SUPPORTING INFORMATION FILE

Identifying the true origins of selectivity in chiral phosphoric acid catalyzed *N*-acyl-azetidine desymmetrizations

by

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Full computational details

Density functional theory (DFT) calculations were performed using Gaussian 16.[1] Geometry optimizations were carried out with the B97D3/6-31G(d,p) level of theory,[2] and the added CPCM implicit solvation[3, 4] model for toluene. This method has been shown to provide good results in previous DFT studies of CPA-catalyzed reactions.[5-10] By default, Gaussian 16 requests an "ultrafine" pruned (99,590) grid for numerical integrations of density, eliminating most orientation-specific issues.[11] Conformational sampling of each stationary point was performed using Grimme's CREST algorithm[12] as implemented in the XTB code.[13] Structures within 6.0 kcal mol^{-1} of the minimum in CREST were selected for full DFT optimization. Normal mode vibrational analysis on the stationary points allowed us to confirm they are minima (zero imaginary frequencies) or transition structures (TS, one imaginary frequency). TSs were followed along their reaction coordinates to verify that they connect the expected minima. ZPE, enthalpy and free energy corrections were obtained using a standard state of 1 atm pressure and 298 K temperature using Goodvibes v2.0.3.[14] Free energies were computed using Grimme's quasiharmonic oscillator approximation, setting all frequencies below 100 cm^{-1} to 100 cm^{-1}.[15] Single-point energy refinements were then performed with the B97D3, ωB97X-D,[16] or M06-2X[17] functionals, using a 6-311+G(2d,2p) or Def2TZVPP basis set and the SMD or CPCM solvation model[18] for toluene. The free energies presented in the manuscript were computed by adding the free energy corrections obtained from the frequency analysis to the single-point electronic energies. Visualizations of the computed structures were prepared using CYLview.[19]

Non-covalent interactions (NCI) were compared through NCI plots[20] using the Multiwfn software,[21] as explained in greater detail in the appropriate section of the SI.

Steric maps were generated using the SambVca 2.1 online tool.[22] The central atom selected is the phosphorus, aligned in the z-axis from the average of the two carbon atoms connecting the binaphthyl backbone. A sphere size of 10 Å was selected, using scaled radii (hydrogens included), and a mesh spacing of 0.05. Superimpositions of the structures optimized with the model catalyst on the structure of the full catalyst were performed using PyMol's pair fitting tool. The five atoms comprising the phosphoric acid core (phosphorus atom + 4 connected oxygen atoms) were selected as the fitted pairs. Atoms comprising the model phosphoric acid catalyst were then removed, resulting in a superimposition of the full catalyst with the transition complex coming from the model-optimized structure.

XYZ coordinates of all computed structures are listed in this document and provided in a .zip archive as a separate Supporting Information file. The Gaussian output files for all optimizations and frequency calculations have been archived and are available for download on Zenodo (DOI: 10.5281/zenodo.4923662).

Low energy conformers of TS 9 (*S*) and TS 9 (*R*) and comparison of computational methods for single-point energies or geometries

For the (*S*)-leading TS 9, 5 structures were within 1.2 kcal mol^{-1} of the global minimum. For the (*R*)-leading TS 9, 13 structures were within 1.2 kcal mol^{-1} of the lowest-energy, none closer than 2.0 kcal mol^{-1} from the best (*S*) structure. All single-point energy methods agree on the relative energy difference between the (*S*) and (*R*) structures, and on the lowest-energy conformer for each enantiomer. Changing the SMD solvation model to the CPCM model (used in the optimizations) reduces the agreement with experimental selectivity (column 2), using a larger Def2TZVPP basis set to eliminate potential basis set superposition errors has no effect (column 3), and using contemporary DFT methods instead of B97D3 do not significantly change the results but encounter more convergence isssues. Therefore the method chosen for the results in the text is the most accurate and convenient for this system.

Table S1: Relative free energy (kcal mol^{-1}) of considered conformers and arrangements of **TS 9 (*S*)** and **TS 9 (*R*)** using various levels of theory.

Structure	**Relative free energy (kcal mol^{-1}) using a given method**				
Pro-(*S*)	**B97D3 6-311+G(2d,2p) SMD (toluene)**	**B97D3 6-311+G(2d,2p) CPCM (toluene)**	**B97D3 Def2TZVPP SMD (toluene)**	**M06-2X Def2TZVPP SMD (toluene)**	**ωB97X-D Def2TZVPP SMD (toluene)**
TS 9 (*S*)	0.0	0.00	0.00	0.00	0.00
Conf 1	0.16	0.13	0.14	0.16	0.10
Conf 2	0.18	0.32	0.16	0.41	0.47
Conf 3	0.36	0.29	0.42	0.43	0.27
Conf 4	0.59	0.66	0.55	1.01	0.90
Pro-(*R*)					
TS 9 (*R*)	2.04	2.31	1.99	2.22	2.07
Conf 1	2.42	2.57	2.46	2.47	2.36
Conf 2	2.54	2.80	2.68	2.81	2.79
Conf 3	2.67	2.89	2.65	3.27	2.83
Conf 4	2.67	2.63	2.58	3.39	2.92
Conf 5	2.69	2.98	2.79	2.86	2.90
Conf 6	2.78	3.02	2.73	3.50	3.13
Conf 7	2.82	3.18	2.81	2.99	2.91
Conf 8	2.85	3.54	2.86	3.16	dnc
Conf 9	2.92	2.31	2.88	4.01	dnc
Conf 10	3.12	3.26	3.07	4.02	3.49
Conf 11	3.14	2.82	3.13	3.62	3.15
Conf 12	3.21	4.01	3.32	2.98	3.31
arr #1	8.70	9.31	8.17	6.69	7.99
arr #3	7.11	7.80	7.05	6.87	7.80
arr #4	9.34	9.34	9.25	9.32	9.92
arr #5	10.88	12.42	9.98	8.26	10.03
arr #6	8.59	9.01	8.89	10.46	10.11
arr #7	10.98	11.81	10.54	10.92	11.49
arr #8	9.80	9.93	9.97	9.39	dnc

dnc: Did not converge

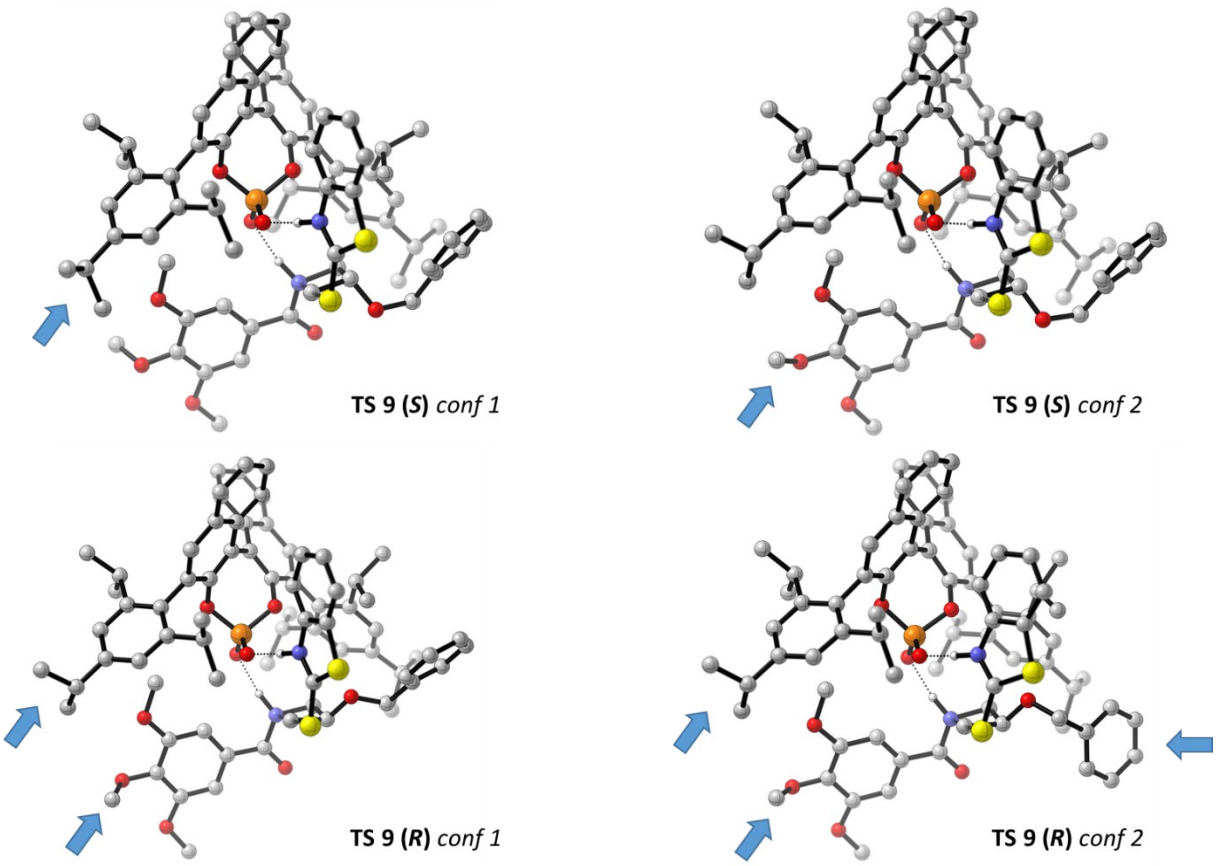


Figure S1.1: Selected structures of conformers of **TS 9 (*S*** and ***R*)**, shown in the Goodman projection. Blue arrows highlight conformational differences between these structures and their corresponding lowest-energy conformer. Non-critical hydrogen atoms hidden.

When re-optimizing the key structures **TS 9 (*S*)** and **TS 9 (*R*)** with M06-2X or ωB97X-D, there are limited changes to the geometry that would warrant performing the whole study with these more expensive methods (Figure S1.2). With M06-2X and a different solvation model, the S_N2 bond lengths at the TS changed slightly from 2.60 and 1.97 to 2.49 and 1.94, while superimposing the two structures gives an RMSD of 0.022. With ωB97X-D and a different solvation model, the bond lengths changed slightly from 2.57 and 1.98 to 2.49 and 1.98, while superimposition gives an RMSD of 0.019. Overall, as the original method captures dispersion and solvation effects, the B97D3 geometries are accurate. This was also the conclusion from Wheeler's work.[7]

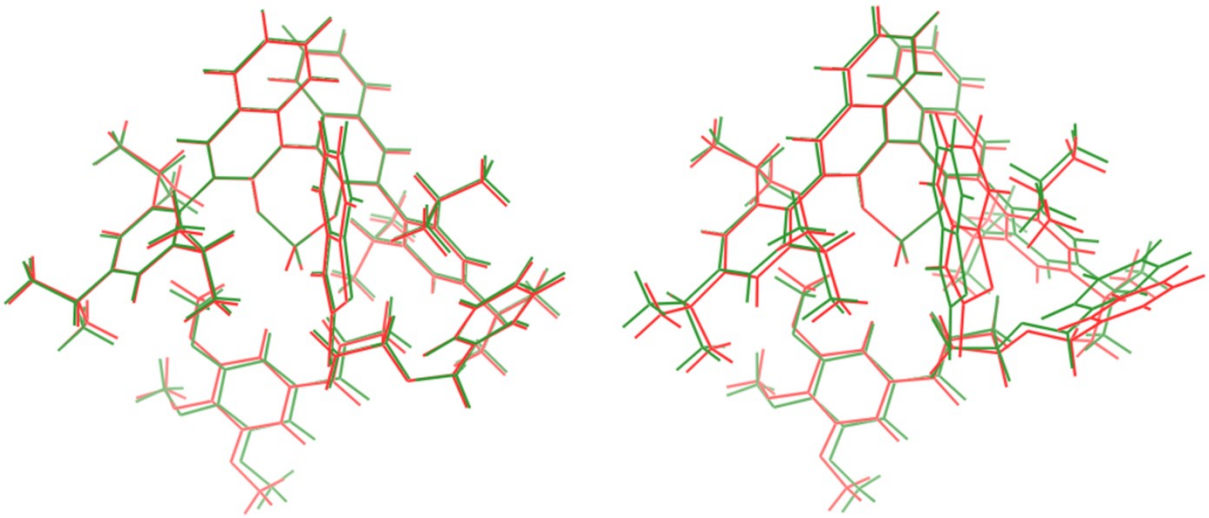


Figure S1.2: left: **TS 9 (*S*)** (green) vs **TS 9 (*S*)** optimized at the ωB97X-D/6-31G(d,p)/SMD(PhMe) level (red). RMSD = 0.019; right: **TS 9 (*R*)** (green) vs **TS 9 (*R*)** optimized at the M06-2X/6-31G(d,p)/SMD(PhMe) level (red). RMSD = 0.022

Activation modes B, C and D with the model catalyst

For modes B, C, and D, only the pro-(*S*) structures were considered. 57 conformers were located for mode B, 40 conformers for mode C, and 55 conformers for mode D. The lowest-energy structures are shown below in **Figure S2**. The modes using the thiol tautomer of the nucleophile (modes C and D) are significantly higher in energy than those using the thione tautomer (see main text). These modes are not considered relevant for the reaction using the full catalyst.

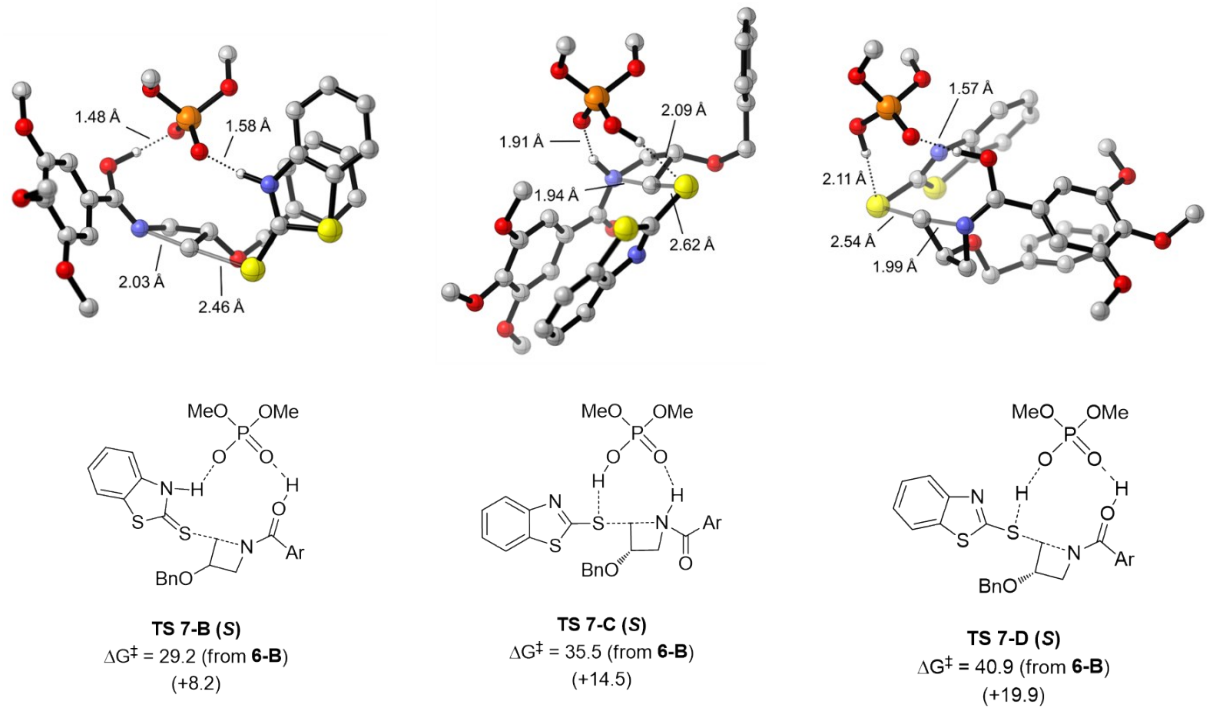


Figure S2: Transition structures leading to the (*S*)-product using model catalyst **5** in modes C (azetidine nitrogen and thiol activation) or mode D (carbonyl and thiol activation). Free energies in kcal mol^{-1}, relative free energies compared to **TS 7-A (*S*)**. Non-critical hydrogen atoms hidden to improve clarity.

Arrangements and conformers of TS 7-A (*S*) and (*R*)

For **TS 7-A (*S*)**, a total of 69 structures were optimized, while 135 structures were optimized for **TS 7-A (*R*)**. The lowest-energy structures, shown in the main text, are replicated in **Figure S3** below.

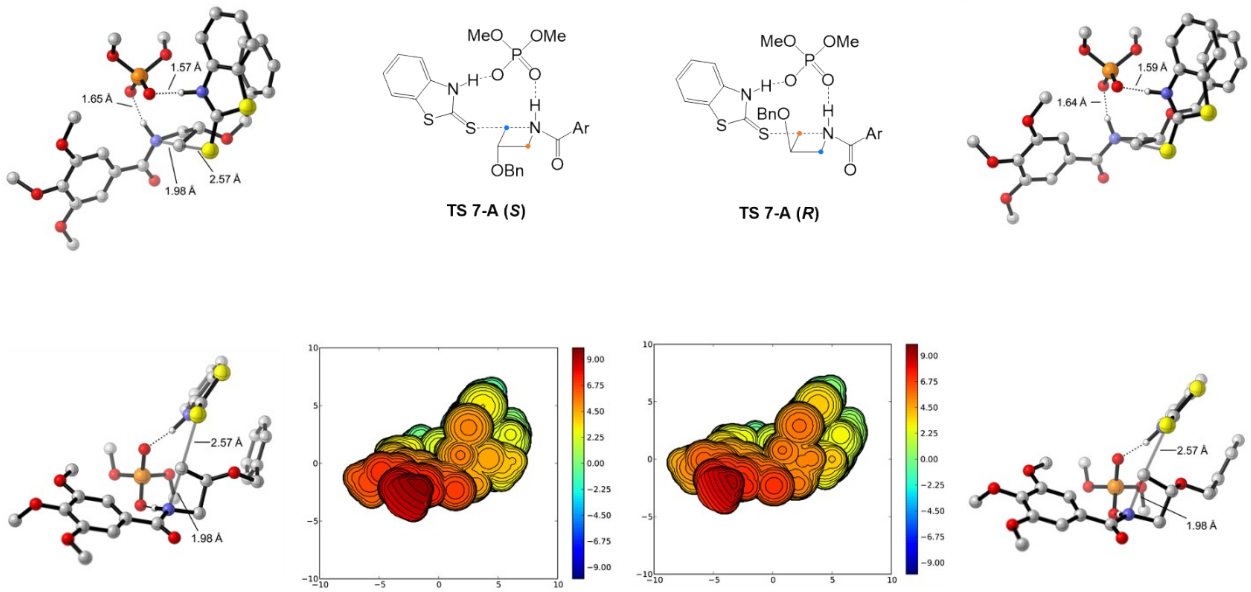
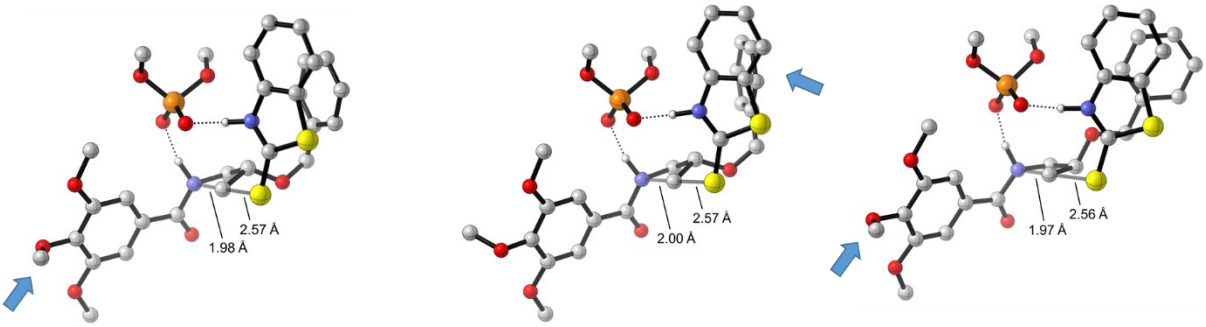


Figure S3: Lowest-energy **TS 7-A (*S*)** and **TS 7-A (*R*)** structures shown in their Goodman and quadrant projections with steric map representations in the quadrant projection. Non-critical hydrogen atoms hidden to improve clarity. Ar = 3,4,5-trimethoxyphenyl

For each arrangement, conformers arising from the rotation around single bonds were also located. Examples of such conformers are shown below in **Figure S4**:



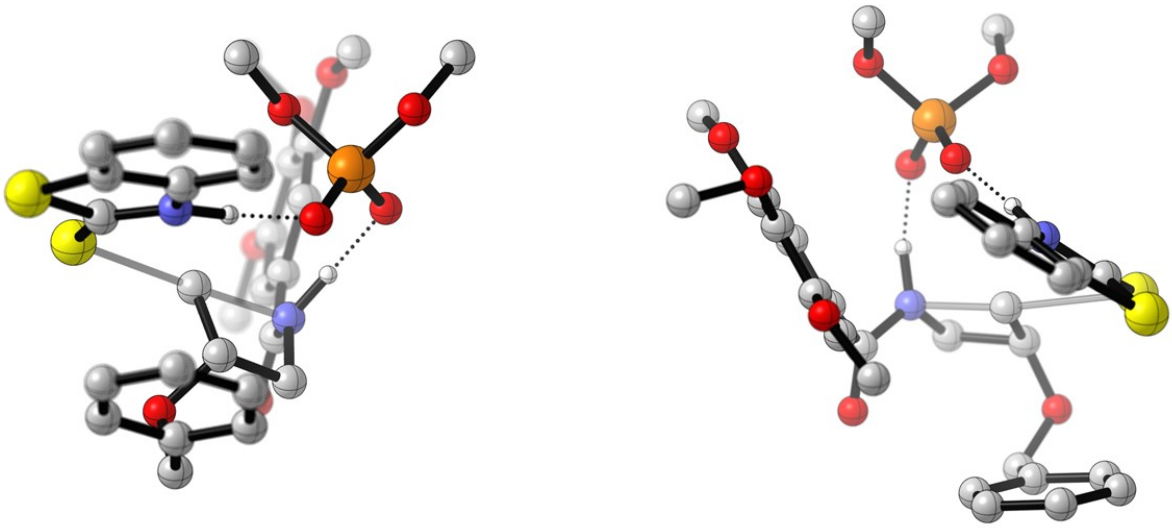
TS 7-A (*S*) (*Conf 1*)
+ 0.2 vs **TS 7-A (*S*)**

TS 7-A (*S*) (*Conf 2*)
+ 0.7 vs **TS 7-A (*S*)**

TS 7-A (*R*) (*Conf 1*)
+ 0.2 vs **TS 7-A (*R*)**

Figure S4: Representative conformers of **TS 7-A (*S*)** and **TS 7-A (*R*)**, shown in their Goodman projection. Non-critical hydrogen atoms hidden to improve clarity. Free energies in kcal mol^{-1} are relative to the lowest-energy structure leading to the same enantiomer. Blue arrows depict the change in conformation vs the lowest-energy structure.

For **TS 7-A (*S*)**, two additional arrangements were located, one of which is within 1.0 kcal mol^{-1} from the lowest-energy structure. Conformational sampling on **TS 7-A (*S*)** led to less arrangements of low energy, therefore is indicative of the stability of the lowest-energy structure.



TS 7-A (*S*) *arr 1*
$\Delta\Delta G$ = 0.7

TS 7-A (*S*) *arr 2*
$\Delta\Delta G$ = 5.9

Figure S5: Lowest-energy conformer of two additional arrangements leading to the (*S*)-product using model catalyst **5**.

Potential energy surface (PES) for the reaction using the full catalyst (*R*)-3b

The potential energy surface for the reaction using the full catalyst is shown below in **Figure S6.** All stationary points on this surface except **TS 9-B (*S*)** were searched for their lowest-energy conformation. Mode B is around 19.0 kcal mol^{-1} higher in energy than mode A, so it is irrelevant with the full catalyst. Of note, the product complexes bind the catalyst more strongly than the reactants, therefore significant catalyst poisoning is expected.

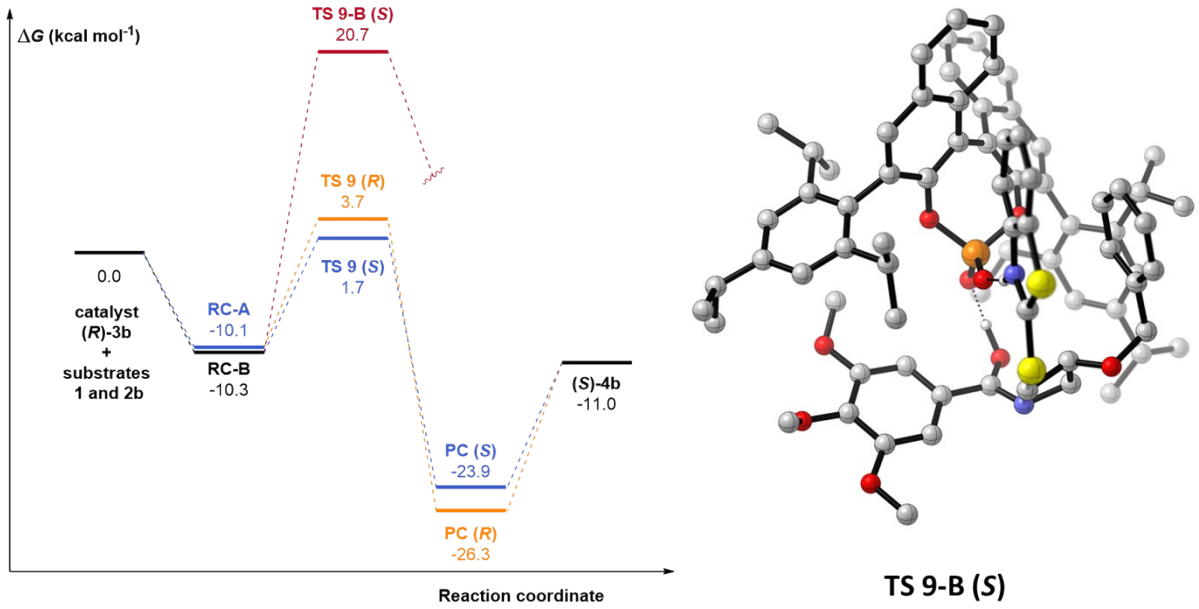


Figure S6: Potential free energy surface (in kcal mol^{-1}) for the reaction of **1** and **2b**, catalyzed by **(*R*)-3b**. Goodman projection of **TS 9-B (*S*)** with non-critical hydrogen atoms hidden.

Other arrangements of TS 9 (*R*) with the full catalyst

Arrangements shown in **Figure 3** of the main text for **TS 7-A (*R*)** were optimized within the full catalyst **(*R*)-3b**, to ensure that the lowest-energy arrangement was truly **TS 9 (*R*)** and that the energy difference between the (*S*) and (*R*) structures did not shrink. The resulting structures are shown below in **Figure S7**. All arrangements are at least 7.1 kcal mol^{-1} higher in free energy than **TS 9 (*S*)**. Arrangement 2 did not yield a unique structure within the full catalyst, instead converging to a structure similar to arrangements 7 and 8.

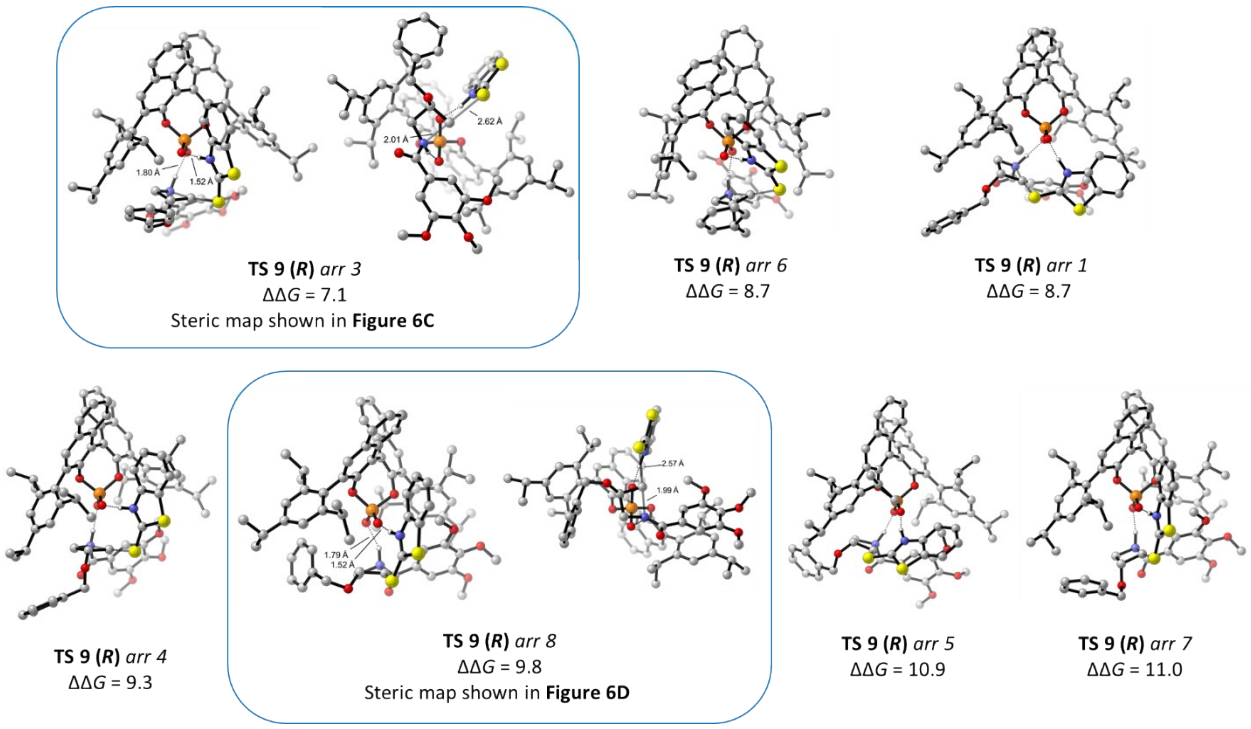


Figure S7: Arrangements leading to the (*R*)-product using catalyst **(*R*)-3b**. Free energies (in kcal mol^{-1}) are relative to **TS 9 (*S*)**, which is 2.0 kcal mol^{-1} more stable than **TS 9 (*R*)**. Structures from arrangements 3 and 8 are shown as steric maps in **Figure 6** of the main text.

Distortion-interaction analysis

Distortion-interaction analysis[23] was performed on **TS 9 (*S*)** and **TS 9 (*R*)** by splitting the full structures as binary complexes between the anionic phosphate catalyst (**cat**) and the cationic transition complex of the azetidinium electrophile + benzothiazole nucleophile (**az + bt**) (**Figure S8**). As the fragments cannot be compared to their ground-state structures due to the completed proton exchange at the TS, only the relative (*R* vs *S*) distortion and interaction energies ($\Delta\Delta E_{dist}$ and $\Delta\Delta E_{int}$) were computed with the following equations:

$\Delta\Delta E_{act} = \Delta E_{full}\ (R) - \Delta E_{full}\ (S)$

$\Delta\Delta E_{dist}$ (for each fragment) $= \Delta E_{fragment}\ (R) - \Delta E_{fragment}\ (S)$

$\Delta E_{int}\ (S) = \Delta E_{full}\ (S) - \Delta E_{cat}\ (S) - \Delta E_{az+bt}\ (S)$

$\Delta\Delta E_{int} = \Delta E_{int}\ (R) - \Delta E_{int}\ (S)$

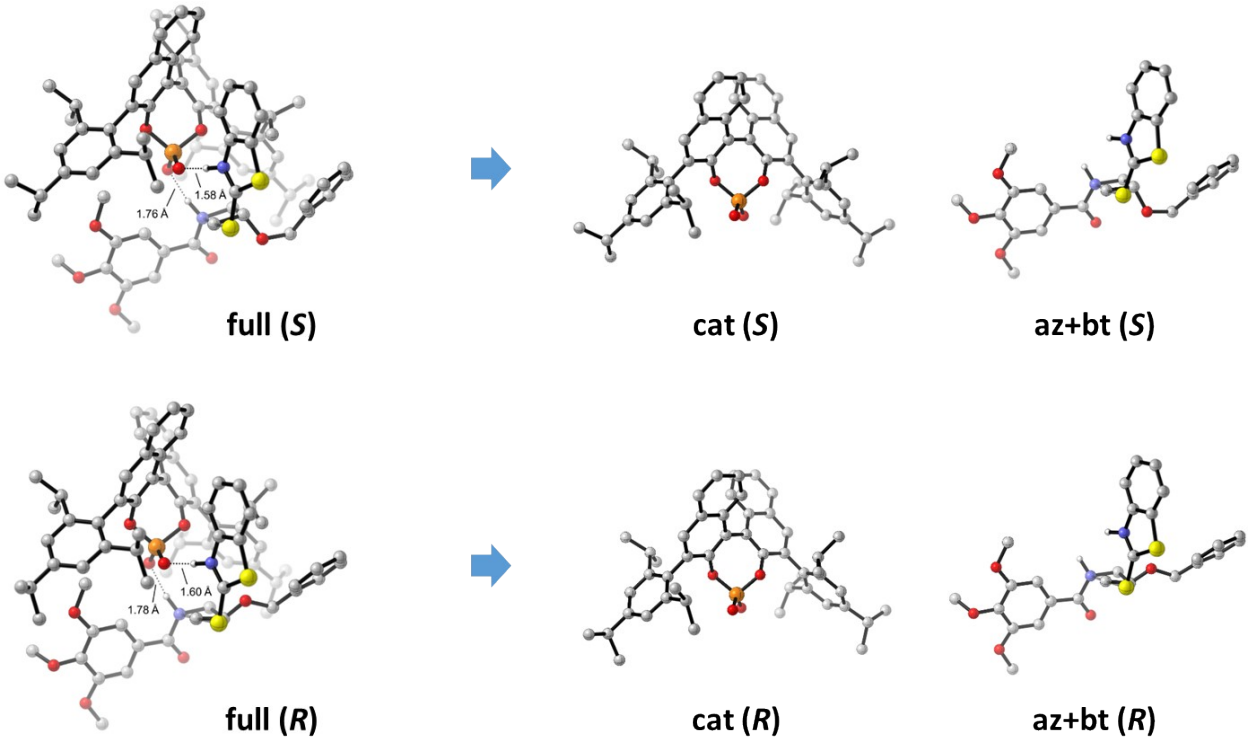


Figure S8: Fragmentation of the TSs for distortion-interaction analysis.

The single-point energy of the isolated fragments was evaluated using four methods:

a) B97D3/6-31G(d,p) (gas phase)

b) B97D3/6-31G(d,p)/CPCM(PhMe), the optimization method
c) B97D3/6-311+G(2d,2p) (gas phase)
d) B97D3/6-311+G(2d,2p)/SMD(PhMe), the single-point energy method

Table S2: Distortion-interaction analysis as a function of computational method

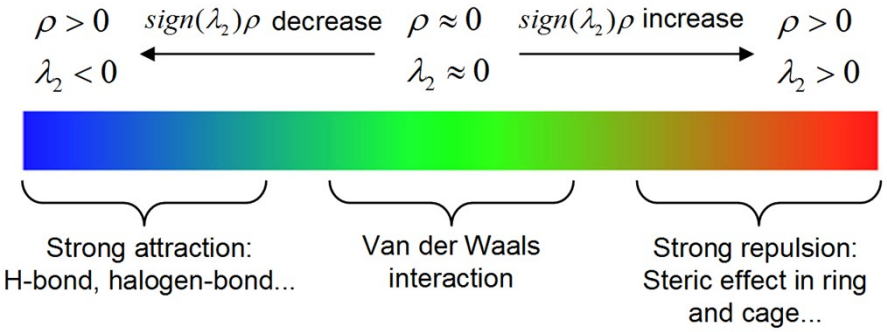
Parameter	**Value (kcal/mol)**			
	B97D3 / 6-31G(d,p)	B97D3 / 6-31G(d,p) / CPCM(PhMe)	B97D3 / 6-311+G(2d,2p)	B97D3 / 6-311+G(2d,2p) / SMD(PhMe)
$\Delta\Delta E_{act}$	3.5	3.5	**3.4**	3.2
$\Delta\Delta E_{dist}$	2.3	2.6	**1.7**	1.5
$\Delta\Delta E_{dist}$ (catalyst)	0.8	0.5	**0.5**	0.2
$\Delta\Delta E_{dist}$ (substrates)	1.5	2.1	**1.2**	1.3
$\Delta\Delta E_{int}$	1.1	0.9	**1.7**	1.7

As can be seen from **Table S2**, although the four methods agree that the overall (*S*) selectivity of the reaction is due to contributions from distortions and interactions, they provide different relative values for each component. With the SPE basis set, the interaction energy is larger, which is unsurprising considering its better ability to account for C-H polarization. As the inclusion of solvation is likely to overstabilize individual fragments (by allowing interactions with solvent in areas which were inaccessible in the full structures), the method with the large basis set but no solvation model (B97D3 / 6-311+G(2d,2p)) is chosen as the best representation and presented in the main text.

The distortion energy of the transition complex (**az+bt**) was further decomposed by computing the SPE of each fragment individually (cationic azetidinium and neutral benzothiazole). It was found that the distortion energy of the benzothiazole nucleophile ($\Delta\Delta E_{dist\text{-}bt}$) is 0.0 for all methods, so that only the distortion energy of the azetidinium substrate ($\Delta\Delta E_{dist\text{-}az}$) affects the global distortion energy of the transition complex. This distortion energy can be tracked down to the puckering of the azetidine ring and partially-eclipsed conformation of the benzyloy substituent, as described in the main text.

Non-covalent interactions (NCI) analysis

NCI plots were generated using the Multiwfn software (http://sobereva.com/multiwfn/),[21] which applies Yang's theory of non-covalent interactions (also called reduced density gradient, RDG).[20] The DFT density of the two competing TSs was first computed using Gaussian 16 at the B97D3/6-31G(d,p)/CPCM(PhMe) level. The formatted checkpoint files (.fchk) were submitted to Multiwfn for NCI analysis using default settings and a high-quality grid (0.12 Bohr). The color-filled visualizations (see below) were generated from the cube files containing the $sign(\lambda_2)\rho$ values with the VMD software (http://www.ks.uiuc.edu/Research/vmd/), using the RGDfill.vmd script provided with Multiwfn. The isosurface is set to 0.5 and the color scale from -0.035 (blue) to 0.02 (red). According to this scale, the non-covalent favorable interactions appear in green:



The resulting NCI plots are shown below in **Figure S9**. A video of the surfaces rotating can also be found in the Zenodo archive at doi.org/10.5281/zenodo.4923662.

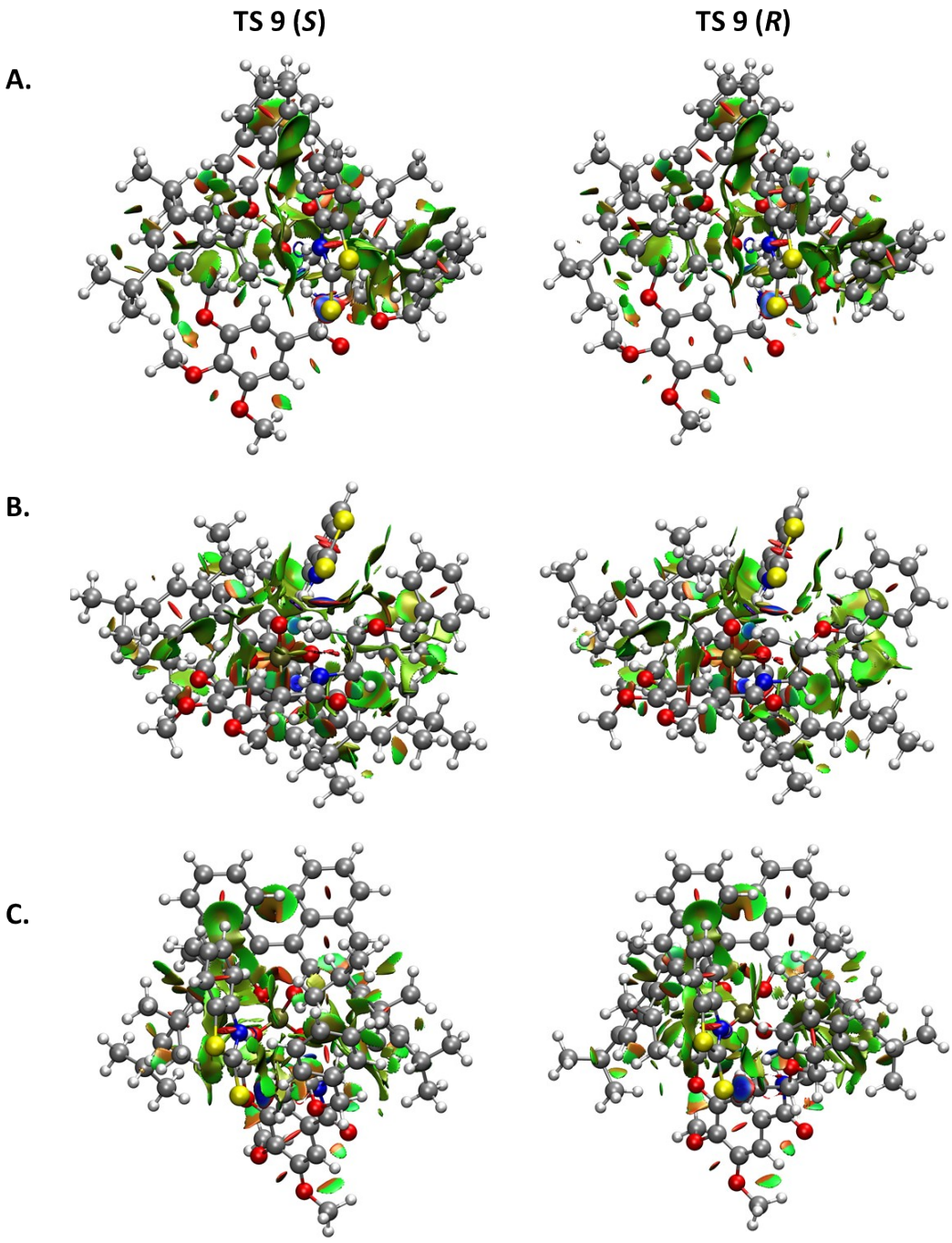


Figure S9: NCI plots for **TS 9 (*S*)** (left) and **TS 9 (*R*)** (right) shown in the **A)** Goodman projection, **B)** quadrant projection and, **C)** Goodman projection rotated 45° in the x axis.

Arrangements optimized with an unsubstituted benzoyl group

The structures of **TS 9 (*S*)**, **TS 9 (*R*)**, and all arrangement of **TS 9 (*R*)** with the full catalyst (**Figure 3** in the main text) were modified by replacing the three methoxy groups on the benzoyl group of the azetidine with hydrogen atoms. The generated structures were then optimized with constraints, fixing all key forming and breaking bond lengths of the TS. Full TS optimizations, followed by single-point energy refinements as described previously, provided the final structures and energies presented below.

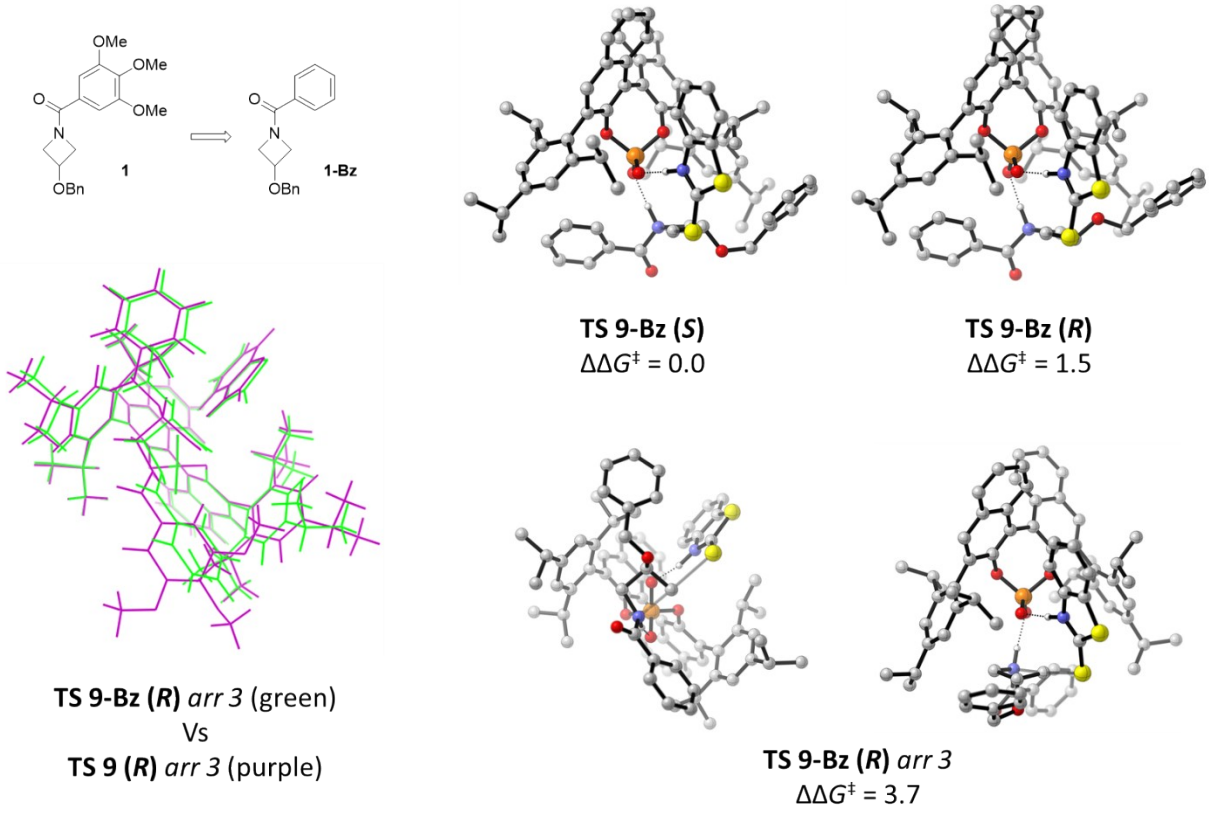


Figure S10: Selected structures optimized with the truncated substrate **1a-Bz**.

As can be seen from the superimposition of *arrangement 3* with substrates **1** or **1-Bz** (**Figure S10**, bottom-left), removal of the methoxy groups allows for less interactions between the benzoyl group and the wall of the catalyst, reducing distortion of the catalyst and of the transition complex. Relative free energy values (**Table S3**) show that reducing the steric bulk of the benzoyl group should result in a lower selectivity, as the difference between pro-(*S*) and pro-(*R*) structures is only 1.5 kcal mol^{-1}. This is in line with the lower selectivity observed experimentally for substrate **1-Bz**. Reducing the steric bulk also greatly lowers the relative free energy of arrangements 3, 6, and 7, while other arrangements become less stable or remain as unstable.

Table S3: Relative free energies (kcal mol^{-1}) of all arrangements computed with substrate **1** or substrate **1-Bz**.

Structure	Relative free energy (kcal mol^{-1})	
	Substrate **1**	Substrate **1-Bz**
TS 9 (*S*)	0.0	0.0
TS 9 (*R*)	2.0	1.5
TS 9 (*R*) *arr 3*	7.1	3.7
TS 9 (*R*) *arr 6*	8.7	4.5
TS 9 (*R*) *arr 1*	8.7	9.8
TS 9 (*R*) *arr 4*	9.3	7.8
TS 9 (*R*) *arr 8*	9.8	8.1
TS 9 (*R*) *arr 5*	10.9	10.4
TS 9 (*R*) *arr 7*	11.0	5.7

Energies, thermochemical corrections, and single-point energy for all reported structures

The "**Opt+Freq**" values correspond to the energy, enthalpy and free energy of the structures optimized at the B97D3/6-31G(d,p)/CPCM(toluene) level of theory. The "**SPE**" value is the B97D3/6-311+G(2d,2p)/SMD(toluene) single-point energy computed on the optimized structures. All values are in hartrees.

Table S4: Reactants and product

	Opt+Freq			SPE
Structure	**E**	**H**	**G (298.15 K)**	**E**
1	-1206.065221	-1205.644617	-1205.723387	-1206.415081
2b-SH	-1120.688043	-1120.579303	-1120.622262	-1120.840442
2b-NH	-1120.706381	-1120.594208	-1120.636385	-1120.857938
(*S*)-4b	-2326.827826	-2326.292298	-2326.38808	-2327.318535

Table S5: Structures with model catalyst **5**

	Opt+Freq			SPE
Structure	**E**	**H**	**G (298.15 K)**	**E**
5	-722.529461	-722.415671	-722.460293	-722.70845
6-A	-3049.364867	-3048.715032	-3048.83333	-3050.029443
6-B	-3049.378763	-3048.728644	-3048.847103	-3050.041512
6-C	-3049.345536	-3048.695725	-3048.813402	-3050.010042
6-D	-3049.353642	-3048.705935	-3048.82271	-3050.015679
TS 7-A (R)	-3049.343326	-3048.694833	-3048.81262	-3050.007945
TS 7-A (R) *conf1*	-3049.34305	-3048.694416	-3048.812349	-3050.007692
TS 7-A (R) *arr #1*	-3049.341603	-3048.693666	-3048.809357	-3050.003977

TS 7-A (R) *arr #2*	-3049.339574	-3048.690949	-3048.808597	-3050.005287
TS 7-A (R) *arr #3*	-3049.335291	-3048.68624	-3048.805984	-3050.002213
TS 7-A (R) *arr #4*	-3049.339697	-3048.690723	-3048.807782	-3050.00492
TS 7-A (R) *arr #5*	-3049.337336	-3048.688167	-3048.806709	-3050.004231
TS 7-A (R) *arr #6*	-3049.338485	-3048.689184	-3048.80672	-3050.004524
TS 7-A (R) *arr #7*	-3049.339151	-3048.6904	-3048.808271	-3050.00517
TS 7-A (R) *arr #8*	-3049.333357	-3048.684903	-3048.802988	-3049.998683
TS 7-A (S)	-3049.343393	-3048.694463	-3048.811616	-3050.008139
TS 7-A (S) *conf1*	-3049.343382	-3048.69429	-3048.811236	-3050.008142
TS 7-A (S) *conf2*	-3049.34212	-3048.693333	-3048.810592	-3050.006824
TS 7-A (S) *arr #1*	-3049.340112	-3048.691094	-3048.809043	-3050.006349
TS 7-A (S) *arr #2*	-3049.337319	-3048.688859	-3048.80488	-3049.999396
TS 7-B (S)	-3049.330037	-3048.682754	-3048.799564	-3049.993794
TS 7-C (S)	-3049.319782	-3048.670969	-3048.788617	-3049.984457
TS 7-D (S)	-3049.31185	-3048.664833	-3048.781428	-3049.975135
8-A (S)	-3049.39823	-3048.746823	-3048.862822	-3050.061266
8-B (S)	-3049.365563	-3048.717116	-3048.834156	-3050.030248
8-C (S)	-3049.390131	-3048.73863	-3048.856422	-3050.054957
8-D (S)	-3049.383313	-3048.732768	-3048.850143	-3050.049341

Table S6: Structures with full catalyst **(*R*)-3b**

	Opt+Freq			SPE
Structure	**E**	**H**	**G (298.15 K)**	**E**
(R)-3b	-2580.751675	-2579.761444	-2579.896972	-2581.389057
RC-A	-4907.627948	-4906.098257	-4906.299087	-4908.740531
RC-B	-4907.625202	-4906.097796	-4906.300105	-4908.737044

TS 9 (S)	-4907.605806	-4906.078126	-4906.279349	-4908.719349
TS 9 (S) *conf 1*	-4907.605884	-4906.078165	-4906.279202	-4908.719321
TS 9 (S) *conf 2*	-4907.605925	-4906.078149	-4906.278773	-4908.719753
TS 9 (S) *conf 3*	-4907.606113	-4906.078187	-4906.278662	-4908.719771
TS 9 (S) *conf 4*	-4907.606168	-4906.078193	-4906.278399	-4908.719722
TS 9 (R)	-4907.60028	-4906.07293	-4906.275709	-4908.714213
TS 9 (R) *conf 1*	-4907.600062	-4906.07274	-4906.274862	-4908.714235
TS 9 (R) *conf 2*	-4907.601135	-4906.073268	-4906.274995	-4908.714983
TS 9 (R) *conf 3*	-4907.601058	-4906.073521	-4906.274791	-4908.714908
TS 9 (R) *conf 4*	-4907.601308	-4906.073696	-4906.275074	-4908.714866
TS 9 (R) *conf 5*	-4907.6013	-4906.07358	-4906.275132	-4908.714778
TS 9 (R) *conf 6*	-4907.601468	-4906.073788	-4906.274868	-4908.715069
TS 9 (R) *conf 7*	-4907.600423	-4906.072919	-4906.274418	-4908.714402
TS 9 (R) *conf 8*	-4907.60056	-4906.073011	-4906.274358	-4908.714553
TS 9 (R) *conf 9*	-4907.601505	-4906.073864	-4906.274664	-4908.715087
TS 9 (R) *conf 10*	-4907.600327	-4906.072626	-4906.27416	-4908.71408
TS 9 (R) *conf 11*	-4907.60099	-4906.07327	-4906.274099	-4908.714796
TS 9 (R) *conf 12*	-4907.598712	-4906.071004	-4906.273019	-4908.713468
TS 9 (R) *arr #8*	-4907.592923	-4906.064909	-4906.264333	-4908.705861
TS 9 (R) *arr #7*	-4907.588158	-4906.060989	-4906.260918	-4908.702641
TS 9 (R) *arr #1*	-4907.587944	-4906.061216	-4906.262879	-4908.704088
TS 9 (R) *arr #5*	-4907.584915	-4906.057282	-4906.259538	-4908.700936
TS 9 (R) *arr #4*	-4907.592095	-4906.064891	-4906.265379	-4908.704727
TS 9 (R) *arr #3*	-4907.59188	-4906.064563	-4906.26549	-4908.707956
TS 9 (R) *arr #6*	-4907.589077	-4906.061913	-4906.263267	-4908.705007
TS 9-B (S)	-4907.58298	-4906.057	-4906.255583	-4908.689927
PC (R)	-4907.648471	-4906.120083	-4906.322571	-4908.763406
PC (S)	-4907.65512	-4906.126237	-4906.325358	-4908.763396

Table S7: Structures with the truncated substrate **1-Bz**

Structure	Opt+Freq			SPE
	E	H	G (298.15 K)	E
TS 9-Bz (S)	-4564.227676	-4562.803873	-4562.988646	-4565.238321
TS 9-Bz (R)	-4564.223819	-4562.800266	-4562.985975	-4565.234786
TS 9-Bz (R) *arr 1*	-4564.209568	-4562.78644	-4562.972152	-4565.221082
TS 9-Bz (R) *arr 3*	-4564.22265	-4562.798841	-4562.9831	-4565.23298
TS 9-Bz (R) *arr 4*	-4564.217899	-4562.794009	-4562.978648	-4565.226134
TS 9-Bz (R) *arr 5*	-4564.207263	-4562.783799	-4562.970685	-4565.219354
TS 9-Bz (R) *arr 6*	-4564.221595	-4562.797974	-4562.982396	-4565.231328
TS 9-Bz (R) *arr 7*	-4564.21901	-4562.795148	-4562.979594	-4565.22955
TS 9-Bz (R) *arr 8*	-4564.213696	-4562.790125	-4562.975678	-4565.224373

XYZ coordinates of all reported structures

For transition structures, the magnitude of the imaginary frequency is provided.

Reactants and product

1

C	1.05878	0.16068	-0.68219
C	1.96250	1.20355	-0.42256
C	3.22489	0.92090	0.14546
C	3.58516	-0.42001	0.41804
C	2.67823	-1.45894	0.16150
C	1.41432	-1.16365	-0.37431
C	0.48765	-2.32155	-0.61307
O	0.90091	-3.48134	-0.77733
N	-0.85325	-2.04141	-0.64551
C	-1.91386	-3.06271	-0.57287
H	-1.60048	-3.97695	-0.05389
H	-2.34005	-3.31916	-1.55245
C	-2.78595	-2.06413	0.22943
O	-4.03334	-1.82232	-0.38921
C	-4.88410	-0.94581	0.37553
C	-4.33524	0.46341	0.46842
C	-3.75036	0.93373	1.65493
C	-3.14136	2.19577	1.70060
C	-3.11460	3.00097	0.55433
C	-3.70567	2.54348	-0.63459
C	-4.31221	1.28358	-0.67470
H	-4.75512	0.91848	-1.60181
H	-3.69124	3.16955	-1.52657
H	-2.64077	3.98171	0.58637
H	-2.68550	2.54665	2.62604
H	-3.75922	0.30092	2.54342
H	-5.03827	-1.36109	1.38703
H	-5.84413	-0.95913	-0.15565
H	-2.92078	-2.34442	1.28689
C	-1.66160	-0.99921	0.02927
H	-1.20258	-0.58534	0.93471
H	-1.96226	-0.18245	-0.63609
H	2.92056	-2.49854	0.35759
O	4.83830	-0.59029	0.93975
C	5.25209	-1.93079	1.22400
H	5.26009	-2.54998	0.31455
H	4.60026	-2.40007	1.97598
H	6.26823	-1.84740	1.62077
O	4.08307	1.95064	0.45660
C	5.04833	2.22249	-0.57782
H	4.54718	2.51848	-1.51144
H	5.68508	1.34516	-0.76134
H	5.66294	3.05249	-0.21251
O	1.71578	2.52396	-0.68360
C	0.40798	2.86312	-1.15646
H	0.20678	2.42062	-2.14430
H	-0.37182	2.54109	-0.45026
H	0.39863	3.95418	-1.24004
H	0.10753	0.37067	-1.15573

2b-NH

C	1.63687	-0.15365	0.00009
C	-0.66065	-0.72938	-0.00013
C	-0.78348	0.67893	0.00010
C	-1.79349	-1.55313	-0.00020
C	-2.04369	1.28475	0.00027
C	-3.05217	-0.94016	-0.00002
H	-1.69108	-2.63689	-0.00035
C	-3.17767	0.46074	0.00020
H	-2.13881	2.36862	0.00037
H	-3.94581	-1.56205	-0.00006
H	-4.16707	0.91495	0.00030
S	0.81439	1.43241	-0.00011
N	0.67243	-1.12745	-0.00014
S	3.28066	-0.39374	0.00006
H	0.96062	-2.09979	-0.00023

2b-SH

H	-3.23323	-1.68344	0.00015
S	-3.25849	-0.33370	0.00005
C	-1.49687	-0.19153	-0.00000
C	0.64834	-0.74431	0.00000
C	0.80951	0.67198	-0.00003
C	1.78780	-1.56888	0.00001
C	2.07617	1.26766	-0.00006
C	3.05243	-0.97515	-0.00003
H	1.66347	-2.65022	0.00003
C	3.19588	0.42696	-0.00006
H	2.18985	2.35000	-0.00008
H	3.94109	-1.60494	-0.00003
H	4.19201	0.86755	-0.00009
S	-0.77325	1.44449	0.00000
N	-0.66927	-1.19599	0.00003

(*S*)-4b

C	-1.17135	0.99340	-1.51155
C	-2.41373	1.40055	-1.00790
C	-3.39684	0.43736	-0.68869
C	-3.12884	-0.93369	-0.89635
C	-1.88299	-1.34043	-1.40020

C	-0.90752	-0.37250	-1.69299
C	0.47363	-0.72971	-2.15270
O	1.17725	0.05890	-2.80432
N	0.93457	-1.97168	-1.77582
H	0.41572	-2.44599	-1.04579
C	2.37508	-2.21400	-1.77505
H	2.55147	-3.29507	-1.71833
H	2.77843	-1.84560	-2.72250
C	3.07302	-1.45849	-0.61308
C	3.26780	-2.27709	0.66827
H	3.62540	-1.62783	1.47356
H	3.99976	-3.07826	0.50091
S	1.77252	-3.17084	1.26183
C	0.70296	-1.81787	1.62583
N	1.04622	-0.56190	1.64308
C	-0.05139	0.25146	1.90865
C	-0.01990	1.65453	1.98277
C	-1.20882	2.33937	2.24595
C	-2.42316	1.64848	2.42213
C	-2.47548	0.25168	2.35432
C	-1.28332	-0.43560	2.10538
S	-1.02438	-2.16880	1.94544
H	-3.42055	-0.27588	2.45758
H	-3.34366	2.20495	2.58655
H	-1.19896	3.42714	2.30216
H	0.92239	2.17411	1.82562
O	4.39305	-1.03558	-0.97990
C	4.38379	0.25684	-1.61889
C	3.92911	1.37041	-0.69295
C	2.93232	2.27436	-1.09601
C	2.53457	3.31786	-0.24860
C	3.11656	3.45486	1.01911
C	4.09314	2.53807	1.43902
C	4.49852	1.50570	0.58593
H	5.25387	0.78945	0.90902
H	4.54009	2.63304	2.42862
H	2.80573	4.26361	1.68060
H	1.76337	4.01636	-0.57407
H	2.45503	2.14133	-2.06547
H	5.42454	0.41372	-1.93398
H	3.74324	0.24063	-2.51347
H	2.46189	-0.58279	-0.36379
H	-1.68265	-2.39091	-1.58589
O	-4.14502	-1.78481	-0.55531
C	-3.91217	-3.18584	-0.72908
H	-3.05883	-3.52738	-0.12470
H	-4.82567	-3.68111	-0.38666
H	-3.73395	-3.43580	-1.78623
O	-4.59119	0.81700	-0.11933
C	-5.57114	1.25715	-1.07851
H	-6.46373	1.52547	-0.50272
H	-5.81759	0.44917	-1.78365
H	-5.21240	2.13580	-1.63320
O	-2.76669	2.69967	-0.77003
C	-1.76649	3.69704	-1.00134
H	-2.22878	4.64835	-0.72133
H	-0.88072	3.51663	-0.37571
H	-1.46849	3.72941	-2.06006
H	-0.38401	1.70203	-1.74387

Structures with model catalyst

5

O	-0.97786	0.49534	-0.83659
O	1.01191	0.36450	0.79806
P	0.01241	-0.54904	-0.09271
O	0.61414	-1.50355	-1.06010
O	-0.84530	-1.19338	1.12712
H	-1.01541	-2.12944	0.93142
C	-1.71950	1.46021	-0.04677
H	-2.28084	2.06861	-0.76134
H	-2.40940	0.94520	0.63255
H	-1.03682	2.09523	0.53151
C	1.96964	1.17544	0.06729
H	1.45228	1.91554	-0.55696
H	2.57470	1.68331	0.82309
H	2.60548	0.54002	-0.56075

6-A

C	0.93976	2.02365	-0.98297
C	0.03448	0.99120	-0.66034
C	-0.09408	0.54696	0.67054
C	0.66713	1.13512	1.68592
C	1.59631	2.16628	1.37348
C	1.70623	2.61140	0.02102
H	1.03957	2.32062	-2.02057
C	-0.74736	0.42076	-1.75284
H	-0.75784	-0.27400	0.91374
O	-0.55960	0.57113	-2.95074
N	-1.93494	-0.37964	-1.32742
C	-3.08502	0.34140	-0.63209
C	-2.88101	-0.86042	-2.40282
C	-4.06895	-0.50340	-1.48994
H	-2.80844	-0.20601	-3.27563
H	-2.71696	-1.90648	-2.67243
H	-4.44343	-1.37168	-0.92582
O	-5.10317	0.16626	-2.16649
H	2.66465	0.28575	-4.64523
O	-0.89057	-4.59784	-0.65662
C	3.11797	0.34912	-3.65722
C	4.18589	1.23908	-3.43594
C	2.62245	-0.45636	-2.62698
H	4.55825	1.85304	-4.25494
H	1.79117	-1.13936	-2.77588
O	-1.68569	-2.36838	0.17934
C	4.78097	1.34878	-2.17010
C	3.21369	-0.34376	-1.36171
C	4.28457	0.55180	-1.13419
N	2.85583	-1.04540	-0.21920
P	-0.38455	-3.17023	-0.03505
H	-1.68953	-1.28395	-0.66432
H	5.60316	2.03992	-1.99531

C	3.56007	-0.78929	0.91360
S	4.79350	0.45947	0.55018
S	3.35630	-1.49258	2.41378
O	0.25660	-3.55945	1.41709
O	0.71323	-2.54532	-0.86698
H	-3.09245	1.39898	-0.90669
H	-3.07646	0.21299	0.45150
H	2.04166	-1.70215	-0.24638
C	-0.62248	-4.11102	2.42057
H	-1.03220	-5.07517	2.09007
H	-0.01338	-4.25495	3.31835
H	-1.44745	-3.41897	2.63384
C	0.13567	-5.55400	-1.00876
H	-0.38079	-6.42336	-1.42807
H	0.82039	-5.12809	-1.75302
H	0.70631	-5.85602	-0.11982
C	-6.27017	0.36989	-1.33757
H	-6.99289	0.86201	-1.99949
H	-6.68186	-0.60677	-1.03086
C	-5.96941	1.21706	-0.11991
C	-5.65597	2.58051	-0.27098
C	-5.90217	0.63984	1.15882
C	-5.27489	3.34858	0.83433
H	-5.69690	3.03082	-1.26325
C	-5.52249	1.40675	2.26934
H	-6.13746	-0.41816	1.28197
C	-5.20377	2.76120	2.10723
H	-5.03135	4.40292	0.70603
H	-5.47090	0.94643	3.25564
H	-4.90308	3.35850	2.96743
O	0.54787	0.79770	3.00291
O	2.36772	2.83148	2.26186
O	2.60755	3.61456	-0.17964
C	-0.15478	-0.41593	3.30957
H	0.27465	-1.26241	2.75843
H	-0.02090	-0.56520	4.38474
H	-1.22837	-0.32166	3.08383
C	2.89021	2.17565	3.44387
H	3.75486	2.78230	3.73280
H	2.14610	2.16824	4.24674
H	3.20337	1.15025	3.21894
C	2.67958	4.17366	-1.49689
H	1.70769	4.58940	-1.80332
H	3.41967	4.97680	-1.43218
H	3.01020	3.42571	-2.23017

6-B

C	-1.62733	0.92224	-0.66362
C	-1.17270	-0.23414	-1.32096
C	-2.08210	-1.23435	-1.70925
C	-3.44737	-1.08112	-1.43843
C	-3.91086	0.06997	-0.75981
C	-2.99297	1.07374	-0.38532
H	-0.93086	1.65622	-0.28840
C	0.26950	-0.50407	-1.58184
H	-1.69237	-2.12298	-2.19147
O	0.63215	-1.68597	-1.87218
N	1.16599	0.49349	-1.53257
C	1.13369	1.95963	-1.35077
C	2.61093	0.45191	-1.82767
C	2.62275	1.99894	-1.81877
H	2.85280	-0.04870	-2.77259
H	3.19921	0.01980	-1.01076
H	2.74016	2.45246	-2.81626
O	3.57795	2.50756	-0.91515
H	-2.86630	-4.78625	0.51980
O	4.19594	-1.66501	0.25888
C	-2.66823	-3.80067	0.93892
C	-3.73718	-3.02586	1.42662
C	-1.35277	-3.32521	0.97401
H	-4.75480	-3.40661	1.36209
H	-0.51575	-3.89835	0.58290
O	2.87734	-2.72590	-1.57897
C	-3.51393	-1.75935	1.98275
C	-1.13143	-2.05705	1.52588
C	-2.19944	-1.28680	2.03929
N	0.08755	-1.39923	1.62066
P	3.22295	-2.93146	-0.05433
H	1.95643	-2.23574	-1.72666
H	-4.34119	-1.15072	2.34018
C	0.08182	-0.15134	2.15503
S	-1.58540	0.24442	2.66047
S	1.38619	0.88650	2.30080
O	4.17131	-4.23911	0.01571
O	2.09535	-3.09156	0.92532
H	0.39758	2.47586	-1.97748
H	1.02109	2.24479	-0.29967
H	0.96546	-1.87277	1.32075
C	5.32767	-4.31513	-0.85499
H	5.84271	-5.24437	-0.59478
H	5.99318	-3.45891	-0.68704
H	5.01280	-4.34104	-1.90521
C	4.54198	-1.41128	1.64775
H	5.28294	-0.60688	1.62792
H	4.97890	-2.30822	2.10556
H	3.65370	-1.08802	2.20191
C	3.63027	3.94761	-0.89447
H	4.49656	4.18119	-0.26300
H	3.82574	4.33096	-1.91145
O	-4.41226	-1.98774	-1.77307
C	-3.98322	-3.18034	-2.43800
H	-3.28251	-3.75127	-1.81291
H	-4.89159	-3.76716	-2.60411
H	-3.50955	-2.95181	-3.40475
O	-5.23699	0.16375	-0.41037
C	-6.00809	1.01468	-1.28064
H	-7.03245	0.99913	-0.89311
H	-5.62379	2.04420	-1.26713
H	-5.99817	0.62759	-2.31052
O	-3.52276	2.14241	0.28513
C	-2.63520	3.22749	0.58673
H	-3.25815	3.99601	1.05374

H	-1.84610	2.92071	1.28720
H	-2.17098	3.63012	-0.32533
C	2.36786	4.57095	-0.33480
C	2.03697	4.38399	1.01970
C	1.47006	5.25841	-1.16730
C	0.82924	4.87036	1.53032
H	2.71732	3.82992	1.66527
C	0.26063	5.75330	-0.65854
H	1.71624	5.39830	-2.22095
C	-0.06132	5.55835	0.69131
H	0.57938	4.70623	2.57778
H	-0.42827	6.28571	-1.31409
H	-1.00064	5.94130	1.08950

6-C

O	-0.96121	3.17862	0.26397
O	-3.37646	2.27520	0.11154
P	-1.82229	1.86137	-0.10265
O	-1.84271	1.61800	-1.65987
O	-1.38540	0.73426	0.80154
H	-0.95083	-0.75891	0.12466
C	-0.78015	4.20418	-0.74854
H	-0.11410	3.82189	-1.52853
H	-1.74381	4.51017	-1.17467
H	-0.31952	5.05251	-0.23360
C	-3.81031	2.54874	1.46587
H	-3.31589	3.44950	1.85240
H	-3.59209	1.69409	2.11839
H	-4.89076	2.70126	1.41029
C	-1.91442	-2.24812	1.23009
C	-3.19718	-1.94869	0.43818
H	-1.76049	-3.32121	1.37591
H	-1.68369	-1.66681	2.12421
C	-2.33306	-1.97675	-0.85416
H	-2.28241	-2.96931	-1.31024
H	-2.43263	-1.18398	-1.59689
H	-1.08766	0.98367	-2.01453
H	-3.56907	-0.93554	0.63945
S	0.17950	-0.31398	-2.68686
C	1.49906	0.54661	-1.98455
C	2.67394	2.07945	-0.84312
C	3.77542	1.25104	-1.22409
C	2.92064	3.22960	-0.06953
C	5.08529	1.54984	-0.83208
C	4.23050	3.53039	0.31484
H	2.08564	3.86092	0.22717
C	5.30461	2.69959	-0.06088
H	5.91371	0.90277	-1.11492
H	4.42328	4.41982	0.91456
H	6.31839	2.94929	0.25090
S	3.18425	-0.08581	-2.18988
N	1.42779	1.65656	-1.27553
O	-4.19721	-2.92113	0.59026
C	-5.33466	-2.67212	-0.27098
H	-5.02528	-2.74864	-1.32704
H	-6.02272	-3.49778	-0.05371
N	-1.10492	-1.79165	0.01311
C	0.15364	-2.59202	-0.32163
O	-0.01174	-3.62816	-0.94221
C	1.37993	-2.07510	0.26056
C	2.56036	-2.81724	0.03544
C	1.42931	-0.88718	1.01693
C	3.77108	-2.36117	0.54528
H	2.49820	-3.72198	-0.55881
C	2.63767	-0.43014	1.55020
H	0.54512	-0.28105	1.16860
C	3.83729	-1.16141	1.32210
C	-5.98709	-1.33102	-0.01456
C	-6.65157	-1.09281	1.20266
C	-5.88641	-0.29077	-0.95263
C	-7.22133	0.15712	1.46655
H	-6.71699	-1.89252	1.94100
C	-6.45507	0.96313	-0.69154
H	-5.35562	-0.46168	-1.89002
C	-7.12801	1.18652	0.51639
H	-7.74150	0.32984	2.40856
H	-6.36268	1.76349	-1.42421
H	-7.57703	2.15864	0.71955
O	4.97341	-2.97955	0.35598
C	4.98515	-4.13687	-0.48593
H	4.37764	-4.94995	-0.06023
H	4.61849	-3.89840	-1.49548
H	6.03153	-4.45134	-0.53797
O	5.08453	-0.84854	1.73515
C	5.37116	0.24187	2.63784
H	6.44848	0.16243	2.81652
H	5.13185	1.20364	2.17704
H	4.82486	0.12547	3.57999
O	2.73337	0.71427	2.28916
C	1.53584	1.47902	2.49170
H	0.80105	0.90983	3.08102
H	1.85342	2.36456	3.04923
H	1.08510	1.77895	1.53941

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C	-2.34422	-0.03481	-1.91696
C	-1.11980	-0.49298	-1.39474
C	-1.06897	-1.63695	-0.57739
C	-2.24932	-2.33317	-0.28711
C	-3.47918	-1.90347	-0.83322
C	-3.52263	-0.73373	-1.62885
H	-2.35688	0.87553	-2.50298
C	0.08137	0.31354	-1.65976
H	-0.15124	-1.92061	-0.08479
O	-0.09957	1.53604	-2.08341
N	1.30400	-0.17829	-1.54076
C	2.62028	0.41120	-1.87405
C	1.86302	-1.52620	-1.28098
C	3.22806	-1.00972	-1.83621
H	1.90522	-1.73657	-0.20882
H	1.35607	-2.32627	-1.82997
H	3.45501	-1.42225	-2.83265

O	4.34912	-1.06932	-0.98952
O	0.65507	4.31120	0.68564
O	1.56293	3.23024	-1.42885
P	1.94789	3.67085	-0.02993
H	0.65180	2.22847	-1.79817
O	3.06106	4.84462	-0.08627
H	2.99967	1.04286	-1.06622
H	2.62800	0.95613	-2.82371
C	2.76284	6.00456	-0.90258
H	3.62516	6.67027	-0.80731
H	2.62730	5.71145	-1.95069
H	1.85960	6.50995	-0.53695
C	0.60826	4.40289	2.13380
H	-0.31349	4.94339	2.36496
H	0.57190	3.39716	2.56398
H	1.47492	4.95641	2.51585
C	4.94132	-2.38223	-0.91654
H	5.20763	-2.73149	-1.92944
H	5.86650	-2.23153	-0.34671
O	2.72109	2.67635	0.91356
H	2.30705	1.76893	1.20491
S	1.79977	0.03228	2.01309
C	0.16409	0.50229	1.77658
S	-1.19867	-0.35462	2.62584
N	-0.24449	1.48024	0.99089
C	-2.33872	0.70268	1.80747
C	-1.62023	1.62902	0.99153
C	-3.73570	0.72145	1.87251
C	-2.33132	2.58999	0.25086
C	-4.42687	1.67954	1.11697
H	-4.27472	0.01187	2.49706
C	-3.72835	2.60677	0.32013
H	-1.77826	3.29397	-0.36580
H	-5.51543	1.70730	1.15477
H	-4.28458	3.35336	-0.24695
O	-4.76428	-0.37489	-2.06518
C	-4.86767	0.83927	-2.81831
H	-5.93321	0.96005	-3.03458
H	-4.50617	1.69642	-2.23345
H	-4.30667	0.77234	-3.76266
O	-4.62417	-2.62543	-0.61064
C	-5.32968	-2.24543	0.58879
H	-5.64378	-1.19425	0.53647
H	-6.20897	-2.89609	0.64214
H	-4.69933	-2.40002	1.47582
O	-2.31232	-3.42679	0.52590
C	-1.06955	-3.93689	1.03021
H	-1.33108	-4.82832	1.60771
H	-0.57138	-3.20714	1.68369
H	-0.39151	-4.21386	0.21027
C	4.03985	-3.38988	-0.23360
C	3.45176	-4.44081	-0.95545
C	3.71319	-3.22604	1.12527
C	2.55413	-5.31981	-0.33220
H	3.69294	-4.56652	-2.01206
C	2.81250	-4.09544	1.74861
H	4.14451	-2.39589	1.68315
C	2.23337	-5.14703	1.02092
H	2.10470	-6.13303	-0.90169
H	2.55811	-3.95060	2.79789
H	1.53576	-5.82804	1.50773

TS 7-A (R)

Imaginary frequency: -446.01 cm^{-1}

C	3.53972	0.20854	-0.04382
C	3.98012	-1.06597	0.36233
C	5.32009	-1.45936	0.18438
C	6.23472	-0.57186	-0.39490
C	5.80344	0.70801	-0.82164
C	4.45169	1.09170	-0.64255
H	2.50909	0.51085	0.09550
C	3.06418	-2.08105	0.94136
H	5.60988	-2.45237	0.51100
O	3.39924	-3.24167	1.18257
N	1.71341	-1.66918	1.12606
C	0.55959	-1.78869	-0.47659
C	0.72639	-2.64424	1.66230
C	-0.29239	-2.59357	0.50224
H	0.32097	-2.29788	2.61862
H	1.21403	-3.61520	1.78075
H	-0.55453	-3.58761	0.10615
O	-1.46093	-1.84897	0.78863
H	-5.29281	3.42023	-0.01011
O	-1.56820	1.55587	1.90756
C	-5.05546	2.55863	-0.63243
C	-6.01765	2.07052	-1.53724
C	-3.80123	1.95396	-0.51012
H	-6.98693	2.56129	-1.61216
H	-3.05760	2.29690	0.20388
O	0.89641	0.68407	2.10275
C	-5.75166	0.95457	-2.34075
C	-3.53208	0.84174	-1.31850
C	-4.50017	0.34242	-2.21864
N	-2.35176	0.10763	-1.34479
P	-0.05164	1.52540	1.26920
H	1.53052	-0.68751	1.47722
H	-6.49759	0.56966	-3.03306
C	-2.32268	-0.94704	-2.17725
S	-3.87093	-1.08313	-3.04086
S	-1.05273	-2.03470	-2.46151
O	0.45926	3.08041	1.45578
O	-0.25016	1.22204	-0.21449
H	0.41047	-0.71825	-0.58489
H	1.26698	-2.29401	-1.12573
H	-1.50464	0.43982	-0.79292
C	-0.24739	4.09751	0.71786
H	-0.29269	3.84430	-0.34924
H	0.30896	5.03043	0.85706
H	-1.26935	4.21895	1.10491
C	-1.68424	1.79133	3.32427
H	-2.75521	1.81932	3.54828
H	-1.22334	2.74968	3.60098

H	-1.20362	0.98247	3.89000
C	-2.45036	-2.60080	1.51277
H	-2.10826	-2.78777	2.54558
H	-2.59835	-3.57839	1.02155
C	-3.72749	-1.80312	1.50387
C	-4.65623	-1.96981	0.46420
C	-3.97420	-0.84029	2.49526
C	-5.81234	-1.18276	0.41212
H	-4.46427	-2.71034	-0.31212
C	-5.12719	-0.04811	2.44346
H	-3.25573	-0.71117	3.30375
C	-6.04646	-0.21608	1.39867
H	-6.52122	-1.31303	-0.40368
H	-5.30845	0.70001	3.21520
H	-6.93844	0.40704	1.34953
O	7.55919	-0.83781	-0.59438
O	6.69874	1.53619	-1.44741
O	4.13485	2.33487	-1.10478
C	8.03629	-2.12291	-0.18217
H	7.90107	-2.27354	0.89955
H	9.10329	-2.13151	-0.42326
H	7.52871	-2.93266	-0.72743
C	7.13937	2.65187	-0.64488
H	6.29653	3.30018	-0.37230
H	7.84896	3.20749	-1.26675
H	7.64593	2.29486	0.26395
C	2.80779	2.81763	-0.83749
H	2.04146	2.18195	-1.30112
H	2.76980	3.81952	-1.27519
H	2.61557	2.87495	0.24122

TS 7-A (R) *conf1*

Imaginary frequency: -455.64 cm^{-1}

C	-3.65733	0.27015	-0.26242
C	-3.99416	-1.05070	-0.61479
C	-5.29570	-1.54573	-0.40608
C	-6.26980	-0.71977	0.16767
C	-5.94617	0.61249	0.52506
C	-4.63536	1.10153	0.30409
H	-2.66080	0.65567	-0.44045
C	-3.00235	-2.00564	-1.16957
H	-5.50291	-2.57460	-0.68035
O	-3.25657	-3.18355	-1.42346
N	-1.66981	-1.51567	-1.30256
C	-0.60793	-1.61488	0.35367
C	-0.61081	-2.42933	-1.81208
C	0.29117	-2.45441	-0.55780
H	-0.11051	-1.98412	-2.67774
H	-1.05703	-3.39300	-2.06970
H	0.43747	-3.46332	-0.14717
O	1.53438	-1.80266	-0.74081
H	5.16661	3.67462	0.28805
O	1.55048	1.77763	-1.78454
C	4.95874	2.71473	0.75862
C	6.00570	2.00248	1.37532
C	3.65630	2.20947	0.73246
H	7.01310	2.41588	1.37487
H	2.84246	2.73021	0.23752
O	-0.90891	0.93588	-2.07558
C	5.77506	0.76321	1.98418
C	3.42384	0.96983	1.34302
C	4.47265	0.25477	1.96420
N	2.20419	0.31106	1.43481
P	0.00713	1.77819	-1.20755
H	-1.52219	-0.51706	-1.60976
H	6.58463	0.20774	2.45228
C	2.21132	-0.86867	2.08130
S	3.85213	-1.25267	2.62884
S	0.89485	-1.88896	2.40933
O	-0.47921	3.33276	-1.43468
O	0.13794	1.48760	0.28648
H	-0.45243	-0.54424	0.45494
H	-1.35583	-2.09169	0.97817
H	1.33941	0.72264	0.96862
C	0.19003	4.35478	-0.66982
H	1.23660	4.45814	-0.99140
H	0.15973	4.12167	0.40241
H	-0.34367	5.29125	-0.86295
C	1.72761	1.94998	-3.20652
H	1.18581	1.17223	-3.75929
H	2.80205	1.86452	-3.39933
H	1.37079	2.93925	-3.52437
C	2.62462	-2.70628	-0.93844
H	2.46532	-3.29329	-1.86349
H	2.67145	-3.42281	-0.09966
C	3.91853	-1.93256	-1.02907
C	5.12644	-2.55974	-0.67928
C	3.94018	-0.60477	-1.48183
C	6.34110	-1.87289	-0.79147
H	5.11436	-3.58575	-0.30839
C	5.15557	0.08192	-1.59064
H	3.00376	-0.10229	-1.70532
C	6.35839	-0.54793	-1.24973
H	7.27082	-2.36750	-0.50985
H	5.15721	1.12083	-1.91709
H	7.30103	-0.00616	-1.32303
O	-7.55506	-1.09805	0.43184
O	-6.92919	1.42142	1.03254
O	-4.42471	2.39667	0.67499
C	-7.92783	-2.43465	0.08029
H	-8.98012	-2.53038	0.36348
H	-7.32906	-3.17648	0.63013
H	-7.81923	-2.60983	-1.00049
C	-6.81157	1.68940	2.44578
H	-5.87154	2.20856	2.67330
H	-6.87035	0.75324	3.02048
H	-7.66115	2.33110	2.70142
C	-3.13449	2.95932	0.38354
H	-2.33010	2.42474	0.90735
H	-3.18115	3.99389	0.73561
H	-2.92968	2.94352	-0.69404

TS 7-A (R) *arr1*

Imaginary frequency: -425.78 cm^{-1}

C	1.58346	-0.67976	0.10817
C	2.67867	-0.12200	0.79081
C	3.99622	-0.48551	0.45813
C	4.22525	-1.43063	-0.54965
C	3.13228	-1.96718	-1.27482
C	1.81331	-1.56866	-0.95271
H	0.57132	-0.39948	0.36726
C	2.52063	0.96423	1.79202
H	4.80950	-0.01470	0.99993
O	3.44962	1.69294	2.13907
N	1.21184	1.14454	2.32489
C	-0.31434	1.96040	1.28513
C	0.95391	2.38117	3.11927
C	0.22450	3.18207	2.03343
H	1.87916	2.84305	3.47202
H	0.29598	2.12398	3.95524
H	-0.57992	3.84259	2.39523
O	1.21394	3.92083	1.32822
H	-4.33081	-3.82657	-1.56189
O	-1.28477	-2.33769	1.48199
C	-4.17640	-2.76397	-1.74209
C	-4.44692	-2.22922	-3.01788
C	-3.70780	-1.95648	-0.70288
H	-4.80818	-2.88222	-3.81069
H	-3.46313	-2.35764	0.27659
O	-0.04156	-0.96557	3.32359
C	-4.25833	-0.86784	-3.28573
C	-3.51075	-0.59340	-0.97018
C	-3.78732	-0.05364	-2.24883
N	-3.04144	0.36257	-0.07749
P	-1.41164	-1.34219	2.79516
H	0.76123	0.25710	2.70632
H	-4.46817	-0.45467	-4.27001
C	-2.94641	1.61976	-0.55287
S	-3.43399	1.67208	-2.25666
S	-2.44199	2.99589	0.29941
O	-2.08981	-2.28901	3.94408
O	-2.39527	-0.25863	2.35126
H	-0.02617	1.74122	0.26461
H	-1.03018	1.31788	1.79027
H	-2.77178	0.10210	0.94037
C	-3.42660	-2.77372	3.70128
H	-4.10940	-1.94169	3.48576
H	-3.74294	-3.28800	4.61459
H	-3.43621	-3.48219	2.86029
C	-0.28921	-3.38408	1.52847
H	-0.53319	-4.11212	2.31374
H	0.70380	-2.95804	1.71314
H	-0.30680	-3.87174	0.54851
C	0.84220	4.43178	0.03329
H	1.47856	5.31784	-0.10248
H	-0.20655	4.76450	0.02465
C	1.09430	3.43212	-1.08419
C	2.28547	2.68453	-1.09751
C	0.14380	3.21849	-2.09695
C	2.50925	1.72182	-2.08769
H	3.01514	2.83023	-0.30342
C	0.36882	2.25621	-3.09203
H	-0.78709	3.78380	-2.08680
C	1.54905	1.49940	-3.08459
H	3.42005	1.12569	-2.06353
H	-0.38519	2.08889	-3.86090
H	1.71522	0.73287	-3.84103
O	5.45579	-1.88414	-0.92770
O	3.38578	-2.80839	-2.32728
O	0.83550	-2.08708	-1.75265
C	6.59165	-1.32427	-0.25903
H	6.65305	-0.23726	-0.41774
H	7.46416	-1.81027	-0.70516
H	6.56472	-1.53276	0.82100
C	2.99756	-4.18001	-2.10467
H	3.53825	-4.59720	-1.24226
H	3.28007	-4.72310	-3.01249
H	1.91512	-4.26489	-1.94227
C	-0.46677	-1.48179	-1.67067
H	-1.07029	-1.97602	-2.43690
H	-0.40383	-0.40479	-1.88288
H	-0.91865	-1.64581	-0.68723

TS 7-A (R) *arr2*

Imaginary frequency: -457.87 cm^{-1}

C	-3.44695	-3.23000	-0.03844
C	-2.33415	-2.38038	0.10532
C	-2.50215	-1.01889	0.42048
C	-3.79405	-0.50392	0.59686
C	-4.92148	-1.34836	0.46012
C	-4.73860	-2.71701	0.13843
H	-3.27121	-4.26781	-0.30137
C	-0.99364	-2.97475	-0.13898
H	-1.64732	-0.37036	0.56540
O	-0.81259	-4.11635	-0.56041
N	0.11050	-2.09906	0.06537
C	0.56081	-0.83671	-1.39963
C	1.50019	-2.55840	-0.19355
C	1.95657	-1.38351	-1.07425
H	1.45259	-3.48265	-0.77571
H	2.06450	-2.70731	0.73112
H	2.51576	-0.63042	-0.50961
O	2.67951	-1.82197	-2.21521
H	-1.09178	5.28756	2.38734
O	1.60692	1.67638	3.17598
C	-1.07004	4.93940	1.35598
C	-1.93711	5.52003	0.40853
C	-0.18088	3.92183	0.99853
H	-2.62072	6.30955	0.71650
H	0.49058	3.46466	1.72183
O	0.15400	0.06695	1.73342
C	-1.93750	5.09751	-0.92669
C	-0.18493	3.49289	-0.33770
C	-1.05465	4.07428	-1.29101

N	0.60396	2.48628	-0.88080
P	1.55723	0.62397	1.91552
H	0.04199	-1.39545	0.83914
H	-2.60877	5.54397	-1.65716
C	0.40705	2.21464	-2.18452
S	-0.83957	3.28670	-2.85346
S	1.16495	0.98482	-3.07649
O	2.47843	-0.64546	2.39176
O	2.24052	1.35922	0.76231
H	0.14289	0.01154	-0.87537
H	-0.02049	-1.29827	-2.19235
H	1.33204	1.96869	-0.25394
C	3.90879	-0.44440	2.48306
H	4.34429	-1.41741	2.72739
H	4.14449	0.27983	3.27500
H	4.31180	-0.09293	1.52786
C	0.95664	1.27200	4.40104
H	1.42516	0.36473	4.80640
H	1.08331	2.09842	5.10795
H	-0.11085	1.08448	4.22872
C	3.92852	-1.13727	-2.40643
H	3.75709	-0.05871	-2.54684
H	4.31714	-1.54232	-3.35143
C	4.92194	-1.36536	-1.28245
C	5.02085	-2.61882	-0.65342
C	5.77490	-0.32767	-0.87206
C	5.95897	-2.83113	0.36357
H	4.35401	-3.42192	-0.96468
C	6.72477	-0.54188	0.13628
H	5.68947	0.65358	-1.34042
C	6.81784	-1.79441	0.75781
H	6.02290	-3.80615	0.84667
H	7.37925	0.27263	0.44601
H	7.54890	-1.96011	1.54876
O	-4.06259	0.79887	0.90751
O	-6.19133	-0.87863	0.67687
O	-5.88840	-3.44255	0.01282
C	-2.94763	1.70488	0.94176
H	-3.36785	2.68549	1.17949
H	-2.44867	1.74856	-0.03678
H	-2.21206	1.41499	1.70368
C	-6.71093	-0.06069	-0.39235
H	-6.76122	-0.63714	-1.32792
H	-6.09450	0.83603	-0.53921
H	-7.72099	0.23003	-0.08540
C	-5.75351	-4.82969	-0.31503
H	-5.26026	-4.96590	-1.28926
H	-6.77397	-5.22083	-0.36272
H	-5.18683	-5.37049	0.45756

TS 7-A (R) *arr3*

Imaginary frequency: -437.81 cm^{-1}

C	-4.04406	-1.86316	-1.40895
C	-2.84254	-1.56815	-0.73651
C	-2.79598	-0.57376	0.25999
C	-3.96923	0.11947	0.59471
C	-5.18206	-0.16597	-0.07775
C	-5.21350	-1.16730	-1.07941
H	-4.03041	-2.64083	-2.16522
C	-1.64886	-2.35630	-1.13797
H	-1.87240	-0.33616	0.77386
O	-1.65356	-3.20715	-2.02684
N	-0.43148	-2.02771	-0.47336
C	0.72206	-0.67732	-1.35618
C	0.78265	-2.86530	-0.66170
C	1.76381	-1.71459	-0.92778
H	0.65119	-3.47523	-1.55903
H	0.99182	-3.49398	0.20897
H	2.24541	-1.36848	-0.00595
O	2.71840	-1.99248	-1.94087
H	0.04460	6.60099	1.66753
O	0.47787	0.91451	3.60715
C	0.54978	6.13654	0.82222
C	1.14027	6.94860	-0.16595
C	0.60069	4.74183	0.73740
H	1.08458	8.03234	-0.07659
H	0.15453	4.09564	1.49025
O	-0.03862	-1.13464	2.07269
C	1.80079	6.38661	-1.26652
C	1.25934	4.17931	-0.36508
C	1.85424	4.99137	-1.35746
N	1.42409	2.82293	-0.61715
P	0.67290	0.20239	2.14348
H	-0.47882	-1.66454	0.50887
H	2.25699	7.01542	-2.02818
C	2.10289	2.49729	-1.73418
S	2.59435	3.97387	-2.59536
S	2.50438	0.94205	-2.27971
O	2.28545	-0.14073	2.07203
O	0.31043	1.29446	1.13754
H	0.30750	-0.74151	-2.35938
H	0.42697	0.14933	-0.72138
H	1.04428	2.10415	0.08020
C	3.20725	0.95517	1.89001
H	2.92727	1.82140	2.50410
H	3.24708	1.24761	0.83266
H	4.19196	0.59213	2.20329
C	0.66140	0.08297	4.77417
H	1.69318	-0.29167	4.82497
H	-0.03393	-0.76578	4.75757
H	0.45786	0.71715	5.64318
C	4.02197	-2.29313	-1.39420
H	4.41244	-1.40847	-0.86438
H	4.65099	-2.48067	-2.27275
C	3.98270	-3.49298	-0.47362
C	3.78860	-4.78071	-1.00602
C	4.02783	-3.33113	0.92135
C	3.64599	-5.88574	-0.16011
H	3.73801	-4.90871	-2.08778
C	3.88220	-4.43576	1.77182
H	4.15467	-2.33416	1.34361
C	3.69068	-5.71448	1.23224

H	3.49734	-6.87907	-0.58315
H	3.91220	-4.29613	2.85215
H	3.57527	-6.57437	1.89168
O	-4.04617	1.08872	1.55122
O	-6.32442	0.54071	0.19799
O	-6.43473	-1.37905	-1.65289
C	-2.85707	1.35284	2.31694
H	-2.04455	1.72934	1.68268
H	-2.51080	0.44731	2.83480
H	-3.14579	2.11206	3.04952
C	-6.98263	0.14295	1.41884
H	-6.32769	0.29434	2.28716
H	-7.29245	-0.91112	1.36336
H	-7.86762	0.78184	1.50650
C	-6.51262	-2.38236	-2.67109
H	-7.55735	-2.39167	-2.99532
H	-6.23879	-3.37376	-2.27977
H	-5.86350	-2.13753	-3.52504

TS 7-A (R) *arr4*

Imaginary frequency: -439.10 cm^{-1}

C	5.13535	1.45385	-0.31796
C	3.85326	1.03740	0.08725
C	3.50035	-0.32504	0.07611
C	4.43947	-1.28004	-0.33528
C	5.73258	-0.87568	-0.74543
C	6.07654	0.49982	-0.72601
H	5.36358	2.51427	-0.29421
C	2.89025	2.09603	0.48611
H	2.52226	-0.65191	0.40570
O	3.12756	3.30263	0.43919
N	1.59512	1.62533	0.84700
C	0.37507	1.40390	-0.72091
C	0.53435	2.57539	1.26636
C	-0.54268	2.16810	0.23725
H	0.88457	3.59618	1.08560
H	0.26915	2.43193	2.31817
H	-1.27853	1.48081	0.67400
O	-1.17889	3.26064	-0.40304
H	-4.90816	-4.35806	0.39750
O	-0.39109	-2.73222	2.48712
C	-4.76115	-3.54683	-0.31362
C	-5.77430	-3.24587	-1.24436
C	-3.56404	-2.82455	-0.28817
H	-6.69818	-3.82197	-1.24128
H	-2.76551	-3.05152	0.41388
O	1.19357	-0.66513	2.25253
C	-5.61135	-2.21940	-2.18439
C	-3.40819	-1.78454	-1.21541
C	-4.41608	-1.49251	-2.16215
N	-2.30322	-0.94906	-1.33416
P	-0.13216	-1.26047	1.81311
H	1.54398	0.71338	1.37259
H	-6.38981	-1.99427	-2.91028
C	-2.35566	-0.02623	-2.31406
S	-3.89959	-0.15629	-3.19102
S	-1.19639	1.13139	-2.72657
O	-1.27438	-0.29255	2.49954
O	-0.39242	-1.46660	0.32249
H	0.98240	1.96527	-1.42474
H	0.41358	0.32179	-0.72955
H	-1.47470	-1.07633	-0.66267
C	-2.66937	-0.60726	2.31082
H	-2.86149	-1.67188	2.49683
H	-2.99896	-0.34120	1.29963
H	-3.22648	-0.00098	3.02955
C	-0.11683	-2.86801	3.89933
H	0.93241	-2.62874	4.11308
H	-0.32323	-3.91191	4.15708
H	-0.76780	-2.20687	4.48805
C	-2.16841	3.88399	0.43078
H	-2.50201	4.75301	-0.15205
H	-1.71358	4.26272	1.36255
C	-3.34585	2.98395	0.76067
C	-3.84280	2.90432	2.07092
C	-3.96961	2.23420	-0.25317
C	-4.95654	2.10421	2.36429
H	-3.35697	3.47265	2.86536
C	-5.06709	1.41765	0.04117
H	-3.58003	2.29045	-1.26764
C	-5.56667	1.35388	1.35102
H	-5.33527	2.05550	3.38513
H	-5.53435	0.83269	-0.74962
H	-6.42293	0.71951	1.57891
O	4.19212	-2.62181	-0.38220
O	6.65135	-1.78442	-1.20333
O	7.35255	0.78464	-1.12120
C	2.91374	-3.06895	0.10357
H	2.76159	-2.77454	1.15105
H	2.93617	-4.15903	0.01798
H	2.08873	-2.66517	-0.49971
C	7.24846	-2.59735	-0.17110
H	7.78772	-1.96643	0.55090
H	7.95626	-3.25898	-0.68125
H	6.48926	-3.19518	0.34980
C	7.74478	2.16115	-1.11953
H	7.68499	2.59463	-0.10975
H	7.12424	2.75564	-1.80669
H	8.78367	2.17127	-1.46211

TS 7-A (R) *arr5*

Imaginary frequency: -458.17 cm^{-1}

C	-5.20135	-1.53089	0.26714
C	-3.94556	-0.90587	0.38764
C	-3.72408	0.38145	-0.13725
C	-4.77625	1.04983	-0.78048
C	-6.04283	0.43208	-0.91100
C	-6.25184	-0.86174	-0.37296
H	-5.32314	-2.52311	0.68833
C	-2.88061	-1.68294	1.07180
H	-2.76123	0.86911	-0.03438
O	-3.03021	-2.83400	1.47964

N	-1.60630	-1.04848	1.17551
C	-0.41122	-1.23022	-0.37173
C	-0.49441	-1.75974	1.87037
C	0.46373	-1.91900	0.66996
H	-0.86105	-2.71973	2.24302
H	-0.10252	-1.13994	2.68088
H	1.39437	-1.36959	0.82226
O	0.71238	-3.26366	0.29488
H	6.10803	2.93655	1.15808
O	0.96129	3.09489	0.37799
C	5.73994	2.33689	0.32690
C	6.56927	2.11483	-0.79015
C	4.45207	1.79704	0.38991
H	7.56989	2.54380	-0.81348
H	3.79536	1.94349	1.24286
O	-1.08442	1.65283	1.13111
C	6.12744	1.34901	-1.87755
C	4.01385	1.02529	-0.69401
C	4.83887	0.80717	-1.81877
N	2.78775	0.37819	-0.79544
P	0.37488	1.96533	1.41997
H	-1.57325	-0.00857	1.29206
H	6.76835	1.17660	-2.73971
C	2.58667	-0.34831	-1.91222
S	4.00273	-0.21898	-2.98143
S	1.24818	-1.28846	-2.33867
O	0.39756	2.71273	2.88091
O	1.41305	0.84625	1.38845
H	-1.04137	-1.82342	-1.02756
H	-0.35649	-0.16267	-0.53454
H	2.09206	0.50387	0.00370
C	1.68962	3.03676	3.43379
H	2.24675	3.70496	2.76159
H	2.27586	2.12480	3.60808
H	1.50447	3.54772	4.38455
C	0.15796	4.26712	0.13877
H	0.74952	4.92726	-0.50441
H	-0.07415	4.78372	1.08052
H	-0.77829	3.99934	-0.36699
C	1.77766	-3.85128	1.07415
H	1.83178	-4.88824	0.72173
H	1.50394	-3.86543	2.14363
C	3.10074	-3.13917	0.88445
C	3.60110	-2.27299	1.87221
C	3.80633	-3.27136	-0.32410
C	4.78130	-1.54902	1.65819
H	3.05241	-2.15507	2.80779
C	4.99226	-2.55950	-0.53583
H	3.41394	-3.92425	-1.10344
C	5.47901	-1.69146	0.45258
H	5.14631	-0.86402	2.42257
H	5.53080	-2.67061	-1.47577
H	6.38626	-1.11575	0.27519
O	-4.67642	2.29983	-1.32121
O	-7.06312	1.05023	-1.58728
O	-7.51252	-1.36118	-0.53119
C	-3.41283	2.96777	-1.19291
H	-3.55565	3.95292	-1.64633
H	-2.62121	2.42401	-1.72958
H	-3.11889	3.07310	-0.13968
C	-7.72908	2.08356	-0.83170
H	-8.51149	2.48000	-1.48720
H	-7.03029	2.88617	-0.56030
H	-8.18607	1.66315	0.07625
C	-7.76822	-2.66862	-0.00648
H	-7.12864	-3.42458	-0.48597
H	-8.81734	-2.87707	-0.23561
H	-7.61468	-2.70096	1.08269

TS 7-A (R) *arr6*

Imaginary frequency: -450.68 cm^{-1}

C	4.90704	-1.69318	0.30016
C	3.89528	-1.03750	-0.42645
C	3.95702	0.34829	-0.66671
C	5.03735	1.08623	-0.15873
C	6.04577	0.44491	0.59853
C	5.97984	-0.95389	0.81576
H	4.82824	-2.76594	0.44160
C	2.78571	-1.88546	-0.93573
H	3.18834	0.85134	-1.24347
O	2.85287	-3.10879	-1.04252
N	1.55493	-1.21622	-1.20537
C	0.23856	-1.41308	0.23311
C	0.49286	-1.90242	-1.99680
C	-0.62157	-1.90795	-0.92820
H	0.82357	-2.91960	-2.22420
H	0.27938	-1.33683	-2.90875
H	-1.41308	-1.18558	-1.15387
O	-1.14336	-3.19644	-0.65546
H	-6.02065	3.37772	-0.99718
O	0.06217	1.81329	0.66114
C	-5.71481	2.66933	-0.22872
C	-6.58797	2.38132	0.83852
C	-4.46371	2.05311	-0.32507
H	-7.55915	2.87126	0.88925
H	-3.78284	2.23480	-1.15198
O	1.17960	1.44924	-1.67797
C	-6.22850	1.46834	1.83931
C	-4.10414	1.14132	0.67591
C	-4.97564	0.85245	1.74837
N	-2.92417	0.40798	0.73148
P	-0.08716	1.92260	-0.98642
H	1.55877	-0.17986	-1.36372
H	-6.90496	1.24120	2.66070
C	-2.80208	-0.45111	1.76282
S	-4.24540	-0.35652	2.80104
S	-1.53990	-1.51399	2.12028
O	-0.16232	3.53611	-1.25588
O	-1.41609	1.22883	-1.26744
H	0.76276	-2.14960	0.83616
H	0.24625	-0.37898	0.55405
H	-2.18073	0.60997	-0.00065

C	-1.30901	4.24411	-0.74051
H	-1.07080	5.31112	-0.80420
H	-1.50517	3.97381	0.30601
H	-2.20024	4.02849	-1.34344
C	1.27819	2.29813	1.26716
H	1.13263	2.23811	2.35064
H	1.46591	3.34150	0.97931
H	2.13460	1.67723	0.97394
C	-2.19856	-3.56485	-1.56917
H	-2.40163	-4.61729	-1.33701
H	-1.84027	-3.50718	-2.61159
C	-3.44460	-2.72336	-1.39600
C	-3.77849	-1.72409	-2.32583
C	-4.25922	-2.89885	-0.26348
C	-4.90778	-0.91714	-2.13291
H	-3.14598	-1.57470	-3.20208
C	-5.39276	-2.10160	-0.07363
H	-3.99356	-3.65691	0.47307
C	-5.71796	-1.10673	-1.00710
H	-5.14627	-0.13408	-2.85172
H	-6.01654	-2.24606	0.80729
H	-6.58483	-0.46817	-0.84389
O	5.19955	2.43045	-0.33411
O	7.07195	1.16329	1.15677
O	7.01361	-1.47942	1.53538
C	4.29535	3.09229	-1.23494
H	4.36685	2.66581	-2.24617
H	4.61520	4.13808	-1.24985
H	3.25467	3.02265	-0.89498
C	8.11761	1.51291	0.22578
H	8.58163	0.60682	-0.19087
H	8.86014	2.07428	0.80237
H	7.72725	2.14011	-0.58692
C	6.99451	-2.89153	1.77307
H	7.89673	-3.10373	2.35396
H	7.02088	-3.45733	0.82977
H	6.10608	-3.18803	2.35033

TS 7-A (R) *arr7*

Imaginary frequency: -435.28 cm^{-1}

C	-3.24082	0.14308	0.59974
C	-3.56528	1.34397	-0.05624
C	-4.88412	1.61934	-0.46168
C	-5.88405	0.66113	-0.24583
C	-5.56765	-0.55957	0.39923
C	-4.24884	-0.80070	0.85163
H	-2.22643	-0.05806	0.91801
C	-2.53465	2.37359	-0.34445
H	-5.09096	2.56899	-0.94400
O	-2.76806	3.57066	-0.49596
N	-1.20540	1.86752	-0.45116
C	-0.00103	1.51351	1.07607
C	-0.10191	2.77901	-0.83743
C	0.96739	2.17329	0.09322
H	-0.35650	3.79639	-0.52557
H	0.09697	2.74788	-1.91390
H	1.54798	1.39602	-0.42337
O	1.81172	3.11908	0.71743
H	4.85332	-3.28388	-2.17738
O	-1.89001	-2.35981	-0.97525
C	4.82404	-2.72259	-1.24472
C	5.99438	-2.59775	-0.47147
C	3.62290	-2.13111	-0.84155
H	6.91698	-3.06792	-0.80842
H	2.71769	-2.19715	-1.44061
O	-0.60546	-0.27415	-1.90389
C	5.99537	-1.86730	0.72395
C	3.62053	-1.41274	0.36119
C	4.79716	-1.27128	1.13084
N	2.53170	-0.75666	0.92529
P	-0.45986	-1.57618	-1.13538
H	-1.11896	0.94832	-0.97696
H	6.90270	-1.75825	1.31439
C	2.77284	-0.07515	2.06553
S	4.47736	-0.25288	2.53264
S	1.67024	0.83877	2.96137
O	0.43111	-2.57229	-2.09791
O	0.11725	-1.55515	0.28287
H	-0.48850	2.13065	1.82585
H	-0.14946	0.44079	1.09145
H	1.53583	-0.98710	0.60255
C	0.59397	-3.93852	-1.65475
H	1.27666	-4.41664	-2.36486
H	-0.37156	-4.46064	-1.65524
H	1.02612	-3.97211	-0.64565
C	-2.86933	-2.22546	-2.02694
H	-3.76645	-2.74349	-1.67437
H	-2.50948	-2.68931	-2.95597
H	-3.09806	-1.16855	-2.20700
C	2.74142	3.72165	-0.21275
H	3.25642	4.48599	0.38073
H	2.19175	4.22858	-1.02405
C	3.72672	2.72852	-0.78726
C	4.83193	2.31116	-0.02525
C	3.52614	2.16502	-2.05956
C	5.72545	1.36110	-0.53102
H	4.98667	2.73309	0.96775
C	4.40921	1.19917	-2.56066
H	2.67356	2.48470	-2.66033
C	5.51301	0.79904	-1.79748
H	6.58042	1.04813	0.06592
H	4.23418	0.76058	-3.54261
H	6.19610	0.04145	-2.17748
O	-7.19238	0.80405	-0.60946
O	-6.54251	-1.51301	0.55660
O	-4.06292	-1.97562	1.51322
C	-7.56298	2.02917	-1.25129
H	-7.37861	2.89572	-0.59870
H	-8.63464	1.94301	-1.45290
H	-7.01950	2.16502	-2.19824
C	-7.15487	-1.50742	1.86279
H	-7.90321	-2.30684	1.85065

H	-7.64792	-0.54310	2.05483
H	-6.41047	-1.70870	2.64531
C	-2.79497	-2.17578	2.16714
H	-1.97445	-2.22065	1.44351
H	-2.89046	-3.13320	2.68791
H	-2.60717	-1.37553	2.89912

TS 7-A (R) *arr8*

Imaginary frequency: -451.35 cm^{-1}

C	-2.95664	-3.38242	-0.48060
C	-1.80456	-2.62509	-0.18677
C	-1.92750	-1.35446	0.40314
C	-3.19761	-0.83931	0.68280
C	-4.35819	-1.59543	0.41500
C	-4.22744	-2.88436	-0.17439
H	-2.82087	-4.35389	-0.94502
C	-0.49676	-3.19134	-0.61693
H	-1.07205	-0.73804	0.65791
O	-0.37437	-4.23833	-1.25040
N	0.62632	-2.37124	-0.33931
C	0.93458	-0.86323	-1.56799
C	1.99593	-2.72938	-0.78529
C	2.36809	-1.31269	-1.23822
H	1.92676	-3.41783	-1.63281
H	2.60669	-3.16137	0.01401
H	2.69932	-0.71967	-0.38258
O	3.30426	-1.28275	-2.29360
H	-2.24223	4.99651	2.01391
O	0.00815	1.22939	2.48137
C	-2.01286	4.67414	0.99935
C	-2.74552	5.20622	-0.08034
C	-0.99872	3.73379	0.79593
H	-3.53355	5.93373	0.10790
H	-0.44441	3.29061	1.61865
O	1.16305	-1.01438	1.87135
C	-2.47677	4.81373	-1.39751
C	-0.73031	3.33649	-0.52225
C	-1.46008	3.87508	-1.60884
N	0.23663	2.42347	-0.93030
P	1.38759	0.48128	1.97799
H	0.66196	-1.85897	0.58483
H	-3.04015	5.22485	-2.23248
C	0.32378	2.20501	-2.25824
S	-0.88582	3.17624	-3.12126
S	1.39484	1.14738	-3.04046
O	2.44633	0.68549	3.21140
O	1.83664	1.30118	0.76884
H	0.42791	-1.28568	-2.43151
H	0.40834	-0.12315	-0.98178
H	0.90836	1.94748	-0.22081
C	2.88694	2.03131	3.48825
H	3.38130	2.46670	2.61054
H	3.59563	1.96126	4.31998
H	2.03914	2.66706	3.78082
C	-0.76870	0.59976	3.52243
H	-0.23377	0.64690	4.48115
H	-0.97509	-0.44646	3.26810
H	-1.70924	1.15439	3.58594
C	4.41236	-0.37430	-2.04505
H	4.03405	0.65624	-1.97575
H	5.03455	-0.46168	-2.94391
C	5.18360	-0.74737	-0.79906
C	6.01474	-1.88242	-0.79258
C	5.00462	-0.02480	0.39418
C	6.66238	-2.28211	0.38174
H	6.14568	-2.45437	-1.71208
C	5.64220	-0.43065	1.57454
H	4.33527	0.83503	0.40547
C	6.47466	-1.55729	1.56912
H	7.30905	-3.15961	0.37479
H	5.47459	0.12462	2.49654
H	6.97193	-1.87456	2.48568
O	-3.28850	0.42315	1.23695
O	-5.62025	-1.11729	0.64997
O	-5.39853	-3.54599	-0.39659
C	-3.79357	1.41932	0.31907
H	-3.76338	2.37050	0.85716
H	-4.82130	1.18681	0.01076
H	-3.14495	1.48387	-0.56621
C	-5.92859	-0.85184	2.03802
H	-5.26158	-0.08739	2.45368
H	-5.84781	-1.77725	2.62583
H	-6.96404	-0.49761	2.04793
C	-5.31341	-4.84638	-0.99231
H	-4.85455	-4.79890	-1.99096
H	-6.34567	-5.19744	-1.07846
H	-4.73849	-5.53907	-0.35980

TS 7-A (S)

Imaginary frequency: -444.02 cm^{-1}

C	-5.17571	-1.55962	-0.05496
C	-3.88783	-1.05495	-0.31536
C	-3.56543	0.28450	-0.02605
C	-4.54073	1.12766	0.52386
C	-5.83961	0.63216	0.79189
C	-6.15298	-0.71721	0.49053
H	-5.37897	-2.59810	-0.29428
C	-2.88977	-2.00381	-0.87150
H	-2.57975	0.67934	-0.23602
O	-3.10946	-3.19565	-1.08502
N	-1.58614	-1.46330	-1.06538
C	-0.40913	-1.53045	0.52618
C	-0.50052	-2.29040	-1.64473
C	0.55929	-2.02087	-0.55426
H	-0.81129	-3.33937	-1.63248
H	-0.25357	-1.97067	-2.66242
H	1.24018	-1.20560	-0.83932
O	1.27593	-3.17089	-0.14841
H	5.46241	3.47034	-0.53873
O	-0.24820	3.32847	-1.52572
C	5.21767	2.68885	0.17922
C	6.19693	2.25433	1.09310

C	3.93676	2.12871	0.16810
H	7.18809	2.70510	1.07889
H	3.18167	2.42305	-0.55490
O	-1.04854	0.99233	-2.01583
C	5.91703	1.24357	2.02185
C	3.65461	1.11973	1.09814
C	4.63641	0.68084	2.01511
N	2.45286	0.43158	1.23404
P	0.03685	1.73505	-1.25903
H	-1.51198	-0.46325	-1.38929
H	6.67412	0.90064	2.72404
C	2.42382	-0.53294	2.17715
S	3.99280	-0.62537	3.00589
S	1.13598	-1.54632	2.58408
O	1.51753	1.46402	-1.93422
O	0.25478	1.47432	0.22971
H	-0.98025	-2.26743	1.08369
H	-0.49671	-0.48045	0.77648
H	1.56509	0.77837	0.75082
C	1.61222	1.49717	-3.37274
H	2.66060	1.30392	-3.61896
H	1.31596	2.48149	-3.76083
H	0.97289	0.72439	-3.81802
C	0.60010	4.28117	-0.85177
H	0.66525	4.05519	0.22014
H	1.60932	4.27773	-1.28806
H	0.14408	5.26560	-0.99936
C	2.28114	-3.55641	-1.11047
H	2.64186	-4.52648	-0.74797
H	1.82448	-3.71058	-2.10309
C	3.41786	-2.56190	-1.20461
C	3.54023	-1.69866	-2.30601
C	4.35336	-2.46746	-0.15848
C	4.58027	-0.76019	-2.36507
H	2.81874	-1.76374	-3.12167
C	5.39829	-1.54058	-0.22125
H	4.25563	-3.12359	0.70624
C	5.51137	-0.68042	-1.32306
H	4.66481	-0.09556	-3.22442
H	6.11967	-1.47935	0.59132
H	6.31315	0.05529	-1.35794
O	-4.32836	2.43712	0.84400
O	-6.79363	1.42204	1.37923
O	-7.43679	-1.09121	0.76770
C	-3.05085	2.99784	0.49382
H	-2.23018	2.49682	1.02577
H	-2.86912	2.93030	-0.58682
H	-3.10086	4.04735	0.79761
C	-7.37795	2.40290	0.49632
H	-7.88107	1.90863	-0.34787
H	-8.11530	2.94625	1.09634
H	-6.61719	3.09985	0.12121
C	-7.79815	-2.44680	0.48334
H	-7.19159	-3.15428	1.06830
H	-8.84900	-2.53786	0.77337
H	-7.68983	-2.67503	-0.58775

TS 7-A (S) *conf1*

Imaginary frequency: -444.67 cm^{-1}

C	-5.20242	-1.49227	-0.17175
C	-3.90849	-1.01334	-0.45008
C	-3.58413	0.34255	-0.25498
C	-4.56379	1.22838	0.21383
C	-5.86663	0.75745	0.50765
C	-6.17816	-0.61216	0.31347
H	-5.40371	-2.54740	-0.32424
C	-2.90708	-2.00517	-0.91793
H	-2.59637	0.71920	-0.48797
O	-3.13530	-3.20583	-1.06250
N	-1.59072	-1.49320	-1.10265
C	-0.46760	-1.47656	0.53068
C	-0.49802	-2.36737	-1.59233
C	0.52861	-2.04495	-0.48451
H	-0.82396	-3.40976	-1.52690
H	-0.21208	-2.11403	-2.61850
H	1.23150	-1.25815	-0.79497
O	1.21403	-3.17711	0.01496
H	5.50830	3.39019	-0.60189
O	-0.16612	3.24918	-1.79409
C	5.22759	2.65220	0.14819
C	6.16958	2.25298	1.11581
C	3.93846	2.11167	0.12471
H	7.16808	2.68744	1.11026
H	3.21201	2.37818	-0.63732
O	-0.97309	0.89481	-2.17240
C	5.84306	1.29821	2.08752
C	3.60972	1.15824	1.09723
C	4.55420	0.75488	2.06824
N	2.39306	0.49615	1.22998
P	0.08964	1.67280	-1.41892
H	-1.48934	-0.51576	-1.48180
H	6.57127	0.98240	2.83172
C	2.31839	-0.41632	2.22087
S	3.85794	-0.48693	3.10494
S	1.00221	-1.38873	2.63787
O	1.59265	1.34717	-2.01586
O	0.24514	1.50255	0.09089
H	-1.06898	-2.17071	1.11084
H	-0.54954	-0.41187	0.71179
H	1.52699	0.82629	0.69723
C	1.74374	1.29152	-3.44899
H	1.11952	0.49342	-3.87035
H	1.46634	2.25034	-3.90820
H	2.80017	1.08210	-3.64127
C	0.66787	4.23410	-1.14951
H	0.69486	4.07215	-0.06444
H	1.69102	4.19721	-1.55033
H	0.22627	5.21129	-1.37071
C	2.24457	-3.63372	-0.88718
H	2.58263	-4.58143	-0.45109
H	1.81783	-3.84814	-1.88191
C	3.39523	-2.65828	-1.00927

C	4.29426	-2.49945	0.06084
C	3.56720	-1.87627	-2.16339
C	5.35216	-1.58965	-0.02886
H	4.15748	-3.09125	0.96573
C	4.62077	-0.95515	-2.25070
H	2.87402	-1.99127	-2.99786
C	5.51534	-0.81114	-1.18385
H	6.04503	-1.47832	0.80291
H	4.74491	-0.35500	-3.15166
H	6.32799	-0.08890	-1.24214
O	-4.35625	2.56265	0.41167
O	-6.85604	1.60850	0.92562
O	-7.45656	-0.96837	0.63529
C	-3.06602	3.08590	0.05040
H	-2.85340	2.91818	-1.01335
H	-3.12033	4.15925	0.25335
H	-2.26339	2.63448	0.65026
C	-6.71091	2.07499	2.28377
H	-5.78011	2.64276	2.41025
H	-7.57138	2.72573	2.47085
H	-6.73010	1.22738	2.98468
C	-7.82019	-2.33962	0.44465
H	-7.72260	-2.63704	-0.61016
H	-7.20770	-3.00816	1.06837
H	-8.86809	-2.41103	0.75043

TS 7-A (S) *conf2*

Imaginary frequency: -436.18 cm^{-1}

C	-5.14343	-1.53462	0.11491
C	-3.84490	-1.07541	-0.17494
C	-3.52969	0.29418	-0.09593
C	-4.52334	1.21295	0.26933
C	-5.83295	0.76392	0.56513
C	-6.13823	-0.61758	0.47770
H	-5.34071	-2.59887	0.04051
C	-2.83025	-2.10102	-0.53172
H	-2.53466	0.65220	-0.32699
O	-3.04904	-3.31218	-0.54932
N	-1.52110	-1.60055	-0.77385
C	-0.37045	-1.43740	0.85278
C	-0.42473	-2.50906	-1.18266
C	0.61782	-2.09204	-0.13629
H	-0.74051	-3.54184	-1.00938
H	-0.13748	-2.36528	-2.22962
H	1.30721	-1.33033	-0.52123
O	1.31149	-3.23691	0.32876
H	5.49368	3.42705	-0.73190
O	-0.07846	3.07081	-1.90143
C	5.23523	2.74028	0.07264
C	6.21533	2.37459	1.01565
C	3.93570	2.22995	0.14195
H	7.22137	2.78333	0.93630
H	3.18169	2.46656	-0.60148
O	-0.91794	0.70418	-2.02340
C	5.91834	1.48261	2.05384
C	3.63290	1.34238	1.18347
C	4.61824	0.97036	2.12772
N	2.41268	0.71057	1.40739
P	0.14197	1.54571	-1.33986
H	-1.42714	-0.65782	-1.23020
H	6.67592	1.19009	2.77769
C	2.37289	-0.14991	2.44402
S	3.95085	-0.20307	3.26095
S	1.07589	-1.11359	2.94735
O	1.65313	1.12463	-1.84410
O	0.25876	1.55135	0.18556
H	-0.96642	-2.08106	1.49451
H	-0.47035	-0.36143	0.93649
H	1.52907	0.99295	0.85940
C	1.85426	0.89063	-3.25497
H	1.65343	1.80454	-3.83094
H	2.89992	0.59271	-3.37068
H	1.19663	0.08608	-3.60656
C	0.75246	4.11759	-1.36027
H	0.80969	4.04565	-0.26661
H	1.76501	4.06563	-1.78591
H	0.28860	5.06726	-1.64666
C	2.73506	-3.09947	0.49961
H	2.96218	-2.49992	1.39147
H	3.07197	-4.12681	0.69556
C	3.44785	-2.52513	-0.70829
C	3.15392	-2.98617	-2.00492
C	4.40914	-1.51567	-0.54752
C	3.80972	-2.44401	-3.11543
H	2.40120	-3.76333	-2.13571
C	5.07087	-0.97184	-1.65630
H	4.64258	-1.15159	0.45109
C	4.77199	-1.43588	-2.94391
H	3.57247	-2.80631	-4.11562
H	5.80373	-0.17901	-1.51065
H	5.28074	-1.01385	-3.81047
O	-4.32010	2.55828	0.37644
O	-6.80687	1.63649	0.97747
O	-7.43278	-0.94554	0.76375
C	-3.02847	3.05860	-0.01149
H	-3.08966	4.14418	0.10743
H	-2.23106	2.65954	0.63052
H	-2.80259	2.80937	-1.05675
C	-7.35577	2.45388	-0.07759
H	-6.58023	3.08243	-0.53449
H	-7.82721	1.82377	-0.84626
H	-8.11458	3.08599	0.39532
C	-7.78713	-2.33043	0.69025
H	-7.20491	-2.93153	1.40462
H	-8.84836	-2.37661	0.95175
H	-7.63949	-2.72951	-0.32466

TS 7-A (S) *arr1*

Imaginary frequency: -446.87 cm^{-1}

C	-3.75048	0.33016	-0.30343
C	-3.89279	-1.06377	-0.44645
C	-5.10458	-1.70378	-0.12315

C	-6.18403	-0.95071	0.35399
C	-6.06117	0.45440	0.48936
C	-4.84059	1.08759	0.15084
H	-2.82179	0.82891	-0.55914
C	-2.79387	-1.93785	-0.93215
H	-5.16257	-2.78047	-0.24204
O	-2.89518	-3.15836	-1.05645
N	-1.54676	-1.29581	-1.18268
C	-0.31096	-1.24602	0.37398
C	-0.42824	-2.07403	-1.78272
C	0.59571	-1.94870	-0.63361
H	-0.74964	-3.10952	-1.92501
H	-0.12346	-1.61993	-2.73021
H	1.43838	-1.30663	-0.90723
O	1.03220	-3.19502	-0.11725
H	6.12269	3.02543	-1.39918
O	-0.39663	2.22179	0.14839
C	5.78359	2.43120	-0.55210
C	6.64982	2.21826	0.53835
C	4.49554	1.88788	-0.56946
H	7.65017	2.64822	0.52478
H	3.81188	2.02679	-1.40341
O	-1.15501	1.25592	-2.04785
C	6.24506	1.46301	1.64751
C	4.09651	1.12328	0.53453
C	4.95543	0.92125	1.63674
N	2.87355	0.47932	0.68468
P	0.08100	1.84424	-1.39074
H	-1.55496	-0.30112	-1.51898
H	6.91366	1.30104	2.49041
C	2.69928	-0.21114	1.82778
S	4.15282	-0.08148	2.84371
S	1.34110	-1.08147	2.33413
O	0.48223	3.29235	-2.04271
O	1.37815	1.04185	-1.35499
H	-0.90035	-1.84951	1.05837
H	-0.34036	-0.17050	0.48648
H	2.13256	0.62389	-0.07555
C	-0.57973	4.25049	-2.23583
H	-0.13117	5.11758	-2.73146
H	-1.37302	3.82874	-2.86591
H	-1.00488	4.55939	-1.27038
C	0.53264	2.88774	1.03174
H	-0.04901	3.58686	1.64320
H	1.02047	2.15370	1.68415
H	1.29250	3.44461	0.46946
C	2.07362	-3.78370	-0.92531
H	2.23179	-4.77459	-0.48310
H	1.72009	-3.92332	-1.96163
C	3.35300	-2.97489	-0.91433
C	4.17477	-2.97121	0.22665
C	3.70945	-2.17173	-2.01124
C	5.33719	-2.19382	0.26218
H	3.89418	-3.57549	1.08937
C	4.86544	-1.38058	-1.97254
H	3.07322	-2.16249	-2.89748
C	5.68285	-1.39327	-0.83607
H	5.96764	-2.20052	1.15012
H	5.12041	-0.74804	-2.82210
H	6.57195	-0.76591	-0.79478
O	-7.39481	-1.46766	0.71657
O	-7.15210	1.17884	0.89412
O	-4.82888	2.44577	0.28940
C	-7.56711	-2.88246	0.58244
H	-8.58873	-3.08696	0.91588
H	-7.44928	-3.20303	-0.46346
H	-6.85530	-3.43548	1.21378
C	-7.05351	1.71336	2.23091
H	-6.20861	2.40872	2.31809
H	-7.99300	2.24608	2.41113
H	-6.94495	0.89938	2.96291
C	-3.62873	3.13297	-0.09993
H	-3.38350	2.93554	-1.15244
H	-3.84368	4.19634	0.04181
H	-2.77298	2.83398	0.51919

TS 7-A (S) *arr2*

Imaginary frequency: -477.66 cm^{-1}

C	2.35840	-0.53390	-1.86471
C	0.98968	-0.37363	-2.12229
C	0.36989	0.88636	-2.07629
C	1.13183	2.00498	-1.70267
C	2.50838	1.85899	-1.41595
C	3.13004	0.59643	-1.54827
H	2.80548	-1.52150	-1.88881
C	0.12249	-1.55452	-2.40856
H	-0.69097	0.96815	-2.28915
O	-0.64911	-1.63959	-3.36217
N	0.14619	-2.52580	-1.38215
C	-1.11902	-2.05122	0.01592
C	-0.68802	-3.75768	-1.46170
C	-1.74621	-3.39658	-0.38356
H	-1.09391	-3.88326	-2.46832
H	-0.07528	-4.62334	-1.19447
H	-1.71312	-4.08499	0.46812
O	-3.10310	-3.39866	-0.78042
H	1.51825	4.50439	1.32074
O	3.90490	-1.46576	1.24602
C	0.60496	3.97112	1.57529
C	-0.56328	4.68894	1.89823
C	0.60910	2.57469	1.54799
H	-0.54109	5.77771	1.90912
H	1.49372	2.00164	1.28642
O	2.11778	-2.98287	0.30669
C	-1.76151	4.02767	2.20137
C	-0.59078	1.91261	1.83955
C	-1.76623	2.62828	2.16641
N	-0.78855	0.53832	1.83955
P	2.32963	-1.91182	1.37031
H	1.03049	-2.62264	-0.78559
H	-2.66264	4.58470	2.44962
C	-2.03614	0.10963	2.12246

S	-3.08953	1.49937	2.45554
S	-2.57961	-1.49307	2.11074
O	2.22371	-2.56260	2.87546
O	1.44287	-0.67911	1.39663
H	-1.50759	-1.11400	-0.36760
H	-0.36275	-2.00744	0.78563
H	0.04903	-0.10534	1.68735
C	2.94329	-3.78826	3.11948
H	4.02487	-3.63629	2.99550
H	2.73030	-4.07627	4.15446
H	2.60789	-4.57907	2.43559
C	4.31856	-0.27220	1.94372
H	5.40930	-0.22696	1.85721
H	3.87611	0.61649	1.47927
H	4.03691	-0.31862	3.00452
C	-3.48059	-2.58815	-1.91521
H	-2.70529	-2.59641	-2.69167
H	-4.36556	-3.10033	-2.31856
C	-3.83794	-1.15462	-1.56910
C	-4.70213	-0.87220	-0.49688
C	-3.35619	-0.09407	-2.35521
C	-5.07030	0.44663	-0.21116
H	-5.07217	-1.69004	0.11792
C	-3.72993	1.22854	-2.07245
H	-2.68660	-0.30681	-3.18746
C	-4.58307	1.50236	-0.99666
H	-5.73560	0.65258	0.62639
H	-3.35840	2.04054	-2.69687
H	-4.86782	2.52946	-0.76948
O	0.64147	3.27289	-1.58321
O	3.23818	2.93262	-0.95829
O	4.47564	0.58133	-1.33178
C	-0.77921	3.43561	-1.64934
H	-1.15843	3.21680	-2.65875
H	-1.28641	2.79171	-0.91790
H	-0.96760	4.48412	-1.40352
C	3.77705	3.75808	-2.00982
H	2.97124	4.19076	-2.61966
H	4.33433	4.56005	-1.51373
H	4.45748	3.17730	-2.64932
C	5.16953	-0.65162	-1.58761
H	4.84557	-1.43215	-0.88943
H	5.01620	-0.97677	-2.62760
H	6.22774	-0.42503	-1.42614

TS 7-B (S)

Imaginary frequency: -404.34 cm^{-1}

C	-4.07266	0.87902	-0.54633
C	-3.39222	-0.20174	-1.13326
C	-3.60684	-1.51988	-0.68895
C	-4.49069	-1.75458	0.37206
C	-5.18848	-0.67615	0.96822
C	-4.97134	0.64190	0.50472
H	-3.85299	1.88031	-0.89755
C	-2.37902	0.07918	-2.17288
H	-3.08404	-2.33215	-1.18048
O	-2.37288	1.31568	-2.67497
N	-1.55720	-0.86666	-2.53722
C	-0.24357	-1.89293	-1.38574
C	-0.38024	-0.66237	-3.37895
C	0.67513	-1.13959	-2.35179
H	-0.23519	0.35372	-3.75909
H	-0.40451	-1.37699	-4.21465
H	1.09829	-0.28458	-1.81613
O	1.68360	-1.96133	-2.91111
H	3.73475	3.00794	3.43094
O	-1.25266	3.08408	-0.06159
C	3.72460	1.94207	3.20752
C	4.65161	1.09139	3.84043
C	2.79415	1.44746	2.28851
H	5.36838	1.50363	4.54904
H	2.09882	2.09721	1.76489
O	-0.10437	2.26645	-2.16076
C	4.66763	-0.28346	3.57134
C	2.81466	0.07365	2.01477
C	3.73650	-0.78342	2.65496
N	1.99886	-0.60023	1.10935
P	0.01198	2.20937	-0.63791
H	-1.41210	1.72120	-2.60209
H	5.38366	-0.94286	4.05745
C	2.21051	-1.92534	0.99452
S	3.51845	-2.43437	2.08254
S	1.42405	-3.05234	0.00795
O	1.33497	3.05601	-0.16026
O	0.08064	0.87471	0.08556
H	-0.60487	-1.42194	-0.48155
H	-0.60161	-2.88527	-1.64041
H	1.24490	-0.06088	0.58757
C	1.55035	4.35723	-0.74707
H	1.66273	4.27419	-1.83498
H	2.47200	4.74848	-0.30373
H	0.71368	5.02986	-0.51477
C	-1.53125	2.97581	1.35058
H	-1.92090	1.97869	1.58908
H	-2.28560	3.73662	1.57773
H	-0.63102	3.17209	1.94990
C	2.79031	-1.18466	-3.42323
H	3.39551	-1.90806	-3.98282
H	2.42475	-0.42110	-4.13033
O	-4.75757	-2.98607	0.90368
C	-4.02797	-4.09804	0.37433
H	-4.25871	-4.25938	-0.68939
H	-2.94268	-3.95790	0.49378
H	-4.35290	-4.96686	0.95413
O	-6.09954	-0.90597	1.97108
C	-5.50015	-1.00537	3.27805
H	-6.32320	-1.18240	3.97871
H	-4.79044	-1.84364	3.32237
H	-4.98596	-0.06921	3.54209
O	-5.67582	1.61501	1.15701
C	-5.56248	2.95081	0.65465
H	-6.22714	3.55672	1.27754

H	-4.53352	3.32914	0.73857
H	-5.88281	3.00996	-0.39615
C	3.60697	-0.53700	-2.32599
C	3.42248	0.81490	-1.98503
C	4.52517	-1.30539	-1.58862
C	4.14859	1.38915	-0.93322
H	2.69478	1.41549	-2.53166
C	5.25631	-0.73178	-0.54289
H	4.65748	-2.35945	-1.83378
C	5.06891	0.61835	-0.21327
H	3.97428	2.42774	-0.66159
H	5.96358	-1.33783	0.02208
H	5.61861	1.05860	0.61755

TS 7-C (S)

Imaginary frequency: -476.16 cm^{-1}

O	1.92024	-2.35446	3.07047
O	3.57078	-1.06123	1.50572
P	2.00607	-1.33952	1.82268
O	1.56741	-2.23667	0.58372
O	1.21961	-0.10382	2.14240
H	0.53193	1.55583	1.50212
C	2.58100	-3.64653	2.98471
H	2.46926	-4.10565	3.97063
H	2.09935	-4.26525	2.21942
H	3.64451	-3.51898	2.74834
C	4.28717	-0.13205	2.36568
H	3.72021	0.79919	2.47755
H	5.23857	0.06065	1.86600
H	4.45267	-0.58625	3.35067
C	1.77611	2.90794	0.46351
C	2.33740	1.82726	-0.47747
H	1.57782	3.82955	-0.09076
H	2.35416	3.12473	1.36758
C	0.99650	1.11564	-0.72060
H	0.32768	1.44895	-1.50742
H	0.72158	0.22409	-0.18664
H	1.69742	-1.83117	-0.33843
H	3.04237	1.14787	0.01826
S	1.52066	-0.95868	-2.22551
C	-0.19580	-1.28262	-2.18961
C	-2.40507	-0.93691	-2.07175
C	-2.44036	-2.36220	-2.00366
C	-3.60657	-0.20958	-2.00203
C	-3.65169	-3.05412	-1.87911
C	-4.81337	-0.90033	-1.87372
H	-3.57122	0.87750	-2.02641
C	-4.83653	-2.30827	-1.81627
H	-3.67425	-4.14136	-1.82807
H	-5.74402	-0.34169	-1.79340
H	-5.78869	-2.82838	-1.71619
S	-0.79963	-2.98753	-2.07747
N	-1.14157	-0.37523	-2.18193
O	2.93033	2.45445	-1.59700
C	3.86908	1.64793	-2.34025
H	3.35232	0.81289	-2.83226
H	4.23560	2.32990	-3.11889
N	0.47274	2.26117	0.75814
C	-0.77131	2.95805	0.60482
O	-0.77250	4.12155	0.20509
C	-1.97602	2.13885	0.83966
C	-3.22582	2.74953	0.61452
C	-1.91819	0.77912	1.19984
C	-4.39814	2.00814	0.75177
H	-3.24305	3.79350	0.32051
C	-3.08812	0.02098	1.32586
H	-0.96943	0.28551	1.37265
C	-4.35595	0.62905	1.11964
C	5.02043	1.13724	-1.49914
C	5.81757	2.03958	-0.77029
C	5.30802	-0.23511	-1.43142
C	6.89644	1.57928	-0.00815
H	5.58298	3.10360	-0.80548
C	6.39104	-0.69997	-0.67219
H	4.68036	-0.94146	-1.97510
C	7.19051	0.20650	0.03648
H	7.51213	2.28725	0.54661
H	6.60320	-1.76780	-0.62784
H	8.03411	-0.15236	0.62585
O	-5.65584	2.49935	0.53507
C	-5.75978	3.86275	0.11522
H	-5.35557	4.54953	0.87428
H	-5.23708	4.02943	-0.83892
H	-6.82983	4.04950	-0.01481
O	-5.57565	0.04298	1.18493
C	-5.77767	-1.31082	1.63752
H	-6.86639	-1.42792	1.65419
H	-5.33027	-2.02821	0.94356
H	-5.36962	-1.45757	2.64342
O	-3.07715	-1.31406	1.62678
C	-1.81072	-1.98559	1.64194
H	-1.17077	-1.62240	2.45831
H	-2.04514	-3.04234	1.79908
H	-1.28719	-1.86711	0.68517

TS 7-D (S)

Imaginary frequency: -451.60 cm^{-1}

C	-1.88979	-0.92929	-1.10443
C	-1.67431	-1.93149	-0.14519
C	-2.74765	-2.61330	0.45211
C	-4.06288	-2.28472	0.08116
C	-4.29633	-1.25846	-0.86398
C	-3.20286	-0.58355	-1.45479
H	-1.03723	-0.40587	-1.52292
C	-0.27335	-2.22758	0.24323
H	-2.54760	-3.41297	1.15783
O	0.56513	-2.27742	-0.78314
N	0.15878	-2.41637	1.46302
C	1.59029	-1.18582	2.08297
C	-0.52609	-1.90247	2.66090
C	0.37634	-0.65462	2.83286
H	-1.59167	-1.67295	2.54125

H	-0.39291	-2.61768	3.48298
H	0.59235	-0.37276	3.87451
O	-0.14633	0.43670	2.08739
O	3.82615	-0.87709	-1.88978
O	3.05978	-2.61839	-0.20092
P	4.23342	-1.76555	-0.60348
H	1.53553	-2.39435	-0.49268
O	5.53653	-2.61673	-1.04642
H	1.82686	-0.81098	1.09684
H	2.23777	-1.92159	2.54401
C	5.35532	-3.58618	-2.10952
H	5.05664	-3.08579	-3.03967
H	6.32533	-4.07280	-2.24296
H	4.59838	-4.32777	-1.82634
C	4.65703	0.25570	-2.25679
H	5.69277	-0.06470	-2.42563
H	4.22959	0.65123	-3.18178
H	4.61469	1.01502	-1.46968
C	-1.14275	1.18188	2.81558
H	-1.77295	0.49431	3.40390
H	-0.63824	1.86690	3.51753
O	4.93142	-0.86089	0.49708
H	4.32107	-0.41239	1.16498
S	3.23391	0.68266	2.60726
C	2.57817	1.54737	1.24870
S	2.08435	3.27349	1.37373
N	2.34292	1.00116	0.07800
C	1.49200	3.18832	-0.27893
C	1.71987	1.87660	-0.79406
C	0.86974	4.17452	-1.05299
C	1.31476	1.56384	-2.10474
C	0.47240	3.84378	-2.35541
H	0.69099	5.17101	-0.65322
C	0.69731	2.55353	-2.87579
H	1.48974	0.55970	-2.48581
H	-0.01835	4.59682	-2.97091
H	0.38232	2.32328	-3.89308
O	-3.52931	0.40662	-2.33388
C	-2.46187	1.25091	-2.79075
H	-1.74206	0.68711	-3.40103
H	-2.93867	2.02084	-3.40408
H	-1.94257	1.72084	-1.94657
O	-5.59055	-0.87711	-1.12586
C	-6.08123	-1.27984	-2.42129
H	-6.06178	-2.37558	-2.51607
H	-7.11579	-0.92498	-2.47528
H	-5.48981	-0.82549	-3.22692
O	-5.18210	-2.89038	0.57708
C	-4.99614	-3.89017	1.58357
H	-4.48461	-3.47835	2.46694
H	-4.42406	-4.74807	1.19886
H	-6.00172	-4.21804	1.86255
C	-2.00047	1.93837	1.83309
C	-3.14235	1.33208	1.28232
C	-1.65644	3.23879	1.43032
C	-3.93626	2.01528	0.35409
H	-3.40629	0.31598	1.57562
C	-2.43940	3.92193	0.49095
H	-0.76873	3.70895	1.85038
C	-3.58159	3.31180	-0.04564
H	-4.80899	1.52741	-0.07514
H	-2.15738	4.92707	0.17904
H	-4.19252	3.84213	-0.77615

8-A (S)

C	1.07823	2.45106	1.56857
C	1.35945	1.11180	1.88075
C	2.59772	0.54091	1.53795
C	3.55521	1.32218	0.87007
C	3.25968	2.65788	0.50169
C	2.01243	3.21798	0.86021
H	0.10838	2.84416	1.85286
C	0.25112	0.34667	2.54515
H	2.82058	-0.48931	1.79423
O	-0.70868	0.93798	3.07872
N	0.32133	-1.01751	2.51206
C	-1.55725	-2.90399	0.71355
C	-0.85920	-1.79071	2.86191
C	-1.88908	-1.78281	1.69115
H	-0.55298	-2.81401	3.11087
H	-1.32459	-1.34094	3.74389
H	-1.79170	-0.81256	1.18597
O	-3.22673	-1.96846	2.14531
H	1.06090	3.57279	-2.00287
O	1.19474	-4.03647	-1.00189
C	0.24677	2.86151	-2.12518
C	-0.92975	3.25527	-2.79634
C	0.37256	1.58127	-1.58234
H	-1.00517	4.26310	-3.20244
H	1.27256	1.27108	-1.05922
O	2.03174	-2.83751	1.06599
C	-2.00780	2.37554	-2.94719
C	-0.70797	0.69220	-1.71047
C	-1.88737	1.09418	-2.39513
N	-0.74738	-0.60720	-1.20719
P	2.10821	-2.81973	-0.43132
H	1.02675	-1.49615	1.94767
H	-2.91668	2.68289	-3.45993
C	-1.90576	-1.18884	-1.44748
S	-3.06756	-0.20208	-2.34227
S	-2.40704	-2.78330	-0.92004
O	3.59432	-3.02950	-1.04463
O	1.70552	-1.49810	-1.20213
H	-1.91092	-3.86374	1.11232
H	-0.48115	-2.98674	0.55357
H	0.71453	-1.22353	-1.08328
C	4.39405	-4.09609	-0.46985
H	5.37008	-4.03715	-0.95893
H	4.50175	-3.95316	0.61177
H	3.93234	-5.07096	-0.67219
C	0.99374	-4.15471	-2.43476
H	1.95748	-4.24054	-2.95207

H	0.40569	-5.06445	-2.58234
H	0.44173	-3.28736	-2.81429
C	-3.82748	-0.74020	2.62012
H	-4.72637	-1.06645	3.15796
H	-3.15434	-0.23774	3.33013
C	-4.19803	0.22040	1.50688
C	-3.39620	1.34312	1.22910
C	-5.36125	0.00817	0.74460
C	-3.76194	2.24513	0.22048
H	-2.49295	1.50826	1.81619
C	-5.73250	0.91358	-0.25586
H	-5.98247	-0.86480	0.94946
C	-4.93428	2.03778	-0.51684
H	-3.12733	3.10499	0.00696
H	-6.64285	0.74516	-0.83142
H	-5.22139	2.74192	-1.29803
O	4.81116	0.89509	0.53708
O	4.18027	3.44326	-0.15090
O	1.80088	4.50424	0.44099
C	5.16834	-0.44958	0.87936
H	4.53593	-1.17555	0.35379
H	6.20728	-0.56646	0.55662
H	5.10017	-0.61608	1.96469
C	4.41881	3.06587	-1.52155
H	3.48824	3.11418	-2.10699
H	5.13516	3.79513	-1.91475
H	4.84196	2.05523	-1.58797
C	0.52629	5.08326	0.74361
H	0.36140	5.14525	1.82936
H	0.55448	6.09132	0.31914
H	-0.29074	4.51000	0.28070

8-B (S)

C	2.87767	0.43373	-1.26357
C	1.80039	-0.42607	-1.53085
C	1.92516	-1.81188	-1.33484
C	3.12107	-2.33521	-0.82905
C	4.20235	-1.47679	-0.52799
C	4.08036	-0.09174	-0.76975
H	2.74296	1.49775	-1.41476
C	0.49160	0.13866	-1.96704
H	1.06441	-2.43586	-1.54892
O	0.58066	1.43016	-2.36830
N	-0.55573	-0.61411	-1.93645
C	-2.86763	-0.19082	-0.09712
C	-1.83367	-0.13343	-2.43645
C	-2.96509	-0.68876	-1.56344
H	-1.98665	-0.52005	-3.45775
H	-1.94417	0.95965	-2.47594
H	-2.92193	-1.78932	-1.58228
O	-4.19433	-0.23034	-2.14092
H	4.02248	2.24389	2.48586
O	-1.78929	4.79453	0.17377
C	3.40298	1.35701	2.36461
C	3.95399	0.08807	2.63210
C	2.08492	1.50185	1.92667
H	4.99641	0.00502	2.93197
H	1.65490	2.46891	1.67956
O	-1.30364	2.97855	-1.50244
C	3.19309	-1.07607	2.48869
C	1.31808	0.33584	1.78554
C	1.86391	-0.93486	2.07664
N	-0.01634	0.26946	1.38878
P	-0.98547	3.39693	-0.08033
H	-0.24764	1.96463	-2.13573
H	3.62730	-2.05680	2.66406
C	-0.51995	-0.95947	1.35279
S	0.65473	-2.18190	1.79923
S	-2.15624	-1.45422	1.05249
O	0.60436	3.79051	0.09226
O	-1.25640	2.44304	1.09267
H	-2.31008	0.74490	-0.00663
H	-3.86940	-0.02278	0.30476
H	-0.59421	1.22463	1.20740
C	1.23880	4.52338	-0.97877
H	2.24418	4.77643	-0.62516
H	0.68705	5.44656	-1.20180
H	1.30590	3.90304	-1.87969
C	-1.70421	5.38882	1.48759
H	-0.66167	5.62854	1.73856
H	-2.11572	4.71103	2.24597
H	-2.29438	6.31005	1.44876
C	-5.25395	-1.20391	-2.11063
H	-6.07122	-0.74020	-2.67768
H	-4.93655	-2.11863	-2.64090
O	3.33509	-3.66258	-0.55457
C	2.29421	-4.57585	-0.91493
H	2.67004	-5.56983	-0.65351
H	1.36900	-4.37391	-0.35521
H	2.07923	-4.53301	-1.99331
O	5.34643	-1.97907	0.05548
C	6.33086	-2.41059	-0.90186
H	7.18318	-2.78173	-0.32164
H	5.93598	-3.21979	-1.53373
H	6.65493	-1.57191	-1.53575
O	5.18493	0.65751	-0.46115
C	5.10078	2.06455	-0.70190
H	4.30467	2.52554	-0.09923
H	6.07074	2.47391	-0.40319
H	4.92036	2.28000	-1.76597
C	-5.70268	-1.54937	-0.70587
C	-5.29002	-2.74276	-0.09109
C	-6.45134	-0.62194	0.04191
C	-5.60609	-3.00279	1.25030
H	-4.70982	-3.46765	-0.66314
C	-6.76918	-0.87735	1.38030
H	-6.76544	0.31113	-0.42692
C	-6.34172	-2.06755	1.98941
H	-5.27391	-3.92995	1.71659
H	-7.34642	-0.14980	1.95043
H	-6.58427	-2.26444	3.03326

8-C (S)

O	3.47855	2.13043	-0.81629
O	1.10036	3.02967	-1.35282
P	1.92445	1.96197	-0.44193
O	1.47633	0.57901	-1.07553
O	1.72564	2.16540	1.03389
H	1.42194	0.36363	1.82446
C	4.02603	1.61071	-2.05622
H	5.11083	1.69571	-1.95622
H	3.74892	0.55922	-2.17876
H	3.66616	2.20401	-2.90628
C	1.16090	4.42522	-0.96220
H	0.50109	4.96164	-1.64976
H	2.18666	4.80541	-1.05653
H	0.81154	4.54837	0.06976
C	-0.34551	-0.73684	2.25097
C	-1.24660	-0.14860	1.12980
H	-0.53135	-1.81112	2.34473
H	-0.61738	-0.26055	3.20387
C	-1.40299	1.36787	1.27557
H	-0.43230	1.87762	1.30593
H	-1.94596	1.57700	2.20377
H	0.61876	0.20215	-0.67479
H	-2.24182	-0.60129	1.20838
S	-2.28871	2.19345	-0.10368
C	-3.88956	1.50089	0.08062
C	-5.59105	0.29895	0.85355
C	-6.23506	0.83006	-0.30092
C	-6.28925	-0.59103	1.68700
C	-7.54880	0.48084	-0.63272
C	-7.60060	-0.94128	1.35647
H	-5.79107	-1.00311	2.56250
C	-8.22388	-0.41336	0.20830
H	-8.03176	0.88517	-1.52036
H	-8.14764	-1.63605	1.99254
H	-9.24614	-0.70230	-0.03271
S	-5.12039	1.87832	-1.16918
N	-4.27508	0.70632	1.04011
O	-0.72421	-0.42954	-0.18135
C	-0.95472	-1.78720	-0.67140
H	-0.45147	-1.79147	-1.64577
H	-0.44910	-2.50240	-0.01001
N	1.07482	-0.58243	1.99428
C	1.80361	-1.64034	1.50706
O	1.34109	-2.79282	1.42997
C	3.19129	-1.32069	1.03338
C	3.90171	-0.19537	1.47729
C	3.73346	-2.17718	0.06137
C	5.14090	0.11456	0.89546
H	3.48520	0.44738	2.24368
C	4.98082	-1.88171	-0.50700
H	3.15347	-3.04440	-0.23630
C	5.67993	-0.71877	-0.10958
C	-2.42611	-2.08460	-0.80583
C	-3.20855	-1.38521	-1.74266
C	-3.04322	-3.02879	0.03132
C	-4.58069	-1.63265	-1.84380
H	-2.73821	-0.63660	-2.37975
C	-4.42003	-3.27391	-0.06569
H	-2.44068	-3.56821	0.76331
C	-5.19000	-2.57518	-1.00289
H	-5.18012	-1.08039	-2.56537
H	-4.89097	-3.99948	0.59699
H	-6.26391	-2.74375	-1.06428
O	5.89302	1.20958	1.21325
C	5.31182	2.16143	2.11602
H	6.01944	2.99514	2.15609
H	4.33835	2.50843	1.74682
H	5.19575	1.73406	3.12398
O	6.84599	-0.37055	-0.75542
C	8.03799	-0.74016	-0.03613
H	8.88196	-0.41578	-0.65481
H	8.08108	-0.23666	0.93997
H	8.08380	-1.83021	0.10618
O	5.59714	-2.63531	-1.46894
C	4.90638	-3.80333	-1.92176
H	5.55600	-4.25632	-2.67676
H	4.74141	-4.51744	-1.10083
H	3.93761	-3.54551	-2.37606

8-D (S)

C	-3.12551	1.70387	-0.40040
C	-1.98332	1.08927	-0.93739
C	-2.09172	-0.01392	-1.79980
C	-3.35932	-0.52789	-2.10691
C	-4.52004	0.09573	-1.59653
C	-4.39794	1.21430	-0.74225
H	-3.02062	2.58403	0.22494
C	-0.60507	1.59746	-0.66340
H	-1.18455	-0.45290	-2.19956
O	0.19557	1.71361	-1.63365
N	-0.24111	1.92665	0.59582
C	0.61051	-0.64739	1.82508
C	-0.86040	1.46546	1.83918
C	-0.80945	-0.06157	2.00786
H	-0.29876	1.92995	2.65807
H	-1.90229	1.78665	1.92067
H	-1.50410	-0.50249	1.27619
O	-1.27966	-0.31639	3.33325
O	3.73952	3.66517	-0.77057
O	2.67969	1.47342	-1.34051
P	3.31142	2.23473	-0.11338
H	1.64549	1.61101	-1.43771
O	4.69604	1.47907	0.22388
H	0.78971	-1.43023	2.56859
H	1.39397	0.11285	1.91768
C	5.63719	1.21479	-0.84848
H	6.00911	2.15745	-1.26970
H	6.45362	0.64704	-0.39613
H	5.16143	0.61459	-1.63102
C	4.30519	4.65245	0.12593
H	4.48914	5.54597	-0.47800

H	3.60222	4.88271	0.93590
H	5.25131	4.29122	0.55130
C	-2.01509	-1.55449	3.44054
H	-1.40276	-2.39987	3.08342
H	-2.18027	-1.68347	4.51755
O	2.48189	2.36927	1.13404
H	0.74819	2.20338	0.70524
S	0.75531	-1.39800	0.14765
C	2.48813	-1.64195	0.06641
S	3.19391	-2.18526	-1.49063
N	3.32739	-1.45767	1.04590
C	4.77211	-2.15184	-0.71383
C	4.62969	-1.72561	0.63912
C	6.02496	-2.45336	-1.26039
C	5.77330	-1.60013	1.44654
C	7.15073	-2.32163	-0.43747
H	6.12454	-2.77532	-2.29532
C	7.02514	-1.89870	0.90124
H	5.66341	-1.26399	2.47569
H	8.13619	-2.54852	-0.84238
H	7.91680	-1.80188	1.51942
O	-5.57526	1.74493	-0.30044
C	-5.49867	2.74474	0.72059
H	-5.01384	3.66215	0.35387
H	-6.53461	2.96677	0.99347
H	-4.95765	2.36624	1.60038
O	-5.76638	-0.41913	-1.86321
C	-6.27014	-0.07985	-3.17036
H	-7.25930	-0.54425	-3.24393
H	-6.36586	1.01078	-3.27787
H	-5.61650	-0.47492	-3.96012
O	-3.58177	-1.63600	-2.87652
C	-2.43023	-2.33983	-3.35812
H	-2.82056	-3.20378	-3.90362
H	-1.79731	-2.68140	-2.52553
H	-1.83239	-1.71427	-4.03723
C	-3.32518	-1.49262	2.68734
C	-3.51616	-2.21544	1.49802
C	-4.34479	-0.63147	3.13411
C	-4.70519	-2.08534	0.76746
H	-2.72197	-2.87109	1.13714
C	-5.53704	-0.50953	2.41298
H	-4.19344	-0.05563	4.04786
C	-5.71840	-1.23561	1.22663
H	-4.82964	-2.61735	-0.17417
H	-6.32267	0.15686	2.76879
H	-6.62550	-1.11087	0.64010

Structures with full catalyst (*R*)-3b

(*R*)-3b

C	0.89121	5.02416	-2.64820
C	0.37608	4.09817	-1.75712
C	3.11647	4.10233	-2.38930
C	2.27541	5.04278	-2.95479
H	0.22308	5.74123	-3.12409
H	-0.68846	4.09201	-1.54272
H	4.17627	4.07905	-2.64407
H	2.66811	5.78277	-3.65120
C	1.22027	3.14450	-1.11932
C	0.73468	2.18085	-0.16015
C	2.61573	3.12378	-1.48372
C	1.61753	1.19681	0.27104
C	-0.69004	2.15023	0.26675
C	3.45080	2.07554	-1.00915
O	1.20394	0.27048	1.24197
C	2.95688	1.07081	-0.19475
C	-1.42864	0.97551	0.11938
H	4.48302	2.02677	-1.35216
P	0.15035	-0.92421	0.86013
C	3.69655	-0.20027	0.07532
O	-0.76688	-0.19795	-0.29290
C	-2.83649	0.89570	0.30896
O	-0.54533	-1.45158	2.05535
O	0.95088	-2.00469	-0.01578
C	3.77420	-1.17407	-0.96609
C	4.21620	-0.48494	1.35933
C	-3.49092	2.05258	0.70585
C	-3.57180	-0.38265	0.06629
H	1.90260	-1.77969	-0.13139
C	4.37177	-2.41349	-0.67874
C	3.27815	-0.88809	-2.38671
C	4.81191	-1.73571	1.58673
C	4.16834	0.54546	2.48096
H	-4.57280	2.03247	0.82706
C	-3.70448	-0.87583	-1.25759
C	-4.14300	-1.09124	1.15297
C	4.88961	-2.71678	0.59033
H	4.42866	-3.16213	-1.46694
C	4.46819	-0.48053	-3.28167
C	2.50716	-2.05802	-3.02862
H	2.58927	-0.03551	-2.33637
H	5.21532	-1.95954	2.57470
C	3.48312	-0.00265	3.74699
C	5.58547	1.07213	2.78785
H	3.57427	1.39728	2.12530
C	-4.41774	-2.06332	-1.46968
C	-3.13419	-0.13306	-2.46362
C	-4.85527	-2.27213	0.88371
C	-4.02051	-0.60982	2.59703
C	5.49870	-4.08072	0.88088
H	5.18216	-1.31152	-3.36974
H	5.00650	0.38125	-2.86885
H	4.11992	-0.21906	-4.29034
H	3.15264	-2.92967	-3.20183
H	1.66010	-2.37510	-2.40983
H	2.11487	-1.74453	-4.00529
H	4.06010	-0.82447	4.19286
H	2.47683	-0.37205	3.51772
H	3.39729	0.79003	4.50282
H	6.23618	0.26395	3.14998
H	6.04839	1.50185	1.88932

H	5.54717	1.84975	3.56318
C	-5.00337	-2.77724	-0.41350
H	-4.52344	-2.43749	-2.48791
C	-2.13904	-1.00233	-3.25723
C	-4.26699	0.39537	-3.36720
H	-2.58391	0.74310	-2.09924
H	-5.30314	-2.82137	1.71238
C	-5.35599	-0.01280	3.08791
C	-3.53750	-1.71954	3.55082
H	-3.26572	0.18594	2.62164
C	4.43834	-5.19450	0.76275
C	6.71417	-4.36791	-0.02247
H	5.85228	-4.06308	1.92355
C	-5.77352	-4.06571	-0.66728
H	-2.63689	-1.87483	-3.70260
H	-1.33310	-1.36166	-2.60678
H	-1.69192	-0.41996	-4.07533
H	-4.85970	-0.43040	-3.78462
H	-4.94751	1.04579	-2.80124
H	-3.85422	0.97332	-4.20617
H	-6.14608	-0.77717	3.08576
H	-5.69050	0.81315	2.44667
H	-5.25511	0.36828	4.11398
H	-4.27695	-2.52710	3.64329
H	-2.59116	-2.14313	3.19975
H	-3.38001	-1.30293	4.55576
H	4.06050	-5.26909	-0.26640
H	3.58293	-4.99531	1.42141
H	4.86822	-6.16809	1.03561
H	6.41825	-4.41964	-1.07943
H	7.47478	-3.58237	0.07713
H	7.17276	-5.33003	0.24394
C	-7.00741	-3.82128	-1.55876
C	-4.86290	-5.15667	-1.26546
H	-6.13259	-4.42795	0.30899
H	-6.70876	-3.47100	-2.55665
H	-7.66675	-3.06131	-1.11888
H	-7.58386	-4.74824	-1.68677
H	-4.48517	-4.85543	-2.25249
H	-3.99701	-5.34483	-0.61722
H	-5.41528	-6.09871	-1.38969
C	-1.36220	3.30646	0.79827
C	-2.78765	3.25248	0.99807
C	-0.66929	4.49363	1.16963
C	-3.46226	4.40143	1.50174
C	-1.35283	5.58683	1.67315
H	0.41199	4.52890	1.06121
C	-2.76245	5.54848	1.82892
H	-4.54260	4.35089	1.63916
H	-0.80229	6.48260	1.95880
H	-3.28838	6.41857	2.22039

RC-A

C	6.61036	-1.60387	-3.44877
C	5.71612	-1.02564	-2.56438
C	5.25226	-3.60877	-3.57800
C	6.38665	-2.91137	-3.95170
C	4.55128	-1.72623	-2.13816
C	3.60198	-1.16513	-1.21319
C	4.30399	-3.03658	-2.68270
C	2.40651	-1.85092	-0.99624
C	3.87329	0.11438	-0.50185
C	3.11412	-3.72696	-2.32533
C	2.14347	-3.14798	-1.52226
C	2.95628	1.16027	-0.57964
C	0.89950	-3.90102	-1.16363
C	3.15540	2.43664	0.02233
C	0.83663	-4.58430	0.07400
C	-0.18140	-3.97541	-2.07892
C	4.32449	2.62383	0.74365
C	2.17397	3.54960	-0.18620
C	-0.29357	-5.37020	0.35553
C	1.96080	-4.49066	1.10256
C	-1.28785	-4.77304	-1.74998
C	-0.15025	-3.22769	-3.40957
C	1.32583	3.97856	0.86770
C	2.12735	4.19928	-1.44534
C	-1.36276	-5.48433	-0.54208
C	1.46806	-3.86878	2.42388
C	2.62581	-5.86150	1.33347
C	0.32504	-4.15479	-4.54779
C	-1.50591	-2.59106	-3.76892
C	0.48523	5.08145	0.64421
C	1.32071	3.29191	2.23182
C	1.25783	5.28763	-1.62136
C	3.02007	3.77728	-2.61005
C	-2.55916	-6.37213	-0.22564
C	0.43823	5.75619	-0.58539
C	2.20768	4.05075	3.24103
C	-0.09543	3.11544	2.81086
C	3.97432	4.91627	-3.02220
C	2.18925	3.27437	-3.80687
C	-3.89751	-5.61305	-0.31379
C	-2.56635	-7.61687	-1.13739
C	-0.42583	7.00229	-0.73989
C	0.42828	8.26166	-0.47581
C	-1.14084	7.10608	-2.09919
C	5.04382	0.29371	0.31747
C	5.26600	1.57542	0.93752
C	5.96885	-0.75612	0.58466
C	6.41877	1.76339	1.75216
C	7.07687	-0.54166	1.38723
C	7.31180	0.72989	1.97044
O	1.44100	-1.29533	-0.15515
O	1.79893	0.96975	-1.32886
O	-0.32182	-0.27001	-1.82192
O	0.04477	0.66679	0.60555
P	0.59885	0.04272	-0.65318
H	7.49110	-1.04658	-3.76668
H	5.89228	-0.01918	-2.19277
H	5.05671	-4.60552	-3.97438
H	7.10195	-3.35680	-4.64232

H	2.95545	-4.73657	-2.70220
H	4.52923	3.59994	1.18025
H	-0.34655	-5.90380	1.30569
H	2.73231	-3.82201	0.70055
H	-2.11554	-4.83839	-2.45420
H	0.57462	-2.40980	-3.30825
H	0.71883	-4.50650	2.91360
H	1.01846	-2.88703	2.24267
H	2.30393	-3.73135	3.12304
H	3.01250	-6.27273	0.39116
H	3.46285	-5.76935	2.03981
H	1.91182	-6.58562	1.74982
H	0.35014	-3.61205	-5.50350
H	-0.35899	-5.00857	-4.65787
H	1.32958	-4.54975	-4.35327
H	-2.25329	-3.34844	-4.04378
H	-1.89811	-2.00648	-2.93139
H	-1.38662	-1.92177	-4.63198
H	-0.15671	5.43133	1.45278
H	1.74640	2.29070	2.09403
H	1.23716	5.78987	-2.58750
H	3.64700	2.94192	-2.27558
H	-2.43913	-6.71911	0.81315
H	2.21667	3.52875	4.20819
H	1.82192	5.06728	3.40426
H	3.24296	4.13599	2.89070
H	-0.05219	2.50897	3.72403
H	-0.54654	4.07960	3.08344
H	-0.75774	2.60859	2.10276
H	3.42122	5.78588	-3.40303
H	4.57808	5.24897	-2.16722
H	4.65548	4.57770	-3.81529
H	1.57669	2.41363	-3.51293
H	1.52686	4.06208	-4.19269
H	2.84897	2.95975	-4.62760
H	-4.09044	-5.26618	-1.33865
H	-3.90040	-4.73587	0.34201
H	-4.72968	-6.27069	-0.02585
H	-1.62617	-8.17753	-1.04848
H	-3.39684	-8.28747	-0.87522
H	-2.68632	-7.32495	-2.19029
H	-1.19899	6.95747	0.04474
H	1.22396	8.34703	-1.22946
H	0.90354	8.21444	0.51278
H	-0.18802	9.17048	-0.52316
H	-1.75812	6.22417	-2.30898
H	-1.79510	7.98843	-2.11199
H	-0.42220	7.22262	-2.92183
H	5.78823	-1.74001	0.16071
H	6.57553	2.73910	2.21259
H	7.76713	-1.36160	1.58272
H	8.18679	0.88488	2.60061
N	-2.27901	1.42107	-2.10540
C	-5.54632	-0.36264	-1.71000
C	-4.15130	-0.15762	-1.66971
C	-3.34923	-0.83461	-0.73071
C	-3.93683	-1.72127	0.17654
C	-5.35002	-1.86705	0.21131
C	-6.14513	-1.19386	-0.76049
C	-3.58942	0.83152	-2.58846
C	-1.85029	2.72053	-2.76313
C	-2.40510	2.16348	-0.76576
C	-2.25655	3.51572	-1.50748
C	-3.99465	4.93893	-0.65124
C	-4.49138	4.00086	0.42553
C	-3.79832	3.87441	1.63967
C	-5.55483	3.12130	0.14684
C	-4.14372	2.87103	2.55535
C	-5.89633	2.11246	1.05430
C	-5.18468	1.98189	2.25731
C	-1.79363	-2.36108	1.01920
C	-5.59660	-2.66062	2.47953
C	-8.33348	-0.73870	-1.59716
O	-4.08023	1.25980	-3.61571
O	-3.45694	4.22094	-1.78587
O	-3.22938	-2.48874	1.04507
O	-6.01161	-2.65977	1.09047
O	-7.48917	-1.40353	-0.65107
H	-6.13275	0.18552	-2.43938
H	-2.27286	-0.71711	-0.73943
H	-3.34742	1.94074	-0.27351
H	-1.55795	1.89444	-0.13030
H	-1.48805	4.17467	-1.08560
H	-1.48673	0.67607	-2.06572
H	-2.42872	2.92389	-3.66679
H	-0.77597	2.69225	-2.95850
H	-3.23220	5.62390	-0.24556
H	-4.81030	5.53714	-1.07614
H	-2.95860	4.53763	1.84991
H	-6.07480	3.19717	-0.80847
H	-3.58047	2.75791	3.47964
H	-6.69969	1.41553	0.81876
H	-5.43436	1.18480	2.95640
H	-1.49879	-1.33597	1.26292
H	-1.43113	-3.04502	1.78699
H	-1.39613	-2.65871	0.04260
H	-6.49044	-2.94947	3.04229
H	-4.78802	-3.37752	2.64897
H	-5.26582	-1.66084	2.78596
H	-9.35354	-1.03985	-1.34240
H	-8.24116	0.35524	-1.51683
H	-8.10286	-1.04871	-2.62724
N	0.27485	-0.21394	3.16074
C	3.93532	-0.74464	3.58333
C	3.91604	-1.24081	4.89998
C	2.75184	-0.37970	2.93302
C	2.71003	-1.37856	5.60186
C	1.54583	-0.51504	3.63309
C	1.52484	-1.00728	4.95857
C	-0.77052	-0.40141	4.01187
S	-0.13548	-1.05419	5.55526
S	-2.37908	-0.07531	3.71119

H	4.88056	-0.64590	3.05591
H	4.85011	-1.52177	5.38463
H	2.75420	-0.01864	1.91000
H	2.69390	-1.76161	6.62042
H	0.12873	0.14384	2.19055

RC-B

C	7.30422	2.00701	-0.34230
C	5.96383	1.89444	-0.01491
C	7.31220	-0.23562	-1.27004
C	7.98886	0.93187	-0.96545
C	5.24264	0.70066	-0.30176
C	3.84868	0.54256	0.01234
C	5.92957	-0.37929	-0.96181
C	3.18667	-0.58645	-0.45123
C	3.12168	1.56073	0.81268
C	5.21669	-1.56890	-1.27515
C	3.85364	-1.69257	-1.04878
C	2.01880	2.21569	0.27897
C	3.15517	-2.99808	-1.26247
C	1.44243	3.37285	0.87362
C	2.96489	-3.84284	-0.14159
C	2.74907	-3.41389	-2.55397
C	1.84947	3.69741	2.15923
C	0.63686	4.34362	0.06619
C	2.37674	-5.10143	-0.33980
C	3.43590	-3.44655	1.25643
C	2.18676	-4.69152	-2.70215
C	2.94475	-2.51339	-3.77064
C	-0.77432	4.34542	0.08287
C	1.35252	5.31840	-0.67773
C	1.99232	-5.55100	-1.60924
C	2.28401	-3.42105	2.27658
C	4.58427	-4.36276	1.72487
C	4.23462	-2.89413	-4.52755
C	1.74019	-2.52527	-4.73021
C	-1.45559	5.36034	-0.60800
C	-1.55501	3.27468	0.83369
C	0.62415	6.29367	-1.37656
C	2.87847	5.29948	-0.76544
C	1.37291	-6.93152	-1.78709
C	-0.77612	6.34483	-1.34018
C	-2.09017	3.80228	2.17902
C	-2.68107	2.69415	-0.03513
C	3.50979	6.69549	-0.61488
C	3.33686	4.61951	-2.07348
C	-0.11847	-6.83871	-2.16934
C	2.15670	-7.78330	-2.80447
C	-1.53050	7.45552	-2.05881
C	-2.53784	6.90259	-3.08492
C	-2.22730	8.39149	-1.05018
C	3.53113	1.89046	2.15156
C	2.84013	2.94429	2.84803
C	4.54839	1.17039	2.84051
C	3.19584	3.23460	4.19492
C	4.86612	1.47511	4.15390
C	4.18691	2.51520	4.83858
O	1.80696	-0.69491	-0.21806
O	1.50370	1.77951	-0.95500
O	-0.55693	0.20384	-0.29076
P	0.75600	0.31471	-0.99562
H	7.83707	2.93206	-0.12443
H	5.44452	2.72608	0.45519
H	7.82441	-1.06263	-1.76227
H	9.04508	1.03305	-1.21251
H	5.76002	-2.41618	-1.69109
H	1.42898	4.58262	2.63540
H	2.22058	-5.75665	0.51740
H	3.84131	-2.42908	1.20565
H	1.88295	-5.01947	-3.69520
H	3.05986	-1.48547	-3.40098
H	1.49550	-2.73247	1.95273
H	2.64617	-3.08166	3.25694
H	1.84089	-4.41695	2.40589
H	4.24918	-5.40532	1.81485
H	5.41918	-4.33700	1.01178
H	4.95832	-4.04102	2.70707
H	4.17448	-3.93052	-4.88947
H	5.11886	-2.81262	-3.88364
H	4.38159	-2.23681	-5.39611
H	1.87269	-1.75504	-5.50207
H	1.64447	-3.49032	-5.24722
H	0.79929	-2.32326	-4.20751
H	-2.54393	5.38095	-0.57281
H	-0.85697	2.45663	1.05446
H	1.15977	7.04455	-1.95787
H	3.25470	4.69093	0.06625
H	1.43248	-7.43887	-0.81113
H	-2.78281	4.64139	2.02178
H	-1.27074	4.15396	2.82038
H	-2.63153	3.00987	2.71416
H	-3.43169	3.45270	-0.29338
H	-2.27541	2.28020	-0.96324
H	-3.20527	1.88559	0.48487
H	3.16387	7.19001	0.30257
H	4.60418	6.60924	-0.56899
H	3.26884	7.34927	-1.46402
H	4.43309	4.54237	-2.10455
H	2.91831	3.61012	-2.16359
H	3.00823	5.20187	-2.94605
H	-0.24351	-6.31760	-3.12954
H	-0.68201	-6.29223	-1.40345
H	-0.55379	-7.84269	-2.27479
H	2.10270	-7.34783	-3.81180
H	3.21633	-7.85670	-2.52578
H	1.74124	-8.79918	-2.85826
H	-0.78536	8.05149	-2.60916
H	-3.33164	6.32945	-2.58706
H	-2.04194	6.23910	-3.80562
H	-3.01534	7.72213	-3.63972
H	-2.98799	7.84633	-0.47404
H	-1.50386	8.81205	-0.33927

H	-2.72668	9.22155	-1.56939
H	5.06098	0.35919	2.32949
H	2.66384	4.03288	4.71255
H	5.63846	0.90423	4.66830
H	4.44498	2.74217	5.87232
N	-1.84709	-0.00963	2.22058
C	1.37065	0.00645	4.10184
C	0.84288	0.03693	5.40463
C	0.53409	-0.00639	2.98063
C	-0.54210	0.04802	5.61988
C	-0.85071	0.00686	3.19329
C	-1.38419	0.03035	4.50301
C	-3.14439	-0.00869	2.64828
S	-3.14744	0.03544	4.43577
S	-4.51790	-0.05856	1.71088
H	2.44765	0.00299	3.95666
H	1.51761	0.05497	6.25914
H	0.93777	-0.02805	1.97435
H	-0.95481	0.07045	6.62653
H	-1.59757	0.04002	1.22383
O	0.80699	0.00822	-2.52721
H	-0.07458	-0.48439	-2.89691
O	-1.26147	-1.02273	-3.36934
C	-2.12379	-1.37995	-2.49891
C	-3.42784	-0.68095	-2.40765
N	-1.85353	-2.36762	-1.63411
C	-4.56166	-1.27091	-1.82405
C	-3.46161	0.64636	-2.86941
C	-2.40035	-2.73233	-0.30507
C	-0.56051	-3.04178	-1.39556
C	-5.71748	-0.50215	-1.62708
H	-4.54132	-2.30847	-1.51695
C	-4.62192	1.41062	-2.69067
H	-2.56527	1.06022	-3.31790
C	-0.97028	-3.21922	0.08305
H	-2.83920	-1.89502	0.24612
H	-3.11644	-3.55940	-0.36262
H	0.32761	-2.44372	-1.60150
H	-0.48735	-3.99154	-1.93460
C	-5.75396	0.84367	-2.05874
O	-6.84904	-0.95464	-1.01174
O	-4.75653	2.71719	-3.06706
H	-0.46364	-2.50318	0.74550
O	-0.81454	-4.54229	0.54004
O	-6.89580	1.58356	-1.87370
C	-6.79741	-2.26277	-0.42709
C	-3.63942	3.33304	-3.71979
C	-1.15061	-4.70957	1.93030
C	-6.83742	2.43583	-0.70959
H	-7.76348	-2.39981	0.06784
H	-6.66840	-3.04133	-1.19461
H	-5.98963	-2.33678	0.31437
H	-3.35629	2.78329	-4.62943
H	-3.97651	4.33736	-3.98916
H	-2.77253	3.40705	-3.04793
H	-0.81176	-5.72551	2.17180
H	-0.57575	-3.99735	2.54388
C	-2.63128	-4.54899	2.19985
H	-7.81225	2.93132	-0.64737
H	-6.66209	1.84142	0.19835
H	-6.04425	3.18887	-0.81559
C	-3.55582	-5.41423	1.58485
C	-3.10566	-3.50685	3.00964
C	-4.92982	-5.23089	1.77019
H	-3.19004	-6.21740	0.94447
C	-4.48175	-3.32481	3.20491
H	-2.39546	-2.82735	3.48129
C	-5.39545	-4.18331	2.58177
H	-5.63895	-5.90168	1.28508
H	-4.83498	-2.50336	3.82509
H	-6.46581	-4.03697	2.72409

TS 9 (*R*)

Imaginary frequency: -445.59 cm^{-1}

C	0.54051	-5.14388	5.15251
C	0.24370	-4.54984	3.93786
C	2.23379	-3.46747	5.60836
C	1.55033	-4.60707	5.99230
C	0.94242	-3.38736	3.50341
C	0.66964	-2.73906	2.24971
C	1.94442	-2.82405	4.37126
C	1.29133	-1.52428	1.97469
C	-0.24790	-3.33825	1.24577
C	2.62357	-1.64082	3.97372
C	2.30313	-0.96444	2.80517
C	-1.34650	-2.61684	0.77927
C	3.07244	0.25280	2.40443
C	-2.32084	-3.17766	-0.09934
C	4.02448	0.15162	1.35894
C	2.93308	1.46224	3.13126
C	-2.11374	-4.47309	-0.54935
C	-3.58636	-2.45669	-0.44705
C	4.85640	1.25229	1.09564
C	4.22625	-1.14535	0.57918
C	3.79768	2.52852	2.83800
C	1.89082	1.62729	4.23485
C	-3.73726	-1.81540	-1.70347
C	-4.66065	-2.49104	0.47363
C	4.77510	2.44102	1.83566
C	4.18378	-0.93345	-0.94405
C	5.53439	-1.83562	1.01644
C	2.56193	1.68274	5.62254
C	0.99534	2.86120	4.00985
C	-4.96612	-1.20860	-2.00206
C	-2.61066	-1.81217	-2.73450
C	-5.87229	-1.87089	0.12359
C	-4.53610	-3.17540	1.83260
C	5.77097	3.57177	1.60695
C	-6.04293	-1.21509	-1.10163
C	-2.76414	-2.98478	-3.72587
C	-2.49706	-0.48501	-3.50330
C	-4.58617	-2.14955	2.98245

C	-5.59627	-4.27923	2.01226	H	4.41913	4.92638	0.53036
C	5.09969	4.94098	1.39122	H	5.85779	5.71485	1.20900
C	6.78021	3.63485	2.77312	H	4.51981	5.24564	2.27276
C	-7.35441	-0.52066	-1.44212	H	6.26761	3.87930	3.71399
C	-7.15163	0.98597	-1.70458	H	7.28587	2.66946	2.90591
C	-8.05486	-1.20232	-2.63496	H	7.54232	4.40526	2.58984
C	0.00630	-4.64518	0.69948	H	-8.01281	-0.62258	-0.56468
C	-0.95180	-5.21614	-0.21012	H	-6.52349	1.14798	-2.59173
C	1.19637	-5.37793	0.97686	H	-6.66486	1.48262	-0.85639
C	-0.70747	-6.50582	-0.76177	H	-8.11818	1.47625	-1.88777
C	1.41131	-6.62439	0.41281	H	-7.44352	-1.12294	-3.54479
C	0.44861	-7.20111	-0.45571	H	-8.22572	-2.26878	-2.43599
O	0.97514	-0.86639	0.78652	H	-9.02491	-0.72773	-2.83905
O	-1.53536	-1.31294	1.24293	H	1.94754	-4.93891	1.62819
O	-0.63616	1.05004	1.60126	H	-1.44508	-6.92704	-1.44519
O	-0.72654	0.06507	-0.82715	H	2.33306	-7.16282	0.63084
P	-0.51638	-0.12761	0.66356	H	0.62956	-8.18344	-0.89059
H	-0.01094	-6.02859	5.46962	N	0.22376	3.36917	0.26824
H	-0.53810	-4.96306	3.30497	C	-2.58143	5.83581	0.45221
H	2.99993	-3.03519	6.25265	C	-1.90115	4.60259	0.46991
H	1.77657	-5.08785	6.94348	C	-2.60872	3.39000	0.55844
H	3.41714	-1.24917	4.60887	C	-4.00661	3.40937	0.64798
H	-2.86702	-4.93543	-1.18558	C	-4.70563	4.64032	0.61820
H	5.60442	1.16871	0.30792	C	-3.98005	5.85610	0.52609
H	3.40781	-1.82710	0.83441	C	-0.42501	4.64158	0.35595
H	3.70916	3.44787	3.41579	C	0.36132	2.81909	-1.61481
H	1.23770	0.74596	4.21065	C	1.70955	3.33744	0.16263
H	3.30460	-0.34982	-1.23575	C	1.80708	3.27806	-1.37447
H	4.14262	-1.90267	-1.45928	C	4.06817	2.96101	-1.98410
H	5.07017	-0.39980	-1.30519	C	4.99095	2.00405	-2.69731
H	6.40495	-1.20352	0.79126	C	4.51901	1.22392	-3.76467
H	5.53066	-2.03727	2.09639	C	6.33346	1.88478	-2.30459
H	5.66167	-2.79039	0.48663	C	5.36495	0.31199	-4.40432
H	3.22513	2.55578	5.70214	C	7.18727	0.98225	-2.95331
H	3.16599	0.78584	5.81123	C	6.70135	0.18455	-3.99810
H	1.80442	1.75937	6.41505	C	-4.08317	1.02824	0.86174
H	1.57622	3.79370	4.00825	C	-6.68373	4.34234	1.89159
H	0.45893	2.77822	3.05985	C	-4.05421	8.23982	0.42865
H	0.24951	2.93596	4.81344	O	0.24011	5.67081	0.24670
H	-5.08735	-0.71067	-2.96229	O	2.76537	2.37055	-1.87152
H	-1.67089	-1.95589	-2.18818	O	-4.77326	2.28926	0.75884
H	-6.70178	-1.88481	0.83213	O	-6.07448	4.68520	0.62767
H	-3.55451	-3.66352	1.87668	O	-4.74282	6.98851	0.52258
H	6.33765	3.32851	0.69423	H	-1.99551	6.74646	0.38611
H	-3.70016	-2.88970	-4.29476	H	-2.09224	2.43878	0.57180
H	-2.77810	-3.95223	-3.21051	H	2.06274	2.40225	0.60540
H	-1.92743	-2.99179	-4.43901	H	2.16905	4.19636	0.65456
H	-3.38014	-0.29638	-4.12864	H	1.95456	4.27936	-1.80866
H	-2.36360	0.35863	-2.81795	H	-0.18288	2.57592	0.80923
H	-1.63191	-0.51866	-4.17662	H	0.05281	1.80067	-1.40777
H	-5.54823	-1.61811	2.99807	H	-0.37891	3.48351	-2.04695
H	-3.78571	-1.40818	2.87456	H	4.47027	3.19840	-0.98752
H	-4.46316	-2.65281	3.95186	H	3.98570	3.91124	-2.54566
H	-6.61357	-3.86443	2.01732	H	3.48307	1.32595	-4.07355
H	-5.53673	-5.01596	1.19981	H	6.71220	2.49341	-1.48290
H	-5.44459	-4.80380	2.96595	H	4.97721	-0.30199	-5.21717

H	8.22515	0.89308	-2.63292
H	7.35932	-0.52999	-4.49224
H	-4.86101	0.28342	1.02443
H	-3.37472	1.03320	1.69925
H	-3.55102	0.79108	-0.06828
H	-6.36235	5.04545	2.67399
H	-6.43396	3.31537	2.18566
H	-7.76365	4.43346	1.73634
H	-3.37700	8.39064	1.28290
H	-4.83460	9.00631	0.43961
H	-3.47976	8.31174	-0.50706
N	0.83160	-0.42998	-2.90173
C	1.60499	-4.04571	-2.49386
C	2.08315	-4.29583	-3.79476
C	1.17128	-2.77106	-2.11806
C	2.13771	-3.27796	-4.75643
C	1.22413	-1.75264	-3.07909
C	1.70079	-2.00155	-4.38511
C	0.95307	0.38627	-3.96859
S	1.62683	-0.52054	-5.34152
S	0.54021	2.02118	-4.08705
H	1.57301	-4.85159	-1.76491
H	2.41734	-5.29730	-4.06175
H	0.81289	-2.56130	-1.11522
H	2.50663	-3.47279	-5.76126
H	0.30144	-0.16063	-2.03010

TS 9 (*R*) *conf1*

Imaginary frequency: -444.95 cm^{-1}

C	-0.42483	-5.29359	-5.00657
C	-0.14333	-4.65668	-3.81014
C	-2.16311	-3.67739	-5.50849
C	-1.44924	-4.80874	-5.86017
C	-0.87280	-3.50124	-3.40884
C	-0.61653	-2.80925	-2.17526
C	-1.89050	-2.99078	-4.29095
C	-1.27137	-1.60500	-1.93382
C	0.31851	-3.35338	-1.15634
C	-2.60228	-1.81631	-3.92588
C	-2.30042	-1.09841	-2.77725
C	1.39915	-2.59003	-0.71538
C	-3.10624	0.10473	-2.40726
C	2.39059	-3.10002	0.17481
C	-3.01180	1.29628	-3.17018
C	-4.04746	0.00352	-1.35178
C	2.21882	-4.38702	0.66268
C	3.64062	-2.34152	0.49814
C	-3.90700	2.34310	-2.89933
C	-1.98540	1.46331	-4.28826
C	-4.91069	1.08527	-1.11194
C	-4.20506	-1.27670	-0.53495
C	3.78310	-1.66898	1.73666
C	4.71543	-2.38168	-0.42474
C	-4.87223	2.25463	-1.88541
C	-1.11852	2.72328	-4.09768
C	-2.67193	1.47264	-5.66948
C	-4.13841	-1.02320	0.98106
C	-5.50547	-2.00722	-0.92759
C	5.00906	-1.04413	2.02071
C	2.65456	-1.64940	2.76519
C	5.92049	-1.74535	-0.09051
C	4.59585	-3.09366	-1.77000
C	-5.89936	3.36126	-1.67784
C	6.08656	-1.06565	1.12508
C	2.52075	-0.29996	3.49082
C	2.81918	-2.78835	3.79322
C	4.64139	-2.08877	-2.93832
C	5.66305	-4.19421	-1.92670
C	-5.26651	4.75428	-1.50190
C	-6.91819	3.36544	-2.83730
C	7.39140	-0.35541	1.45895
C	8.56898	-1.34678	1.54343
C	7.68968	0.77897	0.45732
C	0.09955	-4.64954	-0.57077
C	1.07532	-5.16928	0.35053
C	-1.07284	-5.41952	-0.82098
C	0.86617	-6.44825	0.94027
C	-1.25415	-6.65378	-0.21961
C	-0.27340	-7.18083	0.66027
O	-0.97022	-0.90500	-0.76575
O	1.55193	-1.29555	-1.21699
O	0.58458	1.02932	-1.64397
O	0.71075	0.12139	0.81235
P	0.50100	-0.12235	-0.67118
H	0.15002	-6.17200	-5.29865
H	0.64973	-5.03009	-3.16663
H	-2.94117	-3.28497	-6.16391
H	-1.66300	-5.32284	-6.79671
H	-3.40752	-1.46570	-4.57027
H	2.98625	-4.81097	1.30870
H	-3.85208	3.24774	-3.50397
H	-1.31006	0.59933	-4.25353
H	-5.64961	1.00082	-0.31576
H	-3.37668	-1.94688	-0.78870
H	-1.72318	3.64054	-4.10193
H	-0.38697	2.80357	-4.91371
H	-0.56582	2.66925	-3.15490
H	-1.92439	1.54842	-6.47143
H	-3.25744	0.55830	-5.83167
H	-3.35560	2.32843	-5.76185
H	-5.02862	-0.49746	1.34415
H	-3.26574	-0.41495	1.24025
H	-4.06825	-1.97713	1.52111
H	-6.38599	-1.38998	-0.70002
H	-5.51906	-2.23608	-2.00202
H	-5.59966	-2.95091	-0.37167
H	5.13282	-0.52051	2.96820
H	1.71857	-1.82241	2.22097
H	6.74439	-1.77121	-0.80355
H	3.61739	-3.58854	-1.80588
H	-6.45217	3.12502	-0.75475
H	2.37104	0.51858	2.77878

H	3.40212	-0.07646	4.10694
H	1.65774	-0.32576	4.16720
H	1.97885	-2.78455	4.50215
H	2.84814	-3.77082	3.30775
H	3.75085	-2.66362	4.36349
H	5.59982	-1.55124	-2.96218
H	3.83628	-1.35043	-2.84484
H	4.52272	-2.61020	-3.89859
H	6.67786	-3.77333	-1.93672
H	5.60587	-4.91611	-1.10085
H	5.51721	-4.73725	-2.87089
H	-4.58044	4.78130	-0.64570
H	-6.04533	5.51067	-1.33429
H	-4.70102	5.05239	-2.39495
H	-6.41975	3.60116	-3.78795
H	-7.39605	2.38262	-2.94209
H	-7.70141	4.11753	-2.66734
H	7.26611	0.10130	2.45354
H	8.74941	-1.82598	0.57104
H	8.36657	-2.13880	2.27670
H	9.49221	-0.82872	1.83859
H	7.85613	0.37686	-0.55200
H	6.85677	1.48991	0.39858
H	8.59657	1.32577	0.75211
H	-1.83718	-5.01862	-1.48150
H	1.61718	-6.83083	1.63177
H	-2.16303	-7.22120	-0.41720
H	-0.42770	-8.15438	1.12422
N	-0.34856	3.35654	-0.38421
C	2.48151	3.45585	-0.65590
C	1.73617	4.64848	-0.62960
C	2.37442	5.90370	-0.67012
C	3.77227	5.96350	-0.73409
C	4.53371	4.76881	-0.78108
C	3.87999	3.51492	-0.74135
C	0.25825	4.64473	-0.51873
C	-0.45430	2.86590	1.51791
C	-1.83160	3.28006	-0.26559
C	-1.91641	3.26743	1.27356
C	-4.16043	2.89466	1.91550
C	-5.04349	1.92918	2.66644
C	-4.53618	1.20212	3.75487
C	-6.38314	1.74790	2.28795
C	-5.34367	0.28119	4.43027
C	-7.19874	0.83617	2.97207
C	-6.67701	0.09152	4.03849
C	3.78100	8.35233	-0.72204
C	6.59179	4.93674	0.35232
C	4.03641	1.13505	-0.85258
O	-0.43876	5.65580	-0.44776
O	-2.83933	2.34486	1.80835
O	4.50388	7.11701	-0.76085
O	5.89854	4.82083	-0.90726
O	4.68501	2.42046	-0.79475
H	1.99438	2.48993	-0.62249
H	1.75930	6.79688	-0.63909
H	-2.15753	2.32050	-0.67587
H	-2.32212	4.10742	-0.78096
H	-2.09490	4.27702	1.67590
H	0.08144	2.55932	-0.90192
H	0.26542	3.56991	1.92104
H	-0.11150	1.85243	1.34280
H	-4.57889	3.08787	0.91621
H	-4.10513	3.86382	2.44727
H	-3.50272	1.35229	4.05223
H	-6.78948	2.31485	1.44979
H	-4.92837	-0.29117	5.25970
H	-8.23461	0.69839	2.66257
H	-7.30492	-0.63019	4.56053
H	4.54061	9.13878	-0.75301
H	3.19236	8.44327	0.20317
H	3.11209	8.45107	-1.58984
H	6.36489	4.07945	1.00246
H	6.32224	5.87258	0.86230
H	7.66005	4.94141	0.11173
H	3.49859	0.91647	0.07924
H	4.83831	0.40837	-0.97823
H	3.33858	1.08387	-1.69763
N	-0.81376	-0.35055	2.91303
C	-1.47009	-4.00092	2.62969
C	-1.92061	-4.22564	3.94505
C	-1.08512	-2.72503	2.20795
C	-1.99599	-3.18037	4.87544
C	-1.15891	-1.67921	3.13764
C	-1.60837	-1.90231	4.45781
C	-0.94747	0.49460	3.95535
S	-1.57168	-0.38969	5.36589
S	-0.58699	2.14528	4.01596
H	-1.42133	-4.82789	1.92575
H	-2.21661	-5.22884	4.24819
H	-0.74806	-2.53503	1.19378
H	-2.34355	-3.35568	5.89142
H	-0.30195	-0.09312	2.02661

TS 9 (*R*) *conf2*

Imaginary frequency: -447.45 cm^{-1}

C	2.32701	-5.25157	-4.63870
C	2.29500	-4.48799	-3.48465
C	0.00677	-4.72063	-5.10721
C	1.17212	-5.38013	-5.45323
C	1.10474	-3.81332	-3.08793
C	1.02392	-3.01482	-1.89553
C	-0.05570	-3.91618	-3.93358
C	-0.12539	-2.25934	-1.66811
C	2.13054	-2.98896	-0.90419
C	-1.23516	-3.20866	-3.58026
C	-1.28823	-2.35936	-2.48313
C	2.70919	-1.77636	-0.53257
C	-2.56415	-1.64520	-2.17007
C	3.81810	-1.68621	0.35946
C	-3.38002	-2.10916	-1.10684
C	-3.01537	-0.60008	-3.01586

C	4.29931	-2.86632	0.90698
C	4.50066	-0.38568	0.64666
C	-4.66648	-1.56491	-0.96027
C	-2.91971	-3.24546	-0.19525
C	-4.30989	-0.09242	-2.82704
C	-2.14418	-0.02978	-4.13309
C	4.33969	0.25034	1.90267
C	5.37491	0.16164	-0.32565
C	-5.16070	-0.57589	-1.82265
C	-3.29477	-3.03579	1.28244
C	-3.44523	-4.59618	-0.72335
C	-2.67712	-0.45004	-5.51823
C	-2.01167	1.50305	-4.04255
C	5.07692	1.41806	2.16169
C	3.41976	-0.31616	2.98189
C	6.08695	1.33048	-0.01724
C	5.58826	-0.50080	-1.68442
C	-6.58096	-0.04647	-1.67553
C	5.95571	1.97322	1.22263
C	4.22148	-1.11895	4.02790
C	2.58060	0.76827	3.68071
C	7.05098	-0.95645	-1.85678
C	5.13937	0.41548	-2.83909
C	-6.60148	1.43272	-1.24579
C	-7.39742	-0.26207	-2.96527
C	6.72471	3.24940	1.53695
C	8.24730	3.05069	1.40602
C	6.23961	4.42258	0.66102
C	2.58234	-4.19720	-0.26526
C	3.68857	-4.12378	0.65277
C	1.94796	-5.45829	-0.46078
C	4.13850	-5.31036	1.29886
C	2.40461	-6.59248	0.18982
C	3.51384	-6.52325	1.07171
O	-0.17520	-1.43176	-0.54659
O	2.21287	-0.60062	-1.09894
O	0.25044	0.96711	-1.53507
O	0.86378	0.33115	0.93740
P	0.75230	-0.04123	-0.53101
H	3.24986	-5.75345	-4.92825
H	3.18750	-4.38819	-2.87148
H	-0.88207	-4.79555	-5.73435
H	1.21067	-5.98840	-6.35633
H	-2.12460	-3.32399	-4.19826
H	5.16993	-2.82746	1.55974
H	-5.31172	-1.93179	-0.16396
H	-1.82560	-3.28776	-0.23461
H	-4.66416	0.69886	-3.48713
H	-1.13620	-0.44735	-4.01686
H	-2.79519	-3.78977	1.90495
H	-4.37713	-3.13856	1.44590
H	-2.98945	-2.04116	1.62429
H	-4.54447	-4.61312	-0.71568
H	-3.10915	-4.77236	-1.75379
H	-3.08445	-5.42386	-0.09593
H	-3.68851	-0.05284	-5.68457
H	-2.72648	-1.54224	-5.61452
H	-2.02614	-0.06475	-6.31546
H	-2.98335	2.00526	-4.14436
H	-1.56303	1.79560	-3.08880
H	-1.36115	1.87173	-4.84775
H	4.96631	1.91292	3.12648
H	2.72193	-1.00502	2.48969
H	6.76103	1.74766	-0.76532
H	4.96551	-1.40287	-1.72563
H	-7.06177	-0.62531	-0.87396
H	4.77962	-1.94318	3.56795
H	3.54569	-1.54411	4.78368
H	4.94326	-0.46869	4.54240
H	3.20611	1.45115	4.27148
H	2.01118	1.35532	2.95319
H	1.86961	0.30119	4.37398
H	7.17928	-1.48440	-2.81210
H	7.34775	-1.63423	-1.04494
H	7.74010	-0.10066	-1.85013
H	4.08209	0.68343	-2.73015
H	5.72916	1.34240	-2.86682
H	5.26910	-0.09366	-3.80439
H	-6.11757	1.56432	-0.27125
H	-7.63461	1.79373	-1.15322
H	-6.08553	2.06624	-1.98120
H	-6.98809	0.32630	-3.79818
H	-7.39095	-1.31856	-3.26504
H	-8.44084	0.04985	-2.81711
H	6.51003	3.50652	2.58630
H	8.52877	2.81909	0.36944
H	8.59349	2.22490	2.04158
H	8.78312	3.96353	1.70133
H	6.43555	4.22560	-0.40230
H	5.16038	4.58057	0.77748
H	6.75914	5.35231	0.93265
H	1.08553	-5.52027	-1.11885
H	4.97988	-5.23918	1.98857
H	1.89988	-7.54485	0.03026
H	3.86282	-7.42336	1.57656
N	-1.81908	2.41616	-0.33834
C	0.44791	4.06861	-0.74079
C	-0.84487	4.61423	-0.84622
C	-1.03033	5.97610	-1.15099
C	0.08590	6.79782	-1.35163
C	1.39470	6.25577	-1.26705
C	1.56615	4.88126	-0.97009
C	-2.05904	3.79613	-0.61459
C	-1.59511	2.12159	1.59724
C	-2.98194	1.51314	-0.11726
C	-3.04179	1.60331	1.40986
C	-4.26483	0.38647	3.10309
C	-5.69346	0.61347	2.66759
C	-6.28375	1.88690	2.75284
C	-6.45783	-0.45581	2.16723
C	-7.60591	2.09146	2.33488
C	-7.78135	-0.25856	1.75983

C	-8.35671	1.01841	1.83806
C	-1.27230	8.71913	-1.75171
C	3.30084	7.37779	-0.41015
C	3.04559	3.00865	-0.78920
O	-3.20607	4.23994	-0.57837
O	-3.33308	0.35197	1.99574
O	0.02787	8.13226	-1.63630
O	2.46068	7.07014	-1.54272
O	2.85169	4.42869	-0.94255
H	0.59537	3.02108	-0.51341
H	-2.04431	6.35765	-1.20878
H	-2.69470	0.50656	-0.43156
H	-3.86844	1.84365	-0.65660
H	-3.75118	2.37401	1.73439
H	-1.01822	1.96705	-0.83383
H	-1.38528	3.13898	1.91350
H	-0.74494	1.46512	1.45186
H	-3.94723	1.14584	3.83134
H	-4.15676	-0.59935	3.56904
H	-5.70988	2.71837	3.16398
H	-6.00988	-1.44747	2.11136
H	-8.04964	3.08429	2.40341
H	-8.36570	-1.09852	1.38485
H	-9.38649	1.17369	1.51759
H	-1.09920	9.77375	-1.98526
H	-1.83510	8.63781	-0.80940
H	-1.85225	8.25230	-2.56193
H	3.75770	6.47088	0.00426
H	2.72004	7.89359	0.36881
H	4.08067	8.04604	-0.78969
H	2.73734	2.66540	0.20792
H	4.11659	2.84329	-0.90660
H	2.48830	2.45228	-1.55301
N	-0.34691	-0.79171	3.00425
C	0.29907	-4.43428	2.61735
C	-0.35648	-4.87843	3.78274
C	0.34127	-3.07733	2.28635
C	-0.97889	-3.97474	4.65384
C	-0.28640	-2.17218	3.15299
C	-0.93508	-2.61438	4.32831
C	-0.98955	-0.10683	3.97046
S	-1.60477	-1.23273	5.19540
S	-1.19703	1.57030	4.08985
H	0.78250	-5.15245	1.95897
H	-0.37870	-5.94195	4.01581
H	0.82974	-2.72510	1.38421
H	-1.48113	-4.31831	5.55577
H	0.12149	-0.32237	2.17883

TS 9 (*R*) *conf3*

Imaginary frequency: -437.28 cm^{-1}

C	1.02047	-6.72495	0.09969
C	0.88718	-5.49185	0.71564
C	-1.09492	-6.42826	-1.04886
C	0.01732	-7.20604	-0.78122
C	-0.25684	-4.67598	0.47948
C	-0.42636	-3.37993	1.08289
C	-1.25334	-5.14851	-0.44498
C	-1.47786	-2.57081	0.65226
C	0.52922	-2.89052	2.11074
C	-2.36505	-4.31889	-0.74831
C	-2.48685	-3.03229	-0.24490
C	1.23170	-1.70800	1.89408
C	-3.70942	-2.22620	-0.55835
C	2.28893	-1.26690	2.73986
C	-4.79965	-2.27151	0.34576
C	-3.81260	-1.50373	-1.77221
C	2.56814	-2.02602	3.86777
C	3.14026	-0.08570	2.40137
C	-5.98080	-1.58850	0.01806
C	-4.71774	-3.03216	1.66706
C	-5.01565	-0.83374	-2.05083
C	-2.66497	-1.47992	-2.77916
C	4.06742	-0.18407	1.33319
C	3.10274	1.08043	3.20854
C	-6.10767	-0.85838	-1.17273
C	-5.83228	-4.08924	1.78735
C	-4.72314	-2.06337	2.86655
C	-2.49446	-0.11796	-3.47293
C	-2.82486	-2.59567	-3.83283
C	4.97543	0.86638	1.12930
C	4.15301	-1.41667	0.43705
C	4.03519	2.10144	2.96427
C	2.09208	1.25096	4.34070
C	-7.38616	-0.09805	-1.49791
C	4.99145	2.00645	1.94278
C	3.99334	-1.05280	-1.05019
C	5.46516	-2.18708	0.68752
C	2.78990	1.20994	5.71547
C	1.25918	2.53847	4.18463
C	-8.59006	-1.05075	-1.63801
C	-7.66761	1.00520	-0.45724
C	6.01082	3.11205	1.70153
C	5.34312	4.36798	1.10735
C	6.80872	3.45701	2.97324
C	0.76251	-3.62051	3.32715
C	1.80801	-3.17584	4.21213
C	-0.01489	-4.75108	3.70903
C	2.05885	-3.90122	5.41180
C	0.24652	-5.42661	4.88873
C	1.29800	-5.00740	5.74425
O	-1.58836	-1.28111	1.17433
O	0.95003	-0.96550	0.74782
O	-0.54997	0.99147	1.68352
O	-0.67678	0.17378	-0.80267
P	-0.49199	-0.12918	0.67377
H	1.90881	-7.32737	0.28676
H	1.66859	-5.12745	1.37720
H	-1.86204	-6.77434	-1.74189
H	0.13342	-8.17967	-1.25600
H	-3.14845	-4.70484	-1.39910
H	3.39231	-1.72568	4.51367

H	-6.81618	-1.61657	0.71748
H	-3.76171	-3.56995	1.68914
H	-5.10928	-0.27071	-2.97892
H	-1.74357	-1.67851	-2.21941
H	-6.82792	-3.62552	1.81318
H	-5.71061	-4.66952	2.71260
H	-5.80649	-4.78485	0.93771
H	-4.63260	-2.61932	3.81038
H	-3.88526	-1.35934	2.79919
H	-5.65660	-1.48418	2.90362
H	-1.61497	-0.14223	-4.12796
H	-2.35091	0.68338	-2.74024
H	-3.35701	0.13059	-4.10597
H	-2.87448	-3.58683	-3.36714
H	-3.74411	-2.44765	-4.41752
H	-1.97112	-2.58887	-4.52553
H	5.69591	0.79044	0.31605
H	3.33157	-2.09246	0.70076
H	4.01288	2.99220	3.59166
H	1.39159	0.40785	4.29438
H	-7.23214	0.39276	-2.47203
H	3.09046	-0.45554	-1.21148
H	3.92097	-1.96392	-1.65965
H	4.84565	-0.46978	-1.41598
H	6.33835	-1.57272	0.42690
H	5.55653	-2.47752	1.74311
H	5.49845	-3.09864	0.07391
H	2.05164	1.28738	6.52590
H	3.49786	2.04408	5.82151
H	3.35146	0.27632	5.85106
H	1.89012	3.43777	4.19931
H	0.53891	2.62398	5.01023
H	0.69529	2.51801	3.24696
H	-8.39913	-1.81947	-2.39867
H	-9.49349	-0.49502	-1.92584
H	-8.79901	-1.56165	-0.68770
H	-7.86355	0.56913	0.53254
H	-6.81502	1.68743	-0.35660
H	-8.55280	1.59011	-0.74484
H	6.72653	2.73031	0.95644
H	4.63034	4.80491	1.82076
H	4.79441	4.11804	0.19140
H	6.09218	5.13544	0.86684
H	6.15611	3.87860	3.75002
H	7.29344	2.56377	3.38866
H	7.58567	4.20172	2.75118
H	-0.82906	-5.07403	3.06459
H	2.85830	-3.55827	6.06923
H	-0.36521	-6.28461	5.16623
H	1.49548	-5.55152	6.66731
N	0.41483	3.34314	0.50382
C	-2.41722	3.48692	0.74706
C	-1.65064	4.66606	0.73998
C	-2.26725	5.93160	0.78976
C	-3.66425	6.01548	0.84318
C	-4.44745	4.83422	0.86862
C	-3.81509	3.56972	0.82190
C	-0.17117	4.63727	0.64679
C	0.60476	2.90971	-1.41969
C	1.89839	3.23756	0.43720
C	2.05598	3.32980	-1.08500
C	3.92384	3.06740	-2.57301
C	5.00741	2.07164	-2.89018
C	4.81722	1.11585	-3.90061
C	6.19363	2.04368	-2.13872
C	5.78655	0.13623	-4.14672
C	7.16697	1.06605	-2.38055
C	6.96162	0.10608	-3.38250
C	-3.63012	8.40445	0.86496
C	-6.49064	5.10502	-0.27440
C	-4.01203	1.19222	0.90043
O	0.54335	5.63813	0.60192
O	3.08068	2.48151	-1.55307
O	-4.37522	7.18190	0.88053
O	-5.81251	4.90479	0.98286
O	-4.63880	2.48868	0.85798
H	-1.94769	2.51270	0.70341
H	-1.63617	6.81403	0.77650
H	2.18395	2.24342	0.79209
H	2.39556	4.01117	1.02364
H	2.21674	4.36798	-1.40582
H	-0.04714	2.54001	0.98144
H	-0.11895	3.60438	-1.83516
H	0.27549	1.88763	-1.27225
H	4.35700	4.00708	-2.19093
H	3.32417	3.29122	-3.46735
H	3.90298	1.13898	-4.49021
H	6.35010	2.78921	-1.36017
H	5.62164	-0.60473	-4.92874
H	8.08200	1.05228	-1.78866
H	7.71579	-0.65825	-3.56856
H	-4.37576	9.20391	0.90170
H	-3.03283	8.49801	-0.05439
H	-2.96627	8.47855	1.73906
H	-6.27461	4.27963	-0.96827
H	-6.19764	6.06136	-0.73001
H	-7.56085	5.11811	-0.04297
H	-3.47162	0.97953	-0.03110
H	-4.82698	0.47747	1.00859
H	-3.32108	1.11565	1.74931
N	0.84570	-0.33875	-2.88764
C	1.27136	-4.03107	-2.71606
C	1.72215	-4.24252	-4.03347
C	0.95920	-2.74806	-2.25775
C	1.87423	-3.17534	-4.92845
C	1.10766	-1.67986	-3.15217
C	1.56220	-1.88956	-4.47277
C	1.05596	0.52759	-3.89894
S	1.64170	-0.34938	-5.32922
S	0.79919	2.20002	-3.92222
H	1.16704	-4.87500	-2.03922
H	1.95931	-5.25226	-4.36519

H	0.62456	-2.56988	-1.24087
H	2.22391	-3.33910	-5.94560
H	0.33071	-0.07527	-2.00136

TS 9 (*R*) *conf4*

Imaginary frequency: -436.96 cm^{-1}

C	1.14571	-6.70862	0.29906
C	0.98522	-5.46028	0.87668
C	-0.97073	-6.48979	-0.86487
C	0.15593	-7.23638	-0.57016
C	-0.17419	-4.67541	0.61234
C	-0.37224	-3.36536	1.17556
C	-1.15754	-5.19595	-0.30045
C	-1.43912	-2.59202	0.71784
C	0.56992	-2.82451	2.19013
C	-2.28491	-4.39901	-0.63253
C	-2.43494	-3.10066	-0.16875
C	1.24681	-1.63356	1.94003
C	-3.66975	-2.32519	-0.51020
C	2.29018	-1.14282	2.77565
C	-4.76078	-2.35889	0.39028
C	-3.77713	-1.63399	-1.74436
C	2.58326	-1.86200	3.92602
C	3.11204	0.05031	2.40692
C	-5.94551	-1.68692	0.04326
C	-4.67825	-3.09060	1.72765
C	-4.98052	-0.97762	-2.04135
C	-2.62949	-1.63070	-2.75188
C	4.04657	-0.05288	1.34577
C	3.03882	1.23755	3.18024
C	-6.07304	-0.98211	-1.15977
C	-5.79110	-4.14654	1.87111
C	-4.68436	-2.09777	2.90740
C	-2.47624	-0.29218	-3.49355
C	-2.77721	-2.78384	-3.76647
C	4.92722	1.01559	1.11626
C	4.16871	-1.30754	0.48525
C	3.94588	2.27532	2.91244
C	2.01581	1.41358	4.30048
C	-7.35615	-0.23512	-1.49701
C	4.90988	2.17725	1.89848
C	4.00714	-0.99081	-1.01254
C	5.49936	-2.03575	0.76308
C	2.70350	1.42349	5.68090
C	1.15540	2.67749	4.10571
C	-7.10201	1.27129	-1.71123
C	-8.06028	-0.85851	-2.71925
C	5.90285	3.30118	1.63295
C	5.20854	4.52280	0.99919
C	6.68238	3.70163	2.89977
C	0.81544	-3.51212	3.42863
C	1.84836	-3.01827	4.30229
C	0.06140	-4.64714	3.84287
C	2.11148	-3.70185	5.52372
C	0.33388	-5.28104	5.04295
C	1.37376	-4.81378	5.88766
O	-1.57875	-1.29013	1.20135
O	0.95264	-0.93188	0.77156
O	-0.59224	1.01844	1.64564
O	-0.69332	0.12520	-0.81600
P	-0.50655	-0.12963	0.66894
H	2.04534	-7.28689	0.50717
H	1.75678	-5.05993	1.52892
H	-1.72792	-6.87221	-1.54967
H	0.29356	-8.22130	-1.01496
H	-3.05752	-4.82068	-1.27398
H	3.39794	-1.52369	4.56515
H	-6.78714	-1.69829	0.73732
H	-3.72134	-3.62636	1.76047
H	-5.06877	-0.44135	-2.98428
H	-1.70526	-1.79903	-2.18683
H	-6.78735	-3.68387	1.88953
H	-5.66678	-4.70784	2.80767
H	-5.76581	-4.85918	1.03572
H	-4.59256	-2.63463	3.86213
H	-3.84759	-1.39399	2.82557
H	-5.61906	-1.51987	2.93352
H	-1.59390	-0.32691	-4.14420
H	-2.34865	0.53747	-2.79005
H	-3.33948	-0.07972	-4.13871
H	-2.81466	-3.75921	-3.26760
H	-3.69908	-2.66628	-4.35397
H	-1.92465	-2.79041	-4.46060
H	5.65344	0.93606	0.30848
H	3.36387	-1.99681	0.76485
H	3.89697	3.18215	3.51479
H	1.33484	0.55387	4.27016
H	-8.03025	-0.34179	-0.63213
H	3.09052	-0.42125	-1.19553
H	3.96091	-1.92075	-1.59554
H	4.84650	-0.39756	-1.39139
H	6.35732	-1.40610	0.48871
H	5.59318	-2.29364	1.82688
H	5.55971	-2.96314	0.17582
H	1.95753	1.50619	6.48375
H	3.39257	2.27528	5.76982
H	3.28383	0.50612	5.84515
H	1.76551	3.59117	4.10478
H	0.42542	2.76602	4.92250
H	0.60145	2.62179	3.16359
H	-6.60922	1.72590	-0.84326
H	-8.05023	1.79778	-1.88971
H	-6.45899	1.43974	-2.58646
H	-7.43260	-0.77313	-3.61736
H	-8.26890	-1.92406	-2.55421
H	-9.01109	-0.34639	-2.92323
H	6.63344	2.91695	0.90376
H	4.47909	4.96092	1.69482
H	4.67388	4.23378	0.08648
H	5.93989	5.30220	0.74304
H	6.01390	4.12949	3.65945
H	7.18519	2.83269	3.34422

H	7.44289	4.45829	2.66176
H	-0.74383	-5.00684	3.20673
H	2.90145	-3.32208	6.17231
H	-0.26009	-6.14327	5.34486
H	1.58040	-5.32555	6.82707
N	0.31593	3.35744	0.39205
C	-2.51898	3.44131	0.64525
C	-1.78095	4.63715	0.58515
C	-2.43054	5.88669	0.58295
C	-3.82905	5.94026	0.64315
C	-4.58517	4.74150	0.70593
C	-3.91677	3.49358	0.72186
C	-0.30211	4.64121	0.49112
C	0.52994	2.86816	-1.51521
C	1.80205	3.28617	0.33818
C	1.96823	3.33384	-1.18499
C	3.85336	3.07406	-2.65015
C	4.96207	2.09609	-2.93388
C	4.80016	1.10867	-3.91851
C	6.14457	2.11715	-2.17634
C	5.79340	0.14559	-4.13232
C	7.14187	1.15637	-2.38606
C	6.96450	0.16423	-3.36166
C	-3.84352	8.32659	0.58952
C	-6.58199	4.47680	1.95631
C	-4.05124	1.11227	0.89336
O	0.38841	5.65689	0.41194
O	3.01668	2.49676	-1.61996
O	-4.56364	7.09126	0.65281
O	-5.95293	4.81909	0.70206
O	-4.71097	2.39056	0.80747
H	-2.02672	2.47728	0.64484
H	-1.82160	6.78355	0.53995
H	2.10914	2.31125	0.72671
H	2.27587	4.09017	0.90268
H	2.10577	4.36503	-1.53741
H	-0.12846	2.55900	0.89256
H	-0.20727	3.53159	-1.95722
H	0.22429	1.84354	-1.33800
H	4.26182	4.03376	-2.29135
H	3.25487	3.25939	-3.55398
H	3.88910	1.09415	-4.51325
H	6.27940	2.88761	-1.41823
H	5.65024	-0.62035	-4.89429
H	8.05376	1.18068	-1.78966
H	7.73733	-0.58706	-3.52257
H	-4.60487	9.11190	0.60696
H	-3.25750	8.40168	-0.33875
H	-3.17191	8.44474	1.45329
H	-6.25238	5.16387	2.74947
H	-6.35839	3.44126	2.24139
H	-7.65809	4.59398	1.79208
H	-3.51442	0.88040	-0.03525
H	-4.84790	0.38299	1.03302
H	-3.35233	1.08461	1.73851
N	0.85587	-0.41827	-2.87664
C	1.36625	-4.09236	-2.58469
C	1.83640	-4.33401	-3.89006
C	1.01902	-2.80344	-2.17015
C	1.97304	-3.29191	-4.81651
C	1.15198	-1.76040	-3.09611
C	1.62563	-2.00041	-4.40478
C	1.05668	0.42084	-3.91278
S	1.67804	-0.48654	-5.30863
S	0.76142	2.08495	-3.99185
H	1.27441	-4.91699	-1.88275
H	2.10100	-5.34764	-4.18738
H	0.66942	-2.60157	-1.16281
H	2.33777	-3.47892	-5.82432
H	0.32756	-0.13912	-2.00352

TS 9 (*R*) *conf5*

Imaginary frequency: -448.90 cm^{-1}

C	-2.30196	-5.25380	4.61690
C	-2.26198	-4.49800	3.45797
C	0.00087	-4.68205	5.12174
C	-1.15951	-5.35815	5.45214
C	-1.07584	-3.80743	3.07671
C	-0.98627	-3.01714	1.87947
C	0.07104	-3.88480	3.94363
C	0.15511	-2.24600	1.66701
C	-2.07588	-3.01360	0.86876
C	1.24438	-3.15845	3.60786
C	1.30291	-2.31595	2.50585
C	-2.66706	-1.81189	0.48022
C	2.56838	-1.57487	2.21311
C	-3.76723	-1.74598	-0.42526
C	3.41603	-2.02716	1.17030
C	2.97801	-0.51315	3.05973
C	-4.21918	-2.93659	-0.97493
C	-4.47963	-0.46182	-0.71699
C	4.69301	-1.45567	1.04682
C	3.00204	-3.18007	0.25760
C	4.26496	0.02142	2.89462
C	2.07038	0.04538	4.15376
C	-5.40151	0.04121	0.23503
C	-4.29830	0.20061	-1.95615
C	5.14771	-0.45110	1.91268
C	3.38543	-2.96074	-1.21657
C	3.56615	-4.51142	0.79485
C	2.57705	-0.36120	5.55279
C	1.91330	1.57542	4.05580
C	-6.13439	1.19676	-0.07444
C	-5.62838	-0.64470	1.57993
C	-5.05337	1.35723	-2.21479
C	-3.33808	-0.33078	-3.01774
C	6.56116	0.10332	1.79491
C	-5.97350	1.87322	-1.29291
C	-5.18338	0.25460	2.75008
C	-7.09218	-1.10038	1.73917
C	-2.51509	0.77971	-3.69406
C	-4.09482	-1.15175	-4.08311

C	6.56618	1.58025	1.35766
C	7.35153	-0.09165	3.10408
C	-6.76217	3.13879	-1.60179
C	-8.28023	2.86994	-1.61233
C	-6.40767	4.28118	-0.62736
C	-2.49901	-4.23264	0.23077
C	-3.59084	-4.18226	-0.70582
C	-1.84894	-5.48261	0.44544
C	-4.01103	-5.37954	-1.35217
C	-2.27690	-6.62777	-0.20544
C	-3.37159	-6.58114	-1.10677
O	0.21255	-1.42957	0.53817
O	-2.19523	-0.62470	1.04380
O	-0.25804	0.96921	1.50484
O	-0.82079	0.31069	-0.97381
P	-0.72999	-0.05112	0.49837
H	-3.22166	-5.76824	4.89419
H	-3.14551	-4.41630	2.82937
H	0.87953	-4.73785	5.76501
H	-1.20400	-5.96072	6.35879
H	2.12335	-3.25294	4.24411
H	-5.08210	-2.91571	-1.63877
H	5.36288	-1.81438	0.26729
H	1.90961	-3.25846	0.28606
H	4.58813	0.82460	3.55628
H	1.07284	-0.38984	4.01422
H	2.92168	-3.73462	-1.84233
H	4.47259	-3.02277	-1.36782
H	3.04713	-1.97912	-1.56472
H	4.66538	-4.49258	0.79885
H	3.22520	-4.69557	1.82236
H	3.23926	-5.35223	0.16634
H	3.57754	0.05341	5.74125
H	2.64221	-1.45200	5.65463
H	1.90112	0.01596	6.33303
H	2.87277	2.09502	4.18313
H	1.48532	1.85832	3.08964
H	1.23505	1.93362	4.84274
H	-6.84247	1.58199	0.65924
H	-5.00677	-1.54813	1.61058
H	-4.92189	1.87610	-3.16410
H	-2.63180	-1.00178	-2.51310
H	7.07029	-0.47102	1.00772
H	-4.12446	0.52031	2.65088
H	-5.32136	-0.26592	3.70825
H	-5.77052	1.18314	2.78367
H	-7.22355	-1.64634	2.68386
H	-7.78070	-0.24420	1.74825
H	-7.38834	-1.76197	0.91392
H	-3.14580	1.44453	-4.29971
H	-1.77302	0.33539	-4.36955
H	-1.98114	1.38171	-2.95209
H	-4.63616	-1.99499	-3.63764
H	-4.82609	-0.52062	-4.60799
H	-3.39217	-1.55218	-4.82783
H	6.10239	1.69800	0.37166
H	7.59482	1.95848	1.28633
H	6.02318	2.20835	2.07812
H	6.91298	0.49336	3.92442
H	7.35666	-1.14665	3.40907
H	8.39247	0.23787	2.97813
H	-6.47266	3.46225	-2.61408
H	-8.63273	2.56212	-0.61798
H	-8.53479	2.07129	-2.32174
H	-8.83236	3.77623	-1.89779
H	-6.68032	4.01468	0.40378
H	-5.33394	4.50474	-0.64270
H	-6.95578	5.19649	-0.89167
H	-0.99711	-5.52710	1.11855
H	-4.84173	-5.32582	-2.05624
H	-1.76048	-7.57123	-0.03105
H	-3.69786	-7.48960	-1.61184
N	1.77965	2.49099	0.32910
C	0.79404	6.04579	0.92978
C	0.68846	4.65755	0.71878
C	-0.57124	4.03892	0.62465
C	-1.73540	4.80527	0.76221
C	-1.64580	6.20283	0.97317
C	-0.36830	6.81673	1.05760
C	1.94669	3.89026	0.56097
C	1.60883	2.14525	-1.60361
C	2.98643	1.63717	0.15331
C	3.06759	1.68151	-1.37615
C	4.35532	0.44733	-3.00891
C	5.77019	0.71995	-2.55486
C	6.55773	-0.32088	-2.03115
C	6.32454	2.00926	-2.64501
C	7.86799	-0.08030	-1.60433
C	7.63273	2.25736	-2.20741
C	8.40644	1.21233	-1.68643
C	-3.10661	2.84705	0.65622
C	-3.58128	6.79561	2.21885
C	0.87822	8.82768	1.37164
O	3.07215	4.38683	0.53820
O	3.40460	0.42129	-1.91742
O	-2.99327	4.28405	0.69495
O	-2.75901	6.99626	1.04820
O	-0.38645	8.16483	1.27542
H	1.78465	6.48306	0.99741
H	-0.66127	2.97462	0.45297
H	2.74242	0.62844	0.49591
H	3.84812	2.02723	0.69375
H	3.75766	2.46296	-1.71581
H	0.98918	2.01750	0.81704
H	1.37092	3.14902	-1.94224
H	0.77873	1.46223	-1.46466
H	4.03358	1.17915	-3.76297
H	4.27846	-0.55298	-3.44945
H	6.13892	-1.32508	-1.97245
H	5.73412	2.81893	-3.07571
H	8.47055	-0.89872	-1.21097
H	8.04822	3.26206	-2.27999

H	9.42569	1.40145	-1.35083
H	-4.17150	2.63372	0.74268
H	-2.55545	2.38757	1.48588
H	-2.73699	2.44308	-0.29520
H	-2.99898	6.98868	3.13175
H	-3.99300	5.77960	2.24615
H	-4.39283	7.52618	2.13948
H	1.47221	8.43983	2.21306
H	0.64498	9.88265	1.54303
H	1.45686	8.72443	0.44138
N	0.44271	-0.80946	-3.01187
C	-0.16030	-4.45734	-2.60613
C	0.53704	-4.90329	-3.74630
C	-0.23311	-3.09789	-2.29113
C	1.17232	-3.99919	-4.60759
C	0.40709	-2.19224	-3.14789
C	1.09832	-2.63645	-4.29791
C	1.10546	-0.12499	-3.96500
S	1.77550	-1.25405	-5.15775
S	1.29143	1.55354	-4.09615
H	-0.65255	-5.17615	-1.95508
H	0.58224	-5.96868	-3.96721
H	-0.75379	-2.74394	-1.40789
H	1.70719	-4.34411	-5.49002
H	-0.05132	-0.33932	-2.20228

TS 9 (*R*) *conf6*

Imaginary frequency: -435.71 cm^{-1}

C	0.85456	-6.72818	0.32773
C	0.73398	-5.47189	0.89772
C	-1.22388	-6.42517	-0.88475
C	-0.13675	-7.21738	-0.56209
C	-0.38475	-4.63967	0.60420
C	-0.53954	-3.31979	1.15790
C	-1.36814	-5.12213	-0.32902
C	-1.56047	-2.50252	0.67208
C	0.40215	-2.81713	2.19222
C	-2.45228	-4.27914	-0.68932
C	-2.55695	-2.97300	-0.23444
C	1.13922	-1.66055	1.95218
C	-3.75223	-2.15322	-0.61170
C	2.18745	-1.21613	2.80737
C	-4.86855	-2.14174	0.26113
C	-3.80634	-1.47759	-1.85546
C	2.42136	-1.94251	3.96677
C	3.07557	-0.06780	2.45077
C	-6.02549	-1.44904	-0.12729
C	-4.83767	-2.84642	1.61524
C	-4.98780	-0.79789	-2.19624
C	-2.62842	-1.51247	-2.82662
C	4.02309	-0.22297	1.40747
C	3.05076	1.12362	3.22071
C	-6.10472	-0.76644	-1.35019
C	-5.99355	-3.85391	1.76520
C	-4.82380	-1.82378	2.76944
C	-2.40941	-0.17999	-3.56286
C	-2.77816	-2.66256	-3.84427
C	4.96357	0.79644	1.19338
C	4.09565	-1.48488	0.55202
C	4.01573	2.11177	2.96770
C	2.01756	1.35682	4.32106
C	-7.35566	0.01004	-1.73887
C	4.99221	1.96004	1.97251
C	3.99984	-1.16391	-0.95051
C	5.37096	-2.29054	0.87245
C	2.67965	1.34348	5.71388
C	1.22293	2.65924	4.10193
C	-8.59522	-0.90365	-1.80676
C	-7.59389	1.20246	-0.78889
C	6.04635	3.03039	1.72177
C	5.42697	4.28336	1.07163
C	6.82253	3.39541	3.00130
C	0.58856	-3.50977	3.43815
C	1.62454	-3.06060	4.33198
C	-0.22591	-4.60694	3.83967
C	1.82939	-3.75002	5.56121
C	-0.00885	-5.24743	5.04757
C	1.03317	-4.82489	5.91300
O	-1.65336	-1.19275	1.14544
O	0.90263	-0.95204	0.77466
O	-0.57026	1.06916	1.61148
O	-0.65580	0.17673	-0.85091
P	-0.51545	-0.08357	0.63860
H	1.72397	-7.34306	0.55817
H	1.50676	-5.10210	1.56634
H	-1.98094	-6.77800	-1.58538
H	-0.03086	-8.20911	-1.00039
H	-3.22759	-4.66998	-1.34686
H	3.23787	-1.64042	4.62151
H	-6.87974	-1.43075	0.54921
H	-3.90348	-3.41846	1.67760
H	-5.04338	-0.27060	-3.14803
H	-1.72862	-1.70801	-2.23170
H	-6.97112	-3.35260	1.75917
H	-5.90454	-4.39827	2.71562
H	-5.98511	-4.58566	0.94616
H	-4.77144	-2.33832	3.73934
H	-3.95741	-1.15715	2.68497
H	-5.73423	-1.20773	2.76177
H	-1.51144	-0.24541	-4.18941
H	-2.27113	0.64476	-2.85559
H	-3.24735	0.06238	-4.23031
H	-2.85986	-3.63525	-3.34530
H	-3.67678	-2.51947	-4.46132
H	-1.90437	-2.69575	-4.51066
H	5.69994	0.67627	0.39997
H	3.24275	-2.12387	0.80697
H	4.00290	3.02199	3.56677
H	1.29639	0.53088	4.28387
H	-7.18416	0.41691	-2.74798
H	3.12994	-0.53423	-1.16222
H	3.90809	-2.09120	-1.53228

H	4.88821	-0.63061	-1.30602
H	6.27305	-1.71267	0.62706
H	5.41447	-2.55248	1.93851
H	5.39550	-3.22049	0.28661
H	1.92389	1.46729	6.50214
H	3.40705	2.16185	5.81076
H	3.21215	0.40049	5.89445
H	1.87676	3.54216	4.10292
H	0.48526	2.79065	4.90593
H	0.68174	2.62188	3.15148
H	-8.43145	-1.74151	-2.49752
H	-9.47375	-0.33908	-2.14894
H	-8.83138	-1.32291	-0.81874
H	-7.77606	0.85244	0.23735
H	-6.72784	1.87473	-0.76421
H	-8.47415	1.77883	-1.10715
H	6.76912	2.60617	1.00713
H	4.70918	4.76145	1.75287
H	4.89396	4.01827	0.15069
H	6.20191	5.02289	0.82568
H	6.16306	3.85863	3.74799
H	7.27320	2.50381	3.45666
H	7.62415	4.11220	2.77511
H	-1.03277	-4.93191	3.18706
H	2.62230	-3.40453	6.22521
H	-0.64830	-6.08005	5.33951
H	1.19568	-5.34150	6.85841
N	0.49213	3.36036	0.38145
C	-2.33848	3.56925	0.49459
C	-1.54831	4.73251	0.50445
C	-2.14467	6.00838	0.51379
C	-3.54093	6.12040	0.51748
C	-4.34985	4.95413	0.51318
C	-3.73466	3.67863	0.51120
C	-0.06867	4.67148	0.46738
C	0.71770	2.85513	-1.52271
C	1.97366	3.21991	0.35456
C	2.16971	3.25305	-1.16587
C	4.06556	2.89395	-2.59678
C	5.13155	1.86273	-2.85519
C	4.94175	0.87899	-3.83856
C	6.29987	1.83253	-2.07622
C	5.89344	-0.12951	-4.03096
C	7.25548	0.82600	-2.26425
C	7.05032	-0.16109	-3.23953
C	-3.45226	8.50558	0.53874
C	-6.42411	4.68066	1.64103
C	-3.97459	1.30294	0.64158
O	0.66983	5.65496	0.42265
O	3.18467	2.36443	-1.57783
O	-4.22603	7.30160	0.53247
O	-5.71030	5.09790	0.45628
O	-4.57489	2.60700	0.51555
H	-1.88797	2.58554	0.47761
H	-1.49788	6.87935	0.52404
H	2.22910	2.23371	0.75179
H	2.47424	4.00368	0.92443
H	2.36361	4.27480	-1.51961
H	-0.00086	2.58532	0.87336
H	0.02009	3.55216	-1.97703
H	0.36020	1.84701	-1.34797
H	4.51302	3.83559	-2.23664
H	3.49214	3.10137	-3.51201
H	4.04172	0.90342	-4.44964
H	6.45655	2.59957	-1.31886
H	5.72893	-0.89156	-4.79253
H	8.15660	0.81107	-1.65142
H	7.79062	-0.94767	-3.38389
H	-4.17974	9.32250	0.54945
H	-2.82407	8.58309	-0.36136
H	-2.81404	8.56837	1.43312
H	-6.09434	5.26682	2.51130
H	-6.28162	3.61070	1.83426
H	-7.48019	4.88604	1.43821
H	-3.38712	1.04862	-0.24931
H	-4.80708	0.60628	0.72884
H	-3.33389	1.24954	1.53047
N	0.91081	-0.44318	-2.87320
C	1.24162	-4.13655	-2.56822
C	1.71572	-4.40346	-3.86727
C	0.95147	-2.83153	-2.16032
C	1.91375	-3.37133	-4.79383
C	1.14542	-1.79834	-3.08659
C	1.62352	-2.06366	-4.38878
C	1.16502	0.38300	-3.90786
S	1.75979	-0.55580	-5.29437
S	0.95163	2.05947	-3.99209
H	1.10150	-4.95423	-1.86610
H	1.93505	-5.42931	-4.15947
H	0.59947	-2.61053	-1.15780
H	2.28182	-3.57814	-5.79657
H	0.38034	-0.13751	-2.00999

TS 9 (*R*) *conf7*

Imaginary frequency: -445.43 cm^{-1}

C	0.18621	-5.13766	5.14023
C	-0.04921	-4.53106	3.91835
C	1.94095	-3.54011	5.64461
C	1.19566	-4.64715	6.00831
C	0.71364	-3.40181	3.50477
C	0.50603	-2.74224	2.24453
C	1.71590	-2.88459	4.40052
C	1.19107	-1.55837	1.98713
C	-0.40980	-3.29922	1.21517
C	2.46006	-1.73449	4.02248
C	2.20458	-1.04542	2.84537
C	-1.46302	-2.53004	0.72069
C	3.04207	0.13241	2.46418
C	-2.43981	-3.05043	-0.17973
C	2.94180	1.34947	3.18486
C	4.01493	-0.01707	1.44398
C	-2.27793	-4.35436	-0.62430

C	-3.66979	-2.28447	-0.55818
C	3.86249	2.37308	2.91094
C	1.88169	1.56722	4.26206
C	4.90321	1.04295	1.19857
C	4.17515	-1.32349	0.67041
C	-3.76915	-1.64477	-1.81805
C	-4.77089	-2.28734	0.33425
C	4.85905	2.23689	1.93310
C	1.05008	2.84016	4.01115
C	2.52072	1.59719	5.66559
C	4.13802	-1.11465	-0.85357
C	5.46109	-2.05423	1.10751
C	-4.97933	-1.01520	-2.15474
C	-2.61018	-1.66427	-2.81219
C	-5.95765	-1.64540	-0.05108
C	-4.69598	-2.95895	1.70338
C	5.91143	3.31961	1.72575
C	-6.08176	-0.99879	-1.28974
C	-2.43801	-0.33517	-3.56683
C	-2.75705	-2.82774	-3.81503
C	-4.72245	-1.91284	2.83597
C	-5.80217	-4.01637	1.88305
C	5.30958	4.71752	1.49036
C	6.89422	3.34024	2.91575
C	-7.36531	-0.27623	-1.67603
C	-8.57328	-1.23343	-1.69858
C	-7.62912	0.93182	-0.75294
C	-0.19888	-4.61644	0.67536
C	-1.15798	-5.14665	-0.25733
C	0.95150	-5.39925	0.98181
C	-0.95642	-6.44646	-0.80246
C	1.12652	-6.65419	0.42289
C	0.16107	-7.19029	-0.46841
O	0.93800	-0.88873	0.79047
O	-1.60409	-1.21759	1.17690
O	-0.60368	1.10154	1.56261
O	-0.67423	0.12035	-0.86746
P	-0.51330	-0.08101	0.62842
H	-0.41348	-5.99631	5.44098
H	-0.83082	-4.90848	3.26324
H	2.70796	-3.14320	6.31027
H	1.37323	-5.13748	6.96493
H	3.25345	-1.38015	4.67941
H	-3.03534	-4.78422	-1.27821
H	3.80283	3.29753	3.48428
H	1.18892	0.71723	4.22464
H	5.66546	0.92176	0.42962
H	3.33561	-1.97766	0.92966
H	1.67332	3.74485	4.01984
H	0.28962	2.95323	4.79634
H	0.53316	2.77696	3.04894
H	1.74849	1.71168	6.43910
H	3.07809	0.67421	5.87157
H	3.22131	2.43908	5.75904
H	5.04023	-0.60884	-1.21506
H	3.27668	-0.50550	-1.14625
H	4.06743	-2.08338	-1.36660
H	6.35189	-1.45351	0.87589
H	5.45451	-2.24984	2.18857
H	5.55457	-3.01552	0.58252
H	-5.06967	-0.51653	-3.11925
H	-1.69331	-1.83352	-2.23531
H	-6.80046	-1.63929	0.63989
H	-3.73568	-3.48525	1.77042
H	6.48794	3.04722	0.82747
H	-2.30012	0.49953	-2.87136
H	-3.29731	-0.11718	-4.21519
H	-1.55476	-0.38773	-4.21498
H	-1.89551	-2.85179	-4.49759
H	-2.81222	-3.79669	-3.30512
H	-3.66942	-2.70782	-4.41665
H	-5.66143	-1.34138	2.82427
H	-3.88974	-1.20755	2.73016
H	-4.63773	-2.40403	3.81562
H	-6.80218	-3.56157	1.87063
H	-5.76278	-4.76546	1.08077
H	-5.68331	-4.53403	2.84508
H	4.64874	4.73058	0.61429
H	6.10668	5.45468	1.32305
H	4.72449	5.05253	2.35730
H	6.37098	3.61150	3.84333
H	7.35133	2.35301	3.06316
H	7.69537	4.07397	2.74909
H	-7.22501	0.10965	-2.69811
H	-8.77848	-1.63390	-0.69599
H	-8.39171	-2.08335	-2.36986
H	-9.47642	-0.70876	-2.04020
H	-7.78138	0.60292	0.28509
H	-6.78706	1.63436	-0.76117
H	-8.53436	1.46878	-1.07005
H	1.70453	-4.99216	1.65148
H	-1.69483	-6.83638	-1.50335
H	2.01888	-7.23135	0.66300
H	0.31021	-8.18002	-0.89856
N	0.39904	3.38258	0.25409
C	-2.43601	3.51169	0.40975
C	-1.68021	4.69752	0.38506
C	-2.31362	5.95556	0.37424
C	-3.71227	6.02698	0.39220
C	-4.48694	4.83779	0.42119
C	-3.83464	3.58078	0.43914
C	-0.20087	4.67999	0.32721
C	0.55829	2.82329	-1.62719
C	1.88423	3.29091	0.18381
C	2.01741	3.21385	-1.35028
C	4.27415	2.77934	-1.90707
C	5.16009	1.77167	-2.59686
C	4.67265	1.01982	-3.67765
C	6.48245	1.57513	-2.16860
C	5.48135	0.06046	-4.29563
C	7.29975	0.62441	-2.79524
C	6.79674	-0.14401	-3.85371

C	-3.69308	8.41364	0.36010
C	-6.54294	4.52375	1.57313
C	-4.00382	1.20185	0.61886
O	0.50781	5.68275	0.25074
O	2.94156	2.25518	-1.81539
O	-4.43119	7.18781	0.39072
O	-5.85122	4.94185	0.37553
O	-4.64304	2.48548	0.47415
H	-1.95671	2.54146	0.41243
H	-1.69272	6.84504	0.35747
H	2.19112	2.34773	0.64347
H	2.36464	4.13664	0.67876
H	2.22565	4.20265	-1.78838
H	-0.05409	2.60752	0.78434
H	-0.13912	3.52273	-2.07496
H	0.19630	1.82110	-1.42805
H	4.66933	3.00398	-0.90477
H	4.24978	3.72805	-2.47662
H	3.65300	1.18157	-4.01422
H	6.87359	2.16102	-1.33631
H	5.08099	-0.53015	-5.11957
H	8.32173	0.47542	-2.44722
H	7.42528	-0.89555	-4.33099
H	-4.44409	9.20904	0.36211
H	-3.07870	8.48894	-0.54964
H	-3.04601	8.51521	1.24449
H	-6.22161	5.13223	2.43114
H	-6.36966	3.46127	1.78156
H	-7.60589	4.69740	1.37679
H	-3.41905	0.94694	-0.27368
H	-4.81458	0.48312	0.72940
H	-3.35213	1.18475	1.50108
N	0.89562	-0.44422	-2.91076
C	1.46541	-4.09678	-2.49836
C	1.95094	-4.37061	-3.79175
C	1.09472	-2.80116	-2.12704
C	2.07709	-3.35591	-4.75002
C	1.21898	-1.78587	-3.08480
C	1.70432	-2.05806	-4.38291
C	1.08047	0.36612	-3.97278
S	1.72902	-0.57313	-5.33602
S	0.75911	2.02155	-4.09375
H	1.37787	-4.90078	-1.77198
H	2.23461	-5.38842	-4.05542
H	0.73113	-2.57357	-1.12992
H	2.45195	-3.56925	-5.74887
H	0.36451	-0.14915	-2.04780

TS 9 (*R*) *conf8*

Imaginary frequency: -445.77 cm^{-1}

C	-0.89990	-5.35959	-4.91960
C	-0.54420	-4.72191	-3.74351
C	-2.54541	-3.64386	-5.40355
C	-1.91560	-4.82461	-5.75343
C	-1.18713	-3.51568	-3.34367
C	-0.85257	-2.82137	-2.13031
C	-2.19474	-2.95555	-4.20714
C	-1.42247	-1.57374	-1.89375
C	0.07713	-3.40564	-1.12871
C	-2.81812	-1.73062	-3.84596
C	-2.43790	-1.01426	-2.71997
C	1.21564	-2.70330	-0.73461
C	-3.15066	0.24698	-2.35187
C	2.20214	-3.25853	0.13387
C	-4.07425	0.22530	-1.27680
C	-2.98827	1.41934	-3.13271
C	1.96610	-4.52245	0.65373
C	3.50558	-2.56963	0.39560
C	-4.85484	1.36766	-1.03500
C	-4.29966	-1.02872	-0.43585
C	-3.80255	2.52962	-2.85923
C	-1.97697	1.49710	-4.27403
C	3.72684	-1.86605	1.60727
C	4.54111	-2.69379	-0.56120
C	-4.75098	2.52145	-1.82560
C	-4.16750	-0.75752	1.07284
C	-5.66098	-1.66824	-0.77693
C	-2.69091	1.50953	-5.64136
C	-1.03538	2.70944	-4.13796
C	4.98633	-1.28839	1.82540
C	2.64190	-1.76688	2.67730
C	5.78530	-2.09809	-0.29257
C	4.33875	-3.44652	-1.87404
C	-5.69587	3.69842	-1.61445
C	6.02606	-1.38368	0.88723
C	2.79081	-2.89254	3.72227
C	2.60667	-0.39846	3.37818
C	4.33476	-2.48080	-3.07607
C	5.37785	-4.56984	-2.05523
C	-4.96772	5.04860	-1.47855
C	-6.74012	3.75174	-2.74989
C	7.37175	-0.71674	1.13748
C	7.22808	0.81365	1.27194
C	8.08015	-1.31894	2.36734
C	-0.20227	-4.67547	-0.51200
C	0.76689	-5.23711	0.39175
C	-1.42569	-5.37722	-0.71431
C	0.49721	-6.48923	1.01361
C	-1.66400	-6.58669	-0.08314
C	-0.69238	-7.15571	0.78051
O	-1.04685	-0.87595	-0.74622
O	1.43077	-1.42828	-1.26270
O	0.59760	0.94556	-1.69822
O	0.73813	0.06630	0.76827
P	0.47135	-0.18458	-0.70467
H	-0.39057	-6.27774	-5.21106
H	0.24198	-5.13407	-3.11536
H	-3.31518	-3.21336	-6.04470
H	-2.18849	-5.33972	-6.67391
H	-3.61666	-1.33944	-4.47510
H	2.72578	-4.98221	1.28421
H	-5.58101	1.34533	-0.22305

H	-3.52996	-1.76094	-0.70305
H	-3.69728	3.42024	-3.47776
H	-1.35202	0.59647	-4.22725
H	-3.24658	-0.20820	1.29383
H	-4.14728	-1.70529	1.62775
H	-5.00672	-0.16441	1.45299
H	-6.48715	-0.98511	-0.53433
H	-5.72407	-1.91200	-1.84632
H	-5.80621	-2.59387	-0.20196
H	-3.32778	2.39986	-5.74194
H	-3.32955	0.62578	-5.76792
H	-1.95762	1.52318	-6.45979
H	-1.58478	3.66031	-4.16994
H	-0.47489	2.65745	-3.19979
H	-0.31089	2.71691	-4.96411
H	5.16179	-0.74310	2.75097
H	1.67709	-1.90168	2.17396
H	6.58525	-2.17982	-1.02982
H	3.35222	-3.92552	-1.83993
H	-6.24067	3.51531	-0.67468
H	3.75089	-2.80457	4.25082
H	2.75003	-3.88467	3.25767
H	1.98244	-2.83173	4.46497
H	3.51882	-0.21275	3.96140
H	2.47966	0.41255	2.65326
H	1.76621	-0.36254	4.08189
H	5.29894	-1.96130	-3.16901
H	3.54719	-1.72646	-2.96408
H	4.15648	-3.03136	-4.01058
H	6.39634	-4.16795	-2.14490
H	5.36189	-5.26102	-1.20176
H	5.16449	-5.14326	-2.96807
H	-4.25874	5.04284	-0.64081
H	-5.69011	5.85755	-1.30378
H	-4.40801	5.29513	-2.39073
H	-6.25013	3.93669	-3.71604
H	-7.28551	2.80190	-2.82514
H	-7.46652	4.55801	-2.57601
H	8.00213	-0.91692	0.25656
H	6.62343	1.07323	2.15255
H	6.74061	1.24896	0.39142
H	8.21465	1.28305	1.39384
H	7.50007	-1.13664	3.28278
H	8.20537	-2.40454	2.25867
H	9.07287	-0.86738	2.50330
H	-2.18281	-4.94328	-1.36222
H	1.24322	-6.90409	1.69179
H	-2.61066	-7.10138	-0.24441
H	-0.89209	-8.10894	1.26871
N	-0.11447	3.35456	-0.44507
C	2.78018	5.69623	-0.77762
C	2.05059	4.49114	-0.76470
C	2.70476	3.25016	-0.86757
C	4.10086	3.21007	-0.99276
C	4.84826	4.41231	-0.98894
C	4.17537	5.65682	-0.88516
C	0.58147	4.59419	-0.60250
C	-0.21039	2.89221	1.46405
C	-1.59616	3.38715	-0.29178
C	-1.64698	3.39056	1.24895
C	-3.89524	3.17378	1.94618
C	-4.82146	2.27699	2.72961
C	-4.33622	1.52823	3.81334
C	-6.17944	2.18235	2.38666
C	-5.18580	0.67016	4.51915
C	-7.03638	1.33411	3.10127
C	-6.53846	0.56661	4.16288
C	4.07669	0.82798	-1.15335
C	6.95727	4.62701	0.06134
C	4.35522	8.03973	-0.80067
O	-0.03670	5.65338	-0.50362
O	-2.61758	2.53482	1.81046
O	4.81797	2.06238	-1.12235
O	6.20861	4.34924	-1.14170
O	4.98523	6.75827	-0.90728
H	2.23465	6.63063	-0.69812
H	2.14857	2.32120	-0.86098
H	-2.00030	2.45118	-0.68679
H	-2.03704	4.24490	-0.80252
H	-1.74858	4.41201	1.64785
H	0.24196	2.52222	-0.96210
H	0.05708	1.85536	1.29415
H	0.56505	3.54963	1.84154
H	-4.32619	3.38685	0.95617
H	-3.76052	4.14123	2.46672
H	-3.28771	1.61140	4.08277
H	-6.56794	2.76687	1.55215
H	-4.78843	0.07916	5.34429
H	-8.08668	1.26299	2.81915
H	-7.19963	-0.10628	4.70854
H	4.81845	0.04709	-1.31706
H	3.33731	0.82950	-1.96402
H	3.57079	0.64340	-0.19659
H	6.69451	3.90928	0.85169
H	6.77720	5.65207	0.41095
H	8.01173	4.50568	-0.20730
H	3.66361	8.21481	-1.63795
H	5.16798	8.77079	-0.83682
H	3.80952	8.13970	0.14945
N	-0.75146	-0.27336	2.91920
C	-1.65577	-3.87555	2.71254
C	-2.08564	-4.05031	4.04236
C	-1.19814	-2.63455	2.26035
C	-2.06699	-2.98880	4.95712
C	-1.17780	-1.57265	3.17435
C	-1.60626	-1.74582	4.50896
C	-0.80131	0.59400	3.95058
S	-1.44486	-0.22583	5.39098
S	-0.33249	2.21815	3.97506
H	-1.68055	-4.71411	2.02112
H	-2.43965	-5.02690	4.36923
H	-0.87666	-2.48208	1.23487

H	-2.39865	-3.12546	5.98431
H	-0.24984	-0.06294	2.01473

TS 9 (*R*) *conf9*

Imaginary frequency: -436.65 cm^{-1}

C	-1.34871	-6.69197	0.04388
C	-1.17338	-5.47910	-0.60105
C	0.81042	-6.47701	1.12736
C	-0.34549	-7.20426	0.90692
C	0.01525	-4.71599	-0.41389
C	0.23021	-3.44179	-1.04879
C	1.01392	-5.21897	0.49221
C	1.33329	-2.67869	-0.66587
C	-0.72999	-2.92464	-2.05885
C	2.17401	-4.44034	0.74614
C	2.34485	-3.17229	0.21123
C	-1.36433	-1.70287	-1.84891
C	3.61344	-2.41850	0.46656
C	-2.42052	-1.22384	-2.67510
C	4.67109	-2.53907	-0.46597
C	3.78262	-1.65874	1.65240
C	-2.77201	-1.99114	-3.77705
C	-3.19336	0.01217	-2.34368
C	5.88473	-1.88194	-0.20025
C	4.51973	-3.34612	-1.75326
C	5.01318	-1.02154	1.86904
C	2.67179	-1.56426	2.69591
C	-4.09234	-0.00405	-1.24760
C	-3.11115	1.15402	-3.18186
C	6.07364	-1.11183	0.95359
C	5.62450	-4.40994	-1.89937
C	4.45988	-2.42053	-2.98523
C	2.58465	-0.18335	3.36718
C	2.82015	-2.66547	3.76646
C	-4.93023	1.10361	-1.04570
C	-4.22254	-1.20564	-0.31546
C	-3.97523	2.23381	-2.93949
C	-2.12370	1.23782	-4.34381
C	7.38755	-0.38349	1.20160
C	-4.90509	2.22106	-1.88964
C	-3.99094	-0.81294	1.15491
C	-5.58707	-1.89967	-0.50110
C	-2.85941	1.20446	-5.69883
C	-1.21444	2.47826	-4.24185
C	7.18194	1.14315	1.28744
C	8.10018	-0.92040	2.45904
C	-5.85254	3.38962	-1.65219
C	-5.09767	4.62095	-1.11376
C	-6.66655	3.74443	-2.91094
C	-1.03550	-3.66586	-3.25226
C	-2.08276	-3.18620	-4.11673
C	-0.32723	-4.84170	-3.63192
C	-2.40499	-3.92193	-5.29287
C	-0.65673	-5.52648	-4.78897
C	-1.71072	-5.07176	-5.62298
O	1.49227	-1.40662	-1.21768
O	-1.01237	-0.95249	-0.72779
O	0.55955	0.90620	-1.74314
O	0.71187	0.12924	0.75497
P	0.47143	-0.19075	-0.70949
H	-2.27016	-7.25363	-0.10612
H	-1.95474	-5.08985	-1.24835
H	1.57923	-6.84674	1.80616
H	-0.49519	-8.16142	1.40521
H	2.95637	-4.85255	1.38193
H	-3.59718	-1.66097	-4.40692
H	6.70105	-1.95887	-0.91978
H	3.56349	-3.88196	-1.70410
H	5.14931	-0.43302	2.77448
H	1.72397	-1.73299	2.17163
H	6.61688	-3.95159	-2.00842
H	5.44383	-5.02673	-2.79071
H	5.65250	-5.07060	-1.02239
H	4.31700	-3.00961	-3.90218
H	3.62842	-1.71138	-2.89713
H	5.39154	-1.84735	-3.09349
H	1.72183	-0.15252	4.04371
H	2.46238	0.61053	2.62261
H	3.47383	0.03396	3.97454
H	2.81001	-3.66678	3.32046
H	3.76552	-2.54668	4.31512
H	1.99298	-2.60754	4.48842
H	-5.62868	1.09106	-0.21010
H	-3.45318	-1.93764	-0.58639
H	-3.91937	3.10550	-3.59110
H	-1.47214	0.35658	-4.29354
H	8.03858	-0.58469	0.33608
H	-3.04884	-0.26793	1.26973
H	-3.95325	-1.71018	1.78764
H	-4.79407	-0.16951	1.53051
H	-6.41167	-1.22585	-0.22938
H	-5.73244	-2.21147	-1.54446
H	-5.65476	-2.79101	0.13882
H	-2.14001	1.21942	-6.52954
H	-3.52076	2.07564	-5.80801
H	-3.47722	0.30214	-5.79631
H	-1.79295	3.41194	-4.26864
H	-0.50970	2.49947	-5.08487
H	-0.63160	2.45037	-3.31603
H	6.68788	1.53160	0.38894
H	8.14779	1.65472	1.40550
H	6.55752	1.40524	2.15344
H	7.49814	-0.73581	3.35974
H	8.27117	-2.00263	2.38432
H	9.07139	-0.42464	2.59646
H	-6.56669	3.07024	-0.87690
H	-4.38154	4.99523	-1.85877
H	-4.53850	4.36517	-0.20590
H	-5.79441	5.43713	-0.87636
H	-6.01429	4.10750	-3.71704
H	-7.21187	2.86896	-3.28721
H	-7.39424	4.53742	-2.68910

H	0.48867	-5.19233	-3.00440
H	-3.20500	-3.55193	-5.93479
H	-0.09695	-6.41956	-5.06545
H	-1.96226	-5.62344	-6.52822
N	-0.22272	3.33519	-0.58725
C	2.60767	3.30557	-0.96075
C	1.91441	4.52714	-0.88780
C	2.60726	5.75330	-0.91099
C	4.00438	5.75549	-0.99786
C	4.71701	4.53088	-1.06904
C	4.00595	3.30655	-1.06594
C	0.43952	4.58872	-0.75422
C	-0.40522	2.94107	1.34691
C	-1.70860	3.32343	-0.49296
C	-1.83239	3.44867	1.03001
C	-3.68366	3.33711	2.55459
C	-4.80584	2.40897	2.93546
C	-4.63151	1.47522	3.96904
C	-6.01455	2.41788	2.22019
C	-5.63862	0.55148	4.27250
C	-7.02586	1.49627	2.51956
C	-6.83623	0.55641	3.54342
C	4.10756	8.14446	-0.95705
C	6.80501	4.85510	-0.00068
C	4.05485	0.92290	-1.18903
O	-0.21018	5.63237	-0.69158
O	-2.90081	2.67659	1.53173
O	4.77917	6.88200	-1.03039
O	6.08084	4.50400	-1.19960
O	4.75858	2.17911	-1.16949
H	2.08072	2.35973	-0.94445
H	2.03202	6.67160	-0.85740
H	-2.06231	2.34425	-0.82770
H	-2.16735	4.11825	-1.08255
H	-1.91940	4.50019	1.33511
H	0.17857	2.49724	-1.05859
H	0.36897	3.59413	1.73797
H	-0.14404	1.89818	1.20905
H	-4.07959	4.28525	2.15353
H	-3.04780	3.55803	3.42420
H	-3.69977	1.47143	4.53085
H	-6.15842	3.14725	1.42402
H	-5.48575	-0.17369	5.07158
H	-7.95804	1.51009	1.95505
H	-7.61996	-0.16490	3.77381
H	4.89728	8.90022	-0.99637
H	3.54560	8.24504	-0.01652
H	3.42265	8.28163	-1.80681
H	6.54653	4.16902	0.81855
H	6.59731	5.89071	0.29820
H	7.86564	4.74480	-0.24898
H	3.54462	0.73765	-0.23481
H	4.82181	0.16279	-1.33247
H	3.32473	0.88901	-2.00749
N	-0.78105	-0.26811	2.88653
C	-1.40133	-3.93581	2.80108
C	-1.84685	-4.09494	4.12762
C	-1.02779	-2.68115	2.31129
C	-1.93195	-3.00234	5.00049
C	-1.10885	-1.58776	3.18357
C	-1.55800	-1.74493	4.51332
C	-0.93520	0.62966	3.88034
S	-1.54757	-0.18478	5.33604
S	-0.59516	2.28731	3.86394
H	-1.34993	-4.79827	2.14177
H	-2.13307	-5.08338	4.48388
H	-0.69748	-2.54259	1.28693
H	-2.27822	-3.12544	6.02454
H	-0.27117	-0.04898	1.98507

TS 9 (*R*) *conf10*

Imaginary frequency: -435.78 cm^{-1}

C	1.29152	-6.65571	0.44078
C	1.09044	-5.40352	0.99717
C	-0.80933	-6.50596	-0.76195
C	0.33015	-7.22002	-0.43737
C	-0.08282	-4.65134	0.70104
C	-0.32246	-3.33902	1.24163
C	-1.03762	-5.20914	-0.22017
C	-1.39915	-2.59926	0.75276
C	0.58154	-2.76044	2.27034
C	-2.17868	-4.44546	-0.58298
C	-2.36673	-3.14381	-0.14305
C	1.22731	-1.55178	2.02293
C	-3.60812	-2.39760	-0.52334
C	2.22103	-1.00942	2.88698
C	-4.70540	-2.40376	0.37020
C	-3.71430	-1.76187	-1.78716
C	2.50175	-1.70271	4.05617
C	3.00658	0.21251	2.53340
C	-5.89725	-1.76741	-0.01698
C	-4.62579	-3.07309	1.73979
C	-4.92550	-1.14011	-2.12432
C	-2.55590	-1.77627	-2.78236
C	3.97714	0.14006	1.50177
C	2.86575	1.39853	3.29764
C	-6.02619	-1.12317	-1.25337
C	-5.70961	-4.15538	1.90853
C	-4.68460	-2.03043	2.87411
C	-2.40407	-0.45358	-3.55217
C	-2.68655	-2.95193	-3.77312
C	4.81917	1.24204	1.28361
C	4.18605	-1.12749	0.67673
C	3.75647	2.45872	3.06325
C	1.79098	1.54851	4.37179
C	-7.31717	-0.41176	-1.63459
C	4.75085	2.39681	2.07712
C	4.05612	-0.86597	-0.83341
C	5.54248	-1.77861	1.01626
C	2.41230	1.57886	5.78285
C	0.90916	2.79011	4.13292
C	-7.08439	1.09102	-1.89443

C	-7.99198	-1.08624	-2.84600
C	5.70101	3.57253	1.87563
C	7.13891	3.13299	1.54521
C	5.15724	4.54321	0.80553
C	0.81192	-3.42313	3.52543
C	1.79910	-2.88163	4.42348
C	0.08491	-4.57803	3.93308
C	2.04825	-3.53970	5.66175
C	0.34227	-5.18634	5.14966
C	1.33901	-4.67220	6.01872
O	-1.57961	-1.29382	1.21245
O	0.94966	-0.88039	0.83243
O	-0.66292	1.04727	1.62559
O	-0.68522	0.09782	-0.81782
P	-0.52690	-0.11880	0.67669
H	2.20108	-7.20877	0.67293
H	1.83999	-4.97482	1.65719
H	-1.54488	-6.91699	-1.45376
H	0.49954	-8.20749	-0.86523
H	-2.92941	-4.89549	-1.23097
H	3.28068	-1.32552	4.71764
H	-6.74449	-1.76005	0.67030
H	-3.65438	-3.57775	1.81357
H	-5.01309	-0.64789	-3.09113
H	-1.63580	-1.92610	-2.20519
H	-6.71911	-3.72258	1.88429
H	-5.58979	-4.66971	2.87227
H	-5.64443	-4.90393	1.10739
H	-4.59237	-2.52194	3.85291
H	-3.86924	-1.30434	2.77422
H	-5.63748	-1.48272	2.85996
H	-1.52509	-0.50376	-4.20616
H	-2.27260	0.39011	-2.86635
H	-3.26915	-0.25285	-4.19839
H	-2.72957	-3.91631	-3.25381
H	-3.60021	-2.84963	-4.37610
H	-1.82416	-2.97169	-4.45471
H	5.56044	1.17791	0.48975
H	3.40933	-1.84895	0.95431
H	3.67656	3.36257	3.66916
H	1.13488	0.67112	4.31128
H	-8.00269	-0.50149	-0.77683
H	3.12263	-0.34400	-1.06451
H	4.07072	-1.81514	-1.38644
H	4.88046	-0.24899	-1.20607
H	6.37585	-1.11400	0.74850
H	5.61607	-2.00033	2.08977
H	5.66763	-2.71830	0.45955
H	1.62714	1.64603	6.54893
H	3.07550	2.44737	5.90122
H	3.00550	0.67611	5.97848
H	1.49519	3.71884	4.16516
H	0.13495	2.85775	4.91004
H	0.40782	2.72299	3.16250
H	-6.61652	1.58294	-1.03280
H	-8.03741	1.59527	-2.10785
H	-6.42688	1.24122	-2.76211
H	-7.35331	-1.01815	-3.73777
H	-8.18405	-2.14957	-2.64970
H	-8.94866	-0.59828	-3.07947
H	5.73678	4.12179	2.83015
H	7.20021	2.65070	0.56089
H	7.51622	2.42030	2.29029
H	7.80840	4.00356	1.52739
H	4.94692	4.00480	-0.12666
H	4.22305	5.01404	1.13718
H	5.88141	5.34202	0.59231
H	-0.68748	-4.97422	3.27829
H	2.80388	-3.12364	6.32874
H	-0.23059	-6.06480	5.44552
H	1.53435	-5.16420	6.97102
N	0.30164	3.33581	0.33980
C	-2.52661	3.45933	0.53140
C	-1.77163	4.64614	0.52863
C	-2.40452	5.90317	0.57457
C	-3.80253	5.97249	0.63017
C	-4.57536	4.78237	0.63962
C	-3.92391	3.52587	0.60231
C	-0.29195	4.62997	0.44604
C	0.49846	2.84402	-1.56912
C	1.78453	3.23045	0.28150
C	1.94898	3.27644	-1.24176
C	3.81011	2.96197	-2.73215
C	4.92718	1.98218	-2.97794
C	4.74440	0.91040	-3.86617
C	6.13889	2.08445	-2.27504
C	5.74317	-0.05574	-4.03346
C	7.14238	1.12087	-2.43838
C	6.94238	0.04367	-3.31386
C	-3.78500	8.35878	0.68199
C	-6.58026	4.47873	1.86908
C	-4.08693	1.14212	0.71039
O	0.41575	5.63496	0.38550
O	2.98061	2.41891	-1.67702
O	-4.52189	7.13181	0.68650
O	-5.94154	4.88111	0.63776
O	-4.73183	2.42908	0.63304
H	-2.04730	2.49013	0.48968
H	-1.78371	6.79294	0.57340
H	2.07090	2.24868	0.66879
H	2.27709	4.02109	0.84696
H	2.10866	4.30490	-1.59341
H	-0.15830	2.54976	0.84753
H	-0.22284	3.52621	-2.00917
H	0.16639	1.82871	-1.38661
H	4.21021	3.93907	-2.41396
H	3.20691	3.10542	-3.64045
H	3.81325	0.83228	-4.42304
H	6.29533	2.92336	-1.59832
H	5.58228	-0.88736	-4.71929
H	8.07676	1.21039	-1.88448
H	7.71926	-0.71037	-3.43810

H	-4.53587	9.15284	0.73031
H	-3.19255	8.46708	-0.23890
H	-3.11692	8.42932	1.55369
H	-6.23887	5.11154	2.70145
H	-6.37821	3.42412	2.09375
H	-7.65334	4.62730	1.71059
H	-3.53471	0.91789	-0.21140
H	-4.89272	0.41801	0.82523
H	-3.40345	1.09507	1.56722
N	0.89516	-0.43242	-2.85653
C	1.47407	-4.08892	-2.48863
C	1.86864	-4.36388	-3.81229
C	1.13659	-2.79199	-2.09121
C	1.93831	-3.34809	-4.77494
C	1.20132	-1.77584	-3.05372
C	1.60008	-2.04869	-4.38071
C	1.01887	0.37769	-3.92721
S	1.57417	-0.56176	-5.33054
S	0.69144	2.03357	-4.03651
H	1.43220	-4.89369	-1.75930
H	2.12618	-5.38326	-4.09583
H	0.84057	-2.56406	-1.07201
H	2.24426	-3.56132	-5.79701
H	0.37762	-0.14697	-1.98020

TS 9 (*R*) *conf11*

Imaginary frequency: -436.04 cm^{-1}

C	-0.79134	-6.67952	0.84059
C	-0.72916	-5.54514	0.04869
C	1.33279	-6.12764	1.87278
C	0.25197	-6.98276	1.75339
C	0.38139	-4.65613	0.12958
C	0.47636	-3.45613	-0.66027
C	1.41994	-4.94605	1.08304
C	1.50627	-2.55422	-0.39072
C	-0.52742	-3.15843	-1.71586
C	2.50659	-4.04209	1.21966
C	2.56744	-2.84730	0.51792
C	-1.26971	-1.98246	-1.65220
C	3.79155	-1.98913	0.61608
C	-2.35746	-1.69914	-2.52577
C	3.92865	-1.01404	1.63318
C	4.84714	-2.22505	-0.30075
C	-2.63643	-2.62303	-3.52296
C	-3.22634	-0.49589	-2.34450
C	5.12175	-0.27417	1.69460
C	2.82743	-0.79626	2.66702
C	6.02223	-1.46659	-0.18937
C	4.71673	-3.24865	-1.42674
C	-3.20883	0.54966	-3.30322
C	-4.13821	-0.45413	-1.26027
C	6.17499	-0.47630	0.79200
C	2.66604	0.67526	3.08403
C	3.05230	-1.68496	3.90804
C	4.47673	-2.54294	-2.77770
C	5.92291	-4.20351	-1.49791
C	-4.15010	1.58528	-3.18999
C	-2.21244	0.57010	-4.46043
C	-5.05575	0.60569	-1.19055
C	-4.18472	-1.54217	-0.19092
C	7.45283	0.34631	0.88893
C	-5.09480	1.62160	-2.15374
C	-1.42577	1.89358	-4.52902
C	-2.91921	0.28284	-5.80098
C	-5.51361	-2.32196	-0.24792
C	-3.93878	-0.96168	1.21414
C	8.62090	-0.51705	1.40848
C	7.81590	1.02399	-0.44712
C	-6.12519	2.73883	-2.05725
C	-5.46476	4.07447	-1.66277
C	-6.94681	2.88625	-3.35192
C	-0.76117	-4.06322	-2.80845
C	-1.84418	-3.78673	-3.71697
C	0.05110	-5.20814	-3.04881
C	-2.09573	-4.68596	-4.79235
C	-0.21225	-6.05496	-4.11177
C	-1.30052	-5.80097	-4.98600
O	1.54217	-1.34797	-1.09200
O	-0.99221	-1.07394	-0.63245
O	0.39918	0.79428	-1.87452
O	0.61706	0.33230	0.69364
P	0.41006	-0.17908	-0.72005
H	-1.65474	-7.34010	0.76864
H	-1.54162	-5.31466	-0.63522
H	2.13051	-6.33590	2.58605
H	0.19148	-7.88002	2.36827
H	3.32663	-4.30051	1.88855
H	-3.48324	-2.44522	-4.18465
H	5.23718	0.48741	2.46529
H	1.88574	-1.10693	2.20046
H	6.82977	-1.64050	-0.89955
H	3.83243	-3.86459	-1.22070
H	3.53601	1.03819	3.64862
H	1.79104	0.78412	3.73689
H	2.51813	1.31902	2.21007
H	3.08752	-2.74766	3.63967
H	3.99877	-1.42691	4.40448
H	2.23513	-1.54405	4.63005
H	4.33972	-3.28157	-3.58021
H	5.33375	-1.90765	-3.04344
H	3.58217	-1.91039	-2.73335
H	6.09292	-4.69692	-0.53155
H	5.74716	-4.97958	-2.25562
H	6.84586	-3.67604	-1.77493
H	-4.14529	2.38114	-3.93428
H	-1.48180	-0.22964	-4.28583
H	-5.76326	0.63746	-0.36308
H	-3.38319	-2.26111	-0.39702
H	7.26965	1.14225	1.62859
H	-0.87104	2.05866	-3.60028
H	-2.08641	2.75346	-4.70595
H	-0.70124	1.85752	-5.35458

H	-3.66128	1.06198	-6.02617
H	-2.19184	0.25908	-6.62459
H	-3.44359	-0.68131	-5.77878
H	-6.36662	-1.66554	-0.02639
H	-5.51348	-3.13444	0.49262
H	-5.67159	-2.76100	-1.24249
H	-3.84414	-1.77093	1.95120
H	-3.02038	-0.36655	1.23472
H	-4.76368	-0.31321	1.52863
H	8.37733	-0.96812	2.37971
H	9.53168	0.08719	1.52481
H	8.84244	-1.33174	0.70456
H	8.06668	0.27751	-1.21369
H	6.98620	1.63327	-0.82337
H	8.69449	1.67191	-0.31930
H	-6.82436	2.46113	-1.25281
H	-4.77128	4.41149	-2.44594
H	-4.89562	3.96286	-0.73241
H	-6.21978	4.86030	-1.51992
H	-6.31144	3.19748	-4.19245
H	-7.42565	1.93674	-3.62504
H	-7.73030	3.64671	-3.22753
H	0.89350	-5.40542	-2.39007
H	-2.92348	-4.46931	-5.46823
H	0.42626	-6.92127	-4.28265
H	-1.49911	-6.47873	-5.81564
N	-0.49153	3.30292	-0.95968
C	2.27484	5.78532	-1.06118
C	1.62422	4.54313	-1.19214
C	2.35691	3.34394	-1.25559
C	3.75660	3.38835	-1.18603
C	4.42153	4.62583	-1.01688
C	3.67188	5.82600	-0.95552
C	0.14049	4.56117	-1.18979
C	-0.70086	3.08376	1.00250
C	-1.97759	3.25116	-0.89291
C	-2.14161	3.49166	0.61487
C	-4.01396	3.38772	2.11586
C	-5.04514	2.40457	2.60192
C	-6.24308	2.21477	1.89379
C	-4.79064	1.61695	3.73584
C	-7.16357	1.24043	2.30040
C	-5.70723	0.64220	4.14728
C	-6.89353	0.44771	3.42570
C	3.90901	1.01861	-1.43494
C	6.29340	4.37106	0.38141
C	3.69148	8.20076	-0.71055
O	-0.54219	5.58340	-1.24482
O	-3.17505	2.69913	1.15779
O	4.55784	2.29320	-1.27218
O	5.79094	4.67121	-0.93831
O	4.40749	6.96301	-0.77862
H	1.66701	6.68252	-1.00961
H	1.86081	2.38786	-1.37588
H	-2.29560	2.23830	-1.15569
H	-2.44686	3.98391	-1.55139
H	-2.29414	4.55679	0.83484
H	-0.04831	2.43914	-1.33522
H	0.03998	3.80523	1.33191
H	-0.39517	2.04455	0.96981
H	-4.49442	4.25024	1.62403
H	-3.40046	3.75230	2.95239
H	-6.44985	2.83053	1.01941
H	-3.86736	1.76784	4.29122
H	-8.08788	1.09909	1.74052
H	-5.49204	0.03227	5.02445
H	-7.60642	-0.31426	3.73998
H	3.26739	1.00866	-2.32543
H	3.31609	0.76590	-0.54874
H	4.71577	0.29447	-1.54018
H	7.38522	4.38001	0.30109
H	5.95742	3.37913	0.71333
H	5.96654	5.13622	1.10095
H	2.99513	8.21508	0.14151
H	3.13309	8.39176	-1.63907
H	4.45314	8.97411	-0.57490
N	-0.79053	0.04564	2.90205
C	-1.10859	-3.64685	3.22900
C	-1.57779	-3.69128	4.55611
C	-0.82028	-2.42953	2.60557
C	-1.77311	-2.51799	5.29620
C	-1.01377	-1.25512	3.34434
C	-1.48674	-1.29754	4.67463
C	-1.05625	1.03398	3.77951
S	-1.63152	0.34087	5.31045
S	-0.88210	2.70473	3.56953
H	-0.97223	-4.57128	2.67453
H	-1.79615	-4.65334	5.01722
H	-0.47382	-2.38126	1.57835
H	-2.13822	-2.55227	6.32050
H	-0.30700	0.20625	1.97389

TS 9 (*R*) *conf12*

Imaginary frequency: -455.21 cm^{-1}

C	3.20083	-5.47282	-3.95668
C	2.98016	-4.60511	-2.90101
C	0.88865	-5.27136	-4.66335
C	2.14622	-5.81912	-4.84074
C	1.69226	-4.03909	-2.67824
C	1.41729	-3.13744	-1.59356
C	0.63125	-4.36536	-3.59513
C	0.17675	-2.50525	-1.54193
C	2.41558	-2.88367	-0.52278
C	-0.64853	-3.77724	-3.41144
C	-0.89370	-2.83617	-2.42071
C	2.83022	-1.58188	-0.24543
C	-2.26931	-2.27466	-2.25720
C	3.84006	-1.27987	0.71575
C	-3.07580	-2.72623	-1.18124
C	-2.80572	-1.40021	-3.23569
C	4.37704	-2.33590	1.43744
C	4.38860	0.10231	0.88995

C	-4.42252	-2.33357	-1.14109
C	-2.53822	-3.70157	-0.13596
C	-4.15956	-1.03709	-3.14847
C	-1.96131	-0.85593	-4.38560
C	4.03266	0.88696	2.01445
C	5.34121	0.58043	-0.04467
C	-4.98861	-1.50040	-2.11739
C	-2.92905	-5.14613	-0.50972
C	-2.97026	-3.35177	1.29827
C	-2.40909	-1.45936	-5.73251
C	-1.97923	0.68437	-4.43897
C	4.64793	2.13953	2.17884
C	3.03578	0.38805	3.05774
C	5.92857	1.83667	0.16754
C	5.75193	-0.23570	-1.26778
C	-6.47380	-1.16186	-2.07862
C	5.59458	2.63395	1.27227
C	3.76600	-0.22569	4.27062
C	2.05870	1.48054	3.52675
C	7.26587	-0.52463	-1.27246
C	5.30101	0.44906	-2.57322
C	-6.75303	0.34722	-2.20691
C	-7.23140	-1.95294	-3.16581
C	6.22977	4.00249	1.47696
C	7.75534	3.89399	1.67063
C	5.88306	4.96519	0.32309
C	2.91985	-3.96136	0.28703
C	3.91794	-3.67144	1.28272
C	2.43387	-5.29715	0.18495
C	4.41524	-4.72630	2.09977
C	2.93219	-6.29920	1.00082
C	3.93701	-6.01681	1.96198
O	-0.06220	-1.57560	-0.53082
O	2.26871	-0.53517	-0.97991
O	0.19605	0.73779	-1.75587
O	0.64444	0.44749	0.81338
P	0.70704	-0.09323	-0.60363
H	4.19548	-5.88888	-4.11449
H	3.79641	-4.33780	-2.23401
H	0.07428	-5.51554	-5.34606
H	2.33347	-6.50702	-5.66463
H	-1.46228	-4.06572	-4.07568
H	5.17642	-2.13401	2.14880
H	-5.05810	-2.70320	-0.33688
H	-1.44433	-3.65086	-0.15244
H	-4.57455	-0.37855	-3.91059
H	-0.92185	-1.15984	-4.21011
H	-4.02205	-5.26369	-0.51666
H	-2.51158	-5.85940	0.21520
H	-2.55226	-5.40743	-1.50763
H	-2.43782	-3.98769	2.01701
H	-2.73957	-2.30540	1.52597
H	-4.04712	-3.51066	1.45079
H	-3.44568	-1.17681	-5.96459
H	-2.35705	-2.55585	-5.71651
H	-1.76884	-1.09719	-6.54887
H	-2.99455	1.07708	-4.58666
H	-1.56919	1.10468	-3.51564
H	-1.36013	1.03901	-5.27469
H	4.38334	2.75255	3.04019
H	2.44098	-0.40372	2.58644
H	6.65992	2.20359	-0.55249
H	5.24161	-1.20551	-1.21649
H	-6.85703	-1.49055	-1.09913
H	4.38841	0.53056	4.76991
H	4.41750	-1.05636	3.97413
H	3.03853	-0.60688	5.00149
H	2.57129	2.27354	4.08807
H	1.53590	1.93232	2.67758
H	1.30614	1.04600	4.19676
H	7.53023	-1.16815	-2.12316
H	7.57088	-1.03237	-0.34747
H	7.85222	0.40053	-1.35821
H	4.21396	0.59045	-2.57913
H	5.77719	1.43266	-2.69049
H	5.57511	-0.16420	-3.44319
H	-6.23561	0.92062	-1.42729
H	-7.82962	0.54691	-2.11733
H	-6.42407	0.73609	-3.17991
H	-6.88417	-1.66092	-4.16684
H	-7.06505	-3.03228	-3.05296
H	-8.31185	-1.75948	-3.10958
H	5.80371	4.42239	2.40192
H	8.23808	3.49118	0.76931
H	8.00024	3.22900	2.50949
H	8.19229	4.88202	1.87237
H	6.30803	4.60995	-0.62621
H	4.79803	5.05218	0.18954
H	6.29203	5.96657	0.51826
H	1.65056	-5.52185	-0.53381
H	5.17359	-4.49131	2.84699
H	2.54048	-7.31191	0.91050
H	4.32013	-6.81475	2.59707
N	-2.05080	2.17726	-0.91356
C	0.16317	3.92416	-1.24338
C	-1.14243	4.39725	-1.46923
C	-1.37583	5.74107	-1.81995
C	-0.29181	6.61993	-1.94255
C	1.03012	6.14945	-1.74133
C	1.25091	4.79583	-1.39258
C	-2.32824	3.52128	-1.31548
C	-1.99719	2.04558	1.04231
C	-3.19149	1.23510	-0.73731
C	-3.36637	1.39908	0.78482
C	-4.92240	-0.22658	1.56500
C	-5.77486	0.70744	2.39472
C	-5.47702	0.91002	3.75442
C	-6.85615	1.39727	1.82297
C	-6.24642	1.78591	4.52625
C	-7.63312	2.27278	2.59529
C	-7.32762	2.46946	3.94789
C	-1.70932	8.46510	-2.47700

C	2.60512	7.56528	-0.70820
C	2.80626	3.02555	-0.99899
O	-3.49382	3.89691	-1.42947
O	-3.54088	0.18240	1.48397
O	-0.39408	7.94576	-2.25386
O	2.08893	7.00026	-1.93077
O	2.55057	4.42524	-1.23002
H	0.34598	2.89226	-0.97362
H	-2.40045	6.06385	-1.97177
H	-2.84385	0.22774	-0.97970
H	-4.03971	1.51265	-1.36447
H	-4.16439	2.11193	1.03371
H	-1.18463	1.73306	-1.29004
H	-1.08810	1.45492	1.04800
H	-1.90808	3.09850	1.28634
H	-4.87449	-1.22175	2.02101
H	-5.34445	-0.33905	0.55562
H	-4.63321	0.38431	4.19754
H	-7.09246	1.24577	0.76923
H	-6.00501	1.93669	5.57833
H	-8.46922	2.80298	2.13962
H	-7.92700	3.15215	4.54997
H	-1.57143	9.52492	-2.71018
H	-2.33847	8.36327	-1.57988
H	-2.19993	7.96202	-3.32359
H	2.93015	6.77698	-0.01554
H	1.84561	8.19634	-0.22339
H	3.46517	8.17881	-0.99619
H	2.41738	2.70306	-0.02411
H	3.89083	2.91984	-1.00200
H	2.36123	2.40953	-1.79031
N	-0.62469	-0.54163	2.92074
C	0.52370	-4.07659	3.05785
C	-0.20375	-4.47898	4.19527
C	0.43080	-2.77118	2.56736
C	-1.03759	-3.58284	4.87750
C	-0.40589	-1.87481	3.24590
C	-1.12991	-2.27374	4.39205
C	-1.45723	0.15169	3.72440
S	-2.07308	-0.91426	5.00392
S	-1.88188	1.78351	3.61688
H	1.16781	-4.78799	2.54634
H	-0.11724	-5.50318	4.55504
H	0.97181	-2.45469	1.68196
H	-1.59715	-3.89383	5.75724
H	-0.13665	-0.11440	2.08763

TS 9 (R) *arr1*

Imaginary frequency: -453.03 cm^{-1}

C	0.37377	-4.40415	-3.23825
C	-0.00958	-3.59516	-2.15459
C	0.80439	-3.48459	-1.01387
C	2.02700	-4.16659	-0.96539
C	2.44731	-4.94750	-2.06575
C	1.60521	-5.07493	-3.19869
H	-0.29274	-4.47589	-4.09148
C	-1.29143	-2.84749	-2.26356
H	0.51862	-2.83902	-0.19515
O	-2.20592	-3.14239	-3.02998
N	-1.39646	-1.74183	-1.37766
C	-1.98693	-2.12293	0.49588
C	-2.63233	-0.91140	-1.34726
C	-3.22382	-1.36667	-0.00636
H	-3.27973	-1.14091	-2.19631
H	-2.35732	0.14416	-1.34400
H	-3.48863	-0.53851	0.66327
O	-4.34219	-2.19117	-0.26970
H	4.51299	-0.72030	3.94876
C	3.60779	-1.29116	4.12848
C	3.65234	-2.41041	4.98223
C	2.42453	-0.90683	3.49153
H	4.59184	-2.68502	5.45872
H	2.38666	-0.05647	2.81478
O	0.70280	-0.23172	-0.61848
C	2.51057	-3.18441	5.21966
C	1.27904	-1.67989	3.72940
C	1.32413	-2.81019	4.57989
N	0.01820	-1.48488	3.17400
P	0.40311	0.90783	0.32741
H	-0.51509	-1.19695	-1.20744
H	2.54489	-4.05504	5.87091
C	-0.92528	-2.39077	3.50718
S	-0.25067	-3.59726	4.61511
S	-2.53114	-2.45207	2.96650
O	-0.27692	0.63881	1.65991
H	-1.15809	-1.55440	0.89445
H	-1.93375	-3.20547	0.46871
H	-0.16335	-0.63703	2.54435
C	-5.15783	-2.49951	0.86991
H	-5.26528	-1.60968	1.51117
H	-4.67421	-3.28746	1.47374
C	-6.50968	-2.96686	0.38643
C	-6.61636	-3.80335	-0.73775
C	-7.67629	-2.57400	1.06139
C	-7.87252	-4.22865	-1.18480
H	-5.71367	-4.09496	-1.27204
C	-8.93421	-3.00470	0.61882
H	-7.60037	-1.92036	1.93148
C	-9.03522	-3.83094	-0.50833
H	-7.94505	-4.86883	-2.06397
H	-9.83259	-2.68666	1.14755
H	-10.01283	-4.16060	-0.85944
O	2.88751	-4.11732	0.09203
O	3.69070	-5.52791	-2.08369
O	2.09203	-5.86630	-4.19830
C	2.52721	-3.25536	1.18102
H	3.34271	-3.32995	1.90152
H	1.59038	-3.58966	1.64949
H	2.42915	-2.21678	0.84196
C	3.80863	-6.71349	-1.26950
H	3.11909	-7.49369	-1.62404
H	3.60791	-6.48903	-0.21371

H	4.84222	-7.05606	-1.38504
C	1.29379	-5.99316	-5.38035
H	0.31757	-6.44994	-5.15865
H	1.86102	-6.64708	-6.04903
H	1.13761	-5.01702	-5.86318
O	-0.47406	2.01339	-0.56430
C	-0.65464	3.30084	-0.06052
C	0.43618	4.16743	-0.00210
C	-1.97944	3.70617	0.27542
C	1.72643	3.78068	-0.63032
C	0.26105	5.44996	0.62604
C	-2.15668	4.98543	0.78216
C	-3.15720	2.82401	0.01330
C	2.31884	4.60466	-1.65418
C	2.35613	2.58630	-0.28766
C	-1.06238	5.86008	1.01739
C	1.35065	6.32479	0.90131
H	-3.16464	5.32484	1.01775
C	-3.57556	2.60138	-1.32359
C	-3.90002	2.28111	1.09143
C	1.66966	5.74933	-2.20112
C	3.60989	4.24155	-2.17823
C	3.61415	2.18974	-0.83066
O	1.77441	1.77376	0.68959
C	-1.24560	7.13615	1.62269
C	1.14116	7.55267	1.50517
H	2.35785	6.00967	0.63934
C	-4.72961	1.83584	-1.55582
C	-2.85177	3.22748	-2.51505
C	-5.05557	1.53518	0.80504
C	-3.49177	2.50393	2.54530
C	2.28349	6.52037	-3.17336
H	0.67404	6.01092	-1.85349
C	4.22165	5.06567	-3.16556
C	4.23215	3.04748	-1.72676
C	4.24691	0.89360	-0.43848
C	-0.16779	7.96987	1.85995
H	-2.25462	7.43731	1.90593
H	1.99017	8.20267	1.71518
C	-5.49001	1.29741	-0.50780
H	-5.05062	1.67261	-2.58347
H	-1.99773	3.79972	-2.13373
H	-5.64161	1.12703	1.63004
H	-2.51206	2.99718	2.54399
C	3.57719	6.18862	-3.65110
H	1.76361	7.38724	-3.58047
H	5.20432	4.78114	-3.54301
H	5.21108	2.78199	-2.12290
C	4.14903	-0.22824	-1.30040
C	4.96579	0.80970	0.77662
H	-0.31884	8.94158	2.32916
C	-6.79202	0.54736	-0.75396
H	4.05142	6.80879	-4.41115
C	4.73984	-1.43298	-0.89345
C	3.51581	-0.11043	-2.68544
C	5.55989	-0.41391	1.13021
C	5.21686	2.06934	1.60482
H	-6.96548	-0.09465	0.12193
C	5.44504	-1.55040	0.31585
H	4.65718	-2.31185	-1.53231
H	2.86621	0.77432	-2.67871
H	6.13816	-0.47147	2.05043
H	4.45932	2.81125	1.32085
C	6.12364	-2.87771	0.63937
H	5.44042	-3.66991	0.29700
C	4.62102	0.11787	-3.74036
H	5.22597	1.00413	-3.51307
H	5.29632	-0.74901	-3.77723
H	4.17986	0.24998	-4.73859
C	2.64643	-1.31197	-3.08286
H	2.16305	-1.11706	-4.05052
H	3.23573	-2.23178	-3.19331
H	1.87084	-1.48574	-2.33564
C	5.10379	1.87509	3.12424
H	4.10749	1.51582	3.40735
H	5.85294	1.16772	3.50658
H	5.27225	2.83168	3.63752
C	6.59403	2.65770	1.22841
H	7.39698	1.94938	1.47758
H	6.64921	2.86584	0.15215
H	6.78055	3.59485	1.77197
C	7.43014	-3.00887	-0.17471
H	8.14254	-2.22356	0.11686
H	7.90415	-3.98523	0.00068
H	7.23706	-2.90722	-1.25037
C	6.39931	-3.10161	2.13408
H	5.49408	-2.97113	2.74013
H	6.77898	-4.11884	2.29965
H	7.16008	-2.40390	2.51250
C	-3.77196	4.22936	-3.24257
H	-4.64237	3.72510	-3.68446
H	-4.14265	4.99475	-2.54750
H	-3.22631	4.73300	-4.05273
C	-2.29251	2.17026	-3.48668
H	-1.55292	1.53368	-2.98718
H	-3.08966	1.52906	-3.88779
H	-1.79766	2.66088	-4.33642
C	-4.48979	3.43785	3.25942
H	-4.57764	4.40208	2.74164
H	-5.49120	2.98613	3.29687
H	-4.16640	3.63048	4.29200
C	-3.32740	1.17902	3.30987
H	-2.98295	1.37196	4.33572
H	-4.27327	0.62426	3.37746
H	-2.58953	0.53905	2.81694
C	-7.96600	1.54704	-0.83281
H	-7.84130	2.21821	-1.69474
H	-8.92098	1.01480	-0.94748
H	-8.02027	2.16689	0.07228
C	-6.76197	-0.36536	-1.98984
H	-6.69580	0.21601	-2.92032
H	-5.91425	-1.05663	-1.94148

H	-7.68191	-0.96251	-2.03516

TS 9 (R) *arr3*

Imaginary frequency: -434.93 cm^{-1}

C	-2.32550	5.66096	-1.64766
C	-1.76625	4.59325	-0.92206
C	-2.58194	3.73767	-0.16148
C	-3.96159	3.96862	-0.09601
C	-4.54822	4.99780	-0.87226
C	-3.71365	5.84519	-1.64986
H	-1.66037	6.30678	-2.21117
C	-0.29291	4.44507	-0.92833
H	-2.15069	2.91229	0.38828
O	0.49031	5.33094	-1.26657
N	0.18837	3.17698	-0.47691
C	0.27480	2.71282	1.47401
C	1.66276	2.97898	-0.34672
C	1.75616	2.90755	1.18865
H	2.19258	3.82617	-0.78488
H	1.95456	2.04833	-0.83170
H	2.37908	2.08298	1.54999
O	2.12400	4.14197	1.80386
H	2.17705	-4.88668	1.47368
C	2.03780	-4.12788	2.24157
C	2.29846	-4.43549	3.59198
C	1.59538	-2.85608	1.86686
H	2.64020	-5.43401	3.86044
H	1.38051	-2.60465	0.83353
O	-1.12897	0.78346	-1.20160
C	2.12990	-3.47810	4.60238
C	1.42117	-1.90076	2.87810
C	1.69187	-2.20198	4.23037
N	0.97610	-0.59541	2.70519
P	-0.15224	-0.28634	-0.77806
H	-0.33616	2.35796	-0.85722
H	2.33462	-3.71925	5.64332
C	0.89909	0.17047	3.80804
S	1.38273	-0.77989	5.23229
S	0.43022	1.79810	3.91950
O	0.93648	0.06121	0.22492
H	-0.29859	3.52323	1.91359
H	-0.19575	1.75819	1.29895
H	0.82879	-0.24154	1.70751
C	3.50826	4.46965	1.66413
H	3.58575	5.49434	2.05414
H	3.79775	4.50764	0.60020
C	4.45074	3.54821	2.41963
C	5.76675	3.36057	1.96455
C	4.03742	2.90291	3.59663
C	6.65663	2.54197	2.67312
H	6.09937	3.85766	1.05230
C	4.92079	2.07328	4.29821
H	3.01478	3.03542	3.94429
C	6.23355	1.89198	3.84102
H	7.67320	2.40204	2.30585
H	4.57975	1.56437	5.19976
H	6.91936	1.24266	4.38456
O	-4.80850	3.26790	0.71553
O	-5.88723	5.26986	-0.85048
O	-4.36700	6.81515	-2.35330
C	-4.21027	2.36874	1.66156
H	-5.03612	2.00771	2.27644
H	-3.47681	2.89441	2.29107
H	-3.73524	1.51455	1.16293
C	-6.76682	4.19568	-1.24943
H	-7.74944	4.65796	-1.38916
H	-6.82158	3.41663	-0.48037
H	-6.42774	3.75391	-2.19708
C	-3.56533	7.71183	-3.12952
H	-2.86835	8.27855	-2.49418
H	-4.27070	8.39986	-3.60454
H	-2.99659	7.17417	-3.90315
O	0.52774	-0.90545	-2.15319
C	1.37102	-2.00484	-1.99497
C	0.78399	-3.25219	-1.80090
C	2.78170	-1.79585	-2.05343
C	-0.69628	-3.38941	-1.78610
C	1.63976	-4.38262	-1.55019
C	3.58987	-2.92092	-1.95714
C	3.36855	-0.42305	-2.10584
C	-1.35884	-4.33737	-2.64310
C	-1.47402	-2.61492	-0.92335
C	3.06417	-4.20899	-1.66913
C	1.14451	-5.65156	-1.13378
H	4.66955	-2.80368	-2.03351
C	3.12261	0.43672	-3.20617
C	4.17529	0.02882	-1.02208
C	-0.67930	-5.04553	-3.67582
C	-2.77052	-4.56514	-2.47503
C	-2.86234	-2.85437	-0.71617
O	-0.87854	-1.63912	-0.12998
C	3.92343	-5.31927	-1.42800
C	2.00838	-6.70535	-0.88588
H	0.07446	-5.78152	-0.99532
C	3.67775	1.72669	-3.20591
C	2.33026	-0.00988	-4.43142
C	4.70022	1.32941	-1.07062
C	4.50502	-0.83721	0.19392
C	-1.35028	-5.95350	-4.47675
H	0.37861	-4.85509	-3.83849
C	-3.42856	-5.51535	-3.30714
C	-3.47522	-3.83679	-1.48066
C	-3.64538	-2.12545	0.32707
C	3.40913	-6.54526	-1.04638
H	4.99952	-5.17466	-1.52766
H	1.60845	-7.66424	-0.55753
C	4.46379	2.19707	-2.14734
H	3.48754	2.37447	-4.05935
H	1.91830	-1.00536	-4.23036
H	5.30463	1.68447	-0.23601
H	3.89928	-1.74794	0.14292
C	-2.73416	-6.20177	-4.28646

H	-0.81159	-6.47719	-5.26603
H	-4.49628	-5.68196	-3.16164
H	-4.53321	-4.04352	-1.32178
C	-4.65330	-1.21062	-0.05925
C	-3.43962	-2.43066	1.69912
H	4.07687	-7.38420	-0.85323
C	5.10307	3.58021	-2.15405
H	-3.24845	-6.92300	-4.92084
C	-5.48163	-0.66199	0.93494
C	-4.85400	-0.79124	-1.51376
C	-4.28978	-1.85179	2.65124
C	-2.37160	-3.43223	2.13734
H	5.15261	3.91181	-1.10447
C	-5.32580	-0.97580	2.29040
H	-6.26394	0.04106	0.64524
H	-4.09432	-1.30296	-2.11775
H	-4.15022	-2.10076	3.70106
H	-1.55135	-3.39169	1.41193
C	-6.28845	-0.41597	3.32969
H	-6.81264	0.43389	2.86284
C	4.15811	-0.14335	1.52047
H	4.77578	0.74230	1.69775
H	3.10965	0.16002	1.51834
H	4.31354	-0.83147	2.36256
C	5.98995	-1.25561	0.18114
H	6.20573	-1.92960	1.02226
H	6.26133	-1.76984	-0.75041
H	6.64118	-0.37542	0.27774
C	1.14680	0.93079	-4.72973
H	0.49639	1.02866	-3.85334
H	1.49413	1.93262	-5.01865
H	0.54836	0.53539	-5.56237
C	3.26133	-0.14818	-5.65426
H	4.07995	-0.85059	-5.44653
H	2.70142	-0.51773	-6.52494
H	3.70754	0.81908	-5.92444
C	4.31159	4.63921	-2.93907
H	3.26402	4.69491	-2.61575
H	4.76567	5.62894	-2.79696
H	4.32134	4.42828	-4.01735
C	6.55522	3.48605	-2.67070
H	7.13999	2.77407	-2.07350
H	6.56532	3.14023	-3.71413
H	7.05128	4.46605	-2.62831
C	-2.93892	-4.86720	2.10931
H	-3.31178	-5.12433	1.10968
H	-2.16243	-5.59485	2.38576
H	-3.77141	-4.96517	2.82068
C	-1.75700	-3.11251	3.51100
H	-1.43348	-2.06551	3.56527
H	-2.46516	-3.29316	4.33157
H	-0.88117	-3.74997	3.68535
C	-6.23567	-1.22778	-2.03903
H	-6.37561	-2.31241	-1.93663
H	-7.04578	-0.73145	-1.48635
H	-6.34381	-0.96567	-3.10081
C	-4.63527	0.72381	-1.69802
H	-4.77927	1.00205	-2.75200
H	-5.34218	1.30942	-1.09706
H	-3.61677	1.00599	-1.40825
C	-5.58204	0.10283	4.59620
H	-5.12267	-0.71854	5.16265
H	-4.78969	0.82242	4.35218
H	-6.30394	0.59673	5.26061
C	-7.35379	-1.47280	3.69228
H	-8.08398	-1.06546	4.40583
H	-7.89286	-1.80991	2.79720
H	-6.87960	-2.35155	4.15187

TS 9 (R) *arr4*

Imaginary frequency: -434.41 cm^{-1}

C	1.33933	5.66119	-1.25916
C	1.26791	4.32447	-0.82678
C	0.13603	3.85200	-0.14088
C	-0.91309	4.72542	0.16360
C	-0.86885	6.06600	-0.28720
C	0.25832	6.52167	-1.01972
H	2.23550	5.99313	-1.77276
C	2.46215	3.46254	-0.99651
H	0.06563	2.81758	0.15992
O	3.58079	3.88375	-1.29509
N	2.25827	2.09255	-0.66620
C	2.18947	1.71548	1.29696
C	3.41362	1.15512	-0.60039
C	3.37079	0.80985	0.90905
H	4.32507	1.66952	-0.91166
H	3.24029	0.28886	-1.24347
H	3.09155	-0.23313	1.05417
O	4.55195	0.98812	1.66155
H	-2.74413	-4.35854	2.55008
C	-2.24253	-3.62221	3.17525
C	-2.46479	-3.60923	4.56655
C	-1.37700	-2.70299	2.57579
H	-3.14710	-4.33294	5.00991
H	-1.20242	-2.69478	1.50471
O	-0.06170	0.78418	-1.49436
C	-1.81533	-2.68576	5.39796
C	-0.73595	-1.77264	3.40565
C	-0.93972	-1.77030	4.80317
N	0.15970	-0.79098	2.99930
P	-0.16557	-0.50178	-0.71144
H	1.37370	1.66610	-1.03057
H	-1.98108	-2.68531	6.47322
C	0.72310	-0.04699	3.96835
S	0.05323	-0.51358	5.54971
S	1.94343	1.12255	3.81088
O	0.72762	-0.71461	0.49802
H	2.33690	2.72551	1.66782
H	1.18403	1.32479	1.26108
H	0.40588	-0.70248	1.96137
C	5.21166	2.27247	1.55847
H	5.36548	2.61716	2.59162

H	4.58215	3.01482	1.05058
C	6.53811	2.14512	0.84122
C	6.81619	2.90312	-0.30754
C	7.51223	1.25372	1.32730
C	8.05311	2.77886	-0.95666
H	6.05794	3.58123	-0.69800
C	8.74237	1.12163	0.67486
H	7.29396	0.65454	2.21118
C	9.01745	1.88819	-0.46840
H	8.25762	3.37069	-1.84871
H	9.48783	0.42467	1.05730
H	9.97689	1.78769	-0.97542
O	-1.99351	4.36808	0.91158
O	-1.86412	6.95468	0.02267
O	0.19638	7.82294	-1.42618
C	-1.98551	3.04649	1.47930
H	-2.88536	2.98788	2.09096
H	-1.09263	2.89702	2.10462
H	-2.03609	2.27795	0.69770
C	-3.10044	6.73142	-0.68927
H	-3.48511	5.72337	-0.49884
H	-2.95184	6.87854	-1.76934
H	-3.80698	7.47618	-0.30867
C	1.32057	8.33744	-2.14827
H	2.23525	8.31064	-1.53736
H	1.06801	9.37521	-2.38434
H	1.48903	7.77702	-3.08018
O	0.05699	-1.75083	-1.77158
C	-0.10659	-3.03261	-1.24414
C	-1.40770	-3.49496	-1.08103
C	1.05396	-3.79916	-0.91875
C	-2.55240	-2.64238	-1.49422
C	-1.61159	-4.78302	-0.47252
C	0.84057	-5.09071	-0.45677
C	2.42008	-3.20065	-1.00620
C	-3.53624	-3.14688	-2.41585
C	-2.69701	-1.34360	-0.99692
C	-0.45981	-5.59811	-0.18886
C	-2.89672	-5.26970	-0.09784
H	1.69779	-5.72472	-0.24188
C	2.92659	-2.74725	-2.24937
C	3.20060	-3.03765	0.17619
C	-3.37716	-4.37979	-3.11285
C	-4.71787	-2.36807	-2.67282
C	-3.87630	-0.57530	-1.21707
O	-1.72129	-0.79560	-0.16587
C	-0.64441	-6.88085	0.40226
C	-3.04019	-6.51427	0.49315
H	-3.76951	-4.64573	-0.27192
C	4.18029	-2.11407	-2.29149
C	2.18946	-2.97872	-3.56565
C	4.43893	-2.38885	0.07734
C	2.75856	-3.56331	1.54276
C	-4.34975	-4.83345	-3.98695
H	-2.47084	-4.96031	-2.96086
C	-5.70702	-2.86897	-3.56671
C	-4.86701	-1.11410	-2.02672
C	-4.15427	0.74705	-0.57245
C	-1.90797	-7.33404	0.73558
H	0.23611	-7.49086	0.60576
H	-4.03177	-6.86438	0.77876
C	4.94468	-1.90126	-1.13866
H	4.55569	-1.76988	-3.25261
H	1.19891	-3.38953	-3.33852
H	5.02566	-2.22875	0.98150
H	1.67996	-3.75711	1.49976
C	-5.53196	-4.08082	-4.20922
H	-4.20224	-5.77488	-4.51548
H	-6.60051	-2.26917	-3.74244
H	-5.78361	-0.54527	-2.17949
C	-4.12498	1.92513	-1.35477
C	-4.64421	0.78460	0.75719
H	-2.03573	-8.31301	1.19627
C	6.28277	-1.17218	-1.14812
H	-6.29150	-4.45334	-4.89580
C	-4.68269	3.10013	-0.82397
C	-3.51721	1.94186	-2.75422
C	-5.19571	1.98094	1.23947
C	-4.61136	-0.44667	1.65835
H	6.25934	-0.46806	-0.30340
C	-5.25012	3.14472	0.45559
H	-4.69319	4.00269	-1.43539
H	-3.05087	0.96253	-2.92477
H	-5.60159	2.00238	2.25086
H	-4.03490	-1.22736	1.14775
C	-5.90497	4.41761	0.97607
H	-5.83714	5.16774	0.17239
C	2.99599	-2.57210	2.69655
H	2.53021	-2.95153	3.61643
H	4.06428	-2.42817	2.90508
H	2.56211	-1.59368	2.48148
C	3.47727	-4.89346	1.86054
H	3.11193	-5.31413	2.80809
H	3.33103	-5.64247	1.07271
H	4.55930	-4.72503	1.95650
C	2.92953	-4.03561	-4.41246
H	3.93630	-3.68908	-4.68468
H	3.03591	-4.97797	-3.85814
H	2.37865	-4.24089	-5.34126
C	1.97915	-1.67345	-4.35686
H	1.47060	-0.92305	-3.74123
H	2.93470	-1.25298	-4.70006
H	1.36468	-1.86525	-5.24762
C	6.54651	-0.35621	-2.42142
H	7.46419	0.23074	-2.30085
H	6.67383	-1.00802	-3.29792
H	5.72601	0.34157	-2.63395
C	7.44388	-2.15577	-0.88909
H	8.39547	-1.61194	-0.81468
H	7.29454	-2.71494	0.04373
H	7.52262	-2.88297	-1.71017
C	-3.89039	-0.15464	2.98846

H	-2.87729	0.22425	2.80481
H	-4.43088	0.59134	3.58724
H	-3.80473	-1.07079	3.58641
C	-6.02770	-1.00730	1.89110
H	-6.66408	-0.27296	2.40471
H	-6.50700	-1.26137	0.93606
H	-5.98705	-1.91490	2.51001
C	-4.59853	2.14052	-3.83449
H	-4.14973	2.12161	-4.83748
H	-5.35950	1.35064	-3.78421
H	-5.10685	3.10713	-3.70965
C	-2.40324	3.00069	-2.87384
H	-1.95638	2.96516	-3.87738
H	-2.78965	4.01710	-2.71661
H	-1.61038	2.81348	-2.14244
C	-7.40054	4.19148	1.27592
H	-7.92690	3.80746	0.39199
H	-7.53289	3.46407	2.08895
H	-7.88024	5.13080	1.58469
C	-5.17145	4.98703	2.20684
H	-5.65016	5.91785	2.54226
H	-5.20311	4.27624	3.04493
H	-4.12107	5.19979	1.97689

TS 9 (R) *arr5*

Imaginary frequency: -460.89 cm^{-1}

C	2.30310	-5.03582	-1.44067
C	1.51170	-3.91576	-1.12725
C	1.94453	-2.97076	-0.17964
C	3.18831	-3.13376	0.44487
C	4.00391	-4.24764	0.12619
C	3.54407	-5.20430	-0.81531
H	1.91998	-5.75278	-2.15905
C	0.19786	-3.80251	-1.80296
H	1.35650	-2.08734	0.03284
O	-0.31072	-4.69838	-2.47950
N	-0.51865	-2.60108	-1.54185
C	-1.53929	-2.67167	0.13453
C	-1.86246	-2.40347	-2.14127
C	-2.67993	-2.30743	-0.83244
H	-2.10914	-3.26859	-2.75789
H	-1.88041	-1.50058	-2.75493
H	-3.02030	-1.28785	-0.62260
O	-3.84196	-3.10814	-0.70724
H	2.34431	0.82515	5.74608
C	1.54472	0.09158	5.65723
C	1.17032	-0.67369	6.77921
C	0.90107	-0.06883	4.42726
H	1.68866	-0.53132	7.72603
H	1.15920	0.52753	3.55693
O	0.52904	-0.15865	-1.20589
C	0.13305	-1.61260	6.70266
C	-0.12389	-1.02113	4.34580
C	-0.51330	-1.77825	5.47251
N	-0.88783	-1.31555	3.22209
P	0.05949	0.80983	-0.14358
H	0.02179	-1.70454	-1.44298
H	-0.16252	-2.19449	7.57302
C	-1.86822	-2.22991	3.37785
S	-1.85345	-2.84468	5.04276
S	-2.98175	-2.73636	2.20930
O	-0.32734	0.31704	1.23357
H	-1.32107	-3.70314	0.38895
H	-0.97421	-1.89062	0.62671
H	-0.76382	-0.74775	2.34713
C	-3.79022	-4.43541	-1.25116
H	-4.48351	-5.01803	-0.62826
H	-2.79129	-4.88377	-1.13706
C	-4.22282	-4.48111	-2.70611
C	-5.14293	-3.54429	-3.20641
C	-3.71487	-5.47072	-3.56398
C	-5.55005	-3.59872	-4.54511
H	-5.52341	-2.76864	-2.54428
C	-4.12742	-5.52921	-4.90156
H	-2.97885	-6.18180	-3.18828
C	-5.04599	-4.59283	-5.39589
H	-6.25968	-2.86340	-4.92463
H	-3.72130	-6.29700	-5.55998
H	-5.36067	-4.63275	-6.43850
O	3.69116	-2.27512	1.36985
O	5.19405	-4.38703	0.78754
O	4.38026	-6.26499	-1.02989
C	2.94944	-1.07046	1.61631
H	3.52905	-0.51990	2.35915
H	1.95088	-1.29670	2.01183
H	2.86208	-0.46896	0.70386
C	6.37736	-4.32178	-0.03748
H	6.48530	-5.22373	-0.65145
H	7.21815	-4.23249	0.65752
H	6.34109	-3.43481	-0.68500
C	3.97222	-7.24289	-1.99358
H	3.03329	-7.73070	-1.69308
H	4.77768	-7.98227	-2.02041
H	3.84761	-6.79406	-2.99011
O	-1.17641	1.67048	-0.85288
C	-1.48758	2.97218	-0.47346
C	-0.59393	4.00237	-0.76642
C	-2.76704	3.20398	0.11568
C	0.68997	3.72729	-1.46462
C	-0.92232	5.34099	-0.34396
C	-3.12327	4.51338	0.40144
C	-3.68473	2.07562	0.45674
C	1.05954	4.44672	-2.65574
C	1.58135	2.78313	-0.95620
C	-2.22525	5.59659	0.21324
C	-0.00238	6.42656	-0.42409
H	-4.10653	4.71043	0.82814
C	-4.37789	1.38084	-0.56216
C	-3.88430	1.72698	1.81880
C	0.15064	5.28572	-3.36204
C	2.39281	4.29299	-3.17664
C	2.91341	2.63299	-1.44150

O	1.18838	1.99980	0.12985
C	-2.57384	6.92213	0.60086
C	-0.36542	7.70070	-0.02254
H	1.00148	6.24334	-0.79760
C	-5.24435	0.33134	-0.20778
C	-4.27735	1.80178	-2.02626
C	-4.74943	0.66598	2.11816
C	-3.24098	2.50262	2.96815
C	0.54753	5.96427	-4.50144
H	-0.87024	5.37918	-3.00033
C	2.77475	5.01851	-4.34137
C	3.29786	3.41809	-2.51938
C	3.90244	1.71688	-0.79428
C	-1.66663	7.95864	0.48006
H	-3.56875	7.09808	1.01118
H	0.35899	8.51224	-0.08722
C	-5.44787	-0.04208	1.12742
H	-5.78218	-0.19011	-0.99722
H	-3.60083	2.66446	-2.08111
H	-4.89993	0.38563	3.16159
H	-2.59875	3.27874	2.53632
C	1.87369	5.84240	-4.99089
H	-0.16750	6.59335	-5.03101
H	3.79099	4.89888	-4.71822
H	4.32072	3.34462	-2.88655
C	4.39809	0.59104	-1.50034
C	4.42013	2.03281	0.48936
H	-1.94127	8.96791	0.78530
C	-6.44613	-1.11389	1.55341
H	2.17439	6.38766	-5.88503
C	5.42521	-0.17227	-0.91885
C	3.87706	0.19977	-2.88201
C	5.44453	1.23818	1.02260
C	3.92915	3.23312	1.29537
H	-5.94856	-1.71471	2.33224
C	5.97567	0.14012	0.32992
H	5.82154	-1.02776	-1.46704
H	3.02235	0.84695	-3.11274
H	5.85221	1.49521	2.00024
H	3.17146	3.75863	0.70217
C	7.14868	-0.65099	0.89266
H	7.36979	-1.45606	0.17527
C	4.95190	0.43428	-3.96303
H	5.29744	1.47649	-3.96732
H	5.82806	-0.20700	-3.79173
H	4.55230	0.20112	-4.96003
C	3.36254	-1.25073	-2.91908
H	2.97769	-1.48996	-3.92074
H	4.15267	-1.97671	-2.68266
H	2.55288	-1.38210	-2.19746
C	5.06772	4.23873	1.55853
H	5.85818	3.79844	2.18183
H	5.52559	4.56578	0.61533
H	4.68282	5.12556	2.08128
C	3.25325	2.78647	2.60731
H	2.40702	2.12615	2.38776
H	3.95907	2.24994	3.25738
H	2.87656	3.65649	3.16328
C	6.82127	-1.30852	2.24687
H	7.68712	-1.87821	2.61394
H	6.58051	-0.54830	3.00379
H	5.96714	-1.98695	2.15309
C	8.40644	0.23685	0.99308
H	9.27046	-0.35168	1.33263
H	8.65262	0.68567	0.02142
H	8.25265	1.05412	1.71163
C	-3.67696	0.69564	-2.91228
H	-3.63094	1.02195	-3.96072
H	-2.65855	0.46820	-2.57955
H	-4.27716	-0.22436	-2.87325
C	-5.64802	2.26753	-2.55861
H	-5.55277	2.64521	-3.58635
H	-6.37402	1.44280	-2.56938
H	-6.05945	3.07011	-1.93188
C	-4.31914	3.21652	3.80883
H	-3.85217	3.83138	4.59116
H	-4.94151	3.86988	3.18244
H	-4.98424	2.49263	4.30004
C	-2.33701	1.61819	3.84269
H	-1.92214	2.19874	4.67864
H	-2.88224	0.76288	4.26512
H	-1.50629	1.23760	3.24317
C	-7.68504	-0.44839	2.19406
H	-8.20750	0.17376	1.45298
H	-8.38931	-1.20881	2.56034
H	-7.40531	0.19689	3.03689
C	-6.87118	-2.06860	0.42898
H	-7.45681	-1.54381	-0.34022
H	-5.99887	-2.52645	-0.04922
H	-7.50875	-2.86572	0.83492

TS 9 (R) *arr6*

Imaginary frequency: -470.35 cm^{-1}

C	-4.18059	-0.82099	1.77358
C	-4.35963	-1.74783	0.73471
C	-5.49719	-1.72257	-0.08933
C	-6.44041	-0.69887	0.08497
C	-6.27852	0.24126	1.13111
C	-5.17234	0.14428	2.00585
H	-3.29571	-0.86916	2.39860
C	-3.36047	-2.82852	0.52518
H	-5.60495	-2.47566	-0.86267
O	-3.63925	-4.00230	0.31121
N	-2.00462	-2.38460	0.50517
C	-1.26002	-2.56324	-1.29043
C	-0.88887	-3.33737	0.81876
C	-0.39427	-3.63344	-0.60248
H	-1.28203	-4.23335	1.30604
H	-0.15442	-2.82414	1.44230
H	0.67664	-3.45661	-0.74819
O	-0.74899	-4.96580	-0.93139
H	5.83628	0.49008	-0.51946

C	5.28810	0.00235	-1.32170
C	5.92981	-0.25977	-2.54782
C	3.94893	-0.34344	-1.12081
H	6.97362	0.02176	-2.67891
H	3.42842	-0.13376	-0.19199
O	-1.37170	0.37890	0.63931
C	5.24708	-0.86707	-3.61033
C	3.26961	-0.96362	-2.17751
C	3.90607	-1.21512	-3.41301
N	1.93919	-1.37103	-2.17204
P	0.11771	0.46324	0.42397
H	-1.83690	-1.38038	0.72836
H	5.74100	-1.05773	-4.56085
C	1.46947	-1.90365	-3.31748
S	2.76250	-1.95643	-4.53230
S	-0.09630	-2.44666	-3.65502
O	0.88473	-0.82718	0.16740
H	-2.13701	-2.87076	-1.85201
H	-0.95635	-1.52840	-1.33637
H	1.36330	-1.17082	-1.30180
C	-0.01941	-5.56858	-2.01946
H	-0.21635	-5.04082	-2.96286
H	-0.45218	-6.57561	-2.09020
C	1.47234	-5.64667	-1.76916
C	1.96448	-6.22562	-0.58529
C	2.38357	-5.14424	-2.71100
C	3.34159	-6.30646	-0.35513
H	1.25922	-6.60144	0.15607
C	3.76406	-5.21139	-2.47778
H	2.00732	-4.69646	-3.62879
C	4.24562	-5.79504	-1.29931
H	3.71271	-6.75658	0.56546
H	4.45716	-4.80119	-3.21189
H	5.31796	-5.84788	-1.11236
O	-7.54791	-0.51818	-0.69341
O	-7.17344	1.27323	1.27116
O	-5.15149	1.04343	3.02964
C	-7.76965	-1.46020	-1.74989
H	-8.69658	-1.14280	-2.23597
H	-7.88883	-2.48108	-1.35764
H	-6.94713	-1.44222	-2.47912
C	-8.29151	0.95901	2.12577
H	-8.86907	0.11681	1.71808
H	-8.91774	1.85702	2.15038
H	-7.94944	0.71893	3.14267
C	-4.02955	0.99258	3.92133
H	-3.98664	0.02847	4.45045
H	-4.18849	1.80098	4.64030
H	-3.08837	1.15980	3.38386
O	0.73682	1.31933	1.70278
C	2.11323	1.51692	1.71426
C	2.66168	2.49034	0.88215
C	2.87658	0.70948	2.61305
C	1.76217	3.37116	0.08647
C	4.09778	2.60081	0.83849
C	4.24517	0.92279	2.65683
C	2.16020	-0.35518	3.37807
C	1.87223	4.80886	0.16665
C	0.73595	2.83471	-0.69546
C	4.88658	1.82992	1.76684
C	4.77657	3.40168	-0.12258
H	4.85644	0.34700	3.35078
C	1.13698	0.00532	4.29500
C	2.39156	-1.72197	3.07679
C	2.75594	5.46940	1.06886
C	1.03105	5.62553	-0.67188
C	-0.16778	3.63999	-1.45517
O	0.59515	1.45824	-0.82580
C	6.30594	1.95072	1.73828
C	6.15870	3.47896	-0.13933
H	4.19087	3.94667	-0.85843
C	0.31485	-0.99505	4.82721
C	0.95312	1.44592	4.76516
C	1.53748	-2.68776	3.63885
C	3.53883	-2.18629	2.18471
C	2.85211	6.85041	1.09602
H	3.35654	4.87575	1.75214
C	1.16748	7.04246	-0.63288
C	0.03311	5.00831	-1.47446
C	-1.33076	2.96450	-2.10903
C	6.93279	2.76178	0.80830
H	6.89068	1.37099	2.45305
H	6.65603	4.08976	-0.89205
C	0.47255	-2.34607	4.48151
H	-0.47633	-0.71193	5.52096
H	1.58541	2.09073	4.14212
H	1.69459	-3.73903	3.39478
H	3.96211	-1.30574	1.69058
C	2.06641	7.64786	0.22606
H	3.53320	7.32827	1.79983
H	0.53030	7.64213	-1.28365
H	-0.62119	5.63513	-2.07921
C	-2.54017	2.85101	-1.37931
C	-1.18724	2.34052	-3.36836
H	8.01957	2.83687	0.79067
C	-0.48357	-3.40690	5.00803
H	2.15720	8.73334	0.25163
C	-3.56433	2.04768	-1.90305
C	-2.74571	3.62772	-0.08153
C	-2.23181	1.53303	-3.84450
C	0.07165	2.54630	-4.20609
H	-0.19051	-4.36602	4.55230
C	-3.41714	1.35521	-3.11334
H	-4.49050	1.92855	-1.34115
H	-1.75503	3.79887	0.36146
H	-2.10851	1.02034	-4.79846
H	0.68975	3.29292	-3.68866
C	-4.50441	0.39939	-3.58634
H	-5.37042	0.53851	-2.91969
C	-3.58730	2.88235	0.96187
H	-3.56744	3.42773	1.91521
H	-4.64032	2.79623	0.66443

H	-3.18487	1.87800	1.11844
C	-3.36498	5.00816	-0.38985
H	-2.74044	5.58703	-1.08134
H	-4.35523	4.88488	-0.85142
H	-3.48845	5.59163	0.53380
C	0.90565	1.25875	-4.31821
H	1.17904	0.89686	-3.32234
H	0.34156	0.46500	-4.82541
H	1.82744	1.43892	-4.88921
C	-0.26806	3.11779	-5.59659
H	-0.84921	4.04582	-5.51084
H	0.65223	3.33601	-6.15664
H	-0.85796	2.40473	-6.18904
C	-4.02789	-1.05967	-3.43227
H	-4.80713	-1.76951	-3.74630
H	-3.13275	-1.24416	-4.04213
H	-3.77733	-1.26417	-2.38448
C	-4.96852	0.68626	-5.02596
H	-5.30357	1.72645	-5.13212
H	-4.15754	0.51720	-5.74765
H	-5.80170	0.02450	-5.30177
C	-0.49566	1.94577	4.62143
H	-0.83728	1.83338	3.58694
H	-1.17958	1.39316	5.28078
H	-0.56107	3.00765	4.89648
C	1.45405	1.58971	6.21804
H	2.50345	1.27707	6.30414
H	1.37485	2.63344	6.55354
H	0.85966	0.96632	6.90087
C	3.09041	-3.14828	1.07489
H	2.71868	-4.09988	1.47452
H	2.29631	-2.68799	0.48235
H	3.92960	-3.38408	0.40873
C	4.65839	-2.81347	3.04157
H	5.51109	-3.10101	2.41017
H	5.01630	-2.11310	3.80852
H	4.29714	-3.71519	3.55623
C	-1.93787	-3.11330	4.58499
H	-2.60940	-3.91917	4.91142
H	-2.29691	-2.17550	5.03108
H	-2.02210	-3.01830	3.49506
C	-0.37370	-3.55932	6.53831
H	-1.03359	-4.36080	6.89872
H	0.65587	-3.79753	6.83626
H	-0.66460	-2.62909	7.04599

TS 9 (R) *arr7*

Imaginary frequency: -380.65 cm^{-1}

C	2.19289	-2.65548	0.34096
C	2.25849	-3.60857	-0.69394
C	3.37664	-4.45217	-0.82094
C	4.43451	-4.34166	0.09147
C	4.36569	-3.40489	1.15041
C	3.22588	-2.58139	1.28516
H	1.33268	-2.00901	0.44269
C	1.09020	-3.87344	-1.58383
H	3.37743	-5.19138	-1.61522
O	0.98178	-4.87091	-2.29486
N	0.03686	-2.93336	-1.45629
C	-1.01453	-3.20018	0.29199
C	-1.31227	-3.22283	-2.00816
C	-2.07203	-3.64227	-0.73022
H	-1.27542	-4.02939	-2.74600
H	-1.71279	-2.30808	-2.45456
H	-3.01754	-3.10110	-0.58572
O	-2.28438	-5.04470	-0.78142
H	-1.21671	3.78001	3.98147
C	-1.50619	2.76084	4.22429
C	-2.10080	2.47866	5.46966
C	-1.28331	1.74901	3.28611
H	-2.26508	3.28647	6.18119
H	-0.82801	1.94900	2.32002
O	0.64969	-0.29533	-1.74354
C	-2.49068	1.17704	5.81343
C	-1.67688	0.44853	3.62881
C	-2.27431	0.16165	4.87529
N	-1.55560	-0.68181	2.82646
P	0.07246	0.53474	-0.62803
H	0.32587	-1.92478	-1.50902
H	-2.95163	0.96357	6.77546
C	-2.03121	-1.83360	3.33263
S	-2.65993	-1.56009	4.97010
S	-2.12285	-3.36018	2.59466
O	-0.80131	-0.14356	0.41108
H	-0.32715	-3.91467	0.72938
H	-0.90897	-2.14247	0.50038
H	-1.20154	-0.55263	1.83813
C	-3.27436	-5.55593	0.13136
H	-2.95726	-5.42422	1.17674
H	-3.28812	-6.63379	-0.07826
C	-4.64988	-4.95520	-0.07723
C	-5.22499	-4.95034	-1.36124
C	-5.36436	-4.39393	0.99281
C	-6.49351	-4.39875	-1.56870
H	-4.66442	-5.36835	-2.19712
C	-6.63805	-3.84403	0.78805
H	-4.91420	-4.37345	1.98479
C	-7.20413	-3.84318	-0.49325
H	-6.92614	-4.39456	-2.56823
H	-7.17985	-3.40640	1.62618
H	-8.19133	-3.41150	-0.65625
O	5.57002	-5.10295	0.06293
O	5.40237	-3.26124	2.03831
O	3.19977	-1.78678	2.39134
C	5.64892	-6.13056	-0.93201
H	5.61978	-5.70744	-1.94582
H	4.83442	-6.86045	-0.81497
H	6.61233	-6.62202	-0.76920
C	5.46833	-4.29006	3.04734
H	5.61512	-5.27887	2.59298
H	4.55236	-4.28908	3.65588
H	6.32855	-4.03993	3.67687

C	2.00729	-1.02426	2.63108
H	2.18303	-0.49645	3.57257
H	1.13690	-1.68711	2.74036
H	1.82958	-0.29513	1.83252
O	-0.72771	1.79520	-1.34756
C	-1.28594	2.75011	-0.50267
C	-0.43961	3.65021	0.13815
C	-2.70913	2.79776	-0.40886
C	0.99530	3.69669	-0.25172
C	-1.01307	4.55122	1.10124
C	-3.25760	3.73386	0.45424
C	-3.52288	1.89776	-1.28215
C	1.55695	4.91233	-0.78329
C	1.78436	2.54387	-0.22688
C	-2.44508	4.58385	1.25600
C	-0.21836	5.39064	1.93225
H	-4.33980	3.82202	0.52950
C	-3.45457	2.06122	-2.69078
C	-4.31387	0.85884	-0.72671
C	0.79106	6.09428	-1.00630
C	2.94627	4.92713	-1.15858
C	3.15295	2.53372	-0.62408
O	1.23017	1.35585	0.25243
C	-3.01763	5.47606	2.20645
C	-0.80723	6.24165	2.85323
H	0.86431	5.34814	1.83783
C	-4.15599	1.16568	-3.51084
C	-2.68652	3.20600	-3.34860
C	-4.98972	-0.01611	-1.59291
C	-4.46790	0.67733	0.78042
C	1.37837	7.23874	-1.51764
H	-0.27176	6.09030	-0.78190
C	3.52428	6.12504	-1.66809
C	3.70425	3.73261	-1.05345
C	4.00659	1.30111	-0.63098
C	-2.21891	6.29226	2.98802
H	-4.10246	5.49480	2.31378
H	-0.18110	6.87119	3.48468
C	-4.91408	0.11098	-2.98731
H	-4.10487	1.28641	-4.59373
H	-2.14382	3.75283	-2.56861
H	-5.57959	-0.82599	-1.16728
H	-3.64579	1.21427	1.27080
C	2.76007	7.26441	-1.83798
H	0.76938	8.12704	-1.68380
H	4.58132	6.11800	-1.93566
H	4.75180	3.74871	-1.35114
C	4.14491	0.56785	-1.83355
C	4.76171	0.94411	0.51774
H	-2.67016	6.96625	3.71536
C	-5.57471	-0.89596	-3.91844
H	3.20982	8.17463	-2.23333
C	5.07017	-0.48905	-1.87828
C	3.36505	0.93624	-3.09487
C	5.65795	-0.12933	0.42404
C	4.65530	1.75377	1.81172
H	-5.57325	-0.45434	-4.92774
C	5.84528	-0.84647	-0.77003
H	5.18455	-1.03792	-2.80912
H	2.45399	1.46129	-2.78083
H	6.23039	-0.42581	1.30080
H	3.60979	2.08653	1.90471
C	6.91155	-1.93579	-0.82773
H	6.78403	-2.56220	0.06686
C	5.01269	0.95376	3.07839
H	4.53721	-0.03103	3.08939
H	6.09884	0.80084	3.15407
H	4.70310	1.51373	3.97150
C	5.54757	3.01443	1.75077
H	5.25711	3.68603	0.93665
H	5.48322	3.57446	2.69491
H	6.59645	2.72279	1.59801
C	2.92308	-0.29241	-3.91165
H	3.77310	-0.76990	-4.41949
H	2.43120	-1.03121	-3.27242
H	2.21069	0.01720	-4.68855
C	4.18588	1.89237	-3.98683
H	3.62379	2.14700	-4.89691
H	4.42954	2.82537	-3.46537
H	5.12931	1.41608	-4.29055
C	8.31852	-1.30104	-0.75393
H	9.09633	-2.07810	-0.74405
H	8.49224	-0.65281	-1.62515
H	8.43420	-0.68846	0.14943
C	6.80646	-2.84802	-2.05795
H	7.51372	-3.68274	-1.96910
H	5.79614	-3.26185	-2.16447
H	7.04977	-2.30458	-2.98237
C	-1.64278	2.70356	-4.36510
H	-0.95926	1.98619	-3.89712
H	-2.12213	2.21607	-5.22544
H	-1.05221	3.54733	-4.74879
C	-3.66515	4.20829	-3.99526
H	-4.37676	4.59584	-3.25358
H	-3.11714	5.05826	-4.42587
H	-4.24253	3.73403	-4.80109
C	-5.79795	1.28880	1.27020
H	-6.64956	0.75794	0.82126
H	-5.88099	1.20644	2.36338
H	-5.88662	2.34776	0.99785
C	-4.38352	-0.79465	1.21016
H	-4.39421	-0.87195	2.30490
H	-5.22976	-1.38453	0.83886
H	-3.46314	-1.25751	0.84146
C	-4.73339	-2.18947	-3.97255
H	-4.68000	-2.65409	-2.97986
H	-5.17643	-2.91959	-4.66511
H	-3.70925	-1.97462	-4.30598
C	-7.03679	-1.19515	-3.54059
H	-7.49252	-1.87035	-4.27825
H	-7.10446	-1.68408	-2.56065
H	-7.63156	-0.27283	-3.50295

TS 9 (R) *arr8*

Imaginary frequency: -432.74 cm^{-1}

C	4.75536	-3.40364	-0.34424
C	3.43226	-2.93014	-0.27794
C	3.09361	-1.85288	0.56459
C	4.07742	-1.27582	1.37914
C	5.41700	-1.71749	1.28909
C	5.74840	-2.79290	0.43141
H	4.96687	-4.25256	-0.98585
C	2.40056	-3.70140	-1.01965
H	2.07917	-1.47971	0.61622
O	2.61087	-4.75862	-1.60839
N	1.07477	-3.19347	-0.88258
C	0.22460	-3.57435	0.87873
C	-0.11287	-3.94209	-1.36409
C	-0.95429	-3.74471	-0.08649
H	0.15506	-4.99371	-1.49771
H	-0.52299	-3.52585	-2.28727
H	-1.48361	-2.78594	-0.11535
O	-1.82573	-4.81397	0.22147
H	-1.18013	3.35657	4.02035
C	-1.16837	2.32850	4.37562
C	-1.35895	2.05570	5.74463
C	-0.97154	1.29324	3.45696
H	-1.51212	2.87950	6.44014
H	-0.82886	1.48244	2.39643
O	0.17338	-0.71805	-1.76048
C	-1.36001	0.74157	6.23402
C	-0.97522	-0.02052	3.94760
C	-1.16707	-0.29912	5.31830
N	-0.82535	-1.17593	3.19007
P	-0.35093	0.07061	-0.59025
H	0.94512	-2.17368	-1.06214
H	-1.51047	0.53708	7.29191
C	-0.90339	-2.35125	3.84441
S	-1.13011	-2.04795	5.58267
S	-0.88201	-3.90578	3.17297
O	-0.73140	-0.65945	0.67868
H	0.83618	-4.43422	1.13956
H	0.47303	-2.62230	1.31828
H	-0.77471	-1.07418	2.13939
C	-3.18423	-4.54053	-0.21390
H	-3.60412	-3.71860	0.38384
H	-3.73375	-5.46116	0.01478
C	-3.25262	-4.20156	-1.68481
C	-3.18119	-5.22186	-2.65040
C	-3.26403	-2.85992	-2.10695
C	-3.11937	-4.90902	-4.01320
H	-3.16429	-6.26329	-2.32663
C	-3.18754	-2.54461	-3.46879
H	-3.33557	-2.05889	-1.37313
C	-3.11378	-3.56718	-4.42342
H	-3.06891	-5.70739	-4.75340
H	-3.19299	-1.50298	-3.77918
H	-3.05701	-3.32118	-5.48363
O	3.83793	-0.31954	2.31716
O	6.38421	-1.07334	2.01708
O	7.06377	-3.16386	0.44589
C	2.47237	0.06907	2.53592
H	2.50379	0.80839	3.34078
H	1.87038	-0.79351	2.85579
H	2.03456	0.51982	1.63856
C	6.78777	-1.76823	3.21575
H	7.21193	-2.75229	2.97547
H	5.93297	-1.88392	3.89757
H	7.55143	-1.14008	3.68578
C	7.42686	-4.33431	-0.29724
H	6.87167	-5.21573	0.05572
H	8.49663	-4.47401	-0.11790
H	7.25113	-4.19597	-1.37291
O	0.73153	1.24898	-0.08700
C	0.86169	2.43891	-0.80070
C	-0.19545	3.34627	-0.76905
C	2.08883	2.71055	-1.47312
C	-1.41413	3.05571	0.03034
C	-0.12364	4.53705	-1.57138
C	2.16341	3.88223	-2.21432
C	3.31068	1.84806	-1.36696
C	-1.86784	3.94836	1.06019
C	-2.16336	1.91545	-0.24609
C	1.08326	4.79834	-2.31008
C	-1.21042	5.44890	-1.70771
H	3.09061	4.10790	-2.73965
C	4.25127	2.10221	-0.33100
C	3.59266	0.89016	-2.36668
C	-1.07454	5.02794	1.54220
C	-3.15662	3.71816	1.65769
C	-3.47405	1.70547	0.27853
O	-1.63733	0.97726	-1.13605
C	1.17089	5.96975	-3.11488
C	-1.09725	6.57388	-2.50648
H	-2.14162	5.24701	-1.18456
C	5.46643	1.40520	-0.34548
C	3.98763	3.16561	0.73832
C	4.83646	0.23511	-2.34749
C	2.60784	0.60741	-3.49788
C	-1.53838	5.84963	2.55623
H	-0.08902	5.18955	1.11101
C	-3.61045	4.59112	2.68678
C	-3.94714	2.63040	1.19950
C	-4.35367	0.60424	-0.22036
C	0.10484	6.84561	-3.20961
H	2.09569	6.15714	-3.66135
H	-1.94309	7.25436	-2.60149
C	5.79301	0.48736	-1.35855
H	6.18785	1.57586	0.45140
H	2.90320	3.18369	0.92646
H	5.05506	-0.48375	-3.13267
H	1.60888	0.89453	-3.14770
C	-2.81951	5.63673	3.12934
H	-0.91254	6.66356	2.92094

H	-4.58966	4.40881	3.13013
H	-4.95709	2.51774	1.58849
C	-4.81062	-0.41444	0.65403
C	-4.81070	0.64144	-1.56623
H	0.18046	7.73753	-3.83079
C	7.17949	-0.14943	-1.36653
H	-3.17292	6.29262	3.92423
C	-5.71245	-1.37356	0.16064
C	-4.39281	-0.47597	2.12146
C	-5.70167	-0.34660	-2.00865
C	-4.44330	1.77769	-2.52038
H	7.36294	-0.54085	-0.35497
C	-6.17110	-1.36184	-1.16233
H	-6.07928	-2.15102	0.83134
H	-3.54704	0.20895	2.26069
H	-6.05563	-0.30870	-3.03839
H	-3.76428	2.46161	-1.99883
C	-7.20304	-2.37688	-1.63663
H	-7.32723	-3.11396	-0.82716
C	-5.53803	-0.01162	3.04615
H	-6.39604	-0.69433	2.97037
H	-5.20288	0.00019	4.09292
H	-5.89119	0.99432	2.78866
C	-3.92378	-1.87776	2.54081
H	-3.59618	-1.86959	3.58795
H	-4.72851	-2.62033	2.46026
H	-3.08521	-2.21669	1.92474
C	-3.70421	1.27714	-3.77476
H	-2.78369	0.75232	-3.49420
H	-4.33313	0.59675	-4.36608
H	-3.43228	2.12419	-4.41998
C	-5.69558	2.59835	-2.89278
H	-6.42075	1.99099	-3.45176
H	-6.19672	2.97725	-1.99184
H	-5.41828	3.45650	-3.52096
C	-6.76407	-3.14078	-2.89990
H	-7.53913	-3.86245	-3.19400
H	-6.60840	-2.45681	-3.74519
H	-5.82710	-3.68219	-2.73233
C	-8.56699	-1.68755	-1.85375
H	-8.89633	-1.16846	-0.94374
H	-8.50151	-0.94395	-2.66054
H	-9.33517	-2.42275	-2.13204
C	4.40116	4.56834	0.23750
H	3.83903	4.87134	-0.65144
H	4.23047	5.31952	1.02220
H	5.47135	4.57470	-0.01389
C	4.69510	2.89036	2.07896
H	5.77253	3.09645	2.00605
H	4.29190	3.55639	2.85419
H	4.57590	1.85205	2.40061
C	2.94536	1.45722	-4.74101
H	2.90236	2.53014	-4.51735
H	3.95789	1.22562	-5.10197
H	2.23639	1.24914	-5.55527
C	2.54013	-0.88394	-3.87391
H	3.44950	-1.21699	-4.39358
H	2.40334	-1.50644	-2.98442
H	1.69043	-1.06190	-4.54593
C	8.25416	0.92404	-1.65100
H	9.26155	0.48565	-1.61067
H	8.10772	1.35569	-2.65173
H	8.20741	1.74261	-0.92162
C	7.32589	-1.31454	-2.35474
H	6.53844	-2.06434	-2.21124
H	7.27330	-0.96441	-3.39573
H	8.29878	-1.80446	-2.21879

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Imaginary frequency: -451.48 cm^{-1}

C	-0.89934	-5.04835	5.23655
C	-1.02630	-4.42784	4.00576
C	1.18092	-3.87660	5.66238
C	0.21851	-4.78256	6.06908
C	-0.04011	-3.50879	3.54504
C	-0.12409	-2.84833	2.27025
C	1.07279	-3.20971	4.40851
C	0.79821	-1.84661	1.97213
C	-1.17532	-3.20537	1.28103
C	2.02855	-2.24150	4.00085
C	1.89729	-1.52541	2.81930
C	-2.03129	-2.22385	0.78089
C	2.91015	-0.48115	2.46833
C	-3.12528	-2.51553	-0.08650
C	3.90183	-0.75418	1.49199
C	2.93251	0.74368	3.18363
C	-3.30017	-3.83400	-0.47949
C	-4.11547	-1.46903	-0.49528
C	4.91361	0.19457	1.27384
C	3.89907	-2.04570	0.67845
C	3.98094	1.64780	2.94577
C	1.86281	1.10087	4.21369
C	-4.10646	-0.93926	-1.80953
C	-5.11659	-1.07543	0.42780
C	4.98231	1.39365	1.99969
C	3.55691	-1.76753	-0.79829
C	5.23359	-2.80664	0.80275
C	2.41816	0.97342	5.64741
C	1.27062	2.50527	3.98423
C	-5.11557	-0.03131	-2.17295
C	-3.05262	-1.35504	-2.83347
C	-6.10283	-0.16755	0.01373
C	-5.16321	-1.62394	1.85159
C	6.14452	2.35245	1.77074
C	-6.12117	0.36775	-1.28278
C	-3.58499	-2.46611	-3.76241
C	-2.53212	-0.17431	-3.67150
C	-6.46759	-2.40404	2.10864
C	-4.95552	-0.50596	2.89201
C	5.79059	3.83405	1.98556
C	7.34392	1.94302	2.65290
C	-7.19202	1.36269	-1.71002

C	-8.60193	0.74459	-1.62554
C	-7.11075	2.67132	-0.89706
C	-1.30985	-4.55253	0.79126
C	-2.39808	-4.86316	-0.09825
C	-0.37990	-5.58445	1.10823
C	-2.53906	-6.19190	-0.59039
C	-0.53867	-6.86465	0.60433
C	-1.63202	-7.17727	-0.24433
O	0.68232	-1.17429	0.75672
O	-1.84917	-0.90233	1.19265
O	-0.35844	1.15137	1.41490
O	-0.70026	0.07310	-0.94874
P	-0.55548	-0.07257	0.55598
H	-1.66901	-5.74280	5.57229
H	-1.89170	-4.63198	3.38009
H	2.03336	-3.64595	6.30193
H	0.30794	-5.28242	7.03302
H	2.88181	-2.03917	4.64688
H	-4.15364	-4.08831	-1.10599
H	5.67031	-0.00700	0.51682
H	3.11490	-2.69734	1.08499
H	4.00164	2.57956	3.50702
H	1.04110	0.38238	4.10275
H	2.58803	-1.26453	-0.87521
H	3.49785	-2.70560	-1.36704
H	4.31977	-1.13614	-1.26675
H	6.06014	-2.24089	0.35197
H	5.48478	-2.99847	1.85460
H	5.16969	-3.77150	0.28059
H	3.25110	1.67337	5.80492
H	2.78948	-0.03982	5.84666
H	1.63710	1.20348	6.38557
H	0.47083	2.69495	4.71363
H	2.02462	3.29425	4.11011
H	0.83941	2.58381	2.98197
H	-5.12139	0.38168	-3.18136
H	-2.20064	-1.76270	-2.27601
H	-6.87264	0.13240	0.72474
H	-4.33643	-2.33508	1.97019
H	6.45598	2.23310	0.72055
H	-4.44589	-2.10483	-4.34283
H	-3.90586	-3.34918	-3.19740
H	-2.80270	-2.77951	-4.46848
H	-3.31692	0.25122	-4.31110
H	-2.13375	0.61928	-3.03077
H	-1.72807	-0.51501	-4.33565
H	-6.58774	-3.21629	1.37906
H	-6.46076	-2.84274	3.11625
H	-7.34743	-1.75030	2.03289
H	-4.95633	-0.92330	3.90877
H	-3.99722	0.00056	2.72779
H	-5.75635	0.24468	2.83595
H	5.59021	4.04770	3.04443
H	4.90573	4.13675	1.41043
H	6.63183	4.46972	1.67879
H	7.07873	2.02729	3.71637
H	7.63760	0.90293	2.45948
H	8.21090	2.59119	2.46231
H	-6.99929	1.61332	-2.76511
H	-8.85950	0.49173	-0.58754
H	-8.66609	-0.17524	-2.22192
H	-9.35772	1.45128	-1.99574
H	-7.29967	2.48246	0.16936
H	-6.12244	3.13908	-0.98472
H	-7.86527	3.38952	-1.24755
H	0.47079	-5.35203	1.74316
H	-3.37098	-6.41246	-1.25955
H	0.18927	-7.63599	0.85370
H	-1.74577	-8.18872	-0.63270
N	1.25790	2.93346	-0.01090
C	-0.45076	6.23400	0.33614
C	-0.25401	4.84290	0.24999
C	-1.35170	3.96353	0.23134
C	-2.65393	4.46961	0.32150
C	-2.86843	5.86684	0.40159
C	-1.75321	6.74552	0.40996
C	1.14138	4.34690	0.15535
C	1.13233	2.35268	-1.89714
C	2.59819	2.29975	-0.12355
C	2.58087	1.95646	-1.62540
C	4.81725	2.55255	-2.24502
C	5.30556	1.17805	-2.67079
C	4.67321	0.46606	-3.70372
C	6.43115	0.61497	-2.04599
C	5.14531	-0.79658	-4.08530
C	6.91275	-0.64164	-2.43534
C	6.26393	-1.35546	-3.45227
C	-3.56347	2.25931	0.42936
C	-4.87827	6.15692	1.63282
C	-0.97008	8.99761	0.51982
O	2.14143	5.06215	0.14369
O	3.41791	2.77950	-2.43138
O	-3.76835	3.68299	0.33001
O	-4.12803	6.40402	0.42364
O	-2.06201	8.07253	0.50409
H	0.42202	6.87841	0.35178
H	-1.21197	2.89324	0.16474
H	3.37872	3.00549	0.16240
H	2.62724	1.42169	0.52241
H	2.76866	0.89284	-1.82091
H	0.58619	2.35336	0.53590
H	0.93044	3.31493	-2.35757
H	0.30833	1.67512	-1.70755
H	5.29917	3.33178	-2.85204
H	5.10765	2.73497	-1.19621
H	3.80288	0.90048	-4.19243
H	6.93701	1.16427	-1.25121
H	4.63357	-1.34426	-4.87568
H	7.78389	-1.06635	-1.93681
H	6.62545	-2.34051	-3.74610
H	-2.92332	2.01286	1.28560
H	-4.55502	1.82687	0.56021

H	-3.11541	1.85501	-0.48821
H	-4.34764	6.57039	2.50305
H	-5.83197	6.67862	1.50234
H	-5.05535	5.08429	1.77830
H	-0.37716	8.93377	-0.40492
H	-1.42594	9.98919	0.59535
H	-0.31184	8.82746	1.38524
N	0.65818	-0.94197	-2.96127
C	0.49008	-4.60575	-2.33789
C	0.96956	-5.04380	-3.58760
C	0.36509	-3.24351	-2.05058
C	1.33386	-4.13067	-4.58595
C	0.72624	-2.32912	-3.04882
C	1.20527	-2.76616	-4.30384
C	1.03169	-0.25065	-4.05862
S	1.55753	-1.37363	-5.32837
S	1.01460	1.42356	-4.29067
H	0.21342	-5.33345	-1.57930
H	1.05933	-6.11092	-3.78523
H	0.00904	-2.89240	-1.08733
H	1.70256	-4.47008	-5.55167
H	0.18221	-0.49168	-2.12863

TS 9 (S) *conf1*

Imaginary frequency: -451.01 cm^{-1}

C	-0.76753	-5.03839	5.30766
C	-0.93625	-4.42201	4.07979
C	1.32911	-3.87047	5.65577
C	0.37965	-4.77276	6.09931
C	0.03551	-3.50741	3.58092
C	-0.09150	-2.85193	2.30700
C	1.17830	-3.20775	4.40411
C	0.82066	-1.85137	1.97387
C	-1.17614	-3.21319	1.35610
C	2.12093	-2.24293	3.95982
C	1.94928	-1.53020	2.78151
C	-2.04583	-2.23277	0.87930
C	2.95408	-0.49158	2.39205
C	-3.16643	-2.52370	0.04627
C	3.91893	-0.77814	1.39326
C	2.99862	0.74052	3.09395
C	-3.35906	-3.84344	-0.33302
C	-4.15215	-1.46547	-0.34090
C	4.92820	0.16479	1.13957
C	3.88841	-2.07681	0.59176
C	4.04386	1.63798	2.82053
C	1.95621	1.11014	4.14728
C	-4.17355	-0.94515	-1.66123
C	-5.10462	-1.03316	0.61277
C	5.02005	1.37024	1.85174
C	3.49400	-1.81114	-0.87441
C	5.22622	-2.83740	0.67497
C	2.54250	0.97937	5.56836
C	1.37305	2.52014	3.92992
C	-5.15661	-0.00146	-1.99436
C	-3.17846	-1.40891	-2.72289
C	-6.07046	-0.08876	0.22617
C	-5.12525	-1.57627	2.03909
C	6.18104	2.32158	1.58844
C	-6.11095	0.44502	-1.06753
C	-3.78865	-2.51310	-3.61158
C	-2.65908	-0.25836	-3.60248
C	-4.85586	-0.46465	3.07207
C	-6.44391	-2.31806	2.33495
C	5.82447	3.80958	1.75041
C	7.38020	1.94583	2.48576
C	-7.15420	1.48466	-1.45387
C	-6.50348	2.81239	-1.89368
C	-8.10333	0.94590	-2.54334
C	-1.33079	-4.56243	0.87781
C	-2.44878	-4.87371	0.02595
C	-0.39441	-5.59594	1.16943
C	-2.60998	-6.20451	-0.45427
C	-0.57383	-6.87821	0.67776
C	-1.69535	-7.19127	-0.13304
O	0.66519	-1.18162	0.76154
O	-1.84879	-0.91032	1.28102
O	-0.35863	1.14748	1.43572
O	-0.77651	0.04967	-0.90722
P	-0.58167	-0.08353	0.59287
H	-1.52688	-5.72924	5.67299
H	-1.82449	-4.62540	3.48686
H	2.20397	-3.63936	6.26413
H	0.50175	-5.26949	7.06128
H	2.99748	-2.04102	4.57403
H	-4.23189	-4.09841	-0.93182
H	5.66479	-0.04723	0.36584
H	3.11890	-2.72455	1.03133
H	4.08323	2.57491	3.37228
H	1.12511	0.39968	4.05565
H	4.23871	-1.18203	-1.37414
H	2.52196	-1.31059	-0.92161
H	3.41700	-2.75392	-1.43313
H	6.03599	-2.27761	0.18782
H	5.51594	-3.01838	1.71880
H	5.14246	-3.80764	0.16578
H	3.38713	1.66974	5.70460
H	2.90593	-0.03773	5.76189
H	1.78130	1.22066	6.32350
H	2.13636	3.30208	4.04279
H	0.92424	2.60467	2.93597
H	0.58839	2.71636	4.67379
H	-5.17736	0.40122	-3.00556
H	-2.31603	-1.83737	-2.19785
H	-6.80791	0.24754	0.95658
H	-4.31648	-2.31122	2.13502
H	6.49334	2.16526	0.54341
H	-4.66162	-2.12864	-4.15816
H	-4.11502	-3.37742	-3.02149
H	-3.04989	-2.86214	-4.34719
H	-3.45639	0.17668	-4.21995
H	-2.21634	0.53620	-2.99300

H	-1.89142	-0.63342	-4.29080
H	-5.63754	0.30722	3.04080
H	-4.83736	-0.88269	4.08840
H	-3.88952	0.01555	2.87891
H	-7.30595	-1.63881	2.28315
H	-6.60861	-3.12745	1.61092
H	-6.42081	-2.75550	3.34290
H	5.62038	4.05985	2.80044
H	4.94125	4.09166	1.16257
H	6.66609	4.43523	1.42445
H	7.11418	2.06799	3.54534
H	7.67528	0.89980	2.33005
H	8.24647	2.58791	2.27267
H	-7.75788	1.68893	-0.55526
H	-5.89309	2.67008	-2.79631
H	-5.85369	3.22343	-1.11125
H	-7.27564	3.55874	-2.12748
H	-7.55438	0.73586	-3.47193
H	-8.58686	0.01443	-2.22000
H	-8.88655	1.68132	-2.77468
H	0.47727	-5.36327	1.77514
H	-3.46399	-6.42562	-1.09484
H	0.15928	-7.65081	0.90732
H	-1.82512	-8.20426	-0.51228
N	1.23861	2.89575	-0.04230
C	-0.35947	6.24120	0.38470
C	-0.21058	4.84483	0.28990
C	-1.33327	3.99761	0.33154
C	-2.61220	4.54448	0.49417
C	-2.77838	5.94762	0.58079
C	-1.63956	6.79246	0.52867
C	1.16493	4.31103	0.12806
C	1.04020	2.31664	-1.92032
C	2.55975	2.23057	-0.19729
C	2.49191	1.90147	-1.70002
C	4.71338	2.49208	-2.37827
C	5.18508	1.11648	-2.81884
C	6.32891	0.55169	-2.22977
C	4.51832	0.40452	-3.82987
C	6.79483	-0.70662	-2.63225
C	4.97486	-0.85995	-4.22419
C	6.11182	-1.42060	-3.62644
C	-3.59149	2.36564	0.64466
C	-4.66535	6.34626	1.95531
C	-0.78407	9.01970	0.59609
O	2.18129	5.00064	0.07048
O	3.31032	2.72399	-2.52551
O	-3.75041	3.79662	0.57514
O	-4.02140	6.51642	0.67419
O	-1.90281	8.12786	0.63915
H	0.53268	6.85781	0.35287
H	-1.22834	2.92308	0.26193
H	3.36513	2.91233	0.07581
H	2.58354	1.34521	0.43923
H	2.66237	0.83795	-1.91088
H	0.57190	2.33151	0.52716
H	0.83428	3.27948	-2.37765
H	0.21554	1.64829	-1.70240
H	5.18088	3.27053	-2.99748
H	5.03343	2.67227	-1.33780
H	6.86114	1.10106	-1.45249
H	3.63406	0.84040	-4.29150
H	7.68059	-1.13257	-2.16130
H	4.43684	-1.40763	-4.99689
H	6.46129	-2.40704	-3.93002
H	-3.22077	1.95795	-0.30573
H	-2.90683	2.08289	1.45421
H	-4.58849	1.96761	0.83474
H	-4.06424	6.81079	2.75082
H	-5.62932	6.85938	1.87604
H	-4.82525	5.28410	2.17973
H	-0.24437	8.93963	-0.35943
H	-1.20506	10.02439	0.69639
H	-0.08552	8.82802	1.42459
N	0.52717	-0.97631	-2.95189
C	0.38441	-4.63603	-2.29894
C	0.82790	-5.08183	-3.55917
C	0.26537	-3.27205	-2.01740
C	1.16032	-4.17496	-4.57418
C	0.59521	-2.36388	-3.03202
C	1.03706	-2.80877	-4.29788
C	0.86438	-0.29197	-4.06539
S	1.35406	-1.42279	-5.34255
S	0.83369	1.38027	-4.30855
H	0.13132	-5.35894	-1.52763
H	0.91407	-6.15013	-3.75201
H	-0.06299	-2.91485	-1.04660
H	1.50068	-4.52037	-5.54814
H	0.07423	-0.52135	-2.10904

TS 9 (S) *conf2*

Imaginary frequency: -450.92 cm^{-1}

C	-0.79110	-5.08842	5.23926
C	-0.94611	-4.46217	4.01458
C	1.29107	-3.90786	5.62936
C	0.34197	-4.82122	6.05047
C	0.02586	-3.53562	3.53879
C	-0.08706	-2.86939	2.26917
C	1.15399	-3.23496	4.38157
C	0.82280	-1.85969	1.95833
C	-1.15476	-3.22946	1.29889
C	2.09584	-2.25919	3.96006
C	1.93663	-1.53712	2.78568
C	-2.02422	-2.25075	0.81783
C	2.93922	-0.48733	2.42102
C	-3.12881	-2.54216	-0.03591
C	3.92306	-0.75855	1.43658
C	2.96136	0.73994	3.13226
C	-3.30648	-3.86002	-0.42921
C	-4.11577	-1.48980	-0.43582
C	4.92831	0.19452	1.20650
C	3.91516	-2.05048	0.62377

C	4.00300	1.64836	2.88224
C	1.89858	1.09264	4.17096
C	-4.12645	-0.97614	-1.75671
C	-5.08802	-1.06550	0.50441
C	4.99734	1.39593	1.92801
C	3.53878	-1.77437	-0.84524
C	5.25797	-2.80072	0.71861
C	2.46089	0.94962	5.60056
C	1.31134	2.50176	3.95933
C	-5.12855	-0.05664	-2.10947
C	-3.10367	-1.41914	-2.80059
C	-6.06552	-0.14300	0.10165
C	-5.12201	-1.60763	1.93115
C	6.15271	2.36026	1.68801
C	-6.10626	0.37193	-1.20238
C	-3.67696	-2.52590	-3.71022
C	-2.58302	-0.25374	-3.65993
C	-6.42593	-2.38592	2.19774
C	-4.90583	-0.49020	2.96984
C	5.78239	3.84282	1.86770
C	7.34760	1.98163	2.58979
C	-7.16618	1.38146	-1.62270
C	-8.59271	0.83548	-1.41832
C	-6.97697	2.72828	-0.89490
C	-1.29172	-4.57518	0.80565
C	-2.39450	-4.88701	-0.06553
C	-0.35150	-5.60411	1.10116
C	-2.53828	-6.21438	-0.56058
C	-0.51343	-6.88289	0.59457
C	-1.62055	-7.19696	-0.23545
O	0.67989	-1.18101	0.74924
O	-1.84355	-0.93088	1.23428
O	-0.36852	1.13355	1.43472
O	-0.74560	0.05944	-0.92694
P	-0.57097	-0.08838	0.57461
H	-1.55041	-5.78841	5.58685
H	-1.82346	-4.66713	3.40614
H	2.15492	-3.67573	6.25286
H	0.45342	-5.32563	7.00973
H	2.96145	-2.05626	4.58924
H	-4.16775	-4.11546	-1.04431
H	5.67931	-0.00559	0.44350
H	3.14503	-2.70845	1.04682
H	4.02450	2.58202	3.44029
H	1.07316	0.37878	4.05687
H	2.56391	-1.28028	-0.90080
H	3.47636	-2.71244	-1.41366
H	4.28548	-1.13511	-1.32881
H	6.06967	-2.22989	0.24776
H	5.53484	-2.98883	1.76467
H	5.18938	-3.76694	0.19958
H	3.29952	1.64272	5.75842
H	2.82607	-0.06762	5.78988
H	1.68554	1.17938	6.34481
H	0.51089	2.68408	4.68971
H	2.06730	3.28682	4.09710
H	0.88175	2.59636	2.95793
H	-5.15230	0.34062	-3.12399
H	-2.24619	-1.83808	-2.26010
H	-6.81365	0.17936	0.82593
H	-4.29565	-2.31998	2.04475
H	6.47480	2.22111	0.64345
H	-4.54328	-2.15159	-4.27410
H	-4.00256	-3.39940	-3.13339
H	-2.91645	-2.85821	-4.43126
H	-3.37494	0.17818	-4.28638
H	-2.15967	0.53945	-3.03498
H	-1.79941	-0.61294	-4.33866
H	-6.55109	-3.19984	1.47086
H	-6.41419	-2.82203	3.20645
H	-7.30497	-1.73073	2.12456
H	-4.90015	-0.90847	3.98615
H	-3.94795	0.01487	2.79986
H	-5.70599	0.26164	2.92145
H	5.57004	4.07692	2.91986
H	4.90010	4.12510	1.27859
H	6.62061	4.47991	1.55542
H	7.07178	2.08644	3.64872
H	7.65285	0.94043	2.42176
H	8.21015	2.63390	2.39311
H	-7.02948	1.56418	-2.70031
H	-8.80075	0.65945	-0.35385
H	-8.73123	-0.11507	-1.95024
H	-9.33802	1.55240	-1.78997
H	-7.10910	2.60876	0.18982
H	-5.97256	3.13401	-1.06621
H	-7.71388	3.46543	-1.24395
H	0.50941	-5.37049	1.72171
H	-3.38107	-6.43598	-1.21567
H	0.22244	-7.65187	0.82739
H	-1.73671	-8.20726	-0.62611
N	1.23957	2.90910	-0.00500
C	-0.37042	6.23631	0.51579
C	-0.21444	4.84577	0.35907
C	-1.33995	4.00166	0.35235
C	-2.62208	4.53421	0.53266
C	-2.79840	5.93717	0.64909
C	-1.65113	6.78058	0.65164
C	1.16046	4.32092	0.19435
C	1.06726	2.34864	-1.90087
C	2.56370	2.25031	-0.15493
C	2.51734	1.93870	-1.66181
C	4.74537	2.54918	-2.30165
C	5.23138	1.17994	-2.74645
C	4.58322	0.47252	-3.77266
C	6.36973	0.61665	-2.14548
C	5.05219	-0.78631	-4.17036
C	6.84849	-0.63571	-2.55149
C	6.18370	-1.34545	-3.56095
C	-3.57106	2.33460	0.62986
C	-5.12107	6.13476	0.02152
C	-0.79553	9.00254	0.81421

O	2.17722	5.01354	0.16066
O	3.34342	2.77414	-2.46725
O	-3.74639	3.76398	0.63096
O	-4.00209	6.54802	0.83511
O	-1.91627	8.11368	0.79145
H	0.51849	6.85825	0.50889
H	-1.23263	2.92914	0.26008
H	3.36361	2.93129	0.13594
H	2.58458	1.35684	0.47035
H	2.69649	0.87843	-1.88222
H	0.56910	2.33497	0.54839
H	0.86331	3.31838	-2.34422
H	0.24242	1.67684	-1.69518
H	5.21726	3.33521	-2.90786
H	5.04963	2.72281	-1.25537
H	3.70354	0.90767	-4.24367
H	6.88742	1.16243	-1.35594
H	4.52819	-1.33081	-4.95490
H	7.72978	-1.06064	-2.07131
H	6.54294	-2.32752	-3.86727
H	-2.87258	2.02236	1.41633
H	-4.56097	1.91718	0.81495
H	-3.20776	1.97413	-0.34281
H	-5.60780	5.24574	0.43472
H	-5.81210	6.98480	0.02709
H	-4.79901	5.92837	-1.00804
H	-0.22570	8.95555	-0.12630
H	-1.21741	10.00442	0.93720
H	-0.12325	8.77950	1.65641
N	0.59732	-0.93219	-2.96076
C	0.47120	-4.59943	-2.34728
C	0.92878	-5.02934	-3.60801
C	0.34173	-3.23923	-2.05245
C	1.26531	-4.10993	-4.61031
C	0.67534	-2.31850	-3.05450
C	1.13135	-2.74747	-4.32080
C	0.93938	-0.23475	-4.06438
S	1.44898	-1.34876	-5.34818
S	0.89804	1.43983	-4.29232
H	0.21530	-5.33189	-1.58591
H	1.02295	-6.09502	-3.81128
H	0.00273	-2.89412	-1.08093
H	1.61675	-4.44304	-5.58462
H	0.12979	-0.48960	-2.11869

TS 9 (S) *conf3*

Imaginary frequency: -449.59 cm^{-1}

C	0.43589	-5.33710	-5.08789
C	0.66316	-4.66254	-3.90073
C	-1.63465	-4.12268	-5.43330
C	-0.72789	-5.07700	-5.85683
C	-0.26356	-3.69208	-3.42214
C	-0.07486	-2.97432	-2.19014
C	-1.42295	-3.39996	-4.22440
C	-0.94444	-1.92854	-1.88302
C	1.02838	-3.32065	-1.25544
C	-2.32120	-2.38402	-3.80297
C	-2.08978	-1.61617	-2.67039
C	1.94383	-2.34591	-0.85989
C	-3.05238	-0.53024	-2.30466
C	3.08101	-2.62952	-0.04720
C	-3.98792	-0.73533	-1.25903
C	-3.09048	0.66233	-3.07214
C	3.24403	-3.93307	0.39667
C	4.11268	-1.58696	0.25272
C	-4.96274	0.24773	-1.02331
C	-3.96412	-1.99075	-0.39112
C	-4.10287	1.60104	-2.81439
C	-2.07462	0.94681	-4.17657
C	4.19401	-1.00071	1.54267
C	5.04845	-1.23868	-0.75061
C	-5.05003	1.41372	-1.79899
C	-3.51539	-1.66141	1.04616
C	-5.32294	-2.71798	-0.39280
C	-2.71233	0.76518	-5.56956
C	-1.44332	2.34699	-4.04828
C	5.22186	-0.08069	1.79760
C	3.21498	-1.36912	2.65556
C	6.05998	-0.31348	-0.44240
C	5.00271	-1.85236	-2.14734
C	-6.17758	2.40868	-1.55195
C	6.16314	0.27994	0.82144
C	3.80963	-2.44778	3.58511
C	2.76603	-0.15388	3.48570
C	6.28756	-2.64821	-2.45106
C	4.72893	-0.78463	-3.22457
C	-5.78664	3.87628	-1.79917
C	-7.41168	2.02198	-2.39561
C	7.25523	1.29763	1.12182
C	6.66117	2.67965	1.46429
C	8.19463	0.80505	2.24065
C	1.15571	-4.64712	-0.71018
C	2.29061	-4.95016	0.12202
C	0.17823	-5.66286	-0.91690
C	2.42548	-6.25850	0.66765
C	0.33317	-6.92276	-0.36305
C	1.47018	-7.22987	0.42824
O	-0.72760	-1.19890	-0.71515
O	1.77571	-1.04119	-1.32706
O	0.34877	1.05496	-1.54645
O	0.80873	0.06937	0.83813
P	0.55941	-0.13663	-0.64577
H	1.16159	-6.07026	-5.43886
H	1.56344	-4.86278	-3.32514
H	-2.52163	-3.89629	-6.02569
H	-0.89626	-5.61965	-6.78646
H	-3.21129	-2.18722	-4.39904
H	4.12764	-4.18483	0.98084
H	-5.67649	0.09866	-0.21432
H	-3.22622	-2.68104	-0.81995
H	-4.13882	2.50660	-3.41646
H	-1.26229	0.21599	-4.07672

H	-2.53002	-1.18530	1.03691
H	-3.44348	-2.57648	1.64984
H	-4.22715	-0.98820	1.53641
H	-6.10213	-2.11162	0.08847
H	-5.65048	-2.94520	-1.41622
H	-5.24773	-3.66231	0.16422
H	-3.54022	1.47411	-5.71292
H	-3.11203	-0.24833	-5.70032
H	-1.97024	0.94541	-6.35989
H	-0.67837	2.48266	-4.82534
H	-2.18683	3.14569	-4.17502
H	-0.95937	2.46583	-3.07457
H	5.28902	0.37118	2.78577
H	2.32140	-1.79028	2.17902
H	6.78514	-0.04250	-1.21116
H	4.16991	-2.56581	-2.17803
H	-6.46345	2.31358	-0.49214
H	4.71341	-2.07008	4.08432
H	4.08377	-3.35478	3.03375
H	3.08135	-2.72731	4.35984
H	3.59771	0.28232	4.05519
H	2.33397	0.62329	2.84675
H	2.00682	-0.46146	4.21554
H	6.45540	-3.42513	-1.69295
H	6.21448	-3.13448	-3.43392
H	7.17032	-1.99423	-2.46491
H	4.66083	-1.25104	-4.21746
H	3.78513	-0.26532	-3.02175
H	5.53386	-0.03726	-3.25919
H	-5.60524	4.06770	-2.86560
H	-4.88013	4.16291	-1.25028
H	-6.60192	4.54078	-1.48330
H	-7.17367	2.08433	-3.46698
H	-7.72898	0.99336	-2.17939
H	-8.25449	2.69719	-2.19096
H	7.85603	1.40999	0.20540
H	6.05319	2.62982	2.37833
H	6.01980	3.04833	0.65460
H	7.46227	3.41304	1.63308
H	7.65092	0.69088	3.18879
H	8.63489	-0.16809	1.98566
H	9.01076	1.52225	2.40584
H	-0.70481	-5.43368	-1.50734
H	3.29259	-6.47399	1.29234
H	-0.43096	-7.68164	-0.52819
H	1.58033	-8.22531	0.85692
N	-1.15052	2.92830	-0.12604
C	0.52914	6.20167	-0.74505
C	0.34421	4.81487	-0.59185
C	1.44070	3.93329	-0.62462
C	2.73075	4.43622	-0.83805
C	2.93257	5.82991	-0.97963
C	1.82273	6.71065	-0.92285
C	-1.04202	4.32938	-0.37318
C	-0.91160	2.44285	1.77492
C	-2.48419	2.31155	0.10267
C	-2.38120	2.06292	1.61898
C	-4.56251	2.75504	2.32904
C	-5.05698	1.42371	2.86960
C	-4.37442	0.75412	3.89873
C	-6.23716	0.85962	2.35640
C	-4.85176	-0.46992	4.38537
C	-6.72321	-0.35761	2.85080
C	-6.02483	-1.03095	3.86251
C	3.64595	2.22800	-0.92003
C	5.02254	6.41450	-0.05323
C	1.03595	8.96227	-1.02087
O	-2.03668	5.05065	-0.32712
O	-3.14966	2.95486	2.42014
O	3.84412	3.65535	-0.93456
O	4.18223	6.33882	-1.22365
O	2.12646	8.03558	-1.05505
H	-0.34309	6.84567	-0.70376
H	1.30527	2.86501	-0.51921
H	-3.27835	3.00019	-0.18550
H	-2.55055	1.39386	-0.48296
H	-2.57776	1.01848	1.89320
H	-0.51680	2.31438	-0.68181
H	-0.66248	3.42208	2.17191
H	-0.11474	1.73840	1.56760
H	-4.98958	3.58385	2.91095
H	-4.90968	2.87846	1.28905
H	-3.46233	1.19039	4.30195
H	-6.78208	1.37717	1.56620
H	-4.30195	-0.98594	5.17141
H	-7.63719	-0.78399	2.43770
H	-6.39067	-1.98633	4.23771
H	2.92760	1.92155	-1.69090
H	4.62488	1.79197	-1.12195
H	3.29615	1.88094	0.06224
H	5.16758	5.42282	0.39547
H	5.98484	6.80826	-0.39663
H	4.58700	7.09911	0.68965
H	0.50166	8.91838	-0.05977
H	1.48653	9.95130	-1.14519
H	0.32560	8.77500	-1.83995
N	-0.46034	-0.80429	2.97197
C	-0.44199	-4.49735	2.52305
C	-0.85338	-4.85892	3.82055
C	-0.29494	-3.15531	2.16100
C	-1.12479	-3.88754	4.79311
C	-0.56359	-2.18268	3.13302
C	-0.97325	-2.54307	4.43604
C	-0.73989	-0.04955	4.05533
S	-1.21524	-1.09223	5.41035
S	-0.65438	1.63229	4.20182
H	-0.23667	-5.26933	1.78588
H	-0.96267	-5.91178	4.07628
H	0.00889	-2.86272	1.16105
H	-1.44074	-4.16814	5.79569
H	-0.02251	-0.41025	2.09088

TS 9 (S) *conf4*

Imaginary frequency: -449.22 cm^{-1}

C	0.46457	-5.26714	-5.15275
C	0.68339	-4.61248	-3.95292
C	-1.59333	-4.03267	-5.50209
C	-0.68880	-4.98704	-5.93027
C	-0.24182	-3.64301	-3.46937
C	-0.06191	-2.94596	-2.22417
C	-1.38994	-3.33007	-4.27998
C	-0.92746	-1.89844	-1.91082
C	1.02902	-3.31391	-1.28315
C	-2.28518	-2.31357	-3.85346
C	-2.06081	-1.56481	-2.70683
C	1.94452	-2.35038	-0.86165
C	-3.01836	-0.47616	-2.33566
C	3.07016	-2.65130	-0.03880
C	-3.97065	-0.69082	-1.30727
C	-3.03353	0.73065	-3.08124
C	3.22301	-3.96234	0.38551
C	4.09377	-1.60998	0.29070
C	-4.93894	0.29746	-1.06709
C	-3.96945	-1.96060	-0.46028
C	-4.03954	1.67519	-2.81964
C	-2.00037	1.02383	-4.16718
C	4.15350	-1.03928	1.58893
C	5.03252	-1.23291	-0.69939
C	-5.00294	1.47886	-1.82142
C	-3.53490	-1.65799	0.98721
C	-5.33473	-2.67491	-0.48977
C	-2.62009	0.86584	-5.57116
C	-1.36149	2.41772	-4.01124
C	5.15667	-0.09737	1.86161
C	3.17913	-1.44741	2.69185
C	6.01864	-0.28680	-0.37337
C	5.01742	-1.83886	-2.10026
C	-6.12236	2.48173	-1.56931
C	6.09322	0.30015	0.89540
C	3.79148	-2.53693	3.59728
C	2.71056	-0.26032	3.55109
C	6.31913	-2.61416	-2.38542
C	4.74584	-0.77172	-3.17842
C	-5.71488	3.94858	-1.79295
C	-7.35385	2.11920	-2.42740
C	7.15342	1.34556	1.21385
C	6.52021	2.68895	1.63089
C	8.13648	0.83885	2.28825
C	1.14440	-4.64941	-0.75747
C	2.26856	-4.97064	0.08262
C	0.16494	-5.65735	-0.99122
C	2.39143	-6.28809	0.60880
C	0.30801	-6.92652	-0.45562
C	1.43461	-7.25120	0.34344
O	-0.72027	-1.18905	-0.72901
O	1.78899	-1.03808	-1.31089
O	0.38043	1.07172	-1.50979
O	0.80708	0.04169	0.86319
P	0.57244	-0.13589	-0.62675
H	1.18905	-5.99993	-5.50703
H	1.57607	-4.82783	-3.37102
H	-2.47199	-3.79067	-6.10068
H	-0.85072	-5.51418	-6.86992
H	-3.16679	-2.10080	-4.45664
H	4.09790	-4.22776	0.97660
H	-5.66502	0.14105	-0.27051
H	-3.23270	-2.65073	-0.89137
H	-4.05729	2.59249	-3.40444
H	-1.19439	0.28612	-4.06633
H	-2.54620	-1.18891	0.99647
H	-3.47655	-2.58305	1.57696
H	-4.24725	-0.98724	1.47992
H	-6.11416	-2.06878	-0.00861
H	-5.65176	-2.88324	-1.52050
H	-5.27509	-3.62840	0.05338
H	-3.44153	1.58207	-5.71543
H	-3.02429	-0.14312	-5.72168
H	-1.86623	1.05245	-6.34880
H	-0.58323	2.55736	-4.77429
H	-2.09712	3.22332	-4.14021
H	-0.89260	2.52131	-3.02850
H	5.20632	0.34454	2.85519
H	2.29276	-1.87227	2.20511
H	6.74453	0.00812	-1.13268
H	4.19599	-2.56451	-2.14746
H	-6.41728	2.37480	-0.51306
H	4.68681	-2.15396	4.10759
H	4.08435	-3.42549	3.02609
H	3.06676	-2.84786	4.36332
H	3.53365	0.17054	4.13693
H	2.27274	0.52868	2.93101
H	1.95172	-0.59707	4.26841
H	6.48523	-3.39248	-1.62838
H	6.27078	-3.09621	-3.37189
H	7.19196	-1.94680	-2.38000
H	4.70008	-1.23615	-4.17350
H	3.79180	-0.26630	-2.98926
H	5.54095	-0.01334	-3.19893
H	-5.52532	4.15326	-2.85554
H	-4.80884	4.21797	-1.23472
H	-6.52541	4.61671	-1.47251
H	-7.10703	2.19388	-3.49599
H	-7.68325	1.09099	-2.22789
H	-8.19132	2.80012	-2.21976
H	7.72709	1.51882	0.28945
H	5.95696	2.58409	2.56858
H	5.82893	3.05919	0.86451
H	7.29860	3.44817	1.79202
H	7.61677	0.65741	3.23943
H	8.60883	-0.10256	1.97767
H	8.92731	1.57949	2.47248
H	-0.71023	-5.41487	-1.58802
H	3.25047	-6.51743	1.23969
H	-0.45750	-7.67921	-0.64137

H	1.53558	-8.25375	0.75758
N	-1.12681	2.93333	-0.07112
C	0.54719	6.21620	-0.66045
C	0.36238	4.82777	-0.51662
C	1.46527	3.95539	-0.56566
C	2.75235	4.46054	-0.78608
C	2.95987	5.86030	-0.88484
C	1.83528	6.73166	-0.83412
C	-1.01888	4.33830	-0.30057
C	-0.90557	2.41276	1.83013
C	-2.46186	2.31365	0.13836
C	-2.37510	2.04348	1.65153
C	-4.55953	2.74317	2.34722
C	-5.07169	1.40501	2.85324
C	-4.40878	0.70928	3.87797
C	-6.24841	0.86038	2.31191
C	-4.90183	-0.52079	4.33256
C	-6.75053	-0.36281	2.77462
C	-6.07161	-1.06195	3.78206
C	3.64603	2.24085	-0.94439
C	5.29944	5.99716	-0.31449
C	1.03020	8.97621	-0.93003
O	-2.01629	5.05704	-0.24439
O	-3.14642	2.92841	2.45839
O	3.85350	3.66602	-0.94248
O	4.17315	6.44223	-1.10051
O	2.12856	8.05992	-0.96167
H	-0.32518	6.85925	-0.61089
H	1.33471	2.88397	-0.48673
H	-3.25348	3.00592	-0.14800
H	-2.52398	1.40362	-0.45976
H	-2.58068	0.99649	1.90912
H	-0.49007	2.32799	-0.63065
H	-0.65556	3.38560	2.24188
H	-0.11009	1.70978	1.61303
H	-4.98597	3.56292	2.94232
H	-4.89405	2.89244	1.30650
H	-3.49939	1.13029	4.30304
H	-6.77794	1.39774	1.52448
H	-4.36683	-1.05704	5.11530
H	-7.66163	-0.77374	2.34007
H	-6.44975	-2.02195	4.13244
H	2.90734	1.94953	-1.70175
H	4.61821	1.80419	-1.17553
H	3.31903	1.88104	0.04117
H	5.76057	5.10424	-0.74896
H	6.00774	6.83288	-0.32309
H	4.99419	5.78304	0.71848
H	0.49334	8.92745	0.02958
H	1.47239	9.96937	-1.05231
H	0.32304	8.78366	-1.75087
N	-0.49762	-0.85381	2.96577
C	-0.50368	-4.53856	2.45268
C	-0.93207	-4.91929	3.73918
C	-0.34243	-3.19165	2.11555
C	-1.20646	-3.96278	4.72554
C	-0.61406	-2.23390	3.10145
C	-1.04041	-2.61363	4.39355
C	-0.78126	-0.11617	4.05972
S	-1.28067	-1.17817	5.39071
S	-0.68049	1.56180	4.23833
H	-0.29605	-5.29925	1.70447
H	-1.05226	-5.97554	3.97536
H	-0.02553	-2.88399	1.12422
H	-1.53537	-4.25801	5.71972
H	-0.04531	-0.44883	2.09679

TS 9-B (S)

Imaginary frequency: -424.92 cm^{-1}

C	2.63406	6.31353	-2.16611
C	2.02044	5.30749	-1.43951
C	4.31375	4.76602	-2.97509
C	3.80072	6.04911	-2.92819
C	2.54313	3.98159	-1.43666
C	1.94745	2.89864	-0.69525
C	3.69528	3.70468	-2.25431
C	2.42696	1.60685	-0.89994
C	0.77954	3.15184	0.19190
C	4.16642	2.36964	-2.36897
C	3.53711	1.30287	-1.74602
C	-0.43668	2.50465	-0.03838
C	3.93807	-0.12203	-1.98968
C	-1.66438	2.95627	0.52774
C	4.76334	-0.81396	-1.06099
C	3.43865	-0.78971	-3.13796
C	-1.61136	3.96708	1.47576
C	-2.99201	2.54695	-0.03354
C	4.96434	-2.18982	-1.24314
C	5.48714	-0.06237	0.05967
C	3.68629	-2.16545	-3.27950
C	2.71739	-0.03252	-4.25430
C	-3.70884	1.43866	0.46853
C	-3.56072	3.37817	-1.03594
C	4.40738	-2.89154	-2.32579
C	6.08817	-0.96356	1.15215
C	6.62714	0.80519	-0.52464
C	3.75480	0.51916	-5.25986
C	1.67574	-0.85943	-5.02975
C	-5.02100	1.22019	0.01472
C	-3.09720	0.53473	1.53430
C	-4.87012	3.11236	-1.45976
C	-2.75332	4.50027	-1.68803
C	4.65996	-4.39050	-2.45280
C	-5.63022	2.05912	-0.92821
C	-3.51287	0.99851	2.94494
C	-3.42340	-0.95351	1.31947
C	-3.58280	5.75707	-2.00284
C	-2.04386	3.97459	-2.95586
C	3.61748	-5.12870	-3.30831
C	6.08520	-4.64796	-2.98918
C	-7.06333	1.85790	-1.40944
C	-7.09747	1.00280	-2.69430

C	-7.99592	1.27781	-0.33302
C	0.83688	4.13817	1.23849
C	-0.38253	4.54932	1.88446
C	2.06551	4.69967	1.68907
C	-0.32856	5.53549	2.91011
C	2.08714	5.63938	2.70607
C	0.88048	6.07339	3.31434
O	1.81000	0.56352	-0.20721
O	-0.50641	1.46566	-0.95373
O	-0.22202	-0.79055	0.43612
P	0.31625	0.03320	-0.70688
H	2.21085	7.31766	-2.15791
H	1.12029	5.52538	-0.87159
H	5.19211	4.53969	-3.58024
H	4.27747	6.85248	-3.48880
H	5.02902	2.17855	-3.00420
H	-2.54364	4.34580	1.89377
H	5.56959	-2.74240	-0.52582
H	4.76024	0.61448	0.53445
H	3.27662	-2.68168	-4.14280
H	2.19328	0.81615	-3.79656
H	5.36291	-1.67172	1.56320
H	6.45251	-0.34226	1.98073
H	6.94587	-1.53106	0.76377
H	7.34739	0.16812	-1.05707
H	6.25569	1.55974	-1.22338
H	7.16235	1.32388	0.28337
H	4.30003	-0.31106	-5.73151
H	4.49149	1.17189	-4.77995
H	3.25450	1.09290	-6.05303
H	1.11589	-0.19704	-5.70425
H	2.15331	-1.62611	-5.65628
H	0.96383	-1.35296	-4.36568
H	-5.58465	0.38829	0.42969
H	-2.00835	0.63657	1.45509
H	-5.32598	3.74993	-2.21753
H	-1.96947	4.80318	-0.98249
H	4.61129	-4.80661	-1.43224
H	-4.60532	0.95478	3.05974
H	-3.18962	2.03066	3.13140
H	-3.06105	0.35689	3.71406
H	-4.49365	-1.16116	1.45464
H	-3.13110	-1.28165	0.31588
H	-2.88591	-1.56741	2.05318
H	-4.12564	6.10911	-1.11546
H	-2.92204	6.56479	-2.34610
H	-4.31642	5.57669	-2.80043
H	-1.40460	4.75548	-3.39203
H	-1.41765	3.10390	-2.72918
H	-2.78330	3.67527	-3.71256
H	3.71481	-4.86360	-4.37058
H	2.59399	-4.88932	-2.99565
H	3.76429	-6.21418	-3.22852
H	6.18837	-4.23474	-4.00273
H	6.84238	-4.17182	-2.35251
H	6.29868	-5.72537	-3.03461
H	-7.44753	2.85820	-1.66931
H	-6.65646	0.01477	-2.52211
H	-6.52302	1.48397	-3.49717
H	-8.13196	0.87561	-3.04501
H	-7.73519	0.24026	-0.08832
H	-7.95193	1.86510	0.59401
H	-9.03370	1.27686	-0.69278
H	2.99399	4.36758	1.23033
H	-1.26038	5.84243	3.38534
H	3.03931	6.04584	3.04543
H	0.91108	6.81909	4.10795
N	-0.38383	-1.10281	3.17598
C	0.49662	2.36470	4.21566
C	0.33492	2.20792	5.60429
C	0.24706	1.31217	3.33063
C	-0.07458	0.98522	6.14813
C	-0.14756	0.08434	3.87247
C	-0.30916	-0.07392	5.26571
C	-0.72200	-2.17354	3.92793
S	-0.76072	-1.73195	5.63920
S	-1.10545	-3.75290	3.46290
H	0.83920	3.31625	3.82515
H	0.53619	3.04824	6.26696
H	0.39206	1.42178	2.26136
H	-0.19625	0.85569	7.22145
H	-0.31509	-1.11330	2.13591
O	0.37062	-0.52213	-2.11956
H	0.39401	-1.92006	-2.32460
O	0.45449	-2.96657	-2.42561
C	-0.43462	-3.60919	-1.67663
C	-1.88490	-3.35814	-1.83630
N	-0.04760	-4.48382	-0.78270
C	-2.80637	-4.29385	-1.32743
C	-2.33572	-2.16663	-2.42867
C	-0.54092	-4.16956	1.15802
C	1.32031	-4.43992	-0.26186
C	-4.17998	-4.04234	-1.42194
H	-2.43147	-5.21703	-0.90060
C	-3.70909	-1.88266	-2.46683
H	-1.61882	-1.44055	-2.79106
C	0.95829	-3.85700	1.13119
H	-1.28243	-3.42994	0.88934
H	-0.87477	-5.18509	1.34460
H	2.01456	-3.83650	-0.85701
H	1.71314	-5.45768	-0.13416
C	-4.64758	-2.82351	-1.97460
O	-5.14946	-4.91984	-1.01323
O	-4.22966	-0.72416	-2.95600
H	1.07955	-2.76604	1.12635
O	1.65597	-4.46136	2.20338
O	-5.98291	-2.53886	-2.10437
C	-4.72163	-6.11001	-0.34362
C	-3.31485	0.35641	-3.19904
C	2.98449	-3.91223	2.35482
C	-6.74075	-2.47392	-0.87844
H	-5.63887	-6.63457	-0.06070

H	-4.12228	-6.75015	-1.00800
H	-4.13707	-5.87256	0.55818
H	-2.64252	0.13192	-4.04033
H	-3.94252	1.21589	-3.44253
H	-2.72444	0.58368	-2.30266
H	3.51688	-4.64109	2.97760
H	3.48970	-3.86313	1.37565
C	2.98866	-2.55184	3.01574
H	-7.71314	-2.05469	-1.15539
H	-6.86857	-3.46699	-0.43298
H	-6.24474	-1.80863	-0.15857
C	2.98240	-2.45374	4.41850
C	2.99008	-1.37068	2.25153
C	3.02257	-1.20313	5.04606
H	2.95660	-3.36488	5.01743
C	3.03376	-0.11938	2.87786
H	2.98717	-1.42192	1.16417
C	3.06530	-0.03403	4.27471
H	3.02218	-1.13950	6.13391
H	3.02797	0.78409	2.27190
H	3.08421	0.93973	4.76089

PC (*R*)

C	-6.71714	-2.33456	-3.16991
C	-5.73449	-2.27184	-2.19698
C	-6.45289	0.02785	-3.65027
C	-7.09120	-1.17424	-3.89577
C	-5.07414	-1.04475	-1.90166
C	-4.05275	-0.93308	-0.89439
C	-5.42601	0.12296	-2.66780
C	-3.33865	0.26213	-0.80476
C	-3.75930	-2.04676	0.04790
C	-4.73616	1.34288	-2.43487
C	-3.67435	1.43123	-1.54577
C	-2.45912	-2.52956	0.18405
C	-2.97037	2.73795	-1.35009
C	-2.11267	-3.61659	1.03801
C	-3.20270	3.49538	-0.17545
C	-2.15442	3.26510	-2.38542
C	-3.13720	-4.24006	1.73319
C	-0.69705	-4.08574	1.16580
C	-2.67039	4.79183	-0.09150
C	-4.02777	2.96082	0.99207
C	-1.66074	4.57254	-2.25851
C	-1.79760	2.44554	-3.62408
C	0.07214	-3.72227	2.30148
C	-0.14097	-4.91744	0.16414
C	-1.92249	5.36122	-1.12817
C	-3.15805	2.79266	2.25503
C	-5.25934	3.84618	1.26751
C	-2.58558	2.92085	-4.86148
C	-0.28339	2.46377	-3.91069
C	1.38462	-4.20937	2.40889
C	-0.50794	-2.85475	3.41774
C	1.17226	-5.38407	0.32376
C	-0.93396	-5.31868	-1.07603
C	-1.41337	6.79328	-1.02331
C	1.95641	-5.03528	1.43161
C	-1.08931	-3.73734	4.54373
C	0.50484	-1.86078	4.01654
C	-0.28187	-4.77553	-2.36254
C	-1.13448	-6.84529	-1.14355
C	0.12511	6.85931	-0.95922
C	-1.95843	7.66679	-2.17086
C	3.37337	-5.57895	1.55631
C	4.35071	-4.60275	2.23186
C	3.35799	-6.93851	2.28759
C	-4.79177	-2.61844	0.87404
C	-4.47325	-3.75774	1.69619
C	-6.11335	-2.08996	0.93905
C	-5.49590	-4.35654	2.48619
C	-7.08026	-2.68449	1.73146
C	-6.77742	-3.83708	2.50093
O	-2.29087	0.35519	0.10965
O	-1.44925	-1.97278	-0.60089
O	-0.16709	0.04357	-1.44419
O	-0.17392	-0.48507	1.13202
P	-0.88393	-0.45892	-0.22073
H	-7.20368	-3.28568	-3.38466
H	-5.44881	-3.16840	-1.65241
H	-6.71526	0.92246	-4.21586
H	-7.87076	-1.23668	-4.65445
H	-5.04039	2.23357	-2.98278
H	-2.90857	-5.11106	2.34570
H	-2.84921	5.38041	0.80836
H	-4.40463	1.96753	0.71903
H	-1.04952	4.98234	-3.06209
H	-2.07518	1.40340	-3.42079
H	-3.76147	2.39576	3.08408
H	-2.72481	3.75064	2.57005
H	-2.33274	2.09815	2.06352
H	-5.87607	3.40777	2.06471
H	-4.96552	4.85515	1.58821
H	-5.88010	3.94615	0.36682
H	-2.32293	2.31795	-5.74242
H	-2.35336	3.97135	-5.08782
H	-3.66867	2.84256	-4.70534
H	-0.04438	1.75605	-4.71698
H	0.05890	3.45688	-4.23327
H	0.28508	2.17790	-3.02148
H	1.97718	-3.92556	3.27558
H	-1.32615	-2.26628	2.98367
H	1.60756	-6.02416	-0.44521
H	-1.92997	-4.86452	-1.00001
H	-1.80142	7.20439	-0.07768
H	-0.30000	-4.36459	4.98255
H	-1.88024	-4.39976	4.17458
H	-1.51285	-3.11261	5.34304
H	-0.01404	-1.16102	4.68563
H	1.27502	-2.37007	4.61254
H	1.00190	-1.27916	3.23629
H	0.71747	-5.20671	-2.51661

H	-0.18609	-3.68484	-2.31333
H	-0.89272	-5.02832	-3.24061
H	-0.17416	-7.37073	-1.23990
H	-1.63114	-7.21489	-0.23635
H	-1.75376	-7.11474	-2.01055
H	0.46524	7.90098	-0.87257
H	0.57764	6.43248	-1.86522
H	0.50084	6.29884	-0.09559
H	-1.58114	7.32028	-3.14301
H	-3.05556	7.63397	-2.20490
H	-1.64619	8.71294	-2.04411
H	3.73712	-5.75372	0.53105
H	5.37660	-4.99025	2.16825
H	4.11707	-4.47165	3.29755
H	4.32456	-3.61832	1.75124
H	2.98616	-6.81441	3.31476
H	2.70125	-7.65454	1.77592
H	4.36832	-7.36887	2.33849
H	-6.35675	-1.20231	0.36134
H	-5.24080	-5.22515	3.09411
H	-8.08254	-2.25849	1.76897
H	-7.55030	-4.29917	3.11435
N	1.52072	2.20077	-0.61100
C	4.93329	1.59232	-1.83577
C	3.53356	1.48570	-1.79523
C	2.87407	0.46366	-2.49690
C	3.62330	-0.46954	-3.22957
C	5.03293	-0.39341	-3.24726
C	5.68414	0.64875	-2.54906
C	2.80271	2.50700	-0.96561
C	1.02041	2.23350	2.36257
C	0.65328	3.18928	0.00723
C	1.01674	3.50139	1.46813
C	0.48858	5.42316	2.83549
C	0.88003	4.84333	4.17737
C	-0.11297	4.35840	5.04858
C	2.23054	4.67386	4.52163
C	0.23913	3.70284	6.23327
C	2.58755	4.01907	5.70953
C	1.59224	3.52726	6.56376
C	1.64787	-1.59972	-3.95845
C	5.88315	-1.18180	-5.30073
C	7.74855	1.64775	-1.88807
O	3.35427	3.56088	-0.59849
O	0.01483	4.42373	1.91559
O	3.07982	-1.50663	-3.93623
O	5.78249	-1.36306	-3.87538
O	7.05324	0.62984	-2.61304
H	5.39468	2.40881	-1.29026
H	1.79531	0.37255	-2.46307
H	-0.37375	2.81225	-0.03832
H	0.69011	4.12522	-0.55755
H	2.00642	3.97816	1.48587
H	1.06251	1.35175	-0.95145
H	0.55185	2.45464	3.32428
H	0.48126	1.39377	1.91359
H	-0.35399	6.11899	2.93948
H	1.33882	5.96845	2.39210
H	-1.16311	4.47729	4.77991
H	3.00516	5.04223	3.84836
H	-0.53789	3.32583	6.89790
H	3.63941	3.88702	5.96139
H	1.86706	3.01190	7.48359
H	1.42178	-2.50143	-4.53509
H	1.20163	-0.72130	-4.44770
H	1.23463	-1.68780	-2.94598
H	4.89193	-1.21948	-5.77367
H	6.49948	-2.00835	-5.67137
H	6.37100	-0.22438	-5.53789
H	8.81282	1.45421	-2.05331
H	7.52686	1.59584	-0.81085
H	7.49492	2.65249	-2.25838
N	2.36938	-0.42132	1.09115
C	3.28431	-3.20034	-1.19467
C	4.67866	-3.00667	-1.20152
C	2.43891	-2.37876	-0.44862
C	5.27485	-1.99097	-0.44654
C	3.03113	-1.34783	0.29147
C	4.43346	-1.16736	0.30786
C	3.15924	0.45166	1.71149
S	4.85008	0.19868	1.33766
S	2.71757	1.67968	2.85672
H	2.85069	-4.00592	-1.78082
H	5.30709	-3.64003	-1.82304
H	1.36670	-2.54400	-0.41158
H	6.34961	-1.83105	-0.46845
H	1.26523	-0.42434	1.13123

PC (*S*)

C	-5.57743	2.61436	4.27594
C	-4.70409	2.51482	3.20630
C	-5.78766	0.20044	4.38468
C	-6.13287	1.45030	4.86671
C	-4.34005	1.24408	2.67587
C	-3.43309	1.09776	1.56872
C	-4.88339	0.06312	3.29379
C	-3.00675	-0.18194	1.21713
C	-2.97635	2.27995	0.79283
C	-4.52480	-1.21264	2.78063
C	-3.60044	-1.36215	1.75907
C	-1.61818	2.54177	0.65583
C	-3.36237	-2.68745	1.10568
C	-1.10558	3.70369	0.00858
C	-4.21809	-3.06028	0.03559
C	-2.31179	-3.53991	1.52101
C	-2.02580	4.59072	-0.53084
C	0.36326	3.95945	-0.08152
C	-3.96976	-4.26769	-0.63357
C	-5.44194	-2.21823	-0.33157
C	-2.10705	-4.73795	0.81702
C	-1.45477	-3.18080	2.73260
C	1.01692	3.92740	-1.34139

C	1.09906	4.26517	1.09303	H	3.04219	4.76126	1.88285
C	-2.90170	-5.10396	-0.27893	H	-0.62146	4.10103	2.35466
C	-5.72385	-2.11574	-1.84055	H	-1.64187	-6.76232	-0.69699
C	-6.68319	-2.77243	0.40225	H	-0.35788	5.79989	-2.80604
C	-2.18384	-3.56418	4.03955	H	-0.49583	4.87722	-4.32208
C	-0.05641	-3.81819	2.72042	H	1.09872	5.40487	-3.73510
C	2.39860	4.17801	-1.39010	H	0.89302	1.65286	-3.07072
C	0.26636	3.69375	-2.65187	H	0.36379	2.54763	-4.49219
C	2.47221	4.52377	0.98344	H	1.96280	2.87624	-3.79849
C	0.43694	4.36560	2.46498	H	0.01109	6.50411	2.27859
C	-2.61100	-6.38057	-1.05544	H	-0.03891	5.89506	3.95194
C	3.14772	4.46708	-0.24353	H	1.52226	6.14832	3.14114
C	0.11627	5.02411	-3.42105	H	0.97596	2.34995	3.10721
C	0.92055	2.63201	-3.55139	H	2.10957	3.60684	3.66728
C	0.48612	5.81500	2.98972	H	0.52180	3.43742	4.43793
C	1.05131	3.37893	3.47672	H	-3.44120	-8.39165	-1.29910
C	-3.67637	-7.45824	-0.76841	H	-4.66803	-7.11997	-1.10104
C	-2.48102	-6.11789	-2.56920	H	-3.73773	-7.67641	0.30617
C	4.64191	4.75491	-0.29641	H	-2.14947	-7.02786	-3.08856
C	5.38374	3.96260	-1.38531	H	-3.44764	-5.82477	-3.00275
C	4.88593	6.27115	-0.45475	H	-1.76632	-5.31211	-2.77759
C	-3.91539	3.14228	0.12737	H	5.05771	4.44816	0.67693
C	-3.42139	4.32440	-0.53045	H	6.46825	4.10403	-1.28373
C	-5.30621	2.84850	0.04100	H	5.10321	4.30164	-2.39215
C	-4.33941	5.18217	-1.20110	H	5.16876	2.89032	-1.31240
C	-6.16913	3.69275	-0.63678	H	4.40055	6.83564	0.35237
C	-5.68731	4.87577	-1.25416	H	5.96110	6.49972	-0.44042
O	-2.06288	-0.33826	0.20410	H	4.47260	6.62546	-1.40987
O	-0.71638	1.63250	1.21561	H	-5.68358	1.93918	0.50213
O	0.31683	-0.69282	1.29060	H	-3.95268	6.07661	-1.69033
O	-0.02187	0.49987	-1.02341	H	-7.22753	3.44241	-0.70281
P	-0.49791	0.20220	0.39703	H	-6.37868	5.53302	-1.78050
H	-5.83634	3.59619	4.67144	N	1.33083	-2.81147	-0.45061
H	-4.27637	3.41232	2.76594	C	4.91172	-3.20602	0.27059
H	-6.19798	-0.70290	4.83706	C	3.56777	-2.88610	0.52436
H	-6.82292	1.54370	5.70469	C	3.21437	-2.10746	1.63821
H	-5.00831	-2.09839	3.19007	C	4.21820	-1.62980	2.49372
H	-1.66661	5.50226	-1.00542	C	5.57529	-1.92455	2.23473
H	-4.61465	-4.55484	-1.46232	C	5.91626	-2.72040	1.11799
H	-5.27228	-1.19704	0.03474	C	2.56202	-3.40024	-0.46750
H	-1.28646	-5.39370	1.10460	C	1.35717	-2.52861	-3.47755
H	-1.31756	-2.09086	2.72074	C	0.24019	-3.24703	-1.31140
H	-5.95493	-3.09304	-2.28525	C	0.12230	-2.37212	-2.57693
H	-4.87901	-1.68138	-2.38426	C	-2.22261	-2.06659	-2.94998
H	-6.59568	-1.46855	-2.00791	C	-2.29424	-0.64525	-3.48265
H	-7.56699	-2.15349	0.19234	C	-2.95182	0.35690	-2.74804
H	-6.89558	-3.79874	0.07054	C	-1.74910	-0.32128	-4.73634
H	-6.52829	-2.79447	1.48769	C	-3.07522	1.65519	-3.25885
H	-2.37528	-4.64659	4.06507	C	-1.86600	0.97711	-5.24783
H	-3.14370	-3.04573	4.13758	C	-2.53303	1.96830	-4.51256
H	-1.56659	-3.30596	4.91192	C	2.61960	-0.52946	3.89287
H	-0.10352	-4.90252	2.89549	C	6.77945	-2.03516	4.26310
H	0.46106	-3.64752	1.77174	C	7.64341	-3.69155	-0.21283
H	0.55362	-3.38730	3.52519	O	2.86220	-4.29533	-1.28224
H	2.89840	4.14514	-2.35604	O	-1.03068	-2.76858	-3.33628
H	-0.73782	3.32728	-2.41175	O	3.98768	-0.83662	3.58331

O	6.57580	-1.37046	3.00095
O	7.25765	-2.93047	0.93540
H	5.13063	-3.82046	-0.59622
H	2.18051	-1.84990	1.83122
H	0.40822	-4.29242	-1.59208
H	-0.69312	-3.18626	-0.74264
H	0.00626	-1.32715	-2.26548
H	1.11927	-2.05039	0.19979
H	1.05053	-2.96097	-4.43760
H	2.12525	-3.16915	-3.03319
H	-3.04039	-2.67168	-3.36523
H	-2.34658	-2.06564	-1.85777
H	-3.34328	0.12882	-1.76026
H	-1.22518	-1.09224	-5.30001
H	-3.58000	2.42096	-2.67124
H	-1.43402	1.21717	-6.21974
H	-2.61774	2.98037	-4.90838
H	2.65920	0.14273	4.75511
H	2.11688	-0.03571	3.05217
H	2.06164	-1.43999	4.15659
H	7.59579	-1.50050	4.76094
H	5.87418	-1.98863	4.88382
H	7.06896	-3.08504	4.10642
H	8.73647	-3.73298	-0.18638
H	7.23485	-4.71255	-0.17668
H	7.31467	-3.20579	-1.14466
N	2.45974	0.18367	-1.48304
C	4.10440	1.61282	1.51829
C	5.42176	1.18918	1.24782
C	3.05180	1.30706	0.65970
C	5.72968	0.45617	0.09941
C	3.35238	0.56458	-0.49170
C	4.68054	0.15704	-0.77867
C	3.00152	-0.46562	-2.51110
S	4.71832	-0.69055	-2.31343
S	2.16750	-0.93431	-3.98308
H	3.90119	2.19126	2.41541
H	6.21293	1.40856	1.96050
H	2.04264	1.65750	0.84551
H	6.74286	0.11515	-0.09539
H	1.36364	0.34194	-1.33453

Structures with substrate 1-Bz

TS 9-Bz (S)

Imaginary frequency: -444.73 cm^{-1}

C	-1.93956	5.89640	-3.52752
C	-1.97755	4.86844	-2.60128
C	0.38882	5.42849	-4.01668
C	-0.74422	6.19118	-4.23280
C	-0.81980	4.08358	-2.33060
C	-0.80618	3.01703	-1.36527
C	0.37902	4.35326	-3.08241
C	0.32420	2.20364	-1.28635
C	-1.97420	2.74317	-0.48504
C	1.51415	3.51751	-2.90858
C	1.49715	2.41574	-2.06480
C	-2.53869	1.46669	-0.45752
C	2.67375	1.49206	-2.01739
C	-3.68873	1.13209	0.31556
C	3.54584	1.49147	-0.90242
C	2.96062	0.67841	-3.14615
C	-4.25954	2.14229	1.07673
C	-4.28598	-0.24066	0.30915
C	4.71995	0.72068	-0.95839
C	3.26725	2.32602	0.34393
C	4.15804	-0.05296	-3.16369
C	2.02194	0.58534	-4.34809
C	-4.25417	-1.03087	1.48797
C	-4.95377	-0.72067	-0.84688
C	5.06136	-0.03230	-2.09029
C	3.03591	1.42225	1.56862
C	4.39307	3.34509	0.60985
C	2.59554	1.34771	-5.56051
C	1.70690	-0.87526	-4.72809
C	-4.94872	-2.25198	1.49967
C	-3.48837	-0.60600	2.74004
C	-5.62300	-1.95255	-0.78448
C	-5.00286	0.07104	-2.15043
C	6.40746	-0.73923	-2.17902
C	-5.65245	-2.72572	0.38573
C	-4.43525	-0.08320	3.83986
C	-2.61638	-1.74653	3.29963
C	-6.44678	0.48746	-2.49606
C	-4.34597	-0.71215	-3.30448
C	6.30183	-2.20763	-2.62827
C	7.35686	0.04941	-3.10629
C	-6.44885	-4.02174	0.45999
C	-7.95988	-3.74483	0.31927
C	-5.97926	-5.05957	-0.57708
C	-2.51523	3.75114	0.38844
C	-3.68666	3.43933	1.16572
C	-1.91027	5.02964	0.56053
C	-4.22981	4.42847	2.03474
C	-2.45740	5.96594	1.42192
C	-3.63283	5.66987	2.15950
O	0.32967	1.15395	-0.36905
O	-1.97586	0.46954	-1.25199
O	0.01500	-0.97024	-1.89348
O	-0.75629	-0.90192	0.61391
P	-0.55752	-0.20942	-0.72592
H	-2.83883	6.48019	-3.72214
H	-2.90202	4.64565	-2.07464
H	1.30648	5.62599	-4.57152
H	-0.72731	7.00695	-4.95481
H	2.41465	3.72687	-3.48417
H	-5.16270	1.92785	1.64514
H	5.39738	0.72789	-0.10564
H	2.34645	2.89721	0.17159
H	4.39409	-0.64760	-4.04510
H	1.07254	1.05812	-4.06810
H	2.21177	0.72806	1.37666

H	2.77541	2.02138	2.45204
H	3.93365	0.84220	1.80897
H	5.34039	2.84003	0.84287
H	4.55683	3.99066	-0.26357
H	4.13534	3.98224	1.46756
H	3.55362	0.91092	-5.87661
H	2.77066	2.40550	-5.32730
H	1.90222	1.29531	-6.41172
H	0.97320	-0.89676	-5.54613
H	2.60248	-1.40843	-5.07625
H	1.28319	-1.41155	-3.87382
H	-4.94592	-2.85453	2.40813
H	-2.81662	0.21304	2.45651
H	-6.15014	-2.30704	-1.67006
H	-4.42905	0.99509	-2.01399
H	6.84781	-0.72716	-1.17060
H	-5.13067	-0.87233	4.15931
H	-5.03200	0.76952	3.49458
H	-3.85834	0.23838	4.71864
H	-3.22789	-2.56791	3.69643
H	-1.95464	-2.15115	2.52708
H	-1.99857	-1.37391	4.12706
H	-6.89241	1.07095	-1.67899
H	-6.46204	1.10169	-3.40733
H	-7.08519	-0.38966	-2.67084
H	-4.33154	-0.10350	-4.21951
H	-3.31453	-0.98286	-3.05167
H	-4.89952	-1.63565	-3.52532
H	5.90137	-2.28791	-3.64778
H	5.64489	-2.78520	-1.96663
H	7.29295	-2.68133	-2.62374
H	6.96258	0.07130	-4.13197
H	7.46562	1.08720	-2.76478
H	8.35283	-0.41479	-3.13314
H	-6.27898	-4.45001	1.46043
H	-8.18951	-3.32529	-0.67023
H	-8.30050	-3.02635	1.07653
H	-8.53806	-4.67224	0.43561
H	-6.12838	-4.68858	-1.60079
H	-4.91413	-5.29035	-0.45342
H	-6.54976	-5.99313	-0.47475
H	-0.99929	5.26042	0.01505
H	-5.11948	4.17916	2.61352
H	-1.97362	6.93473	1.54239
H	-4.05333	6.41581	2.83301
N	1.49802	-3.09369	-1.05056
C	-0.57314	-5.48118	-2.99599
C	-0.24190	-4.52528	-2.01456
C	-1.26801	-3.78976	-1.38590
C	-2.60106	-3.98592	-1.75805
C	-2.92020	-4.91770	-2.75575
C	-1.90584	-5.67010	-3.36890
C	1.19923	-4.32987	-1.69355
C	1.41108	-3.05450	0.92144
C	2.91302	-2.70888	-0.79205
C	2.84248	-2.55382	0.74512
C	5.09180	-2.96591	1.42667
C	5.37313	-1.72415	2.25706
C	4.65971	-1.46188	3.43841
C	6.40014	-0.84618	1.87347
C	4.95818	-0.33124	4.20966
C	6.70513	0.28174	2.64681
C	5.97894	0.54537	3.81629
O	2.08183	-5.14860	-1.93671
O	3.73007	-3.40804	1.45440
H	0.22785	-6.05027	-3.46392
H	-1.04545	-3.06960	-0.60535
H	3.55914	-3.54260	-1.08237
H	3.17238	-1.80444	-1.34831
H	2.94870	-1.51120	1.07425
H	0.89463	-2.29335	-1.36934
H	1.25288	-4.11402	1.10041
H	0.56108	-2.38435	0.94008
H	5.66162	-3.81922	1.82058
H	5.42945	-2.80051	0.38913
H	3.85975	-2.13642	3.73632
H	6.96890	-1.04953	0.96586
H	4.38616	-0.13349	5.11545
H	7.50032	0.95664	2.33046
H	6.20423	1.42883	4.41307
N	0.29500	-0.30341	2.95397
C	-0.74606	3.22230	3.52318
C	-0.30689	3.34813	4.85543
C	-0.56820	2.03035	2.81492
C	0.31785	2.28274	5.51725
C	0.05111	0.96204	3.47704
C	0.49009	1.08512	4.81419
C	0.87507	-1.19616	3.78125
S	1.21239	-0.43330	5.34859
S	1.23446	-2.82201	3.48434
H	-1.22907	4.06231	3.02991
H	-0.45444	4.28860	5.38424
H	-0.88779	1.92532	1.78342
H	0.65567	2.38059	6.54683
H	-0.07204	-0.55792	1.99291
H	-2.15516	-6.39843	-4.13975
H	-3.95883	-5.06108	-3.05127
H	-3.38432	-3.40601	-1.27355

TS 9-Bz (R)

Imaginary frequency: -444.46 cm^{-1}

C	-1.26794	6.46089	-2.74705
C	-1.39792	5.32599	-1.96510
C	0.97210	5.80368	-3.40464
C	-0.06981	6.71134	-3.46437
C	-0.33426	4.38454	-1.85949
C	-0.41947	3.19891	-1.05001
C	0.86625	4.61911	-2.62110
C	0.61329	2.26731	-1.12309
C	-1.58632	2.93103	-0.16735
C	1.91095	3.65566	-2.59398
C	1.79474	2.46524	-1.89187

C	-2.30110	1.74036	-0.30556
C	2.88980	1.44687	-1.91392
C	-3.47468	1.44122	0.44646
C	3.73926	1.31149	-0.78955
C	3.10995	0.66467	-3.07661
C	-3.89274	2.38153	1.37754
C	-4.26749	0.18886	0.23634
C	4.82741	0.42665	-0.86572
C	3.52777	2.13400	0.47835
C	4.21847	-0.19592	-3.10786
C	2.20579	0.76358	-4.30346
C	-4.32758	-0.79353	1.26112
C	-5.03042	0.02623	-0.94635
C	5.09782	-0.31982	-2.02119
C	3.30370	1.23919	1.71075
C	4.69669	3.11338	0.70551
C	2.87860	1.60296	-5.41003
C	1.79402	-0.61591	-4.85224
C	-5.19378	-1.88540	1.09944
C	-3.47653	-0.70437	2.52707
C	-5.87478	-1.09094	-1.06152
C	-4.98073	1.02858	-2.09525
C	6.36242	-1.16398	-2.12289
C	-5.98219	-2.05215	-0.04860
C	-4.30894	-0.24897	3.74313
C	-2.76931	-2.03579	2.84395
C	-4.44702	0.36967	-3.38308
C	-6.35386	1.69153	-2.32271
C	6.11794	-2.57817	-2.67965
C	7.42371	-0.42207	-2.96356
C	-6.93053	-3.23473	-0.19117
C	-6.21378	-4.58692	-0.00907
C	-8.11801	-3.10299	0.78478
C	-1.97066	3.84734	0.87275
C	-3.15142	3.56312	1.64602
C	-1.20006	4.99704	1.21076
C	-3.53657	4.45889	2.68398
C	-1.59457	5.84121	2.23537
C	-2.77753	5.57832	2.97384
O	0.52017	1.10620	-0.35714
O	-1.87071	0.80831	-1.24968
O	-0.06222	-0.74826	-2.13548
O	-0.78860	-0.92106	0.38062
P	-0.52519	-0.08620	-0.86307
H	-2.09632	7.16535	-2.81734
H	-2.32369	5.13921	-1.42649
H	1.88965	5.97304	-3.96893
H	0.02080	7.61134	-4.07175
H	2.82312	3.85188	-3.15573
H	-4.80740	2.19730	1.93830
H	5.49100	0.33295	-0.00721
H	2.62414	2.73975	0.34051
H	4.40778	-0.77135	-4.01276
H	1.28615	1.27799	-3.99751
H	2.53071	0.48968	1.51357
H	2.98667	1.84490	2.57099
H	4.22036	0.70979	1.99061
H	5.63875	2.57188	0.87009
H	4.83189	3.77556	-0.16060
H	4.50860	3.73657	1.59133
H	3.81241	1.12691	-5.74206
H	3.12427	2.61266	-5.05822
H	2.21562	1.69588	-6.28182
H	2.65493	-1.17394	-5.24586
H	1.30999	-1.21165	-4.07300
H	1.08096	-0.48926	-5.67876
H	-5.25025	-2.63051	1.89146
H	-2.69704	0.04636	2.35068
H	-6.46712	-1.21676	-1.96880
H	-4.28162	1.82825	-1.82344
H	6.76714	-1.27027	-1.10418
H	-5.10415	-0.97564	3.96268
H	-4.78282	0.72507	3.57202
H	-3.66891	-0.16462	4.63295
H	-3.48608	-2.82662	3.10284
H	-2.17155	-2.37498	1.99179
H	-2.10340	-1.90893	3.70723
H	-5.12661	-0.41768	-3.73829
H	-3.46285	-0.07981	-3.20820
H	-4.35163	1.11692	-4.18338
H	-7.11013	0.95337	-2.62354
H	-6.70828	2.18328	-1.40664
H	-6.28786	2.44799	-3.11723
H	5.38351	-3.12796	-2.07785
H	7.05342	-3.15396	-2.68440
H	5.74526	-2.54438	-3.71209
H	7.06922	-0.28540	-3.99488
H	7.63061	0.57111	-2.54392
H	8.36461	-0.98936	-2.99742
H	-7.33403	-3.20491	-1.21599
H	-5.81983	-4.69284	1.01104
H	-5.37280	-4.68912	-0.70598
H	-6.91203	-5.41737	-0.18335
H	-7.76801	-3.12741	1.82639
H	-8.65119	-2.15546	0.63080
H	-8.83016	-3.92876	0.64704
H	-0.28400	5.19839	0.66164
H	-4.43540	4.23289	3.25819
H	-0.98533	6.70998	2.48276
H	-3.07707	6.25157	3.77629
N	1.02891	-3.20268	-1.65798
C	-1.58994	-4.93053	-3.64348
C	-1.00980	-4.17744	-2.60249
C	-1.82606	-3.35394	-1.80090
C	-3.19557	-3.25863	-2.05990
C	-3.76197	-3.98620	-3.11559
C	-2.95904	-4.82849	-3.90209
C	0.45835	-4.28688	-2.38869
C	0.98259	-3.41240	0.29860
C	2.50007	-3.16932	-1.41843
C	2.49983	-3.45927	0.10252
C	4.54439	-2.74473	1.07994

C	5.06772	-1.88206	2.20275
C	4.33821	-1.75903	3.39708
C	6.28891	-1.20188	2.07677
C	4.80365	-0.94126	4.43167
C	6.76306	-0.38883	3.11584
C	6.01534	-0.24816	4.29228
O	1.15057	-5.22607	-2.77255
O	3.14597	-2.47846	0.88791
H	-0.95047	-5.57294	-4.24598
H	-1.41374	-2.78840	-0.97187
H	2.87880	-2.16561	-1.63621
H	2.99967	-3.91757	-2.03921
H	2.88894	-4.46263	0.33742
H	0.59082	-2.26643	-1.86074
H	0.46799	-2.47223	0.45190
H	0.39630	-4.32283	0.35089
H	5.10705	-2.54919	0.15402
H	4.67462	-3.81475	1.32880
H	3.39966	-2.29643	3.49858
H	6.87065	-1.30196	1.16038
H	4.21607	-0.84127	5.34405
H	7.70794	0.14168	2.99992
H	6.37450	0.39544	5.09502
N	0.33398	-0.93395	2.75602
C	-0.32053	2.54991	3.88230
C	0.00620	2.38470	5.24258
C	-0.22586	1.48331	2.98387
C	0.43054	1.14632	5.74273
C	0.19665	0.24384	3.48363
C	0.51875	0.07398	4.84791
C	0.71383	-2.02882	3.44342
S	0.98501	-1.60170	5.14720
S	0.90115	-3.61494	2.88154
H	-0.65009	3.52010	3.51775
H	-0.07300	3.23234	5.92164
H	-0.46149	1.59871	1.93070
H	0.67919	1.01968	6.79431
H	-0.01637	-0.96076	1.75889
H	-3.40023	-5.39902	-4.71860
H	-4.82865	-3.89830	-3.32154
H	-3.81453	-2.61383	-1.44190

TS 9-Bz (R) *arr1*

Imaginary frequency: -440.84 cm^{-1}

C	0.99924	-4.78550	-3.23002
C	0.45010	-3.89213	-2.28910
C	1.17133	-3.59652	-1.11391
C	2.42415	-4.17526	-0.89223
C	2.97151	-5.04842	-1.84140
C	2.25770	-5.35140	-3.01145
H	0.42887	-5.01367	-4.12816
C	-0.89721	-3.31698	-2.58219
H	0.78072	-2.89485	-0.38632
O	-1.68511	-3.81075	-3.38681
N	-1.24466	-2.17840	-1.81685
C	-1.95602	-2.58266	0.03013
C	-2.59630	-1.56629	-1.94681
C	-3.14739	-1.79441	-0.52509
H	-3.17087	-2.13037	-2.68626
H	-2.52579	-0.51436	-2.23490
H	-3.27590	-0.85743	0.03449
O	-4.36422	-2.51048	-0.60330
H	4.81555	-2.47626	2.31312
C	3.88189	-2.97055	2.55826
C	3.90037	-4.27493	3.08952
C	2.68138	-2.29959	2.31163
H	4.85436	-4.76972	3.26234
H	2.66680	-1.29919	1.88427
O	0.71200	-0.50805	-0.99988
C	2.71255	-4.95268	3.38467
C	1.48952	-2.97453	2.61431
C	1.50527	-4.29099	3.13467
N	0.19637	-2.49638	2.43767
P	0.48996	0.40218	0.18397
H	-0.46392	-1.51456	-1.57921
H	2.72420	-5.96431	3.78440
C	-0.80300	-3.35224	2.73642
S	-0.14293	-4.87751	3.33810
S	-2.46020	-3.07826	2.48971
O	-0.23470	-0.10937	1.41970
H	-1.14770	-2.03161	0.48449
H	-1.91622	-3.66268	-0.05127
H	0.01232	-1.50588	2.07092
C	-5.12184	-2.56066	0.62034
H	-4.77840	-1.77851	1.31008
H	-4.94096	-3.53342	1.10756
C	-6.59438	-2.37306	0.34045
C	-7.18662	-2.89289	-0.82162
C	-7.39203	-1.67030	1.25933
C	-8.54798	-2.68625	-1.07403
H	-6.57049	-3.42983	-1.54006
C	-8.75649	-1.47041	1.01266
H	-6.93955	-1.26471	2.16534
C	-9.33627	-1.97148	-0.16069
H	-8.99339	-3.07966	-1.98770
H	-9.36047	-0.91211	1.72761
H	-10.39432	-1.80619	-0.36241
O	-0.25975	1.73957	-0.44331
C	-0.43293	2.86704	0.35039
C	0.68261	3.62074	0.70850
C	-1.77035	3.25712	0.65031
C	1.99294	3.35059	0.05824
C	0.49651	4.71081	1.62843
C	-1.94571	4.38452	1.44067
C	-2.93046	2.51355	0.07270
C	2.65912	4.40131	-0.67370
C	2.55752	2.07391	0.05446
C	-0.84391	5.09511	1.99022
C	1.58655	5.41722	2.21097
H	-2.95620	4.72641	1.66148
C	-3.11845	2.48917	-1.33621
C	-3.87222	1.87687	0.92173

C	2.07886	5.68447	-0.89634
C	3.95453	4.14002	-1.24456
C	3.81090	1.78652	-0.56140
O	1.92154	1.04104	0.74532
C	-1.03518	6.18874	2.88243
C	1.36647	6.46563	3.08778
H	2.60127	5.11349	1.96380
C	-4.24503	1.83876	-1.85872
C	-2.18706	3.21193	-2.30852
C	-4.98799	1.24319	0.34457
C	-3.71711	1.86233	2.44104
C	2.76412	6.66812	-1.58862
H	1.07845	5.88705	-0.52545
C	4.64238	5.17898	-1.93438
C	4.50175	2.83416	-1.15029
C	4.40400	0.41186	-0.58342
C	0.04580	6.86397	3.42005
H	-2.05463	6.47523	3.14262
H	2.21488	6.98652	3.53082
C	-5.19986	1.21632	-1.04104
H	-4.39665	1.84514	-2.93735
H	-1.36186	3.65311	-1.73891
H	-5.72282	0.76433	0.99199
H	-2.76790	2.35215	2.68692
C	4.06515	6.42447	-2.09802
H	2.29407	7.63789	-1.75004
H	5.62817	4.96314	-2.34754
H	5.48102	2.64029	-1.58622
C	4.17876	-0.43147	-1.69973
C	5.28002	0.01431	0.45538
H	-0.11330	7.69471	4.10688
C	-6.46691	0.61045	-1.62814
H	4.59612	7.21105	-2.63326
C	4.83756	-1.67053	-1.74272
C	3.32324	0.02539	-2.88021
C	5.93926	-1.22148	0.34968
C	5.59413	0.95629	1.61631
H	-6.93123	-0.00148	-0.84482
C	5.72712	-2.08054	-0.74001
H	4.67064	-2.33219	-2.59143
H	2.59067	0.74688	-2.49637
H	6.65428	-1.50563	1.12240
H	4.84657	1.76026	1.60251
C	6.49789	-3.38628	-0.89081
H	6.07461	-3.90919	-1.76287
C	4.20138	0.74150	-3.92982
H	4.70456	1.61984	-3.50981
H	4.97236	0.05732	-4.31270
H	3.58743	1.07364	-4.77917
C	2.53458	-1.11317	-3.54737
H	1.82345	-0.69435	-4.27275
H	3.19251	-1.80120	-4.09683
H	1.97368	-1.68411	-2.80583
C	5.50835	0.28361	2.99731
H	4.51205	-0.13904	3.17419
H	6.24691	-0.52262	3.10771
H	5.70867	1.02037	3.78732
C	6.97567	1.61048	1.40578
H	7.76889	0.84948	1.39793
H	7.01363	2.14691	0.44893
H	7.19520	2.32542	2.21127
C	7.98429	-3.10283	-1.19270
H	8.45882	-2.58178	-0.34920
H	8.53411	-4.03870	-1.36620
H	8.08949	-2.46794	-2.08221
C	6.35387	-4.31984	0.32443
H	5.30171	-4.54895	0.53071
H	6.88521	-5.26536	0.14751
H	6.78095	-3.86518	1.22923
C	-2.92221	4.38011	-2.99815
H	-3.75441	4.01930	-3.61828
H	-3.33303	5.07665	-2.25485
H	-2.23263	4.93629	-3.64864
C	-1.56791	2.24921	-3.34085
H	-1.01224	1.44827	-2.83988
H	-2.33911	1.79676	-3.98023
H	-0.87062	2.79114	-3.99517
C	-4.84588	2.65976	3.12413
H	-4.88614	3.69328	2.75470
H	-5.82573	2.19970	2.93346
H	-4.69279	2.68868	4.21203
C	-3.63229	0.43049	2.99679
H	-3.45346	0.45044	4.08103
H	-4.56635	-0.12412	2.82980
H	-2.81268	-0.12385	2.52734
C	-7.46473	1.72795	-1.99900
H	-7.05412	2.37239	-2.78963
H	-8.40809	1.29713	-2.36351
H	-7.68732	2.36121	-1.12962
C	-6.19272	-0.30842	-2.83076
H	-5.75226	0.24356	-3.67277
H	-5.51314	-1.11950	-2.54784
H	-7.13055	-0.75908	-3.18122
H	2.68296	-6.02877	-3.75110
H	3.95262	-5.49039	-1.67080
H	2.97345	-3.92882	0.01347

TS 9-Bz (R) *arr3*

Imaginary frequency: -447.81 cm^{-1}

C	0.96183	6.18527	-2.78158
C	0.73508	4.94836	-2.14253
C	-0.52639	4.67948	-1.57275
C	-1.53421	5.64726	-1.63734
C	-1.30340	6.87423	-2.27276
C	-0.05301	7.14041	-2.85148
H	1.94371	6.37524	-3.20964
C	1.88566	4.00849	-2.05965
H	-0.73958	3.72872	-1.08942
O	3.02092	4.29100	-2.43414
N	1.62163	2.75371	-1.43698
C	1.60655	2.75088	0.54281

C	2.76880	1.82304	-1.21384
C	2.92845	2.02906	0.30507
H	3.63076	2.14200	-1.80282
H	2.47145	0.80720	-1.47177
H	3.01707	1.09068	0.86267
O	3.96124	2.94480	0.66140
H	-0.87201	-4.37910	2.65415
C	-0.49325	-3.50452	3.17871
C	-0.29407	-3.55206	4.57259
C	-0.21686	-2.34284	2.45195
H	-0.51871	-4.46773	5.11757
H	-0.37333	-2.28563	1.38024
O	-0.74444	1.27182	-1.67673
C	0.18958	-2.44044	5.27633
C	0.26812	-1.23142	3.15464
C	0.47291	-1.27762	4.55083
N	0.59746	0.00575	2.61145
P	-0.50164	0.01047	-0.88103
H	0.71896	2.28400	-1.67556
H	0.34249	-2.48019	6.35276
C	1.05432	0.93912	3.46761
S	1.09361	0.27563	5.11600
S	1.52819	2.53034	3.12763
O	0.71882	-0.07626	0.01981
H	1.60311	3.81748	0.74463
H	0.67786	2.20461	0.59340
H	0.57930	0.11586	1.55232
C	5.28088	2.42089	0.49670
H	5.93856	3.28369	0.67293
H	5.44909	2.09651	-0.54471
C	5.63460	1.29242	1.45009
C	6.56493	0.31253	1.06532
C	5.08188	1.24036	2.74058
C	6.94694	-0.69784	1.95851
H	6.99742	0.34166	0.06427
C	5.45135	0.22319	3.62901
H	4.34850	1.98880	3.03504
C	6.38903	-0.74540	3.24369
H	7.66837	-1.45269	1.64603
H	5.00231	0.18599	4.62152
H	6.67404	-1.53845	3.93450
O	-0.55038	-1.24962	-1.95156
C	-0.50000	-2.53463	-1.41416
C	-1.66662	-3.07152	-0.87144
C	0.74880	-3.22681	-1.45718
C	-2.92329	-2.27395	-0.85842
C	-1.59447	-4.37259	-0.25548
C	0.76321	-4.53200	-0.98709
C	1.99759	-2.51849	-1.87302
C	-4.16056	-2.80664	-1.36876
C	-2.92994	-0.97784	-0.34068
C	-0.36712	-5.11982	-0.35716
C	-2.66182	-4.92933	0.50593
H	1.68856	-5.10333	-1.03528
C	2.13866	-1.99640	-3.18288
C	3.02989	-2.30925	-0.91395
C	-4.23290	-4.04107	-2.07601
C	-5.37560	-2.05381	-1.18612
C	-4.11810	-0.20915	-0.17139
O	-1.75205	-0.41127	0.13056
C	-0.28408	-6.40852	0.24412
C	-2.54244	-6.17704	1.09501
H	-3.57404	-4.35383	0.63607
C	3.28984	-1.26024	-3.50890
C	1.11037	-2.26136	-4.27864
C	4.15538	-1.56204	-1.29010
C	2.97504	-2.86360	0.50855
C	-5.44324	-4.52803	-2.53902
H	-3.31769	-4.59871	-2.25836
C	-6.60618	-2.59020	-1.66195
C	-5.31997	-0.77784	-0.56262
C	-4.02570	1.18094	0.36675
C	-1.34996	-6.93228	0.95330
H	0.64961	-6.96416	0.15324
H	-3.36920	-6.57724	1.68107
C	4.30351	-1.01748	-2.57449
H	3.38584	-0.86581	-4.51837
H	0.24263	-2.75189	-3.82226
H	4.93675	-1.37874	-0.55279
H	1.95649	-3.21620	0.70204
C	-6.64441	-3.80598	-2.32004
H	-5.47196	-5.47160	-3.08330
H	-7.51806	-2.01245	-1.50812
H	-6.24289	-0.21496	-0.42673
C	-4.24218	2.27666	-0.50105
C	-3.67176	1.39924	1.72708
H	-1.27043	-7.91447	1.41801
C	5.56231	-0.22439	-2.90560
H	-7.59114	-4.20350	-2.68443
C	-4.10116	3.57868	0.01290
C	-4.61256	2.09744	-1.97177
C	-3.50438	2.71439	2.17548
C	-3.54306	0.22481	2.69635
H	5.80620	0.36496	-2.00664
C	-3.70270	3.82064	1.33084
H	-4.29936	4.42713	-0.64274
H	-4.53338	1.03020	-2.21013
H	-3.20988	2.88905	3.20805
H	-3.06267	-0.60320	2.16047
C	-3.45939	5.23713	1.83250
H	-3.71363	5.92431	1.00944
C	3.29631	-1.80093	1.57127
H	4.34128	-1.47870	1.53071
H	2.66147	-0.92409	1.43229
H	3.11310	-2.20229	2.57715
C	3.92893	-4.06751	0.65865
H	3.84635	-4.50021	1.66586
H	3.71157	-4.85619	-0.07361
H	4.97152	-3.75268	0.50889
C	0.61334	-0.96278	-4.94236
H	0.22996	-0.26329	-4.19114
H	1.41691	-0.46510	-5.50308

H	-0.19456	-1.18594	-5.65317
C	1.68370	-3.24200	-5.32334
H	1.99474	-4.18285	-4.84926
H	0.93077	-3.47345	-6.09002
H	2.56064	-2.81264	-5.82782
C	5.40055	0.75957	-4.07437
H	4.53970	1.42570	-3.93069
H	6.30093	1.38038	-4.17192
H	5.26285	0.23010	-5.02738
C	6.74607	-1.18373	-3.15544
H	6.90409	-1.84800	-2.29574
H	6.54706	-1.81174	-4.03545
H	7.67400	-0.62279	-3.33598
C	-4.94426	-0.25624	3.13293
H	-5.55138	-0.55150	2.26851
H	-4.86196	-1.12085	3.80692
H	-5.47400	0.54597	3.66615
C	-2.67362	0.52374	3.92800
H	-1.71571	0.97131	3.63993
H	-3.17400	1.21202	4.62353
H	-2.46742	-0.40535	4.47443
C	-6.07357	2.52136	-2.22373
H	-6.76840	1.95478	-1.58926
H	-6.21640	3.58921	-2.00499
H	-6.34946	2.35177	-3.27406
C	-3.64509	2.83898	-2.91448
H	-3.89487	2.61156	-3.96064
H	-3.70967	3.92836	-2.79100
H	-2.61090	2.52981	-2.72642
C	-1.96954	5.44801	2.17631
H	-1.65685	4.78131	2.99181
H	-1.33166	5.23853	1.30819
H	-1.78735	6.48357	2.49634
C	-4.36214	5.59023	3.03056
H	-4.21044	6.63523	3.33484
H	-5.42225	5.45273	2.77949
H	-4.13531	4.95364	3.89683
H	0.12955	8.09206	-3.34902
H	-2.09575	7.62094	-2.31650
H	-2.49858	5.43664	-1.18524

TS 9-Bz (R) *arr4*

Imaginary frequency: -448.55 cm^{-1}

C	3.38778	5.08736	-2.39989
C	2.62721	4.08004	-1.76883
C	1.25223	4.28862	-1.53445
C	0.66236	5.49761	-1.91707
C	1.42213	6.49442	-2.54283
C	2.78748	6.28461	-2.79053
H	4.44787	4.90965	-2.56685
C	3.35670	2.86297	-1.32624
H	0.63316	3.52442	-1.07079
O	4.58148	2.75036	-1.39196
N	2.57392	1.84123	-0.71903
C	2.10134	2.10017	1.17138
C	3.26736	0.63202	-0.17475
C	2.98790	0.85367	1.32803
H	4.31963	0.64849	-0.45757
H	2.78930	-0.26992	-0.55407
H	2.40849	0.03135	1.74250
O	4.07088	1.03532	2.22388
H	-2.62040	-3.94006	2.70240
C	-2.18445	-3.13356	3.28750
C	-2.39495	-3.08337	4.67957
C	-1.42494	-2.15537	2.63900
H	-2.99308	-3.85540	5.16142
H	-1.25953	-2.17134	1.56695
O	-0.05708	1.22889	-1.49579
C	-1.84804	-2.05653	5.46143
C	-0.87840	-1.12791	3.42057
C	-1.08157	-1.07867	4.81696
N	-0.10285	-0.06846	2.96037
P	-0.42689	0.00825	-0.68427
H	1.63863	1.65041	-1.14759
H	-2.01144	-2.02121	6.53649
C	0.32967	0.81246	3.88499
S	-0.25132	0.32482	5.49359
S	1.26586	2.20353	3.65102
O	0.48538	-0.42655	0.44917
H	2.50423	3.09252	1.35880
H	1.03731	2.01860	0.99754
H	0.13334	-0.03560	1.92556
C	5.28347	1.60540	1.71554
H	5.72772	2.12985	2.57444
H	5.09586	2.35632	0.93482
C	6.25300	0.54989	1.20987
C	7.17303	0.85663	0.19388
C	6.27642	-0.72926	1.79234
C	8.11981	-0.09230	-0.21592
H	7.13817	1.83558	-0.28377
C	7.21828	-1.67947	1.37900
H	5.54802	-0.96990	2.56488
C	8.14912	-1.36054	0.37940
H	8.82598	0.15555	-1.00817
H	7.22443	-2.66970	1.83457
H	8.87982	-2.10076	0.05549
O	-0.68564	-1.22403	-1.75653
C	-1.13096	-2.43028	-1.21822
C	-2.47952	-2.54941	-0.88833
C	-0.17148	-3.47536	-1.04505
C	-3.40900	-1.41305	-1.13441
C	-2.91802	-3.76689	-0.25466
C	-0.63939	-4.68648	-0.55633
C	1.27638	-3.20472	-1.29510
C	-4.63284	-1.58922	-1.87485
C	-3.10273	-0.13440	-0.66616
C	-1.98316	-4.85525	-0.12244
C	-4.21854	-3.92182	0.30441
H	0.05344	-5.51881	-0.44310
C	1.71818	-2.80669	-2.58328
C	2.20396	-3.25755	-0.21562
C	-4.95879	-2.80262	-2.54652

C	-5.55768	-0.48834	-1.97282
C	-3.99094	0.97458	-0.78383
O	-1.92398	0.08966	0.03434
C	-2.40637	-6.06350	0.50223
C	-4.59337	-5.10358	0.92136
H	-4.91565	-3.08974	0.25706
C	3.05549	-2.42122	-2.76124
C	0.80562	-2.85311	-3.80583
C	3.52982	-2.86166	-0.45023
C	1.82990	-3.75083	1.18207
C	-6.15188	-2.93918	-3.23536
H	-4.25072	-3.62688	-2.52083
C	-6.78282	-0.66673	-2.67667
C	-5.21486	0.76575	-1.39840
C	-3.55204	2.31670	-0.29790
C	-3.68653	-6.19067	1.01138
H	-1.69003	-6.88074	0.59029
H	-5.59047	-5.19457	1.35102
C	3.97305	-2.41363	-1.70384
H	3.38140	-2.11122	-3.75220
H	-0.21911	-3.03964	-3.46386
H	4.24284	-2.87241	0.37462
H	0.73862	-3.82527	1.24089
C	-7.08123	-1.86919	-3.29120
H	-6.37507	-3.87560	-3.74597
H	-7.47556	0.17347	-2.73333
H	-5.91563	1.59574	-1.48320
C	-3.19977	3.31325	-1.23722
C	-3.42876	2.56483	1.09608
H	-3.99462	-7.11650	1.49604
C	5.41866	-1.96957	-1.87516
H	-8.01936	-1.99191	-3.83153
C	-2.72775	4.54901	-0.75871
C	-3.30924	3.09077	-2.74392
C	-2.91504	3.79660	1.51776
C	-3.90862	1.52992	2.11174
H	5.73916	-1.55390	-0.91074
C	-2.54532	4.79984	0.60480
H	-2.48572	5.33355	-1.47625
H	-3.53353	2.03027	-2.90969
H	-2.79281	3.98389	2.58250
H	-3.66563	0.53514	1.71761
C	-1.93130	6.10619	1.08843
H	-1.77251	6.74130	0.20201
C	2.26198	-2.79383	2.30622
H	1.93085	-3.18128	3.27948
H	3.35171	-2.66587	2.35066
H	1.80370	-1.81346	2.15810
C	2.40971	-5.16167	1.41765
H	2.08953	-5.55422	2.39319
H	2.08609	-5.86542	0.63921
H	3.50858	-5.13635	1.40404
C	1.19937	-4.03999	-4.71083
H	2.22264	-3.91965	-5.09346
H	1.15604	-4.98739	-4.15651
H	0.52015	-4.11165	-5.57219
C	0.79739	-1.52876	-4.59259
H	0.55383	-0.68664	-3.93542
H	1.77139	-1.33295	-5.06238
H	0.04849	-1.57138	-5.39575
C	5.61538	-0.87468	-2.93567
H	6.65230	-0.51557	-2.90808
H	5.42106	-1.24945	-3.95046
H	4.95638	-0.01510	-2.75786
C	6.32076	-3.18632	-2.16839
H	7.37424	-2.88073	-2.23057
H	6.22903	-3.94290	-1.37782
H	6.03836	-3.65524	-3.12215
C	-3.23046	1.64452	3.48544
H	-2.14187	1.71095	3.38408
H	-3.57317	2.52999	4.03885
H	-3.46601	0.76308	4.09545
C	-5.44402	1.60728	2.25794
H	-5.74188	2.59568	2.63591
H	-5.94380	1.44433	1.29510
H	-5.80317	0.84620	2.96530
C	-4.47635	3.90898	-3.33250
H	-4.57843	3.71739	-4.41000
H	-5.42730	3.65423	-2.84570
H	-4.30822	4.98667	-3.19473
C	-1.99029	3.38978	-3.48200
H	-2.08799	3.12340	-4.54407
H	-1.72881	4.45551	-3.43481
H	-1.16654	2.81101	-3.04967
C	-2.86673	6.86804	2.04720
H	-3.84209	7.05681	1.57945
H	-3.03972	6.29528	2.96869
H	-2.42597	7.83357	2.33198
C	-0.55361	5.85453	1.73755
H	-0.09173	6.80196	2.04933
H	-0.64926	5.21496	2.62581
H	0.12613	5.35451	1.03583
H	3.38090	7.05569	-3.28010
H	0.95157	7.43219	-2.83674
H	-0.39361	5.65540	-1.71980

TS 9-Bz (R) *arr5*

Imaginary frequency: -464.88 cm^{-1}

C	-0.89044	-5.33524	-1.89993
C	-0.98030	-3.99914	-1.45989
C	-0.09248	-3.53406	-0.46794
C	0.86370	-4.39579	0.07480
C	0.94690	-5.72281	-0.36657
C	0.07318	-6.18968	-1.36075
H	-1.58644	-5.68114	-2.66118
C	-2.06676	-3.15880	-2.03657
H	-0.12252	-2.50303	-0.13360
O	-3.00035	-3.61819	-2.69416
N	-2.03341	-1.78449	-1.68477
C	-2.75807	-1.48154	0.11922
C	-3.16344	-0.89672	-2.07735
C	-3.72124	-0.58213	-0.66438

H	-3.85426	-1.45098	-2.71479
H	-2.78994	-0.02052	-2.61188
H	-3.55737	0.46215	-0.37568
O	-5.09510	-0.81314	-0.41097
H	3.35403	-3.19340	3.58917
C	2.28547	-3.21515	3.78700
C	1.77346	-4.08704	4.76847
C	1.44112	-2.37921	3.05189
H	2.45408	-4.73208	5.32172
H	1.81898	-1.70817	2.28451
O	0.27497	-0.42936	-1.39900
C	0.40119	-4.14228	5.04704
C	0.06875	-2.43647	3.33088
C	-0.45096	-3.30648	4.31565
N	-0.92061	-1.68483	2.71595
P	0.50359	0.48969	-0.22065
H	-1.09221	-1.31214	-1.63194
H	0.00962	-4.81665	5.80552
C	-2.18959	-1.89428	3.12468
S	-2.20717	-3.13400	4.39669
S	-3.57522	-1.14560	2.49738
O	-0.15457	0.21033	1.11554
H	-2.98937	-2.51507	0.34691
H	-1.84489	-1.04329	0.49495
H	-0.65096	-0.91988	2.02909
C	-5.66871	-2.01692	-0.94235
H	-6.46437	-2.28466	-0.23258
H	-4.94313	-2.84444	-0.94538
C	-6.24880	-1.83231	-2.33396
C	-6.72018	-0.57881	-2.75829
C	-6.33972	-2.93046	-3.20578
C	-7.27694	-0.42752	-4.03450
H	-6.63483	0.27606	-2.08993
C	-6.90277	-2.78062	-4.47936
H	-5.94924	-3.89862	-2.89296
C	-7.37306	-1.52801	-4.89767
H	-7.63473	0.55089	-4.35549
H	-6.96145	-3.63846	-5.14917
H	-7.80402	-1.40896	-5.89155
O	0.11484	2.00438	-0.76638
C	0.63061	3.13532	-0.14098
C	1.97097	3.46346	-0.33906
C	-0.27055	3.93750	0.61821
C	2.85107	2.57830	-1.14997
C	2.49039	4.63854	0.31418
C	0.21153	5.12999	1.13592
C	-1.66516	3.47863	0.90226
C	3.64285	3.08647	-2.24020
C	2.94303	1.21932	-0.84923
C	1.57794	5.50173	1.02067
C	3.87540	4.97313	0.32463
H	-0.46580	5.77841	1.69023
C	-2.64988	3.48522	-0.11213
C	-1.99847	3.04746	2.21478
C	3.48853	4.40713	-2.75069
C	4.60827	2.21991	-2.86676
C	3.90216	0.34945	-1.44501
O	2.11584	0.67958	0.13625
C	2.07279	6.68683	1.63681
C	4.32696	6.12372	0.94825
H	4.58437	4.30707	-0.15954
C	-3.96062	3.08151	0.20163
C	-2.34367	3.97509	-1.52436
C	-3.31730	2.65396	2.47555
C	-0.98309	3.04337	3.35694
C	4.27188	4.86207	-3.79746
H	2.73500	5.05616	-2.31152
C	5.40948	2.72463	-3.93058
C	4.73703	0.87746	-2.41752
C	4.03131	-1.06760	-0.98483
C	3.41919	6.99958	1.59685
H	1.36677	7.33426	2.15784
H	5.39197	6.35458	0.94630
C	-4.31971	2.67215	1.49276
H	-4.71509	3.10462	-0.58271
H	-1.28444	4.25985	-1.56005
H	-3.58165	2.32328	3.48010
H	0.01125	3.20928	2.92470
C	5.25078	4.02088	-4.38616
H	4.13069	5.87379	-4.17681
H	6.14305	2.06047	-4.38867
H	5.50038	0.24188	-2.86443
C	3.62955	-2.13521	-1.82534
C	4.59334	-1.33486	0.29006
H	3.78727	7.90567	2.07719
C	-5.74901	2.31945	1.89237
H	5.86524	4.39368	-5.20510
C	3.80800	-3.45128	-1.36999
C	3.06425	-1.89812	-3.22387
C	4.74110	-2.66871	0.70239
C	5.13035	-0.21559	1.18083
H	-5.68685	1.42714	2.53728
C	4.36061	-3.74331	-0.11582
H	3.50931	-4.27936	-2.01275
H	2.83491	-0.82918	-3.31355
H	5.19933	-2.87043	1.67052
H	4.92203	0.74071	0.68634
C	4.62823	-5.19071	0.27734
H	4.01952	-5.82128	-0.38948
C	4.11884	-2.24868	-4.29451
H	5.04515	-1.67738	-4.15026
H	4.37533	-3.31689	-4.25176
H	3.73440	-2.03173	-5.30115
C	1.75324	-2.66349	-3.47629
H	1.36785	-2.42676	-4.47813
H	1.89211	-3.75182	-3.42344
H	1.00170	-2.37530	-2.73818
C	6.66335	-0.32383	1.31709
H	6.95386	-1.25155	1.82966
H	7.14407	-0.32001	0.32962
H	7.05913	0.52122	1.89779
C	4.44599	-0.17018	2.55876

H	3.36737	-0.00958	2.45103
H	4.60691	-1.10046	3.12086
H	4.85435	0.65421	3.15994
C	4.23667	-5.52658	1.72674
H	4.37968	-6.59846	1.92108
H	4.86006	-4.97894	2.44688
H	3.18934	-5.27708	1.93545
C	6.11045	-5.53841	0.01963
H	6.31057	-6.59630	0.24173
H	6.38197	-5.34512	-1.02640
H	6.76403	-4.92528	0.65630
C	-2.55559	2.86722	-2.57355
H	-2.31863	3.23808	-3.58061
H	-1.89865	2.01681	-2.35800
H	-3.59802	2.51800	-2.58192
C	-3.16368	5.23657	-1.86295
H	-2.88803	5.62058	-2.85520
H	-4.24127	5.02183	-1.87242
H	-2.98491	6.02904	-1.12382
C	-1.26950	4.20347	4.33348
H	-0.51320	4.23452	5.13062
H	-1.26514	5.17280	3.81842
H	-2.25521	4.07995	4.80417
C	-0.92843	1.70071	4.10823
H	-0.15984	1.74110	4.89310
H	-1.88430	1.45928	4.59230
H	-0.67634	0.89273	3.41751
C	-6.34907	3.46491	2.73879
H	-6.42158	4.38249	2.13719
H	-7.35777	3.20347	3.08869
H	-5.72589	3.68568	3.61497
C	-6.67430	1.98150	0.71492
H	-6.83713	2.85733	0.07021
H	-6.26201	1.16715	0.10927
H	-7.65740	1.66641	1.09028
H	0.14085	-7.21969	-1.70875
H	1.69161	-6.39179	0.06216
H	1.54778	-4.02393	0.83252

TS 9-Bz (R) *arr6*

Imaginary frequency: -416.63 cm^{-1}

C	-0.48724	4.67287	-1.54581
C	0.73100	4.91827	-2.21183
C	0.92099	6.14221	-2.88593
C	-0.08801	7.10645	-2.89721
C	-1.29511	6.86266	-2.22435
C	-1.48935	5.64874	-1.55252
H	-0.67191	3.73249	-1.03182
C	1.87644	3.96488	-2.19877
H	1.87023	6.31504	-3.38856
O	2.98813	4.23683	-2.64522
N	1.63394	2.71855	-1.56133
C	1.79250	2.70125	0.45293
C	2.76563	1.75437	-1.41201
C	3.08545	1.95871	0.07437
H	3.59869	2.03875	-2.05734
H	2.41613	0.74672	-1.63221
H	3.20945	1.02564	0.63523
O	4.23992	2.78290	0.16465
H	-1.04818	-4.33469	2.69606
C	-0.61808	-3.47527	3.20599
C	-0.38674	-3.52419	4.59489
C	-0.30796	-2.33133	2.46495
H	-0.63890	-4.42576	5.15119
H	-0.48921	-2.27340	1.39722
O	-0.76649	1.27526	-1.68844
C	0.16580	-2.43264	5.27893
C	0.24397	-1.23908	3.14788
C	0.48415	-1.28845	4.53857
N	0.61369	-0.02078	2.58901
P	-0.51596	0.02010	-0.88755
H	0.70389	2.27432	-1.72650
H	0.34514	-2.47409	6.35119
C	1.14667	0.88743	3.42541
S	1.19625	0.23473	5.07671
S	1.70618	2.44708	3.06159
O	0.71080	-0.06214	0.00626
H	1.80610	3.76780	0.66039
H	0.86247	2.16053	0.54055
H	0.58371	0.08904	1.52666
C	4.86471	2.82083	1.45992
H	4.16053	3.16616	2.23042
H	5.64868	3.58262	1.35074
C	5.47728	1.49632	1.87084
C	6.32829	0.81086	0.98518
C	5.23901	0.95510	3.14431
C	6.94059	-0.38697	1.37022
H	6.50976	1.22689	-0.00509
C	5.86067	-0.23862	3.53754
H	4.56118	1.47007	3.82506
C	6.71285	-0.91155	2.65240
H	7.59838	-0.90794	0.67460
H	5.66606	-0.64976	4.52787
H	7.18887	-1.84444	2.95332
O	-0.56392	-1.24732	-1.95009
C	-0.52529	-2.52979	-1.40599
C	-1.69970	-3.05609	-0.86912
C	0.71863	-3.23152	-1.43658
C	-2.94895	-2.24666	-0.86043
C	-1.64304	-4.35659	-0.25030
C	0.71915	-4.53501	-0.96164
C	1.97776	-2.53848	-1.84844
C	-4.18991	-2.76653	-1.37430
C	-2.94482	-0.95238	-0.33821
C	-0.42062	-5.11317	-0.34004
C	-2.72133	-4.90460	0.50226
H	1.64022	-5.11362	-1.00149
C	2.14067	-2.03977	-3.16409
C	3.00118	-2.32409	-0.88070
C	-4.27181	-3.99775	-2.08600
C	-5.39845	-2.00379	-1.18994
C	-4.12616	-0.17446	-0.16500

O	-1.76040	-0.39816	0.13278
C	-0.35268	-6.40191	0.26297
C	-2.61680	-6.15300	1.09290
H	-3.63039	-4.32235	0.62398
C	3.30579	-1.32395	-3.48931
C	1.11679	-2.30128	-4.26465
C	4.13820	-1.59497	-1.25484
C	2.92108	-2.85191	0.55059
C	-5.48570	-4.47229	-2.55251
H	-3.36103	-4.56250	-2.26888
C	-6.63300	-2.52762	-1.66952
C	-5.33250	-0.73161	-0.55974
C	-4.02702	1.21094	0.38441
C	-1.42883	-6.91733	0.96253
H	0.57755	-6.96466	0.18074
H	-3.45210	-6.54668	1.67124
C	4.30977	-1.07402	-2.54672
H	3.41555	-0.94571	-4.50332
H	0.24064	-2.77848	-3.80995
H	4.90882	-1.40139	-0.50938
H	1.89106	-3.17113	0.74285
C	-6.68078	-3.74044	-2.33245
H	-5.52205	-5.41353	-3.10036
H	-7.54011	-1.94268	-1.51462
H	-6.25091	-0.16228	-0.42046
C	-4.24373	2.31504	-0.47294
C	-3.67519	1.41653	1.74731
H	-1.36106	-7.89990	1.42829
C	5.56882	-0.27115	-2.85807
H	-7.63042	-4.12824	-2.69972
C	-4.11009	3.61222	0.05497
C	-4.60796	2.15066	-1.94693
C	-3.51804	2.72782	2.21079
C	-3.53902	0.23325	2.70480
H	5.70991	0.42218	-2.01282
C	-3.72107	3.84203	1.37793
H	-4.30634	4.46673	-0.59342
H	-4.52365	1.08643	-2.19703
H	-3.22883	2.89266	3.24656
H	-3.06658	-0.59124	2.15694
C	-3.49546	5.25506	1.89746
H	-3.74403	5.94863	1.07794
C	-3.63971	2.90713	-2.87696
H	-3.88887	2.69637	-3.92675
H	-3.70343	3.99442	-2.73569
H	-2.60595	2.59450	-2.69318
C	-6.06952	2.57235	-2.19982
H	-6.76510	1.99711	-1.57404
H	-6.21651	3.63742	-1.97056
H	-6.34086	2.41285	-3.25290
C	-2.65469	0.51890	3.92934
H	-1.69721	0.96363	3.63412
H	-3.14410	1.20395	4.63576
H	-2.44717	-0.41552	4.46610
C	-4.93663	-0.24874	3.15134
H	-5.55305	-0.53338	2.28982
H	-4.84971	-1.12062	3.81535
H	-5.45909	0.54913	3.69809
C	-2.01301	5.47558	2.26562
H	-1.84446	6.51038	2.59540
H	-1.70831	4.80630	3.08205
H	-1.35913	5.27668	1.40685
C	-4.41883	5.58790	3.08567
H	-5.47389	5.44526	2.81694
H	-4.20019	4.94280	3.94778
H	-4.27988	6.63046	3.40415
C	0.63884	-1.00053	-4.93844
H	0.25728	-0.29342	-4.19337
H	1.45222	-0.51414	-5.49483
H	-0.16609	-1.21807	-5.65437
C	1.68417	-3.29460	-5.30035
H	1.98141	-4.23630	-4.81914
H	0.93285	-3.52158	-6.06994
H	2.56887	-2.87869	-5.80250
C	3.27055	-1.78075	1.59588
H	4.32797	-1.50176	1.56188
H	2.67456	-0.88131	1.43237
H	3.06084	-2.15360	2.60770
C	3.84028	-4.07877	0.72989
H	3.74071	-4.48907	1.74496
H	3.60623	-4.87590	0.01246
H	4.89154	-3.79440	0.57970
C	5.47988	0.57338	-4.13747
H	6.37385	1.20306	-4.23561
H	5.42391	-0.06157	-5.03297
H	4.60005	1.23025	-4.13227
C	6.80279	-1.19820	-2.90175
H	7.72267	-0.61651	-3.05502
H	6.90621	-1.76764	-1.96913
H	6.70966	-1.91793	-3.72752
H	0.06580	8.04783	-3.42331
H	-2.08214	7.61633	-2.22358
H	-2.42074	5.45325	-1.02947

TS 9-Bz (R) *arr7*

Imaginary frequency: -415.73 cm^{-1}

C	-1.34156	4.42786	-1.53437
C	-0.21290	4.95170	-2.19637
C	-0.30626	6.19856	-2.84807
C	-1.50811	6.90892	-2.84158
C	-2.62833	6.38434	-2.17783
C	-2.54074	5.14591	-1.52899
H	-1.30666	3.46296	-1.03536
C	1.11237	4.26973	-2.20384
H	0.57682	6.59049	-3.34840
O	2.13773	4.78099	-2.64711
N	1.14211	2.99226	-1.58437
C	1.34197	3.02477	0.43095
C	2.44601	2.27692	-1.45693
C	2.74052	2.52131	0.03069
H	3.19125	2.74256	-2.10207
H	2.31307	1.22153	-1.69759

H	3.02692	1.62036	0.58408
O	3.74400	3.52423	0.11392
H	-0.06673	-4.40858	2.68396
C	0.19864	-3.48246	3.18906
C	0.46693	-3.48759	4.57217
C	0.26183	-2.29868	2.44849
H	0.40880	-4.42218	5.12808
H	0.04791	-2.27519	1.38539
O	-0.96568	1.14372	-1.71394
C	0.81022	-2.31032	5.25100
C	0.60572	-1.12111	3.12589
C	0.88200	-1.12466	4.51082
N	0.71699	0.14663	2.56634
P	-0.47629	-0.03125	-0.90226
H	0.31475	2.37540	-1.73674
H	1.01816	-2.31803	6.31888
C	1.07816	1.14053	3.39676
S	1.29423	0.50781	5.04183
S	1.30736	2.78170	3.03186
O	0.74979	0.12980	-0.01789
H	1.16658	4.07950	0.62471
H	0.52435	2.32858	0.53331
H	0.63553	0.25014	1.50631
C	4.34156	3.69438	1.41280
H	3.58096	3.94325	2.16637
H	4.99357	4.56916	1.28615
C	5.15547	2.50066	1.87355
C	6.17184	1.97799	1.05277
C	4.94085	1.92939	3.13850
C	6.96720	0.91541	1.49651
H	6.34295	2.41680	0.07038
C	5.73872	0.86726	3.58665
H	4.14362	2.31895	3.77077
C	6.75457	0.35909	2.76771
H	7.75923	0.52519	0.85756
H	5.55794	0.43172	4.56914
H	7.37310	-0.46961	3.11138
O	-0.27571	-1.29097	-1.95515
C	0.00741	-2.53959	-1.40443
C	-1.04442	-3.26978	-0.85219
C	1.35597	-3.00470	-1.44960
C	-2.42491	-2.71476	-0.84583
C	-0.74545	-4.53106	-0.22248
C	1.59848	-4.28280	-0.96483
C	2.48269	-2.13151	-1.90182
C	-3.53792	-3.47625	-1.35055
C	-2.67484	-1.44234	-0.32820
C	0.59328	-5.05241	-0.32098
C	-1.69788	-5.25963	0.54674
H	2.60924	-4.68370	-1.01694
C	2.56269	-1.66834	-3.24069
C	3.50290	-1.78262	-0.97370
C	-3.37402	-4.69945	-2.06216
C	-4.87397	-2.97629	-1.15296
C	-3.98813	-0.92471	-0.13696
O	-1.61990	-0.66012	0.12906
C	0.90292	-6.30069	0.29176
C	-1.36027	-6.46168	1.14599
H	-2.69679	-4.85238	0.67529
C	3.66768	-0.89470	-3.62725
C	1.53194	-2.04830	-4.29976
C	4.58226	-0.99647	-1.41179
C	3.49570	-2.23577	0.48613
C	-4.47046	-5.41116	-2.51750
H	-2.36926	-5.06737	-2.25434
C	-5.98131	-3.74043	-1.62060
C	-5.05934	-1.72016	-0.51668
C	-4.21074	0.43608	0.44026
C	-0.05359	-6.99703	1.00809
H	1.91962	-6.68433	0.20306
H	-2.10323	-6.99559	1.73769
C	4.69821	-0.55813	-2.73758
H	3.74497	-0.56425	-4.66418
H	0.73218	-2.61684	-3.81189
H	5.35739	-0.73637	-0.69382
H	2.53178	-2.71098	0.69593
C	-5.78748	-4.93770	-2.28491
H	-4.31996	-6.34045	-3.06626
H	-6.98683	-3.35222	-1.45574
H	-6.07250	-1.35321	-0.35655
C	-4.72297	1.46771	-0.38640
C	-3.95658	0.67850	1.81530
H	0.19755	-7.94565	1.48136
C	5.88830	0.25846	-3.23135
H	-6.64171	-5.51101	-2.64366
C	-5.01078	2.71694	0.19075
C	-4.99194	1.25367	-1.87546
C	-4.25249	1.94528	2.33885
C	-3.46657	-0.43881	2.73519
H	6.01989	0.00838	-4.29676
C	-4.79158	2.97414	1.55142
H	-5.43527	3.49884	-0.43936
H	-4.62559	0.25515	-2.14160
H	-4.07958	2.13933	3.39688
H	-2.83582	-1.11170	2.14335
C	-5.18980	4.29723	2.19396
H	-4.79673	4.28579	3.22286
C	-2.60446	0.05780	3.90831
H	-1.80934	0.72802	3.55981
H	-3.20040	0.59720	4.65735
H	-2.13600	-0.79610	4.41445
C	-4.66566	-1.26481	3.24801
H	-5.24061	-1.68504	2.41304
H	-4.32068	-2.09460	3.88140
H	-5.33964	-0.63358	3.84450
C	-4.23039	2.25793	-2.76021
H	-4.57243	3.28804	-2.59363
H	-3.15415	2.21253	-2.56088
H	-4.39703	2.02317	-3.82116
C	-6.50471	1.28639	-2.17289
H	-6.69279	1.08276	-3.23640
H	-7.04537	0.53770	-1.57869

H	-6.93158	2.27153	-1.93722
C	-6.72642	4.41019	2.28179
H	-7.02191	5.33543	2.79647
H	-7.17099	4.42319	1.27658
H	-7.15278	3.55796	2.82722
C	-4.59027	5.52375	1.48297
H	-4.82899	6.44219	2.03688
H	-3.49893	5.44436	1.40020
H	-5.00038	5.63687	0.46980
C	0.88937	-0.80503	-4.94467
H	0.44080	-0.15873	-4.18171
H	1.63015	-0.21825	-5.50572
H	0.10136	-1.10590	-5.64925
C	2.15646	-2.97586	-5.36271
H	2.58174	-3.87528	-4.89702
H	1.39708	-3.29082	-6.09229
H	2.96148	-2.46759	-5.91137
C	4.60181	-3.27806	0.75084
H	5.59661	-2.83706	0.59609
H	4.54866	-3.63688	1.78857
H	4.51479	-4.14513	0.08298
C	3.63768	-1.05295	1.45637
H	3.53838	-1.39492	2.49536
H	4.60940	-0.55846	1.36377
H	2.85657	-0.31611	1.26220
C	5.59786	1.77152	-3.15007
H	5.42291	2.07628	-2.10968
H	6.44599	2.35282	-3.53839
H	4.70726	2.03430	-3.73529
C	7.20367	-0.07997	-2.50992
H	8.04494	0.43430	-2.99352
H	7.17860	0.24639	-1.46204
H	7.40272	-1.15965	-2.52340
H	-1.57308	7.87057	-3.34933
H	-3.56631	6.93913	-2.16660
H	-3.40182	4.72877	-1.01596

TS 9-Bz (R) *arr8*

Imaginary frequency: -435.37 cm^{-1}

C	4.20401	-4.83244	0.43531
C	3.18188	-3.91133	0.12885
C	3.23121	-2.61162	0.67483
C	4.25352	-2.26837	1.56171
C	5.24610	-3.20071	1.89150
C	5.23273	-4.47696	1.31044
H	4.14882	-5.83089	0.00679
C	2.00688	-4.43185	-0.62526
H	2.49401	-1.85774	0.41008
O	1.94004	-5.55554	-1.11258
N	0.85470	-3.59379	-0.55971
C	0.05860	-3.52929	1.25052
C	-0.49565	-4.10184	-0.91157
C	-1.19756	-3.61242	0.37399
H	-0.46813	-5.19376	-0.95276
H	-0.86347	-3.68855	-1.85326
H	-1.57530	-2.59257	0.25287
O	-2.19591	-4.48466	0.86764
H	0.06112	3.93264	3.44117
C	-0.05515	2.97084	3.93650
C	-0.16498	2.91018	5.33974
C	-0.10164	1.80898	3.16032
H	-0.12537	3.82934	5.92247
H	-0.01927	1.83785	2.07767
O	0.42996	-1.06970	-1.60421
C	-0.33248	1.68762	6.00535
C	-0.26953	0.58613	3.82618
C	-0.38901	0.52233	5.23215
N	-0.37792	-0.66349	3.22714
P	-0.05174	-0.07421	-0.58008
H	0.94856	-2.59418	-0.84659
H	-0.42424	1.64663	7.08874
C	-0.61351	-1.70842	4.04318
S	-0.63095	-1.15558	5.73457
S	-0.94204	-3.31036	3.59767
O	-0.72063	-0.55629	0.69163
H	0.51133	-4.44022	1.63213
H	0.50991	-2.58851	1.52698
H	-0.45746	-0.70911	2.16543
C	-3.52070	-4.06722	0.44555
H	-3.77245	-3.10733	0.91947
H	-4.18950	-4.84256	0.83735
C	-3.62618	-3.95038	-1.05783
C	-3.78257	-5.10347	-1.84788
C	-3.44619	-2.70730	-1.69103
C	-3.75687	-5.01890	-3.24477
H	-3.91470	-6.07041	-1.36077
C	-3.40667	-2.62251	-3.08796
H	-3.33695	-1.80360	-1.09412
C	-3.56008	-3.77675	-3.86682
H	-3.88343	-5.91835	-3.84713
H	-3.26489	-1.65499	-3.56252
H	-3.53220	-3.70952	-4.95426
O	1.20369	0.91976	-0.07371
C	1.63811	1.95740	-0.89927
C	0.80091	3.05509	-1.09384
C	2.95527	1.90219	-1.43771
C	-0.50631	3.12673	-0.39448
C	1.20890	4.10246	-1.98938
C	3.37293	2.95564	-2.24054
C	3.95629	0.84184	-1.09852
C	-0.81819	4.21506	0.49048
C	-1.44555	2.11618	-0.58199
C	2.52619	4.04713	-2.56520
C	0.35444	5.18238	-2.35615
H	4.39123	2.94415	-2.62796
C	4.77191	1.02022	0.04792
C	4.20680	-0.21943	-1.99721
C	0.14352	5.19043	0.88123
C	-2.14299	4.29498	1.04494
C	-2.77494	2.19280	-0.07029
O	-1.06836	1.00327	-1.34148
C	2.94982	5.08626	-3.44204

C	0.79163	6.17080	-3.22089
H	-0.65594	5.21734	-1.95623
C	5.86131	0.15886	0.23475
C	4.46431	2.11051	1.07279
C	5.31776	-1.05008	-1.77069
C	3.32829	-0.43634	-3.22594
C	-0.19445	6.20645	1.75981
H	1.15569	5.11916	0.49056
C	-2.46202	5.35995	1.93475
C	-3.09776	3.30218	0.70021
C	-3.82010	1.17022	-0.38064
C	2.10296	6.13163	-3.76208
H	3.95391	5.03387	-3.86393
H	0.11968	6.98399	-3.49414
C	6.16922	-0.86615	-0.67546
H	6.49539	0.28419	1.11368
H	3.74064	2.79821	0.61688
H	5.51752	-1.85465	-2.47409
H	2.37175	0.06790	-3.03893
C	-1.50922	6.29905	2.28660
H	0.55789	6.93734	2.05479
H	-3.47053	5.41016	2.34593
H	-4.11545	3.40420	1.07184
C	-4.38649	0.38961	0.66004
C	-4.32378	1.06285	-1.70393
H	2.43442	6.91934	-4.43792
C	7.42096	-1.70671	-0.45256
H	-1.76137	7.10443	2.97561
C	-5.45338	-0.47170	0.35093
C	-3.90494	0.48487	2.10669
C	-5.38431	0.18093	-1.95855
C	-3.81232	1.94993	-2.83756
H	7.45797	-1.94174	0.62382
C	-5.97212	-0.58998	-0.94483
H	-5.90527	-1.06278	1.14819
H	-2.96211	1.04507	2.11137
H	-5.77625	0.11166	-2.97284
H	-3.00407	2.57734	-2.44424
C	-7.18574	-1.46986	-1.21643
H	-7.37875	-2.04610	-0.29738
C	-4.91985	1.24801	2.98378
H	-5.87365	0.70405	3.03405
H	-4.53501	1.35503	4.00784
H	-5.12974	2.25058	2.59153
C	-3.61838	-0.89390	2.72214
H	-3.22481	-0.77840	3.74024
H	-4.52588	-1.50814	2.79381
H	-2.87796	-1.44128	2.13209
C	-3.22425	1.13227	-4.00176
H	-2.39850	0.50238	-3.65036
H	-3.98606	0.48960	-4.46511
H	-2.83597	1.80235	-4.78151
C	-4.92167	2.90625	-3.32177
H	-5.76442	2.35229	-3.75790
H	-5.30919	3.50821	-2.48878
H	-4.53233	3.58902	-4.09002
C	-6.96557	-2.47729	-2.36005
H	-7.86900	-3.08592	-2.50638
H	-6.75343	-1.96459	-3.30810
H	-6.12457	-3.14506	-2.14632
C	-8.42636	-0.59156	-1.48595
H	-8.60467	0.10515	-0.65597
H	-8.28871	0.00253	-2.40048
H	-9.32330	-1.21323	-1.61703
C	5.70264	2.94436	1.44773
H	6.17497	3.37152	0.55309
H	5.41764	3.76951	2.11512
H	6.45635	2.34152	1.97266
C	3.79000	1.51233	2.32556
H	4.48625	0.85600	2.86802
H	3.47442	2.30796	3.01520
H	2.90232	0.92963	2.05097
C	3.96957	0.19516	-4.47899
H	4.11603	1.27481	-4.35191
H	4.95000	-0.25966	-4.68124
H	3.33168	0.03775	-5.36034
C	3.01149	-1.92196	-3.47465
H	3.89799	-2.48192	-3.80303
H	2.62298	-2.39622	-2.56830
H	2.24976	-2.01651	-4.25963
C	8.67988	-0.87687	-0.79002
H	9.59396	-1.44961	-0.57842
H	8.68279	-0.60786	-1.85597
H	8.71274	0.05360	-0.20848
C	7.43196	-3.03700	-1.21899
H	6.52531	-3.62129	-1.02201
H	7.50773	-2.87227	-2.30313
H	8.30079	-3.63765	-0.91793
H	4.27563	-1.27096	1.98793
H	6.03326	-2.92932	2.59393
H	6.01282	-5.19748	1.55235

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