80741800	-2.89199600	1.65452500
H	1.28213800	-2.12672700	2.22472800
H	1.37823700	-3.86663900	1.88366200
H	2.85943100	-2.88589900	1.94479300
C	2.37574200	-3.73986500	-0.65641000
H	2.31301800	-3.54819500	-1.72735400
H	3.42809100	-3.81058300	-0.37683700
H	1.88656200	-4.68827500	-0.43072300
H	-2.34038000	-2.85266100	0.86924800
H	3.59817400	0.58232800	-2.17417200
C	-2.68039300	-0.97820300	-0.95946500
C	-3.93762700	-1.13304000	-0.37774400
C	-2.30151300	0.28507300	-1.41143000
C	-4.78676400	-0.04041100	-0.22668700
H	-4.26516500	-2.10755400	-0.03170900
C	-3.13893200	1.38141100	-1.24585500
H	-1.32928300	0.40156100	-1.87171100
C	-4.38637900	1.22186900	-0.64953600
H	-5.75816600	-0.17623800	0.23367700
H	-2.81125600	2.36150700	-1.57386000
H	-5.04050700	2.07469300	-0.51442700
C	2.00766600	1.93122100	-0.58301100
C	2.07887700	3.23091700	-0.09072100
C	1.07237800	1.62788500	-1.57478700
C	1.23223200	4.22053200	-0.58123200
H	2.79490700	3.46758700	0.68894100
C	0.23052200	2.61696700	-2.06994700
H	0.99861800	0.60701500	-1.94541500
C	0.30874000	3.91593400	-1.57352000
H	1.29199500	5.22694300	-0.18467000

H	-0.48619300	2.37781200	-2.84795700
H	-0.34915500	4.68529200	-1.95978100
C	-0.51934400	0.21897100	1.34003700
C	-0.33647400	1.52952200	2.12305200
F	0.94408100	1.75549600	2.42623900
F	-1.03010300	1.52160700	3.25802300
F	-0.76575900	2.55090400	1.37232600
O	-0.92127700	-0.76763800	1.88365100
H	-0.29339600	0.29090200	0.27135800

COM4-5

C	1.32457900	-2.81194000	-0.48496900
C	2.29518100	-1.67228900	-0.29479400
O	3.37591000	-1.70330900	-1.10884300
C	3.34390900	0.15947600	0.33600500
C	4.07542900	-0.46311400	-0.88476100
H	3.96776500	0.09627200	1.23263900
H	5.12418200	-0.68750400	-0.70031400
C	0.13680600	-2.53289400	0.40529600
O	0.27244800	-2.88254900	1.70166600
C	-1.76996100	-1.79796500	1.24271400
C	-0.97918200	-2.55927100	2.33729500
H	-2.75258300	-2.24269700	1.07668300
H	-1.46017400	-3.49275600	2.63045700
N	2.18001500	-0.71471600	0.52361800
N	-0.94346400	-1.98710800	0.03248700
C	0.88471500	-2.84477800	-1.95547400
H	0.43474300	-1.89605000	-2.24917500
H	1.74883000	-3.04203200	-2.58948600
H	0.14415400	-3.63246300	-2.09864800
C	2.00636700	-4.13344000	-0.09423000
H	2.32971400	-4.11286800	0.94604900
H	1.30668700	-4.96108700	-0.22577000
H	2.87137000	-4.29957700	-0.73688400
H	3.97522100	0.15141200	-1.78084100
H	-0.76984600	-1.95337800	3.21726500
C	2.95571700	1.60572000	0.12165700
C	3.90537500	2.60807100	0.32493700
C	1.67834000	1.95819000	-0.30910000
C	3.58582400	3.94075600	0.09349200
H	4.89889900	2.34290100	0.67385100
C	1.35282600	3.29340400	-0.53081300
H	0.92548400	1.19017100	-0.44577000
C	2.30638100	4.28625000	-0.33376800
H	4.33145000	4.71018100	0.25582000
H	0.34683000	3.54203300	-0.84660100
H	2.05368700	5.32576500	-0.50569400
C	-1.93881000	-0.31929700	1.52894600
C	-3.20080100	0.27258600	1.54321600
C	-0.80920000	0.47230800	1.75796300
C	-3.33677300	1.64028500	1.76877000
H	-4.07972400	-0.33592500	1.35867400
C	-0.94615100	1.83538700	1.98413600
H	0.18095100	0.02419300	1.71984900
C	-2.20998600	2.42307700	1.98561400
H	-4.32134800	2.09205100	1.75927300

H	-0.06264300	2.44432700	2.13675500
H	-2.31245400	3.48936300	2.14744600
C	-1.86948400	0.83973400	-1.28168200
C	-3.26441800	0.35708600	-1.71548300
F	-3.27591000	0.22987700	-3.05042400
F	-4.22033700	1.21250700	-1.37414600
F	-3.55900700	-0.84010600	-1.20121200
O	-1.65775400	2.00591600	-1.13355700
H	-1.12469000	0.03542000	-1.18019700

COM4-6

C	1.08102300	-0.61914800	2.15463500
C	0.15524600	-1.41617900	1.26965700
O	0.00353400	-2.70796400	1.61707100
C	-1.24320700	-2.09508800	-0.28954100
C	-0.93880400	-3.26926600	0.68265100
H	-0.84192900	-2.32168300	-1.28288000
H	-0.46312900	-4.11686900	0.19309800
C	1.29117700	0.71199500	1.48152400
O	2.02328900	0.67958800	0.33149200
C	1.18705700	2.82165200	0.84988000
C	2.12046800	2.04812500	-0.11623500
H	1.71034500	3.65627000	1.31959100
H	3.16414500	2.35394200	-0.04099000
N	-0.48073100	-0.97418500	0.26717200
N	0.84212500	1.82322000	1.87779700
C	0.39868200	-0.42581500	3.51559000
H	-0.54168600	0.11333100	3.40216600
H	0.20971600	-1.40096900	3.96582100
H	1.04820500	0.15420600	4.17218800
C	2.42149500	-1.35524200	2.32091000
H	2.90132500	-1.54112400	1.36113100
H	3.09063400	-0.74999000	2.93574800
H	2.25226600	-2.31010800	2.81820100
H	-1.81901700	-3.59438800	1.23821900
H	1.79323100	2.09490400	-1.15339900
C	-2.71757900	-1.78319000	-0.42753300
C	-3.52325600	-2.62260800	-1.19879100
C	-3.29519100	-0.69067600	0.21591800
C	-4.88597700	-2.37981500	-1.31961600
H	-3.07755900	-3.46909800	-1.71272700
C	-4.65974400	-0.44289700	0.08898300
H	-2.67153500	-0.02934800	0.80635800
C	-5.45811100	-1.28595800	-0.67557400
H	-5.50047700	-3.03865000	-1.92167800
H	-5.09673500	0.41366000	0.58897300
H	-6.51942700	-1.09150200	-0.77315700
C	-0.06920400	3.33832800	0.17908900
C	-0.30434500	4.70369200	0.05349300
C	-0.99954400	2.43216200	-0.33679500
C	-1.45443300	5.16653400	-0.58228500
H	0.41171400	5.41101000	0.45901100
C	-2.14794000	2.89362700	-0.96779400
H	-0.82776400	1.36344900	-0.23307400
C	-2.37811400	4.26264300	-1.09252900
H	-1.62901700	6.23222500	-0.67222900

H	-2.86703100	2.18197600	-1.35829100
H	-3.27541600	4.62103800	-1.58297400
C	1.99756400	-1.40847000	-1.40542100
C	3.40872000	-0.89721100	-1.74344600
F	3.38447700	0.38298400	-2.12197300
F	3.90749600	-1.61066500	-2.75812400
F	4.23513300	-1.01874000	-0.71027600
O	1.87279800	-2.47467800	-0.88224000
H	1.16256800	-0.75648100	-1.70173700

COM4-7

C	0.65402200	-2.02803400	0.19448400
C	0.77023800	-0.65268600	0.80595700
O	1.97367000	-0.04096100	0.63746300
C	0.39563200	1.30904100	1.73027400
C	1.90620100	1.16920600	1.42031900
H	0.23804300	1.54115100	2.78462200
H	2.50674700	1.02085600	2.31864800
C	-0.82209900	-2.34720400	0.14852600
O	-1.35618800	-2.84020700	1.28632100
C	-2.94921800	-2.47086200	-0.41637600
C	-2.76163100	-3.01255100	1.02715200
H	-3.36093400	-3.23790200	-1.07567000
H	-2.99664400	-4.07290900	1.11790900
N	-0.13353300	-0.02825700	1.43233500
N	-1.57505600	-2.15167200	-0.84934300
C	1.22745700	-2.01096700	-1.22850200
H	0.74598800	-1.24730200	-1.83989000
H	2.30112000	-1.83030300	-1.18487300
H	1.05364600	-2.97926200	-1.69884700
C	1.42247200	-3.02973200	1.07214100
H	1.01194200	-3.05676000	2.08085200
H	1.35217700	-4.02919800	0.63842900
H	2.47331200	-2.73948300	1.11443300
H	2.31263000	1.98862600	0.82950200
H	-3.31776500	-2.44208100	1.77011900
C	-0.29494900	2.36428700	0.88640700
C	-0.39024200	3.67156300	1.36470900
C	-0.80420900	2.06492300	-0.37686600
C	-0.97625900	4.66732500	0.59192500
H	-0.00799200	3.90863000	2.35266600
C	-1.39392700	3.06084100	-1.14973400
H	-0.77629100	1.04508900	-0.74610600
C	-1.47951100	4.36305100	-0.66977500
H	-1.04752900	5.67764400	0.97705500
H	-1.79988000	2.81167200	-2.12299400
H	-1.94299100	5.13584700	-1.27123200
C	-3.82475400	-1.23819200	-0.49045400
C	-5.01007800	-1.23953200	-1.21918000
C	-3.43409000	-0.07612600	0.17866400
C	-5.80126400	-0.09472700	-1.28151500
H	-5.31435400	-2.13762800	-1.74676600
C	-4.21733300	1.06909000	0.10955500
H	-2.50367600	-0.06696400	0.74086100
C	-5.40470800	1.06156500	-0.61979200
H	-6.72211100	-0.10587800	-1.85275000

H	-3.89289300	1.97110100	0.61687500
H	-6.01538100	1.95507300	-0.67400300
C	4.07419800	0.44458500	-1.57606500
C	4.88182700	-0.14456300	-0.40541600
F	4.72543900	0.61268000	0.68686300
F	6.17417300	-0.20633500	-0.68908700
F	4.45493400	-1.37873300	-0.11570800
O	4.61620600	0.74999100	-2.59219400
H	2.99588900	0.54859400	-1.37974800

COM4-8

C	-0.73166500	-2.70467700	0.06315500
C	0.07709900	-1.86854700	-0.90807800
O	-0.47656900	-0.67149000	-1.23675100
C	1.65275500	-0.98321000	-2.15677200
C	0.38010600	-0.10700100	-2.24719300
H	1.98117100	-1.29681800	-3.14970900
H	-0.13083300	-0.19826100	-3.20747800
C	-0.62912500	-1.93937200	1.36506200
O	0.52308100	-2.13657600	2.05770100
C	-0.76349500	-0.38394400	2.91366500
C	0.39428600	-1.34140400	3.25207400
H	-1.44975500	-0.25533000	3.75069800
H	0.15201500	-2.00940200	4.08039600
N	1.20925500	-2.15842600	-1.39225100
N	-1.44622500	-1.07053800	1.78957600
C	-2.19165000	-2.77517100	-0.39616100
H	-2.64643000	-1.78861700	-0.41466500
H	-2.23985400	-3.21387600	-1.39483700
H	-2.75717400	-3.40561400	0.29182900
C	-0.12011700	-4.10054900	0.19399600
H	0.92815600	-4.04729300	0.47939400
H	-0.66876800	-4.66839400	0.94796500
H	-0.19425600	-4.62017700	-0.76204000
H	0.54944900	0.94161800	-2.00741100
H	1.34289400	-0.84026400	3.43600300
C	2.79894100	-0.26204200	-1.46678000
C	3.35616700	0.85892000	-2.08833100
C	3.28658900	-0.65808000	-0.22437600
C	4.36807100	1.58250700	-1.47120100
H	2.99010400	1.16918000	-3.06272400
C	4.29768000	0.07154200	0.39840600
H	2.86467200	-1.53191700	0.25893300
C	4.83841400	1.19248900	-0.21893600
H	4.78891100	2.45058300	-1.96464700
H	4.66202100	-0.24079200	1.37012000
H	5.62354000	1.75831800	0.26786200
C	-0.30886400	0.96471300	2.39503500
C	-0.95742400	2.14087300	2.75375400
C	0.71381200	1.01471100	1.44245000
C	-0.59821500	3.35060000	2.15872800
H	-1.75797700	2.11155100	3.48545700
C	1.07856200	2.21600900	0.85247200
H	1.22016900	0.10303300	1.14352200
C	0.41334000	3.38945400	1.20680000
H	-1.11547300	4.26112900	2.43715200

H	1.87435100	2.22891400	0.11388300
H	0.67998800	4.32780400	0.73627000
C	-1.96323800	1.57060200	-0.77090900
C	-3.27226400	0.94855000	-1.29362500
F	-3.03093600	0.08567900	-2.28455800
F	-4.08494200	1.89280100	-1.76803200
F	-3.91353900	0.29668200	-0.32159500
O	-1.40511100	2.38523400	-1.44342500
H	-1.62316700	1.21171100	0.21079900

COM4-9

C	2.52428300	2.15271500	-0.14936100
C	1.04774700	2.38969900	-0.35284300
O	0.72956700	3.55206400	-0.96958900
C	-1.15454200	2.34206500	-0.28674900
C	-0.69023300	3.47716700	-1.21933200
H	-1.53878000	2.75161600	0.65239700
H	-1.13248600	4.44449700	-0.99496700
C	2.70608900	0.71223400	0.26480400
O	2.31879800	0.39432800	1.52790100
C	3.09464900	-1.45761000	0.29455900
C	2.65346000	-0.99493400	1.70738600
H	4.07759400	-1.93079600	0.32470600
H	3.45537900	-1.05940200	2.44338100
N	0.10321100	1.63425000	0.02258800
N	3.18582800	-0.19955700	-0.46733700
C	3.27889100	2.42151200	-1.45629600
H	2.92453400	1.76612900	-2.25164600
H	3.13631800	3.46035100	-1.75243000
H	4.34195100	2.22926700	-1.30835500
C	3.01450600	3.09589600	0.96552400
H	2.47810300	2.91011600	1.89583800
H	4.08119400	2.93720500	1.13590100
H	2.85899200	4.13161000	0.66111000
H	-0.83776800	3.23017000	-2.27349300
H	1.77094800	-1.52089700	2.07246500
C	-2.18306200	1.40000600	-0.86021900
C	-3.44034000	1.28394500	-0.27432800
C	-1.85819100	0.58828400	-1.94842600
C	-4.36847200	0.37286000	-0.77162700
H	-3.68404900	1.88985100	0.59215200
C	-2.78387700	-0.31820400	-2.44775100
H	-0.86722100	0.65050900	-2.38776100
C	-4.04214100	-0.42820700	-1.85857800
H	-5.33971000	0.28216400	-0.30031500
H	-2.52201300	-0.94710700	-3.29084700
H	-4.76089700	-1.14180800	-2.24332400
C	2.11309900	-2.40097300	-0.36704600
C	2.48682700	-3.69959400	-0.69976000
C	0.81228700	-1.97166100	-0.63904100
C	1.57535800	-4.56555100	-1.29826400
H	3.49796300	-4.03511500	-0.49395400
C	-0.09847900	-2.83570100	-1.23467100
H	0.51100900	-0.95481000	-0.39360500
C	0.28214000	-4.13395300	-1.56728400
H	1.87754800	-5.57394600	-1.55532800

H	-1.10735800	-2.49270000	-1.43158500
H	-0.42889000	-4.80588900	-2.03318300
C	-1.13208000	0.26807100	2.22780900
C	-1.92558000	-1.00896800	1.90608900
F	-1.87772900	-1.29209000	0.60390000
F	-3.19726100	-0.90449800	2.26771600
F	-1.37688000	-2.03980000	2.56524100
O	-1.69555400	1.24539100	2.62047900
H	-0.04532800	0.19477800	2.07648000

COM4-10

C	2.45518100	0.92579200	1.40651500
C	1.98841000	-0.46226100	1.03106400
O	2.50591300	-1.46120700	1.77250800
C	0.95429400	-2.21913400	0.17181700
C	2.02936000	-2.68856800	1.18035300
H	1.12742000	-2.65652300	-0.81234900
H	2.87381800	-3.17412800	0.69084900
C	1.42867400	1.89973200	0.87458400
O	1.53608400	2.23449200	-0.43569600
C	-0.35469500	3.16472200	0.61234500
C	0.51754600	3.22943800	-0.66755300
H	-0.52664700	4.16320400	1.01781400
H	1.01304200	4.19479700	-0.78334700
N	1.17489100	-0.76066400	0.10262100
N	0.47954300	2.39162900	1.54958900
C	2.53522700	1.04980500	2.93381400
H	1.56135900	0.87400300	3.38932400
H	3.25413300	0.33086300	3.32464200
H	2.85502200	2.05925800	3.19509100
C	3.83826700	1.16393700	0.77611900
H	3.80574900	1.06023900	-0.30824500
H	4.18573800	2.16981200	1.01898900
H	4.54908900	0.44125700	1.17942500
H	1.63706000	-3.31969000	1.97538200
H	-0.02049200	2.96670500	-1.57473800
C	-0.46846000	-2.50583900	0.60535400
C	-1.29707600	-3.32115600	-0.16045800
C	-0.96131500	-1.95852400	1.79164300
C	-2.59729900	-3.59708200	0.25600000
H	-0.92532900	-3.73525200	-1.09143400
C	-2.25660100	-2.23259700	2.21012300
H	-0.33156500	-1.30147400	2.38502200
C	-3.07770300	-3.05597100	1.44294700
H	-3.23355000	-4.23167300	-0.34947100
H	-2.63040900	-1.79498100	3.12789100
H	-4.08986600	-3.26683600	1.76689300
C	-1.69100400	2.48233100	0.39630500
C	-2.87021900	3.22278000	0.36157200
C	-1.74644400	1.10300700	0.19378300
C	-4.08976000	2.59563200	0.12020400
H	-2.83682600	4.29481700	0.52827800
C	-2.96174700	0.47521700	-0.04920600
H	-0.83583500	0.51479100	0.21571000
C	-4.13742200	1.22086000	-0.08622300
H	-5.00174000	3.18076700	0.09888400

H	-2.98265100	-0.59894400	-0.20359100
H	-5.08693800	0.73267600	-0.27209700
C	1.87210900	-0.38169200	-2.38540500
C	0.39176900	-0.33848500	-2.80002900
F	-0.27584000	-1.42177200	-2.41077300
F	0.32110900	-0.27662400	-4.13800000
F	-0.22180900	0.73894400	-2.31584500
O	2.50406600	-1.38549400	-2.53201000
H	2.27218100	0.58062900	-2.03524800

COM4-11

C	-0.31740300	-2.60251000	0.28106000
C	0.39167600	-1.51639200	1.05308500
O	1.73859700	-1.68027300	1.17776900
C	0.94345800	0.26896800	2.21710100
C	2.15844000	-0.68837000	2.13767800
H	0.69277200	0.47684200	3.25946500
H	2.34508900	-1.19815500	3.08424100
C	-1.74384900	-2.14659500	0.08079200
O	-2.57265800	-2.33259900	1.13305600
C	-3.59717800	-1.22781600	-0.67895100
C	-3.86692800	-1.87023000	0.70716500
H	-4.24788000	-1.65274300	-1.44545400
H	-4.53303800	-2.73182200	0.64999400
N	-0.13950400	-0.51273300	1.60853600
N	-2.19918300	-1.60510100	-0.96798700
C	0.35690600	-2.81675600	-1.07938700
H	0.32163300	-1.91045600	-1.68039900
H	1.39298500	-3.12554700	-0.93238300
H	-0.16824000	-3.60617000	-1.61863400
C	-0.27051900	-3.89697300	1.11268900
H	-0.73840100	-3.75228200	2.08595200
H	-0.80210400	-4.69114000	0.58498900
H	0.76708100	-4.20262600	1.25204600
H	3.06787600	-0.21355500	1.77553900
H	-4.23740000	-1.15983500	1.44458200
C	1.16763000	1.58798200	1.50099100
C	2.06194300	2.50592500	2.05561000
C	0.53829700	1.89504100	0.29884300
C	2.33715300	3.70402500	1.41086300
H	2.54846700	2.27753400	2.99964300
C	0.80871000	3.10016700	-0.34562700
H	-0.15642600	1.19012900	-0.14118200
C	1.70961400	4.00386900	0.20368900
H	3.03655800	4.40580700	1.84963600
H	0.31118800	3.32630600	-1.28154900
H	1.92141500	4.93867100	-0.30145500
C	-3.74613600	0.27847800	-0.68401400
C	-4.65245500	0.91040900	-1.52932300
C	-2.95871100	1.04881700	0.17477900
C	-4.77548300	2.29808300	-1.52147200
H	-5.26218100	0.31629100	-2.20208400
C	-3.07495500	2.43309500	0.17798500
H	-2.24035500	0.56002200	0.82906800
C	-3.98575900	3.06104300	-0.66979400
H	-5.48348100	2.78064100	-2.18493500

H	-2.44786600	3.02259600	0.83723700
H	-4.07590800	4.14086600	-0.66676800
C	3.81731200	-1.42148200	-1.28270700
C	3.22581500	-0.01000100	-1.42409600
F	1.89142700	-0.07811700	-1.45332000
F	3.64488600	0.59597300	-2.52263600
F	3.57530000	0.73175300	-0.36575700
O	4.54482300	-1.86922800	-2.11333800
H	3.50293200	-1.94888700	-0.36762100

COM4-12

C	-0.32510400	3.09024400	-0.21114100
C	-1.09835900	2.01000300	-0.94448200
O	-0.34170900	1.17949200	-1.70001100
C	-2.61929000	0.58179400	-1.64738900
C	-1.23246900	0.17518300	-2.22349100
H	-3.31131800	0.84184700	-2.45337200
H	-1.18751700	0.21910000	-3.31110900
C	0.33085200	2.32709900	0.92217100
O	-0.39226200	2.22396200	2.06334400
C	1.48972000	0.83252100	2.04658300
C	0.43454200	1.47040600	2.97351200
H	2.49052900	0.86986300	2.47696400
H	0.87720000	2.16909500	3.68561900
N	-2.34152500	1.79201200	-0.86200800
N	1.41878200	1.68381800	0.83799000
C	0.74755700	3.68889700	-1.12829400
H	1.44831700	2.92602900	-1.46075500
H	0.27233000	4.14420000	-1.99931500
H	1.29818600	4.45972800	-0.58687900
C	-1.27691600	4.16492200	0.31309700
H	-2.05939900	3.72943100	0.93045000
H	-0.71768500	4.89224200	0.90458500
H	-1.74256700	4.67853800	-0.52906900
H	-0.88358400	-0.79733500	-1.87405700
H	-0.19407700	0.74836200	3.49039300
C	-3.25184800	-0.51506600	-0.81333500
C	-3.55189200	-1.73571800	-1.42316400
C	-3.51777300	-0.35269300	0.54364200
C	-4.09219000	-2.78190600	-0.68606900
H	-3.35575200	-1.86940300	-2.48296800
C	-4.05580800	-1.40291900	1.28432600
H	-3.29389600	0.59641000	1.01598700
C	-4.34190900	-2.61870100	0.67484000
H	-4.31716100	-3.72418100	-1.17144800
H	-4.24982100	-1.26783200	2.34183700
H	-4.75843700	-3.43442600	1.25334100
C	1.15270900	-0.59329700	1.65053500
C	2.08121600	-1.62319400	1.78058800
C	-0.11069500	-0.88179000	1.12237600
C	1.76096700	-2.91833700	1.37690800
H	3.06487100	-1.40949300	2.18446600
C	-0.43614100	-2.17226700	0.73090900
H	-0.85055000	-0.09235200	1.02009800
C	0.50657500	-3.19313600	0.84972500
H	2.49925000	-3.70610700	1.46534800

H	-1.42226000	-2.37923700	0.32828500
H	0.26040700	-4.19788200	0.52854300
C	2.15986100	-0.69698400	-1.24985900
C	3.66340600	-0.81611200	-0.94779800
F	4.35203300	-0.34654700	-1.99859400
F	4.04160300	-2.07176300	-0.73640200
F	4.01297700	-0.08195000	0.11385100
O	1.57245200	-1.62193100	-1.72914100
H	1.72269600	0.28905700	-1.03719800

COM5-1

C	6.07841300	-2.72407900	0.00865200
C	4.97090000	-1.92512000	0.25845200
C	4.36390900	-1.22029100	-0.78437800
C	4.87031800	-1.33872700	-2.08067100
C	5.98033600	-2.13601900	-2.32597700
C	6.58706600	-2.82872300	-1.28292800
H	6.54075400	-3.27187000	0.82074400
H	4.56141800	-1.87099200	1.25970400
H	4.39419000	-0.79048500	-2.88309800
H	6.37365800	-2.21533400	-3.33208500
H	7.45160300	-3.45259200	-1.47586900
C	3.18174600	-0.36684100	-0.54464300
O	2.45822500	-0.13198200	-1.63079900
C	2.85324100	0.13746200	0.67825000
H	1.69464500	0.43332700	-1.35480500
H	3.46429100	-0.05661700	1.54491700
C	1.58075400	0.81071100	0.86379600
O	0.82642100	1.09821000	-0.06372800
O	1.28819800	1.09104000	2.12668100
H	0.30094600	1.17985300	2.20288600
C	-3.01275200	1.92660900	1.30630000
C	-3.59721800	1.53240000	-0.02817100
O	-2.77299900	0.78543700	-0.80464000
C	-4.87510800	1.16939700	-1.77981400
C	-3.43994600	0.65951300	-2.07383200
H	-5.19177900	1.89936900	-2.52615300
H	-2.91348900	1.28513600	-2.79585200
C	-2.47966000	0.66329600	1.93050700
O	-3.35828100	-0.35622200	2.00140600
C	-1.22417200	-0.93935600	2.81459100
C	-2.69081200	-1.42658200	2.70091300
H	-0.87442100	-0.98052200	3.84729300
H	-3.17208700	-1.54436800	3.67176900
N	-4.74259800	1.83312700	-0.46892100
N	-1.31298100	0.47376100	2.38845800
C	-1.87189300	2.92673900	1.07988700
H	-1.08680700	2.49092100	0.46071600
H	-2.27055200	3.81912600	0.59411600
H	-1.44248900	3.21567300	2.04112800
C	-4.10615400	2.51007200	2.20900800
H	-4.91244800	1.79226200	2.35772500
H	-3.67506800	2.78014500	3.17489400
H	-4.52375500	3.40121700	1.74081400
H	-3.40372500	-0.38372700	-2.38190500
H	-2.79673100	-2.33677600	2.11377800

C	-5.89534900	0.05185000	-1.71559600
C	-6.82313700	-0.11840200	-2.73948200
C	-5.88358900	-0.84917900	-0.64907300
C	-7.72726000	-1.17660800	-2.70658600
H	-6.84182900	0.58357100	-3.56672700
C	-6.78501500	-1.90586900	-0.61597900
H	-5.17248600	-0.71596200	0.16070000
C	-7.70902900	-2.07288400	-1.64468600
H	-8.44735700	-1.29608700	-3.50739500
H	-6.77146000	-2.59927200	0.21677400
H	-8.41355700	-2.89543700	-1.61486500
C	-0.25828700	-1.70543200	1.93236800
C	0.78466400	-2.44112800	2.48923500
C	-0.41690700	-1.68566300	0.54518700
C	1.65670100	-3.15790100	1.67407200
H	0.91858100	-2.44857800	3.56594600
C	0.45751200	-2.39504400	-0.26924800
H	-1.20589500	-1.08515300	0.10033400
C	1.49499900	-3.13480000	0.29346400
H	2.46612800	-3.72690700	2.11677500
H	0.34153200	-2.35730800	-1.34572600
H	2.18390700	-3.67707900	-0.34404400
C	3.63717300	2.74768400	-0.43331000
C	5.12945600	2.37843000	-0.45345900
F	5.85033900	3.50839100	-0.48486900
F	5.43886500	1.65696200	-1.52155400
F	5.49044600	1.70700000	0.64200900
O	3.00320700	2.76066700	-1.44317900
H	3.25288500	3.05479400	0.55347200

COM5-2

C	-7.38988300	-1.58657700	0.09254500
C	-6.06170100	-1.30713900	-0.19853700
C	-5.15750100	-1.04399400	0.83389300
C	-5.59769100	-1.07712200	2.15972000
C	-6.92947300	-1.35043300	2.44593400
C	-7.82736900	-1.60468300	1.41429900
H	-8.08344000	-1.79843300	-0.71201100
H	-5.72151300	-1.31692300	-1.22696800
H	-4.88834200	-0.88163100	2.95391800
H	-7.26590900	-1.36688000	3.47544600
H	-8.86458600	-1.82279900	1.63859300
C	-3.74181200	-0.71678600	0.55701800
O	-2.92557500	-0.96412400	1.57148100
C	-3.31776600	-0.15706300	-0.60935900
H	-2.02319000	-0.65351500	1.29506700
H	-4.00470200	0.05720900	-1.41272800
C	-1.90226200	0.13098200	-0.79655600
O	-1.07267000	-0.00075900	0.10109300
O	-1.58177600	0.56408500	-2.00251600
H	-0.58546300	0.57222600	-2.08741000
C	2.49459300	1.73966400	-1.17606700
C	3.18803600	1.37092000	0.11306000
O	2.51263500	0.47749400	0.87693500
C	4.58239200	1.10489700	1.79050600
C	3.24208500	0.39413900	2.11391800
H	4.83625900	1.83217900	2.56300200
H	2.66754800	0.91521800	2.88110300
C	2.17317100	0.44230000	-1.87086500
O	3.19577900	-0.43362000	-1.96919700
C	1.17818100	-1.31917100	-2.77774200
C	2.70218700	-1.54617500	-2.74482500
H	0.77604600	-1.43687200	-3.78458600
H	3.15218600	-1.48929200	-3.73634900
N	4.30012600	1.80862600	0.52509800
N	1.05416000	0.09660400	-2.35521500
C	1.19829100	2.49304800	-0.85046200
H	0.53716400	1.88347200	-0.23302600
H	1.44162800	3.41580300	-0.32042300
H	0.67662500	2.75064400	-1.77405000
C	3.43002800	2.56914400	-2.06269500
H	4.34307700	2.01831300	-2.28797700
H	2.91811100	2.82429700	-2.99236500
H	3.70463100	3.48572400	-1.54086000
H	3.35789600	-0.65542200	2.37823200
H	2.99804000	-2.46878100	-2.24938800

C	5.73456300	0.13522800	1.62546900
C	6.69189600	0.00093200	2.62787400
C	5.81881000	-0.67247300	0.48996300
C	7.71911000	-0.93056800	2.50564300
H	6.63643900	0.63229000	3.50873900
C	6.84394500	-1.60276600	0.36766700
H	5.08617900	-0.56335400	-0.30352200
C	7.79640300	-1.73516100	1.37493200
H	8.46056400	-1.02222800	3.29050700
H	6.90441500	-2.22338900	-0.51879200
H	8.59698000	-2.45838400	1.27537200
C	0.37802600	-2.15760600	-1.80215800
C	-0.88733100	-2.62198300	-2.14733400
C	0.84817700	-2.35155100	-0.50255100
C	-1.68481700	-3.26104200	-1.20136700
H	-1.26374700	-2.45510000	-3.15128400
C	0.06110300	-3.00289800	0.43654800
H	1.81226300	-1.94640900	-0.20853400
C	-1.21179900	-3.45069700	0.09211700
H	-2.67704400	-3.60220500	-1.47285000
H	0.42781500	-3.13714500	1.44718900
H	-1.83600600	-3.93603300	0.83262900
C	-3.45353700	2.25514500	1.16572600
C	-3.12127500	3.14912200	-0.04112300
F	-3.80362100	2.77986400	-1.12675300
F	-1.82615500	3.13757700	-0.32275000
F	-3.47920900	4.40827500	0.24733900
O	-2.61344300	1.96403400	1.95983600
H	-4.51934700	1.98468700	1.25139300

COM5-3

C	-5.64386600	2.60541500	-2.09953800
C	-4.88128200	1.58386900	-1.55190100
C	-4.60396800	1.57171300	-0.18241600
C	-5.11730600	2.58361100	0.63174000
C	-5.87500200	3.60846300	0.07860300
C	-6.13682000	3.62356200	-1.28722700
H	-5.86237700	2.60315400	-3.16039700
H	-4.52752500	0.77914100	-2.18451700
H	-4.91558000	2.55790300	1.69477300
H	-6.26428000	4.39367600	0.71522800
H	-6.73137500	4.42050300	-1.71754400
C	-3.76052700	0.52009700	0.42238200
O	-3.90254200	0.39705600	1.73310300
C	-2.87010000	-0.22727900	-0.29176100
H	-3.25000200	-0.28516600	2.03185900
H	-2.71642300	-0.05385100	-1.34458200
C	-1.93022500	-1.08411800	0.40431400
O	-1.96825600	-1.29486000	1.61733500
O	-0.99342200	-1.61638100	-0.36902400
H	-0.21042900	-1.81778500	0.20945300
C	3.18704800	-2.34180400	0.12081100
C	4.06321100	-1.47837900	-0.75345000
O	3.40115900	-0.48208400	-1.39671600
C	5.71823800	-0.47947800	-1.80233500
C	4.37097000	0.14210400	-2.25883900
H	6.27616400	-0.87196000	-2.65382500
H	4.12052400	-0.11056600	-3.28990700
C	2.44582600	-1.40047900	1.03622100
O	3.22188100	-0.55698600	1.74381700
C	0.91910900	-0.19957200	2.10585400
C	2.33468300	0.18759200	2.60584900
H	0.28671100	-0.55208800	2.92095400
H	2.51967400	-0.13114300	3.63165000
N	5.30790000	-1.59580500	-0.93021300
N	1.19046200	-1.32658100	1.19147600
C	2.19539400	-3.10960800	-0.76143700
H	1.58643200	-2.42523500	-1.35319200
H	2.74674400	-3.76898400	-1.43376600
H	1.53694500	-3.71608200	-0.13763700
C	4.04764500	-3.29234000	0.96020000
H	4.75097500	-2.73436300	1.57722800
H	3.40314500	-3.89880500	1.59922600
H	4.61585100	-3.94709500	0.29954600
H	4.32024800	1.21947200	-2.11210700
H	2.55813600	1.24655200	2.49235900

C	6.59259500	0.49961800	-1.04717500
C	7.73168500	1.03467900	-1.64236500
C	6.23703400	0.91027100	0.23896100
C	8.50689900	1.97420300	-0.96820300
H	8.01781200	0.71138100	-2.63793500
C	7.01026400	1.84788900	0.91209400
H	5.35913700	0.48570900	0.71664300
C	8.14665200	2.38300200	0.31026700
H	9.39351300	2.38079700	-1.44007600
H	6.72988900	2.15914300	1.91153900
H	8.75003500	3.11139400	0.83862700
C	0.20120100	0.92670500	1.38667400
C	-0.80925200	1.63268800	2.03712700
C	0.54319800	1.27405800	0.07940900
C	-1.47127500	2.67308800	1.39466900
H	-1.09747300	1.34770800	3.04368000
C	-0.12231700	2.31263700	-0.56456300
H	1.31454400	0.71688700	-0.44380800
C	-1.13181200	3.01269300	0.08912700
H	-2.26726600	3.20281800	1.90508500
H	0.14095300	2.56760700	-1.58439300
H	-1.66254700	3.80897900	-0.41966500
C	-4.62228900	-2.55510400	0.26990400
C	-5.55204200	-2.12277000	-0.87550000
F	-4.86185200	-1.82898500	-1.98280600
F	-6.28893600	-1.07350800	-0.54041500
F	-6.37369900	-3.13682300	-1.17679700
O	-4.92208400	-2.34419500	1.40414700
H	-3.72559800	-3.11169600	-0.04944900

COM5-4

C	2.95760500	-2.62130700	-0.09153600
C	3.55301900	-1.63181200	-1.07016600
O	3.26905500	-1.84261700	-2.37542200
C	4.45585600	0.14914400	-1.99220900
C	4.01031200	-0.83810000	-3.09788900
H	5.50723800	0.41791400	-2.10203100
H	4.85639200	-1.32730300	-3.58330100
C	2.64974500	-1.81690600	1.15277400
O	3.52699700	-1.86951600	2.16232500
C	1.77562700	-0.33677100	2.56759500
C	2.97735900	-1.05412100	3.22401800
H	0.85855500	-0.46143900	3.14292200
H	2.67701100	-1.72233100	4.03082200
N	4.25699600	-0.62883900	-0.75428700
N	1.63440800	-1.06685100	1.29192200
C	1.65475500	-3.21320200	-0.64902400
H	0.93465700	-2.43435200	-0.90136000
H	1.87191600	-3.78946500	-1.54795400
H	1.20512600	-3.87004900	0.09725700
C	3.98596900	-3.72628800	0.18915200
H	4.90372400	-3.30570100	0.59815700
H	3.57802800	-4.44483400	0.90226300
H	4.21305500	-4.24857700	-0.74181600
H	3.35037600	-0.39540100	-3.84100500
H	3.75596700	-0.37539900	3.56595600
C	3.61618700	1.41010500	-1.92967600
C	4.17539800	2.65975700	-2.17611900
C	2.25714700	1.32287800	-1.61803200
C	3.39014500	3.80981000	-2.11161900
H	5.23154800	2.73754500	-2.41387100
C	1.47378400	2.46515400	-1.54842200
H	1.80508100	0.35891200	-1.40820900
C	2.04068100	3.71400500	-1.79542300
H	3.83719600	4.77870000	-2.30182900
H	0.42646100	2.37647800	-1.28381100
H	1.43245900	4.60865800	-1.73173100
C	1.99475100	1.13436400	2.28359400
C	1.02234300	2.07305600	2.61661500
C	3.16506000	1.55224600	1.64544600
C	1.22245200	3.42167100	2.33065000
H	0.10139200	1.74089200	3.08237600
C	3.36358700	2.89629300	1.36056200
H	3.90331300	0.81834800	1.33346600
C	2.39381000	3.83405100	1.70646000
H	0.46087100	4.14681400	2.59269800

H	4.26427900	3.21022600	0.84624200
H	2.54705800	4.88185900	1.47505400
C	-6.42214300	1.25956600	-2.08556300
C	-5.23152400	0.86104700	-1.49365700
C	-4.97336700	1.17476000	-0.15576200
C	-5.93147200	1.87269200	0.58385000
C	-7.11912100	2.27374900	-0.01444100
C	-7.36594100	1.97062600	-1.34943200
H	-6.61733900	1.00823800	-3.12087000
H	-4.51439900	0.28535100	-2.06549100
H	-5.73288600	2.09924600	1.62326500
H	-7.85334000	2.82242400	0.56275500
H	-8.29403100	2.28086900	-1.81430000
C	-3.71189700	0.76530300	0.50038900
O	-3.78567300	0.72301500	1.82643500
C	-2.57850000	0.43929500	-0.17884800
H	-2.89722900	0.42235200	2.15090300
H	-2.52677800	0.51523000	-1.25340100
C	-1.37520800	0.05129400	0.54642200
O	-1.33655800	-0.02606200	1.77771300
O	-0.33876600	-0.21344000	-0.21480500
H	0.43210800	-0.55390200	0.36174900
C	-3.86207400	-2.18754600	0.72172000
C	-3.22650900	-2.77889800	-0.54714000
F	-3.63569000	-4.04484200	-0.69582800
F	-1.90215800	-2.77361100	-0.48190900
F	-3.60837200	-2.10570800	-1.63774100
O	-3.31133700	-2.28285900	1.77408200
H	-4.85841900	-1.73768200	0.57259000

COM5-5

C	4.10440900	-1.57933400	-1.26445500
C	4.18678100	-0.07964100	-1.10785900
O	4.66577700	0.57372700	-2.19419000
C	4.17827800	2.00004700	-0.39914300
C	4.44109900	1.97149200	-1.92220600
H	5.09493100	2.25797700	0.14227300
H	5.31834100	2.53269100	-2.23572600
C	3.53660400	-2.12022400	0.02126500
O	4.34220200	-2.08135500	1.09192500
C	2.16667500	-2.83726000	1.61622300
C	3.57748200	-2.58384700	2.20649100
H	1.85503500	-3.87345200	1.76038500
H	4.05905400	-3.49402100	2.56231000
N	3.86086900	0.59734400	-0.09008200
N	2.36560400	-2.58523500	0.17419100
C	3.17396800	-1.90283700	-2.44103900
H	2.19394300	-1.44648300	-2.29237200
H	3.61217200	-1.51577600	-3.36088900
H	3.05509800	-2.98400100	-2.52996500
C	5.51519700	-2.14534500	-1.50278700
H	6.17622300	-1.91198300	-0.66815600
H	5.46035200	-3.22989500	-1.61577100
H	5.92714300	-1.71785900	-2.41692100
H	3.56258200	2.29238100	-2.48692700
H	3.58089100	-1.82557600	2.98775100
C	3.09618700	2.97175800	0.00281200
C	3.43486600	4.29662900	0.27598000
C	1.75881000	2.58081400	0.06718700
C	2.45264900	5.22516200	0.60215000
H	4.47646500	4.60073300	0.24085300
C	0.77594100	3.50903400	0.40175200
H	1.49491600	1.54618400	-0.13367100
C	1.12036900	4.83120300	0.66684800
H	2.72845200	6.25146800	0.81396300
H	-0.25930000	3.19272300	0.45499500
H	0.35291100	5.55021500	0.92754000
C	1.09247500	-1.91587300	2.16210000
C	-0.03321000	-2.43017700	2.79970400
C	1.22438100	-0.53269500	2.01376900
C	-1.01537000	-1.57604100	3.29527300
H	-0.14542300	-3.50436500	2.90415800
C	0.23914400	0.31911500	2.49994800
H	2.09224300	-0.12305900	1.50084500
C	-0.88157100	-0.20055700	3.14458800
H	-1.88624600	-1.98665300	3.79366000

H	0.34743500	1.39025600	2.37135000
H	-1.65274200	0.46468000	3.51613200
C	-5.38750800	0.05523000	2.04491700
C	-4.15294200	-0.28204500	1.50957200
C	-3.49527700	0.60409300	0.65141400
C	-4.07893100	1.83759600	0.35242000
C	-5.31584000	2.16973400	0.88944200
C	-5.97286600	1.27966100	1.73210100
H	-5.89213500	-0.63375300	2.71119000
H	-3.68772300	-1.22521000	1.77009500
H	-3.56789600	2.51288600	-0.32122500
H	-5.77098200	3.12125900	0.64326800
H	-6.93852100	1.53969500	2.14905900
C	-2.20263500	0.24964600	0.03458100
O	-1.48364800	1.29875700	-0.35342200
C	-1.79379500	-1.03139600	-0.16789200
H	-0.66171700	0.94051800	-0.77389300
H	-2.40002400	-1.86795200	0.13987100
C	-0.46639800	-1.29223400	-0.69343700
O	0.29399900	-0.40173100	-1.08395300
O	-0.12134100	-2.56731700	-0.71221400
H	0.87798200	-2.61525800	-0.66570800
C	-3.65310800	-0.30708900	-2.61108800
C	-4.92618200	-0.95361800	-2.03816800
F	-5.57933900	-1.55902200	-3.04063300
F	-5.73557400	-0.06701000	-1.48451500
F	-4.62798100	-1.89251700	-1.13494300
O	-3.54659200	0.87663100	-2.70100200
H	-2.90397900	-1.03190500	-2.96832700

COM5-6

C	-4.35846800	-0.54736400	1.57827200
C	-3.90856300	-0.95744900	0.19491500
O	-4.88824900	-1.30831800	-0.65734200
C	-2.77678800	-1.26662700	-1.68801000
C	-4.22306500	-1.78308100	-1.85095100
H	-2.03754800	-2.02647600	-1.93893400
H	-4.27945900	-2.87259700	-1.85215400
C	-3.20050600	0.19446800	2.20849800
O	-2.26254000	-0.57455200	2.80144400
C	-1.69967100	1.70929700	2.74365800
C	-1.29388000	0.33998100	3.35201800
H	-1.78303800	2.46778500	3.52498600
H	-1.39829400	0.32111400	4.43793000
N	-2.71409300	-0.97585400	-0.23970900
N	-3.03111700	1.44809700	2.17342200
C	-5.56792000	0.39003500	1.45643700
H	-5.30957400	1.28439500	0.88984800
H	-6.39022400	-0.12896000	0.96513400
H	-5.88178900	0.69981700	2.45399600
C	-4.72475900	-1.80830300	2.37787200
H	-3.86891000	-2.47640700	2.46776800
H	-5.05216500	-1.52417000	3.37964200
H	-5.54172700	-2.33086700	1.87824900
H	-4.74235300	-1.37303400	-2.71387600
H	-0.30527900	0.00342300	3.05036500
C	-2.49248700	-0.01282200	-2.49330500
C	-1.52005900	-0.01660900	-3.48962500
C	-3.22347800	1.15362900	-2.26430400
C	-1.28234000	1.12443300	-4.24983300
H	-0.93052800	-0.91143900	-3.65174200
C	-2.98340300	2.29787700	-3.01606300
H	-3.97847900	1.17677000	-1.48329300
C	-2.01227000	2.28468800	-4.01340900
H	-0.51913000	1.10942400	-5.01893700
H	-3.54969700	3.20017900	-2.81921400
H	-1.82174700	3.17667400	-4.59814300
C	-0.73111600	2.21300100	1.68667600
C	0.41522000	2.90945600	2.07430900
C	-0.94707800	1.97210500	0.33202900
C	1.32820100	3.35304300	1.12276100
H	0.58798000	3.11645400	3.12663700
C	-0.03570600	2.41434900	-0.62246300
H	-1.82837200	1.42810900	0.01908800
C	1.10551400	3.10528800	-0.22961000
H	2.21428400	3.89440100	1.43487900

H	-0.22062900	2.19569400	-1.66954700
H	1.82468200	3.43825700	-0.96924200
C	5.51797700	1.84784800	1.63500900
C	4.26426500	1.37915500	1.26526600
C	4.05872500	0.87250300	-0.02079100
C	5.11590900	0.84821800	-0.93389500
C	6.37028400	1.31139400	-0.55573300
C	6.57313600	1.81126000	0.72687400
H	5.67128800	2.24979700	2.62919700
H	3.43393900	1.43289900	1.95962900
H	4.94383700	0.44937800	-1.92557900
H	7.19015800	1.28237400	-1.26309100
H	7.55052700	2.17708600	1.01799400
C	2.74654500	0.33183600	-0.43037200
O	2.51143800	0.41452400	-1.73230200
C	1.88232000	-0.25541800	0.44002100
H	1.63172900	-0.01504300	-1.88863400
H	2.10370100	-0.31323300	1.49461100
C	0.59136800	-0.72450000	-0.03758800
O	0.28271700	-0.75084200	-1.22928000
O	-0.23723300	-1.10798800	0.91334900
H	-1.16211400	-1.14599400	0.53890400
C	3.81629500	-2.42855800	-0.36157700
C	2.78525700	-3.40594900	0.22775400
F	3.32934700	-4.62864100	0.28853100
F	1.68931300	-3.47525200	-0.51607900
F	2.44287300	-3.05726200	1.46957900
O	3.90621300	-2.27696900	-1.54111600
H	4.47607900	-1.95105500	0.38219400

COM5-7

C	4.52618900	1.03383300	-1.35615000
C	4.04178300	-0.36626500	-1.05796800
O	4.99889600	-1.30640700	-0.96428000
C	2.86867600	-2.14142900	-0.42851000
C	4.30384100	-2.56547200	-0.80943700
H	2.11401700	-2.70618000	-0.97466800
H	4.34490900	-3.08779700	-1.76640100
C	3.38908200	1.96917100	-1.00974700
O	2.45342300	2.13738600	-1.96929200
C	1.91365300	3.19864700	0.05938300
C	1.50954000	3.08705900	-1.43489700
H	2.01589200	4.24552500	0.35307600
H	1.64325900	4.02724400	-1.97226900
N	2.83867100	-0.72799700	-0.86287600
N	3.23251900	2.54733000	0.10483800
C	5.74012100	1.34382900	-0.46929500
H	5.47776200	1.27340500	0.58606600
H	6.54789700	0.64745900	-0.69172400
H	6.07678000	2.36200800	-0.66772900
C	4.90143000	1.12622500	-2.84418800
H	4.04290000	0.90784700	-3.47837000
H	5.25476600	2.13385900	-3.07062000
H	5.70227200	0.41811000	-3.06173700
H	4.81208100	-3.14035800	-0.03898600
H	0.50954600	2.68940300	-1.58815900
C	2.58617900	-2.24599300	1.05809900
C	1.59054000	-3.09599400	1.53199100
C	3.34281400	-1.51173600	1.97227800
C	1.35522200	-3.21565600	2.89829900
H	0.98042700	-3.64499700	0.82421200
C	3.10516800	-1.62233500	3.33724400
H	4.11720300	-0.83672400	1.61829600
C	2.11075500	-2.47780400	3.80363600
H	0.57365700	-3.87666700	3.25379500
H	3.69168100	-1.03733600	4.03535900
H	1.92212100	-2.56275400	4.86714200
C	0.92833400	2.52843000	1.00254100
C	-0.22650600	3.21041600	1.39139200
C	1.13485700	1.23253000	1.46869400
C	-1.15801400	2.60365300	2.22738600
H	-0.39240400	4.22667900	1.04507700
C	0.20292000	0.62114700	2.30288200
H	2.02348600	0.69195900	1.17111800
C	-0.94599100	1.30519000	2.68475500
H	-2.05235800	3.14137200	2.52146900

H	0.37895100	-0.39772300	2.63352600
H	-1.68176300	0.82627400	3.32081600
C	-5.27318900	2.48013700	0.77769400
C	-4.07291100	1.86506400	0.44896200
C	-3.87559700	0.51185700	0.73597200
C	-4.88913600	-0.21154200	1.36879300
C	-6.08944800	0.40644000	1.69376500
C	-6.28467100	1.75174200	1.39786800
H	-5.41717800	3.53100500	0.55777300
H	-3.27649900	2.44442900	-0.00172300
H	-4.72975000	-1.25974700	1.58577000
H	-6.87431100	-0.16314400	2.17628200
H	-7.22059100	2.23383300	1.65388600
C	-2.61189600	-0.17056900	0.38854200
O	-2.39238500	-1.28066600	1.08015400
C	-1.74381000	0.28539800	-0.55763300
H	-1.53501300	-1.65772500	0.76055400
H	-1.94677300	1.18731600	-1.11291100
C	-0.45851000	-0.36728800	-0.73180700
O	-0.16701900	-1.44064100	-0.20380100
O	0.38594800	0.28282800	-1.51302300
H	1.30658900	-0.07614000	-1.36009100
C	-2.71188800	-2.00117300	-2.15240600
C	-4.06849600	-1.33979800	-2.44540600
F	-3.94528700	-0.02971100	-2.66859000
F	-4.92868700	-1.52877700	-1.45565500
F	-4.57867700	-1.88746700	-3.55828000
O	-2.62900600	-2.89187300	-1.36376700
H	-1.87912800	-1.63346600	-2.77416700

COM5-8

C	-4.55614200	-0.53310600	-0.86068800
C	-3.81714300	0.64073700	-0.26388700
O	-4.60234500	1.61986100	0.23201400
C	-2.31123100	2.02730200	0.58559700
C	-3.71264900	2.67762700	0.64683300
H	-1.60735700	2.64859000	0.03198400
H	-3.82003400	3.50247200	-0.05812100
C	-3.56109300	-1.66149600	-0.99723000
O	-2.73421800	-1.59561000	-2.06285700
C	-2.23585400	-3.36463300	-0.61684100
C	-1.99870800	-2.83613600	-2.05168600
H	-2.44200900	-4.43658100	-0.62148700
H	-2.43940200	-3.49082900	-2.80705500
N	-2.56003600	0.78313000	-0.17356100
N	-3.43099200	-2.62333100	-0.18314200
C	-5.68962100	-0.95063500	0.08570100
H	-5.29746100	-1.22568200	1.06481100
H	-6.39908600	-0.13108000	0.19542700
H	-6.20167100	-1.81942500	-0.32925000
C	-5.11619300	-0.11879100	-2.23217100
H	-4.31354500	0.17834300	-2.90622600
H	-5.65317100	-0.95901400	-2.67666900
H	-5.81094400	0.71280400	-2.10620500
H	-4.00368200	2.99533200	1.64617100
H	-0.95883700	-2.61500600	-2.27327200
C	-1.71883300	1.69702700	1.94025300
C	-0.46332900	2.17583700	2.30269800
C	-2.43154600	0.90369500	2.84097900
C	0.06882500	1.88104500	3.55562600
H	0.10234800	2.77178600	1.59545700
C	-1.90052400	0.60188800	4.08874000
H	-3.40695600	0.51385500	2.56100800
C	-0.64881200	1.09561800	4.45070600
H	1.04579200	2.26182500	3.82957500
H	-2.45955500	-0.01985900	4.77757600
H	-0.23432300	0.86163000	5.42399200
C	-1.04881800	-3.08568900	0.28873900
C	0.08933300	-3.88489500	0.17580000
C	-1.02818000	-1.99792800	1.15688300
C	1.24177900	-3.57990100	0.88884600
H	0.08006500	-4.73881800	-0.49547400
C	0.12363500	-1.69117800	1.87672900
H	-1.90462000	-1.37117500	1.25516800
C	1.26386800	-2.47467100	1.73724300
H	2.12646300	-4.19569200	0.77742000

H	0.12588600	-0.82401700	2.52940600
H	2.16800800	-2.22656900	2.28187500
C	6.33707200	0.38081000	1.42781600
C	5.03184800	0.19691400	0.99283900
C	4.75960800	-0.66921600	-0.07006800
C	5.81100200	-1.36139100	-0.67614100
C	7.11642000	-1.17082600	-0.24133400
C	7.38283100	-0.29850600	0.80884900
H	6.53807800	1.04743600	2.25754600
H	4.22133700	0.70710200	1.49895600
H	5.59428300	-2.04249400	-1.48875900
H	7.92642100	-1.70587500	-0.72191000
H	8.40068900	-0.15398000	1.15053100
C	3.38000900	-0.87570900	-0.56191700
O	3.21442900	-2.01272800	-1.22922200
C	2.37010000	0.01189700	-0.36264600
H	2.26301800	-2.05446900	-1.49400000
H	2.52514100	0.92518000	0.18969100
C	1.03224400	-0.29054900	-0.84427600
O	0.75131700	-1.28803000	-1.49910100
O	0.13766700	0.63701700	-0.53217700
H	-0.78409800	0.34300700	-0.71924700
C	1.85177500	2.23699900	-2.54326000
C	1.23353300	3.32775200	-1.65451200
F	1.60012900	3.17274300	-0.37671300
F	-0.08863000	3.34459000	-1.72205400
F	1.69235200	4.52067300	-2.05596800
O	1.18954700	1.62778400	-3.32247700
H	2.93935500	2.11485000	-2.41412800

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C	-6.33589700	2.09467700	-0.17703800
C	-5.19161700	1.34683300	0.08037100
C	-4.52586200	0.70512900	-0.96388400
C	-5.01811800	0.81670400	-2.26587600
C	-6.16624800	1.55219100	-2.51963000
C	-6.82602700	2.19516600	-1.47428300
H	-6.84409400	2.59822500	0.63636800
H	-4.81045500	1.29604800	1.09243600
H	-4.48611700	0.31160600	-3.06253400
H	-6.54997300	1.62481300	-3.53008400
H	-7.72114200	2.77302200	-1.67167100
C	-3.25101000	-0.05994900	-0.77418000
O	-2.50418000	-0.25307000	-1.71608600
C	-2.94183000	-0.59585300	0.57208000
H	-1.10807800	-1.47655200	-0.63781700
H	-3.58538200	-0.31316100	1.39303700
C	-1.55714600	-0.57962000	0.92853200
O	-0.65413000	-0.96526200	0.08808600
O	-1.18733800	-0.25851400	2.11029900
H	-0.14664200	-0.08946000	2.19037000
C	2.95273500	-1.17001900	1.94501000
C	3.56844400	-1.32685600	0.57533200
O	2.76592900	-0.93481400	-0.44444600
C	4.88208400	-1.67221900	-1.14988200
C	3.45622800	-1.31898800	-1.64952700
H	5.20822100	-2.63400100	-1.54808400
H	2.93722700	-2.17839400	-2.07569400
C	2.40207300	0.23028500	1.99645600
O	3.28698900	1.20639400	1.76476400
C	1.12096000	2.05433300	2.17110100
C	2.55398900	2.45220500	1.74586100
H	0.88571200	2.43193600	3.16850800
H	3.03566200	3.13784300	2.43881800
N	4.71869600	-1.77654200	0.31260400
N	1.20318700	0.57697200	2.24220800
C	1.82785700	-2.19863300	2.11296100
H	1.08869200	-2.10490700	1.31757700
H	2.25717600	-3.20100800	2.08202900
H	1.33713800	-2.06033700	3.07821900
C	4.02349500	-1.32686100	3.03148900
H	4.82216300	-0.59751200	2.90128500
H	3.56889600	-1.19961200	4.01578000
H	4.45622100	-2.32445500	2.96315200
H	3.43253300	-0.48143000	-2.34366300
H	2.59584200	2.85028500	0.73216800

C	5.90730800	-0.61550100	-1.50661400
C	6.78939500	-0.82522900	-2.56382600
C	5.94387400	0.59891800	-0.81975600
C	7.69410800	0.16387400	-2.93788700
H	6.77120100	-1.77067000	-3.09604900
C	6.84749900	1.58703300	-1.19254900
H	5.27044500	0.76639700	0.01494400
C	7.72430900	1.37285500	-2.25265200
H	8.37784100	-0.01325400	-3.75956200
H	6.87243100	2.52561100	-0.65133300
H	8.43043600	2.14307700	-2.53878300
C	0.02861500	2.46961900	1.21092300
C	-1.07364300	3.19247400	1.65807100
C	0.08388600	2.05436400	-0.12060100
C	-2.11425500	3.49773100	0.78493200
H	-1.12670300	3.50237800	2.69630800
C	-0.95432400	2.35686700	-0.99243800
H	0.91995700	1.45196400	-0.46540000
C	-2.05706900	3.07802900	-0.53953900
H	-2.97405900	4.05276400	1.14120000
H	-0.92372000	1.99918800	-2.01364800
H	-2.87660700	3.29616900	-1.21466000
C	-3.06387700	-2.52099400	0.27033800
C	-4.56279400	-2.67444000	-0.01554500
F	-4.88981200	-3.97343400	0.06651400
F	-4.89758700	-2.25492100	-1.23517300
F	-5.33727800	-2.02506100	0.87108300
O	-2.27933300	-2.84887500	-0.65093800
H	-2.87225500	-2.81045900	1.32135500

Value of Imaginary Frequency= -423.7 cm^{-1}

ts1-1-(*R*)

C	7.50842800	-0.07549800	-0.31920900
C	6.13878400	0.13687800	-0.20824400
C	5.24242800	-0.75775000	-0.79691500
C	5.73195000	-1.85914100	-1.50149900
C	7.09852600	-2.07878300	-1.59649700
C	7.98895000	-1.18603700	-1.00484300
H	8.19945300	0.62769600	0.12918400
H	5.78110500	1.01607200	0.31516400
H	5.02145300	-2.52951800	-1.96929500
H	7.47201100	-2.94101600	-2.13549800
H	9.05662000	-1.35294800	-1.08332900
C	3.75342900	-0.57155100	-0.74748400
O	3.03405300	-1.14776600	-1.54204900
C	3.22225900	0.37806800	0.25180600
H	1.25452200	0.12737300	-1.07751500
H	3.87444100	0.64935800	1.07091700
C	1.87302100	0.17321500	0.67914800
O	0.93607600	-0.09595000	-0.16603200
O	1.54572000	0.31320800	1.90842600
H	0.51021300	0.17285300	2.06484900
C	-2.37290500	1.54343600	1.45302600
C	-3.09313900	1.34664400	0.14085500
O	-2.44753400	0.53514400	-0.73128600
C	-4.50070000	1.33608000	-1.54498800
C	-3.18808600	0.62124400	-1.96296300
H	-4.72345400	2.16687400	-2.21592500
H	-2.59899700	1.20614800	-2.67023700
C	-2.04355100	0.16590200	1.96446500
O	-3.07597000	-0.68714200	2.04218600
C	-1.04479000	-1.71963500	2.61246300
C	-2.57342700	-1.89460300	2.65758400
H	-0.58855000	-1.94345600	3.57714000
H	-2.95681500	-1.93098200	3.67712100
N	-4.19448500	1.86206400	-0.20096100
N	-0.90544200	-0.26965200	2.32836300
C	-1.09088100	2.34605200	1.19867000
H	-0.47411400	1.87773400	0.43150300
H	-1.35974100	3.34911900	0.86391100
H	-0.50940100	2.43403000	2.11824000
C	-3.28782700	2.24370600	2.46478200
H	-4.19478700	1.66459100	2.63619100
H	-2.75485700	2.37796500	3.40795900
H	-3.57368800	3.21939700	2.07294200
H	-3.34359300	-0.38627800	-2.34422300
H	-2.93687200	-2.74713700	2.08817700

C	-5.69117500	0.40078700	-1.50474400
C	-6.64148600	0.43138100	-2.52209300
C	-5.82079100	-0.53707500	-0.47907000
C	-7.70653400	-0.46466000	-2.52326700
H	-6.55019700	1.16404300	-3.31729200
C	-6.88420800	-1.43200500	-0.47938800
H	-5.09358100	-0.55668700	0.32671200
C	-7.82934500	-1.39891500	-1.50145300
H	-8.44181800	-0.42791400	-3.31828100
H	-6.98032600	-2.15422400	0.32292300
H	-8.65962000	-2.09490600	-1.49723500
C	-0.32259300	-2.46972100	1.51370200
C	0.98328400	-2.90873300	1.71835500
C	-0.89795600	-2.59517400	0.24966700
C	1.71356300	-3.45572000	0.66802900
H	1.43856800	-2.79893800	2.69747200
C	-0.17538100	-3.15688100	-0.79475800
H	-1.89780900	-2.21235200	0.06608500
C	1.13405600	-3.57953800	-0.58945500
H	2.73546200	-3.77827700	0.82973600
H	-0.62462100	-3.24117800	-1.77686100
H	1.70725200	-3.98794200	-1.41231700
C	2.98029400	1.86136600	-1.05269700
C	2.92181200	3.03358700	-0.06836400
F	4.01697800	3.10222900	0.70896100
F	1.85520800	2.97382500	0.73812800
F	2.84940400	4.18868300	-0.74037100
O	1.96582600	1.63804400	-1.74799400
H	3.99548800	1.79512300	-1.48422200

Value of Imaginary Frequency = -404.4 cm^{-1}

ts1-2-(*S*)

C	-4.75712500	3.38041900	-2.06975300
C	-4.21195100	2.25174700	-1.47510800
C	-4.74861900	1.76786800	-0.27740100
C	-5.82505300	2.42989500	0.32345400
C	-6.36929400	3.55433400	-0.27919400
C	-5.83682700	4.02879900	-1.47531100
H	-4.33597200	3.75978400	-2.99239900
H	-3.34658500	1.77225500	-1.91579200
H	-6.22748900	2.04759100	1.25276800
H	-7.20875800	4.06064000	0.18058600
H	-6.26109100	4.90888800	-1.94357000
C	-4.18359100	0.58244000	0.38048800
O	-4.45405700	0.43549300	1.63401700
C	-3.49057000	-0.43475200	-0.30841800
H	-4.49038500	-0.57155800	1.82417500
H	-3.37173500	-0.30791900	-1.37567900
C	-2.30604000	-1.01970700	0.38955100
O	-2.22919200	-1.15681200	1.58683700
O	-1.34642200	-1.32951000	-0.46973200
H	-0.50930100	-1.49090900	0.04937200
C	2.88992100	-2.20621800	0.01279400
C	3.86440600	-1.35676500	-0.76520800
O	3.30115200	-0.29115400	-1.39286300
C	5.63310100	-0.41347900	-1.66982700
C	4.35281300	0.30260700	-2.17668200
H	6.22164500	-0.79871600	-2.50384200
H	4.14797800	0.09876800	-3.22856500
C	2.14645400	-1.26739500	0.92769300
O	2.92039600	-0.49738600	1.71657000
C	0.61670000	-0.04916700	1.97879700
C	2.02354700	0.27666200	2.54301200
H	-0.05396300	-0.42558800	2.75085800
H	2.15017900	-0.05235000	3.57387900
N	5.10829000	-1.54169200	-0.87910000
N	0.88994600	-1.13609200	1.01748900
C	1.91249800	-2.87546400	-0.96101300
H	1.37988400	-2.13092500	-1.55350100
H	2.46610600	-3.53615800	-1.63018600
H	1.18298600	-3.46739700	-0.40647200
C	3.64237800	-3.24199700	0.85571700
H	4.33484800	-2.75478600	1.54132000
H	2.92560000	-3.83793200	1.42359300
H	4.21405700	-3.89804500	0.19942300
H	4.35627100	1.37569300	-1.99438700
H	2.29382600	1.32674500	2.44610700

C	6.50940200	0.48175500	-0.81868900
C	7.69476500	1.00102100	-1.33233600
C	6.11179500	0.83554500	0.47188300
C	8.47467100	1.86866700	-0.57296100
H	8.01303200	0.72147100	-2.33138400
C	6.88987400	1.70185000	1.23011500
H	5.19733400	0.42220600	0.88631200
C	8.07263700	2.22136200	0.70988000
H	9.39748200	2.26276700	-0.98182100
H	6.57658000	1.96863400	2.23265000
H	8.67966800	2.89314400	1.30486800
C	-0.04944900	1.11718700	1.27673700
C	-1.19010900	1.70780600	1.81733800
C	0.47190300	1.60580400	0.07839000
C	-1.80133900	2.77899100	1.17310700
H	-1.62068300	1.30339300	2.72660100
C	-0.13795900	2.67732300	-0.56532100
H	1.34518900	1.13308600	-0.36293400
C	-1.27496200	3.26664000	-0.01915300
H	-2.69601200	3.22336100	1.59504500
H	0.27132200	3.04838500	-1.49764100
H	-1.75682400	4.09530200	-0.52517500
C	-4.88036900	-1.82305100	0.03480200
C	-4.27113900	-3.00573600	-0.72765500
F	-5.20749700	-3.96057700	-0.83489200
F	-3.22432500	-3.53682000	-0.10482400
F	-3.90110900	-2.68151300	-1.97432300
O	-4.99481600	-1.94840400	1.27870400
H	-5.67774600	-1.36292500	-0.57322800

Value of Imaginary Frequency= -537.9 cm^{-1}

ts1-2-(*R*)

C	-4.54704800	3.25202100	-1.76304800
C	-3.99920400	2.08835300	-1.24177600
C	-4.55176600	1.51195800	-0.09456400
C	-5.65036500	2.11249800	0.52934000
C	-6.19515300	3.27335100	0.00241600
C	-5.64478000	3.84283900	-1.14367200
H	-4.11474000	3.70185000	-2.64813700
H	-3.12161300	1.65168300	-1.70216400
H	-6.07209000	1.65033700	1.41262500
H	-7.05184600	3.73256700	0.47958200
H	-6.07185300	4.75016600	-1.55379100
C	-3.98189100	0.28818800	0.48325800
O	-4.28015600	0.03480700	1.71373700
C	-3.23340700	-0.64997600	-0.25635400
H	-4.28011400	-0.97908100	1.83163500
H	-3.08981900	-0.44764900	-1.30832600
C	-2.05737700	-1.27202900	0.41621400
O	-1.97820400	-1.47098400	1.60480900
O	-1.10779200	-1.57420300	-0.45999400
H	-0.26397400	-1.74577700	0.04764100
C	3.14135000	-2.34814200	-0.11518800
C	4.05656500	-1.41907100	-0.87484500
O	3.43046500	-0.35023100	-1.43349100
C	5.75705000	-0.35437200	-1.77558200
C	4.43360400	0.32977500	-2.21099000
H	6.33642600	-0.67186300	-2.64385300
H	4.20840000	0.17250400	-3.26662200
C	2.39441900	-1.49022700	0.87391200
O	3.16576200	-0.73713900	1.68092100
C	0.86074800	-0.37168500	2.02502300
C	2.26931300	-0.06238500	2.59098300
H	0.20021800	-0.78999200	2.78380400
H	2.42352100	-0.48259800	3.58461000
N	5.30357900	-1.54240400	-1.02948100
N	1.13713000	-1.40714000	1.00757100
C	2.15776100	-3.00090000	-1.09375400
H	1.57718100	-2.24665800	-1.62583900
H	2.71304600	-3.60065700	-1.81673400
H	1.47164400	-3.65205700	-0.55017600
C	3.96131900	-3.39789300	0.64300600
H	4.65749000	-2.92190300	1.33259700
H	3.28831900	-4.05334300	1.19874200
H	4.53528000	-3.99252700	-0.06759000
H	4.39602100	1.39093700	-1.97142700
H	2.51468000	0.99788200	2.58622200

C	6.61950200	0.53556400	-0.90493200
C	7.75505400	1.14589000	-1.43117400
C	6.25659500	0.79391400	0.41795100
C	8.51943700	2.00957300	-0.65194600
H	8.04665400	0.94093600	-2.45611900
C	7.01971900	1.65590400	1.19627800
H	5.38171000	0.31012600	0.84127700
C	8.15231700	2.26652500	0.66374200
H	9.40341300	2.47520700	-1.07126000
H	6.73409300	1.84815200	2.22383200
H	8.74779800	2.93477100	1.27416900
C	0.18193900	0.82300300	1.38421600
C	-0.95563300	1.38437500	1.96218100
C	0.69289900	1.37058200	0.20708200
C	-1.57302600	2.48506100	1.37617600
H	-1.37826900	0.93512800	2.85408500
C	0.07729600	2.47234200	-0.37755100
H	1.56338200	0.92320900	-0.26466700
C	-1.05555800	3.03246000	0.20607900
H	-2.46566900	2.90613100	1.82523700
H	0.47921700	2.89027200	-1.29311500
H	-1.54233900	3.88463400	-0.25397000
C	-4.44230900	-2.22080400	-0.03705400
C	-5.60654900	-1.83845800	-0.95847100
F	-5.20501900	-1.41467400	-2.16493200
F	-6.37094400	-0.88456400	-0.42043600
F	-6.38012200	-2.91325900	-1.15591700
O	-4.70912600	-2.34353800	1.18217200
H	-3.75087400	-2.91221800	-0.54429400

Value of Imaginary Frequency= -517.6 cm^{-1}

ts1-3-(*S*)

C	-4.05121000	-0.15646000	-1.75068300
C	-3.77751400	0.53854700	-0.43565300
O	-4.85246500	0.79907800	0.32734600
C	-2.83823800	1.33667700	1.40755300
C	-4.36299700	1.57206800	1.44855700
H	-2.27467700	2.25388300	1.57361100
H	-4.62865900	2.61577200	1.27359200
C	-2.76590700	-0.85401200	-2.14114400
O	-1.86500100	-0.09559400	-2.80214800
C	-1.07253900	-2.25748700	-2.28876500
C	-0.73041700	-0.94705200	-3.05076000
H	-1.03066200	-3.12095400	-2.95582500
H	-0.64907100	-1.09364000	-4.12812100
N	-2.63738400	0.87224100	0.01826600
N	-2.46724600	-2.04962400	-1.85379300
C	-5.16584600	-1.19379800	-1.56366700
H	-4.88093200	-1.94347400	-0.82610800
H	-6.08219400	-0.69932000	-1.24354200
H	-5.34283500	-1.70104500	-2.51287700
C	-4.45943500	0.89951400	-2.79141000
H	-3.67020700	1.63748300	-2.93019100
H	-4.65702400	0.41391000	-3.74883800
H	-5.37009600	1.40132300	-2.46041300
H	-4.84291400	1.20075200	2.35072900
H	0.15201700	-0.43974700	-2.66449800
C	-2.36941000	0.27922100	2.38997300
C	-1.51700000	0.61977900	3.43711800
C	-2.81087400	-1.03975700	2.27584600
C	-1.12165900	-0.33799700	4.36578100
H	-1.13934900	1.63320600	3.50565900
C	-2.41430400	-1.99945200	3.19954500
H	-3.45231700	-1.33019900	1.44882500
C	-1.57094000	-1.64936000	4.24971700
H	-0.45314800	-0.06099100	5.17237600
H	-2.75427200	-3.02238600	3.09169700
H	-1.25745400	-2.39804400	4.96754200
C	-0.16924400	-2.51443100	-1.09826800
C	0.78059800	-3.53365600	-1.11837000
C	-0.27716300	-1.71248400	0.03876400
C	1.60939000	-3.74810200	-0.01849600
H	0.86604000	-4.17134800	-1.99285400
C	0.54723300	-1.92190800	1.13798800
H	-1.03139000	-0.93534200	0.07975600
C	1.49483200	-2.94368400	1.11012100
H	2.34596700	-4.54293500	-0.04584600

H	0.43900100	-1.28231200	2.00851600
H	2.14221200	-3.10944400	1.96363800
C	4.44079200	-2.31876100	-1.67309900
C	3.58372300	-1.30984500	-1.25849300
C	3.74292200	-0.73603800	0.00612600
C	4.75568900	-1.19246600	0.85788300
C	5.60933700	-2.20020600	0.43774100
C	5.45371200	-2.76187500	-0.82822700
H	4.30805800	-2.77163800	-2.64774100
H	2.76185100	-1.00676200	-1.89518100
H	4.86110300	-0.74782600	1.83918700
H	6.39716500	-2.54916700	1.09358200
H	6.12041100	-3.55173800	-1.15323000
C	2.81691400	0.29682900	0.48016700
O	2.77515300	0.49088200	1.75645000
C	2.05994300	1.12169300	-0.37841200
H	2.47386400	1.44420600	1.92055000
H	2.21261200	0.98277400	-1.43989700
C	0.63924400	1.33624000	0.02289400
O	0.26512500	1.43437100	1.16690300
O	-0.15594200	1.36134700	-1.03705000
H	-1.10059900	1.26078600	-0.73147200
C	2.90913400	2.83309400	0.19195800
C	2.18382200	3.80681300	-0.74499500
F	2.19803600	3.40541400	-2.02400100
F	2.82021000	4.98698700	-0.70030800
F	0.92009400	4.01833300	-0.38866800
O	2.70757200	2.97183400	1.42074900
H	3.91375900	2.61409900	-0.20889500

Value of Imaginary Frequency= -517.9 cm^{-1}

ts1-3-(*R*)

C	4.32822800	0.11761900	-1.79314600
C	3.97740100	-0.84777100	-0.68329800
O	5.01438600	-1.37846900	-0.01451000
C	2.94722500	-1.97809900	0.92155700
C	4.44389000	-2.35267100	0.89052500
H	2.30201900	-2.85399000	0.87082300
H	4.61770600	-3.34248700	0.46545800
C	3.12323500	1.01604900	-1.97323800
O	2.15899800	0.54688100	-2.79452100
C	1.58332500	2.57557600	-1.73691500
C	1.12359700	1.54825900	-2.80853000
H	1.64100800	3.58121800	-2.15819500
H	1.08107700	1.97455200	-3.81115800
N	2.80572600	-1.17938300	-0.31519100
N	2.94211400	2.12118500	-1.38415000
C	5.54303300	0.95958700	-1.38202300
H	5.33381500	1.53051900	-0.47799800
H	6.40216800	0.31197900	-1.21130400
H	5.77567400	1.66319700	-2.18229800
C	4.63066900	-0.68617500	-3.06887000
H	3.77012600	-1.28293100	-3.36885300
H	4.88316200	-0.00333400	-3.88215100
H	5.48244100	-1.34405900	-2.88881800
H	4.94338400	-2.25536800	1.85129300
H	0.18502500	1.05574600	-2.56093900
C	2.56498600	-1.14858600	2.13374800
C	1.69133300	-1.66154600	3.08932300
C	3.10885800	0.12232100	2.32471800
C	1.37446000	-0.92341600	4.22529900
H	1.23632500	-2.63169300	2.92681300
C	2.79116200	0.86345100	3.45667700
H	3.76658700	0.55253100	1.57512400
C	1.92516300	0.34026200	4.41203000
H	0.68792000	-1.33165600	4.95753000
H	3.20962200	1.85438800	3.58522400
H	1.67241900	0.91995600	5.29186000
C	0.68679800	2.60734200	-0.51474000
C	-0.15837100	3.68789100	-0.26716500
C	0.68748800	1.53210100	0.37395800
C	-0.99110600	3.69033600	0.84974100
H	-0.15745700	4.53677500	-0.94383000
C	-0.14611000	1.52713600	1.48701100
H	1.36386600	0.70119300	0.21200500
C	-0.98941200	2.60998000	1.72635300
H	-1.64489000	4.53535200	1.03247100

H	-0.12359700	0.67507200	2.16006100
H	-1.64510600	2.60985400	2.58956400
C	-4.13277900	2.88244100	-0.72569100
C	-3.29684500	1.77722400	-0.65348300
C	-3.53161200	0.79007400	0.30635400
C	-4.59836500	0.92163700	1.20170500
C	-5.43177900	2.02586200	1.12270800
C	-5.20017500	3.00525400	0.15830700
H	-3.94181200	3.65521200	-1.45997800
H	-2.43231400	1.70965100	-1.30349600
H	-4.76653100	0.14721000	1.93911700
H	-6.26436700	2.12485600	1.80795300
H	-5.85175600	3.86905700	0.10027600
C	-2.63870500	-0.36689600	0.41881800
O	-2.62467400	-0.98096300	1.55471100
C	-1.88630300	-0.87667500	-0.65954200
H	-2.36378100	-1.94582100	1.38885400
H	-2.01492900	-0.39010900	-1.61665100
C	-0.49190800	-1.30732800	-0.36751100
O	-0.12341300	-1.75865200	0.69046000
O	0.29545800	-1.12729900	-1.42068100
H	1.24608300	-1.19990200	-1.12265000
C	-2.65946700	-2.71210800	-0.73391900
C	-4.05146200	-2.42550900	-1.30975700
F	-4.02139700	-1.62809000	-2.38701700
F	-4.85684400	-1.86334900	-0.40439600
F	-4.61461300	-3.57916300	-1.69028600
O	-2.61836900	-3.20388200	0.41768000
H	-1.97087200	-3.04681000	-1.52658300

Value of Imaginary Frequency= -508.2 cm^{-1}

ts1-4-(*S*)

C	-3.94127200	-1.53316100	0.95598700
C	-3.88109300	-0.02295900	0.94054600
O	-4.25615400	0.56243800	2.10385700
C	-3.75050500	2.10716700	0.41952100
C	-3.91651100	1.95467000	1.94641900
H	-4.68265800	2.46343500	-0.03239800
H	-4.71381200	2.55861600	2.37314900
C	-3.37356600	-2.00285500	-0.35730500
O	-4.13892800	-1.81343900	-1.43976400
C	-2.00105800	-2.65771600	-1.97762200
C	-3.37007700	-2.25067400	-2.57816600
H	-1.75226200	-3.69291700	-2.21837900
H	-3.89649300	-3.08503900	-3.04010500
N	-3.54854300	0.71794500	-0.02965900
N	-2.23202700	-2.53500700	-0.52406900
C	-3.10499100	-2.06124400	2.12826400
H	-2.09080500	-1.66328200	2.08628700
H	-3.56551500	-1.74850000	3.06504100
H	-3.06775600	-3.15129000	2.09417500
C	-5.41093500	-1.97240700	1.08753000
H	-6.00596200	-1.60023200	0.25373600
H	-5.46854200	-3.06264400	1.10325400
H	-5.82011300	-1.58676800	2.02143600
H	-2.97573600	2.13724400	2.47141800
H	-3.29716000	-1.41795000	-3.27590200
C	-2.63867400	3.04691200	0.02447600
C	-2.94040800	4.35873800	-0.33702500
C	-1.30551300	2.63365300	0.05523200
C	-1.92752600	5.25603700	-0.66009300
H	-3.97702900	4.67868900	-0.37169600
C	-0.29368900	3.53161500	-0.27248600
H	-1.05900100	1.61076100	0.32728300
C	-0.60077700	4.84212400	-0.62929300
H	-2.17559500	6.27282200	-0.94093100
H	0.73749000	3.19938800	-0.24575400
H	0.19116600	5.53665600	-0.88375500
C	-0.84903200	-1.75980000	-2.38525100
C	0.28439800	-2.28839600	-2.99803000
C	-0.90794200	-0.39064300	-2.11434100
C	1.34734200	-1.46049300	-3.34900900
H	0.33852500	-3.35385000	-3.19609200
C	0.15538200	0.43553500	-2.46197800
H	-1.77448000	0.02924100	-1.60723000
C	1.28303700	-0.09661100	-3.08297500
H	2.22534800	-1.87993600	-3.82716700

H	0.10052300	1.49568700	-2.24175100
H	2.11398500	0.54764800	-3.34858100
C	5.20866100	-0.40468300	-2.21374900
C	4.12455400	-0.64424100	-1.38240400
C	3.57729100	0.39950200	-0.62929700
C	4.12742700	1.68253400	-0.71833700
C	5.20804000	1.91794900	-1.55506400
C	5.74908300	0.87552400	-2.30312400
H	5.62816000	-1.21396600	-2.79829900
H	3.68659300	-1.63325300	-1.34789100
H	3.70570000	2.48017200	-0.12059800
H	5.63336800	2.91158300	-1.62040200
H	6.59343200	1.06052200	-2.95631800
C	2.41292200	0.18340900	0.23906100
O	1.84363000	1.24155100	0.71723100
C	1.95903500	-1.08327600	0.65417100
H	1.44911600	1.00110400	1.62887500
H	2.50872500	-1.94941200	0.31572500
C	0.48527600	-1.29575500	0.74457100
O	-0.31549400	-0.42003600	0.97883000
O	0.16962800	-2.56697200	0.55814400
H	-0.81661400	-2.61443900	0.34688100
C	2.23645900	-0.85388500	2.61607200
C	3.76597800	-0.90256500	2.71571500
F	4.11561400	-1.07567300	3.99647400
F	4.32611300	0.23329100	2.29375400
F	4.30694000	-1.91298100	2.01980500
O	1.68358800	0.21604100	2.96657200
H	1.79533500	-1.83308300	2.86075900

Value of Imaginary Frequency= -515.4 cm^{-1}

ts1-4-(*R*)

C	3.71105900	-1.33339200	0.24495400
C	3.42843000	-0.08696500	-0.56718600
O	3.53072800	-0.26406500	-1.90570900
C	3.17105600	1.96069900	-1.30993900
C	3.03541700	0.96273500	-2.47482400
H	4.14351100	2.46468500	-1.35093500
H	3.63098000	1.20835200	-3.35071100
C	3.07394700	-1.14225500	1.59633700
O	3.69818500	-0.32492900	2.45359500
C	1.62502300	-1.08623900	3.27963500
C	2.89082400	-0.27525200	3.64687500
H	1.43615100	-1.88036300	4.00379000
H	3.46119000	-0.72844000	4.45728200
N	3.18904200	1.07550100	-0.12637700
N	1.98803100	-1.68222400	1.97861900
C	3.12705200	-2.56641500	-0.45439000
H	2.07517000	-2.41988500	-0.69655300
H	3.66741900	-2.74015800	-1.38418400
H	3.23204400	-3.44039700	0.19009300
C	5.23907100	-1.46460400	0.39299300
H	5.65411100	-0.59816600	0.90671100
H	5.48100600	-2.36561500	0.96064700
H	5.68891700	-1.54599800	-0.59739600
H	1.98876700	0.80585500	-2.74935900
H	2.68241000	0.76931700	3.87158800
C	2.09060100	3.01112300	-1.28672400
C	2.39041200	4.33420400	-1.60295000
C	0.77184600	2.66048500	-0.99319600
C	1.38868100	5.30023400	-1.63379500
H	3.41585400	4.61186100	-1.82442600
C	-0.22951700	3.62493700	-1.02895000
H	0.53772200	1.63111400	-0.73687600
C	0.07547900	4.94616900	-1.34804300
H	1.63528900	6.32644400	-1.87947800
H	-1.25224400	3.33676800	-0.81337200
H	-0.70742400	5.69496700	-1.37386600
C	0.36955200	-0.25414600	3.10899600
C	-0.81201800	-0.60890400	3.75479000
C	0.37996200	0.84969600	2.25293500
C	-1.97376600	0.13290700	3.55945700
H	-0.82527300	-1.47539300	4.40760600
C	-0.77891700	1.59387800	2.06231300
H	1.28654400	1.11412800	1.71067400
C	-1.95708500	1.23828300	2.71544000
H	-2.88941100	-0.15108900	4.06567000

H	-0.75879000	2.45154700	1.40063000
H	-2.86109500	1.81724200	2.56093700
C	-5.65681400	0.05556500	1.50858400
C	-4.42618700	-0.35051600	1.01463400
C	-3.80945700	0.37846900	-0.00834200
C	-4.43397200	1.52022700	-0.52295600
C	-5.66514900	1.92121100	-0.02516900
C	-6.27679000	1.18976800	0.98946300
H	-6.12939000	-0.50555800	2.30504800
H	-3.92749600	-1.20653500	1.45121500
H	-3.94816200	2.07682200	-1.31421600
H	-6.14967500	2.80168900	-0.42824400
H	-7.23690100	1.50560700	1.37961600
C	-2.48984400	-0.00691900	-0.52530600
O	-1.86493500	0.88579800	-1.22096400
C	-1.94000100	-1.29630300	-0.39381100
H	-1.29018400	0.39611300	-1.91445400
H	-2.54380600	-2.03825500	0.10951300
C	-0.47943700	-1.37543200	-0.08745600
O	0.34397700	-0.59910000	-0.51726800
O	-0.21361700	-2.38794100	0.71695900
H	0.71373600	-2.25363400	1.09793900
C	-1.92768700	-1.67436500	-2.37049100
C	-1.37517600	-3.10496700	-2.36253800
F	-2.00729500	-3.89908100	-1.48875400
F	-0.07164500	-3.15289300	-2.10573600
F	-1.56811100	-3.63235500	-3.58076500
O	-1.22230800	-0.79515300	-2.91980700
H	-3.02283000	-1.69739100	-2.49579700

Value of Imaginary Frequency= -492.5 cm^{-1}

ts1-5-(*S*)

C	-4.05121000	-0.15646000	-1.75068300
C	-3.77751400	0.53854700	-0.43565300
O	-4.85246500	0.79907800	0.32734600
C	-2.83823800	1.33667700	1.40755300
C	-4.36299700	1.57206800	1.44855700
H	-2.27467700	2.25388300	1.57361100
H	-4.62865900	2.61577200	1.27359200
C	-2.76590700	-0.85401200	-2.14114400
O	-1.86500100	-0.09559400	-2.80214800
C	-1.07253900	-2.25748700	-2.28876500
C	-0.73041700	-0.94705200	-3.05076000
H	-1.03066200	-3.12095400	-2.95582500
H	-0.64907100	-1.09364000	-4.12812100
N	-2.63738400	0.87224100	0.01826600
N	-2.46724600	-2.04962400	-1.85379300
C	-5.16584600	-1.19379800	-1.56366700
H	-4.88093200	-1.94347400	-0.82610800
H	-6.08219400	-0.69932000	-1.24354200
H	-5.34283500	-1.70104500	-2.51287700
C	-4.45943500	0.89951400	-2.79141000
H	-3.67020700	1.63748300	-2.93019100
H	-4.65702400	0.41391000	-3.74883800
H	-5.37009600	1.40132300	-2.46041300
H	-4.84291400	1.20075200	2.35072900
H	0.15201700	-0.43974700	-2.66449800
C	-2.36941000	0.27922100	2.38997300
C	-1.51700000	0.61977900	3.43711800
C	-2.81087400	-1.03975700	2.27584600
C	-1.12165900	-0.33799700	4.36578100
H	-1.13934900	1.63320600	3.50565900
C	-2.41430400	-1.99945200	3.19954500
H	-3.45231700	-1.33019900	1.44882500
C	-1.57094000	-1.64936000	4.24971700
H	-0.45314800	-0.06099100	5.17237600
H	-2.75427200	-3.02238600	3.09169700
H	-1.25745400	-2.39804400	4.96754200
C	-0.16924400	-2.51443100	-1.09826800
C	0.78059800	-3.53365600	-1.11837000
C	-0.27716300	-1.71248400	0.03876400
C	1.60939000	-3.74810200	-0.01849600
H	0.86604000	-4.17134800	-1.99285400
C	0.54723300	-1.92190800	1.13798800
H	-1.03139000	-0.93534200	0.07975600
C	1.49483200	-2.94368400	1.11012100
H	2.34596700	-4.54293500	-0.04584600

H	0.43900100	-1.28231200	2.00851600
H	2.14221200	-3.10944400	1.96363800
C	4.44079200	-2.31876100	-1.67309900
C	3.58372300	-1.30984500	-1.25849300
C	3.74292200	-0.73603800	0.00612600
C	4.75568900	-1.19246600	0.85788300
C	5.60933700	-2.20020600	0.43774100
C	5.45371200	-2.76187500	-0.82822700
H	4.30805800	-2.77163800	-2.64774100
H	2.76185100	-1.00676200	-1.89518100
H	4.86110300	-0.74782600	1.83918700
H	6.39716500	-2.54916700	1.09358200
H	6.12041100	-3.55173800	-1.15323000
C	2.81691400	0.29682900	0.48016700
O	2.77515300	0.49088200	1.75645000
C	2.05994300	1.12169300	-0.37841200
H	2.47386400	1.44420600	1.92055000
H	2.21261200	0.98277400	-1.43989700
C	0.63924400	1.33624000	0.02289400
O	0.26512500	1.43437100	1.16690300
O	-0.15594200	1.36134700	-1.03705000
H	-1.10059900	1.26078600	-0.73147200
C	2.90913400	2.83309400	0.19195800
C	2.18382200	3.80681300	-0.74499500
F	2.19803600	3.40541400	-2.02400100
F	2.82021000	4.98698700	-0.70030800
F	0.92009400	4.01833300	-0.38866800
O	2.70757200	2.97183400	1.42074900
H	3.91375900	2.61409900	-0.20889500

Value of Imaginary Frequency= -492.9 cm^{-1}

ts1-5-(*R*)

C	4.32822800	0.11761900	-1.79314600
C	3.97740100	-0.84777100	-0.68329800
O	5.01438600	-1.37846900	-0.01451000
C	2.94722500	-1.97809900	0.92155700
C	4.44389000	-2.35267100	0.89052500
H	2.30201900	-2.85399000	0.87082300
H	4.61770600	-3.34248700	0.46545800
C	3.12323500	1.01604900	-1.97323800
O	2.15899800	0.54688100	-2.79452100
C	1.58332500	2.57557600	-1.73691500
C	1.12359700	1.54825900	-2.80853000
H	1.64100800	3.58121800	-2.15819500
H	1.08107700	1.97455200	-3.81115800
N	2.80572600	-1.17938300	-0.31519100
N	2.94211400	2.12118500	-1.38415000
C	5.54303300	0.95958700	-1.38202300
H	5.33381500	1.53051900	-0.47799800
H	6.40216800	0.31197900	-1.21130400
H	5.77567400	1.66319700	-2.18229800
C	4.63066900	-0.68617500	-3.06887000
H	3.77012600	-1.28293100	-3.36885300
H	4.88316200	-0.00333400	-3.88215100
H	5.48244100	-1.34405900	-2.88881800
H	4.94338400	-2.25536800	1.85129300
H	0.18502500	1.05574600	-2.56093900
C	2.56498600	-1.14858600	2.13374800
C	1.69133300	-1.66154600	3.08932300
C	3.10885800	0.12232100	2.32471800
C	1.37446000	-0.92341600	4.22529900
H	1.23632500	-2.63169300	2.92681300
C	2.79116200	0.86345100	3.45667700
H	3.76658700	0.55253100	1.57512400
C	1.92516300	0.34026200	4.41203000
H	0.68792000	-1.33165600	4.95753000
H	3.20962200	1.85438800	3.58522400
H	1.67241900	0.91995600	5.29186000
C	0.68679800	2.60734200	-0.51474000
C	-0.15837100	3.68789100	-0.26716500
C	0.68748800	1.53210100	0.37395800
C	-0.99110600	3.69033600	0.84974100
H	-0.15745700	4.53677500	-0.94383000
C	-0.14611000	1.52713600	1.48701100
H	1.36386600	0.70119300	0.21200500
C	-0.98941200	2.60998000	1.72635300
H	-1.64489000	4.53535200	1.03247100

H	-0.12359700	0.67507200	2.16006100
H	-1.64510600	2.60985400	2.58956400
C	-4.13277900	2.88244100	-0.72569100
C	-3.29684500	1.77722400	-0.65348300
C	-3.53161200	0.79007400	0.30635400
C	-4.59836500	0.92163700	1.20170500
C	-5.43177900	2.02586200	1.12270800
C	-5.20017500	3.00525400	0.15830700
H	-3.94181200	3.65521200	-1.45997800
H	-2.43231400	1.70965100	-1.30349600
H	-4.76653100	0.14721000	1.93911700
H	-6.26436700	2.12485600	1.80795300
H	-5.85175600	3.86905700	0.10027600
C	-2.63870500	-0.36689600	0.41881800
O	-2.62467400	-0.98096300	1.55471100
C	-1.88630300	-0.87667500	-0.65954200
H	-2.36378100	-1.94582100	1.38885400
H	-2.01492900	-0.39010900	-1.61665100
C	-0.49190800	-1.30732800	-0.36751100
O	-0.12341300	-1.75865200	0.69046000
O	0.29545800	-1.12729900	-1.42068100
H	1.24608300	-1.19990200	-1.12265000
C	-2.65946700	-2.71210800	-0.73391900
C	-4.05146200	-2.42550900	-1.30975700
F	-4.02139700	-1.62809000	-2.38701700
F	-4.85684400	-1.86334900	-0.40439600
F	-4.61461300	-3.57916300	-1.69028600
O	-2.61836900	-3.20388200	0.41768000
H	-1.97087200	-3.04681000	-1.52658300

Value of Imaginary Frequency= --495.4 cm^{-1}

ts1-6-(*S*)

C	-4.97199200	0.63587400	0.36846800
C	-4.13464600	-0.41354500	1.05776600
O	-4.81483600	-1.43872600	1.60815700
C	-2.47480500	-1.66642200	1.82804200
C	-3.83374600	-2.26968400	2.26568300
H	-1.85453000	-1.41929800	2.69094900
H	-3.99773800	-2.19639600	3.34042200
C	-4.02673200	1.46121500	-0.47375100
O	-3.27624800	2.36970600	0.19065100
C	-2.74032600	2.21459800	-2.08167900
C	-2.58397900	3.11590600	-0.83378000
H	-2.99719900	2.80612400	-2.96212200
H	-3.09801300	4.07208100	-0.95277700
N	-2.87054500	-0.41678000	1.15120800
N	-3.86641200	1.33724100	-1.72354000
C	-6.00981700	-0.05108800	-0.52760200
H	-5.52411200	-0.68113400	-1.27270600
H	-6.67746800	-0.65878700	0.08260700
H	-6.59028000	0.70778300	-1.05310800
C	-5.66051900	1.50272200	1.43655800
H	-4.92468200	1.99523700	2.07141900
H	-6.26930400	2.26665200	0.94907500
H	-6.31014300	0.87814600	2.05135000
H	-3.98043200	-3.29598400	1.93367300
H	-1.55350500	3.25532700	-0.51836400
C	-1.67399400	-2.54366000	0.88691900
C	-0.35948900	-2.89417400	1.18315300
C	-2.25175000	-3.01185300	-0.29416000
C	0.36281600	-3.71935800	0.32407800
H	0.09888500	-2.52047600	2.09251100
C	-1.53208200	-3.82879800	-1.15784800
H	-3.27221600	-2.73134200	-0.54264100
C	-0.22252400	-4.18913300	-0.84712500
H	1.37970500	-4.00050100	0.57522300
H	-1.99020200	-4.18231500	-2.07361400
H	0.33695600	-4.83119500	-1.51706600
C	-1.48237300	1.41636900	-2.37457300
C	-0.44566800	2.02820600	-3.07996000
C	-1.30377900	0.12086300	-1.89610400
C	0.75157600	1.36127900	-3.30013100
H	-0.57591200	3.03998600	-3.45170700
C	-0.10154500	-0.54957000	-2.11087100
H	-2.09909800	-0.36621400	-1.34619500
C	0.92553400	0.06565700	-2.81927200
H	1.55040900	1.84912500	-3.84609100

H	0.02134000	-1.55678100	-1.72411000
H	1.85485300	-0.46084200	-3.00422200
C	4.22159300	-2.53712900	-1.46526800
C	3.38275300	-1.59114000	-0.89419600
C	3.76910500	-0.24750700	-0.86138500
C	4.99310200	0.14347600	-1.41095500
C	5.83104000	-0.80824300	-1.97287000
C	5.44677300	-2.14686100	-1.99982600
H	3.91713400	-3.57596000	-1.50234900
H	2.41096600	-1.88622100	-0.51412300
H	5.27788300	1.18734000	-1.37574200
H	6.78512600	-0.50925300	-2.38857000
H	6.10195800	-2.88698700	-2.44333700
C	2.87835000	0.76515700	-0.28230300
O	3.04983100	1.98288400	-0.67112900
C	1.94050700	0.47227800	0.72678100
H	2.73886200	2.59882400	0.07198500
H	1.91955800	-0.54588800	1.09085800
C	0.59974300	1.11219000	0.63694100
O	0.37451700	2.17296700	0.11414600
O	-0.30163800	0.34757700	1.24754200
H	-1.22966900	0.60252200	1.04874800
C	2.63350200	1.68804200	2.15343600
C	3.90415500	0.94602100	2.58328500
F	4.36446700	1.48379900	3.71948000
F	4.87267500	1.04570900	1.66891400
F	3.69401900	-0.35698600	2.82152600
O	2.78633600	2.82714400	1.65584100
H	1.80072800	1.46796700	2.84069500

Value of Imaginary Frequency= -498.7 cm^{-1}

ts1-6-(*R*)

C	4.76758900	0.23789600	0.38956200
C	3.95559500	-0.04983000	-0.84932500
O	4.64213600	-0.53201500	-1.90442400
C	2.32065300	-0.35999800	-2.31577200
C	3.68626100	-0.67957600	-2.97741300
H	1.80621500	0.44962000	-2.83620600
H	3.94912000	0.02977700	-3.76128200
C	3.77900900	0.45519900	1.51184700
O	3.13853300	1.64591900	1.51491000
C	2.36947700	0.17718800	3.16976100
C	2.35578100	1.66130700	2.72787800
H	2.57175600	0.08970300	4.23878300
H	2.86568400	2.30788300	3.44481800
N	2.70512200	0.11093800	-0.97240600
N	3.48794100	-0.39523600	2.40353100
C	5.66103300	-0.96911200	0.69983900
H	5.06213400	-1.86761700	0.84911600
H	6.35871300	-1.13020100	-0.12173000
H	6.21957800	-0.77901300	1.61687400
C	5.61441900	1.49928100	0.14861800
H	4.97982000	2.35695600	-0.07251500
H	6.20279300	1.72019500	1.04130600
H	6.29590100	1.32821400	-0.68578400
H	3.75596500	-1.69798300	-3.35627300
H	1.36424100	2.03923000	2.49100400
C	1.37971800	-1.54295800	-2.20902800
C	0.08553500	-1.47001200	-2.71756500
C	1.80016500	-2.71838600	-1.58601700
C	-0.77119600	-2.56401200	-2.62565400
H	-0.25288700	-0.54776700	-3.17798600
C	0.94499400	-3.80973100	-1.48421100
H	2.80293400	-2.77851800	-1.17055500
C	-0.34316700	-3.73605800	-2.00926800
H	-1.77050100	-2.50242200	-3.04285300
H	1.28112500	-4.71545100	-0.99399600
H	-1.00805600	-4.58885600	-1.93731700
C	1.06222000	-0.53027100	2.86016000
C	0.00037700	-0.40929300	3.75759700
C	0.87078600	-1.23810400	1.67615700
C	-1.23113200	-0.98673600	3.48033200
H	0.14027800	0.14635300	4.67976000
C	-0.36596100	-1.81294200	1.39156200
H	1.68334900	-1.33497400	0.96649100
C	-1.41588900	-1.69766000	2.29682100
H	-2.04743400	-0.88556600	4.18578100

H	-0.49674500	-2.35448800	0.45911600
H	-2.37199500	-2.16421800	2.08907100
C	-4.64558300	-2.70728500	-0.47297500
C	-3.73822600	-1.66803500	-0.33331800
C	-4.07045800	-0.55271500	0.44425800
C	-5.30964800	-0.49333800	1.08915300
C	-6.21648600	-1.53265700	0.93788100
C	-5.88605800	-2.63743400	0.15748400
H	-4.38325700	-3.57652000	-1.06360800
H	-2.75650600	-1.74046200	-0.78781300
H	-5.54956000	0.37110800	1.69509300
H	-7.18040900	-1.48341300	1.42864800
H	-6.59392200	-3.44997900	0.04592400
C	-3.11145200	0.54461600	0.61966800
O	-3.28776700	1.31002300	1.64219400
C	-2.11438200	0.85141900	-0.32812500
H	-2.91667100	2.22887000	1.41237500
H	-2.08169400	0.23126000	-1.21412300
C	-0.77396100	1.23286100	0.20392700
O	-0.58681400	1.78529900	1.25764600
O	0.16702200	0.86717700	-0.65639200
H	1.07815600	0.93091600	-0.29770700
C	-2.86675600	2.63379300	-0.79818900
C	-1.89493600	3.05716600	-1.90803000
F	-1.67258600	2.08818700	-2.81076400
F	-0.72321400	3.46453600	-1.43473700
F	-2.44436100	4.08466500	-2.57357800
O	-2.87114900	3.32948400	0.24543300
H	-3.80371900	2.26636900	-1.25117800

Value of Imaginary Frequency= -512.1 cm^{-1}

im1-1-(*S*)

C	-4.70841900	2.78299300	1.14327700
C	-4.10495200	1.56270100	0.85777600
C	-4.21217000	1.02073500	-0.42277700
C	-4.92616400	1.70043000	-1.41221500
C	-5.54726600	2.90407500	-1.11675200
C	-5.43461700	3.44805800	0.16203400
H	-4.60973000	3.21351100	2.13239200
H	-3.51736900	1.06313800	1.61943100
H	-4.98160600	1.26756400	-2.40397100
H	-6.11648900	3.42211300	-1.87909000
H	-5.91464400	4.39217200	0.39163100
C	-3.49993200	-0.23085400	-0.81140100
O	-3.14606800	-0.42840400	-1.94623100
C	-3.18149200	-1.25434300	0.29762300
H	-2.08078900	-2.65079400	-1.41573100
H	-3.75035700	-1.02921600	1.19788800
C	-1.69846200	-1.10440400	0.60092300
O	-0.85256500	-1.57410300	-0.12819000
O	-1.46727500	-0.40736500	1.68738600
H	-0.48756900	-0.13602500	1.76365500
C	2.74409500	-0.99198100	2.04214500
C	3.55220700	-1.30003200	0.80474100
O	2.89457900	-1.07665400	-0.35956800
C	5.10509200	-1.81204100	-0.66189900
C	3.75832500	-1.57864200	-1.39645500
H	5.50283200	-2.80412200	-0.88037000
H	3.32443200	-2.50336900	-1.77896800
C	2.14737200	0.37188700	1.81651700
O	3.03246600	1.35311200	1.57763200
C	0.80471400	2.12581900	1.55042700
C	2.26503600	2.52181600	1.21775600
H	0.45916900	2.62488500	2.45971400
H	2.63441300	3.36567600	1.79564100
N	4.73798600	-1.73332900	0.76472200
N	0.91590400	0.68084700	1.82829500
C	1.63662900	-2.04225600	2.18979300
H	1.00850100	-2.07468600	1.29878700
H	2.09372300	-3.02088400	2.34481400
H	1.01484700	-1.80658200	3.05572900
C	3.65318400	-0.95212600	3.27564600
H	4.43692800	-0.20422200	3.15963500
H	3.05834600	-0.72241500	4.16174700
H	4.12532400	-1.92582800	3.40356000
H	3.81721900	-0.83412800	-2.18781900
H	2.40700500	2.70023100	0.15109400

C	6.15047400	-0.77249700	-1.00984200
C	7.19324000	-1.08882600	-1.87689300
C	6.05018900	0.52684000	-0.50983900
C	8.12344500	-0.12217000	-2.24780800
H	7.28070000	-2.09959600	-2.26189200
C	6.97872700	1.49251500	-0.87970200
H	5.24861100	0.77910400	0.17756400
C	8.01722600	1.17114900	-1.74984800
H	8.93248300	-0.38168200	-2.92025400
H	6.89590100	2.49815800	-0.48440900
H	8.74200500	1.92471700	-2.03376800
C	-0.16265400	2.41527700	0.42532800
C	-0.99308300	3.53108000	0.47918500
C	-0.19324200	1.58827700	-0.70032200
C	-1.83702700	3.83208600	-0.58706900
H	-0.98330200	4.16622300	1.35929100
C	-1.04031100	1.88534700	-1.76074500
H	0.43280500	0.70156900	-0.73650200
C	-1.85799700	3.01230200	-1.70859400
H	-2.48725300	4.69731000	-0.53418800
H	-1.07846900	1.22630500	-2.61909300
H	-2.52303500	3.23763800	-2.53344900
C	-3.48050700	-2.71108100	-0.10950200
C	-4.98199900	-2.91335100	-0.23026600
F	-5.27618600	-4.15905900	-0.60023700
F	-5.54340200	-2.08227200	-1.11606300
F	-5.57848500	-2.69075300	0.95398800
O	-2.91494200	-3.12763300	-1.31174200
H	-3.16671600	-3.35496000	0.72487200

im1-1-(*R*)

C	7.60525700	0.45058700	0.39160900
C	6.21882400	0.52832100	0.32907900
C	5.50861400	-0.31013700	-0.53411400
C	6.20262600	-1.22398100	-1.33170100
C	7.58526300	-1.29973400	-1.26764400
C	8.28820200	-0.46171900	-0.40494700
H	8.15022400	1.10194000	1.06338300
H	5.70831100	1.24714600	0.95908400
H	5.63544900	-1.86653700	-1.99341800
H	8.11734600	-2.01019000	-1.88819100
H	9.36883900	-0.52016200	-0.35408400
C	4.01619700	-0.28870300	-0.65183000
O	3.42560400	-1.07768000	-1.34587200
C	3.25082600	0.79581700	0.11625800
H	1.91622500	1.67255300	-1.77722000
H	3.66499500	0.89846000	1.11912900
C	1.79705200	0.36793000	0.24898100
O	0.97475000	0.56009500	-0.62356000
O	1.55407800	-0.22372100	1.38931500
H	0.58439200	-0.52028300	1.45753400
C	-2.41946900	0.88933500	1.73118800
C	-3.28360500	1.23905800	0.54461700
O	-2.78468900	0.82907300	-0.64665800
C	-4.86934500	1.89832400	-0.82537800
C	-3.65588800	1.38790400	-1.64696700
H	-5.12020300	2.92538300	-1.09459500
H	-3.12095000	2.19548000	-2.14847900
C	-2.09114500	-0.57503000	1.60163800
O	-3.15864000	-1.38595000	1.47467800
C	-1.15044800	-2.58272900	1.58044700
C	-2.62820700	-2.68928300	1.15595600
H	-1.01101200	-2.97305000	2.59369200
H	-3.19704600	-3.43902200	1.69985500
N	-4.38372100	1.86012900	0.56710300
N	-0.94400500	-1.12066100	1.63362600
C	-1.14558700	1.74056000	1.68863100
H	-0.62094900	1.60633200	0.74315500
H	-1.41575300	2.79197500	1.80047700
H	-0.48026400	1.46326100	2.50835400
C	-3.19591700	1.10479700	3.03656500
H	-4.10032100	0.49756100	3.05861600
H	-2.56079100	0.84578200	3.88586700
H	-3.48500600	2.15273200	3.11127500
H	-3.91068700	0.60572900	-2.35933900
H	-2.72635500	-2.83894700	0.07841700

C	-6.09880500	1.02944900	-0.99141100
C	-7.17255200	1.46794200	-1.76174800
C	-6.14776100	-0.24069400	-0.41400700
C	-8.28151900	0.65052400	-1.96100800
H	-7.14336800	2.45761100	-2.20584100
C	-7.25427600	-1.05733600	-0.61274900
H	-5.32112700	-0.58504100	0.19995900
C	-8.32398000	-0.61442300	-1.38682100
H	-9.11258300	1.00494500	-2.55920400
H	-7.28590100	-2.04072900	-0.15842900
H	-9.18729700	-1.25154700	-1.53711500
C	-0.20032700	-3.29133600	0.64732300
C	0.18870000	-4.60101600	0.92360100
C	0.26871500	-2.66313500	-0.50564300
C	1.03354100	-5.28110200	0.05334600
H	-0.16407600	-5.08715400	1.82769000
C	1.12922100	-3.33735700	-1.36519600
H	-0.01767300	-1.63873400	-0.72063800
C	1.50802300	-4.64770300	-1.09072900
H	1.33156600	-6.29879100	0.27599600
H	1.51877700	-2.82621800	-2.23623900
H	2.17981900	-5.17018500	-1.76122500
C	3.39626100	2.13082900	-0.64783700
C	2.90733600	3.28421000	0.22015800
F	3.62698400	3.35238200	1.35538500
F	1.62064200	3.15174200	0.57537000
F	3.03205100	4.45247600	-0.40612600
O	2.76509000	2.13314100	-1.88738500
H	4.45787700	2.33332600	-0.81735100

im1-2-(*S*)

C	-2.59686600	3.07713200	-2.07377300
C	-3.05708500	1.91157900	-1.47460100
C	-4.13005900	1.96654600	-0.58018200
C	-4.72194200	3.19636200	-0.27949300
C	-4.26041700	4.35698600	-0.88184200
C	-3.20177300	4.29566900	-1.78545600
H	-1.76018200	3.03338400	-2.75987400
H	-2.56637000	0.97272200	-1.70232900
H	-5.54887600	3.21718900	0.41960200
H	-4.72721900	5.30768200	-0.65452400
H	-2.84410400	5.20170000	-2.26085000
C	-4.70071000	0.74526600	0.05636000
O	-5.60740800	0.81333500	0.85804500
C	-4.11938900	-0.61379600	-0.33146500
H	-5.50014200	-1.01113200	1.81800700
H	-3.98769700	-0.66723600	-1.41273400
C	-2.75299700	-0.72774100	0.34577200
O	-2.60360600	-0.47082300	1.51488800
O	-1.79941900	-1.09048700	-0.48566300
H	-0.90754900	-1.07305400	0.00293700
C	2.24388300	-2.20091900	-0.20679400
C	3.39643000	-1.49333600	-0.87670600
O	3.07757800	-0.28497600	-1.41050900
C	5.35084800	-0.83620500	-1.63953400
C	4.25348900	0.15067100	-2.11814000
H	5.89932500	-1.25180800	-2.48604700
H	4.05508600	0.06825600	-3.18773800
C	1.66635300	-1.22349500	0.78396000
O	2.54025900	-0.71089900	1.66852800
C	0.36946400	0.17738200	1.92628300
C	1.76944400	0.10287500	2.58184800
H	-0.42119500	-0.10570500	2.61886200
H	1.75426500	-0.40418500	3.54632900
N	4.58479500	-1.90817600	-0.97731700
N	0.45898500	-0.84462000	0.86267600
C	1.19122200	-2.56899200	-1.25943500
H	0.83557700	-1.68166400	-1.78368800
H	1.63034200	-3.25946900	-1.98123400
H	0.33951300	-3.05633100	-0.78207200
C	2.74592300	-3.43994100	0.54353800
H	3.49547800	-3.16677000	1.28532700
H	1.90578800	-3.93195200	1.03694300
H	3.20092700	-4.13198100	-0.16486300
H	4.45481100	1.18639200	-1.85083000
H	2.25931400	1.07049400	2.67048900

C	6.33312300	-0.19959400	-0.67814200
C	7.61293700	0.14385300	-1.10604500
C	5.94838900	0.09766200	0.63041200
C	8.49990800	0.78188500	-0.24362300
H	7.92008400	-0.09342000	-2.11943200
C	6.83367200	0.73471900	1.49161500
H	4.95870300	-0.18147800	0.97854500
C	8.11102700	1.07928100	1.05723400
H	9.49473800	1.03991500	-0.58682700
H	6.52904700	0.95813000	2.50734700
H	8.80066500	1.57184600	1.73218200
C	0.04583000	1.52806700	1.32288600
C	-1.07285400	2.24543400	1.73934900
C	0.89274200	2.07571300	0.35664600
C	-1.32955500	3.51056500	1.21792300
H	-1.75007200	1.80259000	2.46077400
C	0.63839400	3.33967500	-0.16090100
H	1.75209400	1.50816500	0.00779300
C	-0.46942000	4.06209000	0.27620400
H	-2.20715200	4.05912600	1.53964200
H	1.30315700	3.76195800	-0.90549600
H	-0.67064800	5.04657200	-0.12988300
C	-5.08563400	-1.73075200	0.10447700
C	-4.61986800	-3.08101500	-0.40863100
F	-5.51579800	-4.03325900	-0.14088200
F	-3.45863700	-3.45505200	0.13669000
F	-4.45045600	-3.05091100	-1.74030700
O	-5.21167100	-1.86971000	1.48555300
H	-6.05305400	-1.54062800	-0.37857200

im1-2-(*R*)

C	-2.26032900	2.79421500	-2.14909600
C	-2.64238000	1.64593200	-1.46382900
C	-3.60579400	1.73084200	-0.45829900
C	-4.18796500	2.96274600	-0.14643500
C	-3.82315400	4.09900600	-0.85060300
C	-2.85441200	4.01492400	-1.85046700
H	-1.49825800	2.73325100	-2.91626900
H	-2.15957300	0.70170400	-1.68740800
H	-4.92716500	3.00520000	0.64433600
H	-4.28781000	5.05067100	-0.62299000
H	-2.56432600	4.90482100	-2.39668900
C	-4.00020100	0.54994100	0.35426900
O	-4.47643900	0.68188300	1.46229700
C	-3.77597900	-0.85120000	-0.22943700
H	-5.10965300	-1.04625000	1.85646700
H	-3.69136300	-0.79251200	-1.31302800
C	-2.44853100	-1.36229500	0.33007000
O	-2.30611500	-1.66603500	1.48615400
O	-1.50239900	-1.39485300	-0.58991900
H	-0.60731300	-1.56419400	-0.14235300
C	2.67575300	-2.34639200	-0.61856300
C	3.69505000	-1.36720500	-1.14803700
O	3.19527900	-0.13468500	-1.42633200
C	5.51182600	-0.30844300	-1.79087600
C	4.27491900	0.59531700	-2.03917600
H	6.06889900	-0.47041600	-2.71481300
H	4.04696300	0.71010600	-3.09975000
C	2.01865600	-1.67711600	0.56100300
O	2.85681100	-1.22731800	1.51104000
C	0.60063100	-0.72160000	1.98358300
C	2.03058900	-0.70540900	2.57669200
H	-0.10198400	-1.24656500	2.62946800
H	2.13705000	-1.36809700	3.43501000
N	4.92311300	-1.58455000	-1.34427100
N	0.77596100	-1.49844700	0.73846500
C	1.63519900	-2.63466700	-1.70725100
H	1.14471400	-1.71654000	-2.03177300
H	2.12802800	-3.09885300	-2.56296000
H	0.87733400	-3.32007500	-1.32477900
C	3.36842800	-3.63025900	-0.14736500
H	4.10834300	-3.41141900	0.62160000
H	2.62302700	-4.32176000	0.24964900
H	3.87790300	-4.09712300	-0.99022300
H	4.34806000	1.57061500	-1.56148300
H	2.38560500	0.29338100	2.82292800

C	6.44797300	0.25309600	-0.74097900
C	7.65435500	0.83874700	-1.11571000
C	6.08712500	0.23621200	0.60738300
C	8.49120400	1.40807700	-0.16014400
H	7.94404700	0.84597500	-2.16142100
C	6.92240100	0.80437300	1.56163600
H	5.15634000	-0.23320000	0.91073100
C	8.12583400	1.39252700	1.18074800
H	9.42941300	1.85731900	-0.46346300
H	6.63732900	0.78373800	2.60695200
H	8.77699700	1.83137900	1.92716800
C	0.05175100	0.65335900	1.66241200
C	-1.10046200	1.12192300	2.28866700
C	0.71499400	1.47015800	0.74332600
C	-1.57440300	2.40358100	2.01912100
H	-1.63972400	0.47414300	2.97107600
C	0.24064900	2.74832000	0.47574500
H	1.59878600	1.09961400	0.23017600
C	-0.90201000	3.21962700	1.11783800
H	-2.48345700	2.74972700	2.49727600
H	0.75641700	3.37627500	-0.24155600
H	-1.27992600	4.21082200	0.89643500
C	-4.92208000	-1.82727000	0.11383100
C	-6.15549900	-1.45772200	-0.70556400
F	-5.89617100	-1.52465400	-2.02302900
F	-6.57704900	-0.20956200	-0.44976300
F	-7.16973200	-2.28365200	-0.45452600
O	-5.25842600	-1.91697800	1.45959200
H	-4.63617000	-2.82612000	-0.23142100

im1-3-(*S*)

C	3.01455300	-2.48163300	0.55605700
C	3.68158100	-1.42822800	-0.29850100
O	4.03607700	-1.82112100	-1.54153200
C	4.44355300	0.46396500	-1.13090300
C	4.70354000	-0.68866300	-2.13630400
H	5.37256400	0.97168600	-0.86749400
H	5.76266100	-0.93083400	-2.22790500
C	2.28450400	-1.71806800	1.63656200
O	2.95253900	-1.45718000	2.76363500
C	0.80230100	-0.46061100	2.72869400
C	2.07637200	-0.65637300	3.59121500
H	-0.08534900	-0.86983800	3.21083800
H	1.88879300	-1.21032100	4.50961100
N	3.90758400	-0.23269500	0.05003900
N	1.10166800	-1.26882900	1.53234900
C	2.01488200	-3.28488600	-0.28929000
H	1.28101400	-2.64013100	-0.77413500
H	2.55365700	-3.83618600	-1.05924400
H	1.48087900	-3.99017800	0.34904500
C	4.09040300	-3.40458500	1.14902300
H	4.79364100	-2.83986900	1.76003500
H	3.62176500	-4.17098500	1.76897300
H	4.62964500	-3.89410700	0.33692800
H	4.27027500	-0.51539600	-3.11964400
H	2.58886500	0.27862400	3.81176900
C	3.44051600	1.49009700	-1.61983700
C	3.81954900	2.81242700	-1.83348300
C	2.12033100	1.11137300	-1.87417300
C	2.90045100	3.74534400	-2.30890400
H	4.84097800	3.11554700	-1.62845200
C	1.20479700	2.03700600	-2.35606100
H	1.80234300	0.08967100	-1.68747100
C	1.59310700	3.35738700	-2.57598600
H	3.20867200	4.77110500	-2.47282900
H	0.18695500	1.72807800	-2.56549300
H	0.87919700	4.07826100	-2.95789200
C	0.53413400	0.97773600	2.33765600
C	-0.62981900	1.62495400	2.74788300
C	1.46744300	1.66658300	1.56123900
C	-0.84267400	2.95930300	2.41587300
H	-1.37552400	1.07598000	3.31205000
C	1.24863000	2.99626700	1.21838900
H	2.36204100	1.15682200	1.21414700
C	0.10015000	3.64791600	1.65927200
H	-1.75465000	3.45500600	2.72897000

H	1.97336200	3.51476900	0.59910200
H	-0.07347600	4.68471400	1.39373900
C	-1.90326900	3.35190600	-0.81765300
C	-2.26231400	2.01498900	-0.70211600
C	-3.51635900	1.67305300	-0.18921100
C	-4.39443900	2.67788900	0.22593400
C	-4.03139700	4.01110100	0.11013700
C	-2.78728400	4.34842300	-0.41938000
H	-0.92035300	3.60979300	-1.19304000
H	-1.54834100	1.25191400	-0.99132300
H	-5.35822600	2.39126900	0.62810400
H	-4.71638300	4.78811300	0.42685100
H	-2.50402900	5.39058100	-0.51171700
C	-3.97460700	0.25796300	-0.08534600
O	-5.04712500	-0.02681100	0.40265600
C	-3.05971600	-0.83540100	-0.63107800
H	-4.79271600	-2.01711000	0.89109300
H	-2.69547100	-0.55146900	-1.61955400
C	-1.87014300	-0.96664300	0.32011400
O	-2.01593900	-0.97605400	1.51759800
O	-0.71969000	-1.04524000	-0.31289300
H	0.03038800	-1.16309200	0.38013800
C	-3.84485100	-2.15404300	-0.75529200
C	-3.01129100	-3.23214500	-1.42519600
F	-3.75050200	-4.31298300	-1.68913500
F	-1.98412400	-3.62494000	-0.66686800
F	-2.51108200	-2.79375900	-2.59132400
O	-4.24783700	-2.69113900	0.46700900
H	-4.69656900	-1.97266900	-1.42375700

im1-3-(*R*)

C	3.92594300	-1.91218000	0.78664400
C	4.09504200	-1.12322100	-0.49407500
O	4.08665700	-1.84375400	-1.63805700
C	4.15253200	0.47521700	-2.00260100
C	4.35361400	-0.89555400	-2.69196900
H	4.95448600	1.16867400	-2.25824900
H	5.38137000	-1.04413900	-3.02710200
C	3.17460100	-0.99695800	1.72967900
O	3.89575100	-0.28899700	2.60419100
C	1.59877700	0.25924800	2.68268800
C	2.95371500	0.47085500	3.39681500
H	0.82682700	-0.09201800	3.36684000
H	2.96584700	0.06049700	4.40622000
N	4.20959600	0.13494800	-0.56806200
N	1.91448800	-0.82622100	1.72719400
C	3.09650200	-3.17825100	0.53064100
H	2.12828400	-2.94187300	0.08810600
H	3.63535200	-3.83523500	-0.15114500
H	2.92979600	-3.70051800	1.47370300
C	5.31387200	-2.27152100	1.33753400
H	5.89770600	-1.37275000	1.53134600
H	5.21317800	-2.83488000	2.26691000
H	5.83805600	-2.89149800	0.60833500
H	3.65727700	-1.08476100	-3.50612300
H	3.28132500	1.50825200	3.40655000
C	2.81227800	1.11602500	-2.30842800
C	2.72744100	2.30104600	-3.03307700
C	1.63758700	0.51251800	-1.85553900
C	1.48724800	2.87775400	-3.30270600
H	3.63513700	2.78170900	-3.38348800
C	0.40398900	1.08858900	-2.11488400
H	1.68018200	-0.39824000	-1.26837600
C	0.32372700	2.27418100	-2.84073900
H	1.43434800	3.80262800	-3.86504700
H	-0.48806300	0.61865200	-1.71898500
H	-0.63987800	2.73049700	-3.03593100
C	1.08795300	1.47317000	1.93355800
C	-0.21838600	1.92230800	2.11221000
C	1.92596200	2.13749300	1.03510700
C	-0.68806200	3.01919300	1.39465000
H	-0.87616200	1.39804300	2.79589300
C	1.45910200	3.23593300	0.32474400
H	2.93330900	1.76889600	0.85964100
C	0.14977300	3.67633400	0.50061300
H	-1.71048400	3.35187300	1.53185700

H	2.10880300	3.72922700	-0.38913600
H	-0.21962900	4.52339700	-0.06672600
C	-3.46144800	3.04436900	-0.88032600
C	-3.25952000	1.67953300	-0.70418300
C	-3.69273800	1.05382400	0.46647400
C	-4.32302600	1.80967400	1.46035900
C	-4.50927700	3.17278500	1.28892100
C	-4.08175800	3.79105000	0.11451900
H	-3.13857400	3.52195400	-1.79714900
H	-2.79855600	1.11300000	-1.50338100
H	-4.66031900	1.30612200	2.35779400
H	-4.99128300	3.75472800	2.06487600
H	-4.23475500	4.85480800	-0.02365900
C	-3.56333600	-0.41465500	0.70137000
O	-4.27311400	-0.97609100	1.50692800
C	-2.46529200	-1.18448000	-0.02434300
H	-3.75465800	-2.82211600	1.35966800
H	-2.20161700	-0.72482800	-0.97497600
C	-1.21902400	-1.14667100	0.86625600
O	-1.26922300	-0.93628300	2.05159700
O	-0.12244700	-1.38345400	0.17914400
H	0.69459400	-1.25705500	0.78892100
C	-2.81140900	-2.66017900	-0.30059500
C	-3.90108500	-2.76714600	-1.36031300
F	-5.06342600	-2.23901200	-0.95696100
F	-4.13016800	-4.03889800	-1.68727100
F	-3.53924900	-2.11920400	-2.48271900
O	-3.15971500	-3.38242100	0.83860300
H	-1.92995100	-3.13382600	-0.74183100

im1-4-(*S*)

C	-3.90026200	-1.89010200	0.46435000
C	-4.11291700	-0.43556200	0.82558900
O	-4.46878500	-0.22320100	2.11365000
C	-4.15044500	1.76953200	0.89153300
C	-4.65411200	1.20119200	2.24436000
H	-4.90232100	2.41155000	0.42945500
H	-5.71499300	1.38996600	2.41005700
C	-3.25800200	-1.90204300	-0.89864300
O	-4.03604000	-1.55143000	-1.93046100
C	-1.77665900	-1.81782200	-2.55182900
C	-3.19500400	-1.54060400	-3.10265900
H	-1.30672000	-2.66212200	-3.05909900
H	-3.54721800	-2.32122400	-3.77632300
N	-3.96418600	0.56355700	0.06429400
N	-2.03971700	-2.17144900	-1.13953500
C	-2.95589500	-2.52220900	1.49548600
H	-2.02156200	-1.96072100	1.55847200
H	-3.43490400	-2.52213400	2.47385000
H	-2.73030800	-3.54982900	1.20639400
C	-5.25719800	-2.61273200	0.43279600
H	-5.91776200	-2.16617200	-0.31031800
H	-5.10926300	-3.66614300	0.18688400
H	-5.72470600	-2.54572200	1.41564800
H	-4.07324300	1.54330500	3.09915100
H	-3.28718000	-0.56419700	-3.57521700
C	-2.84123200	2.52543700	0.98945700
C	-2.74184000	3.85833800	0.59907800
C	-1.70721200	1.86797600	1.46505300
C	-1.52575300	4.53120000	0.69801200
H	-3.61676000	4.37284700	0.21527200
C	-0.49170900	2.53222500	1.56083600
H	-1.75830500	0.81874600	1.73363200
C	-0.40135900	3.87014800	1.18201500
H	-1.45796700	5.56921000	0.39410500
H	0.37575100	1.98752400	1.91638900
H	0.54357100	4.39687000	1.25493600
C	-0.83718200	-0.62787700	-2.56936700
C	0.44988900	-0.73839900	-3.08955800
C	-1.23465400	0.56727900	-1.96795400
C	1.33353200	0.33451700	-3.00574000
H	0.76760800	-1.67107000	-3.54461300
C	-0.35273600	1.63781900	-1.88245000
H	-2.22250300	0.65052500	-1.52207300
C	0.93566300	1.52171900	-2.39683100
H	2.33644500	0.24269800	-3.40781800

H	-0.66682800	2.55105700	-1.38820600
H	1.63434800	2.34750400	-2.31297300
C	4.53021200	2.02065400	-1.81293500
C	4.00541000	0.99119900	-1.04082700
C	3.24053400	1.28846200	0.08793200
C	3.02005600	2.61918300	0.44779500
C	3.51859500	3.64544900	-0.34144600
C	4.27315000	3.34581900	-1.47394500
H	5.13692100	1.78925500	-2.67981300
H	4.21804700	-0.03706300	-1.30901300
H	2.45333800	2.82898500	1.34641400
H	3.32727800	4.67746000	-0.07341700
H	4.66881300	4.14645600	-2.08742300
C	2.66796500	0.22652100	0.95908100
O	2.46125500	0.42878000	2.13749300
C	2.29867700	-1.12438200	0.35379800
H	2.52754000	-1.40826900	2.78870700
H	2.58756800	-1.19593800	-0.69560800
C	0.77485300	-1.29233300	0.38128400
O	0.01961100	-0.49234100	0.86642900
O	0.41315500	-2.42228700	-0.19586100
H	-0.58384900	-2.40044100	-0.36542200
C	2.92773300	-2.29987400	1.12566200
C	4.44167600	-2.28476600	0.97159200
F	5.00800600	-3.32182600	1.58376500
F	4.99056700	-1.16810600	1.47391800
F	4.78742100	-2.34200400	-0.32916300
O	2.57630900	-2.32391700	2.47516700
H	2.58585000	-3.23087300	0.66748700

im1-4-(*R*)

C	3.00713600	1.33439800	1.79392500
C	3.13597900	0.54194700	0.50608700
O	3.54512800	-0.73283300	0.67676100
C	3.37856700	-0.12379700	-1.56947100
C	3.41295800	-1.34070400	-0.62373700
H	4.38815200	0.10969600	-1.92647300
H	4.26000400	-2.00370200	-0.78458600
C	1.89915100	2.34009300	1.60249500
O	2.22286900	3.48334700	0.98999500
C	-0.08015000	3.34475200	1.46497000
C	1.03258800	4.29535500	0.95880800
H	-0.64289500	3.79665600	2.28344900
H	1.19260900	5.14775100	1.61925300
N	2.97336900	0.98158900	-0.67031200
N	0.68843500	2.19348100	1.97292700
C	2.68739900	0.41266300	2.97614000
H	1.80868200	-0.19941400	2.78292100
H	3.52939900	-0.25677700	3.14769100
H	2.51774000	1.01165200	3.87227300
C	4.34554500	2.05928600	2.03103500
H	4.57282000	2.72930200	1.20351000
H	4.30083400	2.63639600	2.95713700
H	5.13988700	1.31669300	2.12184700
H	2.47315400	-1.89784400	-0.63079700
H	0.87797200	4.63210900	-0.06415900
C	2.49257100	-0.32043100	-2.77585200
C	3.04033900	-0.30095300	-4.05651200
C	1.12550900	-0.56909700	-2.62916200
C	2.24439100	-0.53219900	-5.17559300
H	4.10010400	-0.10365200	-4.18066900
C	0.33013300	-0.80628700	-3.74487100
H	0.69183000	-0.57514800	-1.63460300
C	0.88755200	-0.78867100	-5.02173500
H	2.68647300	-0.51348400	-6.16483600
H	-0.72620000	-1.00974900	-3.60848200
H	0.26654600	-0.97460900	-5.89007300
C	-1.04071600	2.91410400	0.37573200
C	-2.37065900	3.32217300	0.40868300
C	-0.58000100	2.15099800	-0.70271200
C	-3.23713900	2.99237500	-0.63104100
H	-2.73072900	3.90690900	1.24926900
C	-1.44655600	1.82112100	-1.73757600
H	0.45603400	1.81916500	-0.73825900
C	-2.77360500	2.24718100	-1.70708400
H	-4.27139000	3.31378400	-0.59605400

H	-1.07946500	1.23843700	-2.57412700
H	-3.44462800	1.99016600	-2.51799100
C	-4.97378100	0.63724400	1.17291700
C	-3.77248600	-0.05346500	1.05773400
C	-3.45322600	-0.68981500	-0.14322600
C	-4.34076700	-0.63131300	-1.22238500
C	-5.54497300	0.04199600	-1.09589200
C	-5.86129000	0.67797500	0.10374900
H	-5.21566700	1.14246700	2.09990300
H	-3.08065900	-0.06684000	1.89100400
H	-4.06973200	-1.12456000	-2.14789800
H	-6.23828800	0.07397000	-1.92754000
H	-6.80218800	1.20661300	0.20279100
C	-2.18144700	-1.43596200	-0.33334300
O	-1.78913200	-1.74341000	-1.44109500
C	-1.36644900	-1.85221900	0.89628500
H	-0.08427300	-2.74288500	-1.15098300
H	-2.03052300	-1.97953700	1.75069300
C	-0.38251800	-0.72107800	1.20196400
O	0.58635100	-0.51274100	0.51688100
O	-0.72394600	-0.00146900	2.24926200
H	-0.12534900	0.83247600	2.26032300
C	-0.66926700	-3.20100800	0.61422300
C	0.01871500	-3.70760700	1.87065500
F	-0.87080700	-3.84361100	2.86832100
F	0.97376400	-2.87540200	2.30048100
F	0.58123500	-4.89828700	1.66789500
O	0.30445100	-3.18606500	-0.38418000
H	-1.45738500	-3.93478000	0.39463900

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C	-4.45020400	-1.15972800	0.53819800
C	-3.87715900	-0.38654200	-0.62615600
O	-4.78438100	0.13672000	-1.46966900
C	-2.58010500	0.73221600	-2.04531600
C	-4.03488300	0.72251200	-2.55901700
H	-1.88834600	0.30756600	-2.77143000
H	-4.16311700	0.08251900	-3.43200000
C	-3.31984800	-1.38139300	1.51253900
O	-2.42433900	-2.33196800	1.16059000
C	-1.79526000	-1.12722800	3.06421700
C	-1.50598500	-2.42205500	2.26630200
H	-1.83478000	-1.32734200	4.13673800
H	-1.75169100	-3.32233200	2.83320800
N	-2.65006100	-0.17136600	-0.87523400
N	-3.12290700	-0.72387300	2.57583300
C	-5.55598300	-0.32544200	1.19740800
H	-5.16765100	0.63349600	1.54122000
H	-6.36304000	-0.15666600	0.48519500
H	-5.94366400	-0.86315300	2.06322200
C	-5.00688100	-2.49725100	0.02072700
H	-4.22271700	-3.08989400	-0.44938400
H	-5.42312400	-3.06519600	0.85493200
H	-5.80006200	-2.30685100	-0.70322400
H	-4.43909100	1.71331500	-2.75558600
H	-0.49684500	-2.47837500	1.86463300
C	-2.06906100	2.08757400	-1.60184300
C	-0.79552000	2.51336100	-1.96559200
C	-2.86446100	2.91088900	-0.80017900
C	-0.33059900	3.76279200	-1.55961700
H	-0.15498600	1.86004700	-2.54641400
C	-2.40400200	4.15765600	-0.39798400
H	-3.85244600	2.57623200	-0.49362500
C	-1.13662600	4.59050800	-0.78792500
H	0.66654600	4.07653400	-1.84357500
H	-3.03004900	4.79271900	0.21747900
H	-0.77833800	5.56477400	-0.47674400
C	-0.76214800	-0.04646700	2.78605400
C	0.55853900	-0.26558700	3.18192800
C	-1.07163600	1.10643500	2.07170900
C	1.55888800	0.63528300	2.83937400
H	0.80767000	-1.15685700	3.75132900
C	-0.07073000	2.00884200	1.72240500
H	-2.09097500	1.28415200	1.75220500
C	1.24634100	1.77373800	2.09706100
H	2.58260100	0.45491900	3.14876800

H	-0.32558300	2.88621800	1.13961300
H	2.02845700	2.47093500	1.81746900
C	5.65164300	0.31535600	1.68438900
C	4.49820200	-0.00489300	0.97734700
C	3.91087000	0.93793800	0.12976200
C	4.49606000	2.19956500	-0.00403500
C	5.64579000	2.51796000	0.70292300
C	6.22444400	1.57538600	1.54961200
H	6.10104200	-0.41923600	2.34104800
H	4.06598700	-0.99077000	1.10345200
H	4.02905400	2.91772900	-0.66655400
H	6.09315000	3.49840800	0.59521600
H	7.12237100	1.82278800	2.10301800
C	2.65593900	0.67531300	-0.64814200
O	2.12713800	1.54439200	-1.29479000
C	2.08892800	-0.74902200	-0.62209100
H	1.93519600	-1.05650800	-3.06089400
H	2.11703700	-1.12575300	0.40109300
C	0.63533500	-0.72436500	-1.07105700
O	0.31110200	-0.62083100	-2.23828500
O	-0.19065000	-0.81671900	-0.06719700
H	-1.15376500	-0.66720300	-0.35003400
C	2.95940900	-1.63311900	-1.54201300
C	2.61732400	-3.10185500	-1.32643100
F	3.37508800	-3.89522800	-2.08159600
F	1.33705600	-3.37513000	-1.60903800
F	2.82380100	-3.44782100	-0.04104700
O	2.86231300	-1.29149500	-2.88775100
H	4.00924000	-1.53695600	-1.24998000

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C	-4.16230800	-1.84294500	0.79349600
C	-3.79689200	-1.08721200	-0.46363600
O	-4.79895800	-0.91363200	-1.34359900
C	-2.83069300	0.19473700	-1.99834600
C	-4.20372400	-0.29583400	-2.50819200
H	-2.02541100	-0.05356600	-2.68905200
H	-4.11311400	-1.06067900	-3.28052600
C	-2.99639500	-1.68198500	1.73897300
O	-1.94606100	-2.50319400	1.51436700
C	-1.50401300	-0.85375500	3.11144200
C	-0.99999400	-2.20783000	2.56008100
H	-1.46729500	-0.83659200	4.20236700
H	-1.06318900	-3.00567200	3.30295500
N	-2.66572800	-0.58273000	-0.75054300
N	-2.90128400	-0.80856100	2.64986900
C	-5.42201900	-1.21065500	1.40160100
H	-5.25247300	-0.16130400	1.64337200
H	-6.25114500	-1.29435900	0.69960300
H	-5.67653300	-1.73358100	2.32424000
C	-4.40626000	-3.31925600	0.44179800
H	-3.51608600	-3.76897700	0.00306600
H	-4.66633400	-3.87180900	1.34655200
H	-5.23424100	-3.39373400	-0.26410900
H	-4.86029100	0.50496700	-2.84028500
H	-0.00860600	-2.16450900	2.11611600
C	-2.79164600	1.68104900	-1.70341300
C	-1.89013100	2.51283800	-2.36078800
C	-3.68482400	2.23555800	-0.78452900
C	-1.88687500	3.88297100	-2.11276800
H	-1.17135200	2.08113300	-3.04648000
C	-3.67722200	3.60085200	-0.52770400
H	-4.39040100	1.59548200	-0.26154000
C	-2.77847000	4.42931000	-1.19636700
H	-1.17885200	4.52052700	-2.62872600
H	-4.37013100	4.01891500	0.19263100
H	-2.77140300	5.49440300	-0.99774400
C	-0.71668900	0.32764200	2.56103200
C	0.62818600	0.47380200	2.90893000
C	-1.28675800	1.23744700	1.67479700
C	1.39165300	1.50016100	2.36347100
H	1.08251600	-0.22080600	3.61038200
C	-0.52203000	2.25833000	1.11704200
H	-2.32697200	1.13503500	1.39862700
C	0.81873300	2.38972600	1.45578400
H	2.43370600	1.61075500	2.64311800

H	-0.97998400	2.93722600	0.40601500
H	1.41978100	3.17939800	1.02016000
C	5.16170000	0.79067500	2.21227500
C	4.39636500	0.21387100	1.20567500
C	3.88942600	1.00919500	0.17695600
C	4.15918400	2.37813700	0.15469400
C	4.89084300	2.95720500	1.18189300
C	5.39346200	2.16282600	2.21066700
H	5.57072200	0.17110000	3.00074700
H	4.22205800	-0.85563000	1.21471900
H	3.77097200	2.97337200	-0.66324800
H	5.07696900	4.02416400	1.17952700
H	5.97229900	2.61365300	3.00784900
C	3.07913700	0.43625600	-0.93436100
O	3.12203100	0.90604400	-2.05051900
C	2.16220200	-0.74467600	-0.64223800
H	2.54159500	-0.65441900	-3.05418200
H	2.26459100	-1.09509000	0.38369200
C	0.69242300	-0.34815600	-0.84065200
O	0.31692100	0.52930200	-1.57049700
O	-0.08595600	-1.16109700	-0.15368300
H	-1.05387900	-0.92599100	-0.29622200
C	2.41615700	-1.92392000	-1.60777700
C	3.79538500	-2.52233100	-1.36776600
F	3.91465800	-2.94229000	-0.09306300
F	4.77823800	-1.63627000	-1.58284900
F	4.01698200	-3.57036600	-2.15743300
O	2.26611700	-1.57857900	-2.94958300
H	1.70242400	-2.71900200	-1.37310300

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C	-4.62992600	-1.19625300	0.10572300
C	-3.84183000	-0.69702200	-1.07961500
O	-4.56957200	-0.41817800	-2.17770400
C	-2.27220900	0.04322400	-2.46266300
C	-3.63757500	0.00448900	-3.19505800
H	-1.54318200	-0.60701700	-2.94940000
H	-3.66359300	-0.72743000	-4.00123500
C	-3.71126100	-1.15334200	1.30355200
O	-2.79262500	-2.14274800	1.38290400
C	-2.56960800	-0.53856700	3.07046200
C	-2.16938300	-1.97949300	2.67489200
H	-2.87263300	-0.48897900	4.11771100
H	-2.60048900	-2.72379700	3.34797900
N	-2.58787700	-0.51179200	-1.13248300
N	-3.72536800	-0.26177500	2.20224900
C	-5.83342400	-0.27288300	0.33477400
H	-5.50843900	0.75145100	0.51714700
H	-6.48708400	-0.29756300	-0.53664300
H	-6.38553600	-0.61263600	1.21144800
C	-5.09301200	-2.63581400	-0.17907800
H	-4.24028500	-3.29340600	-0.34520700
H	-5.66167400	-3.01034900	0.67420100
H	-5.73637600	-2.64588100	-1.05979300
H	-3.95594200	0.97847000	-3.56353900
H	-1.09859900	-2.12125400	2.55992700
C	-1.67460200	1.42673300	-2.32165200
C	-0.41810100	1.71596600	-2.84530700
C	-2.38240000	2.42846900	-1.65547200
C	0.12127000	2.99381600	-2.72038300
H	0.14092900	0.93657800	-3.35266500
C	-1.84477800	3.70241000	-1.52237600
H	-3.35810200	2.20731200	-1.23100000
C	-0.59075300	3.98848600	-2.05845200
H	1.09625500	3.20942200	-3.14332300
H	-2.39969200	4.47079500	-0.99787300
H	-0.17363900	4.98394100	-1.95966300
C	-1.44216700	0.44915600	2.83272500
C	-0.43796300	0.56570500	3.79275300
C	-1.33561900	1.17515900	1.64847000
C	0.66348200	1.38200200	3.56984000
H	-0.51409300	0.00248300	4.71804900
C	-0.22953200	1.98901200	1.41997700
H	-2.11081700	1.09718500	0.89620100
C	0.77231700	2.09509600	2.37987800
H	1.43979500	1.46018100	4.32201700

H	-0.15522400	2.53856400	0.48572500
H	1.63398200	2.72922900	2.20390100
C	2.78111600	3.23065600	-0.30786400
C	2.63382000	1.84817900	-0.31503700
C	3.41610200	1.06134600	0.53409400
C	4.33747400	1.67027300	1.39084000
C	4.48620300	3.04853700	1.39083500
C	3.70842900	3.83005000	0.53800200
H	2.15952400	3.83957800	-0.95258000
H	1.87458700	1.40777400	-0.95320300
H	4.92465500	1.04260300	2.04947000
H	5.20405400	3.51623900	2.05328500
H	3.82126500	4.90769700	0.53867600
C	3.28709500	-0.42221200	0.60387700
O	3.87752500	-1.06404300	1.44504200
C	2.36438600	-1.11141500	-0.39780300
H	3.37954100	-2.86722700	1.08587700
H	2.35123200	-0.57152800	-1.34312000
C	0.94902900	-1.11279800	0.17975300
O	0.70815400	-1.37182500	1.32530700
O	0.05892400	-0.83889800	-0.76210000
H	-0.87448200	-0.84235900	-0.43603000
C	2.75429400	-2.57517500	-0.69930300
C	4.01196000	-2.62020700	-1.56144700
F	4.32491000	-3.87439100	-1.88586000
F	5.07532800	-2.08348100	-0.95042500
F	3.82779500	-1.94072600	-2.70799200
O	2.89868000	-3.38415800	0.42223700
H	1.96877600	-3.01041800	-1.32532000

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C	4.45858000	0.42789100	0.53511100
C	3.68962700	0.21907400	-0.74528000
O	4.44435400	0.04723200	-1.84761800
C	2.12867300	-0.10272900	-2.28878200
C	3.53091500	-0.13535300	-2.95001200
H	1.52236300	0.71528100	-2.68263600
H	3.68566500	0.67935900	-3.65556700
C	3.45960700	0.38100100	1.66619900
O	2.68826100	1.48027800	1.81692000
C	2.11213300	-0.25989100	3.27132000
C	1.93903200	1.25922700	3.03026500
H	2.32695000	-0.46881400	4.32085000
H	2.40108000	1.85568100	3.81985500
N	2.42874000	0.17705100	-0.87263200
N	3.28035500	-0.60169900	2.44436300
C	5.48414100	-0.70255000	0.68965400
H	4.99068300	-1.67443600	0.70867400
H	6.19338700	-0.67032900	-0.13708100
H	6.01974600	-0.57760000	1.63114400
C	5.15832800	1.79697900	0.48000000
H	4.43213300	2.60076300	0.36239900
H	5.71200000	1.95923900	1.40679700
H	5.85937500	1.81656300	-0.35515700
H	3.75811800	-1.08930700	-3.42433600
H	0.90959000	1.56091500	2.85689700
C	1.34616600	-1.39243000	-2.41059800
C	0.12042000	-1.42105100	-3.06910900
C	1.84670400	-2.56851900	-1.85035300
C	-0.59163600	-2.61233300	-3.18230500
H	-0.28006900	-0.50432500	-3.48947700
C	1.13606200	-3.75785100	-1.95527600
H	2.79455100	-2.55075000	-1.31937500
C	-0.08505600	-3.78221100	-2.62550200
H	-1.54169700	-2.62414800	-3.70495500
H	1.53082700	-4.66393600	-1.51166800
H	-0.63715000	-4.71089200	-2.71270800
C	0.88189300	-1.04321700	2.85166900
C	-0.20508500	-1.10263900	3.72288500
C	0.77388300	-1.62775800	1.59189900
C	-1.38765100	-1.72055300	3.33793700
H	-0.12793400	-0.64887600	4.70645500
C	-0.41274400	-2.24247800	1.20158700
H	1.61300100	-1.59246000	0.90787100
C	-1.49622200	-2.29008300	2.07287900
H	-2.22755300	-1.75491900	4.02210700

H	-0.48566400	-2.67962400	0.20962400
H	-2.42132400	-2.76741900	1.77013400
C	-3.34599600	-2.77874900	-0.87391400
C	-3.04483100	-1.43200000	-0.70347900
C	-3.80801700	-0.65549500	0.17224000
C	-4.86226600	-1.24011700	0.88010600
C	-5.16002100	-2.58279400	0.70668800
C	-4.40312400	-3.35241300	-0.17549900
H	-2.74281200	-3.38159500	-1.54141200
H	-2.19189700	-1.01630700	-1.23063400
H	-5.43410100	-0.62228400	1.56124200
H	-5.97858400	-3.03181100	1.25556200
H	-4.63391400	-4.40229500	-0.31187000
C	-3.54140000	0.79282100	0.39993800
O	-4.19443300	1.44062300	1.18922900
C	-2.42636800	1.46186500	-0.39765400
H	-3.10719200	3.17748800	1.39708500
H	-2.41528900	1.08122400	-1.41849700
C	-1.09050000	1.13351300	0.27239400
O	-0.91350200	1.23531900	1.45457700
O	-0.19402600	0.74521600	-0.61971000
H	0.69754100	0.57754600	-0.22948000
C	-2.67510600	2.98291800	-0.44800900
C	-1.70804500	3.66277200	-1.40127500
F	-1.74554700	3.08111800	-2.61309700
F	-0.44661400	3.60821700	-0.96875200
F	-2.02272300	4.94900900	-1.56721400
O	-2.51917100	3.62707000	0.77720400
H	-3.67598800	3.14051800	-0.87157600

ts2'-1-(*S*)

C	3.79088800	-3.10574400	0.98618300
C	3.44555000	-1.76744000	0.82073200
C	3.91610200	-1.04389400	-0.27605400
C	4.75579700	-1.68338600	-1.19102000
C	5.11848200	-3.01294300	-1.01678300
C	4.62742000	-3.73445200	0.06872700
H	3.41138900	-3.65930700	1.83845900
H	2.79237800	-1.28481300	1.53696700
H	5.10545900	-1.11235200	-2.04261800
H	5.78209600	-3.49047900	-1.72922600
H	4.90322800	-4.77413500	0.20385800
C	3.54721400	0.39555300	-0.54777400
O	3.58222600	0.75779900	-1.76610200
C	3.20667900	1.21648500	0.52307900
H	3.04418900	2.33328700	-1.55250900
H	3.41275900	0.88100500	1.53163400
C	0.72887800	0.80726600	0.82789000
O	0.36234400	1.65938800	0.13323500
O	0.76017000	-0.07622900	1.60221000
H	-0.43490600	-1.71241600	1.72077400
C	-3.01637500	-0.93364600	2.47004100
C	-3.28995700	0.30785400	1.64390000
O	-2.23330300	0.70562200	0.89574500
C	-4.15508100	2.02089200	0.58839400
C	-2.62700400	1.97606500	0.32234900
H	-4.44814800	2.97988000	1.01634700
H	-2.07949600	2.75926700	0.84570600
C	-2.45414700	-1.90931600	1.47256300
O	-3.27186800	-2.50178300	0.65122300
C	-1.02912200	-3.13321300	0.13858200
C	-2.49275400	-3.22043800	-0.35579200
H	-0.68331000	-4.09257800	0.52571200
H	-2.87985600	-4.23344800	-0.40271000
N	-4.36847800	0.95496400	1.59098800
N	-1.21124500	-2.21157100	1.28442200
C	-1.98627800	-0.60414300	3.56014800
H	-1.08490300	-0.15169500	3.14591800
H	-2.43608400	0.10726900	4.25279400
H	-1.72177200	-1.50468000	4.11758500
C	-4.31550300	-1.48633000	3.06374300
H	-5.04314700	-1.70831200	2.28516100
H	-4.10867600	-2.38766000	3.64290200
H	-4.73961600	-0.72928900	3.72179700
H	-2.35749800	1.97302700	-0.73109700
H	-2.64296200	-2.70000800	-1.30038700

C	-4.97439900	1.76157400	-0.65939000
C	-5.48950000	2.83629800	-1.38113100
C	-5.16713900	0.46589400	-1.13851200
C	-6.18097800	2.62351900	-2.56894300
H	-5.34885600	3.84642300	-1.01098400
C	-5.86016900	0.25206000	-2.32469200
H	-4.78998900	-0.38101900	-0.57476100
C	-6.36721200	1.32996700	-3.04365500
H	-6.57759800	3.46758100	-3.12012700
H	-6.01013700	-0.75814800	-2.68693500
H	-6.90841600	1.16193400	-3.96678400
C	-0.04768700	-2.58955400	-0.86485800
C	0.93444500	-3.42069800	-1.39257800
C	-0.11183100	-1.24805900	-1.24920700
C	1.85047200	-2.91350600	-2.30821300
H	0.99784200	-4.45629600	-1.07537700
C	0.83391700	-0.73382000	-2.12510700
H	-0.87493600	-0.59409000	-0.83273300
C	1.81168700	-1.57033900	-2.65921400
H	2.62807200	-3.55572600	-2.70222300
H	0.84668300	0.32381300	-2.35862200
H	2.57280700	-1.14531700	-3.29995300
C	3.10704900	2.70823900	0.31016000
C	4.44046500	3.38062500	0.61743900
F	4.36330900	4.71991800	0.50965700
F	5.42467000	2.98235000	-0.19676500
F	4.84045300	3.12491800	1.88121200
O	2.72171500	3.07449500	-0.98635400
H	2.40583700	3.16730800	1.02091600

Value of Imaginary Frequency= -258.0 cm^{-1}

ts2'-1-(*R*)

C	-5.62046300	-0.71008500	0.69556800
C	-4.34092500	-1.24736600	0.78289700
C	-3.84506900	-2.07665300	-0.22772100
C	-4.65655300	-2.33757900	-1.33411000
C	-5.93966200	-1.80827900	-1.41975900
C	-6.42835500	-0.99278800	-0.40270200
H	-5.98822900	-0.06742500	1.48765600
H	-3.72028000	-1.00079700	1.63546200
H	-4.25047300	-2.96670700	-2.11631100
H	-6.56030400	-2.03335400	-2.27999700
H	-7.42908500	-0.58024300	-0.46492000
C	-2.45774800	-2.68513900	-0.21578900
O	-2.06109400	-3.21115300	-1.29867800
C	-1.66078600	-2.55565100	0.91365700
H	-0.40235200	-3.26263400	-0.96059400
H	-2.07643000	-2.26327400	1.86716900
C	-1.15277200	-0.28952000	0.06057500
O	-0.81476200	-0.55728100	-1.01729600
O	-1.42401400	0.32721700	1.02671400
H	-0.91075400	2.24490300	1.49408300
C	1.86242800	2.26223100	1.62602800
C	2.37190700	1.13906800	0.74483500
O	1.51948500	0.74770800	-0.22185600
C	3.43036700	-0.61983200	-0.01150000
C	2.17451400	-0.36771000	-0.88854000
H	3.28905900	-1.52642600	0.58342900
H	1.48475300	-1.20837000	-0.90415500
C	0.84797400	3.03523400	0.83179400
O	1.23721600	3.87479900	-0.08343700
C	-1.14509500	3.87191700	0.02561000
C	0.06242300	4.38120400	-0.79231000
H	-1.59546800	4.68011000	0.60393400
H	0.14166700	5.46342600	-0.81397500
N	3.45233200	0.51862900	0.92627000
N	-0.43640600	2.98138900	0.97334400
C	1.20196700	1.62399200	2.86078800
H	0.43296600	0.90165900	2.58019100
H	1.97239600	1.08640900	3.41223400
H	0.77609400	2.39392200	3.50758300
C	3.01327700	3.19340500	2.02997700
H	3.46751700	3.66162000	1.15733600
H	2.65462900	3.96625200	2.71209100
H	3.76688800	2.59052300	2.53440700
H	2.42916000	-0.04348600	-1.89829900
H	0.10028400	3.97368800	-1.80045700

C	4.69447700	-0.76227000	-0.82382800
C	4.94120000	-1.97207600	-1.47448100
C	5.59109700	0.29132800	-0.98002900
C	6.06543300	-2.12328000	-2.27689500
H	4.24761400	-2.79757000	-1.34677400
C	6.72085300	0.13754800	-1.77852000
H	5.40792700	1.22466800	-0.46086400
C	6.95948900	-1.06725600	-2.43030900
H	6.24750500	-3.06723800	-2.77666600
H	7.41818700	0.95994500	-1.88809900
H	7.83986100	-1.18586900	-3.05055300
C	-2.21845700	3.11050500	-0.71159500
C	-3.55194000	3.29554500	-0.34871700
C	-1.88297300	2.12630000	-1.63778400
C	-4.54042000	2.48468000	-0.89323500
H	-3.81252000	4.05768000	0.37820600
C	-2.87306900	1.31498300	-2.18062500
H	-0.84484900	1.93638200	-1.89232200
C	-4.19959700	1.48668000	-1.80093700
H	-5.57302600	2.61487700	-0.59307800
H	-2.59969200	0.51827200	-2.86082900
H	-4.96274700	0.82425700	-2.19115000
C	-0.31518800	-3.23858000	0.93147800
C	0.62618400	-2.56583900	1.90892900
F	0.11780000	-2.52176900	3.14972200
F	0.90973100	-1.28836200	1.56362300
F	1.80772500	-3.19624500	1.98785600
O	0.34406300	-3.21490300	-0.31276300
H	-0.39334600	-4.27734100	1.29919700

Value of Imaginary Frequency= -265.2 cm^{-1}

ts2'-2-(*S*)

C	-2.07285000	2.86823300	-2.31020600
C	-2.71725200	1.83993900	-1.62739200
C	-3.66893700	2.12716100	-0.64821300
C	-3.97044300	3.46390500	-0.37520600
C	-3.34947700	4.49018900	-1.07514300
C	-2.38874000	4.19601700	-2.04076000
H	-1.32315300	2.63156700	-3.05728600
H	-2.47278100	0.80590600	-1.84277700
H	-4.69872300	3.67646000	0.39906000
H	-3.60849300	5.52222900	-0.86514100
H	-1.89387500	4.99546400	-2.58038800
C	-4.38833800	1.06326300	0.14407600
O	-4.57379300	1.30296400	1.38662000
C	-4.82022400	-0.05929200	-0.53545500
H	-5.34159400	-0.18688500	1.74570600
H	-4.71627200	-0.10287900	-1.61232400
C	-2.57301900	-1.26513300	0.39174200
O	-2.89675300	-1.29329400	1.49871900
O	-2.01547900	-1.34160100	-0.63457400
H	-0.08297400	-1.32869100	-0.20542900
C	2.52130600	-2.19810300	-0.74267600
C	3.64312100	-1.26085000	-1.12867700
O	3.25836600	0.03285600	-1.24978000
C	5.55622700	-0.31951700	-1.64959200
C	4.42084500	0.73837800	-1.74093700
H	6.06686400	-0.42718400	-2.60726200
H	4.21486000	1.05145100	-2.76402100
C	1.85120200	-1.55959300	0.43833700
O	2.55910200	-1.27907600	1.49390000
C	0.31584100	-0.51940500	1.80619900
C	1.68273200	-0.69883900	2.51199900
H	-0.47658400	-1.04255200	2.34077700
H	1.64928500	-1.40558100	3.33722600
N	4.84237400	-1.57670300	-1.34396500
N	0.60432000	-1.24274700	0.54350700
C	1.53881900	-2.32874000	-1.91481100
H	1.15110100	-1.35616200	-2.22310100
H	2.06416400	-2.77255700	-2.76015600
H	0.70898000	-2.98807400	-1.65059700
C	3.07754900	-3.56175000	-0.30999000
H	3.78037300	-3.45262200	0.51485900
H	2.25957000	-4.22123100	-0.01589900
H	3.60598800	-4.00081400	-1.15504400
H	4.58785400	1.60615700	-1.10586100
H	2.12687900	0.24347600	2.82097200

C	6.57577800	-0.00471000	-0.57611700
C	7.84778300	0.44146500	-0.92293800
C	6.23474400	-0.11348400	0.77280600
C	8.76936700	0.78174100	0.06326200
H	8.12152700	0.52016100	-1.96975900
C	7.15376400	0.22467400	1.75793400
H	5.25007000	-0.47542500	1.05260300
C	8.42367600	0.67423900	1.40489800
H	9.75762400	1.12503400	-0.21798100
H	6.88333000	0.13338600	2.80314900
H	9.14073700	0.93496100	2.17378300
C	-0.08319000	0.90706300	1.52500600
C	-1.30560900	1.39476600	1.97528400
C	0.78652100	1.73695700	0.81074600
C	-1.65421500	2.71954100	1.72784700
H	-2.00888400	0.75325200	2.49340600
C	0.43377600	3.05608700	0.56827400
H	1.73064200	1.35072000	0.43338400
C	-0.78494800	3.54899700	1.03309400
H	-2.62898500	3.06511700	2.04594400
H	1.10185100	3.69966700	0.00865500
H	-1.06724200	4.57343600	0.82478600
C	-5.83866000	-0.97947600	0.08969900
C	-5.69909800	-2.39937100	-0.42576500
F	-6.63252700	-3.21352700	0.08680700
F	-4.50762400	-2.96339200	-0.14270600
F	-5.83339100	-2.44464600	-1.76467600
O	-5.76856600	-1.03821500	1.48904200
H	-6.85845000	-0.69274100	-0.22823300

Value of Imaginary Frequency= -50.2 cm^{-1}

ts2'-2-(*R*)

C	6.94656000	0.10754400	0.44166100
C	5.66876500	-0.43270900	0.51902900
C	4.80185500	-0.36378300	-0.57407900
C	5.23641100	0.27104800	-1.73911700
C	6.51650400	0.80629400	-1.82033800
C	7.37633600	0.72521300	-0.72957300
H	7.60667000	0.05291500	1.29940300
H	5.34049000	-0.89248800	1.44331900
H	4.54978500	0.32908100	-2.57428700
H	6.84420100	1.28642100	-2.73515300
H	8.37400900	1.14428900	-0.78857100
C	3.40863800	-0.92683700	-0.55592000
O	2.60106100	-0.46859700	-1.43122600
C	3.04254300	-1.84076100	0.42972400
H	1.22588200	-1.15182100	-0.87219900
H	3.80256900	-2.34046600	1.01497200
C	2.36420000	-0.24655400	2.08741700
O	1.77369500	-0.98990900	2.77716100
O	2.77478700	0.78651400	1.71222600
H	0.33051800	1.34910200	1.86065900
C	-1.88595400	-0.35097200	1.85452500
C	-3.32665600	-0.02061500	1.54147600
O	-3.56051400	1.30517900	1.36985100
C	-5.47055300	-0.04263300	1.07507000
C	-4.98953000	1.42928600	1.21036800
H	-6.27349000	-0.25559000	1.78228400
H	-5.38564000	1.92190900	2.09868300
C	-1.07838100	0.32544200	0.78687900
O	-1.41242100	0.16240500	-0.45442500
C	0.54548500	1.52270200	-0.32135200
C	-0.47997200	0.90385200	-1.30011000
H	1.50978700	1.02642500	-0.43137100
H	-0.02250900	0.19394600	-1.98457700
N	-4.28266600	-0.83465100	1.44144700
N	-0.05988000	1.10503300	0.95919900
C	-1.52797800	0.19686200	3.24359100
H	-1.68594100	1.27511400	3.30436300
H	-2.16806900	-0.28765600	3.98126600
H	-0.49264600	-0.04881600	3.49039600
C	-1.63217700	-1.86454300	1.77284000
H	-1.77543400	-2.23644300	0.75966600
H	-0.60822300	-2.07144000	2.08367200
H	-2.33436200	-2.36033300	2.44236200
H	-5.18649900	2.03042800	0.32495000
H	-1.06492700	1.64709000	-1.83841800

C	-5.94536400	-0.37777400	-0.32383000
C	-7.30351100	-0.30364400	-0.62767000
C	-5.03772300	-0.70331700	-1.33126800
C	-7.75170300	-0.54334700	-1.92232600
H	-8.01563500	-0.06254100	0.15507100
C	-5.48596200	-0.94614400	-2.62501100
H	-3.98103900	-0.78349500	-1.10049400
C	-6.84246000	-0.86505900	-2.92427000
H	-8.81039400	-0.48740400	-2.14581100
H	-4.77469900	-1.20733400	-3.39953300
H	-7.18973200	-1.05896100	-3.93191500
C	0.70902900	3.01700800	-0.40632600
C	1.97190200	3.54694000	-0.65281400
C	-0.38431600	3.86740000	-0.23562500
C	2.14045100	4.92581700	-0.73983300
H	2.81652800	2.87610000	-0.77306600
C	-0.21310700	5.24271400	-0.31719700
H	-1.36806900	3.45361600	-0.03030300
C	1.05043800	5.77189700	-0.57255400
H	3.12362500	5.33648500	-0.93377900
H	-1.06147300	5.90248600	-0.18221400
H	1.18281200	6.84508800	-0.63794400
C	1.69692200	-2.50641100	0.34951700
C	1.71662600	-3.76732800	-0.50112100
F	2.60745800	-4.65605200	-0.02879400
F	2.02822900	-3.52743000	-1.78031000
F	0.51868500	-4.37968600	-0.49863400
O	0.71086300	-1.63960600	-0.17457100
H	1.37672900	-2.84329000	1.34096300

Value of Imaginary Frequency= -289.6 cm^{-1}

ts2'-3-(*S*)

C	3.31463900	-2.71832100	0.18070100
C	3.85002400	-1.55708600	-0.63289300
O	4.00685400	-1.77345200	-1.94854700
C	4.46670400	0.44995200	-1.28847500
C	4.56888900	-0.54579400	-2.47501500
H	5.42637000	0.93166300	-1.09809500
H	5.59898600	-0.75016500	-2.76538000
C	2.53167800	-2.05901800	1.28747200
O	3.00461300	-1.98754700	2.49033800
C	0.94421800	-0.77784700	2.36982600
C	2.04351400	-1.27401500	3.33695100
H	-0.03580700	-1.14131200	2.67034200
H	1.67410500	-1.99583800	4.06066400
N	4.11770000	-0.42159800	-0.14653200
N	1.36592900	-1.51033700	1.14909100
C	2.38042700	-3.60088800	-0.66381900
H	1.58310200	-3.02948200	-1.14271800
H	2.96557200	-4.07002100	-1.45322000
H	1.93610900	-4.37795500	-0.04101500
C	4.48369700	-3.53330000	0.75063200
H	5.13061700	-2.90835500	1.36501900
H	4.10864700	-4.36331400	1.35125700
H	5.06196300	-3.93695800	-0.08084200
H	3.98043600	-0.25146700	-3.34134000
H	2.58454100	-0.47095700	3.82948000
C	3.39913400	1.51033800	-1.45808700
C	3.73528900	2.85786700	-1.52618900
C	2.05453800	1.14051900	-1.53854800
C	2.74217100	3.82565800	-1.66879100
H	4.77704600	3.15500900	-1.46276600
C	1.06120100	2.10017000	-1.66133500
H	1.77568000	0.09107600	-1.50514800
C	1.40686400	3.44884300	-1.72712900
H	3.01491200	4.87317100	-1.72027900
H	0.02091300	1.79823300	-1.68206800
H	0.63066200	4.20106900	-1.80573900
C	0.90199500	0.70457100	2.09470800
C	-0.32479800	1.35804500	1.98068700
C	2.09494000	1.40669100	1.90252500
C	-0.34877500	2.72109000	1.69346600
H	-1.26454900	0.82327100	2.11471900
C	2.06263400	2.76540000	1.62786200
H	3.04885700	0.88828900	1.93134100
C	0.83884200	3.42225000	1.52913900
H	-1.30004700	3.22752600	1.59602300

H	2.98772500	3.30635200	1.47027600
H	0.81094500	4.48185900	1.30244800
C	-2.33303700	3.51555300	-1.34884200
C	-2.64527800	2.19100700	-1.05945700
C	-3.37896700	1.86626600	0.08380000
C	-3.78904800	2.89641500	0.93342800
C	-3.49845200	4.22341400	0.63371800
C	-2.76242200	4.53823100	-0.50635200
H	-1.76335800	3.75029100	-2.24190900
H	-2.30999900	1.39781600	-1.71877600
H	-4.33973200	2.62819800	1.82706900
H	-3.84114800	5.01346800	1.29251500
H	-2.53058800	5.57110200	-0.73944500
C	-3.76496700	0.45298900	0.44709700
O	-3.88711900	0.19959100	1.69351700
C	-3.96422300	-0.44696700	-0.58129100
H	-4.25580800	-1.44751300	1.51106200
H	-3.95143200	-0.10438600	-1.60762800
C	-1.41418100	-1.11762200	0.03479700
O	-1.68614800	-1.58381700	1.05753500
O	-0.86113600	-0.72210900	-0.91590200
H	0.92482900	-1.36299400	0.24579800
C	-4.62900100	-1.77679000	-0.32860500
C	-4.08414600	-2.84947300	-1.25494500
F	-4.69736800	-4.02753100	-1.07365300
F	-2.76501900	-3.08102700	-1.09792100
F	-4.26084100	-2.51107200	-2.54599300
O	-4.48852400	-2.24916200	0.98292400
H	-5.69882400	-1.72437300	-0.60258700

Value of Imaginary Frequency= -61.0 cm^{-1}

ts2'-3-(*R*)

C	-4.12211100	-1.92140500	-0.70163400
C	-4.00491200	-1.29999200	0.67685000
O	-3.78917000	-2.14741700	1.69517500
C	-3.74938600	0.12779800	2.32968000
C	-3.77621900	-1.32067200	2.88512800
H	-4.51787400	0.74270300	2.79918300
H	-4.68251600	-1.53829800	3.44982500
C	-3.51032700	-0.89593800	-1.62121400
O	-4.24982700	-0.13961500	-2.37183700
C	-1.96583400	0.52872000	-2.56507000
C	-3.37805100	0.73402900	-3.16009100
H	-1.24461900	0.26030100	-3.33690800
H	-3.45760900	0.40102800	-4.19220200
N	-4.06810400	-0.05685100	0.89680600
N	-2.24115900	-0.66921000	-1.73686600
C	-3.32104200	-3.23115200	-0.78882000
H	-2.27630000	-3.10185500	-0.49942800
H	-3.76440100	-3.95625000	-0.10830000
H	-3.36379000	-3.62586700	-1.80461800
C	-5.60162800	-2.14718700	-1.03981500
H	-6.15686500	-1.21096900	-0.99797900
H	-5.70102100	-2.58134500	-2.03570100
H	-6.02069500	-2.84305200	-0.31236900
H	-2.89364400	-1.58094600	3.46508800
H	-3.75003500	1.74819000	-3.04712800
C	-2.40485300	0.81258400	2.46048100
C	-2.24798200	1.94295800	3.25498600
C	-1.30126700	0.30940700	1.76831900
C	-1.00433800	2.56512900	3.35560900
H	-3.09979500	2.34251500	3.79584800
C	-0.06857600	0.93982700	1.84293300
H	-1.40100700	-0.58235500	1.15763900
C	0.08118900	2.07064100	2.64394900
H	-0.89125400	3.44356200	3.98011400
H	0.76506100	0.56159000	1.26107000
H	1.04161600	2.57033900	2.69575900
C	-1.43709100	1.66149600	-1.71895600
C	-0.11027300	2.06479800	-1.84903400
C	-2.27013800	2.28808300	-0.78869200
C	0.38606500	3.09229100	-1.05210800
H	0.54276000	1.57797500	-2.56456300
C	-1.77656300	3.32243800	-0.00681200
H	-3.29144800	1.94699300	-0.64593300
C	-0.44922500	3.72355900	-0.13914400
H	1.42382700	3.38800300	-1.14354600

H	-2.41937500	3.79820600	0.72372300
H	-0.05922600	4.51862300	0.48603500
C	3.39697100	3.33087400	0.97716700
C	3.32376800	1.94676800	0.85434200
C	3.61177700	1.32115600	-0.36213300
C	3.97748700	2.11744200	-1.44965600
C	4.05424100	3.50129500	-1.32993600
C	3.76414300	4.11485700	-0.11398400
H	3.19096100	3.79898300	1.93370900
H	3.07747100	1.35091200	1.72601500
H	4.22088500	1.61338400	-2.37685500
H	4.34854500	4.10209700	-2.18316900
H	3.83427400	5.19179300	-0.01324600
C	3.60316700	-0.18086400	-0.56527800
O	4.14992900	-0.61148300	-1.62135000
C	2.92070800	-0.98380400	0.33963600
H	3.50398800	-2.22135000	-1.60135100
H	2.53521200	-0.59298900	1.26916400
C	0.92820600	-1.16038100	-1.30157600
O	1.35827700	-0.73407900	-2.28754700
O	0.18683500	-1.60393200	-0.50074200
H	-1.52315200	-1.12123500	-1.16742700
C	2.98918100	-2.47887900	0.20892400
C	4.21628700	-3.06464300	0.89388500
F	5.36796600	-2.64448900	0.36156100
F	4.22615900	-4.40987600	0.83340100
F	4.23880600	-2.74362700	2.20301900
O	2.97380400	-2.91081900	-1.13410200
H	2.13945600	-2.94496900	0.72176400

Value of Imaginary Frequency= -218.5 cm^{-1}

ts2'-4-(*S*)

C	3.67236800	1.75453800	-0.97190200
C	3.66129800	1.21297900	0.44356400
O	3.72035500	2.15010500	1.40367600
C	3.55860700	-0.06300700	2.23927100
C	3.61993400	1.43157500	2.65868100
H	4.44701900	-0.60121900	2.57681800
H	4.49677000	1.67595000	3.25462600
C	3.36094600	0.57196200	-1.84672900
O	4.27045900	-0.32394600	-2.08803700
C	2.17575900	-1.06138900	-2.94713500
C	3.68792200	-1.37015900	-2.92570500
H	1.79003100	-1.02600000	-3.96519000
H	4.15295000	-1.28243700	-3.90504200
N	3.59122300	-0.00715700	0.76132800
N	2.21949800	0.31824900	-2.40018800
C	2.59467300	2.84027000	-1.11264200
H	1.61226800	2.49913900	-0.77656700
H	2.87286900	3.68712200	-0.48792500
H	2.52608700	3.17792500	-2.14842300
C	5.06888600	2.30457400	-1.30901400
H	5.82739700	1.52772600	-1.21643000
H	5.08256600	2.70110600	-2.32565000
H	5.29906400	3.11273600	-0.61539800
H	2.71547600	1.76697700	3.16420200
H	3.92638400	-2.32461800	-2.46526600
C	2.32591400	-0.79997300	2.71485700
C	2.43607800	-1.99040500	3.43052700
C	1.06024200	-0.30488700	2.40653500
C	1.29127100	-2.67158400	3.83729900
H	3.41807300	-2.38457700	3.67156800
C	-0.08777800	-0.98612200	2.79426900
H	0.95900800	0.61413300	1.83693600
C	0.03234000	-2.17129000	3.51708700
H	1.38450000	-3.59296200	4.40041000
H	-1.06137100	-0.59546500	2.50908800
H	-0.85795000	-2.70540400	3.82917100
C	1.30270400	-1.92250200	-2.06433600
C	0.00873000	-2.25048400	-2.46908500
C	1.75056300	-2.28982800	-0.79475100
C	-0.83652300	-2.93953700	-1.60401000
H	-0.34499900	-1.94768700	-3.44956600
C	0.90868000	-2.98486000	0.06263600
H	2.73299700	-1.98848400	-0.44497800
C	-0.38172400	-3.30940500	-0.34239000
H	-1.85598200	-3.16606100	-1.89760200

H	1.25032000	-3.23927300	1.05965100
H	-1.04954300	-3.82636400	0.33543500
C	-4.77351900	-2.61486100	-1.65904000
C	-4.37553300	-1.32673200	-1.31955800
C	-3.71136200	-1.07641700	-0.11488500
C	-3.47775600	-2.14717400	0.74883800
C	-3.87582400	-3.43743300	0.41387800
C	-4.51997800	-3.67884000	-0.79551200
H	-5.29371500	-2.78836600	-2.59430400
H	-4.60259400	-0.50959600	-1.99325300
H	-2.97984400	-1.93649900	1.68757700
H	-3.68708500	-4.25680300	1.09934100
H	-4.83515400	-4.68212100	-1.05811600
C	-3.21062700	0.28905300	0.30249700
O	-2.82270300	0.41297200	1.50668900
C	-3.05675900	1.26952200	-0.66210400
H	-1.80923000	1.80467000	1.29285400
H	-3.41241400	1.14198900	-1.67315600
C	-0.64187100	0.50695000	-0.97201600
O	-0.49983400	-0.19663400	-0.06892200
O	-0.45480000	1.14140200	-1.94815200
H	1.37173100	0.87749000	-2.27996200
C	-2.49534400	2.61051000	-0.28311200
C	-3.56214400	3.57730800	0.20995900
F	-3.04779100	4.79511400	0.47076600
F	-4.16995100	3.16710600	1.32670500
F	-4.51642400	3.76081300	-0.72329300
O	-1.48086100	2.52203800	0.69870000
H	-2.06516100	3.10044800	-1.16388400

Value of Imaginary Frequency= -193.3 cm^{-1}

ts2'-4-(*R*)

C	3.40483000	-0.37820000	-1.69943000
C	3.19631800	0.16804400	-0.29164800
O	3.23490200	1.50214500	-0.19468500
C	3.04550000	0.42666600	1.87802600
C	2.82889800	1.78253700	1.17587900
H	4.05060800	0.38615900	2.31253800
H	3.46504200	2.57743200	1.55630100
C	2.69906500	-1.69975900	-1.68206000
O	3.25114500	-2.72435300	-1.11374200
C	1.02638300	-3.28635300	-1.76334500
C	2.24945800	-3.77247900	-0.95081600
H	0.88255200	-3.87812500	-2.66791200
H	2.68158000	-4.69620900	-1.32270600
N	3.04897200	-0.53821000	0.74701200
N	1.51314400	-1.94165900	-2.15014900
C	2.81623300	0.55864700	-2.75860200
H	1.77239600	0.80893400	-2.56761800
H	3.36630300	1.49772900	-2.73621200
H	2.91443000	0.11612900	-3.75169300
C	4.91357000	-0.58904000	-1.92257400
H	5.32095400	-1.27856900	-1.18455500
H	5.09876100	-0.97606900	-2.92608500
H	5.41256800	0.37505900	-1.82317200
H	1.78588400	2.10420100	1.14379700
H	2.04164900	-3.83760600	0.11579000
C	2.05757300	0.07283000	2.96371100
C	2.52142400	-0.43750200	4.17583100
C	0.68417900	0.23259500	2.77835300
C	1.63073600	-0.78333700	5.18739500
H	3.58830000	-0.56320100	4.33018100
C	-0.20788900	-0.10319700	3.79103500
H	0.28687600	0.62643300	1.85267600
C	0.26308700	-0.61498900	4.99690500
H	2.00620100	-1.17660500	6.12494400
H	-1.26487300	0.06049300	3.61446400
H	-0.43105500	-0.87399000	5.78790600
C	-0.26748200	-3.16063300	-0.99997100
C	-1.42812900	-3.73850700	-1.50483200
C	-0.31743100	-2.37513200	0.15516500
C	-2.64205100	-3.52910700	-0.85923800
H	-1.38547600	-4.33750600	-2.40844000
C	-1.53813700	-2.13124100	0.77183500
H	0.58280300	-1.90668600	0.54909800
C	-2.69798400	-2.71556900	0.26559100
H	-3.54873900	-3.97247100	-1.25266500

H	-1.58896600	-1.45129900	1.61607500
H	-3.65231700	-2.50950900	0.73422900
C	-5.12138700	-0.73289500	-1.41693700
C	-4.01392300	0.07624900	-1.18628200
C	-3.69683500	0.49106000	0.10904800
C	-4.51126800	0.07817000	1.16606100
C	-5.63261200	-0.71077800	0.93404200
C	-5.93863300	-1.12517300	-0.35985600
H	-5.34733400	-1.05952700	-2.42578100
H	-3.37575900	0.36443200	-2.01335600
H	-4.24557100	0.39494000	2.16714700
H	-6.26598300	-1.00725700	1.76266000
H	-6.80738200	-1.74682200	-0.54347800
C	-2.51773800	1.37114200	0.43549500
O	-2.02136700	1.24256500	1.60956000
C	-2.06728800	2.26464200	-0.51819000
H	-0.82969100	2.37206300	1.47240300
H	-2.63447500	2.41419000	-1.42763700
C	-0.38120400	0.39597700	-1.25672500
O	0.31722400	0.49622500	-0.33741900
O	-0.84633000	0.09197900	-2.28495500
H	0.91315600	-1.25229300	-2.59572600
C	-1.12529500	3.37476400	-0.11660900
C	-0.22510200	3.80715300	-1.25958700
F	-0.95316600	4.21795200	-2.31318400
F	0.59089400	2.83444100	-1.71551100
F	0.56897800	4.82688000	-0.90732900
O	-0.30160600	3.05136800	0.97388600
H	-1.70053600	4.29222800	0.10584200

Value of Imaginary Frequency= -152.5 cm^{-1}

ts2'-5-(*S*)

C	-3.58185900	-1.97832700	-1.00399700
C	-3.00348500	-0.68073800	-1.49589800
O	-3.57828800	-0.06018700	-2.48717900
C	-1.76370400	1.25294500	-1.65893100
C	-2.80347200	1.14259300	-2.80006400
H	-0.74885000	1.28572200	-2.05661900
H	-2.34699100	0.97658400	-3.77250200
C	-2.70220900	-2.42496500	0.14011700
O	-1.45667700	-2.80569200	-0.22483400
C	-1.71018800	-2.58998400	2.07756700
C	-0.83992600	-3.26857300	1.00182000
H	-1.86855900	-3.23822600	2.93979200
H	-0.92290600	-4.35673400	1.02134500
N	-1.98070300	-0.05648500	-1.01437700
N	-2.98685400	-2.35346200	1.36861000
C	-5.01168300	-1.69678800	-0.51793100
H	-5.01651200	-0.94576700	0.27258200
H	-5.62683800	-1.36104200	-1.35262300
H	-5.42657100	-2.61872400	-0.11139800
C	-3.56473500	-2.99895000	-2.15616600
H	-2.54895400	-3.18069900	-2.50571300
H	-3.98126200	-3.93816200	-1.79010900
H	-4.17866500	-2.64004200	-2.98219000
H	-3.49903200	1.97663100	-2.83403100
H	0.19992400	-2.95613200	0.99547400
C	-1.98274200	2.37028400	-0.66798400
C	-0.91762900	3.17138800	-0.26902500
C	-3.25423500	2.57572100	-0.12753700
C	-1.13630300	4.20111500	0.64374100
H	0.08207600	2.99942600	-0.65993800
C	-3.46680500	3.59675300	0.78778000
H	-4.08519700	1.93974600	-0.42361200
C	-2.40553600	4.41778200	1.16592000
H	-0.30627100	4.82666000	0.94504900
H	-4.45461100	3.75622700	1.20211900
H	-2.57053900	5.22097200	1.87387300
C	-1.10871500	-1.25766000	2.51222200
C	0.18682900	-1.24195900	3.03269000
C	-1.77887200	-0.04868200	2.33480500
C	0.81305700	-0.04060100	3.33249000
H	0.72501700	-2.17363100	3.17373700
C	-1.14880400	1.15842300	2.63083400
H	-2.79686800	-0.04562300	1.96253800
C	0.15059600	1.16638300	3.11914900
H	1.82566200	-0.04637400	3.71946000

H	-1.67899700	2.09026700	2.47150700
H	0.64496000	2.10629500	3.33472700
C	2.35730600	3.68292600	1.10134600
C	2.76352600	2.38217800	0.82397100
C	3.12101800	2.00866900	-0.47546400
C	3.03493600	2.96509100	-1.49036900
C	2.62077700	4.26494400	-1.21727400
C	2.29213600	4.63283900	0.08395400
H	2.10872400	3.96289600	2.11958700
H	2.82778900	1.66456500	1.63284200
H	3.32864400	2.66082800	-2.48710100
H	2.57235800	4.99627400	-2.01621900
H	1.99734800	5.65271300	0.30560800
C	3.63837900	0.63491300	-0.85703700
O	4.16366000	0.53938400	-2.01208700
C	3.44008800	-0.42293900	0.00948100
H	4.35431400	-1.08513100	-2.02342400
H	3.03435300	-0.27157700	0.99942600
C	1.07465600	-0.43207700	-1.00128800
O	1.27865300	-0.48812300	-2.14100700
O	0.55255200	-0.35415200	0.04593500
H	-1.39085600	-0.37765600	-0.24219700
C	4.03805300	-1.77716800	-0.27456100
C	3.08404900	-2.88753400	0.13191200
F	3.63774300	-4.10065600	0.01014900
F	1.95254100	-2.91040100	-0.60025900
F	2.69443000	-2.76884600	1.42249200
O	4.34292300	-1.99457200	-1.62309000
H	4.92815800	-1.95280800	0.35740500

Value of Imaginary Frequency= -185.0 cm^{-1}

ts2'-5-(*R*)

C	3.92403200	1.53613300	1.43226300
C	3.81750000	1.08153600	0.00255500
O	4.89565700	1.05077600	-0.73470000
C	3.05624900	0.17484900	-1.96451700
C	4.51337100	0.66791800	-2.09473700
H	2.40033600	0.67531200	-2.67600000
H	4.60116100	1.56208000	-2.70766900
C	2.59689300	1.23380800	2.08769600
O	1.54970200	1.92592100	1.57618000
C	0.91283000	0.26273100	3.09060200
C	0.41426000	1.54838600	2.39013200
H	0.62501600	0.24677700	4.14253300
H	0.22348900	2.36396300	3.08909200
N	2.75649900	0.68401000	-0.61267800
N	2.38183000	0.36030200	2.97138000
C	5.05780900	0.75371600	2.10756800
H	4.87734600	-0.32054900	2.06128700
H	6.00750600	0.98815600	1.62747400
H	5.10056600	1.04337900	3.15687300
C	4.20717600	3.05193400	1.43532700
H	3.39902900	3.60418800	0.95678600
H	4.29338500	3.38377200	2.47072400
H	5.14701100	3.25648300	0.92205200
H	5.20809400	-0.09800600	-2.42675600
H	-0.43268900	1.39060000	1.72664000
C	2.84294600	-1.32011700	-2.01440100
C	1.71089100	-1.83004200	-2.64205000
C	3.74422500	-2.18725800	-1.39390900
C	1.48691900	-3.20308100	-2.66825000
H	0.99855900	-1.15728000	-3.10728400
C	3.52834500	-3.55847500	-1.43391100
H	4.62078200	-1.79824900	-0.88178000
C	2.40122800	-4.06670700	-2.07703200
H	0.59818900	-3.59033200	-3.15042100
H	4.23504600	-4.23046500	-0.96252600
H	2.23329300	-5.13658100	-2.10626600
C	0.40449400	-0.99073300	2.39296100
C	-0.97223900	-1.22639100	2.36168300
C	1.25438200	-1.85873700	1.71410200
C	-1.49301300	-2.29982300	1.65104800
H	-1.65143400	-0.55440500	2.88015700
C	0.73399700	-2.93333600	0.99565800
H	2.32515000	-1.69578800	1.73795800
C	-0.63649500	-3.15307400	0.95796800
H	-2.56490000	-2.45834500	1.62079200

H	1.40661200	-3.59100600	0.45860800
H	-1.04335100	-3.97589100	0.38230100
C	-5.06260300	-1.39069500	2.23947600
C	-4.47276200	-0.41788800	1.43808700
C	-4.19941100	-0.67691100	0.09383600
C	-4.54732400	-1.91719200	-0.44141400
C	-5.12188600	-2.89681000	0.36059700
C	-5.37886000	-2.63729200	1.70515800
H	-5.28183100	-1.17547000	3.27913700
H	-4.24165100	0.55757200	1.85162000
H	-4.34850800	-2.08856000	-1.49244300
H	-5.37515000	-3.86265800	-0.06168400
H	-5.83303800	-3.39750400	2.33002800
C	-3.52616800	0.32254700	-0.81236300
O	-3.81632300	0.29003600	-2.03645800
C	-2.50715700	1.09993700	-0.26056400
H	-2.45935800	1.23844800	-2.62534000
H	-2.36101900	1.11451800	0.81054700
C	-0.79601400	-0.45464700	-0.98344900
O	-1.34573900	-1.25657700	-1.62049600
O	0.10348400	0.12353400	-0.48121400
H	1.81200700	0.62392800	-0.21933300
C	-1.85661700	2.17330900	-1.08286300
C	-2.63724300	3.47870000	-1.06487600
F	-2.78154800	3.93693600	0.19617600
F	-3.85981500	3.36896200	-1.59123900
F	-2.00266800	4.45050600	-1.74895600
O	-1.66343300	1.78297100	-2.42515900
H	-0.87699100	2.43304700	-0.66136900

Value of Imaginary Frequency= -285.0 cm^{-1}

ts2'-6-(*S*)

C	4.78597100	0.07601100	-0.10291700
C	3.89368400	-1.08741200	0.22482300
O	4.37576600	-2.04866100	0.96171300
C	2.08199500	-2.47207000	0.48742400
C	3.36745400	-3.10002400	1.07893000
H	1.65943800	-3.10225700	-0.29463500
H	3.73079000	-3.94966100	0.50520000
C	3.92687400	1.19544800	-0.64155600
O	3.30065500	0.91715000	-1.81153600
C	2.74043800	3.01885700	-0.92293000
C	2.67540900	2.15973100	-2.21251700
H	3.10440900	4.02337700	-1.14110800
H	3.26868200	2.57779700	-3.02643600
N	2.66439400	-1.26744100	-0.13197400
N	3.73305800	2.31203300	-0.08933800
C	5.51375600	0.51934100	1.17257000
H	4.80763700	0.83635400	1.94009600
H	6.13055700	-0.29433100	1.55222000
H	6.14703700	1.37097900	0.92760000
C	5.78763600	-0.39471000	-1.18043000
H	5.27148300	-0.71154900	-2.08611200
H	6.44562200	0.44031100	-1.42454300
H	6.39169200	-1.21563200	-0.79303000
H	3.27902400	-3.34832500	2.13273800
H	1.66322900	1.94736600	-2.54885100
C	1.02115100	-2.11917600	1.50360700
C	-0.16165800	-2.84871600	1.53741700
C	1.23136800	-1.09515800	2.42915800
C	-1.13817000	-2.55410100	2.48474400
H	-0.33900400	-3.63651000	0.81419500
C	0.25641400	-0.79929500	3.37234700
H	2.15240700	-0.51947900	2.41923200
C	-0.93116900	-1.52865400	3.39897200
H	-2.06730800	-3.10978700	2.48067300
H	0.41939300	0.00358500	4.08115200
H	-1.69511200	-1.29083800	4.12953900
C	1.39745700	3.11455000	-0.22683700
C	0.53849600	4.16292300	-0.55298400
C	0.96015200	2.13064900	0.65811000
C	-0.74037600	4.22111700	-0.01222700
H	0.87159200	4.93350400	-1.24103100
C	-0.32379700	2.18180700	1.19080900
H	1.61814500	1.31267700	0.92880500
C	-1.17623100	3.22910900	0.85894100
H	-1.40268400	5.03617300	-0.27863400

H	-0.66681200	1.39519800	1.85452600
H	-2.17729300	3.26328100	1.26971300
C	-4.09334200	1.73401200	2.45816000
C	-3.59118600	0.80982400	1.54731800
C	-3.70543600	1.03101800	0.17300800
C	-4.34424400	2.18928800	-0.27130500
C	-4.84334500	3.11742100	0.63578600
C	-4.71962200	2.89299900	2.00500900
H	-4.00843300	1.54542500	3.52262500
H	-3.12870000	-0.10312300	1.90635700
H	-4.44288900	2.33246300	-1.34036400
H	-5.33504400	4.01459900	0.27703200
H	-5.11535300	3.61085200	2.71420600
C	-3.21389800	0.04781200	-0.86223300
O	-3.73416100	0.12002100	-2.00869000
C	-2.16569800	-0.81066900	-0.53088000
H	-2.63427600	-0.92035200	-2.85268600
H	-1.76654300	-0.84577700	0.47259300
C	-0.42198700	0.53503100	-1.61493000
O	-0.98537400	1.44543200	-2.06118800
O	0.46995000	-0.19223900	-1.34953500
H	2.11001000	-0.62808700	-0.71392800
C	-1.82369400	-1.93214400	-1.46723100
C	-2.72100400	-3.14960800	-1.28223000
F	-2.33996300	-4.17361300	-2.07069300
F	-4.00624800	-2.91148000	-1.54548900
F	-2.65799800	-3.62018000	-0.01195800
O	-1.87740200	-1.55177800	-2.82319000
H	-0.81184500	-2.30358900	-1.26083500

Value of Imaginary Frequency= -286.6 cm^{-1}

ts2'-6-(*R*)

C	-4.27279900	-0.56168500	0.11991500
C	-3.44767500	0.57984300	0.64178900
O	-3.98092900	1.35296400	1.54746100
C	-1.72616100	1.99495100	1.16543600
C	-3.04717600	2.43788000	1.83817700
H	-1.32496500	2.78328200	0.53310800
H	-3.46658100	3.33998500	1.39721500
C	-3.38838200	-1.47137100	-0.69814000
O	-2.84030200	-0.89287200	-1.79314800
C	-2.14983100	-3.11105700	-1.46106900
C	-2.20542100	-1.97505800	-2.51325400
H	-2.47722600	-4.05750100	-1.89509100
H	-2.84476500	-2.22105200	-3.36220700
N	-2.24102500	0.90889900	0.31788200
N	-3.12921600	-2.67909400	-0.44482500
C	-4.87020800	-1.31913100	1.31355100
H	-4.08822800	-1.70978100	1.96523500
H	-5.52497000	-0.66008000	1.88234300
H	-5.44352100	-2.16343400	0.93325400
C	-5.38449200	0.03283200	-0.77251600
H	-4.96173800	0.57525800	-1.61755900
H	-5.99584300	-0.78727400	-1.15125200
H	-6.01579700	0.69971400	-0.18493500
H	-2.97425100	2.52542700	2.91821300
H	-1.23148300	-1.63489400	-2.85788500
C	-0.67288800	1.51427700	2.13824300
C	0.30189700	2.41854300	2.55701700
C	-0.70823300	0.23233200	2.68467800
C	1.21223800	2.05628700	3.54372000
H	0.35510600	3.40111100	2.10093700
C	0.20387800	-0.12745100	3.67092700
H	-1.43147300	-0.49790100	2.33621000
C	1.15499600	0.78790100	4.11111500
H	1.97214800	2.76018000	3.85902200
H	0.17307600	-1.12529200	4.09248800
H	1.86606500	0.50604200	4.87815900
C	-0.76512800	-3.27481100	-0.85590900
C	0.31019900	-3.51124200	-1.71176800
C	-0.52603300	-3.12230800	0.50771600
C	1.61071600	-3.53959800	-1.22296700
H	0.13784300	-3.63684500	-2.77665500
C	0.77599200	-3.15071700	0.99629300
H	-1.35923600	-2.95445100	1.17930000
C	1.84889800	-3.34276400	0.13278300
H	2.43999900	-3.68337200	-1.90493900

H	0.96041300	-2.99576300	2.05342700
H	2.86423100	-3.32069800	0.51045100
C	3.42743400	-1.18890700	2.30652600
C	2.96085100	-0.32290000	1.32372300
C	3.65652800	-0.17343500	0.12029500
C	4.80675700	-0.93687900	-0.08568200
C	5.27242000	-1.80751700	0.89400700
C	4.58820600	-1.93051900	2.10012500
H	2.87790600	-1.29132300	3.23582400
H	2.04077100	0.22427100	1.49586200
H	5.32295200	-0.81682800	-1.02986100
H	6.17261700	-2.38606100	0.71950600
H	4.95134200	-2.60234900	2.86953500
C	3.24729600	0.78662900	-0.97781300
O	3.90890000	0.75093600	-2.05406100
C	2.14922600	1.61672200	-0.78528100
H	2.71759100	1.60068500	-3.11102400
H	1.69191700	1.73563300	0.18707400
C	0.74683200	-0.27928700	-1.61510400
O	1.26565200	-0.54590500	-2.61673700
O	-0.01894600	-0.28926300	-0.71964000
H	-1.64126900	0.40562500	-0.34641000
C	1.90519800	2.69396700	-1.80860400
C	0.52496800	3.28491900	-1.64289300
F	0.38484600	3.86123200	-0.42170700
F	-0.46636000	2.37056400	-1.73009900
F	0.25032200	4.23058700	-2.54295200
O	1.97543100	2.23986000	-3.13785000
H	2.59072900	3.54915800	-1.66634500

Value of Imaginary Frequency= -267.6 cm^{-1}

im2-1-(*S*)

C	-4.11721300	2.87857800	1.92348700
C	-3.70822400	1.59260900	1.59188200
C	-3.50250400	1.25675000	0.25140200
C	-3.71196700	2.20790300	-0.74958100
C	-4.15202500	3.48189100	-0.41542700
C	-4.35062800	3.81808900	0.92136800
H	-4.26056900	3.14674800	2.96297700
H	-3.49619400	0.86513600	2.36623500
H	-3.53696400	1.92897700	-1.78142800
H	-4.33524200	4.21268700	-1.19368500
H	-4.68801000	4.81382300	1.18402200
C	-3.02121100	-0.09407100	-0.15369200
O	-2.36416500	-0.20806300	-1.18452100
C	-3.32197000	-1.29643600	0.70201400
H	-2.64561200	-2.04293600	-1.59281200
H	-4.11258900	-1.05780300	1.41690300
C	-2.02543800	-1.61095600	1.56549900
O	-1.37685400	-0.59163400	1.89869200
O	-1.80954700	-2.79637500	1.80710000
H	-0.38746600	0.03523700	-0.93120600
C	1.41928000	-1.89188200	0.00342800
C	2.80123400	-1.72346700	-0.59140700
O	2.88940300	-0.75134000	-1.53824600
C	4.93848100	-1.80290600	-1.08027700
C	4.21395300	-0.87843800	-2.09356400
H	5.47279400	-2.60262500	-1.59446900
H	4.12259400	-1.33270000	-3.08112600
C	1.02028100	-0.51339700	0.44727400
O	1.55699100	-0.02395800	1.52360900
C	0.01430800	1.53801800	0.60115100
C	0.92881800	1.25688400	1.81808100
H	-1.02473300	1.55555600	0.92375500
H	0.35841200	1.11471600	2.73091700
N	3.83530000	-2.37897000	-0.29058100
N	0.22624200	0.30153600	-0.16495200
C	0.45383500	-2.41126500	-1.07209800
H	0.42380700	-1.75646900	-1.94572800
H	0.79955300	-3.39218900	-1.39955600
H	-0.54699100	-2.53285200	-0.65223000
C	1.45060000	-2.82522800	1.21926700
H	2.16988500	-2.47516300	1.95806600
H	0.45228900	-2.88052800	1.65862300
H	1.75801400	-3.81437200	0.88062400
H	4.65370500	0.11370800	-2.17173800
H	1.72453300	1.98867500	1.93680000

C	5.90907800	-1.04796300	-0.19436400
C	7.26078600	-1.00619400	-0.53147900
C	5.46409300	-0.33901400	0.92122100
C	8.15661900	-0.26094800	0.22767500
H	7.61544500	-1.56567300	-1.39108800
C	6.35954300	0.40510900	1.68167200
H	4.41888600	-0.38351600	1.20821000
C	7.70674200	0.44780000	1.33646600
H	9.20582100	-0.24083100	-0.04191700
H	6.00599100	0.94644600	2.55122800
H	8.40336600	1.02405800	1.93328300
C	0.35521800	2.77058200	-0.19460900
C	-0.50185100	3.86617300	-0.14701100
C	1.52561300	2.83434700	-0.95176300
C	-0.18888800	5.02702800	-0.84782600
H	-1.41787300	3.80456200	0.43292000
C	1.83434200	3.99265100	-1.65344100
H	2.18444600	1.97181300	-1.00447100
C	0.97837100	5.09053600	-1.60026200
H	-0.85995100	5.87672200	-0.81036100
H	2.74059100	4.04015200	-2.24494000
H	1.22094400	5.99199300	-2.14983800
C	-3.76499200	-2.52209600	-0.10190100
C	-5.17911000	-2.33051100	-0.62626400
F	-5.60617600	-3.38953000	-1.31576600
F	-5.26411800	-1.26345300	-1.44587900
F	-6.05082100	-2.12485700	0.37466700
O	-2.92674300	-2.86671400	-1.17123900
H	-3.78336700	-3.36713900	0.58886200

im2-1-(*R*)

C	-2.36592100	4.40867600	0.15698500
C	-2.72889800	3.06643400	0.11526300
C	-2.18390200	2.22901700	-0.86362900
C	-1.27136900	2.74935400	-1.78740700
C	-0.92127300	4.09151100	-1.74910500
C	-1.47225200	4.92400300	-0.77761400
H	-2.78525100	5.05281700	0.92015300
H	-3.39258400	2.66250700	0.86920900
H	-0.85880000	2.08797800	-2.53966500
H	-0.22333300	4.49001000	-2.47533500
H	-1.20376000	5.97359400	-0.74773600
C	-2.52635400	0.77011000	-0.97272600
O	-1.86316800	0.05014500	-1.69766300
C	-3.65601300	0.20641100	-0.14618800
H	-3.17168500	-2.14049100	-0.01609400
H	-4.37902200	0.98905800	0.07557300
C	-2.98142400	-0.20580100	1.23098600
O	-2.93500300	0.67665800	2.09040900
O	-2.48342200	-1.35870200	1.27447200
H	-0.04123500	-0.18153600	-0.61919100
C	0.55258100	-2.73629300	0.17440100
C	1.77386200	-2.36195600	-0.64602500
O	1.52125700	-1.56893500	-1.71525900
C	3.80729800	-1.99201200	-1.38722500
C	2.80882900	-1.09187700	-2.15821700
H	4.20601600	-2.77414300	-2.04219700
H	2.85496900	-1.19206500	-3.23993600
C	0.28576200	-1.46266100	0.93428000
O	0.40189900	-1.42130000	2.22223600
C	0.11967800	0.78129700	1.37336100
C	0.07661500	-0.06368000	2.66440100
H	-0.78558300	1.38335200	1.31124200
H	-0.93564300	-0.10025800	3.06411300
N	2.97126200	-2.64695600	-0.36711600
N	0.07529400	-0.30902900	0.38383800
C	-0.64490500	-3.07551500	-0.73278700
H	-1.01011200	-2.21749500	-1.29708300
H	-0.34161100	-3.85961300	-1.42818100
H	-1.45813600	-3.44901000	-0.11279600
C	0.86867600	-3.87983600	1.13545100
H	1.74371800	-3.65899500	1.74383900
H	0.01063500	-4.05712700	1.78401500
H	1.06749500	-4.77966800	0.55321100
H	2.89948700	-0.04174000	-1.86755500
H	0.81922700	0.22046500	3.40453600

C	4.97116500	-1.23338800	-0.78579000
C	5.67504800	-0.32252600	-1.57602400
C	5.37446000	-1.44228200	0.53158900
C	6.76359200	0.36982500	-1.05873000
H	5.37535300	-0.15391800	-2.60594500
C	6.46483000	-0.74798800	1.05002500
H	4.83144200	-2.15093900	1.14415200
C	7.16256400	0.15787500	0.25832200
H	7.30093800	1.07288900	-1.68384900
H	6.76892800	-0.91764400	2.07609700
H	8.01125100	0.69559200	0.66339900
C	1.34634400	1.62621500	1.12881000
C	1.20617700	2.99601900	0.93244400
C	2.61095900	1.03793800	1.04008400
C	2.32408300	3.77951400	0.65821500
H	0.21883800	3.44500500	0.97984000
C	3.72585900	1.81837100	0.76231900
H	2.73469400	-0.03494400	1.17603500
C	3.58084600	3.19206100	0.57254400
H	2.20818500	4.84558600	0.50278600
H	4.70271400	1.35418700	0.68921400
H	4.45028800	3.80029000	0.35339500
C	-4.36437300	-0.94748800	-0.88526400
C	-5.75636200	-1.12465700	-0.29385600
F	-6.49345600	-0.00432400	-0.42344200
F	-5.71339100	-1.41983300	1.01259300
F	-6.42659700	-2.10609800	-0.90377900
O	-3.70140500	-2.16990200	-0.84697000
H	-4.52066700	-0.66329400	-1.93180400

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C	-5.91825100	-1.85207200	1.22547600
C	-5.10211000	-0.81388100	0.79345300
C	-4.27526500	-0.99909200	-0.31928100
C	-4.28287600	-2.22106900	-0.99796300
C	-5.10752900	-3.24802500	-0.56948500
C	-5.92339600	-3.06506200	0.54487200
H	-6.55178800	-1.71098500	2.09215900
H	-5.10801500	0.12276500	1.33743100
H	-3.62988600	-2.34762900	-1.85201600
H	-5.10717700	-4.19557800	-1.09437000
H	-6.56476500	-3.87031700	0.88327800
C	-3.36985200	0.06595200	-0.82193500
O	-2.60438900	-0.13343500	-1.74515700
C	-3.42175200	1.44950200	-0.16791300
H	-1.23372700	1.39131000	-1.61635300
H	-4.46636000	1.74581800	-0.06142400
C	-2.86460600	1.41151300	1.26727700
O	-1.64232700	0.93739500	1.43347400
O	-3.53020200	1.77666000	2.19658800
H	-1.13340300	0.67946600	0.62073600
C	2.01016500	1.49582800	-0.01592400
C	3.32505300	1.13331900	0.62773700
O	3.22220400	0.22251400	1.62704500
C	5.43359500	0.91052600	1.21000500
C	4.53842600	0.11491700	2.19890800
H	6.03489800	1.65239000	1.73816300
H	4.51380200	0.56074900	3.19400100
C	1.37023900	0.20204900	-0.45350100
O	2.21200200	-0.64734200	-1.07778600
C	0.01892400	-1.44131200	-1.05976600
C	1.48523600	-1.88017100	-1.23221600
H	-0.43772700	-1.23692500	-2.03360100
H	1.71558800	-2.30107200	-2.20782800
N	4.46346100	1.59952400	0.33994800
N	0.15098200	-0.14987200	-0.35273700
C	1.14733100	2.23916100	1.01045900
H	0.91975000	1.60720900	1.86868300
H	1.69430000	3.12002200	1.35224200
H	0.21562300	2.56425900	0.54936300
C	2.24338400	2.35950600	-1.26363400
H	2.84934200	1.82991400	-1.99892200
H	1.27868400	2.62964400	-1.69708900
H	2.77314400	3.26741300	-0.97563400
H	4.80099600	-0.93937600	2.26651500
H	1.79853800	-2.56095100	-0.43723200

C	6.35218500	0.01904200	0.40089000
C	7.71087800	-0.04828700	0.69766500
C	5.83653800	-0.78120800	-0.62015100
C	8.54814500	-0.90664500	-0.00934900
H	8.11839900	0.57848000	1.48422200
C	6.67186600	-1.63802000	-1.32645500
H	4.78083300	-0.72192900	-0.86617800
C	8.02949800	-1.70385600	-1.02289200
H	9.60460900	-0.94703500	0.22813000
H	6.26513400	-2.25299200	-2.12078800
H	8.67947300	-2.36972200	-1.57789400
C	-0.82532000	-2.47128300	-0.35061400
C	-1.14261400	-3.64897300	-1.03283200
C	-1.25780000	-2.30916400	0.96242700
C	-1.87459200	-4.65114400	-0.41010000
H	-0.81582900	-3.77779400	-2.06071800
C	-2.01115600	-3.30624700	1.57920300
H	-1.00945700	-1.40703700	1.50714000
C	-2.31624500	-4.47835100	0.89953000
H	-2.10971600	-5.56196800	-0.94852500
H	-2.35638700	-3.16174200	2.59607100
H	-2.90098700	-5.25185600	1.38314500
C	-2.72415400	2.47541200	-1.07902700
C	-2.86788800	3.88609100	-0.53549500
F	-2.40708300	4.78295800	-1.40940600
F	-2.19186800	4.05064300	0.60550800
F	-4.15344900	4.17509500	-0.29510300
O	-1.34817700	2.26655100	-1.22163900
H	-3.23664100	2.46716000	-2.04859300

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C	-5.07848000	-3.43005500	0.29414200
C	-4.44020400	-2.21241500	0.49279500
C	-3.85653200	-1.55110300	-0.58992900
C	-3.91571400	-2.11562300	-1.86663600
C	-4.57016400	-3.32289400	-2.06366700
C	-5.15071300	-3.98090200	-0.98201700
H	-5.51655500	-3.95149900	1.13620200
H	-4.34290800	-1.80555000	1.49102100
H	-3.45068200	-1.58980800	-2.69147500
H	-4.62839700	-3.75240300	-3.05630400
H	-5.65786000	-4.92646600	-1.13361000
C	-3.12972200	-0.26405200	-0.42715700
O	-2.30289200	0.07001400	-1.27129000
C	-3.39655500	0.60874100	0.77619200
H	-2.15400300	1.94403600	-0.98682500
H	-4.36391900	0.35096500	1.21272800
C	-2.30857300	0.26563400	1.88213100
O	-1.96380900	-0.93304200	1.91803600
O	-1.91593400	1.21915600	2.56140300
H	-0.36013700	0.27097100	-0.56801800
C	0.65350900	-2.04692500	0.63962700
C	1.96744900	-2.07927900	-0.12880700
O	1.90790000	-1.50826400	-1.35398100
C	4.06267900	-2.25646200	-0.76682900
C	3.22426300	-1.63787700	-1.92262500
H	4.51255900	-3.20159100	-1.08049700
H	3.15241800	-2.28862300	-2.79357500
C	0.57073300	-0.59427900	1.03399800
O	1.15546000	-0.21669800	2.13077300
C	0.57662700	1.69581100	0.85214200
C	1.02693600	1.23672800	2.25326500
H	-0.29252400	2.34800100	0.91248600
H	0.25726000	1.41426900	2.99805200
N	3.07166000	-2.53189100	0.28458900
N	0.15815900	0.38977200	0.29888000
C	-0.49581000	-2.47925200	-0.28078500
H	-0.59815300	-1.83982800	-1.15761800
H	-0.28974100	-3.49352700	-0.62725600
H	-1.42378200	-2.46693000	0.28772400
C	0.71467300	-2.91878000	1.89308600
H	1.58448400	-2.67893300	2.50101900
H	-0.19740100	-2.75326800	2.46726200
H	0.77791200	-3.96422300	1.59095400
H	3.56579700	-0.64623500	-2.21954500
H	2.00248400	1.61885500	2.54217000

C	5.16836600	-1.33435300	-0.28772400
C	6.19162400	-0.99841200	-1.17788600
C	5.18266200	-0.79430000	0.99539900
C	7.20181200	-0.12378500	-0.79841500
H	6.19657000	-1.42577000	-2.17636000
C	6.19192800	0.08849700	1.37438100
H	4.40018600	-1.06602900	1.69442500
C	7.20075400	0.42779300	0.48097500
H	7.98949500	0.12732600	-1.49876600
H	6.18874700	0.50836700	2.37324600
H	7.98474700	1.11344100	0.77862500
C	1.67521200	2.27439500	-0.00835500
C	1.49592600	3.47589800	-0.68389100
C	2.88284300	1.58359000	-0.13477200
C	2.52395100	3.98905600	-1.47315000
H	0.55320200	4.00514600	-0.59301100
C	3.91018000	2.09471900	-0.91427600
H	3.03238400	0.64314700	0.38928200
C	3.72748300	3.30311400	-1.58678000
H	2.38229800	4.92652100	-1.99707400
H	4.84874000	1.55430000	-0.98719000
H	4.52577600	3.70880900	-2.19655400
C	-3.40284400	2.10739900	0.46354400
C	-4.66467400	2.50534000	-0.28376000
F	-5.76760600	2.18532700	0.41090700
F	-4.75385100	1.88541400	-1.47554400
F	-4.70925000	3.81864500	-0.52024200
O	-2.28531900	2.56593900	-0.25692400
H	-3.41237500	2.63425600	1.41866700

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C	-2.06841000	2.77835500	-0.89954600
C	-1.13290800	3.06757800	0.25462800
O	-1.72776800	3.45455400	1.40248900
C	0.63389400	3.50768400	1.50158000
C	-0.65832000	3.70542600	2.33819100
H	1.14700700	4.46119700	1.35071300
H	-0.77098500	4.71958100	2.71725800
C	-1.27028800	1.97029300	-1.90167600
O	-0.80426300	2.63127300	-2.96555900
C	-0.04935600	0.40830600	-2.89437100
C	-0.15791000	1.65361600	-3.80484300
H	-0.38969100	-0.48732500	-3.41640100
H	-0.79993400	1.48609200	-4.67081100
N	0.13014600	3.05765600	0.18947600
N	-0.98484600	0.73061400	-1.80197500
C	-3.31525100	2.00282400	-0.44842800
H	-3.07258400	1.03667000	-0.01269600
H	-3.85381900	2.59710700	0.28965100
H	-3.96575100	1.83714300	-1.30953700
C	-2.48865600	4.13536300	-1.49284600
H	-1.61994900	4.70589000	-1.81922300
H	-3.14929600	3.98117100	-2.34744700
H	-3.02606200	4.70118900	-0.73085300
H	-0.75004100	2.99249800	3.15709900
H	0.80479300	2.05295300	-4.11578800
C	1.62685600	2.52204600	2.08319200
C	2.98146800	2.83881600	2.15221800
C	1.20012200	1.27189200	2.53479600
C	3.89817900	1.92598500	2.66935700
H	3.32322000	3.80615100	1.79914900
C	2.11295500	0.35493700	3.04129800
H	0.15274300	1.00158300	2.48603700
C	3.46594700	0.68109600	3.11374400
H	4.94821600	2.18869200	2.72277800
H	1.75622200	-0.60815500	3.38853600
H	4.17799000	-0.03018100	3.51613300
C	1.36316600	0.16651900	-2.39263300
C	2.32111300	-0.28762100	-3.30340300
C	1.74470900	0.42388100	-1.07908300
C	3.64165300	-0.46276700	-2.91164500
H	2.02982100	-0.49983900	-4.32849800
C	3.06671600	0.23246000	-0.68099900
H	1.02764900	0.80485100	-0.36356900
C	4.01742400	-0.20227000	-1.59500100
H	4.37650900	-0.80789900	-3.63008300

H	3.34101800	0.43482500	0.34874000
H	5.04587400	-0.34712400	-1.28478700
C	2.95903900	-3.10590200	1.36164700
C	1.62617400	-2.83331800	1.07817700
C	1.18955300	-2.81659300	-0.24973700
C	2.08783400	-3.09477600	-1.28351900
C	3.40919400	-3.39038200	-0.99272200
C	3.84745200	-3.38885000	0.32974500
H	3.30053200	-3.10415000	2.38961800
H	0.94368100	-2.62468800	1.89296800
H	1.73305200	-3.06282100	-2.30586400
H	4.10416600	-3.60309500	-1.79590400
H	4.88436200	-3.60850600	0.55556000
C	-0.21307400	-2.49519200	-0.61876000
O	-0.54860700	-2.33786600	-1.77558600
C	-1.26625700	-2.39527300	0.49028800
H	-2.36802700	-1.27223900	-1.62488300
H	-1.14619800	-3.24884900	1.15955300
C	-1.06159000	-1.15180500	1.36960400
O	-0.90319600	-1.24967400	2.55885200
O	-1.06562700	0.02148800	0.77068700
H	-1.11917800	0.04599400	-0.23190900
C	-2.67087500	-2.45930200	-0.13957700
C	-3.74743800	-2.55971200	0.92661300
F	-4.94514200	-2.77199300	0.37772800
F	-3.83045100	-1.44514800	1.65881600
F	-3.49788900	-3.57845500	1.76134600
O	-3.00636900	-1.33751200	-0.90229600
H	-2.73313800	-3.38424700	-0.72550800

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C	0.51283500	-3.66920200	0.06730400
C	1.42099500	-2.86769900	-0.84391500
O	1.21747000	-3.01044000	-2.16113500
C	3.05485300	-1.64839400	-1.65526800
C	2.03683300	-1.98219400	-2.76704800
H	3.97368400	-2.23136300	-1.78253900
H	2.48428600	-2.38941800	-3.67040500
C	0.26259300	-2.82213200	1.28801400
O	0.55658100	-3.29456400	2.47525700
C	-0.33332700	-1.09217300	2.63251700
C	0.14538900	-2.31159300	3.46486400
H	-1.36635400	-0.83725700	2.87046700
H	-0.64855500	-2.76442200	4.05506900
N	2.37970700	-2.14884900	-0.43527700
N	-0.27288900	-1.65234000	1.27777000
C	-0.84551900	-3.96781500	-0.59157300
H	-1.35658800	-3.04676000	-0.86830300
H	-0.67644900	-4.56679100	-1.48577200
H	-1.47192300	-4.53251100	0.10190800
C	1.23857400	-4.96909400	0.44466100
H	2.18102400	-4.75498300	0.94804200
H	0.61311200	-5.57971600	1.09698400
H	1.44341700	-5.52835900	-0.46928100
H	1.37711500	-1.14172700	-2.99474300
H	1.00997300	-2.09068800	4.08595900
C	3.42757700	-0.18812300	-1.56255200
C	4.75329800	0.21375600	-1.70987800
C	2.44816300	0.77589800	-1.31479800
C	5.10129400	1.55882600	-1.61476300
H	5.52028300	-0.53060400	-1.89748400
C	2.79481400	2.11687800	-1.21008300
H	1.41747600	0.46280100	-1.18447500
C	4.12185900	2.51288100	-1.36302000
H	6.13605700	1.85807500	-1.73387900
H	2.02611600	2.85075200	-0.99860700
H	4.38989700	3.56020400	-1.28432300
C	0.53262500	0.13647700	2.79679500
C	0.23926400	1.02879900	3.82824200
C	1.63571300	0.36149900	1.97721500
C	1.05137300	2.13509500	4.04733100
H	-0.63380400	0.86503800	4.45199100
C	2.44003100	1.47871700	2.19144500
H	1.87581900	-0.32911100	1.17387000
C	2.15399900	2.36184600	3.22625900
H	0.81828700	2.82448900	4.85022400

H	3.28771000	1.65237500	1.53858200
H	2.78439500	3.22757900	3.39172800
C	-0.15429400	4.33556700	-1.61242600
C	-0.85059400	3.13901500	-1.48475300
C	-1.02468700	2.56709600	-0.21962600
C	-0.45652800	3.17842800	0.90180900
C	0.24671500	4.36614500	0.76779600
C	0.38345700	4.95478700	-0.48797400
H	-0.02499400	4.77863200	-2.59199100
H	-1.23093500	2.65148300	-2.37387200
H	-0.57763100	2.70690700	1.86954500
H	0.68620200	4.83268900	1.64139700
H	0.92233400	5.88928700	-0.59261500
C	-1.81446200	1.31848500	-0.00546400
O	-1.95956300	0.86431600	1.11770800
C	-2.33754100	0.59351300	-1.22673500
H	-2.82611400	-0.78217000	0.83959200
H	-2.73465200	1.29739100	-1.95584800
C	-1.09672900	-0.09718500	-1.87828100
O	-0.88834600	0.07994700	-3.06653600
O	-0.39807200	-0.79077900	-1.07028800
H	-0.47131700	-1.13890300	0.30809300
C	-3.41795000	-0.46475400	-0.94485800
C	-4.77234100	0.19249300	-0.70956700
F	-4.76927700	0.98395800	0.37343900
F	-5.72946400	-0.72110600	-0.53061400
F	-5.13187000	0.95153200	-1.75634900
O	-3.13367900	-1.34092700	0.11033000
H	-3.54490500	-1.06951500	-1.84777100

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C	3.46231900	1.42254400	0.95990800
C	2.43835900	0.67821000	1.80266800
O	1.47219800	1.39868100	2.40249200
C	1.32395500	-0.92945400	2.81892200
C	0.72629600	0.45100700	3.21055700
H	1.69555000	-1.45356000	3.70152800
H	0.89962900	0.70449500	4.25593800
C	3.41746000	0.74322400	-0.38635700
O	4.51057100	0.20877200	-0.86788800
C	2.67053200	-0.37324900	-2.23585800
C	4.20703000	-0.31288300	-2.19938500
H	2.25425300	0.02419400	-3.15720900
H	4.62215900	0.39617600	-2.91422100
N	2.47438300	-0.57477300	1.96642400
N	2.38260200	0.58041800	-1.13915900
C	3.15911800	2.92147800	0.80712000
H	2.17186700	3.09669600	0.38604600
H	3.20451900	3.38394700	1.79347700
H	3.92099000	3.38017100	0.17410800
C	4.84436900	1.22088900	1.60230100
H	5.07737000	0.16194100	1.70042400
H	5.61456300	1.70929500	1.00447000
H	4.83119700	1.67353100	2.59464000
H	-0.32698900	0.55166500	2.95680400
H	4.68744500	-1.28274500	-2.28565500
C	0.34531600	-1.82990400	2.09745000
C	-0.13463500	-2.97965000	2.71701400
C	-0.12238800	-1.49698500	0.82443000
C	-1.08166700	-3.78194100	2.08255000
H	0.23070300	-3.24916400	3.70290300
C	-1.06979700	-2.28900100	0.18981500
H	0.24882200	-0.60691200	0.32339900
C	-1.55203600	-3.43362100	0.82337900
H	-1.44965700	-4.67403800	2.57611800
H	-1.43242700	-2.01118600	-0.79399600
H	-2.29554800	-4.04853600	0.32943200
C	2.09294400	-1.74065300	-1.93751400
C	1.04739500	-2.24075800	-2.70941400
C	2.61292900	-2.50912800	-0.89403000
C	0.54994700	-3.51526800	-2.46068400
H	0.59382800	-1.61209500	-3.46510800
C	2.10527200	-3.77695300	-0.63995600
H	3.39552000	-2.11378900	-0.25337500
C	1.08083100	-4.28570900	-1.43202200
H	-0.27037800	-3.89368000	-3.05868400

H	2.50124400	-4.36055800	0.18230400
H	0.68015600	-5.27208400	-1.23002000
C	-5.55054000	-0.88908500	-0.86663300
C	-4.41663900	-0.08903200	-0.94275800
C	-3.56958200	0.02549200	0.16083200
C	-3.86174300	-0.68155200	1.33167500
C	-4.98758600	-1.48672400	1.40187600
C	-5.83729900	-1.58612300	0.30213800
H	-6.20478400	-0.97590500	-1.72534600
H	-4.17632800	0.40758000	-1.87163300
H	-3.18031100	-0.60070200	2.16981100
H	-5.20214800	-2.04040600	2.30789500
H	-6.71977500	-2.21324200	0.35463200
C	-2.34809100	0.88156600	0.16398000
O	-1.74342000	1.05584100	1.21291600
C	-1.85030700	1.50271500	-1.12325800
H	-0.16436800	1.94698400	0.77037700
H	-2.70278200	1.89078600	-1.68488500
C	-1.18963600	0.39283800	-2.07385800
O	-1.93944000	-0.48687400	-2.49066100
O	0.02715600	0.57420200	-2.29802100
H	1.42406900	0.94445600	-0.99668500
C	-0.84083400	2.62986300	-0.90455700
C	-1.47123300	3.92436900	-0.41875800
F	-0.56008800	4.90571400	-0.35797200
F	-2.02380400	3.82815800	0.79627300
F	-2.43414200	4.32860800	-1.26419400
O	0.22754700	2.28262500	-0.05394900
H	-0.40223100	2.86975100	-1.87385000

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C	1.36511100	-3.27393900	-0.03667900
C	2.64741700	-2.55317500	-0.39275900
O	3.25260500	-2.98247500	-1.51533600
C	4.36147300	-1.16743400	-0.47393100
C	4.41667700	-2.14053800	-1.68402300
H	5.22635900	-1.30754300	0.17761200
H	5.29743900	-2.77985000	-1.67607600
C	0.85325000	-2.54891100	1.17659800
O	1.43638300	-2.73881000	2.32733100
C	-0.19134800	-0.99763400	2.50472400
C	0.87435700	-1.79832300	3.29211100
H	-1.19579700	-1.13417600	2.89756200
H	0.45465500	-2.38642700	4.10404100
N	3.15677200	-1.59704900	0.25871300
N	-0.10428600	-1.69008800	1.20074900
C	0.37652900	-3.16183700	-1.20636900
H	0.21986000	-2.12110300	-1.49843100
H	0.78399800	-3.70720700	-2.05665700
H	-0.59136700	-3.58362100	-0.93297700
C	1.66538800	-4.74183900	0.30880900
H	2.36004400	-4.81556300	1.14540500
H	0.73960800	-5.25935600	0.56504900
H	2.10483800	-5.22290400	-0.56455300
H	4.33187900	-1.63501600	-2.64513300
H	1.69546700	-1.17838300	3.64523100
C	4.26596900	0.29793800	-0.84144500
C	5.15522200	1.22204200	-0.29952000
C	3.27485100	0.74132700	-1.71882700
C	5.06969100	2.57039600	-0.63741900
H	5.92219800	0.88527800	0.38978400
C	3.19873200	2.08329100	-2.07155600
H	2.55893700	0.03423600	-2.12945200
C	4.09553500	3.00158700	-1.52997700
H	5.76865800	3.27904000	-0.20963700
H	2.44136100	2.41519900	-2.77247700
H	4.03621000	4.04724600	-1.80803400
C	0.10167000	0.47670100	2.33838700
C	-0.84427900	1.42064700	2.72469000
C	1.31571300	0.88888900	1.78023700
C	-0.56378300	2.77909200	2.58159400
H	-1.80875600	1.09845500	3.10175800
C	1.58747800	2.24160800	1.63450000
H	2.03990800	0.15361400	1.43913500
C	0.65012100	3.18919100	2.04704200
H	-1.30849400	3.51067100	2.87110100

H	2.52316500	2.55291200	1.18034700
H	0.85690900	4.24559700	1.92196800
C	-2.03455300	4.59716100	-0.42383400
C	-2.34587400	3.24251300	-0.39541900
C	-1.37489300	2.30501900	-0.75672500
C	-0.10328200	2.73341000	-1.14190400
C	0.19677100	4.08574800	-1.18956300
C	-0.77138300	5.01999700	-0.82853000
H	-2.78146900	5.32481000	-0.13059200
H	-3.31649400	2.91351600	-0.04511800
H	0.64116300	1.98439200	-1.37760000
H	1.18690900	4.41149800	-1.48885500
H	-0.54037700	6.07869800	-0.85777100
C	-1.62263700	0.83544500	-0.73670100
O	-0.68965600	0.05986000	-0.88402200
C	-3.02581300	0.30723900	-0.54870800
H	-2.75479700	-1.82053100	0.51044700
H	-3.73649900	0.99243600	-1.00950900
C	-3.33291200	0.30338400	1.01153600
O	-3.87906700	1.29232200	1.47640500
O	-2.92360900	-0.72912100	1.61787600
H	-0.65383000	-1.40398400	0.38010200
C	-3.14318800	-1.08789200	-1.19923600
C	-4.60382600	-1.40143400	-1.48282600
F	-5.14998200	-0.48772200	-2.30591200
F	-5.34160100	-1.42263000	-0.36580200
F	-4.74044300	-2.59342200	-2.07408200
O	-2.59929100	-2.12292300	-0.43253800
H	-2.64487300	-1.07685800	-2.17411000

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C	0.27259600	3.45344000	0.20416900
C	1.66260500	2.93861600	-0.03457500
O	2.64431300	3.70993200	0.37595300
C	3.51594900	1.64748100	-0.39944200
C	3.90973400	3.06965700	0.05405900
H	3.93020400	1.40431300	-1.37683600
H	4.37169700	3.65586800	-0.73756700
C	-0.76233400	2.74167400	-0.63318700
O	-0.33796000	2.26693700	-1.82215800
C	-2.65896300	2.05704000	-1.50685100
C	-1.49007000	1.60269400	-2.40612700
H	-3.22790000	2.85366600	-1.99903700
H	-1.58068100	1.93814600	-3.43676300
N	2.05856500	1.81796200	-0.52948500
N	-1.98648300	2.67983100	-0.34017500
C	-0.02643500	3.25956900	1.70324100
H	0.00263900	2.19990100	1.95979200
H	0.69296000	3.81892600	2.30324300
H	-1.03033600	3.63664500	1.89517500
C	0.22464800	4.95018300	-0.17088600
H	0.44345000	5.09442300	-1.23051800
H	-0.78244300	5.31306500	0.03192700
H	0.93977200	5.51727000	0.42377700
H	4.52245000	3.07989100	0.95152400
H	-1.28724800	0.53395400	-2.37489600
C	3.83528300	0.55151300	0.58790300
C	4.68665200	-0.48452800	0.22428300
C	3.23773100	0.54974100	1.84989600
C	4.93152100	-1.53005000	1.11035000
H	5.12406100	-0.49987500	-0.76724700
C	3.48128300	-0.49285800	2.73321300
H	2.55521700	1.34517300	2.13525300
C	4.32601000	-1.53742200	2.36071600
H	5.57430200	-2.34845500	0.81095800
H	3.00329000	-0.49985900	3.70496500
H	4.50227500	-2.35966800	3.04322700
C	-3.64212100	0.99603500	-1.05402100
C	-3.50590300	-0.35636900	-1.34663400
C	-4.72502700	1.41532000	-0.27405000
C	-4.41246300	-1.28367900	-0.83185500
H	-2.70110100	-0.72779100	-1.96842300
C	-5.63946200	0.49786800	0.21881500
H	-4.83185300	2.47035600	-0.04301100
C	-5.47763200	-0.86131400	-0.05086300
H	-4.24975700	-2.33396600	-1.04318300

H	-6.47208500	0.83702000	0.82488100
H	-6.17729900	-1.58328200	0.35425600
C	-3.27593800	-2.71781100	2.44564000
C	-2.16587200	-2.51149300	1.63485300
C	-1.70947400	-1.21317400	1.39668800
C	-2.39745700	-0.12547700	1.94539100
C	-3.50785000	-0.33619500	2.74711600
C	-3.94068800	-1.63449200	3.00844500
H	-3.62646300	-3.72624300	2.62874000
H	-1.68935700	-3.35783900	1.16047300
H	-2.06826600	0.87838300	1.70110100
H	-4.04873500	0.50986000	3.15379300
H	-4.80926000	-1.79945000	3.63580800
C	-0.50290100	-0.92284500	0.56892800
O	-0.04821300	0.21031200	0.51984900
C	0.13529900	-2.03787300	-0.22769400
H	0.83075300	-0.86511100	-2.16057100
H	0.13231600	-2.96132700	0.34948900
C	-0.79483400	-2.26955800	-1.48995200
O	-0.52921700	-1.51056800	-2.46882400
O	-1.69201600	-3.09050000	-1.37783600
H	1.46860500	1.02700700	-0.84828900
C	1.57605800	-1.66649400	-0.60199400
C	2.32418500	-2.90822100	-1.06650900
F	3.55616800	-2.61794600	-1.50615300
F	1.69798100	-3.54904500	-2.05961100
F	2.46385500	-3.78251600	-0.05198800
O	1.65245400	-0.67513800	-1.59226400
H	2.10250700	-1.32365800	0.29319800

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C	0.51294000	-3.66920900	0.06698400
C	0.26265400	-2.82229800	1.28780200
O	0.55681400	-3.29479600	2.47497800
C	-0.33359700	-1.09264200	2.63249000
C	0.14511300	-2.31215700	3.46471300
H	-1.36663900	-0.83778000	2.87042600
H	-0.64894100	-2.76530700	4.05453000
C	1.42102200	-2.86754800	-0.84417400
O	1.21737200	-3.01005400	-2.16141200
C	3.05480000	-1.64809900	-1.65548900
C	2.03665100	-1.98166100	-2.76720400
H	3.97360600	-2.23106300	-1.78297100
H	2.48399300	-2.38868700	-3.67070500
N	-0.27306500	-1.65261100	1.27768600
N	2.37977700	-2.14877300	-0.43550400
C	1.23875600	-4.96909900	0.44417400
H	2.18119800	-4.75498200	0.94756900
H	0.61334600	-5.57983800	1.09643800
H	1.44363100	-5.52825300	-0.46982900
C	-0.84542300	-3.96783300	-0.59189100
H	-1.35660500	-3.04679100	-0.86845500
H	-0.67633300	-4.56665000	-1.48619300
H	-1.47174300	-4.53270800	0.10152100
H	1.00944700	-2.09123300	4.08614300
H	1.37691300	-1.14113400	-2.99463100
C	0.53233200	0.13599200	2.79705300
C	0.23881300	1.02821600	3.82853400
C	1.63558300	0.36106800	1.97770200
C	1.05090600	2.13448400	4.04787500
H	-0.63436100	0.86443100	4.45212900
C	2.43990300	1.47822700	2.19220500
H	1.87584300	-0.32951000	1.17437600
C	2.15369600	2.36127700	3.22704200
H	0.81767400	2.82380200	4.85078900
H	3.28774600	1.65189400	1.53956000
H	2.78409500	3.22696900	3.39270500
C	3.42753300	-0.18785400	-1.56256100
C	4.75313700	0.21414900	-1.71061500
C	2.44821300	0.77603900	-1.31397300
C	5.10109500	1.55921900	-1.61539100
H	5.52006000	-0.53011200	-1.89887200
C	2.79483900	2.11701600	-1.20911800
H	1.41761900	0.46284400	-1.18313000
C	4.12175600	2.51314900	-1.36278600
H	6.13576100	1.85857200	-1.73509900

H	2.02621300	2.85077000	-0.99696600
H	4.38976300	3.56046600	-1.28396900
C	-0.15401600	4.33567800	-1.61219700
C	-0.85043200	3.13918500	-1.48461500
C	-1.02459900	2.56718200	-0.21953900
C	-0.45631700	3.17833300	0.90194000
C	0.24703200	4.36599500	0.76802000
C	0.38379400	4.95475000	-0.48769900
H	-0.02466700	4.77879900	-2.59173000
H	-1.23077300	2.65174300	-2.37378100
H	-0.57737800	2.70670400	1.86963100
H	0.68662900	4.83240800	1.64163100
H	0.92275500	5.88921200	-0.59225700
C	-1.81440300	1.31856800	-0.00547500
O	-1.95962000	0.86438700	1.11767300
C	-2.33739200	0.59361500	-1.22679300
H	-2.82635800	-0.78212600	0.83947900
H	-2.73438300	1.29749000	-1.95597200
C	-1.09652500	-0.09716000	-1.87818700
O	-0.39800700	-0.79079700	-1.07009300
O	-0.88793900	0.07997100	-3.06639300
H	-0.47176100	-1.13913900	0.30790000
C	-3.41790100	-0.46457500	-0.94506000
C	-4.77226100	0.19274600	-0.70984700
F	-5.13160000	0.95194700	-1.75657200
F	-4.76927700	0.98405400	0.37325700
F	-5.72947900	-0.72081900	-0.53114700
O	-3.13380800	-1.34083300	0.11013200
H	-3.54482900	-1.06930200	-1.84799800

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C	-0.33188500	3.24352000	0.07923800
C	0.52712900	2.42573900	-0.84910500
O	0.86971200	2.94373800	-1.98994000
C	1.73682300	0.72824100	-1.80678400
C	1.61425200	1.94674400	-2.75421200
H	1.16589400	-0.10525600	-2.21241800
H	1.00931900	1.71594700	-3.62461600
C	-0.35780500	2.52855400	1.41508300
O	-1.54466900	2.11703800	1.88954800
C	0.29619500	1.39516900	3.18463100
C	-1.25115700	1.31851200	3.06056100
H	0.58360100	1.87506500	4.12466600
H	-1.77630300	1.76113400	3.90454900
N	1.00783000	1.24538000	-0.64391800
N	0.69221800	2.26120100	2.06702000
C	0.33404500	4.62247800	0.25414600
H	1.33310800	4.51876400	0.67793100
H	0.38993500	5.13212700	-0.70746600
H	-0.27505500	5.21820200	0.93487400
C	-1.72545800	3.38315200	-0.55390700
H	-2.23432900	2.42687800	-0.64896000
H	-2.33056800	4.03030200	0.08235500
H	-1.63508000	3.83046100	-1.54353300
H	2.57119800	2.39393000	-3.01545800
H	-1.61547300	0.30959900	2.86651700
C	3.12553600	0.29388300	-1.40798000
C	3.54260900	-1.00214700	-1.69147200
C	3.97509300	1.15699500	-0.71360600
C	4.80411400	-1.43566300	-1.29235000
H	2.87111000	-1.67535100	-2.21356500
C	5.23173600	0.72442700	-0.31043700
H	3.64665300	2.16420900	-0.47169900
C	5.64821400	-0.57381500	-0.60188000
H	5.12161100	-2.44732700	-1.51538400
H	5.88581500	1.39569000	0.23259100
H	6.62866900	-0.91012400	-0.28670300
C	1.02509200	0.06298200	3.09042700
C	0.55576800	-1.05551300	3.77929900
C	2.20477500	-0.04770200	2.35049500
C	1.25381000	-2.25845600	3.73269000
H	-0.35665500	-0.99212500	4.36346400
C	2.89782600	-1.25357100	2.29291000
H	2.58537700	0.81839300	1.82300200
C	2.42843700	-2.36081300	2.99190400
H	0.87780300	-3.11742200	4.27555800

H	3.80274600	-1.31791900	1.69718100
H	2.96986900	-3.29911100	2.95991900
C	0.61473300	-3.46038100	-2.53551900
C	-0.29642500	-2.45809100	-2.22718600
C	-0.35487000	-1.94684400	-0.92715000
C	0.51590800	-2.43233500	0.05075900
C	1.41745600	-3.44361900	-0.25870100
C	1.46175000	-3.96312900	-1.54879800
H	0.66168100	-3.85358900	-3.54376000
H	-0.93746100	-2.05178100	-2.99985900
H	0.45887200	-2.02551300	1.05446200
H	2.07979300	-3.82504000	0.50909300
H	2.15954800	-4.75666800	-1.79017500
C	-1.33107500	-0.89087400	-0.52563200
O	-1.11128600	-0.22546400	0.48001100
C	-2.55405800	-0.64436500	-1.36192100
H	-2.79619700	0.74311800	0.72991800
H	-2.78411900	-1.52378900	-1.96705800
C	-2.21072200	0.52388600	-2.39749200
O	-3.17571400	1.09384500	-2.89039300
O	-0.98167300	0.70121500	-2.57657900
H	0.78205100	0.68061900	0.17261000
C	-3.80684000	-0.29218200	-0.56076800
C	-4.32390100	-1.49356400	0.21369100
F	-5.46387400	-1.21867900	0.85368600
F	-3.44461200	-1.91560100	1.14314000
F	-4.56415400	-2.53723400	-0.59820100
O	-3.67091900	0.79044800	0.31826800
H	-4.57623000	-0.02974800	-1.2903110

im2-6-(*R*)

C	0.12997600	2.81635100	-1.84245400
C	-0.49658600	2.53660600	-0.50816200
O	-0.61346400	3.50685200	0.34510800
C	-1.59966000	1.52838200	1.23192700
C	-1.12716100	2.95515400	1.59641400
H	-1.09125400	0.80836600	1.87348300
H	-0.28597200	2.91645000	2.28653900
C	0.45893400	1.48783700	-2.49635100
O	1.75479700	1.18508000	-2.62455900
C	0.32718200	-0.45746100	-3.50981000
C	1.79839600	-0.17447600	-3.12417100
H	0.20622100	-0.37855300	-4.59705400
H	2.48288000	-0.19355500	-3.96942900
N	-1.04891400	1.42892400	-0.13161400
N	-0.41516500	0.67458700	-2.92072400
C	-0.94829300	3.54036200	-2.68070100
H	-1.81799800	2.90025400	-2.82569500
H	-1.24227000	4.46668700	-2.18510200
H	-0.52559000	3.78262300	-3.65650600
C	1.36851200	3.70247100	-1.66305000
H	2.08624700	3.23584200	-0.99191800
H	1.82844900	3.86229900	-2.63832200
H	1.06853000	4.66463300	-1.24820700
H	-1.92562500	3.60837800	1.93824100
H	2.16594600	-0.79126400	-2.30797500
C	-3.08636700	1.27337200	1.23386700
C	-3.58121000	0.12770900	1.84849300
C	-3.96315900	2.15090100	0.59460700
C	-4.94716400	-0.13950200	1.83161900
H	-2.89519100	-0.55696400	2.33697400
C	-5.32575400	1.88531500	0.57905300
H	-3.58083900	3.04263800	0.10524800
C	-5.81889200	0.73884400	1.19928400
H	-5.32601100	-1.03347400	2.31248800
H	-6.00442200	2.56946300	0.08447300
H	-6.88246200	0.53338100	1.18679100
C	-0.25109400	-1.79658600	-3.09937600
C	0.55520000	-2.91438000	-2.89621500
C	-1.63561900	-1.93488700	-2.98765400
C	-0.01005900	-4.14693800	-2.58046000
H	1.63327500	-2.83253200	-2.97884400
C	-2.20228300	-3.16697700	-2.67836700
H	-2.26507600	-1.06619500	-3.13968200
C	-1.39051600	-4.27901600	-2.47277000
H	0.63145600	-5.00513100	-2.41889500

H	-3.27931900	-3.25708600	-2.59553100
H	-1.82899900	-5.23934900	-2.22888300
C	-1.31760300	-2.47031500	3.53478900
C	-0.30622500	-1.75690100	2.89928200
C	-0.20159800	-1.79998400	1.50565000
C	-1.11726900	-2.54640100	0.75868900
C	-2.11535800	-3.26770300	1.39902100
C	-2.21343300	-3.23280100	2.78872500
H	-1.40562200	-2.43083800	4.61364200
H	0.36687200	-1.13420800	3.47730900
H	-1.02073600	-2.56098500	-0.32115400
H	-2.81251300	-3.85741200	0.81531500
H	-2.98999800	-3.79727500	3.29174400
C	0.85077400	-1.05216600	0.74463000
O	0.69839000	-0.84532900	-0.44465900
C	2.04427900	-0.49720900	1.47922200
H	2.80356100	0.93649300	-0.31159600
H	2.18409000	-1.00615800	2.42999000
C	1.60660300	0.99147600	1.77422500
O	1.11649500	1.20100700	2.88649100
O	1.70638300	1.77502500	0.79686200
H	-1.00186600	0.57732500	-0.69028900
C	3.33432900	-0.62802600	0.65059000
C	4.53166900	-0.33417600	1.54563100
F	4.58599500	-1.18694700	2.58644500
F	4.49557000	0.90508700	2.04893900
F	5.68138700	-0.46102200	0.87538900
O	3.40593400	0.18207100	-0.47866400
H	3.45461900	-1.67339800	0.34055300

ts2-1-(*S*)

C	-4.09071800	3.15702800	1.18865400
C	-3.79614900	1.79898700	1.13745400
C	-3.28165000	1.23870100	-0.03528100
C	-3.05458800	2.05634800	-1.14531900
C	-3.37780700	3.40617100	-1.10042700
C	-3.89690500	3.95802900	0.06647200
H	-4.48307400	3.58739800	2.10245300
H	-3.95904300	1.17482300	2.01006300
H	-2.64186300	1.61201100	-2.04300400
H	-3.21400600	4.02953100	-1.97138100
H	-4.14184400	5.01316600	0.10540900
C	-2.99861500	-0.22450300	-0.17591200
O	-2.02839000	-0.56433100	-0.92859300
C	-3.74700800	-1.13926400	0.57549800
H	-2.26939500	-2.36375400	-0.89665000
H	-4.64783400	-0.76474700	1.04436900
C	-2.48116300	-1.24110300	2.22915200
O	-1.36153900	-1.33799000	1.82841500
O	-3.22800800	-1.19801300	3.14868000
H	-0.64414800	-0.07740300	-0.38087500
C	1.57494100	-1.79608700	0.20844500
C	2.89884700	-1.62764000	-0.50127200
O	2.89605900	-0.66897900	-1.46181800
C	4.98384200	-1.71657300	-1.18114000
C	4.17820400	-0.77224900	-2.11428900
H	5.44628200	-2.52420300	-1.75006500
H	4.01796700	-1.19916600	-3.10484100
C	1.17133100	-0.41012500	0.62067500
O	1.91375700	0.18079100	1.52683000
C	0.07677100	1.55254600	0.93854900
C	1.40544100	1.52493900	1.72860400
H	-0.78826500	1.46364500	1.60211800
H	1.28702700	1.67910800	2.79728500
N	3.95707600	-2.27803500	-0.28418900
N	0.18704400	0.29532800	0.18556800
C	0.54608300	-2.40834200	-0.74698200
H	0.36929100	-1.77436300	-1.61734500
H	0.92036100	-3.37452300	-1.08694900
H	-0.38831200	-2.56286700	-0.20809100
C	1.73725500	-2.65947300	1.46656600
H	2.50315600	-2.25378600	2.12578900
H	0.78180900	-2.71153000	1.98956600
H	2.04097000	-3.65961200	1.15968300
H	4.60468100	0.22540000	-2.19641200
H	2.14008200	2.21492800	1.31525900

C	6.05598900	-0.98939300	-0.39580600
C	7.37853500	-1.02042000	-0.83269300
C	5.72939700	-0.23689500	0.73251500
C	8.36310300	-0.30466500	-0.15900000
H	7.64076200	-1.61312300	-1.70306500
C	6.71286900	0.47745500	1.40720000
H	4.70621200	-0.22282700	1.09329400
C	8.03143000	0.44678800	0.96281900
H	9.38883800	-0.34067400	-0.50605300
H	6.45165400	1.05390700	2.28682300
H	8.79709100	1.00038500	1.49278500
C	-0.05710300	2.78105700	0.07493400
C	-0.53721800	3.95022100	0.65878400
C	0.34601700	2.78474700	-1.25853200
C	-0.61043900	5.12175900	-0.08506500
H	-0.87404600	3.93936600	1.69057300
C	0.25360100	3.95378400	-2.00570300
H	0.72152000	1.87504700	-1.71450600
C	-0.21961300	5.12400300	-1.41978600
H	-0.98990900	6.02738800	0.37284800
H	0.55460200	3.95063200	-3.04634900
H	-0.28696300	6.03402900	-2.00371800
C	-3.83174500	-2.59714100	0.17236100
C	-4.99093000	-2.79154400	-0.80122000
F	-5.14915000	-4.08042000	-1.12746300
F	-4.80364000	-2.11429700	-1.94269400
F	-6.15318300	-2.37324600	-0.27231700
O	-2.67324300	-3.11304100	-0.42460000
H	-4.07978400	-3.21796500	1.04075900

Value of Imaginary Frequency= -354.2 cm^{-1}

ts2-1-(*R*)

C	-2.38875300	4.45962100	0.01907600
C	-2.80366100	3.13298900	0.00776800
C	-2.22562600	2.22349400	-0.88582700
C	-1.21960500	2.66447200	-1.74979500
C	-0.82079900	3.99628300	-1.74914900
C	-1.40705800	4.89813700	-0.86749900
H	-2.83922500	5.15514200	0.71719200
H	-3.56035600	2.80015400	0.70758900
H	-0.77513500	1.95193800	-2.43385300
H	-0.05102600	4.32846300	-2.43559000
H	-1.09966100	5.93741700	-0.86634200
C	-2.66351900	0.78922600	-0.99742800
O	-1.84768300	-0.02627900	-1.53597500
C	-3.90522100	0.39230500	-0.47961500
H	-2.83155800	-1.56539900	-1.40644300
H	-4.61207600	1.17318300	-0.22880100
C	-3.11566500	-0.04537300	1.43917800
O	-3.52784900	0.81910500	2.14043900
O	-2.45227100	-1.02434000	1.31452900
H	-0.46984400	-0.19606500	-0.61564200
C	0.57238000	-2.72540100	0.08304500
C	1.86671000	-2.42341900	-0.65671700
O	1.72634400	-1.70400800	-1.78998800
C	3.96845500	-2.12360100	-1.21811600
C	3.05769600	-1.29913300	-2.16710800
H	4.44153700	-2.94999800	-1.75856500
H	3.19557600	-1.52223200	-3.22270000
C	0.35507400	-1.43781800	0.83356400
O	0.62678900	-1.38092800	2.10867600
C	0.11329000	0.77842800	1.29143100
C	0.27822400	-0.04748800	2.58394700
H	-0.81941900	1.34387300	1.30368000
H	-0.65256100	-0.14568700	3.13946000
N	3.02842300	-2.70131600	-0.24433000
N	0.02723200	-0.30977900	0.30296100
C	-0.59431900	-2.97171800	-0.88544800
H	-0.67267500	-2.18336800	-1.63304900
H	-0.42682000	-3.91984700	-1.39785700
H	-1.52908100	-3.02751400	-0.32518000
C	0.75404700	-3.89074700	1.05401500
H	1.59024200	-3.71906600	1.72833500
H	-0.15956000	-4.02894400	1.63348300
H	0.94920100	-4.79602400	0.47924200
H	3.14646400	-0.22435200	-1.99222000
H	1.09039200	0.29744900	3.21753000

C	5.05568100	-1.29686800	-0.56436700
C	5.90694500	-0.53840700	-1.37134000
C	5.23549100	-1.27833300	0.81682300
C	6.91869600	0.22924900	-0.80728400
H	5.78116100	-0.55062000	-2.44989500
C	6.24775800	-0.50644000	1.38239300
H	4.58006100	-1.87110500	1.44284900
C	7.09136600	0.24766200	0.57467700
H	7.57257700	0.81165900	-1.44533500
H	6.37614300	-0.49708900	2.45823700
H	7.87904200	0.84572500	1.01662600
C	1.27770200	1.68069000	0.95759400
C	1.09223300	3.05415100	0.86496700
C	2.54353000	1.13277400	0.73297800
C	2.16755100	3.88148600	0.55028600
H	0.10331800	3.47392800	1.01995400
C	3.61576400	1.95607100	0.41707000
H	2.70227500	0.05846900	0.80185400
C	3.42529200	3.33465300	0.32554500
H	2.01570600	4.95150400	0.47155600
H	4.59417100	1.52155500	0.24290600
H	4.25985900	3.97907700	0.07651900
C	-4.55260900	-0.87090400	-1.01647100
C	-5.68565600	-1.33292200	-0.11911400
F	-6.60911600	-0.36364600	0.01209600
F	-5.28474200	-1.66446700	1.11335200
F	-6.30479600	-2.40223100	-0.63304000
O	-3.68802000	-1.96226200	-1.17637800
H	-5.04725400	-0.63047900	-1.97253400

Value of Imaginary Frequency= -351.3 cm^{-1}

ts2-2-(*S*)

C	-6.58976400	-1.57775400	0.30854200
C	-5.57267700	-0.63648800	0.19004400
C	-4.66257700	-0.71247000	-0.86684400
C	-4.80181600	-1.73553600	-1.80763900
C	-5.82476300	-2.66883700	-1.69572600
C	-6.71979500	-2.59540500	-0.63170900
H	-7.28054700	-1.51735300	1.14121800
H	-5.47293600	0.14047000	0.93801600
H	-4.09308900	-1.78143100	-2.62606800
H	-5.92618500	-3.45201500	-2.43803300
H	-7.51591500	-3.32460000	-0.53780300
C	-3.52257800	0.25348800	-1.03977300
O	-2.51426600	-0.15956900	-1.69487400
C	-3.59456400	1.52454600	-0.45585800
H	-1.56189900	1.20862800	-1.65817800
H	-4.56053600	1.88320400	-0.12482200
C	-2.82604000	0.87124100	1.55213100
O	-1.74164700	0.44764300	1.32789600
O	-3.71541600	1.14915200	2.26520800
H	-0.56029200	0.29455500	-0.03734100
C	2.04127700	1.34885200	-0.14979800
C	3.39003600	1.03119900	0.44618100
O	3.34319800	0.15944700	1.48297000
C	5.52399300	0.87507300	0.94468500
C	4.69114100	0.08016500	1.98928600
H	6.11059700	1.65790800	1.42787500
H	4.70722900	0.53737200	2.97859700
C	1.42507300	0.03844800	-0.53943600
O	2.18270300	-0.89880100	-1.05317700
C	-0.07609300	-1.65489300	-0.92413500
C	1.36355100	-2.08460000	-1.29002000
H	-0.72614600	-1.59144900	-1.79471600
H	1.47740000	-2.35090100	-2.33689800
N	4.50255700	1.50249600	0.08491500
N	0.18290200	-0.28012000	-0.45662600
C	1.16879100	2.05979100	0.89684000
H	1.01313000	1.43401400	1.77630900
H	1.67369300	2.97829900	1.19891300
H	0.20383000	2.32155500	0.46248800
C	2.17872700	2.19693300	-1.42470800
H	2.77191600	1.68075400	-2.17988100
H	1.18362500	2.42623000	-1.80961300
H	2.68922500	3.12391200	-1.16543000
H	4.97307100	-0.96914900	2.05475200
H	1.75136400	-2.87384500	-0.64874100

C	6.45150800	-0.00683700	0.13601400
C	7.81828100	-0.01908200	0.40121600
C	5.94032100	-0.85372700	-0.84830900
C	8.66701500	-0.86954800	-0.30136000
H	8.22284300	0.64378800	1.15901600
C	6.78686400	-1.70207900	-1.55126800
H	4.87814100	-0.83816100	-1.07072400
C	8.15240800	-1.71302600	-1.27882100
H	9.72941200	-0.86753500	-0.08885800
H	6.38319800	-2.35272800	-2.31809000
H	8.81158200	-2.37250000	-1.83035600
C	-0.76240000	-2.44480900	0.16281100
C	-2.06700800	-2.87834800	-0.04082900
C	-0.14114900	-2.65737100	1.39285100
C	-2.75713500	-3.52302200	0.98019500
H	-2.55133200	-2.67252400	-0.98640200
C	-0.82590500	-3.30989500	2.40950900
H	0.86631000	-2.29014300	1.57024400
C	-2.13546700	-3.74020000	2.20455500
H	-3.78264300	-3.83530200	0.81782000
H	-0.34601300	-3.46936600	3.36732200
H	-2.67160000	-4.23478800	3.00554500
C	-2.65387900	2.59201500	-0.97487200
C	-2.47204700	3.73471400	0.00411000
F	-1.70517600	4.70334200	-0.51644800
F	-1.88516000	3.35860200	1.15226100
F	-3.65175200	4.28399000	0.32348100
O	-1.36573200	2.10015200	-1.27775700
H	-3.08755700	3.07364700	-1.86715400

Value of Imaginary Frequency= -317.8 cm^{-1}

ts2-2-(*R*)

C	3.04437500	-4.75322200	0.59924800
C	3.20320700	-3.47675800	0.07198400
C	2.87117300	-2.35523900	0.83655800
C	2.38259100	-2.53154100	2.13278700
C	2.23909300	-3.80710300	2.66314500
C	2.56640800	-4.92143800	1.89546700
H	3.29026100	-5.61800600	-0.00524800
H	3.55530200	-3.35734900	-0.94657100
H	2.12010100	-1.65269700	2.70906400
H	1.87135700	-3.93387100	3.67456800
H	2.44802900	-5.91767900	2.30487700
C	2.97392600	-0.95672500	0.30699100
O	2.19378500	-0.08974900	0.81532100
C	3.82584500	-0.69084600	-0.77247600
H	2.76302400	1.38232800	-0.08176700
H	4.58749100	-1.42527500	-0.99826300
C	2.46072600	-1.14459400	-2.31889200
O	1.41484600	-0.65249900	-2.02797400
O	3.12359800	-1.75436400	-3.08587100
H	0.68055700	0.16872400	0.33294600
C	-1.58676600	-1.37913400	-0.43937600
C	-2.92924100	-1.28427700	0.24692000
O	-2.95801000	-0.42345800	1.29601200
C	-5.03222200	-1.44376900	0.85636500
C	-4.25706600	-0.59429400	1.89961900
H	-5.50771900	-2.30381900	1.32961900
H	-4.12140400	-1.11603400	2.84752200
C	-1.14812300	0.03669500	-0.67256500
O	-1.86724100	0.77965800	-1.47995200
C	0.04971100	1.97258300	-0.73964900
C	-1.27082900	2.10745400	-1.53230800
H	0.92091100	1.92909100	-1.39679000
H	-1.12663300	2.36028700	-2.57855700
N	-3.97723100	-1.91398700	-0.06109900
N	-0.12714500	0.62744700	-0.16801200
C	-0.58503700	-2.10225500	0.46923200
H	-0.45552300	-1.58760900	1.42282700
H	-0.94537200	-3.11325200	0.66211400
H	0.38130600	-2.16910400	-0.03253000
C	-1.71625200	-2.08236100	-1.79710500
H	-2.45698800	-1.58777800	-2.42393200
H	-0.74711700	-2.07935900	-2.29759000
H	-2.03889000	-3.10876500	-1.62630900
H	-4.69130900	0.38908300	2.06793300
H	-1.97176200	2.79483900	-1.06099700

C	-6.08229100	-0.64528000	0.11198400
C	-7.42572100	-0.76323300	0.46011500
C	-5.71441300	0.25516200	-0.88841500
C	-8.39148800	0.01107000	-0.17544900
H	-7.71926900	-1.46921500	1.23010600
C	-6.67836900	1.02826800	-1.52449200
H	-4.67261000	0.34139300	-1.18011000
C	-8.01907100	0.90910300	-1.16910100
H	-9.43390400	-0.09294900	0.10097400
H	-6.38472000	1.72076400	-2.30447600
H	-8.76957600	1.50917100	-1.66930000
C	0.24081200	3.01972100	0.33044700
C	1.30386500	3.91415100	0.25303400
C	-0.66275300	3.10178800	1.39167500
C	1.45510800	4.89726000	1.22795000
H	2.02462000	3.82246300	-0.55175600
C	-0.50661700	4.07935100	2.36403700
H	-1.47896700	2.38834300	1.46477200
C	0.55146700	4.98209200	2.27959300
H	2.28633800	5.58890600	1.16757600
H	-1.20514800	4.13637900	3.18994600
H	0.67393800	5.74426500	3.03959800
C	4.21461100	0.72712100	-1.13047100
C	5.45972900	1.14494500	-0.35458300
F	6.48200100	0.30391600	-0.58001700
F	5.24198400	1.16872600	0.96694500
F	5.87262900	2.36987100	-0.70890800
O	3.21365700	1.68578100	-0.89205300
H	4.50138400	0.78875000	-2.18610500

Value of Imaginary Frequency= -338.4 cm^{-1}

ts2-3-(*S*)

C	1.43032900	2.91614700	1.18931200
C	0.67175000	3.10347000	-0.10816900
O	1.40037600	3.53936400	-1.14998800
C	-0.91930800	3.38486700	-1.60811700
C	0.45523600	3.77068000	-2.21994900
H	-1.57106600	4.25923900	-1.54495800
H	0.51447300	4.82210900	-2.49583000
C	0.47766400	2.15838100	2.07608500
O	-0.28228200	2.81975000	2.90539300
C	-0.83455000	0.51037000	2.95756300
C	-1.09276000	1.86742200	3.65409500
H	-0.50712700	-0.25327900	3.66301800
H	-0.74132700	1.89774900	4.68373200
N	-0.58077700	2.98037300	-0.22756300
N	0.30166000	0.88155800	2.10944700
C	2.75609100	2.16138000	1.01191100
H	2.63097400	1.14210900	0.65447800
H	3.36432000	2.70549900	0.28950400
H	3.28745900	2.13621600	1.96513500
C	1.69428100	4.31808800	1.77062000
H	0.76728900	4.87811500	1.88936700
H	2.18860600	4.23578900	2.73961700
H	2.35237500	4.85363500	1.08655100
H	0.74359000	3.15069900	-3.06703900
H	-2.12666900	2.19383200	3.58414300
C	-1.66578300	2.28859200	-2.33906500
C	-3.03658500	2.39524800	-2.56072500
C	-0.99723400	1.14560700	-2.77698900
C	-3.72749000	1.38147800	-3.21961900
H	-3.56710100	3.27763100	-2.21878900
C	-1.68375400	0.12380400	-3.42163600
H	0.07017000	1.05339300	-2.61867300
C	-3.05271000	0.24458300	-3.65123200
H	-4.79246200	1.48055000	-3.39328000
H	-1.14383200	-0.75874000	-3.74323600
H	-3.58970400	-0.54594600	-4.16197300
C	-2.01134600	-0.00286900	2.15428000
C	-3.09302900	-0.54041500	2.85319600
C	-2.04977900	0.06238000	0.76528900
C	-4.21253600	-0.99375800	2.16797700
H	-3.05722000	-0.61057900	3.93665500
C	-3.16991100	-0.40093300	0.08063400
H	-1.22197100	0.47899700	0.20471300
C	-4.25108300	-0.92513100	0.77753100
H	-5.04856600	-1.41047700	2.71736200

H	-3.18393400	-0.34974900	-1.00187500
H	-5.11847700	-1.29033700	0.24045400
C	-1.94456300	-4.11567500	-1.22716000
C	-0.72443000	-3.51265600	-0.94252700
C	-0.43422900	-3.08542800	0.35632400
C	-1.38839400	-3.27070000	1.35836600
C	-2.59942000	-3.88883200	1.07682200
C	-2.88276700	-4.31153000	-0.21824500
H	-2.16257500	-4.43243700	-2.24046400
H	-0.01035700	-3.35365400	-1.74136900
H	-1.16235500	-2.91517200	2.35577100
H	-3.32920800	-4.02785000	1.86604000
H	-3.83113800	-4.78618800	-0.44202400
C	0.85605100	-2.41114500	0.72943200
O	0.83900500	-1.68560300	1.78348900
C	1.96869200	-2.53242100	-0.09491000
H	2.47919200	-1.25468000	1.83882000
H	1.96129500	-3.28329000	-0.87350200
C	1.20408300	-0.77187500	-1.34322900
O	1.19313400	-1.23556300	-2.42117900
O	1.05556500	0.09314100	-0.55139200
H	0.75725400	0.15472500	1.53613300
C	3.34655900	-2.15117300	0.40463500
C	4.24266800	-1.64244000	-0.71154800
F	5.50146400	-1.47305200	-0.28395000
F	3.84444600	-0.46111700	-1.21056300
F	4.28325500	-2.51100500	-1.73393600
O	3.35507600	-1.16467200	1.40463400
H	3.86197800	-3.05929000	0.76098800

Value of Imaginary Frequency= -284.0 cm^{-1}

ts2-3-(*R*)

C	0.78356300	-3.59873700	-0.06908700
C	1.58658600	-2.70494500	-0.98586700
O	1.44486700	-2.93549300	-2.30067800
C	3.05861800	-1.29747700	-1.80389400
C	2.18783100	-1.87714900	-2.94661600
H	4.07590100	-1.69938000	-1.85471000
H	2.75862000	-2.30834900	-3.76550700
C	0.65280800	-2.86519600	1.23875800
O	1.12627200	-3.40863200	2.32657700
C	0.12841200	-1.30313900	2.83334400
C	0.82427400	-2.53887600	3.45801700
H	-0.89089000	-1.18295700	3.20029600
H	0.18280400	-3.10364100	4.12990500
N	2.42230800	-1.84132600	-0.59130000
N	0.06617000	-1.73222100	1.42889200
C	-0.62587200	-3.89696000	-0.61432500
H	-1.23278000	-2.99774900	-0.71158500
H	-0.52164600	-4.36506400	-1.59274700
H	-1.12994400	-4.59518400	0.05662400
C	1.57451500	-4.90399900	0.12045000
H	2.56565800	-4.70666700	0.52873700
H	1.03895800	-5.57708100	0.79052900
H	1.67862400	-5.38504500	-0.85246000
H	1.47171000	-1.14404500	-3.32317900
H	1.76923100	-2.29563100	3.93727100
C	3.13793700	0.21004400	-1.81652600
C	4.16319600	0.83658100	-2.52473300
C	2.18503200	0.99197400	-1.16396300
C	4.23347800	2.22413200	-2.58833700
H	4.91464000	0.23353400	-3.02499300
C	2.26195600	2.37962900	-1.21581000
H	1.38941300	0.51900100	-0.59797300
C	3.28262100	2.99817700	-1.93105900
H	5.03442300	2.69860500	-3.14304000
H	1.52463300	2.97356700	-0.69075700
H	3.33660000	4.07980100	-1.97208100
C	0.88719300	-0.00963900	3.01099200
C	0.51282200	0.86254300	4.03013100
C	1.96698700	0.30334200	2.18781600
C	1.21426800	2.04785100	4.22557800
H	-0.34056800	0.62713000	4.65743500
C	2.65099200	1.50061300	2.37060300
H	2.26204400	-0.37058800	1.38842000
C	2.28005300	2.37075600	3.39099000
H	0.91599100	2.72578900	5.01632100

H	3.46765700	1.75396000	1.70474000
H	2.81503200	3.30267300	3.53032300
C	-0.66670400	4.57384500	-1.07875900
C	-1.23572400	3.30718400	-1.13511500
C	-1.19277500	2.46140700	-0.02141100
C	-0.54023600	2.89905700	1.13326000
C	0.02251900	4.16942400	1.19140300
C	-0.04592800	5.01463600	0.08795600
H	-0.70336000	5.21668100	-1.95026100
H	-1.69011300	2.97330300	-2.05948600
H	-0.49028100	2.22788400	1.98140000
H	0.51678100	4.49443100	2.09995400
H	0.38967300	6.00613500	0.13054700
C	-1.82573100	1.09610800	0.00697200
O	-1.49129100	0.32704900	0.97232800
C	-2.65754000	0.69701400	-1.03186600
H	-2.52420400	-1.00544200	0.61780900
H	-3.00746500	1.43038800	-1.74377500
C	-0.86348400	-0.06445600	-2.17376200
O	-0.88628600	0.58112800	-3.15276600
O	-0.45190700	-0.91420400	-1.46117900
H	-0.37930600	-1.11219800	0.72979000
C	-3.51224000	-0.54742500	-0.93782800
C	-4.92906800	-0.17227700	-0.51426500
F	-4.96419800	0.36197900	0.71295900
F	-5.73971600	-1.24108400	-0.50180000
F	-5.47364300	0.72130800	-1.35834700
O	-3.04054400	-1.51830400	-0.03814300
H	-3.63019000	-1.01545000	-1.92338600

Value of Imaginary Frequency= -277.5 cm^{-1}

ts2-4-(*S*)

C	3.38244700	1.45457100	0.99248700
C	2.41106300	0.65271900	1.84502600
O	1.46505700	1.32070900	2.51618900
C	1.36688900	-1.03117600	2.81321000
C	0.69462800	0.31030700	3.22223000
H	1.79127700	-1.53714400	3.68334700
H	0.77930600	0.51906800	4.28728700
C	3.32204500	0.79788600	-0.36508000
O	4.41389000	0.31301000	-0.89356900
C	2.54674100	-0.27512000	-2.22806800
C	4.08664300	-0.19025100	-2.22315200
H	2.12206800	0.15273300	-3.13286000
H	4.47520800	0.53446100	-2.93704500
N	2.47722600	-0.60791600	1.93671300
N	2.26213200	0.62108200	-1.08444500
C	3.00421800	2.94007200	0.87641700
H	1.99597600	3.07162800	0.48982900
H	3.05619500	3.38513300	1.87028000
H	3.72349800	3.44727600	0.23062000
C	4.79054800	1.30124200	1.58820000
H	5.07218200	0.25170400	1.65795500
H	5.52069500	1.83418000	0.97800500
H	4.78852000	1.73418400	2.58931400
H	-0.33940100	0.39573000	2.88994500
H	4.57498100	-1.15344300	-2.33666600
C	0.44284800	-1.99344500	2.09892700
C	0.23026100	-3.27358700	2.60097400
C	-0.21692500	-1.60170900	0.93173700
C	-0.64322500	-4.14975300	1.95895800
H	0.74385500	-3.58609800	3.50458800
C	-1.09969400	-2.46505700	0.29794500
H	-0.06145100	-0.60443300	0.53233900
C	-1.31428800	-3.74218300	0.81325100
H	-0.80474800	-5.14270900	2.36228600
H	-1.62931400	-2.14561100	-0.59181700
H	-2.00610700	-4.41395500	0.31852800
C	2.01053600	-1.67218500	-1.99915400
C	1.14202200	-2.24798500	-2.92286300
C	2.41844500	-2.40642300	-0.88409900
C	0.68587900	-3.54896200	-2.73678300
H	0.81084900	-1.67194100	-3.77939200
C	1.96207900	-3.70502800	-0.69984900
H	3.05784500	-1.95848300	-0.12976800
C	1.09794900	-4.27832300	-1.62705300
H	0.00209600	-3.98619200	-3.45412100

H	2.25953200	-4.25805300	0.18302700
H	0.73107400	-5.28618100	-1.47349000
C	-5.89075000	-0.38681200	-0.57291900
C	-4.75091500	0.40322800	-0.65491000
C	-3.71598300	0.25240500	0.27011100
C	-3.84639100	-0.70354900	1.27974200
C	-4.98024700	-1.50262900	1.35573800
C	-6.00708100	-1.34498800	0.42990300
H	-6.68940000	-0.25555600	-1.29343200
H	-4.67782500	1.14402000	-1.44096000
H	-3.03589200	-0.81279200	1.98957000
H	-5.06295200	-2.24862800	2.13763100
H	-6.89498700	-1.96368600	0.48953800
C	-2.45217000	1.06024800	0.22701000
O	-1.71546000	1.02965000	1.26377400
C	-2.07600100	1.72538500	-0.94759400
H	-0.39733600	1.61957900	0.69398500
H	-2.80716700	1.95813600	-1.70898300
C	-1.35179600	0.01990800	-2.30565200
O	-2.27768000	-0.68793200	-2.41861500
O	-0.25308800	0.39902500	-2.51952600
H	1.31974200	0.98749700	-0.80711800
C	-0.83588900	2.57275400	-0.90723900
C	-1.08922600	3.99096500	-0.42029100
F	0.04267700	4.72289800	-0.44026600
F	-1.56456700	4.04588900	0.82555900
F	-1.96897800	4.61738200	-1.21973100
O	0.15333200	1.99519800	-0.07228500
H	-0.41236300	2.68946700	-1.90907200

Value of Imaginary Frequency= -286.8 cm^{-1}

ts2-4-(*R*)

C	1.25227400	-3.25490600	0.11471100
C	2.57834900	-2.67884000	-0.33353300
O	3.05633900	-3.15895400	-1.49560400
C	4.41534100	-1.47747000	-0.53587000
C	4.33513400	-2.51192900	-1.69137100
H	5.31747600	-1.62535500	0.05979100
H	5.10922900	-3.27557200	-1.62736500
C	0.84875400	-2.37043200	1.26375500
O	1.34282700	-2.61881700	2.44878300
C	0.08203900	-0.59990300	2.48459500
C	1.01184600	-1.50401700	3.32626300
H	-0.93914500	-0.60158100	2.85815000
H	0.52809100	-1.91692900	4.20687600
N	3.23743800	-1.79826600	0.29155100
N	0.10028200	-1.32818600	1.20087000
C	0.23269000	-3.19127700	-1.03056200
H	0.10608900	-2.17808500	-1.41516000
H	0.58321900	-3.82703900	-1.84261500
H	-0.73532900	-3.56511900	-0.69041300
C	1.45671200	-4.70247900	0.59045300
H	2.17877300	-4.75188900	1.40475000
H	0.50705000	-5.11942300	0.92866300
H	1.81988600	-5.29612800	-0.24832700
H	4.33654400	-2.05754300	-2.68052700
H	1.94993600	-1.01935900	3.59119000
C	4.35157700	-0.03291600	-0.98397300
C	5.33823100	0.87485000	-0.61078900
C	3.28782300	0.40356200	-1.77609300
C	5.27422500	2.20144600	-1.03209800
H	6.16416300	0.54295200	0.00945100
C	3.22667200	1.72252200	-2.20583000
H	2.50291000	-0.29290100	-2.06098200
C	4.22098100	2.62540800	-1.83323800
H	6.04971300	2.89872200	-0.73813600
H	2.40410200	2.04799200	-2.83221300
H	4.17368100	3.65402800	-2.17124100
C	0.56193500	0.81625800	2.27533100
C	-0.28713500	1.88670100	2.54066800
C	1.84593100	1.04946300	1.77592300
C	0.15980200	3.19068300	2.34622100
H	-1.29799500	1.70097300	2.88993700
C	2.28639500	2.35073800	1.57600300
H	2.49252000	0.21343900	1.52164200
C	1.44663600	3.42146200	1.87516700
H	-0.50471500	4.02243100	2.54626700

H	3.27833400	2.52421800	1.17281600
H	1.78641400	4.43782900	1.71300200
C	-1.75215700	4.47408000	-0.57433300
C	-2.25636100	3.17984600	-0.56773500
C	-1.41743500	2.09685000	-0.85297100
C	-0.06666400	2.33255300	-1.11310400
C	0.43032400	3.62919500	-1.13601600
C	-0.41224400	4.70413400	-0.87434700
H	-2.40864700	5.30563300	-0.34704600
H	-3.29456100	3.01380000	-0.30987300
H	0.58255300	1.48394600	-1.29075100
H	1.48286500	3.79821800	-1.33476900
H	-0.02494600	5.71645200	-0.88928500
C	-1.91091000	0.68414200	-0.91605200
O	-1.04716100	-0.24989600	-0.91345900
C	-3.28966500	0.41455900	-0.90147600
H	-2.20178400	-1.71910000	-0.71918300
H	-3.96161200	1.23001500	-1.13325800
C	-3.36761200	0.43134300	1.14777900
O	-4.06586600	1.34762500	1.43991000
O	-2.68876800	-0.47596300	1.52818700
H	-0.35439000	-0.90727600	0.34160800
C	-3.78293700	-0.93173500	-1.40102400
C	-5.24121600	-1.13916200	-1.03612400
F	-6.00412600	-0.14761000	-1.52840600
F	-5.44683500	-1.18261500	0.28390900
F	-5.70834600	-2.28618400	-1.54675100
O	-3.09099900	-2.04938800	-0.90751200
H	-3.76769400	-0.92975300	-2.50312800

Value of Imaginary Frequency= -358.4 cm^{-1}

ts2-5-(*S*)

C	0.09144600	3.82869700	-0.16957300
C	1.39560700	3.08126000	-0.11970500
O	2.47175000	3.79360000	0.16482600
C	2.98880500	1.48882100	0.01407800
C	3.61345900	2.89759700	0.16023000
H	3.39143800	0.96248600	-0.85271100
H	4.23733300	3.17468100	-0.68733700
C	-0.96757800	2.98123700	-0.82864800
O	-0.61866400	2.48639000	-2.03554000
C	-2.82320200	1.97002900	-1.42066000
C	-1.71036100	1.62615500	-2.43450500
H	-3.56149200	2.63499000	-1.88368000
H	-1.96963100	1.86564700	-3.46365200
N	1.58947500	1.82358700	-0.26679800
N	-2.12818500	2.76885100	-0.38374100
C	-0.30365100	4.16391100	1.27644700
H	-0.44670000	3.25391500	1.86116900
H	0.46812300	4.78027900	1.73880900
H	-1.24654500	4.70917400	1.26381300
C	0.27410400	5.11328100	-1.00172000
H	0.57821600	4.87636500	-2.02170300
H	-0.67889200	5.64294500	-1.03370100
H	1.02357900	5.75674700	-0.54182700
H	4.15090700	3.03601200	1.09544100
H	-1.35239000	0.60216200	-2.35442000
C	3.12521500	0.61119500	1.24362700
C	4.36227700	0.01301800	1.49391900
C	2.05815700	0.36114600	2.10338500
C	4.52836500	-0.82549400	2.58768900
H	5.19232500	0.18891200	0.81632400
C	2.22300200	-0.49142100	3.19265800
H	1.08548500	0.80179500	1.91697700
C	3.45481400	-1.08449100	3.43721000
H	5.49016600	-1.28943300	2.76947400
H	1.37845000	-0.69562300	3.84009800
H	3.57939300	-1.75215700	4.28086800
C	-3.57502300	0.80778200	-0.80358800
C	-3.43005700	-0.50692900	-1.23327300
C	-4.47150500	1.08481700	0.23204500
C	-4.13590000	-1.53665100	-0.61171000
H	-2.76494000	-0.75250800	-2.05145600
C	-5.18884700	0.06459000	0.83848200
H	-4.58268700	2.10928900	0.57042400
C	-5.01289000	-1.25498800	0.42591400
H	-3.97947900	-2.55771800	-0.93976900

H	-5.87394900	0.29347300	1.64701700
H	-5.55269400	-2.05642100	0.91636100
C	-2.41579600	-2.99503700	2.62111900
C	-1.53242100	-2.71861100	1.58641700
C	-1.24402700	-1.39364800	1.24235100
C	-1.87363200	-0.35726900	1.93618300
C	-2.74211100	-0.63801300	2.98329000
C	-3.01115500	-1.95667700	3.33249100
H	-2.64008100	-4.02471500	2.87299400
H	-1.10024300	-3.53744500	1.02665800
H	-1.68838700	0.66463700	1.62484700
H	-3.22502700	0.17487300	3.51303600
H	-3.69298000	-2.17674400	4.14582600
C	-0.24949900	-1.01816900	0.18888100
O	-0.26730100	0.20111800	-0.18473000
C	0.59724400	-1.99886700	-0.34968700
H	1.02386800	-0.68234100	-2.43812400
H	0.64513900	-2.93795100	0.18501300
C	-0.75370300	-2.47123100	-1.85926800
O	-0.58835600	-1.63020500	-2.69687100
O	-1.32880500	-3.44281400	-1.51047600
H	0.76579300	0.99989300	-0.38068700
C	1.90676300	-1.63411700	-1.01655500
C	2.53107600	-2.85240800	-1.68469300
F	3.73978900	-2.55798400	-2.17988200
F	1.79326100	-3.32442800	-2.69734000
F	2.69571200	-3.85540200	-0.80679000
O	1.85212500	-0.58070000	-1.94379300
H	2.63815000	-1.34816600	-0.25051600

Value of Imaginary Frequency= -507.1 cm^{-1}

ts2-5-(*R*)

C	1.41958200	-3.29518900	-0.56075900
C	1.20814700	-2.72220100	0.81258200
O	1.65612100	-3.36918400	1.85839100
C	0.64848300	-1.33513300	2.54460700
C	1.15809700	-2.69459800	3.05531600
H	-0.35154200	-1.10480800	2.90520700
H	0.35966700	-3.31734800	3.45423600
C	1.94820900	-2.18059100	-1.43465600
O	1.59971600	-2.24237500	-2.73099000
C	2.98906800	-0.41215100	-2.20426600
C	2.11548200	-1.03387600	-3.32803400
H	4.05185600	-0.52102500	-2.44693700
H	2.67428900	-1.31026700	-4.21996000
N	0.56631100	-1.64344400	1.10430400
N	2.70804600	-1.25587300	-1.03328100
C	2.46035000	-4.42455800	-0.52412500
H	3.41039600	-4.06786700	-0.12576100
H	2.10139600	-5.25253200	0.08760400
H	2.61491800	-4.78110700	-1.54316600
C	0.05827900	-3.81524500	-1.06198900
H	-0.68426800	-3.01828800	-1.09268100
H	0.19475300	-4.23263500	-2.05892800
H	-0.30111800	-4.59929600	-0.39270000
H	1.98188900	-2.62343100	3.75958200
H	1.26739800	-0.40081600	-3.59312500
C	1.57205300	-0.15858100	2.76417100
C	1.02797400	1.09582100	3.02582000
C	2.95491900	-0.30638300	2.64541300
C	1.86538200	2.19712700	3.17900200
H	-0.05014100	1.20578700	3.06418800
C	3.78894300	0.79365700	2.79973000
H	3.38717900	-1.27456600	2.40981700
C	3.24385000	2.04674600	3.06941500
H	1.43585900	3.17255700	3.37734700
H	4.86100000	0.67639900	2.70058200
H	3.89492600	2.90498000	3.18619000
C	2.71798100	1.05594900	-1.95182900
C	2.66068400	1.93200300	-3.03692000
C	2.57184500	1.56215100	-0.66196600
C	2.45676700	3.29259000	-2.84041500
H	2.77656100	1.55071700	-4.04716100
C	2.38291000	2.92733600	-0.46695500
H	2.60364000	0.88712800	0.18563900
C	2.32011700	3.79539800	-1.55064500
H	2.40434900	3.95839400	-3.69351300

H	2.27763100	3.30680900	0.54331500
H	2.15768200	4.85507100	-1.39327400
C	-3.02710200	4.51455800	0.10219100
C	-3.15563800	3.12985100	0.08050700
C	-2.05538200	2.31681000	0.35470600
C	-0.82589300	2.90717000	0.64659200
C	-0.69291100	4.29007000	0.65147600
C	-1.79566400	5.09756000	0.38524700
H	-3.88953800	5.13918300	-0.09851900
H	-4.11814700	2.67548700	-0.12560100
H	0.02190100	2.26317900	0.84746700
H	0.27122800	4.74116400	0.85980900
H	-1.69599700	6.17660500	0.39744000
C	-2.15301800	0.81910300	0.36558400
O	-1.45020900	0.19440100	1.22807500
C	-2.88598500	0.19979500	-0.64121900
H	-1.97302000	-1.38284000	0.83656200
H	-3.48455900	0.80809100	-1.30490900
C	-1.04802900	0.12834900	-2.00984500
O	-0.23611800	-0.42400800	-1.34890400
O	-1.46365900	0.62090700	-2.98649600
H	0.14238400	-0.98900900	0.43339700
C	-3.25848500	-1.26066700	-0.56040000
C	-4.65186600	-1.41745500	0.03874800
F	-5.56970300	-0.73739300	-0.67041500
F	-4.71241200	-0.97364400	1.30097200
F	-5.04396100	-2.70110100	0.05442200
O	-2.36985900	-2.03059200	0.21293800
H	-3.33120900	-1.70693900	-1.56074100

Value of Imaginary Frequency= -260.8 cm^{-1}

ts2-6-(*S*)

C	-0.24681200	3.17098600	1.14437500
C	0.79439900	2.73097200	0.15804300
O	1.55726600	3.63522500	-0.40672300
C	2.02120600	1.47375100	-1.28507200
C	2.28282600	2.98687600	-1.49301000
H	1.59502300	1.02673700	-2.18474400
H	1.85517700	3.35930500	-2.42153200
C	-0.60831100	1.97551400	2.00460800
O	-1.91733100	1.68821700	2.10460600
C	-0.53605500	0.18922600	3.28818900
C	-1.99549700	0.44467800	2.83949200
H	-0.43940900	0.34641900	4.36780600
H	-2.68597800	0.58812700	3.66771800
N	0.97728200	1.53337300	-0.26369000
N	0.23256000	1.25690900	2.61492700
C	0.31023600	4.29045200	2.03799100
H	1.17549900	3.94060700	2.60138400
H	0.59290900	5.15092200	1.43152500
H	-0.46685700	4.59445300	2.74059300
C	-1.44588600	3.66388500	0.31048200
H	-1.82413000	2.87659800	-0.34244400
H	-2.24274300	3.97420400	0.98581700
H	-1.13704300	4.51511800	-0.29779100
H	3.33010600	3.26162700	-1.40082900
H	-2.37491300	-0.30412200	2.14764500
C	3.21865400	0.67869500	-0.81296900
C	4.13452200	0.22264900	-1.75885400
C	3.41344100	0.38731700	0.53534400
C	5.24064600	-0.51779700	-1.36129900
H	3.96725800	0.42546000	-2.81204300
C	4.51887600	-0.36008000	0.93023500
H	2.68863700	0.71389300	1.27488000
C	5.43344600	-0.81307600	-0.01442400
H	5.94534600	-0.87492500	-2.10271400
H	4.66280900	-0.58883400	1.97997500
H	6.29231100	-1.39616100	0.29566700
C	0.05162700	-1.17519800	2.97025100
C	-0.72810700	-2.27639700	2.62400900
C	1.43678600	-1.33565900	3.06491700
C	-0.13443000	-3.51028600	2.36761500
H	-1.80379100	-2.19018200	2.53632600
C	2.03041500	-2.56550600	2.80653800
H	2.04682000	-0.48125800	3.33663400
C	1.24422900	-3.65952200	2.45452000
H	-0.75575700	-4.35261300	2.08821300

H	3.10699800	-2.67067500	2.87813400
H	1.70335200	-4.61838200	2.24571000
C	1.53797600	-2.29295700	-3.31799700
C	0.37637700	-1.64742000	-2.91310900
C	0.12486800	-1.44595200	-1.55190600
C	1.05600700	-1.89153500	-0.61084700
C	2.20723900	-2.55573200	-1.01731700
C	2.45129200	-2.75471600	-2.37096200
H	1.73262500	-2.43590400	-4.37429200
H	-0.32537700	-1.28522300	-3.65619100
H	0.86334500	-1.71680200	0.44121800
H	2.92024500	-2.89343600	-0.27316900
H	3.35615900	-3.25772600	-2.69191000
C	-1.09447000	-0.74013000	-1.04780600
O	-0.98909700	-0.13506900	0.06045000
C	-2.23738300	-0.64163700	-1.85979000
H	-2.65408900	0.83291200	0.10612300
H	-2.33912900	-1.36144800	-2.66284200
C	-1.76014500	1.05095900	-2.92456200
O	-2.55503400	1.03794400	-3.80643800
O	-0.84200700	1.62119800	-2.40863100
H	0.31541600	0.73582900	-0.01127700
C	-3.54696300	-0.18769500	-1.25930500
C	-4.21667400	-1.30976900	-0.47629000
F	-5.41581000	-0.94531300	-0.00652600
F	-3.48628900	-1.69850100	0.58888200
F	-4.40324100	-2.39665000	-1.24024800
O	-3.45217400	0.94690800	-0.43416900
H	-4.24064100	0.05292700	-2.07052900

Value of Imaginary Frequency= -372.6 cm^{-1}

ts2-6-(*R*)

C	0.66226600	2.31943500	2.26913000
C	-0.00595600	0.98253300	2.41875800
O	-0.10230200	0.46730100	3.61595500
C	-0.99107400	-1.02631200	1.98816800
C	-0.64166900	-0.88060800	3.49212600
H	-0.40887600	-1.83228500	1.53777300
H	0.14244900	-1.56393200	3.80826600
C	0.36026800	2.83393400	0.87505200
O	1.41291000	3.05322400	0.06899200
C	-0.66281300	3.47720500	-0.96326700
C	0.86034800	3.36808800	-1.22893700
H	-0.98556400	4.52213900	-1.02603300
H	1.31345800	4.29632300	-1.56994200
N	-0.49474000	0.25241900	1.47914400
N	-0.80682100	3.04868200	0.44058000
C	0.06306900	3.28920500	3.30502200
H	-1.00756400	3.41480200	3.14372100
H	0.24360800	2.91774700	4.31361000
H	0.54934100	4.25913100	3.19363400
C	2.17132200	2.12328400	2.50820500
H	2.60646400	1.41944600	1.79954400
H	2.66597700	3.08895100	2.40204200
H	2.32784200	1.75049300	3.52106100
H	-1.51105200	-0.94592300	4.14180200
H	1.11836000	2.54187600	-1.88933100
C	-2.45582400	-1.22847600	1.67468200
C	-2.97464000	-2.52091400	1.69644300
C	-3.28449400	-0.15521900	1.35414300
C	-4.31557200	-2.73998400	1.40513300
H	-2.32229200	-3.36038100	1.91496300
C	-4.62385900	-0.37798400	1.05248300
H	-2.87809400	0.84990500	1.31227800
C	-5.14179800	-1.66898500	1.07850900
H	-4.71148000	-3.74840800	1.41711000
H	-5.26234000	0.45964100	0.79644600
H	-6.18505500	-1.84091700	0.84227600
C	-1.56250200	2.65914000	-1.87182500
C	-1.18194800	2.30624800	-3.16495900
C	-2.82941600	2.28500700	-1.41795700
C	-2.04127400	1.57729900	-3.98249400
H	-0.20900200	2.59120200	-3.54821200
C	-3.68928100	1.55854300	-2.23399600
H	-3.13100000	2.56333200	-0.41545000
C	-3.29582000	1.19798500	-3.51957600
H	-1.72446300	1.30092000	-4.98093900

H	-4.66584700	1.26847200	-1.86313000
H	-3.95999500	0.62357800	-4.15423700
C	-1.25785400	-3.90931600	-1.31670000
C	-0.12509900	-3.12162300	-1.15200400
C	-0.21636800	-1.72981100	-1.27295500
C	-1.45474800	-1.14999400	-1.56279500
C	-2.58275900	-1.94254200	-1.73939800
C	-2.48669100	-3.32347500	-1.61557800
H	-1.18101900	-4.98510200	-1.21158600
H	0.82059700	-3.58694300	-0.90178100
H	-1.52017500	-0.07216600	-1.65554700
H	-3.53542200	-1.47423100	-1.96001800
H	-3.36653700	-3.94376100	-1.74196700
C	0.95662800	-0.81144500	-1.08959600
O	0.69588900	0.41059000	-0.84843200
C	2.26781200	-1.31192600	-1.08156300
H	2.41242700	1.07494700	-0.44261100
H	2.43515700	-2.28112000	-1.53396800
C	2.23868500	-1.89524700	0.93010700
O	2.40728800	-3.06961000	0.90274700
O	2.04540000	-0.91719400	1.58569500
H	-0.28215300	0.43262500	0.46138800
C	3.41093000	-0.33258900	-1.27441000
C	4.74357500	-0.98106100	-0.94986200
F	4.92435800	-2.09663500	-1.67723900
F	4.85466400	-1.32278500	0.33841600
F	5.76366000	-0.15927800	-1.22870600
O	3.35029500	0.83210700	-0.49470700
H	3.48256800	-0.07351400	-2.34398800

Value of Imaginary Frequency= -364.5 cm^{-1}

im3-1-(*S*)

C	3.45128200	2.93060400	-2.58113500
C	3.49190900	1.60094600	-2.17696400
C	3.34244500	1.27182000	-0.82838300
C	3.13957300	2.28811900	0.10891700
C	3.12054800	3.61737500	-0.29522900
C	3.27143000	3.94199100	-1.64057800
H	3.55874500	3.17795000	-3.63053600
H	3.61925100	0.80891500	-2.90593800
H	3.00452100	2.03022300	1.15322300
H	2.97868000	4.39869500	0.44190900
H	3.24929000	4.97847900	-1.95581800
C	3.39685200	-0.13634400	-0.36403700
O	2.48156600	-0.47564600	0.58872000
C	4.32348400	-1.00346200	-0.78425300
H	2.71645700	-2.36391300	0.55499900
H	5.09412900	-0.64617800	-1.45492100
H	1.60668600	-0.09962200	0.31004900
C	-1.10091100	-1.61977600	-1.01313200
C	-2.35310500	-1.82316900	-0.19475700
O	-2.30422700	-1.27016600	1.04459500
C	-4.36565700	-2.29161000	0.55623200
C	-3.52149700	-1.67024000	1.70163000
H	-4.73951300	-3.27732800	0.83737500
H	-3.26645500	-2.39586000	2.47496500
C	-0.84992300	-0.13215500	-1.01699500
O	-1.84771200	0.60065100	-1.54678800
C	-0.09237400	1.92773600	-0.71942300
C	-1.38506700	1.96515100	-1.57263000
H	0.74009300	2.39361800	-1.25207600
H	-1.19346800	2.23344200	-2.61192900
N	-3.40092600	-2.43162200	-0.54968000
N	0.16819300	0.48439900	-0.57411700
C	0.06288800	-2.36592800	-0.35485300
H	0.21754700	-2.02801700	0.67078000
H	-0.15547100	-3.43511500	-0.34431400
H	0.98087600	-2.20900600	-0.92246400
C	-1.32284400	-2.10128500	-2.45131900
H	-2.16277200	-1.58263900	-2.91090900
H	-0.41863800	-1.92528900	-3.03718800
H	-1.53984800	-3.16929000	-2.44401600
H	-3.97836900	-0.78851000	2.14736600
H	-2.16312700	2.60023700	-1.15393300
C	-5.53412900	-1.41843800	0.14808700
C	-6.82688800	-1.74088500	0.55308700
C	-5.32165500	-0.25505300	-0.59322400

C	-7.89703000	-0.91156300	0.23021500
H	-6.99877600	-2.64925400	1.12136300
C	-6.38996700	0.57299300	-0.91626000
H	-4.31952300	-0.00441500	-0.92695800
C	-7.67995600	0.24789600	-0.50500200
H	-8.89897000	-1.17524000	0.54751800
H	-6.21748300	1.47233800	-1.49581700
H	-8.51162800	0.89320900	-0.76131400
C	-0.25581200	2.60036000	0.62847600
C	-0.04498400	3.97632000	0.72865600
C	-0.66538500	1.88950500	1.75467100
C	-0.23665100	4.63460700	1.93682500
H	0.28239700	4.52998800	-0.14606000
C	-0.85184400	2.54933600	2.96711400
H	-0.83907200	0.82127600	1.68598900
C	-0.63803000	3.91928500	3.06224300
H	-0.06667200	5.70276100	2.00340000
H	-1.16406600	1.98790900	3.83974900
H	-0.78099100	4.42868300	4.00762400
C	4.41982900	-2.43524600	-0.32459200
C	5.39917600	-2.54171000	0.83939300
F	5.60339300	-3.81447100	1.19810600
F	4.95067300	-1.89113200	1.92040000
F	6.59486900	-2.02207500	0.51908400
O	3.20715900	-3.03032500	0.05263100
H	4.84632600	-3.04757300	-1.12380800

im3-1-(*R*)

C	-3.66271400	4.03459700	0.58005100
C	-3.79899900	2.65423200	0.51343100
C	-3.30569400	1.94509700	-0.58826200
C	-2.63861200	2.64268500	-1.59837400
C	-2.50219700	4.02476900	-1.52858000
C	-3.02034900	4.72580500	-0.44558600
H	-4.05094200	4.57190600	1.43715200
H	-4.27859200	2.12187200	1.32685300
H	-2.23917900	2.09288700	-2.44099200
H	-1.98729900	4.55310600	-2.32193000
H	-2.91544100	5.80293200	-0.39224400
C	-3.47593400	0.47495700	-0.70985100
O	-2.58829000	-0.15643600	-1.53911800
C	-4.46210600	-0.21587500	-0.12687600
H	-3.46354200	-1.73878100	-1.75810600
H	-5.21375400	0.31127500	0.44500300
H	-1.67961600	-0.13262000	-1.11124400
C	0.56245600	-2.45795500	-0.50106200
C	1.97146300	-2.17181300	-0.98020800
O	2.05695700	-1.22980700	-1.95075600
C	4.14049700	-1.89968500	-1.13582200
C	3.44607900	-1.18219800	-2.31708200
H	4.90991300	-2.58723300	-1.49175400
H	3.56599800	-1.72181100	-3.25865500
C	0.23869700	-1.24794000	0.34735600
O	0.79575100	-1.23150600	1.57214100
C	-0.32306700	0.77117800	1.07350200
C	0.28655700	-0.05225900	2.22908900
H	-1.31574800	1.14672000	1.32863200
H	-0.46243600	-0.37308300	2.95407700
N	3.04278900	-2.65462900	-0.50966100
N	-0.43287900	-0.23075800	-0.00714200
C	-0.40330400	-2.55585900	-1.68578600
H	-0.37871100	-1.65275100	-2.29352200
H	-0.12141000	-3.40575000	-2.30981200
H	-1.41751000	-2.71443600	-1.31650700
C	0.52780600	-3.72931100	0.35077100
H	1.23744800	-3.67079600	1.17300600
H	-0.47966800	-3.86878500	0.74678500
H	0.78498900	-4.58658300	-0.27243600
H	3.73521800	-0.13977500	-2.43748200
H	1.11594500	0.44502700	2.72833500
C	4.76657900	-0.91849800	-0.15594400
C	5.83590000	-0.12984900	-0.58908000
C	4.28898400	-0.75534700	1.14212400

C	6.40804400	0.81493400	0.25267000
H	6.22333200	-0.25800400	-1.59569800
C	4.86074400	0.19570300	1.98550200
H	3.46021300	-1.36308700	1.48566400
C	5.91673900	0.98343500	1.54544500
H	7.23676000	1.41881100	-0.09784100
H	4.47515800	0.31940300	2.99087700
H	6.35760000	1.72271500	2.20323500
C	0.55625500	1.91469900	0.61841900
C	0.08785100	3.22302600	0.61525200
C	1.86490100	1.65257000	0.20810200
C	0.92247700	4.26426800	0.21357600
H	-0.93456400	3.42756200	0.91727900
C	2.70348000	2.68837800	-0.17807500
H	2.23562000	0.63271500	0.19183800
C	2.23007800	4.00019400	-0.17724200
H	0.54655500	5.28094800	0.20695900
H	3.72358900	2.46768900	-0.47444400
H	2.87962200	4.81192500	-0.48273400
C	-4.59068000	-1.71859700	-0.20645500
C	-3.82807500	-2.35441500	0.95290100
F	-4.26109400	-1.88805100	2.13476900
F	-2.50756500	-2.09917500	0.88715400
F	-3.96584500	-3.68272100	0.97116300
O	-4.16399500	-2.30834300	-1.40424300
H	-5.63487500	-2.00358200	-0.04807200

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C	-5.55978600	-2.64410000	0.58705800
C	-5.08300700	-1.34381700	0.50074200
C	-4.52787900	-0.87173700	-0.69139800
C	-4.50207300	-1.71236300	-1.80783400
C	-4.97828700	-3.01582800	-1.71864300
C	-5.49924000	-3.48904600	-0.51874700
H	-5.98468700	-2.99875700	1.51856400
H	-5.14421000	-0.69182200	1.36354500
H	-4.09976100	-1.33646200	-2.74002500
H	-4.94432800	-3.66130200	-2.58826800
H	-5.87109900	-4.50424700	-0.44886400
C	-3.93016500	0.47810400	-0.78492600
O	-3.84626800	0.92764500	-2.06329900
C	-3.46632000	1.16693500	0.26871200
H	-3.24318600	1.69057200	-2.07698700
H	-3.49271000	0.72445400	1.25521700
H	-1.37000900	1.91176300	-0.98241600
C	1.87946500	1.62763000	-1.51896800
C	3.01388000	1.34588800	-0.56377100
O	2.62066800	1.11870700	0.71524600
C	4.94327600	0.92064800	0.40219800
C	3.83137500	0.99062000	1.48345800
H	5.73557300	1.64180400	0.60862600
H	3.92202400	1.86990500	2.12228500
C	0.92751800	0.46426400	-1.38959300
O	1.47862400	-0.74572000	-1.61123500
C	-0.77698200	-0.88916800	-0.98485800
C	0.38507900	-1.68605600	-1.62290600
H	-1.69935600	-1.01079500	-1.55695500
H	0.18772200	-1.95524300	-2.66180200
N	4.24548500	1.30346700	-0.83978200
N	-0.30693300	0.50613500	-1.09621600
C	1.19602500	2.93821400	-1.11192000
H	0.79728100	2.87733900	-0.09940900
H	1.92518500	3.74885600	-1.16130100
H	0.37598300	3.16557500	-1.79397200
C	2.40408100	1.69179900	-2.95779800
H	2.90645600	0.76438500	-3.22959000
H	1.57189700	1.87163000	-3.64110100
H	3.12046600	2.50857900	-3.04524100
H	3.76051200	0.08957900	2.09018700
H	0.67799700	-2.56295500	-1.05029000
C	5.55279500	-0.45953800	0.27300100
C	6.83861900	-0.71163500	0.74330100
C	4.81088100	-1.50504500	-0.27982100

C	7.38021900	-1.99207300	0.66991000
H	7.42275500	0.09947800	1.16566700
C	5.35073000	-2.78302400	-0.35300100
H	3.81306000	-1.31378200	-0.66300700
C	6.63655100	-3.03029700	0.12195300
H	8.38356900	-2.17529100	1.03574000
H	4.76960500	-3.58874300	-0.78604200
H	7.05668600	-4.02707700	0.06063500
C	-1.02871000	-1.28598400	0.45692800
C	-1.93982300	-2.30514100	0.73431000
C	-0.32167300	-0.69759300	1.50442700
C	-2.15427200	-2.72117600	2.04372100
H	-2.50066000	-2.76554500	-0.07416800
C	-0.54188700	-1.11104000	2.81424400
H	0.38617000	0.09716300	1.30128900
C	-1.45868500	-2.12111600	3.08839900
H	-2.87587100	-3.50462300	2.24454300
H	0.00271400	-0.63819200	3.62314900
H	-1.63094400	-2.43779400	4.11027900
C	-2.87688300	2.54325000	0.09697000
C	-2.10313100	2.97152000	1.33098600
F	-1.66901500	4.23161800	1.22178700
F	-1.02453000	2.20141300	1.53571400
F	-2.86328200	2.89987300	2.43286300
O	-2.03587900	2.64622600	-1.03163000
H	-3.66455400	3.29476700	-0.03103600

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C	-1.93420600	4.40501100	-0.76356300
C	-2.37260000	3.10164600	-0.97447400
C	-2.81446400	2.32846900	0.09955900
C	-2.80439700	2.86999300	1.38810400
C	-2.37971900	4.17665400	1.59353200
C	-1.94035900	4.94547600	0.51894800
H	-1.58180000	4.99672300	-1.60017700
H	-2.35577800	2.66934000	-1.96869400
H	-3.14063100	2.26216400	2.21997400
H	-2.38745100	4.59459700	2.59301200
H	-1.59971700	5.96100600	0.68092300
C	-3.29598000	0.93967700	-0.09398600
O	-2.85375700	0.02990600	0.82734000
C	-4.16200300	0.59460500	-1.05077000
H	-3.40613200	-1.59667700	-0.05504700
H	-4.56959500	1.37606400	-1.67906100
H	-1.88192100	0.14921500	0.90179000
C	1.57506000	1.72319800	0.08939800
C	2.93462900	1.29407800	0.58232100
O	2.90609900	0.28607600	1.49288400
C	5.08301500	0.97969500	0.93474600
C	4.26681400	0.11071800	1.92898800
H	5.75791000	1.65231800	1.46641500
H	4.34222000	0.46763100	2.95699000
C	0.88891900	0.47384000	-0.40201800
O	1.58981000	-0.22425800	-1.32054400
C	-0.44219000	-1.26183300	-0.74883500
C	0.73957300	-1.30680300	-1.74846000
H	-1.40135000	-1.24514900	-1.27037600
H	0.42951300	-1.10605500	-2.77425100
N	4.05229700	1.77105200	0.23831300
N	-0.24260600	0.02450600	-0.04875900
C	0.78597000	2.34545900	1.24447800
H	0.65683700	1.63410200	2.06055000
H	1.31755900	3.22505800	1.61283700
H	-0.19614400	2.65283700	0.88706000
C	1.71712500	2.70885500	-1.07615100
H	2.28163400	2.26536900	-1.89563800
H	0.72323600	2.99703700	-1.42511100
H	2.24713600	3.59840700	-0.73530600
H	4.51177400	-0.94873400	1.87927700
H	1.31100400	-2.23172700	-1.70031400
C	5.88465200	0.15236900	-0.04836300
C	7.26554500	0.03813300	0.08790700
C	5.23988400	-0.54329900	-1.07268700

C	7.99827900	-0.76453000	-0.78192800
H	7.77264000	0.58404000	0.87683100
C	5.97088000	-1.34467200	-1.94109100
H	4.16529700	-0.44753300	-1.19524600
C	7.35157000	-1.45807600	-1.79797500
H	9.07305900	-0.84230500	-0.66836300
H	5.46361400	-1.87896000	-2.73584900
H	7.91968300	-2.08060700	-2.47879400
C	-0.43702300	-2.41335700	0.23597200
C	-1.30235200	-3.49095400	0.05313600
C	0.46509500	-2.43049200	1.30180500
C	-1.26825200	-4.57536900	0.92549800
H	-2.01425500	-3.47373900	-0.76516200
C	0.49752400	-3.51510500	2.17046200
H	1.13678800	-1.59152500	1.45592400
C	-0.36860900	-4.58941300	1.98499600
H	-1.95035600	-5.40435900	0.77931200
H	1.19761600	-3.52042900	2.99767100
H	-0.34479700	-5.43070400	2.66730100
C	-4.67198400	-0.80533300	-1.27357000
C	-5.98522000	-1.01121600	-0.52625100
F	-6.88505800	-0.07391900	-0.86061100
F	-5.81022200	-0.95256000	0.79948200
F	-6.52804700	-2.20166400	-0.80433400
O	-3.78405600	-1.83237100	-0.91633900
H	-4.91132400	-0.94239200	-2.33126600

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C	-0.09105400	2.85383100	0.36155700
C	-0.26404600	2.09841800	1.65636400
O	-1.24415100	2.56470400	2.46479700
C	-0.34348600	0.52314800	3.19242200
C	-1.20909800	1.72367800	3.63594600
H	0.39821500	0.26400000	3.94879500
H	-0.74697700	2.29216200	4.44426500
C	1.27228700	2.51371100	-0.19245600
O	2.29155800	3.20659000	0.34664800
C	3.02157900	1.66329500	-1.25833900
C	3.44594500	2.92136900	-0.46502500
H	3.27722900	1.75948900	-2.31471100
H	3.62195200	3.78449700	-1.10966700
N	0.33616000	1.03297900	1.98238100
N	1.55190000	1.67595400	-1.10851700
C	-1.20313800	2.36351700	-0.57687400
H	-1.20117100	1.27654600	-0.64954700
H	-2.17265600	2.67479600	-0.18579600
H	-1.07487200	2.79221300	-1.57169400
C	-0.19924000	4.36988200	0.58376400
H	0.55124300	4.72272700	1.28998500
H	-0.05757700	4.88941900	-0.36601600
H	-1.19021100	4.60713000	0.96845700
H	-2.23088100	1.45716000	3.89816600
H	4.29731000	2.75474700	0.19032200
C	-1.15038100	-0.70767600	2.83347700
C	-0.78920400	-1.96561900	3.30612500
C	-2.26538000	-0.58794800	1.99988000
C	-1.53641300	-3.09086300	2.96377800
H	0.08186700	-2.06686900	3.94522100
C	-3.01657700	-1.70650900	1.66166400
H	-2.54894500	0.38460200	1.60719800
C	-2.65312700	-2.96223100	2.14581900
H	-1.24699600	-4.06554800	3.33920300
H	-3.87983900	-1.59917000	1.01690300
H	-3.23715600	-3.83559700	1.88146200
C	3.66421700	0.41318900	-0.69422900
C	4.81970400	-0.08867300	-1.28980100
C	3.18851800	-0.16412300	0.48342400
C	5.51478100	-1.14208900	-0.70279200
H	5.18382900	0.35200100	-2.21275100
C	3.88890600	-1.21188300	1.06909300
H	2.26978400	0.19613200	0.93667800
C	5.05510200	-1.69859600	0.48529800
H	6.41372600	-1.52415000	-1.17254000

H	3.51099900	-1.66109800	1.98048500
H	5.59565200	-2.51679800	0.94699800
C	1.09776000	-3.31458700	0.31191800
C	0.17863300	-2.39582800	-0.17985900
C	0.42230600	-1.73962600	-1.38757000
C	1.61951000	-1.97703100	-2.06873400
C	2.53258700	-2.90017200	-1.57749800
C	2.26809200	-3.57915100	-0.39235200
H	0.89799500	-3.81555100	1.25234500
H	-0.72456200	-2.17585900	0.37658700
H	1.81636900	-1.44963900	-2.99512700
H	3.45618200	-3.08253500	-2.11379200
H	2.98655100	-4.29307500	-0.00622800
C	-0.59095400	-0.84514000	-1.99706200
O	-0.10354200	0.22370200	-2.69805700
C	-1.90181200	-1.11188800	-1.95952500
H	-1.67768400	1.01134300	-3.09771200
H	-2.21879700	-2.03336700	-1.48588300
H	0.55457800	0.71701300	-2.12971200
C	-2.99258700	-0.30266300	-2.61119400
C	-4.15924700	-0.14022400	-1.64971300
F	-5.16483900	0.53746800	-2.20781300
F	-3.81902100	0.50776900	-0.52600900
F	-4.64514400	-1.34060100	-1.27992000
O	-2.64355700	0.99075500	-3.02287100
H	-3.40810500	-0.87609300	-3.45443600

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C	0.14917800	-2.42331000	1.22671400
C	1.51080600	-2.53729200	0.58575300
O	1.69149700	-3.64037600	-0.17611300
C	3.55747900	-2.20642700	-0.15165900
C	2.93526300	-3.42970400	-0.87430600
H	4.35697500	-2.52315900	0.52526600
H	3.53079400	-4.33707200	-0.80156000
C	0.18103400	-1.18830700	2.09301100
O	0.91904800	-1.28126100	3.20814800
C	0.02494300	0.87487100	2.89790400
C	0.76460400	-0.03296300	3.91197500
H	-0.85569100	1.33560500	3.34939800
H	0.17946500	-0.22521400	4.81168300
N	2.44920100	-1.69299800	0.66191900
N	-0.40375100	-0.08314400	1.85797300
C	-0.88171900	-2.28454900	0.09883400
H	-0.65763100	-1.41402100	-0.52081000
H	-0.84764400	-3.17747400	-0.52547500
H	-1.89038100	-2.18008300	0.50044500
C	-0.13886800	-3.66682500	2.08424100
H	0.60485200	-3.78114900	2.87253400
H	-1.12620700	-3.57445700	2.54056800
H	-0.12873900	-4.55319800	1.45022400
H	2.70614400	-3.21187600	-1.91936500
H	1.75429400	0.33467600	4.17451200
C	4.11481400	-1.17293800	-1.10257600
C	5.42146200	-1.31096900	-1.57067900
C	3.33737500	-0.10588400	-1.55383200
C	5.94764500	-0.40327600	-2.48264700
H	6.03377900	-2.13230700	-1.21152000
C	3.86845400	0.80617100	-2.46129700
H	2.32374300	0.02383300	-1.18573700
C	5.17045200	0.66051100	-2.92932500
H	6.96482600	-0.52132800	-2.83676000
H	3.26004700	1.63658800	-2.79812000
H	5.57899100	1.37451000	-3.63438300
C	0.91123300	1.95671000	2.31372100
C	0.67199800	3.29818200	2.59964600
C	2.00819200	1.60817000	1.52263800
C	1.52715800	4.28607800	2.11501100
H	-0.18322100	3.57403400	3.20839100
C	2.85593000	2.59414100	1.03283600
H	2.19933200	0.56451500	1.28647100
C	2.62180500	3.93479600	1.33297500
H	1.33490500	5.32691800	2.34774400

H	3.70033200	2.31160300	0.41368900
H	3.28739800	4.70195900	0.95491800
C	0.27040200	1.57577300	-2.92592600
C	-0.80392800	0.82131600	-2.46929500
C	-1.45547300	1.16999900	-1.28326300
C	-0.99540200	2.26537800	-0.54867600
C	0.07511000	3.02020800	-1.00721700
C	0.70664900	2.68083100	-2.19910300
H	0.77301300	1.29422200	-3.84421800
H	-1.13038600	-0.05298400	-3.02113600
H	-1.48738700	2.53076900	0.37995700
H	0.42097400	3.86654500	-0.42660300
H	1.53954300	3.27564900	-2.55631300
C	-2.62014500	0.40129200	-0.78188700
O	-2.74160400	0.33106200	0.57211000
C	-3.53416500	-0.16149500	-1.58110900
H	-3.99638500	-1.05946600	0.69802400
H	-3.46761100	0.00889100	-2.64723700
H	-1.83961400	0.23423100	0.98934400
C	-4.69649000	-0.98155700	-1.08286900
C	-5.93061300	-0.10118400	-0.92007500
F	-5.75979600	0.81800400	0.03875900
F	-7.01079500	-0.82020000	-0.59131900
F	-6.21789300	0.54861200	-2.05909500
O	-4.47454900	-1.67142800	0.11978600
H	-4.96653100	-1.72597600	-1.83684000

im3-4-(*S*)

C	2.81190700	-2.13364500	1.39453800
C	1.51055200	-2.57020800	0.76193800
O	0.69678500	-3.27858800	1.57563900
C	-0.08860100	-3.14301000	-0.63432600
C	-0.50113600	-3.52751500	0.80790000
H	0.14687200	-4.03982600	-1.21742200
H	-0.77155100	-4.57463700	0.92506400
C	3.40306500	-1.06077600	0.50811000
O	4.27427000	-1.45447300	-0.43076400
C	3.83466900	0.86476300	-0.51427200
C	4.69977400	-0.26401300	-1.12769400
H	4.45507100	1.65839500	-0.09456800
H	5.76413100	-0.12976400	-0.93967600
N	1.16846600	-2.39890400	-0.44511600
N	3.12842400	0.17760700	0.58411200
C	2.57076600	-1.58288800	2.80774300
H	1.88052300	-0.74005700	2.80539400
H	2.15473400	-2.37159600	3.43376500
H	3.51859000	-1.25229500	3.23522900
C	3.73579400	-3.36344800	1.45662800
H	3.91593100	-3.76635600	0.46063700
H	4.69305600	-3.08621100	1.90156400
H	3.26883000	-4.12906400	2.07700000
H	-1.28882300	-2.87744400	1.19198900
H	4.52345700	-0.41267800	-2.19167200
C	-1.15459700	-2.36513100	-1.36669700
C	-2.21292700	-3.04606000	-1.97113800
C	-1.12473500	-0.97529500	-1.41524200
C	-3.22696500	-2.34527300	-2.61426500
H	-2.23744100	-4.13137600	-1.94455000
C	-2.13287500	-0.27328200	-2.06927200
H	-0.30793500	-0.44765100	-0.93445700
C	-3.18568100	-0.95466000	-2.66892400
H	-4.04465100	-2.88364900	-3.07894800
H	-2.09750600	0.81054800	-2.09135200
H	-3.97589100	-0.40620400	-3.16746900
C	2.82280800	1.47379700	-1.45956400
C	2.70319400	2.85591900	-1.57857600
C	1.94653800	0.64428700	-2.16297100
C	1.71502300	3.41063000	-2.38764500
H	3.36914700	3.50166500	-1.01696200
C	0.96923400	1.19756800	-2.98268600
H	2.00128400	-0.43505800	-2.03821000
C	0.84842900	2.58163300	-3.09197000
H	1.61953500	4.48719400	-2.46100300

H	0.28966300	0.54728700	-3.52045900
H	0.07914000	3.01046400	-3.72318300
C	-5.81529300	1.42864500	0.90641700
C	-4.44948400	1.57428700	1.11688600
C	-3.59446100	0.47984800	0.97619500
C	-4.12808700	-0.76583400	0.63771800
C	-5.49314400	-0.90767100	0.42324000
C	-6.34053400	0.18808000	0.55683400
H	-6.47176100	2.28220100	1.02680800
H	-4.04479600	2.53500500	1.41380000
H	-3.45941400	-1.61032300	0.51370500
H	-5.89496500	-1.87514200	0.14562800
H	-7.40595800	0.07554700	0.39465100
C	-2.12823700	0.61058500	1.14423200
O	-1.56580200	-0.51038200	1.65475900
C	-1.45473000	1.69953500	0.74244000
H	-0.60586200	-0.34722700	1.70821400
H	-2.01385400	2.50953000	0.29235200
H	1.60174100	0.69737500	1.17048100
C	0.03867500	1.85279100	0.74231300
C	0.45268300	3.18784200	1.34335800
F	1.79143100	3.30516600	1.36373300
F	0.02503100	3.34877800	2.59655500
F	-0.02631900	4.21054300	0.61575500
O	0.66390200	0.82605400	1.47201900
H	0.40618400	1.88015100	-0.29440400

im3-4-(*R*)

C	1.06577100	-3.04714200	0.59799100
C	2.39381900	-2.71126900	-0.03989800
O	2.68091100	-3.38968400	-1.17426200
C	4.28406500	-1.75168600	-0.63896500
C	4.00645500	-2.96774100	-1.55728200
H	5.26095600	-1.83122800	-0.16064600
H	4.69170000	-3.79496700	-1.36931200
C	0.74176400	-1.89565700	1.52464200
O	1.24722400	-1.96788900	2.76150200
C	0.10709000	0.05834800	2.36988300
C	0.76367900	-0.81004400	3.47355500
H	-0.91154300	0.34076900	2.64389200
H	0.05018400	-1.15358800	4.22289200
N	3.22078700	-1.84954900	0.37745800
N	0.06046300	-0.86514900	1.21830500
C	-0.00530500	-3.17225000	-0.49343200
H	-0.06640400	-2.27070300	-1.10321100
H	0.23515700	-4.01493200	-1.14035200
H	-0.98130900	-3.34134900	-0.03571800
C	1.20009800	-4.36550000	1.37739800
H	1.95758700	-4.28265200	2.15567100
H	0.24543800	-4.62168200	1.84071600
H	1.47741500	-5.16280300	0.68661000
H	3.99348200	-2.72230800	-2.61751400
H	1.61281600	-0.32607300	3.95103300
C	4.17669500	-0.41061400	-1.33732700
C	5.24402200	0.48154500	-1.35326800
C	2.98200700	-0.05217900	-1.96701800
C	5.12518900	1.71565800	-1.99069000
H	6.17343300	0.21278400	-0.86226200
C	2.86180400	1.17337500	-2.60725200
H	2.13994300	-0.73904500	-1.95383000
C	3.93473600	2.06387500	-2.61657600
H	5.96318300	2.40262700	-1.99522500
H	1.93186700	1.43731800	-3.09824500
H	3.84011700	3.02216700	-3.11332400
C	0.90250200	1.30890900	2.05806200
C	0.46124100	2.55047200	2.50617300
C	2.11566700	1.21647400	1.37337700
C	1.23052400	3.68999500	2.28737400
H	-0.49055800	2.63036600	3.02165600
C	2.87551200	2.35655300	1.14172100
H	2.46779600	0.25230900	1.02123700
C	2.43776700	3.59587300	1.60431600
H	0.87649800	4.65296200	2.63709400

H	3.80795300	2.27166600	0.59342800
H	3.03198300	4.48487300	1.42670700
C	-1.77050900	4.08406900	-0.11135000
C	-2.47764800	2.88985600	-0.12142500
C	-1.87182100	1.71033800	-0.56678800
C	-0.52999400	1.74425000	-0.95822800
C	0.17585700	2.94095500	-0.94527000
C	-0.44418100	4.11399800	-0.53242800
H	-2.25207200	4.99037400	0.23640400
H	-3.50245600	2.86401100	0.22987700
H	-0.03583300	0.83130700	-1.27374900
H	1.21994700	2.94942000	-1.23461200
H	0.11294200	5.04323500	-0.51253700
C	-2.64393300	0.44859800	-0.66085000
O	-1.94083000	-0.71592100	-0.58291400
C	-3.95957200	0.40556500	-0.89977700
H	-3.36035400	-1.84858000	-0.09778800
H	-4.49015800	1.32831900	-1.09123700
H	-1.15413400	-0.65901400	0.02839800
C	-4.74088300	-0.88040400	-0.99426600
C	-6.19492200	-0.61594500	-0.65346300
F	-6.72328200	0.28979300	-1.49561800
F	-6.34967900	-0.14107300	0.58665300
F	-6.93260300	-1.72604600	-0.75213300
O	-4.32514500	-1.89019500	-0.10906700
H	-4.74649800	-1.24689600	-2.03221900

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C	3.70466300	0.55256600	-0.70260100
C	3.15595800	-0.84229500	-0.54190200
O	4.06035100	-1.81926500	-0.36053500
C	1.85154600	-2.63884400	-0.38702400
C	3.30452200	-3.00588700	-0.01689600
H	1.57615100	-3.05204500	-1.36157000
H	3.70692300	-3.84177600	-0.58286300
C	2.57968200	1.47049200	-1.12519300
O	2.03734300	1.19932200	-2.33264500
C	1.06278500	3.06666100	-1.27515700
C	0.96510200	2.14913800	-2.51850700
H	1.40921400	4.06237200	-1.57140400
H	1.14376200	2.67725200	-3.45358100
N	1.93089000	-1.17265000	-0.53357600
N	2.14333500	2.45735100	-0.46748600
C	4.28511800	0.99655600	0.64678300
H	3.51622000	0.99371900	1.42117300
H	5.09200300	0.32186200	0.93543900
H	4.67423300	2.01092200	0.55972600
C	4.79373000	0.55071900	-1.79115500
H	4.38890000	0.21705800	-2.74662700
H	5.18291100	1.56349500	-1.90975000
H	5.60950600	-0.10932500	-1.49661100
H	3.42415300	-3.18138100	1.05393700
H	0.03875900	1.58262200	-2.56937500
C	0.79966400	-3.03668400	0.62056800
C	-0.23067000	-3.90261200	0.26243100
C	0.81479800	-2.48304400	1.89973700
C	-1.23581900	-4.21052000	1.17310100
H	-0.26385600	-4.30705900	-0.74283700
C	-0.19746600	-2.77471900	2.80541400
H	1.59860500	-1.78466800	2.17712900
C	-1.22501900	-3.64030600	2.44259700
H	-2.03532000	-4.88384900	0.88631700
H	-0.19383100	-2.30935400	3.78436200
H	-2.01754500	-3.86608300	3.14638600
C	-0.19790300	3.24661300	-0.44284400
C	-1.46533000	2.88079400	-0.88831500
C	-0.07152800	3.81250200	0.82647500
C	-2.57864100	3.04385500	-0.06923800
H	-1.60545900	2.43201400	-1.86278800
C	-1.18064400	3.97937700	1.64566000
H	0.91594000	4.08035000	1.18536300
C	-2.43983500	3.58772000	1.20222600
H	-3.55142400	2.72438700	-0.42570100

H	-1.05850500	4.39539200	2.63900200
H	-3.30408000	3.69810700	1.84673500
C	-1.75289900	0.85888500	3.82114600
C	-2.01498400	0.38110300	2.54540300
C	-1.00542200	0.33591300	1.57766200
C	0.25930800	0.81912600	1.91221500
C	0.52587800	1.29033000	3.19333900
C	-0.47575500	1.30573800	4.15568400
H	-2.54935600	0.89222800	4.55538700
H	-3.01945300	0.06135400	2.29544500
H	1.03997900	0.84596500	1.16336100
H	1.51618100	1.66321300	3.43040200
H	-0.27234300	1.67861300	5.15268300
C	-1.24049300	-0.24600700	0.23201300
O	-0.35877500	0.10843400	-0.75594200
C	-2.24034700	-1.08986300	-0.04298400
H	-0.73128000	-1.22107400	-2.03511100
H	-2.94009700	-1.36164800	0.73465500
H	0.54874500	-0.29187900	-0.59621000
C	-2.45686800	-1.72462600	-1.39352000
C	-3.37590200	-0.84905500	-2.23877200
F	-3.70814600	-1.44323800	-3.39086700
F	-2.79649700	0.32110900	-2.55317300
F	-4.51864000	-0.56874600	-1.59259200
O	-1.29694100	-2.00048900	-2.13607800
H	-2.98885400	-2.67158500	-1.26444500

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C	0.29997300	-1.35972200	-2.57031300
C	0.05857000	-2.21181700	-1.34973100
O	0.43785300	-3.49840200	-1.40701800
C	-0.35067500	-2.90754000	0.71236300
C	-0.07111900	-4.10780000	-0.20071000
H	-1.30396700	-3.02095600	1.23151400
H	-0.98961600	-4.63607000	-0.46037700
C	1.61058600	-0.65172800	-2.33404300
O	1.89735800	0.32501800	-3.22329900
C	3.53877400	0.05594900	-1.55334500
C	3.09327300	0.96238100	-2.73516000
H	4.43664500	-0.51098800	-1.82102300
H	3.81220600	1.01032700	-3.55091600
N	-0.45670000	-1.79929300	-0.26445300
N	2.42794300	-0.89045200	-1.39966800
C	0.39752800	-2.21372200	-3.84299200
H	1.17707000	-2.96934900	-3.74998800
H	-0.55482100	-2.71419300	-4.02710600
H	0.62341800	-1.56630800	-4.69067000
C	-0.82108100	-0.31479000	-2.69907900
H	-0.77524000	0.41211500	-1.88817100
H	-0.71026200	0.22249600	-3.64064900
H	-1.79642300	-0.80353800	-2.66836300
H	0.66678400	-4.81158800	0.17404300
H	2.82918700	1.96913700	-2.40578100
C	0.72521400	-2.55938800	1.72301000
C	0.39727500	-1.68728800	2.76266800
C	2.03367000	-3.02661000	1.61475800
C	1.35377200	-1.31709400	3.70049800
H	-0.61229000	-1.29334800	2.82908100
C	2.99033400	-2.66163800	2.55785100
H	2.32439800	-3.65972700	0.78466400
C	2.65087900	-1.81483200	3.60632800
H	1.08498000	-0.64451600	4.50665000
H	4.00409000	-3.03223200	2.46525400
H	3.39703400	-1.53245600	4.33968100
C	3.81930200	0.82672300	-0.28044200
C	4.68676800	1.92105700	-0.32862100
C	3.22365600	0.48388900	0.93174200
C	4.94014900	2.67549000	0.81031700
H	5.16340100	2.19086800	-1.26668100
C	3.47971600	1.24108900	2.07317800
H	2.54696100	-0.36236900	0.97504900
C	4.33122600	2.33808800	2.01676200
H	5.60950300	3.52597600	0.75668500

H	2.99662200	0.97369900	3.00509800
H	4.51933300	2.92933300	2.90487800
C	-0.72844600	4.65542900	-0.14134600
C	-1.68249800	3.65020500	-0.08111300
C	-1.30385700	2.31299000	0.08391400
C	0.05529000	2.00963500	0.21866800
C	1.01120000	3.02029000	0.15233200
C	0.62319400	4.34228100	-0.03211800
H	-1.04163200	5.68580200	-0.26073000
H	-2.73281000	3.90927800	-0.13443600
H	0.37695300	0.98325600	0.37576400
H	2.06090200	2.77512300	0.25766900
H	1.37029200	5.12586800	-0.07498700
C	-2.32220700	1.23040700	0.10493000
O	-1.98716400	0.08924600	0.78267700
C	-3.51275300	1.33260400	-0.49701800
H	-3.30350500	-1.09588200	0.06720600
H	-3.77097300	2.25057600	-1.00656200
H	-1.27226600	-0.43597600	0.32252800
C	-4.53887300	0.22766600	-0.53613500
C	-5.48528100	0.33771600	0.65401300
F	-6.04133000	1.55807700	0.71991200
F	-4.85560300	0.11628800	1.81401400
F	-6.48503000	-0.54882600	0.57079700
O	-4.01662400	-1.07458900	-0.58616900
H	-5.16973200	0.35430200	-1.41951600

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C	0.31230100	3.38349400	-0.20155700
C	1.43635200	2.57799000	-0.81130400
O	2.53771400	3.25799500	-1.16507300
C	2.69927600	0.95736700	-1.63932000
C	3.35351500	2.33480400	-1.91820700
H	2.54810400	0.39997300	-2.56574700
H	3.29412200	2.62125900	-2.96896100
C	-0.33925100	2.54879100	0.88069000
O	-1.68802500	2.57451900	0.90887500
C	-0.74631600	1.19461300	2.57292900
C	-2.08534300	1.66315600	1.95552800
H	-0.65223100	1.57221100	3.59593400
H	-2.70977500	2.21041800	2.65917000
N	1.39672800	1.33530900	-1.07507800
N	0.27786000	1.86996000	1.74913600
C	0.83965800	4.67624100	0.43995900
H	1.58069400	4.45047500	1.20701300
H	1.29395300	5.31465800	-0.31778200
H	0.00591500	5.20997300	0.89957000
C	-0.68133000	3.70421000	-1.33278700
H	-1.10558900	2.79033500	-1.75144200
H	-1.49517400	4.31830300	-0.94749700
H	-0.16412100	4.25318500	-2.12210200
H	4.37733300	2.41222100	-1.55948800
H	-2.66712300	0.87326100	1.48651200
C	3.50823700	0.10573500	-0.68071400
C	4.52271800	-0.70570500	-1.18919300
C	3.28329300	0.14246000	0.69387600
C	5.31069600	-1.46957500	-0.33698600
H	4.68627800	-0.75075200	-2.26155700
C	4.07213000	-0.62686400	1.54606600
H	2.47540200	0.74765900	1.09584700
C	5.08639900	-1.43114000	1.03690000
H	6.09285100	-2.09983100	-0.74348000
H	3.89114400	-0.59657800	2.61454100
H	5.69664100	-2.02776600	1.70453200
C	-0.46830100	-0.30083800	2.61251400
C	-1.38121200	-1.27743800	2.22324200
C	0.79032200	-0.70467500	3.06752500
C	-1.04050500	-2.62737200	2.28097700
H	-2.36271500	-1.01193100	1.85510300
C	1.13286100	-2.04953800	3.12300900
H	1.50696700	0.05390400	3.36616700
C	0.21447800	-3.01880600	2.72778100
H	-1.76090700	-3.37062400	1.96015600

H	2.11709900	-2.34277200	3.47008600
H	0.48009900	-4.06862000	2.76009200
C	0.80376100	-3.69181600	-2.61562000
C	-0.23694800	-2.78478600	-2.46934700
C	-0.25007400	-1.89379300	-1.39117500
C	0.80557800	-1.91660600	-0.47710700
C	1.84922100	-2.82217000	-0.62813000
C	1.85036000	-3.71306200	-1.69526400
H	0.80708700	-4.37412300	-3.45740300
H	-1.03113500	-2.74780700	-3.20585900
H	0.80855700	-1.23032700	0.36268400
H	2.66309600	-2.81610900	0.08956400
H	2.66612200	-4.41601600	-1.81716900
C	-1.34948300	-0.91462900	-1.20597200
O	-1.01279900	0.23576100	-0.56795400
C	-2.61268800	-1.13935800	-1.58952000
H	-2.58164000	1.20153000	-0.76885700
H	-2.85739600	-2.11048100	-1.99919600
H	-0.06298200	0.49578000	-0.74065800
C	-3.75354500	-0.15842400	-1.51972800
C	-4.80311100	-0.63984900	-0.52323600
F	-5.89085900	0.13594100	-0.53970400
F	-4.34460800	-0.64212300	0.74194700
F	-5.19977200	-1.89122400	-0.80142100
O	-3.43795400	1.17313400	-1.22031500
H	-4.27541800	-0.16739500	-2.48481100

im3-6-(*R*)

C	1.20598200	-2.75081300	-1.72594900
C	0.70625100	-1.36423900	-2.05256700
O	0.88969300	-0.98306100	-3.32615500
C	-0.20404600	0.65569800	-2.02184900
C	0.36673100	0.35756900	-3.43591100
H	0.31739200	1.50302700	-1.56880500
H	1.18863000	1.01677800	-3.71001300
C	0.87430100	-2.99539900	-0.27690300
O	1.68390100	-2.36880000	0.61580800
C	-0.13527600	-3.44860700	1.61994600
C	1.22523700	-2.77580000	1.92217700
H	-0.20867700	-4.41172900	2.13025900
H	1.95578000	-3.47759900	2.32619300
N	0.13049300	-0.55739100	-1.25843000
N	-0.09764400	-3.66929500	0.16598900
C	0.47103000	-3.76183300	-2.61593200
H	-0.60551700	-3.71431000	-2.45059100
H	0.68761300	-3.54986700	-3.66274800
H	0.80937600	-4.77033300	-2.37528100
C	2.72538200	-2.80980100	-1.96400700
H	3.25136500	-2.05298600	-1.38106900
H	3.09903200	-3.79586500	-1.68168500
H	2.93106800	-2.64561900	-3.02181300
H	-0.39748100	0.36117200	-4.21190400
H	1.15303500	-1.88515800	2.54187500
C	-1.69098300	0.93614300	-2.02183400
C	-2.14277700	2.24163000	-2.20257900
C	-2.62030300	-0.09431800	-1.88935900
C	-3.50445600	2.51507700	-2.25882000
H	-1.42401100	3.05122300	-2.27934000
C	-3.98307000	0.17941700	-1.93961200
H	-2.27200400	-1.10883500	-1.73322200
C	-4.42887300	1.48430300	-2.12622100
H	-3.84324300	3.53626900	-2.38935800
H	-4.69847800	-0.62864700	-1.83620100
H	-5.49068200	1.69686900	-2.16419500
C	-1.34245000	-2.60783600	2.01266400
C	-1.46146400	-2.15312700	3.32796400
C	-2.35467000	-2.30912200	1.10339900
C	-2.57302500	-1.42294600	3.72855200
H	-0.68061000	-2.37580800	4.04868900
C	-3.47217800	-1.57946100	1.50446900
H	-2.26533300	-2.66064200	0.08382300
C	-3.58775100	-1.13921900	2.81730700
H	-2.64912800	-1.07588000	4.75204600

H	-4.24784200	-1.34909800	0.78297500
H	-4.45641000	-0.57204700	3.13051100
C	-1.86373300	4.20073300	0.68987900
C	-0.63567200	3.55798600	0.74824400
C	-0.56060800	2.20253900	1.09042300
C	-1.74319300	1.50608000	1.35116100
C	-2.97385600	2.14784700	1.27243400
C	-3.03832900	3.49752900	0.95035400
H	-1.90676300	5.25198800	0.42992300
H	0.26544700	4.11479000	0.51990200
H	-1.69685900	0.45796200	1.61965600
H	-3.88047100	1.58477600	1.46315500
H	-3.99685500	3.99941400	0.88890200
C	0.72861000	1.47525200	1.15928100
O	0.64224600	0.12455100	1.37536200
C	1.94460300	2.01469900	1.04096600
H	2.46096500	-0.53832000	0.30698500
H	2.07474600	3.08543000	0.95973400
H	0.22786000	-0.28872900	0.58298600
C	3.16352400	1.12504200	0.99830800
C	4.39080600	1.94735700	0.66718000
F	4.55544100	2.93564600	1.56279400
F	4.30045600	2.51970900	-0.53995800
F	5.50446500	1.21059300	0.67877300
O	3.10380100	0.12145100	0.01059200
H	3.35327600	0.68764000	1.98738100

(*S*)-enol-P

C	-1.96935700	0.15295300	-0.92800700
C	-2.73335200	-0.49817200	0.21850800
F	-4.03779500	-0.16081100	0.15845500
F	-2.28462400	-0.10630400	1.41217100
F	-2.65949200	-1.82912200	0.15984900
O	-2.16646700	1.55613600	-0.84798000
H	-3.11028800	1.74788200	-0.86567000
H	-2.40437400	-0.24804600	-1.84931900
C	3.57750400	-1.52572300	-0.14445000
C	2.23014100	-1.19667100	-0.20537700
C	1.81998400	0.13064800	-0.05661400
C	2.77902600	1.11738400	0.18139700
C	4.12710800	0.78527200	0.24116900
C	4.53058900	-0.53512900	0.07486900
H	3.88355200	-2.55905700	-0.25469200
H	1.49144200	-1.97751300	-0.34097800
H	2.45799100	2.14217700	0.31539800
H	4.86337800	1.55975800	0.41952900
H	5.58137900	-0.79392900	0.12572100
C	0.38926100	0.51048200	-0.13741500
O	0.11433200	1.63384400	0.55817100
C	-0.50965000	-0.17858800	-0.86035900
H	-0.77968100	1.92933500	0.32776600
H	-0.17663600	-1.02905400	-1.43588900

(*R*)-enol-P

C	-1.96935700	0.15295300	0.92800700
C	-2.73335200	-0.49817200	-0.21850800
F	-4.03779500	-0.16081100	-0.15845500
F	-2.28462400	-0.10630400	-1.41217100
F	-2.65949200	-1.82912200	-0.15984900
O	-2.16646700	1.55613600	0.84798000
H	-3.11028800	1.74788200	0.86567000
H	-2.40437400	-0.24804600	1.84931900
C	3.57750400	-1.52572300	0.14445000
C	2.23014100	-1.19667100	0.20537700
C	1.81998400	0.13064800	0.05661400
C	2.77902600	1.11738400	-0.18139700
C	4.12710800	0.78527200	-0.24116900
C	4.53058900	-0.53512900	-0.07486900
H	3.88355200	-2.55905700	0.25469200
H	1.49144200	-1.97751300	0.34097800
H	2.45799100	2.14217700	-0.31539800
H	4.86337800	1.55975800	-0.41952900
H	5.58137900	-0.79392900	-0.12572100
C	0.38926100	0.51048200	0.13741500
O	0.11433200	1.63384400	-0.55817100
C	-0.50965000	-0.17858800	0.86035900
H	-0.77968100	1.92933500	-0.32776600
H	-0.17663600	-1.02905400	1.43588900

TS_T-*S*

C	-7.00689700	0.44526200	1.23996800
C	-5.63202800	0.41496000	1.05311000
C	-5.08085700	-0.30995300	-0.00712800
C	-5.92962000	-0.98759100	-0.88587400
C	-7.30504100	-0.95870400	-0.69318700
C	-7.84680300	-0.24483800	0.37024400
H	-7.42452300	1.01540200	2.06082100
H	-4.98953100	0.97623000	1.72003800
H	-5.50118400	-1.53728100	-1.71360100
H	-7.95446000	-1.49349900	-1.37557500
H	-8.91977800	-0.21951800	0.51794700
C	-3.61772300	-0.37290200	-0.22474500
O	-3.28453500	-0.71579200	-1.46751700
C	-2.70721900	-0.13039200	0.75378100
H	-2.30318400	-0.75434500	-1.50219600
H	-3.02659300	0.10061500	1.75721000
C	-1.27231200	-0.20050300	0.52174500
O	-0.84992800	-0.52650400	-0.63543200
O	-0.50514000	0.05862500	1.50138300
H	0.70921800	0.17463400	1.20993600
C	1.62837400	1.91189300	0.23737200
C	2.90641400	2.59696400	-0.23238300
F	2.63534700	3.80168500	-0.75976200
F	3.54719900	1.88770300	-1.16588700
F	3.75998500	2.78678100	0.78553200
O	0.74445400	1.81942000	-0.84567600
H	0.43219400	2.69970900	-1.07565500
H	1.22488500	2.53371700	1.04593700
C	5.73444200	-1.68077500	0.84653700
C	4.61736300	-0.87023400	0.69730800
C	3.46469600	-1.37687600	0.09029100
C	3.44433900	-2.69485700	-0.37688200
C	4.55779300	-3.50469500	-0.21333200
C	5.70199100	-2.99809100	0.39893700
H	6.63120700	-1.28415400	1.30578600
H	4.65163000	0.16341400	1.02029300
H	2.54816900	-3.06876300	-0.85537800
H	4.53738400	-4.52943600	-0.56280800
H	6.57303200	-3.63063400	0.52197100
C	2.27694500	-0.52177400	-0.10536800
O	1.50746900	-0.86023300	-1.06670700
C	1.95448200	0.53636100	0.79204600
H	0.47251600	-0.56385800	-0.91709400
H	2.62765800	0.60857100	1.64036400

Value of Imaginary Frequency= -1384.3 cm^{-1}

TS_T-*R*

C	-7.00689700	0.44526200	-1.23996800
C	-5.63202800	0.41496000	-1.05311000
C	-5.08085700	-0.30995300	0.00712800
C	-5.92962000	-0.98759100	0.88587400
C	-7.30504100	-0.95870400	0.69318700
C	-7.84680300	-0.24483800	-0.37024400
H	-7.42452300	1.01540200	-2.06082100
H	-4.98953100	0.97623000	-1.72003800
H	-5.50118400	-1.53728100	1.71360100
H	-7.95446000	-1.49349900	1.37557500
H	-8.91977800	-0.21951800	-0.51794700
C	-3.61772300	-0.37290200	0.22474500
O	-3.28453500	-0.71579200	1.46751700
C	-2.70721900	-0.13039200	-0.75378100
H	-2.30318400	-0.75434500	1.50219600
H	-3.02659300	0.10061500	-1.75721000
C	-1.27231200	-0.20050300	-0.52174500
O	-0.84992800	-0.52650400	0.63543200
O	-0.50514000	0.05862500	-1.50138300
H	0.70921800	0.17463400	-1.20993600
C	1.62837400	1.91189300	-0.23737200
C	2.90641400	2.59696400	0.23238300
F	2.63534700	3.80168500	0.75976200
F	3.54719900	1.88770300	1.16588700
F	3.75998500	2.78678100	-0.78553200
O	0.74445400	1.81942000	0.84567600
H	0.43219400	2.69970900	1.07565500
H	1.22488500	2.53371700	-1.04593700
C	5.73444200	-1.68077500	-0.84653700
C	4.61736300	-0.87023400	-0.69730800
C	3.46469600	-1.37687600	-0.09029100
C	3.44433900	-2.69485700	0.37688200
C	4.55779300	-3.50469500	0.21333200
C	5.70199100	-2.99809100	-0.39893700
H	6.63120700	-1.28415400	-1.30578600
H	4.65163000	0.16341400	-1.02029300
H	2.54816900	-3.06876300	0.85537800
H	4.53738400	-4.52943600	0.56280800
H	6.57303200	-3.63063400	-0.52197100
C	2.27694500	-0.52177400	0.10536800
O	1.50746900	-0.86023300	1.06670700
C	1.95448200	0.53636100	-0.79204600
H	0.47251600	-0.56385800	0.91709400
H	2.62765800	0.60857100	-1.64036400

Value of Imaginary Frequency= -1384.3 cm^{-1}

TS_T-*S'*

C	2.16137600	0.56471100	0.47814600
C	2.06040700	-0.81725900	-0.15655600
F	3.20493300	-1.14032100	-0.79046600
F	1.07901500	-0.89430400	-1.06121500
F	1.83781500	-1.76884200	0.76321500
O	2.44100400	1.48649900	-0.55030600
H	3.26876000	1.23743400	-0.97338400
H	2.98358700	0.49931500	1.20094100
C	-2.68355200	-1.63310700	0.35581700
C	-1.52992700	-0.89560800	0.58002900
C	-1.48591800	0.45280600	0.21314200
C	-2.59986900	1.05845500	-0.37932500
C	-3.74590900	0.31441700	-0.61148500
C	-3.78701900	-1.02865600	-0.24088800
H	-2.72223100	-2.67792100	0.63695300
H	-0.65661000	-1.35989600	1.02255800
H	-2.54802900	2.10698000	-0.64524100
H	-4.60952900	0.77708000	-1.07252000
H	-4.68578700	-1.60746400	-0.41800000
C	-0.27599800	1.23706900	0.44741100
O	-0.16777400	2.42695800	0.00216700
C	0.90741600	0.95135800	1.23620600
H	0.78642800	2.38575900	0.77098900
H	0.77566300	0.33716100	2.12403100

Value of Imaginary Frequency= -2061.7 cm^{-1}

TS_T-*R'*

C	2.16137600	0.56471100	-0.47814600
C	2.06040700	-0.81725900	0.15655600
F	3.20493300	-1.14032100	0.79046600
F	1.07901500	-0.89430400	1.06121500
F	1.83781500	-1.76884200	-0.76321500
O	2.44100400	1.48649900	0.55030600
H	3.26876000	1.23743400	0.97338400
H	2.98358700	0.49931500	-1.20094100
C	-2.68355200	-1.63310700	-0.35581700
C	-1.52992700	-0.89560800	-0.58002900
C	-1.48591800	0.45280600	-0.21314200
C	-2.59986900	1.05845500	0.37932500
C	-3.74590900	0.31441700	0.61148500
C	-3.78701900	-1.02865600	0.24088800
H	-2.72223100	-2.67792100	-0.63695300
H	-0.65661000	-1.35989600	-1.02255800
H	-2.54802900	2.10698000	0.64524100
H	-4.60952900	0.77708000	1.07252000
H	-4.68578700	-1.60746400	0.41800000
C	-0.27599800	1.23706900	-0.44741100
O	-0.16777400	2.42695800	-0.00216700
C	0.90741600	0.95135800	-1.23620600
H	0.78642800	2.38575900	-0.77098900
H	0.77566300	0.33716100	-2.12403100

Value of Imaginary Frequency= -2061.7 cm^{-1}

(*S*)-P

C	2.06495900	0.15909100	-0.93332700
C	2.64962500	0.36873700	0.45796500
F	2.46219200	1.63838300	0.86242700
F	2.09667100	-0.42588000	1.38265300
F	3.96401700	0.13705000	0.46773800
O	2.36675800	-1.12182500	-1.40295700
H	2.60400400	0.86912000	-1.56606700
C	-3.65829900	1.34612600	-0.33336400
C	-2.31588900	1.06244400	-0.55585900
C	-1.78170500	-0.16028300	-0.14385400
C	-2.60388100	-1.09388200	0.49271100
C	-3.94045400	-0.80547700	0.72106900
C	-4.46877700	0.41533000	0.30722400
H	-4.06978100	2.29341900	-0.65931800
H	-1.69868400	1.79688900	-1.05848700
H	-2.17350500	-2.03838600	0.80177600
H	-4.57277800	-1.52951900	1.21996400
H	-5.51392700	0.63995100	0.48420200
C	-0.35297500	-0.53170100	-0.37463800
O	0.03888600	-1.65053000	-0.11389900
C	0.57456900	0.51124500	-0.97800500
H	1.78004300	-1.73107200	-0.93283700
H	0.28142400	0.62267000	-2.02736300
H	0.40909100	1.48000500	-0.50191800

(*R*)-P

C	2.06495900	0.15909100	0.93332700
C	2.64962500	0.36873700	-0.45796500
F	2.46219200	1.63838300	-0.86242700
F	2.09667100	-0.42588000	-1.38265300
F	3.96401700	0.13705000	-0.46773800
O	2.36675800	-1.12182500	1.40295700
H	2.60400400	0.86912000	1.56606700
C	-3.65829900	1.34612600	0.33336400
C	-2.31588900	1.06244400	0.55585900
C	-1.78170500	-0.16028300	0.14385400
C	-2.60388100	-1.09388200	-0.49271100
C	-3.94045400	-0.80547700	-0.72106900
C	-4.46877700	0.41533000	-0.30722400
H	-4.06978100	2.29341900	0.65931800
H	-1.69868400	1.79688900	1.05848700
H	-2.17350500	-2.03838600	-0.80177600
H	-4.57277800	-1.52951900	-1.21996400
H	-5.51392700	0.63995100	-0.48420200
C	-0.35297500	-0.53170100	0.37463800
O	0.03888600	-1.65053000	0.11389900
C	0.57456900	0.51124500	0.97800500
H	1.78004300	-1.73107200	0.93283700
H	0.28142400	0.62267000	2.02736300
H	0.40909100	1.48000500	0.50191800

18. Cartesian coordinates of all the optimized structures of the reactant, intermediates, transition states and products in the uncatalyzed reaction between *β*-CA_1 and CF_3CHO.

CF_3CHO

C	-1.06110300	-0.58379300	-0.00065700
C	0.35783200	0.00155600	-0.00014700
F	1.01905700	-0.42695200	1.07979000
F	0.34914900	1.32406200	0.00060400
F	1.02006000	-0.42578000	-1.07963900
O	-2.02291900	0.11715800	-0.00005900
H	-1.09140800	-1.68580700	-0.00149700

***β*-CA$_1$**

C	2.83152000	-1.43088500	-0.17563400
C	1.46390000	-1.20272600	-0.22958300
C	0.95775400	0.08590300	-0.03746900
C	1.84201800	1.14265100	0.19315300
C	3.20993500	0.90926900	0.25121300
C	3.70737100	-0.37665200	0.06908800
H	3.21562700	-2.43129400	-0.33281200
H	0.79345000	-2.02524400	-0.44546900
H	1.44751800	2.14082400	0.33025000
H	3.88802200	1.73304600	0.43769900
H	4.77472700	-0.55737700	0.11089700
C	-0.49509400	0.35785400	-0.07579700
O	-0.79281300	1.63653400	-0.27840300
C	-1.44581900	-0.59942500	0.10378700
H	-1.77390100	1.71864500	-0.26456800
H	-1.18277200	-1.62362500	0.31067500
C	-2.84431700	-0.23885800	0.05808300
O	-3.27390200	0.89372900	-0.12705000
O	-3.67682600	-1.26976400	0.24429200
H	-4.57795200	-0.92175200	0.20158300

^{uncat}TS1-*S*

C	1.94661900	0.73171500	0.08671000
O	2.18479900	0.62400100	1.31361900
C	-3.41028800	-0.74074800	-1.31382400
C	-2.06422700	-0.94123300	-1.04381000
C	-1.54534200	-0.59280600	0.20708000
C	-2.38555300	-0.04918200	1.18577200
C	-3.72784800	0.15216300	0.90849700
C	-4.24017600	-0.19228000	-0.34058300
H	-3.81323300	-1.01642500	-2.28009700
H	-1.42746200	-1.39103100	-1.79515300
H	-1.96834400	0.22221800	2.14679100
H	-4.37618300	0.58139800	1.66191500
H	-5.29038000	-0.03450600	-0.55481000
C	-0.12658100	-0.79148200	0.52022600
O	0.20556500	-0.77312900	1.76448700
C	0.88603700	-0.87952100	-0.46311600
H	1.15818400	-0.39314500	1.83302500
H	0.59458300	-0.76638600	-1.49763600
C	2.00248600	-1.82675700	-0.23339500
O	2.34589500	-2.27803500	0.82469200
O	2.62940900	-2.10236700	-1.39175900
H	3.36372600	-2.69743900	-1.18596800
H	2.73091700	0.55779500	-0.66602000
C	1.01734800	1.87386000	-0.34260100
F	1.70427900	3.02136800	-0.32972200
F	-0.01579400	2.00940000	0.49141100
F	0.53240200	1.71494100	-1.58125600

Value of Imaginary Frequency= -493.9 cm^{-1}

^{uncat}TS1-*R*

C	1.28307700	-0.89085800	-0.65273600
C	2.51029400	-1.09915900	0.24187100
F	2.19145700	-1.23569300	1.53490000
F	3.39571200	-0.11376300	0.12897300
F	3.11352900	-2.23425900	-0.13636100
O	1.49107100	-0.42833800	-1.80095600
H	0.54792500	-1.69320500	-0.47680700
C	-3.84891000	-0.20089500	1.56834400
C	-2.56100300	0.18548700	1.22802900
C	-2.15299200	0.14888400	-0.11003700
C	-3.04927800	-0.26634400	-1.10246700
C	-4.33256700	-0.65768000	-0.75442000
C	-4.73189600	-0.62626100	0.57961400
H	-4.16708500	-0.16367300	2.60245500
H	-1.88677900	0.54295200	1.99613800
H	-2.72326500	-0.28414600	-2.13438100
H	-5.02286300	-0.98711000	-1.52067500
H	-5.73671700	-0.92865700	0.84900600
C	-0.79843600	0.55590400	-0.50126300
O	-0.61090600	0.83408500	-1.74325000
C	0.30746200	0.53415500	0.38250500
H	0.36114000	0.56629600	-1.98193500
H	0.13185300	0.18078000	1.38885800
C	1.28204700	1.64701400	0.26630400
O	1.52819300	2.25966400	-0.73680100
O	1.86851900	1.89141600	1.44990000
H	2.52771100	2.58409700	1.30412600

Value of Imaginary Frequency= -527.0 cm^{-1}

^{uncat}IM1-*S*

C	1.30973800	-0.41862100	-0.71757800
O	0.49444500	-1.50598500	-1.06553800
C	-3.39158100	-1.56197700	0.88897700
C	-2.15227300	-1.00550300	0.59985200
C	-2.08094000	0.19515200	-0.11085200
C	-3.25439600	0.82972900	-0.53133100
C	-4.48850200	0.27860200	-0.22573900
C	-4.55663400	-0.91781700	0.48536300
H	-3.44761300	-2.49864100	1.42915900
H	-1.25082800	-1.52957500	0.88858200
H	-3.17686800	1.75487300	-1.08882300
H	-5.39704700	0.77700500	-0.53991000
H	-5.52133800	-1.35048200	0.72213100
C	-0.79098900	0.82938600	-0.46896700
O	-0.71836300	1.67767100	-1.33845500
C	0.49332100	0.43198800	0.26566900
H	0.91913800	-2.01177800	-1.76642200
H	0.29028800	-0.16126500	1.15346500
C	1.29044000	1.65635900	0.74567800
O	1.76017300	1.70028700	1.84294200
O	1.46344800	2.62939700	-0.14692600
H	0.85286100	2.49488400	-0.89618600
H	1.59334000	0.18364400	-1.58902500
C	2.59910400	-0.93614100	-0.09254000
F	3.15460400	-1.84797600	-0.90698700
F	2.38977800	-1.52529100	1.08430900
F	3.48636500	0.04475900	0.08041700

^{uncat}IM1-*R*

C	1.88560100	-0.29709400	-0.28363900
C	1.38193400	-1.73081300	-0.26925700
F	2.25884700	-2.56106400	-0.82461900
F	1.14165500	-2.15601600	0.97615200
F	0.23174300	-1.82807300	-0.95450900
O	3.08858700	-0.30638500	0.42761800
H	3.67591000	0.37131700	0.08090200
H	2.01839500	-0.02155800	-1.33519700
C	-3.21368900	-0.87615800	1.26884900
C	-1.92329200	-0.47976500	0.94248200
C	-1.71361800	0.38629300	-0.13389000
C	-2.80334900	0.84511000	-0.88139700
C	-4.08978000	0.45686100	-0.54414700
C	-4.29493800	-0.40398500	0.53220500
H	-3.37429200	-1.55418600	2.09743000
H	-1.09261100	-0.87338100	1.51437300
H	-2.61953200	1.50784700	-1.71766800
H	-4.93302000	0.82116500	-1.11748900
H	-5.30055400	-0.70981500	0.79490900
C	-0.36302400	0.83369400	-0.54802900
O	-0.17531500	1.38641200	-1.61731700
C	0.84183000	0.64251700	0.37244700
H	1.38062500	2.32331900	-1.23867500
H	0.58255300	0.25924100	1.35534100
C	1.55668200	1.97822300	0.62027300
O	1.89762800	2.65584600	-0.48110300
O	1.86237200	2.34576700	1.71298500

^{uncat}TS2-*S*

C	1.53610600	-0.42059100	-0.73539200
O	1.10727400	-1.64430600	-1.28874500
C	-3.58135500	-1.58512100	0.87424700
C	-2.30046000	-1.18017200	0.53133200
C	-2.11631200	0.00951000	-0.18381000
C	-3.22321600	0.77985700	-0.56498700
C	-4.49860600	0.37343100	-0.20945500
C	-4.67675500	-0.80639000	0.51080100
H	-3.72716900	-2.50932600	1.41857900
H	-1.44872200	-1.80024700	0.78056100
H	-3.06617300	1.69418900	-1.12249300
H	-5.35514400	0.97318100	-0.48987800
H	-5.67588900	-1.12314400	0.78507500
C	-0.77614700	0.43931200	-0.56393600
O	-0.70225100	1.26732800	-1.56722200
C	0.40299000	0.08936300	0.13540400
H	1.80071700	-1.98643600	-1.86405000
H	0.24427600	-0.52059200	1.01649600
C	0.98709000	1.77061500	0.72294500
O	1.11138700	1.76632600	1.90411300
O	1.13652300	2.46425700	-0.26939600
H	0.13164300	1.80358100	-1.44205900
H	1.80075400	0.30835100	-1.50873200
C	2.80077000	-0.66856300	0.07879600
F	3.68883900	-1.34568900	-0.67074500
F	2.56577100	-1.39840500	1.17056100
F	3.38401300	0.46899500	0.45805300

Value of Imaginary Frequency= -400.5 cm^{-1}

^{uncat}TS2-*R*

C	1.93643200	-0.04097700	-0.27008300
C	1.86694600	-1.56584800	-0.25387000
F	2.94816600	-2.11574500	-0.79975400
F	1.76318200	-2.03112200	1.00163400
F	0.79568600	-2.00543300	-0.93246800
O	3.09882600	0.36627000	0.39222200
H	2.92374100	0.42207700	1.33891500
H	2.03722900	0.25786200	-1.31588300
C	-3.26301000	-1.33369500	1.08667800
C	-1.98755800	-0.89253400	0.76972000
C	-1.82135700	0.14965000	-0.15089200
C	-2.93935400	0.73221800	-0.76225800
C	-4.21072300	0.29130500	-0.43364200
C	-4.37206200	-0.73880500	0.49078700
H	-3.39356500	-2.14521700	1.79101500
H	-1.12340600	-1.37743200	1.20721300
H	-2.79547800	1.53202500	-1.47714300
H	-5.07721600	0.74808500	-0.89466900
H	-5.36753000	-1.08385600	0.74317900
C	-0.48517200	0.61574200	-0.50609300
O	-0.37860200	1.24942000	-1.63903400
C	0.64576600	0.50431700	0.33244300
H	0.39166500	1.88515600	-1.54346600
H	0.43784600	0.10054000	1.31831300
C	1.18944700	2.28155200	0.59123100
O	1.22909500	2.82692900	-0.49398000
O	1.43159000	2.43411900	1.74625400

Value of Imaginary Frequency= -430.6 cm^{-1}

(*S*)-enol-P

C	-1.96935700	0.15295300	-0.92800700
C	-2.73335200	-0.49817200	0.21850800
F	-4.03779500	-0.16081100	0.15845500
F	-2.28462400	-0.10630400	1.41217100
F	-2.65949200	-1.82912200	0.15984900
O	-2.16646700	1.55613600	-0.84798000
H	-3.11028800	1.74788200	-0.86567000
H	-2.40437400	-0.24804600	-1.84931900
C	3.57750400	-1.52572300	-0.14445000
C	2.23014100	-1.19667100	-0.20537700
C	1.81998400	0.13064800	-0.05661400
C	2.77902600	1.11738400	0.18139700
C	4.12710800	0.78527200	0.24116900
C	4.53058900	-0.53512900	0.07486900
H	3.88355200	-2.55905700	-0.25469200
H	1.49144200	-1.97751300	-0.34097800
H	2.45799100	2.14217700	0.31539800
H	4.86337800	1.55975800	0.41952900
H	5.58137900	-0.79392900	0.12572100
C	0.38926100	0.51048200	-0.13741500
O	0.11433200	1.63384400	0.55817100
C	-0.50965000	-0.17858800	-0.86035900
H	-0.77968100	1.92933500	0.32776600
H	-0.17663600	-1.02905400	-1.43588900

(*R*)-enol-P

C	-1.96935700	0.15295300	0.92800700
C	-2.73335200	-0.49817200	-0.21850800
F	-4.03779500	-0.16081100	-0.15845500
F	-2.28462400	-0.10630400	-1.41217100
F	-2.65949200	-1.82912200	-0.15984900
O	-2.16646700	1.55613600	0.84798000
H	-3.11028800	1.74788200	0.86567000
H	-2.40437400	-0.24804600	1.84931900
C	3.57750400	-1.52572300	0.14445000
C	2.23014100	-1.19667100	0.20537700
C	1.81998400	0.13064800	0.05661400
C	2.77902600	1.11738400	-0.18139700
C	4.12710800	0.78527200	-0.24116900
C	4.53058900	-0.53512900	-0.07486900
H	3.88355200	-2.55905700	0.25469200
H	1.49144200	-1.97751300	0.34097800
H	2.45799100	2.14217700	-0.31539800
H	4.86337800	1.55975800	-0.41952900
H	5.58137900	-0.79392900	-0.12572100
C	0.38926100	0.51048200	0.13741500
O	0.11433200	1.63384400	-0.55817100
C	-0.50965000	-0.17858800	0.86035900
H	-0.77968100	1.92933500	-0.32776600
H	-0.17663600	-1.02905400	1.43588900

$^{uncat}TS_T$-*S*

C	-7.00689700	0.44526200	1.23996800
C	-5.63202800	0.41496000	1.05311000
C	-5.08085700	-0.30995300	-0.00712800
C	-5.92962000	-0.98759100	-0.88587400
C	-7.30504100	-0.95870400	-0.69318700
C	-7.84680300	-0.24483800	0.37024400
H	-7.42452300	1.01540200	2.06082100
H	-4.98953100	0.97623000	1.72003800
H	-5.50118400	-1.53728100	-1.71360100
H	-7.95446000	-1.49349900	-1.37557500
H	-8.91977800	-0.21951800	0.51794700
C	-3.61772300	-0.37290200	-0.22474500
O	-3.28453500	-0.71579200	-1.46751700
C	-2.70721900	-0.13039200	0.75378100
H	-2.30318400	-0.75434500	-1.50219600
H	-3.02659300	0.10061500	1.75721000
C	-1.27231200	-0.20050300	0.52174500
O	-0.84992800	-0.52650400	-0.63543200
O	-0.50514000	0.05862500	1.50138300
H	0.70921800	0.17463400	1.20993600
C	1.62837400	1.91189300	0.23737200
C	2.90641400	2.59696400	-0.23238300
F	2.63534700	3.80168500	-0.75976200
F	3.54719900	1.88770300	-1.16588700
F	3.75998500	2.78678100	0.78553200
O	0.74445400	1.81942000	-0.84567600
H	0.43219400	2.69970900	-1.07565500
H	1.22488500	2.53371700	1.04593700
C	5.73444200	-1.68077500	0.84653700
C	4.61736300	-0.87023400	0.69730800
C	3.46469600	-1.37687600	0.09029100
C	3.44433900	-2.69485700	-0.37688200
C	4.55779300	-3.50469500	-0.21333200
C	5.70199100	-2.99809100	0.39893700
H	6.63120700	-1.28415400	1.30578600
H	4.65163000	0.16341400	1.02029300
H	2.54816900	-3.06876300	-0.85537800
H	4.53738400	-4.52943600	-0.56280800
H	6.57303200	-3.63063400	0.52197100
C	2.27694500	-0.52177400	-0.10536800
O	1.50746900	-0.86023300	-1.06670700
C	1.95448200	0.53636100	0.79204600
H	0.47251600	-0.56385800	-0.91709400
H	2.62765800	0.60857100	1.64036400

Value of Imaginary Frequency= -1384.3 cm^{-1}

$^{uncat}TS_T$-*R*

C	-7.00689700	0.44526200	-1.23996800
C	-5.63202800	0.41496000	-1.05311000
C	-5.08085700	-0.30995300	0.00712800
C	-5.92962000	-0.98759100	0.88587400
C	-7.30504100	-0.95870400	0.69318700
C	-7.84680300	-0.24483800	-0.37024400
H	-7.42452300	1.01540200	-2.06082100
H	-4.98953100	0.97623000	-1.72003800
H	-5.50118400	-1.53728100	1.71360100
H	-7.95446000	-1.49349900	1.37557500
H	-8.91977800	-0.21951800	-0.51794700
C	-3.61772300	-0.37290200	0.22474500
O	-3.28453500	-0.71579200	1.46751700
C	-2.70721900	-0.13039200	-0.75378100
H	-2.30318400	-0.75434500	1.50219600
H	-3.02659300	0.10061500	-1.75721000
C	-1.27231200	-0.20050300	-0.52174500
O	-0.84992800	-0.52650400	0.63543200
O	-0.50514000	0.05862500	-1.50138300
H	0.70921800	0.17463400	-1.20993600
C	1.62837400	1.91189300	-0.23737200
C	2.90641400	2.59696400	0.23238300
F	2.63534700	3.80168500	0.75976200
F	3.54719900	1.88770300	1.16588700
F	3.75998500	2.78678100	-0.78553200
O	0.74445400	1.81942000	0.84567600
H	0.43219400	2.69970900	1.07565500
H	1.22488500	2.53371700	-1.04593700
C	5.73444200	-1.68077500	-0.84653700
C	4.61736300	-0.87023400	-0.69730800
C	3.46469600	-1.37687600	-0.09029100
C	3.44433900	-2.69485700	0.37688200
C	4.55779300	-3.50469500	0.21333200
C	5.70199100	-2.99809100	-0.39893700
H	6.63120700	-1.28415400	-1.30578600
H	4.65163000	0.16341400	-1.02029300
H	2.54816900	-3.06876300	0.85537800
H	4.53738400	-4.52943600	0.56280800
H	6.57303200	-3.63063400	-0.52197100
C	2.27694500	-0.52177400	0.10536800
O	1.50746900	-0.86023300	1.06670700
C	1.95448200	0.53636100	-0.79204600
H	0.47251600	-0.56385800	0.91709400
H	2.62765800	0.60857100	-1.64036400

Value of Imaginary Frequency= -1384.3 cm^{-1}

$^{uncat}TS_T$-*S'*

C	2.16137600	0.56471100	0.47814600
C	2.06040700	-0.81725900	-0.15655600
F	3.20493300	-1.14032100	-0.79046600
F	1.07901500	-0.89430400	-1.06121500
F	1.83781500	-1.76884200	0.76321500
O	2.44100400	1.48649900	-0.55030600
H	3.26876000	1.23743400	-0.97338400
H	2.98358700	0.49931500	1.20094100
C	-2.68355200	-1.63310700	0.35581700
C	-1.52992700	-0.89560800	0.58002900
C	-1.48591800	0.45280600	0.21314200
C	-2.59986900	1.05845500	-0.37932500
C	-3.74590900	0.31441700	-0.61148500
C	-3.78701900	-1.02865600	-0.24088800
H	-2.72223100	-2.67792100	0.63695300
H	-0.65661000	-1.35989600	1.02255800
H	-2.54802900	2.10698000	-0.64524100
H	-4.60952900	0.77708000	-1.07252000
H	-4.68578700	-1.60746400	-0.41800000
C	-0.27599800	1.23706900	0.44741100
O	-0.16777400	2.42695800	0.00216700
C	0.90741600	0.95135800	1.23620600
H	0.78642800	2.38575900	0.77098900
H	0.77566300	0.33716100	2.12403100

Value of Imaginary Frequency= -2061.7 cm^{-1}

$^{uncat}TS_T$-*R*'

C	2.16137600	0.56471100	-0.47814600
C	2.06040700	-0.81725900	0.15655600
F	3.20493300	-1.14032100	0.79046600
F	1.07901500	-0.89430400	1.06121500
F	1.83781500	-1.76884200	-0.76321500
O	2.44100400	1.48649900	0.55030600
H	3.26876000	1.23743400	0.97338400
H	2.98358700	0.49931500	-1.20094100
C	-2.68355200	-1.63310700	-0.35581700
C	-1.52992700	-0.89560800	-0.58002900
C	-1.48591800	0.45280600	-0.21314200
C	-2.59986900	1.05845500	0.37932500
C	-3.74590900	0.31441700	0.61148500
C	-3.78701900	-1.02865600	0.24088800
H	-2.72223100	-2.67792100	-0.63695300
H	-0.65661000	-1.35989600	-1.02255800
H	-2.54802900	2.10698000	0.64524100
H	-4.60952900	0.77708000	1.07252000
H	-4.68578700	-1.60746400	0.41800000
C	-0.27599800	1.23706900	-0.44741100
O	-0.16777400	2.42695800	-0.00216700
C	0.90741600	0.95135800	-1.23620600
H	0.78642800	2.38575900	-0.77098900
H	0.77566300	0.33716100	-2.12403100

Value of Imaginary Frequency= -2061.7 cm^{-1}

(*S*)-P

C	2.06495900	0.15909100	-0.93332700
C	2.64962500	0.36873700	0.45796500
F	2.46219200	1.63838300	0.86242700
F	2.09667100	-0.42588000	1.38265300
F	3.96401700	0.13705000	0.46773800
O	2.36675800	-1.12182500	-1.40295700
H	2.60400400	0.86912000	-1.56606700
C	-3.65829900	1.34612600	-0.33336400
C	-2.31588900	1.06244400	-0.55585900
C	-1.78170500	-0.16028300	-0.14385400
C	-2.60388100	-1.09388200	0.49271100
C	-3.94045400	-0.80547700	0.72106900
C	-4.46877700	0.41533000	0.30722400
H	-4.06978100	2.29341900	-0.65931800
H	-1.69868400	1.79688900	-1.05848700
H	-2.17350500	-2.03838600	0.80177600
H	-4.57277800	-1.52951900	1.21996400
H	-5.51392700	0.63995100	0.48420200
C	-0.35297500	-0.53170100	-0.37463800
O	0.03888600	-1.65053000	-0.11389900
C	0.57456900	0.51124500	-0.97800500
H	1.78004300	-1.73107200	-0.93283700
H	0.28142400	0.62267000	-2.02736300
H	0.40909100	1.48000500	-0.50191800

(*R*)-P

C	2.06495900	0.15909100	0.93332700
C	2.64962500	0.36873700	-0.45796500
F	2.46219200	1.63838300	-0.86242700
F	2.09667100	-0.42588000	-1.38265300
F	3.96401700	0.13705000	-0.46773800
O	2.36675800	-1.12182500	1.40295700
H	2.60400400	0.86912000	1.56606700
C	-3.65829900	1.34612600	0.33336400
C	-2.31588900	1.06244400	0.55585900
C	-1.78170500	-0.16028300	0.14385400
C	-2.60388100	-1.09388200	-0.49271100
C	-3.94045400	-0.80547700	-0.72106900
C	-4.46877700	0.41533000	-0.30722400
H	-4.06978100	2.29341900	0.65931800
H	-1.69868400	1.79688900	1.05848700
H	-2.17350500	-2.03838600	-0.80177600
H	-4.57277800	-1.52951900	-1.21996400
H	-5.51392700	0.63995100	-0.48420200
C	-0.35297500	-0.53170100	0.37463800
O	0.03888600	-1.65053000	0.11389900
C	0.57456900	0.51124500	0.97800500
H	1.78004300	-1.73107200	0.93283700
H	0.28142400	0.62267000	2.02736300
H	0.40909100	1.48000500	0.50191800