Electronic Supplementary Material (ESI) for Faraday Discussions.

Electronic Supplementary Information

Successes and Challenges in Multiscale Modelling of Artificial Metalloenzymes: the Case Study of POP-Rh_2 Cyclopropanase

José-Emilio Sánchez-Aparicio,‡[a] Giuseppe Sciortino,‡[a,§] Eric Mates-Torres,[a,+] Agustí Lledós*[a] and Jean-Didier Maréchal*[a]

[a] *Insilichem, Department of Chemistry, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain. E-mails: agusti@klingon.uab.cat, jeandidier.marechal@uab.cat*
[§] *Current address: Institute of Chemical Research of Catalonia (ICIQ), The Barcelona Institute of Science and Technology, 43007 Tarragona, Spain*
[+] *Current address: School of Chemistry, Trinity College Dublin, College Green, Dublin, 2, Ireland*

‡ *These authors have contributed equally to this work*

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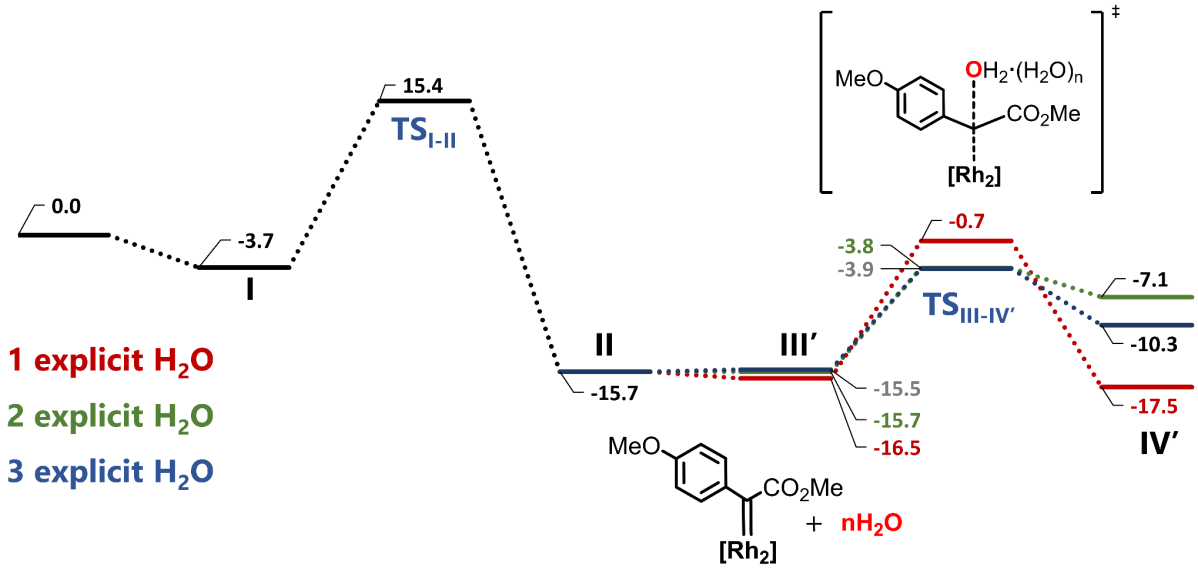
1. Supplementary scheme



Scheme S1. Gibbs energy profile for the side reaction (carbene insertion into the O-H bond of water) of the complete cofactor in water. All Gibbs energy values are given in kcal·mol^{-1}. Profiles for one, two and three explicit water molecules are shown in red, green and blue, respectively.

2. Supplementary tables

Table S1. Residues interacting with the carbene molecule along the MD simulation of the GSH variant.

Amino acid	Location	Mean of PyContact score along the MD simulation[a]
His592	Loop at the peptidase/barrel interface	2.864
Gly594	Loop at the peptidase/barrel interface	2.296
Met593	Loop at the peptidase/barrel interface	1.847
Trp142	Propeller domain, blade b3	1.131
Ser99[b]	**Propeller domain, blade b2**	**0.947**
Gln98	Propeller domain, blade b2	0.706
Met53	Propeller domain, blade b1	0.547
Asn143	Propeller domain, blade b3	0.406
Ile406	Loop at the peptidase/barrel interface	0.171
Thr101	Propeller domain, blade b2	0.122
Phe156	Propeller domain, blade b3	0.121
Arg55	Propeller domain, blade b1	0.110

[a] PyContact scores were obtained using the version 1.0.4 of the software, with the default parameters. Only residues with mean of PyContact score > 0.1 are reported.

[b] Mutated amino acid in the GSH variant.

Table S2. Residues interacting with the carbene molecule along the MD simulation of the HFF variant.

Amino acid	Location	Mean of PyContact score along the MD simulation[a]
Met411	Loop connecting strands 3 and 4 at the peptidase domain	1.779
Phe412	Loop connecting strands 3 and 4 at the peptidase domain	0.319
Phe413	Loop connecting strands 3 and 4 at the peptidase domain	0.290
Arg600	Peptidase domain	0.285
Leu408	Loop connecting strands 3 and 4 at the peptidase domain	0.145
Arg476	Peptidase domain, end of the strand 5	0.140
Ser324	Propeller domain, blade b7	0.119
Thr409	Loop connecting strands 3 and 4 at the peptidase domain	0.114

[a] PyContact scores were obtained using the version 1.0.4 of the software, with the default parameters. Only residues with mean of PyContact score > 0.1 are reported.

Table S3. Residues interacting with the carbene molecule along the MD simulation of the RFY variant.

Amino acid	Location	Mean of PyContact score along the MD simulation[a]
Gly52	Propeller domain, blade b1	6.232
Met53	Propeller domain, blade b1	5.374
Phe99[b]	**Propeller domain, blade b2**	**3.983**
Arg338	Propeller domain, blade b7	2.563
Arg98[b]	**Propeller domain, blade b2**	**1.724**
Leu328	Propeller domain, blade b6	1.499
Ser64	Propeller domain, blade b1	1.262
Tyr326	Propeller domain, blade b7	0.973
Ile51	Propeller domain, blade b1	0.786
Val71	Propeller domain, blade b1	0.746
Tyr65	Propeller domain, blade b1	0.558
Ser66	Propeller domain, blade b1	0.389
Trp142	Propeller domain, blade b3	0.361
Pro327	Propeller domain, blade b7	0.355
Thr50	Propeller domain, blade b1	0.335
Arg55	Propeller domain, blade b1	0.210

[a] PyContact scores were obtained using the version 1.0.4 of the software, with the default parameters. Only residues with mean of PyContact score > 0.1 are reported.

[b] Mutated amino acid in the RFY variant.

Table S4. Result of the refinement docking experiment in the HFF variant. Best-scored solution for each enantiomer is highlighted in bold letters.

Enantiomer	POP structure	Intermediate II structure	F_{max}	F_{mean}
S,R	1	11	72.3	66.5
S,R	1	16	72.7	61.9
S,R	**3**	**9**	**86.3**[a]	**74.0**
S,R	3	14	81.5	68.0
S,R	3	17	80.1	73.4
S,R	4	9	70.6	58.7
S,R	5	9	21.6	21.2
S,R	5	16	47.3	34.6
R,S	1	3	79.4	69.1
R,S	1	9	64.8	58.9
R,S	1	10	78.1	68.1
R,S	3	3	81.4	73.1
R,S	6	9	76.5	57.5
R,S	**6**	**16**	**82.6**[a]	**67.6**

[a] ΔF_{max}(SR/RS) = -3.7

3. Supplementary figures

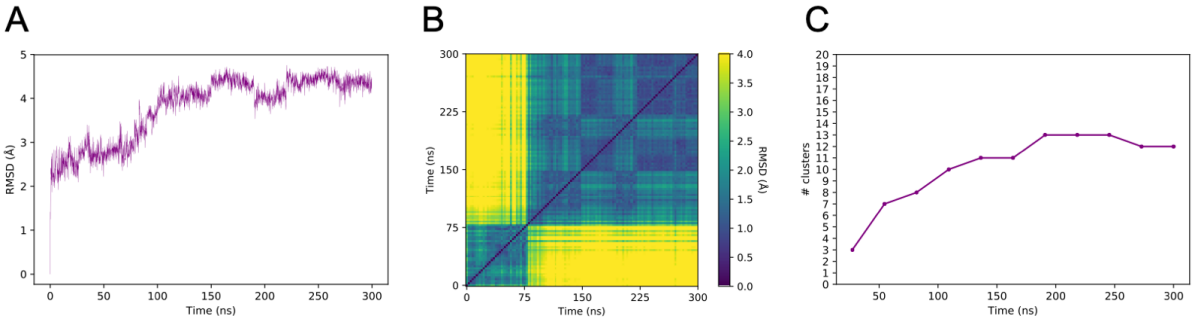


Figure S1. Convergence analyses for the MD simulation of the GSH variant, considering all the atoms of the cofactor and the carbene. (A) Scalar RMSD from the initial frame of the trajectory. (B) All-to-all frames RMSD. The RMSD with respect to all other frames is plotted in the indicated colour scale. (C) Cluster counting study with a cut-off of 1.5 Å.

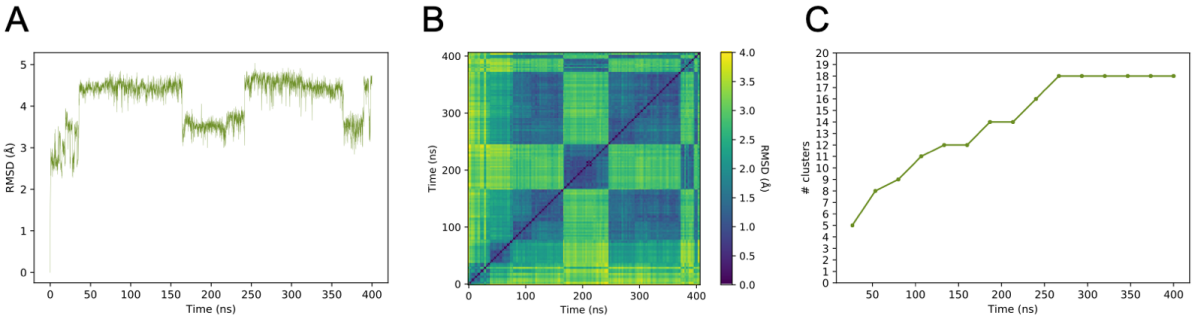


Figure S2. Convergence analyses for the MD simulation of the HFF variant, considering all the atoms of the cofactor and the carbene. (A) Scalar RMSD from the initial frame of the trajectory. (B) All-to-all frames RMSD. The RMSD with respect to all other frames is plotted in the indicated colour scale. (C) Cluster counting study with a cut-off of 1.5 Å.

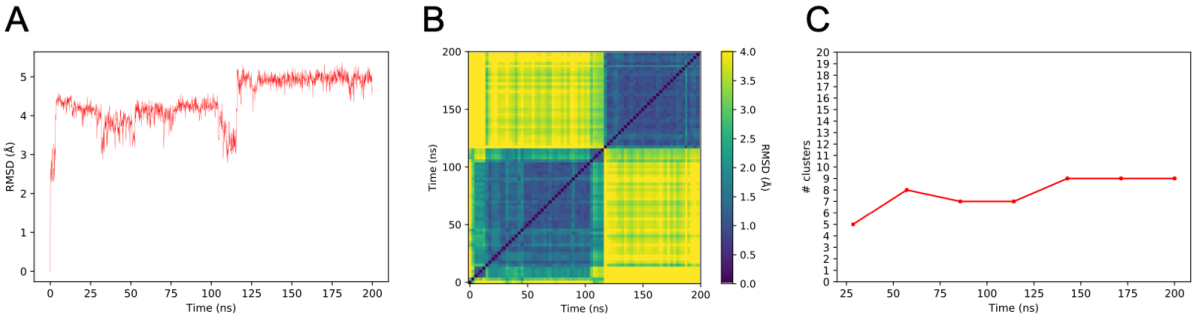


Figure S3. Convergence analyses for the MD simulation of the RFY variant, considering all the atoms of the cofactor and the carbene. (A) Scalar RMSD from the initial frame of the trajectory. (B) All-to-all frames RMSD. The RMSD with respect to all other frames is plotted in the indicated colour scale. (C) Cluster counting study with a cut-off of 1.5 Å.

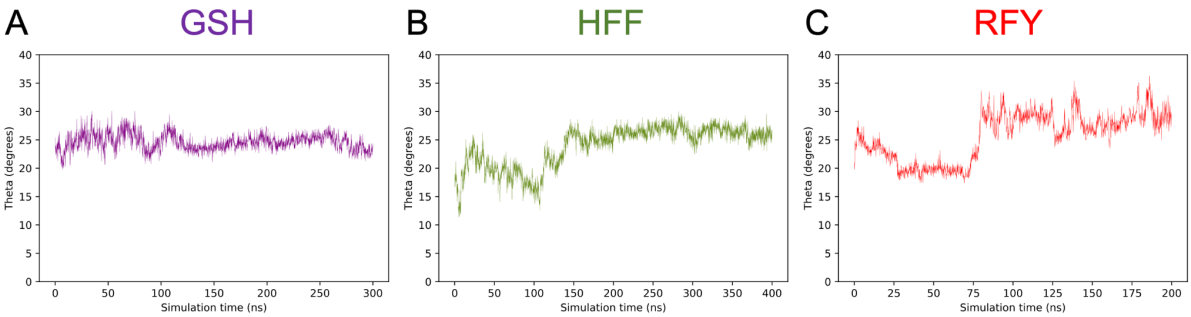


Figure S4. Evolution of the interdomain angle θ along the MD simulations. (A) GSH variant. (B) HFF variant. (C) RFY variant.

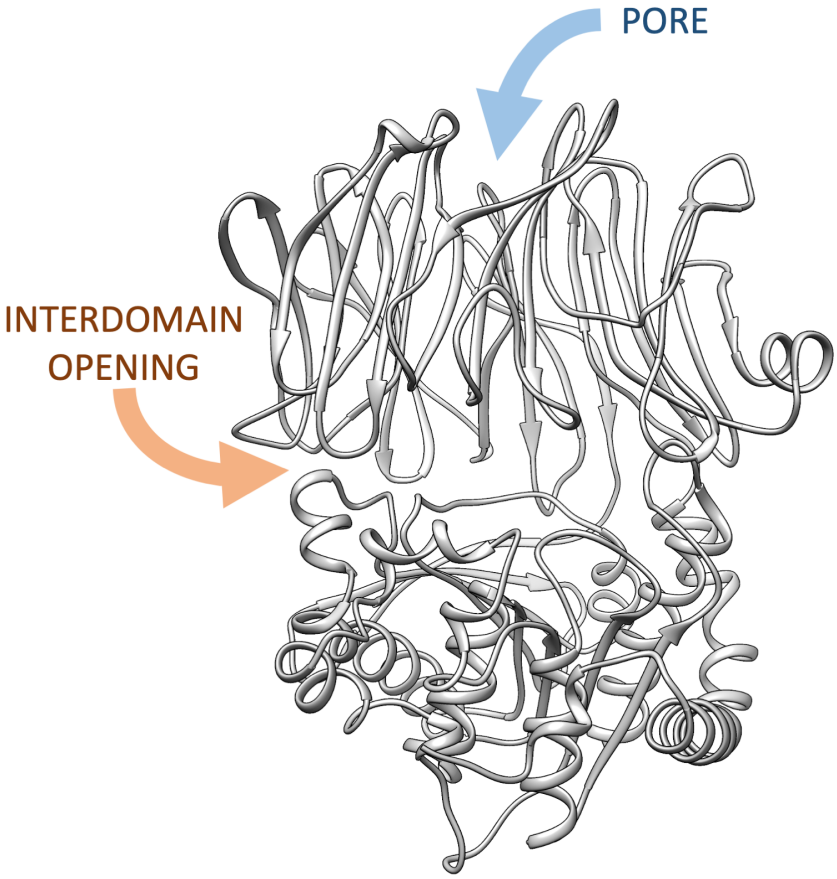


Figure S5. Entrance channels of the POP protein. Pore at the propeller domain is indicated with a blue arrow, while interdomain opening is indicated with an orange arrow.

4. Details of computational methods

DFT simulations

The mechanistic analysis in water was performed considering the whole Rh_2-cofactor at DFT level of theory using Gaussian09 software.[1] The structures of all the intermediates and transition states were optimized in water, using the B3LYP functional[2] combined with the Grimme's D3 correction for dispersion[3] and the SMD continuum solvent model.[4] The BS1 basis set was used for the optimizations. BS1 includes the 6-31G(d,p) basis set for the main group elements,[5] and the scalar relativistic Stuttgart-Dresden SDD pseudopotential and its associated double-ζ basis set,[6] complemented with a set of *f* polarization functions,[7] for the rhodium atom. Frequency calculations were carried out for all the optimized geometries to characterize the stationary points as either minima or transition states. It was confirmed that transition states connect with the corresponding intermediates by usual intrinsic reaction coordinate (IRC) calculations and subsequent optimization to minima.

Final Gibbs energies were obtained by adding the thermal and entropic corrections obtained with BS1 to the potential energies obtained in water with single point calculations using an extended basis set (BS2). BS2 consists in the triple-ζ def2-TZVP basis set for the main group elements and the quadruple-ζ def2-QZVP basis set for Rh.[8] A correction of 1.9 kcal·mol^{-1} was applied to all Gibbs values to change the standard state from the gas phase (1 atm) to solution (1 M) at 298.15 K.[9]

The Cartesian coordinates of the optimised geometries are provided in section 7 of this ESI. The report was generated with ESIGen v0.0.5.[10]

Docking of the intermediate **II**

Exploratory docking

Four structures of the POP protein scaffold were considered in order to cover the whole range of interdomain angles previously reported in the literature[11] (Table S5): the two structures representing intermediate interdomain angles were obtained from the PDB (codes 5t88 and 6can), whereas the two structures representing the completely opened and closed conformations were generated by Normal Mode Analysis (NMA) from the 5t88 PDB code. In the case of NMA, the Gaussian network model of the ProDy algorithm[12] was used (setup partially supported by the Tangram suite of UCSF Chimera graphical interfaces[13]) with the following parameters: i) group by 15 residues, ii) normal mode amplitude of 500 for the opened conformation and 400 for the closed conformation, and iii) the first normal mode was selected. In order to avoid unfeasible structures, the resulting conformations from NMA were further submitted to 100 steps of minimization using OpenMM[14] and the AMBER14SB force field.[15] By means of UCSF Chimera,[16] small crystallographic molecules were removed from these four conformations of the POP protein, hydrogen atoms were added, and the three variants –

GSH, HFF, RFY – were built by mutating the necessary sidechains. The following possibilities of coordination with the Rh atom were tested: His326 for the GSH variant; His328 for the HFF variant; and Glu241, Glu283, Tyr239 and His591 for the RFY variant. The Rh_2-cofactor was restrained to be covalently anchored to the 413/477 Cα and allowed to freely rotate all the other rotatable bonds (Figure S6). The side chain of the amino acid implicated in the possible coordination bond was allowed to freely rotate, as were the side chains of the mutated amino acids. Ten runs of the GaudiMM multi-objective genetic algorithm were carried out for each variant/test-case, defining a population of 52 individuals, which were evolved during 200 generations. The objectives used to guide the evolution were: i) coordination score with the tested amino acid; ii) distance of the coordination bond; iii) minimization of steric clashes. The input .yaml files used in each calculation with GaudiMM[17] v.0.0.7 are provided in section 5 of this ESI.

Table S5. Pool of POP protein structures considered in the exploratory docking experiment of the intermediate **II**.

Structure	Source	PDB code	Interdomain angle θ (degrees)
1. Closed	NMA		16
2	PDB	5t88	29
3	PDB	6can	32
4. Open	NMA		48

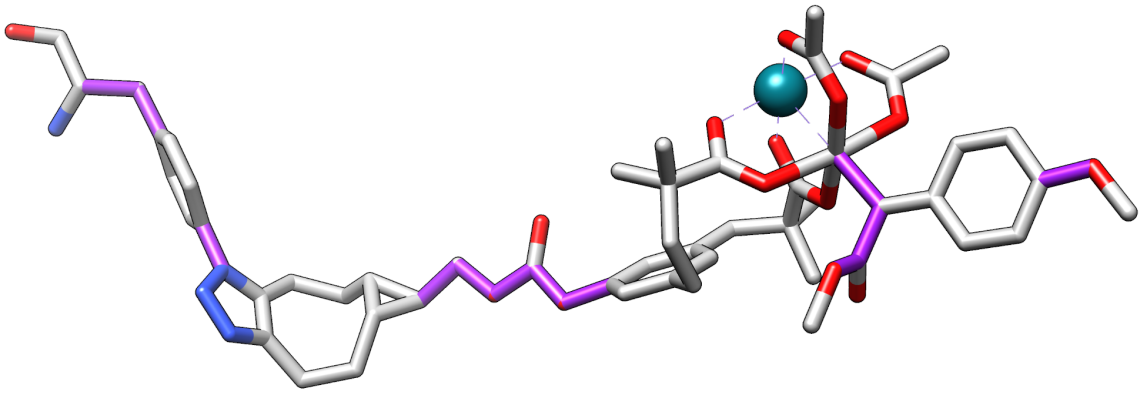


Figure S6. Structure of the intermediate **II**. Bonds allowed to rotate are shown in purple.

Refinement docking

The POP protein structures were treated as rigid (except for the coordinating His residues, allowed to freely rotate) and were selected from the best solutions of the previous exploratory dockings: PDB 5t88 for the GSH and RFY variants and closed conformation for the HFF variant. For each system, 50 docking solutions were generated into the covalent docking framework with a minimum of 100,000 building operations, considering the $Cα_{(477/413)}$-$Cβ_{cofactor}$ bond formation. The evaluation sphere was set to a radius of 15 Å from the centre of mass of

the protein. Full flexibility according to the GOLD implemented algorithm was allowed for the Rh_2-cofactor. The solutions were analysed by means of the GaudiView GUI extension for Chimera and the structures with best GoldScore were selected as initial frames for the further Molecular Dynamics (MD) simulations.

Molecular dynamics

Molecular Dynamics (MD) simulations were set up with *xleap*, which was instructed to solvate the protein with a cubic box of pre-equilibrated TIP3P water molecules and balance the total charge with Na+ ions (*ions94.lib* library). The AMBER14SB force field[15] was used for the standard residues, while the GAFF force field was adopted for the remaining atoms. Rh-bonding force constants and equilibrium parameters were obtained through the Seminario's method,[18] using Gaussian09[1] to compute the geometry and harmonic frequencies at BS1 DFT level. Point charges of the Rh_2-cofactor were derived using the RESP (Restrained ElectroStatic Potential) model.[19] The force field building operations were carried out using MCPB.py.[20] For all the MDs, the solvent and the whole system were sequentially submitted to 3000 energy minimization steps to relax possible steric clashes. Then, thermalization of water molecules and side chains was achieved by increasing the temperature from 100 K up to 300 K. Simulations were carried out with the OpenMM engine[14] through OMMProtocol[21] and analysed by means of CPPTraj implemented in AmberTools18.[22] The convergence of the trajectories was assessed by RMSD, all-to-all RMSD and cluster counting analyses.[23,24]

Clustering analysis

Representative orientations of the carbene were obtained with a Quality Threshold (QT) clustering[25] of the MDs trajectories (considering the relative orientations of the carbene with a RMSD cut-off of 3.0 Å), which resulted on three representative orientations for the GSH variant and two orientations for each of the HFF and RFY variants.

Interaction analysis

Interaction between the carbene and the POP protein was assessed along the three trajectories. The PyContact software[26] (version 1.0.4) was configured with the standard parameters to assess the interactions with a frequency of 10 frames per nanosecond of simulation.

Interdomain angle analysis

The interdomain angle θ was analysed by means of CPPTraj implemented in AmberTools18.[22] The same definition of interdomain angle reported in previous studies[11,27] was used: average of two angles (θ_1 and θ_2), each one defined by three groups of Cα atoms. For θ_1, the three groups of Cα atoms are from residues R158-E160, F412-Q415 and H510-L512. The centroid of each group is computed and named as P_1, P_2 and P_3. θ_1 is then computed as the angle between vectors $\mathbf{P_2P_1}$ and $\mathbf{P_2P_3}$. For θ_2, its definition is analogue, by using the following three groups of residues: G117-D119, F412-Q415 and D560-R562.

Styrene diffusion pathways

Allowed conformations for the POP protein scaffold were extracted from the previous MDs trajectories by means of a QT clustering[25] (considering alpha carbons and a RMSD cut-off of 1.0 Å), which resulted on 194, 272 and 167 representative structures of the scaffold for the GSH, HFF and RFY variants, respectively. The styrene molecule was treated as flexible applying the GPathFinder implemented algorithm. Twenty runs of the GPathFinder multi-objective genetic algorithm were carried out for each variant/carbene orientation/face, defining a population of 12 individuals, which were evolved during 750 generations (recommended parameters for two objectives). The objectives used to guide the evolution were: i) vina docking score and ii) minimization of steric clashes along the binding route. The input .yaml file used with GPathFinder[28] v.1.3.0 is provided in section 6 of this ESI.

NCI Plot analysis

The Non Covalent Interaction (NCI) analyses along the diffusion pathways of the styrene have been performed through ligand mode NCI calculations with NCIPLOT4.[29,30] The electron density ρ(r) has been integrated for each frame of the pathway within two ranges, corresponding to attractive (sign(λ_2)ρ(r) between −0.1 and −0.02) and vdW interactions (sign(λ_2)ρ(r) between −0.02 and 0.02).

Docking of the intermediate **III**

Exploratory docking

The GaudiMM platform[17] was used to perform the exploratory docking study to filter what conformations from the MD simulation have the possibility of accommodating the styrene to form the intermediate **III**. The flexibility of the POP protein scaffold was considered by selecting six representative structures from the MD simulation, through a QT clustering[25] (considering alpha carbons and a RMSD cut-off of 2.0 Å). The flexibility of the cofactor+carbene+styrene adduct (intermediate **III**) was taken into account by selecting 18 representative structures of the intermediate **II** from the MD simulation (through a QT clustering[25] considering the intermediate **II** atoms and a RMSD cut-off of 2.0 Å) and adding the styrene molecule in both *Re* and *Si* faces of the carbene by means of the Chimera software.[16] The side chains of the following amino acids, ubicated in a distance up to 5 Å from any atom of the cofactor+carbene adduct, were treated as flexible: Met53, Phe99, Ser324, Tyr326, His328, Arg338, Thr340, Ile406, Met411 and Arg562. Ten runs of the GaudiMM multi-objective genetic algorithm were carried out for each of the six global conformations of the POP protein, defining a population of 52 individuals, which were evolved during 200 generations. The objectives used to guide the evolution were: i) coordination score between the Rh atom and His328; ii) distance of the coordination bond; iii) minimization of steric clashes; and iv) optimization of the LigScore.[31] Solutions with steric clashes < 150 Å^3, LigScore < 10 and coordination score < 1.0 were considered valid and provided the representative structures of the POP protein backbone and intermediate **II** for the further refinement dockings. The input .yaml file used with GaudiMM[17] v.0.0.7 is provided in section 5 of this ESI.

Refinement docking

Gold5.8,[32] with our recent version of GoldScore accounting for binding with coordination,[33,34] was used to carry out the refinement docking study to evaluate the affinities of the intermediate **III** into the HFF variant. The following constraints were introduced in the exploration: i) representative structures of the POP protein backbone were selected from the previous exploratory dockings; ii) representative structures of the cofactor+carbene adduct (intermediate **II**) were selected from the previous exploratory dockings; and iii) the side chains of the following amino acids, ubicated in a distance up to 5 Å from any atom of the cofactor+carbene adduct, were treated as flexible: Met53, Phe99, Ser324, Tyr326, His328, Arg338, Thr340, Ile406, Met411 and Arg562. The flexibility of these side chains were taken into account by applying the rotamer conformations found during MDs, extracted with a rotamer dynamics analysis[35] (Table S6). For each POP backbone/intermediate **II** case, 50 docking solutions were generated into the covalent docking framework with a minimum of 100,000 building operations, considering the $C\alpha_{477}$-$C\beta_{cofactor}$ bond formation. The evaluation sphere was set to a radius of 15 Å from the centre of mass of the protein. Full flexibility according to the GOLD implemented algorithm was allowed for the Rh_2-cofactor. The solutions were analysed by means of the GaudiView GUI extension for Chimera.[16]

Table S6. Selected rotamers for each flexible residue in the refinement docking of the intermediate **III**.

Residue	Selected rotamers (following [35] nomenclature)
Met53	ptm, tpp, tpt, ttm, mtp, 0
Phe99	t80, 0
Ser324	t, m
Tyr326	t80, m-85, 0
His328	Free rotation
Arg338	ttt85, ttt-85, 0
Thr340	t
Ile406	tp, tt, mt, mm
Met411	ptp, 0
Arg562	ptp180, ttm-85, mtm180, mmt-85, 0

5. GaudiMM input files

Intermediate **II**, GSH variant

```
ga:
    cx_pb: 0.5
    mu: 1
    mut_indpb: 1.0
    mut_pb: 0.5
    population: 52
    generations: 200

output:
    check_every: 0
    name: gsh_477Z_H326
    pareto: true
    path: ./gsh_477Z_H326

genes:
-   module: gaudi.genes.molecule
    name: Protein
    path: <path_to_the_POP_protein_folder>

-   module: gaudi.genes.molecule
    name: Intermediate_II
    path: <path_to_the_intermediate_II.mol2>

-   module: gaudi.genes.torsion
    name: Torsion_HIS
    target: Protein
    rotatable_bonds: [[5247, 5251, 5247], [5251, 5252, 5251]]

-   module: gaudi.genes.rotamers
    name: Rotamers
    library: dunbrack
    residues: [Protein/99, Protein/301]

-   module: gaudi.genes.torsion
    name: Torsion
    target: Intermediate_II #Bonds allowed to rotate as defined in Fig S6
    rotatable_bonds: [[87, 89, 87], [89, 90, 89], [95, 97, 95], [66, 63,
66], [63, 12, 63], [12, 10, 12], [10, 9, 10], [9, 1, 9], [36, 108, 36],
[108, 109, 108], [109, 111, 109], [123, 126, 123] ]

objectives:
-   module: gaudi.objectives.contacts
    name: Clashes
    probes: [Intermediate_II]
    which: clashes
    weight: -1.0

-   module: gaudi.objectives.coordination
```

```
    name: Coordination
    weight: -1.0
    probe: Intermediate_II/35
    residues: [Protein/326]
    radius: 4.0
    atom_names: [NE2]
    prevent_intruders: True
    distance_correction: True

-   module: gaudi.objectives.distance
    name: Distance
    weight: -1.0
    target: Protein/5256  # Serial number of the coordinant atom
    probes: [Intermediate_II/35]  # Serial number of the Rh atom
    threshold: 2.0

similarity:
    args: [[Intermediate_II], 0.2]
    kwargs: {}
    module: gaudi.similarity.rmsd
```

Intermediate **II**, HFF variant

```
ga:
    cx_pb: 0.5
    mu: 1
    mut_indpb: 1.0
    mut_pb: 0.5
    population: 52
    generations: 200

output:
    check_every: 0
    name: hff_477Z_H328
    pareto: true
    path: ./hff_477Z_H328

genes:
-   module: gaudi.genes.molecule
    name: Protein
    path: <path_to_the_POP_protein_folder>

-   module: gaudi.genes.molecule
    name: Intermediate_II
    path: <path_to_the_intermediate_II.mol2>

-   module: gaudi.genes.torsion
    name: Torsion_HIS
    target: Protein
    rotatable_bonds: [[5295, 5299, 5295], [5299, 5300, 5299]]

-   module: gaudi.genes.rotamers
    name: Rotamers
```

```
    library: dunbrack
    residues: [Protein/99, Protein/594]

-   module: gaudi.genes.torsion
    name: Torsion
    target: Intermediate_II #Bonds allowed to rotate as defined in Fig S6
    rotatable_bonds: [[87, 89, 87], [89, 90, 89], [95, 97, 95], [66, 63,
66], [63, 12, 63], [12, 10, 12], [10, 9, 10], [9, 1, 9], [36, 108, 36],
[108, 109, 108], [109, 111, 109], [123, 126, 123] ]

objectives:
-   module: gaudi.objectives.contacts
    name: Clashes
    probes: [Intermediate_II]
    which: clashes
    weight: -1.0

-   module: gaudi.objectives.coordination
    name: Coordination
    weight: -1.0
    probe: Intermediate_II/35
    residues: [Protein/328]
    radius: 4.0
    atom_names: [NE2]
    prevent_intruders: True
    distance_correction: True

-   module: gaudi.objectives.distance
    name: Distance
    weight: -1.0
    target: Protein/5304  # Serial number of the coordinant atom
    probes: [Intermediate_II/35]  # Serial number of the Rh atom
    threshold: 2.0

similarity:
    args: [[Intermediate_II], 0.2]
    kwargs: {}
    module: gaudi.similarity.rmsd
```

Intermediate **II**, RFY variant

```
ga:
    cx_pb: 0.5
    mu: 1
    mut_indpb: 1.0
    mut_pb: 0.5
    population: 52
    generations: 200

output:
    check_every: 0
    name: rfy_413Z_E241 # rfy_413Z_E283, rfy_413Z_Y239, rfy_413Z_H591
```

```
    pareto: true
    path: ./rfy_413Z_E241 # rfy_413Z_E283, rfy_413Z_Y239, rfy_413Z_H591

genes:
-   module: gaudi.genes.molecule
    name: Protein
    path: <path_to_the_POP_protein_folder>

-   module: gaudi.genes.molecule
    name: Intermediate_II
    path: <path_to_the_intermediate_II.mol2>

-   module: gaudi.genes.torsion
    name: Torsion_E241 # Torsion_E283, Torsion_Y239, Torsion_H591
    target: Protein
    rotatable_bonds: [[3909, 3912, 3909], [3912, 3913, 3912], [3913, 3914,
3913]]

-   module: gaudi.genes.rotamers
    name: Rotamers
    library: dunbrack
    residues: [Protein/98, Protein/99, Protein/239]

-   module: gaudi.genes.torsion
    name: Torsion
    target: Intermediate_II #Bonds allowed to rotate as defined in Fig S6
    rotatable_bonds: [[86, 87, 86], [87, 88, 87], [93, 94, 93], [66, 63,
66], [63, 12, 63], [12, 10, 12], [10, 9, 10], [9, 1, 9], [36, 103, 36],
[103, 104, 103], [104, 106, 104], [118, 121, 118] ]

objectives:
-   module: gaudi.objectives.contacts
    name: Clashes
    probes: [Intermediate_II]
    which: clashes
    weight: -1.0

-   module: gaudi.objectives.coordination
    name: Coordination
    weight: -1.0
    probe: Intermediate_II/35
    residues: [Protein/241]  # [Protein/283], [Protein/239], [Protein/591]
    radius: 4.0
    atom_names: [OE1]  # Name of the coordinant atom in each case
    prevent_intruders: True
    distance_correction: True

-   module: gaudi.objectives.distance
    name: Distance
    weight: -1.0
    target: Protein/3915  # Serial number of the coordinant atom
    probes: [Intermediate_II/35] # Serial number of the Rh atom
    threshold: 2.0
```

```
similarity:
    args: [[Intermediate_II], 0.2]
    kwargs: {}
    module: gaudi.similarity.rmsd
```

Intermediate **III**, HFF variant

```
ga:
    cx_pb: 0.5
    mu: 1
    mut_indpb: 1.0
    mut_pb: 0.5
    population: 52
    generations: 200

output:
    check_every: 0
    name: hff_POP1_RS  # hff_POP2_RS, hff_POP3_RS, hff_POP4_RS,
# hff_POP5_RS, hff_POP6_RS, hff_POP1_SR, hff_POP2_SR, hff_POP3_SR,
# hff_POP4_SR, hff_POP5_SR, hff_POP6_SR
    pareto: true
    path: ./hff_POP1_RS  # And the rest of POP representatives

genes:
-   module: gaudi.genes.molecule
    name: Protein
    path: <path_to_the_POP_represntative.mol2 file>

-   module: gaudi.genes.molecule
    name: IntermediateIII
    path: <path_to_the_folder_with_IntermediateIII_representatives>

-   module: gaudi.genes.torsion
    name: Torsion_HIS328
    target: Protein
    rotatable_bonds: [[5266, 5269, 5266], [5269, 5270, 5269]]

-   module: gaudi.genes.rotamers
    name: Rotamers
    library: dunbrack
    residues: [Protein/53, Protein/99, Protein/324, Protein/326,
Protein/338, Protein/340, Protein/406, Protein/411, Protein/562]

objectives:
-   module: gaudi.objectives.contacts
    name: Clashes
    probes: [IntermediateIII]
    which: clashes
    weight: -1.0

-   module: gaudi.objectives.coordination
```

```
    name: Coordination
    weight: -1.0
    probe: IntermediateIII/106  #Serial number of the Rh atom
    residues: [Protein/328]
    radius: 4.0
    atom_names: [NE2]
    prevent_intruders: True
    distance_correction: True

-   module: gaudi.objectives.distance
    name: Distance
    weight: -1.0
    target: Protein/5273  #Serial number of the HIS328 NE2 atom
    probes: [IntermediateIII/106]  #Serial number of the Rh atom
    threshold: 2.0

-   module: gaudi.objectives.ligscore
    name: LigScore
    weight: -1.0
    proteins: [Protein]
    ligands: [IntermediateIII]

similarity:
    args: [[IntermediateIII], 0.2]
    kwargs: {}
    module: gaudi.similarity.rmsd
```

6. GPathFinder input file

```
ga:         # Section to configure the Genetic Algorithm parameters
    mut_pb: 0.8
    cx_pb: 0.2
    mut_indpb: 1
    generations: 750
    population: 12

output:
    check_every: 0
    # One .yaml file per variant/carbene representative/face
    name: gsh_carbene1_RS  # variant_carbeneRepresentative_face
    pareto: False
    path: ./gsh_carbene1_RS

genes:      # Section to configure the genes
-   module: gpath.genes.molecule
    name: Ligand
    path: <path_to_the_final_position_of_styrene.mol2 file>
-   module: gpath.genes.molecule
    name: Protein
    path: <path_to_the_folder_with_POP_IntermediateII_representatives>
    first_frame: <path_to_final_position_of_POP_IntermediateII.mol2 file>
-   module: gpath.genes.path_torsion
    name: T
    target: Ligand
    anchor: Ligand/4  # Serial number of the central atom of the styrene
-   module: gpath.genes.path
    name: Pathway
    ligand: Ligand
    protein: Protein
    torsion_gene: T
    min_step_increment: 0

objectives:     # Section to configure the evaluation of the pathways
-   module: gpath.objectives.path_scoring
    name: Clashes
    probe: Pathway
    which: clashes
    method: max
    weight: -1.0
-   module: gpath.objectives.path_scoring
    name: Vina
    probe: Pathway
    which: vina
    method: max
    weight: -1.0

similarity:
    args:
    - Pathway
    - 1.0
```

```
kwargs: {}
module: gpath.path_similarity.pathways_rmsd
```

7. Cartesian coordinates obtained from DFT calculations

Rh2_co-factor

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3011.080316
Thermal and entropic correction, BS1 (a.u.)	0.790856
Electronic Energy, BS2 (a.u.)	-3012.196581
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	1.177050	-2.845123	-0.044301
C	1.742330	-2.460156	-1.256117
C	3.098920	-2.113682	-1.304173
C	3.837896	-2.189041	-0.117201
C	3.270426	-2.596809	1.096687
C	1.911633	-2.930895	1.132083
H	1.128963	-2.427539	-2.150465
H	1.426556	-3.244276	2.050866
O	-0.170789	-3.248643	0.010725
C	-1.111439	-2.380545	-0.440238
O	-0.916660	-1.230842	-0.783408
O	-2.278844	-3.017702	-0.430410
H	4.889340	-1.941623	-0.109862
C	3.666514	-1.635642	-2.631986
H	3.259249	-0.637438	-2.829957
H	3.275383	-2.281329	-3.426825
C	5.206890	-1.569897	-2.819228
C	5.490243	-1.021043	-4.237752
H	5.033411	-0.038251	-4.381969
H	6.568076	-0.930735	-4.408831
H	5.082798	-1.706347	-4.987632
C	5.800797	-0.557724	-1.830003
C	5.850704	-2.957308	-2.682255
H	6.926296	-2.909526	-2.873230
H	5.701076	-3.391398	-1.691775
H	5.403753	-3.632599	-3.418737
O	5.274262	0.605481	-1.826143
O	6.766876	-0.921307	-1.079468
C	4.138379	-2.637257	2.333700
H	5.182954	-2.664413	2.013747
H	3.951052	-3.569121	2.879765
C	3.963017	-1.477587	3.344639

H	3.062883	-1.654617	3.943797
H	4.808096	-1.543460	4.038531
Rh	5.897694	1.999313	-0.434888
Rh	7.466540	0.372825	0.395686
O	6.594923	3.293271	1.037802
O	8.069091	1.753111	1.812830
C	7.497599	2.895254	1.850773
C	7.887199	3.829846	2.963343
H	7.819062	4.867772	2.632449
H	7.184006	3.686432	3.791689
H	8.894065	3.608225	3.320347
O	7.359908	2.650907	-1.753294
O	8.837467	1.117021	-0.971821
C	8.506913	2.088271	-1.735741
C	9.559277	2.629787	-2.664910
H	9.100432	3.016766	-3.576531
H	10.074714	3.455720	-2.161839
H	10.293396	1.859019	-2.904812
C	3.852265	-0.015345	2.828852
C	4.202871	0.929300	4.009195
H	5.226852	0.762318	4.358062
H	4.103069	1.978395	3.712878
H	3.520054	0.741383	4.844280
C	2.421571	0.313773	2.354158
H	2.311836	1.383636	2.160743
H	2.152537	-0.224640	1.443755
H	1.708598	0.036761	3.136826
C	4.867298	0.331187	1.736178
O	4.531415	1.254532	0.918355
O	6.007409	-0.243029	1.750949
C	-3.402024	-2.270039	-1.005361
H	-3.160927	-2.068876	-2.053785
H	-3.495838	-1.318058	-0.475843
C	-4.631875	-3.107435	-0.855038
H	-4.585844	-4.079728	-1.343177
C	-5.975188	-2.423982	-0.877307
C	-5.463108	-3.044267	0.411281
H	-5.122843	-2.302715	1.131324
H	-5.939414	-1.334572	-0.891499
C	-6.013873	-4.316198	1.060847
H	-5.639816	-4.334385	2.089654
H	-5.595096	-5.201691	0.571136
C	-7.560861	-4.491581	1.104020
H	-7.896471	-5.011787	0.203008
H	-7.813693	-5.142438	1.946899
C	-8.335913	-3.219917	1.230990
C	-7.137295	-2.989996	-1.665833
H	-7.175663	-4.076678	-1.555237
H	-6.990582	-2.794993	-2.734705
C	-8.481147	-2.351722	-1.254952
H	-8.504131	-1.316263	-1.610532
H	-9.303452	-2.867496	-1.765776
C	-8.721206	-2.345972	0.225729
N	-14.046879	2.956910	0.159837

C	-12.938117	3.952681	-0.073808
C	-13.610956	5.253717	-0.596945
O	-14.870824	5.208115	-0.730650
C	-11.891402	3.419173	-1.061054
C	-11.201678	2.165304	-0.574850
C	-10.286532	2.223988	0.487977
C	-11.492481	0.918562	-1.143015
C	-9.669306	1.072227	0.966167
C	-10.892767	-0.247299	-0.664689
C	-9.979683	-0.162739	0.387108
O	-12.840568	6.210834	-0.838698
N	-9.363995	-1.343399	0.897578
H	-12.473201	4.158549	0.891746
H	-11.170500	4.228790	-1.202251
H	-12.375198	3.237197	-2.027118
H	-10.048887	3.183918	0.937855
H	-12.201077	0.855994	-1.964260
H	-8.950514	1.119422	1.776697
H	-11.139042	-1.211694	-1.095440
H	-13.937819	2.095412	-0.381406
H	-14.893818	3.482708	-0.156215
H	-14.142667	2.703254	1.144897
N	-9.375288	-1.581857	2.236898
N	-8.749481	-2.715427	2.429520

(4-methoxyphenyl)methyldiazoacetate (1)

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-722.231769
Thermal and entropic correction, BS1 (a.u.)	0.147887
Electronic Energy, BS2 (a.u.)	-722.518789
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	1.517555	0.645017	0.113266
C	2.580009	-0.354952	0.005451
O	3.776094	-0.106399	0.138247
O	2.098549	-1.580101	-0.272576
C	3.089745	-2.623300	-0.406998
H	3.752108	-2.411955	-1.249970
H	3.677494	-2.713910	0.509402
C	0.051920	0.463774	0.025557
C	-0.573506	-0.663409	0.577678
C	-0.753213	1.440035	-0.591370

C	-1.956348	-0.832771	0.499645
H	0.022373	-1.421961	1.071287
C	-2.131470	1.290078	-0.655705
H	-0.297216	2.323792	-1.028301
C	-2.743576	0.148263	-0.116784
H	-2.403200	-1.719995	0.930868
H	-2.751590	2.042487	-1.132259
O	-4.105531	0.086338	-0.243342
C	-4.777702	-1.062280	0.283355
H	-5.837358	-0.909622	0.073438
H	-4.438069	-1.982220	-0.206266
H	-4.630894	-1.149076	1.366015
N	1.980039	1.867189	0.282354
N	2.364109	2.929580	0.413457
H	2.523949	-3.536366	-0.588088

Intermediate I

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3733.351277
Thermal and entropic correction, BS1 (a.u.)	0.963329
Electronic Energy, BS2 (a.u.)	-3734.742739
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	-0.208104	2.272757	1.148113
C	0.249066	1.484152	2.199102
C	1.579500	1.046043	2.204651
C	2.406213	1.443846	1.145934
C	1.947392	2.255298	0.100583
C	0.612110	2.676396	0.102551
H	-0.429737	1.210651	3.000338
H	0.211034	3.296265	-0.692803
O	-1.531005	2.756558	1.159808
C	-2.529199	1.838581	1.205103
O	-2.395382	0.635055	1.097932
O	-3.672576	2.494915	1.382633
H	3.441079	1.135982	1.110530
C	2.019859	0.127743	3.335065
H	1.530800	-0.841943	3.185879
H	1.621564	0.522824	4.276881
C	3.534345	-0.130428	3.554626
C	3.686137	-1.134016	4.721943
H	3.151119	-2.065190	4.516808

H	4.742012	-1.369947	4.891851
H	3.282628	-0.697234	5.640827
C	4.121692	-0.809493	2.312118
C	4.284855	1.163818	3.905226
H	5.340726	0.963099	4.106152
H	4.230513	1.907574	3.107925
H	3.842905	1.599302	4.807103
O	3.529133	-1.859750	1.889620
O	5.154574	-0.296012	1.770678
C	2.895182	2.625166	-1.016330
H	3.918864	2.453939	-0.677169
H	2.810868	3.697894	-1.227748
C	2.684158	1.884683	-2.356171
H	1.799682	2.296316	-2.855333
H	3.534368	2.141115	-2.993060
Rh	4.218461	-2.761570	0.164571
Rh	5.910364	-1.079372	-0.001988
O	4.987321	-3.568806	-1.593993
O	6.585062	-1.970086	-1.737716
C	5.978916	-3.006142	-2.173010
C	6.441849	-3.578200	-3.484422
H	6.227250	-4.646803	-3.536714
H	5.895008	-3.073983	-4.289374
H	7.508296	-3.394809	-3.627172
O	5.539841	-3.913588	1.278435
O	7.146292	-2.322919	1.116127
C	6.710845	-3.458350	1.510604
C	7.666480	-4.336063	2.271353
H	7.124563	-5.048942	2.894599
H	8.271795	-4.894181	1.548080
H	8.337668	-3.728907	2.881829
C	2.497566	0.339319	-2.361035
C	2.909008	-0.175952	-3.765675
H	3.963148	0.038522	-3.969153
H	2.748263	-1.255515	-3.850931
H	2.303798	0.323215	-4.529598
C	1.026156	-0.047830	-2.105773
H	0.869160	-1.117689	-2.262405
H	0.706195	0.198859	-1.091281
H	0.383428	0.494927	-2.805793
C	3.415735	-0.410214	-1.389580
O	2.983748	-1.529248	-0.943233
O	4.574906	0.059608	-1.144587
C	-4.849248	1.642751	1.581699
H	-4.639363	0.982729	2.428776
H	-4.993302	1.031381	0.686490
C	-6.024260	2.531566	1.841248
H	-5.910719	3.196041	2.696404
C	-7.403532	1.964588	1.623089
C	-6.881564	3.054460	0.704361
H	-6.598627	2.686951	-0.279982
H	-7.428202	0.972509	1.171920
C	-7.385151	4.498482	0.699017
H	-6.980912	4.974132	-0.200377

H	-6.962407	5.047769	1.546592
C	-8.929407	4.719771	0.719453
H	-9.265590	4.843600	1.752560
H	-9.155540	5.660504	0.208094
C	-9.737980	3.629602	0.093279
C	-8.525190	2.195414	2.613272
H	-8.514414	3.231982	2.960363
H	-8.374540	1.571209	3.501750
C	-9.899931	1.830757	2.012744
H	-9.963546	0.741598	1.920915
H	-10.696300	2.125488	2.706999
C	-10.147362	2.432772	0.661138
N	-15.545845	-2.579220	-1.048789
C	-14.416347	-3.510677	-1.402831
C	-15.000324	-4.951000	-1.374977
O	-16.154483	-5.067032	-0.865883
C	-13.257791	-3.386447	-0.399970
C	-12.618225	-2.017181	-0.380497
C	-11.765543	-1.615213	-1.420778
C	-12.884139	-1.114204	0.656856
C	-11.171284	-0.357160	-1.413969
C	-12.311142	0.158298	0.667245
C	-11.443937	0.525005	-0.362611
O	-14.254261	-5.851220	-1.824699
N	-10.822339	1.808350	-0.352144
H	-14.075827	-3.263390	-2.408608
H	-12.527182	-4.145409	-0.692379
H	-13.626180	-3.649941	0.597549
H	-11.551890	-2.303711	-2.233562
H	-13.545553	-1.408125	1.467256
H	-10.491584	-0.057575	-2.203683
H	-12.534795	0.856651	1.465900
H	-15.276747	-1.831104	-0.404199
H	-16.253361	-3.214352	-0.622371
H	-15.959009	-2.151000	-1.880429
N	-10.826570	2.571085	-1.478411
N	-10.168177	3.668123	-1.200990
C	8.180755	1.123158	-0.377445
N	9.000268	0.150348	-0.725461
N	9.693880	-0.691988	-1.043953
C	7.960680	1.271271	1.064100
O	8.710488	0.407740	1.783576
O	7.176258	2.067231	1.567414
C	8.419180	0.341623	3.198187
H	9.141152	-0.364156	3.607139
H	8.540862	1.322386	3.662702
H	7.401752	-0.024886	3.351195
C	7.450487	1.839511	-1.443711
C	6.894352	3.105465	-1.215960
C	7.250260	1.237185	-2.701724
C	6.124009	3.739436	-2.193198
H	7.041793	3.597977	-0.263803
C	6.498618	1.867472	-3.681658
H	7.648483	0.248669	-2.905591

C	5.913598	3.117177	-3.428029
H	5.692593	4.707851	-1.972848
H	6.326634	1.390663	-4.641178
O	5.139909	3.629995	-4.436155
C	4.407172	4.830066	-4.168278
H	3.735844	4.701492	-3.311552
H	5.078916	5.676494	-3.985386
H	3.817196	5.025858	-5.064779

TS I-II

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3733.321493
Thermal and entropic correction, BS1 (a.u.)	0.959988
Electronic Energy, BS2 (a.u.)	-3734.708916
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-469.4i

Molecular Geometry in Cartesian Coordinates

C	-0.209542	-2.081379	-1.475830
C	0.309821	-1.256096	-2.468183
C	1.632396	-0.804680	-2.366203
C	2.389282	-1.227620	-1.265571
C	1.866167	-2.069023	-0.275185
C	0.539938	-2.503208	-0.384851
H	-0.313489	-0.965380	-3.307161
H	0.090421	-3.148112	0.363384
O	-1.518859	-2.587670	-1.588915
C	-2.535363	-1.694894	-1.690926
O	-2.435410	-0.486005	-1.611736
O	-3.654706	-2.387131	-1.882972
H	3.417357	-0.916048	-1.154600
C	2.140161	0.162570	-3.424718
H	1.701275	1.145828	-3.217560
H	1.739250	-0.146460	-4.396870
C	3.670872	0.354196	-3.605011
C	3.893506	1.373955	-4.746004
H	3.391660	2.322037	-4.534745
H	4.961992	1.570534	-4.884500
H	3.496534	0.973344	-5.684001
C	4.258235	0.980362	-2.331639
C	4.362139	-0.967503	-3.970108
H	5.428545	-0.813393	-4.155313
H	4.262164	-1.720383	-3.186372
H	3.911052	-1.365065	-4.885042

O	3.724418	2.064408	-1.924811
O	5.229988	0.385636	-1.760655
C	2.726379	-2.441221	0.910262
H	3.774909	-2.305418	0.636920
H	2.594594	-3.504926	1.140591
C	2.446370	-1.659961	2.218177
H	1.540333	-2.061798	2.685790
H	3.271851	-1.896381	2.897605
Rh	4.379866	2.887090	-0.142243
Rh	5.938455	1.024522	0.097861
O	5.096336	3.589308	1.684395
O	6.559067	1.867271	1.876528
C	6.007412	2.941883	2.297025
C	6.454027	3.446102	3.642482
H	6.234111	4.509029	3.751351
H	5.908231	2.892508	4.414979
H	7.520850	3.260656	3.783127
O	5.922074	3.897876	-1.124294
O	7.358749	2.154693	-0.915666
C	7.058893	3.343050	-1.282827
C	8.158451	4.153852	-1.915204
H	7.747817	4.991467	-2.480368
H	8.797585	4.545895	-1.116032
H	8.774089	3.523525	-2.560416
C	2.253996	-0.115417	2.180899
C	2.530410	0.419373	3.611493
H	3.561930	0.213050	3.915921
H	2.358993	1.499141	3.666227
H	1.859047	-0.072221	4.323261
C	0.817308	0.274861	1.779471
H	0.655771	1.347572	1.910970
H	0.596772	0.022167	0.740833
H	0.104265	-0.256551	2.417462
C	3.266398	0.613006	1.293224
O	2.947688	1.771019	0.860805
O	4.396832	0.057832	1.107275
C	-4.860028	-1.581081	-2.102345
H	-4.724687	-1.034609	-3.040853
H	-4.951945	-0.861055	-1.284965
C	-6.028185	-2.513812	-2.148256
H	-5.983154	-3.265207	-2.934916
C	-7.397809	-1.968629	-1.831207
C	-6.729503	-2.934958	-0.871447
H	-6.352600	-2.453366	0.028646
H	-7.415242	-0.934758	-1.486447
C	-7.160245	-4.385826	-0.654911
H	-6.628621	-4.746793	0.231445
H	-6.816548	-5.008452	-1.487393
C	-8.683366	-4.659446	-0.460805
H	-9.132369	-4.913999	-1.424769
H	-8.802910	-5.541275	0.175983
C	-9.465356	-3.532526	0.133368
C	-8.612999	-2.342098	-2.654057
H	-8.592571	-3.407674	-2.897518

H	-8.594939	-1.808207	-3.611358
C	-9.928698	-1.967698	-1.937519
H	-10.039313	-0.878347	-1.954514
H	-10.780460	-2.369514	-2.499737
C	-9.995779	-2.424410	-0.509950
N	-15.580376	2.238886	1.375919
C	-14.533575	3.320449	1.478923
C	-15.291228	4.678127	1.442223
O	-16.548326	4.604587	1.297019
C	-13.500355	3.225141	0.347015
C	-12.716491	1.933284	0.361808
C	-11.724617	1.714515	1.330700
C	-12.988446	0.914973	-0.560424
C	-11.013137	0.519313	1.371885
C	-12.298040	-0.297010	-0.519143
C	-11.305631	-0.485971	0.443647
O	-14.582474	5.704744	1.551251
N	-10.587552	-1.716568	0.500439
H	-14.041522	3.212040	2.446841
H	-12.834187	4.082018	0.476005
H	-14.014816	3.348514	-0.612465
H	-11.499205	2.495011	2.052144
H	-13.754636	1.065146	-1.316084
H	-10.232913	0.360204	2.107734
H	-12.535037	-1.088140	-1.221684
H	-15.439377	1.611968	0.579611
H	-16.462845	2.787800	1.257425
H	-15.638382	1.669573	2.222403
N	-10.428265	-2.346766	1.695936
N	-9.747545	-3.440527	1.465042
C	7.169502	-0.794045	0.373171
N	8.691310	-0.102250	0.870602
N	9.244511	0.657664	1.470716
C	7.435157	-1.304903	-0.994986
O	8.480060	-0.731579	-1.614398
O	6.671178	-2.088531	-1.546846
C	8.623748	-1.040587	-3.021363
H	9.524135	-0.516787	-3.339283
H	8.737176	-2.116867	-3.167206
H	7.754365	-0.676913	-3.573842
C	6.812212	-1.736623	1.440457
C	6.790033	-3.132322	1.246151
C	6.419484	-1.238738	2.706204
C	6.331533	-3.995488	2.235816
H	7.106467	-3.553730	0.300072
C	5.999295	-2.088528	3.710426
H	6.446151	-0.171548	2.886759
C	5.927983	-3.475141	3.475823
H	6.302453	-5.060023	2.040740
H	5.694380	-1.705693	4.678707
O	5.461053	-4.222096	4.507957
C	5.356848	-5.642804	4.334093
H	4.672441	-5.890610	3.515823

H	6.338353	-6.090113	4.144753
H	4.956678	-6.025935	5.273225

Intermediate II

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3623.830793
Thermal and entropic correction, BS1 (a.u.)	0.957163
Electronic Energy, BS2 (a.u.)	-3625.172680
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	0.101913	-2.799944	0.966711
C	0.936464	-3.449532	0.067418
C	2.278084	-3.051422	-0.038473
C	2.712184	-1.994902	0.771680
C	1.862293	-1.341814	1.675780
C	0.534656	-1.765879	1.786214
H	0.535902	-4.248832	-0.548696
H	-0.163230	-1.281459	2.461533
O	-1.241455	-3.221533	1.058113
C	-2.112823	-2.567437	0.250159
O	-1.829216	-1.659254	-0.508363
O	-3.315778	-3.099185	0.438332
H	3.732418	-1.644082	0.715527
C	3.146111	-3.755136	-1.071811
H	2.751095	-3.500529	-2.062011
H	3.005210	-4.836894	-0.961995
C	4.677946	-3.499749	-1.090665
C	5.273979	-4.275308	-2.289229
H	4.806355	-3.972486	-3.229894
H	6.352070	-4.098075	-2.364558
H	5.113557	-5.349220	-2.151770
C	4.941495	-2.010957	-1.355213
C	5.354079	-3.984747	0.200559
H	6.437501	-3.856377	0.140589
H	4.998915	-3.452995	1.085093
H	5.142927	-5.050216	0.336655
O	4.384854	-1.501039	-2.380462
O	5.693653	-1.378901	-0.538940
C	2.377848	-0.156158	2.456460
H	3.469574	-0.167891	2.423469
H	2.090561	-0.256181	3.509756
C	1.877451	1.232421	1.981111

H	0.869217	1.403132	2.374501
H	2.524533	1.973277	2.463833
Rh	4.589397	0.531994	-2.743167
Rh	5.909230	0.691903	-0.680345
O	4.826368	2.587559	-2.953361
O	6.028396	2.732943	-1.034771
C	5.452218	3.242669	-2.058969
C	5.492986	4.742489	-2.176095
H	5.308615	5.054416	-3.204999
H	4.706216	5.156598	-1.535350
H	6.452890	5.128464	-1.827012
O	6.358475	0.179933	-3.775835
O	7.587294	0.342657	-1.871150
C	7.453632	0.130013	-3.127847
C	8.703942	-0.247155	-3.877087
H	8.578514	-0.083218	-4.948198
H	9.558321	0.319916	-3.501812
H	8.900233	-1.310928	-3.701765
C	1.801574	1.557558	0.460422
C	1.796310	3.102783	0.317297
H	2.714690	3.539829	0.723778
H	1.706050	3.398174	-0.732725
H	0.945509	3.518719	0.866873
C	0.522182	0.997634	-0.195104
H	0.394372	1.404346	-1.201608
H	0.537787	-0.089560	-0.270101
H	-0.350345	1.285176	0.399480
C	3.034291	1.099743	-0.319912
O	2.905957	0.895986	-1.570987
O	4.133958	1.024431	0.323342
C	-4.386077	-2.543065	-0.396786
H	-4.098434	-2.677877	-1.443562
H	-4.465181	-1.472894	-0.185626
C	-5.646589	-3.269905	-0.052019
H	-5.634107	-4.335310	-0.277096
C	-6.973511	-2.578968	-0.238999
C	-6.461256	-2.871810	1.162406
H	-6.093142	-1.978812	1.663299
H	-6.912729	-1.527152	-0.518681
C	-7.010456	-3.923368	2.132373
H	-6.721177	-3.606252	3.139749
H	-6.515007	-4.885904	1.964598
C	-8.542198	-4.179071	2.138616
H	-8.806847	-4.883246	1.346221
H	-8.803663	-4.667344	3.082965
C	-9.376261	-2.947915	1.990051
C	-8.144095	-3.292200	-0.882791
H	-8.185615	-4.333001	-0.552978
H	-7.996473	-3.323067	-1.968916
C	-9.486139	-2.579250	-0.620903
H	-9.491162	-1.625754	-1.160386
H	-10.302901	-3.173144	-1.049329
C	-9.764388	-2.301041	0.826774
N	-15.297874	2.516600	-0.447807

C	-14.270046	3.562609	-0.791431
C	-15.026062	4.720282	-1.505411
O	-16.288805	4.687132	-1.408219
C	-13.120179	2.970319	-1.610500
C	-12.397809	1.861589	-0.879654
C	-11.551926	2.157837	0.200377
C	-12.594255	0.520017	-1.229699
C	-10.908273	1.145721	0.905915
C	-11.967692	-0.506911	-0.522841
C	-11.120736	-0.187497	0.539666
O	-14.315892	5.582080	-2.073618
N	-10.474191	-1.221751	1.278819
H	-13.893590	3.947990	0.159923
H	-12.440893	3.797428	-1.830504
H	-13.514551	2.605307	-2.565242
H	-11.389629	3.194120	0.483663
H	-13.252143	0.272791	-2.058122
H	-10.241906	1.377026	1.729283
H	-12.143675	-1.544098	-0.785701
H	-15.321893	1.767131	-1.145295
H	-16.198784	3.033507	-0.493796
H	-15.147626	2.092601	0.469393
N	-10.519667	-1.202090	2.638318
N	-9.851509	-2.245153	3.059377
C	6.921877	0.777121	1.087021
C	7.931758	-0.290368	1.213826
O	9.055366	-0.207777	0.726669
O	7.466292	-1.382030	1.843003
C	8.343982	-2.536147	1.850952
H	7.775699	-3.328861	2.334175
H	8.604689	-2.818894	0.829005
H	9.250100	-2.315820	2.419704
C	6.714196	1.641220	2.183821
C	7.386915	1.445581	3.432362
C	5.781174	2.727973	2.107758
C	7.137443	2.241423	4.529265
H	8.108222	0.640585	3.530227
C	5.524347	3.523726	3.196856
H	5.272658	2.917502	1.173875
C	6.188971	3.284488	4.422754
H	7.659921	2.059380	5.459555
H	4.813653	4.341623	3.145810
O	5.853531	4.101506	5.428949
C	6.475268	3.932313	6.718708
H	6.026262	4.692545	7.357077
H	6.265177	2.937132	7.121207
H	7.555001	4.093732	6.651160

Intermediate III

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.521953
Thermal and entropic correction, BS1 (a.u.)	1.083048
Electronic Energy, BS2 (a.u.)	-3934.96995
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	1.176715	-2.214907	-0.171288
C	0.672667	-1.844101	1.071556
C	-0.663491	-1.438141	1.181635
C	-1.449657	-1.445035	0.021681
C	-0.941777	-1.833626	-1.225378
C	0.398775	-2.224892	-1.321904
H	1.320151	-1.867202	1.942263
H	0.834996	-2.526956	-2.268560
O	2.502145	-2.678209	-0.280454
C	3.493002	-1.852657	0.142934
O	3.361859	-0.688280	0.466231
O	4.625030	-2.550791	0.134754
H	-2.489737	-1.155145	0.060494
C	-1.152044	-0.967042	2.543219
H	-0.706321	0.015984	2.735392
H	-0.742230	-1.637005	3.307953
C	-2.677990	-0.857299	2.804636
C	-2.881202	-0.338188	4.247307
H	-2.388105	0.626211	4.395976
H	-3.947432	-0.219648	4.467176
H	-2.464186	-1.055343	4.961393
C	-3.278422	0.202857	1.869644
C	-3.371784	-2.220070	2.662131
H	-4.434184	-2.146279	2.906893
H	-3.281931	-2.630593	1.655224
H	-2.910845	-2.927830	3.358739
O	-2.731789	1.352508	1.877445
O	-4.281033	-0.128453	1.154094
C	-1.849342	-1.796401	-2.432290
H	-2.882354	-1.810657	-2.084398
H	-1.703425	-2.707560	-3.024242
C	-1.681529	-0.598349	-3.399543
H	-0.816982	-0.775700	-4.049061
H	-2.561105	-0.609402	-4.052778
Rh	-3.397090	2.805419	0.554797
Rh	-5.042832	1.181866	-0.266012
O	-4.161531	4.148910	-0.833053
O	-5.675044	2.638505	-1.595471

C	-5.117769	3.791872	-1.592989
C	-5.634323	4.781827	-2.602405
H	-5.255587	5.782966	-2.394200
H	-5.302700	4.471296	-3.599028
H	-6.727199	4.782166	-2.598650
O	-4.797564	3.411774	1.968120
O	-6.324875	1.933712	1.177018
C	-5.935293	2.840092	1.988702
C	-6.898707	3.229900	3.078247
H	-6.801976	4.292743	3.308627
H	-7.924543	2.992173	2.793959
H	-6.645028	2.659348	3.978603
C	-1.500791	0.836847	-2.832367
C	-1.854421	1.837079	-3.964700
H	-2.897486	1.726111	-4.278433
H	-1.697466	2.869459	-3.636493
H	-1.212998	1.650794	-4.832430
C	-0.044512	1.095952	-2.393087
H	0.110742	2.153262	-2.165045
H	0.231946	0.514486	-1.511845
H	0.633508	0.822555	-3.207583
C	-2.464908	1.181811	-1.692055
O	-2.092348	2.088644	-0.879021
O	-3.605026	0.606084	-1.671737
C	5.791058	-1.854905	0.688811
H	5.524286	-1.509056	1.691964
H	6.008870	-0.985877	0.061602
C	6.930040	-2.823854	0.710871
H	6.746442	-3.725747	1.292759
C	8.335566	-2.283081	0.764335
C	7.843121	-2.987766	-0.488182
H	7.633642	-2.299762	-1.304779
H	8.419076	-1.200988	0.662131
C	8.291240	-4.373623	-0.960152
H	7.997052	-4.461045	-2.011187
H	7.736322	-5.152200	-0.425943
C	9.805096	-4.720064	-0.851147
H	10.010265	-5.164077	0.126483
H	10.038730	-5.490415	-1.592725
C	10.734925	-3.566808	-1.050303
C	9.372291	-2.871857	1.697871
H	9.292816	-3.961931	1.713415
H	9.179032	-2.536174	2.723534
C	10.803451	-2.429957	1.327501
H	10.914673	-1.366538	1.564951
H	11.526180	-2.959812	1.960113
C	11.149363	-2.627761	-0.118391
N	17.037395	2.070639	0.193774
C	16.035673	3.186139	0.043813
C	16.733834	4.482999	0.541188
O	17.843116	4.320647	1.131147
C	14.764995	2.912820	0.865024
C	14.020426	1.673429	0.426972
C	13.266609	1.675280	-0.757213

C	14.093138	0.491022	1.174194
C	12.584766	0.536176	-1.174106
C	13.431604	-0.665238	0.757998
C	12.668646	-0.632936	-0.409724
O	16.112737	5.551043	0.334679
N	11.963870	-1.796010	-0.837849
H	15.788592	3.277550	-1.014304
H	14.136921	3.799777	0.746311
H	15.035717	2.839032	1.923833
H	13.200395	2.584115	-1.348819
H	14.675429	0.470383	2.091408
H	11.982188	0.546518	-2.075342
H	13.511646	-1.580835	1.333023
H	16.643843	1.210133	0.584669
H	17.756483	2.482373	0.826249
H	17.485992	1.841255	-0.695533
N	12.044634	-2.195130	-2.136071
N	11.297820	-3.263183	-2.255758
C	-6.397714	-0.186453	-0.944806
C	-5.770438	-1.465888	-1.334793
O	-5.369402	-1.683701	-2.475386
O	-5.634122	-2.321292	-0.315498
C	-4.941357	-3.565109	-0.580574
H	-5.029967	-4.141038	0.339225
H	-5.413535	-4.094520	-1.410698
H	-3.891415	-3.369513	-0.806415
C	-7.791797	-0.070620	-1.115280
C	-8.588152	-1.183346	-1.536375
C	-8.479322	1.149704	-0.814106
C	-9.959297	-1.105626	-1.631306
H	-8.105246	-2.124627	-1.777401
C	-9.847793	1.230133	-0.886226
H	-7.904139	2.013683	-0.512622
C	-10.604765	0.099498	-1.275807
H	-10.529198	-1.972597	-1.936522
H	-10.376918	2.144769	-0.641204
O	-11.933090	0.268018	-1.274005
C	-12.785626	-0.824565	-1.672055
H	-13.802566	-0.443832	-1.582630
H	-12.585102	-1.110460	-2.708593
H	-12.647691	-1.682059	-1.008188
C	-11.105106	-2.976434	1.050863
C	-9.921194	-3.697648	0.878800
C	-8.704400	-3.151445	1.288720
C	-8.647433	-1.885838	1.903042
C	-9.846404	-1.162131	2.050182
C	-11.059949	-1.702000	1.628019
H	-12.053457	-3.395035	0.727120
H	-9.943418	-4.680803	0.417575
H	-7.783246	-3.709412	1.140621
H	-9.824863	-0.165158	2.479615
H	-11.972780	-1.123099	1.735129
C	-7.341964	-1.372020	2.350902
H	-6.482483	-1.891455	1.935939

C	-7.125268	-0.358499	3.200415
H	-7.931288	0.200578	3.668011
H	-6.113229	-0.052875	3.446417

TS III-IVa

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.507321
Thermal and entropic correction, BS1 (a.u.)	1.084266
Electronic Energy, BS2 (a.u.)	-3934.952306
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-242.8i

Molecular Geometry in Cartesian Coordinates

C	1.234253	-2.203658	0.398473
C	0.713748	-1.858883	1.642178
C	-0.647128	-1.544891	1.755612
C	-1.432328	-1.604785	0.598115
C	-0.907896	-1.968535	-0.648216
C	0.454104	-2.273369	-0.749176
H	1.364620	-1.836541	2.510288
H	0.905594	-2.556136	-1.694590
O	2.583866	-2.587580	0.281667
C	3.530883	-1.699932	0.675930
O	3.335293	-0.546304	1.005753
O	4.704388	-2.323034	0.624269
H	-2.488721	-1.382839	0.637288
C	-1.176831	-1.124176	3.117754
H	-0.763290	-0.135338	3.346816
H	-0.766163	-1.803152	3.874256
C	-2.711863	-1.064537	3.342546
C	-2.964551	-0.546358	4.778146
H	-2.508196	0.435293	4.931834
H	-4.038730	-0.463619	4.974795
H	-2.538431	-1.244970	5.505156
C	-3.328068	-0.028429	2.391267
C	-3.363157	-2.447488	3.191091
H	-4.432788	-2.400317	3.413713
H	-3.246428	-2.857978	2.186261
H	-2.898320	-3.141772	3.898305
O	-2.794010	1.127507	2.384423
O	-4.328049	-0.378920	1.680986
C	-1.836928	-2.013424	-1.838706
H	-2.858820	-2.053055	-1.456868
H	-1.671871	-2.945139	-2.392905

C	-1.735894	-0.856935	-2.860975
H	-0.867920	-1.022109	-3.508933
H	-2.616899	-0.939443	-3.506249
Rh	-3.468341	2.564549	1.055582
Rh	-5.125453	0.931128	0.278437
O	-4.228146	3.905968	-0.330439
O	-5.752831	2.390273	-1.056580
C	-5.189175	3.536493	-1.081547
C	-5.700503	4.509043	-2.111409
H	-5.319403	5.513437	-1.923844
H	-5.368026	4.177226	-3.100932
H	-6.793444	4.511875	-2.109781
O	-4.851561	3.192477	2.474821
O	-6.365560	1.650837	1.787126
C	-5.972478	2.594347	2.554707
C	-6.918958	2.999767	3.654402
H	-6.613555	3.946779	4.100866
H	-7.936727	3.075400	3.264040
H	-6.911431	2.221150	4.424851
C	-1.623667	0.608640	-2.357143
C	-2.076808	1.540547	-3.512088
H	-3.119883	1.350520	-3.784270
H	-1.976847	2.593081	-3.227842
H	-1.452790	1.362505	-4.394129
C	-0.170701	0.964593	-1.981957
H	-0.067754	2.034253	-1.784061
H	0.169899	0.421346	-1.098769
H	0.491357	0.709066	-2.815279
C	-2.568749	0.937923	-1.195530
O	-2.182242	1.841191	-0.383697
O	-3.704746	0.356645	-1.157612
C	5.856165	-1.535637	1.075041
H	5.631945	-1.157292	2.076629
H	5.983690	-0.687489	0.396223
C	7.045950	-2.441832	1.065212
H	6.954953	-3.310807	1.715709
C	8.428907	-1.851387	0.965638
C	7.858487	-2.652048	-0.195956
H	7.550552	-2.013065	-1.021133
H	8.465160	-0.777350	0.783129
C	8.291608	-4.050003	-0.652215
H	8.076069	-4.115070	-1.723830
H	7.666857	-4.810974	-0.171460
C	9.772096	-4.462394	-0.446541
H	9.934972	-4.776258	0.587138
H	9.968727	-5.341671	-1.068718
C	10.766355	-3.402645	-0.797966
C	9.535886	-2.332330	1.880709
H	9.467492	-3.413220	2.025415
H	9.398833	-1.884534	2.872343
C	10.940443	-1.935870	1.388618
H	11.043733	-0.846415	1.446728
H	11.691014	-2.348259	2.074220
C	11.247240	-2.364142	-0.015680

N	17.530181	1.709290	-0.413950
C	16.665046	2.886083	-0.785464
C	17.520559	4.161917	-0.546067
O	18.631457	3.981300	0.036361
C	15.379263	2.925165	0.055249
C	14.490844	1.721877	-0.160012
C	13.728031	1.599377	-1.332086
C	14.444976	0.685083	0.780602
C	12.930127	0.481378	-1.554327
C	13.666590	-0.452357	0.562028
C	12.904546	-0.545339	-0.603407
O	17.012755	5.239762	-0.932117
N	12.105610	-1.700148	-0.851051
H	16.420511	2.801817	-1.844914
H	14.861176	3.843966	-0.231947
H	15.651194	3.014760	1.112704
H	13.750577	2.395533	-2.071067
H	15.029491	0.762047	1.693378
H	12.325928	0.397863	-2.450569
H	13.663064	-1.261157	1.283809
H	17.061176	1.026586	0.187188
H	18.333569	2.156858	0.079237
H	17.883254	1.218330	-1.238067
N	12.147062	-2.290673	-2.076088
N	11.334438	-3.314268	-2.036711
C	-6.609661	-0.415878	-0.514369
C	-5.904177	-1.519845	-1.222648
O	-5.365646	-2.500487	-0.718983
O	-5.812412	-1.254313	-2.550404
C	-5.230152	-2.287036	-3.377244
H	-5.157629	-1.855117	-4.374621
H	-4.245559	-2.582327	-3.018145
H	-5.889000	-3.159866	-3.391807
C	-7.879845	0.036552	-1.036237
C	-8.626495	-0.699941	-1.994889
C	-8.476311	1.231229	-0.543985
C	-9.856789	-0.268204	-2.465434
H	-8.233661	-1.635306	-2.375425
C	-9.703649	1.669112	-0.998687
H	-7.957598	1.801089	0.214417
C	-10.413773	0.915329	-1.952739
H	-10.391866	-0.869581	-3.188948
H	-10.156695	2.575407	-0.610330
O	-11.632220	1.398332	-2.297232
C	-12.457261	0.613458	-3.171124
H	-13.393517	1.164187	-3.265190
H	-11.996314	0.503337	-4.158196
H	-12.651402	-0.374120	-2.738142
C	-12.014311	-2.101760	-0.341425
C	-11.235841	-3.199126	-0.727692
C	-9.924048	-3.308685	-0.280091
C	-9.359363	-2.320561	0.559547
C	-10.171346	-1.237756	0.966299
C	-11.480248	-1.129413	0.513675

H	-13.036711	-2.009428	-0.695389
H	-11.651288	-3.957667	-1.383873
H	-9.308607	-4.147788	-0.592723
H	-9.769745	-0.478512	1.627612
H	-12.087751	-0.282244	0.816195
C	-7.957099	-2.415459	0.896131
H	-7.458084	-3.330211	0.587192
C	-7.183491	-1.412680	1.419669
H	-7.620530	-0.507174	1.822525
H	-6.165414	-1.623642	1.716014

TS III-IVb

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.507788
Thermal and entropic correction, BS1 (a.u.)	1.084924
Electronic Energy, BS2 (a.u.)	-3934.953057
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-241.1i

Molecular Geometry in Cartesian Coordinates

C	1.229318	-2.343386	0.758862
C	0.700631	-1.899364	1.966529
C	-0.645769	-1.515559	2.029170
C	-1.410337	-1.610113	0.859108
C	-0.875987	-2.067948	-0.352510
C	0.471238	-2.443511	-0.400689
H	1.335154	-1.854726	2.845836
H	0.929748	-2.799766	-1.317483
O	2.562369	-2.793230	0.698259
C	3.541952	-1.906612	1.004878
O	3.386886	-0.723917	1.239986
O	4.694281	-2.569843	0.992539
H	-2.456350	-1.340876	0.864227
C	-1.174935	-0.979082	3.350948
H	-0.754186	0.022191	3.499413
H	-0.769845	-1.597079	4.160757
C	-2.709796	-0.892379	3.572630
C	-2.957059	-0.290595	4.975764
H	-2.486184	0.690980	5.075982
H	-4.030253	-0.180551	5.164429
H	-2.543352	-0.953798	5.741997
C	-3.318094	0.091536	2.560808
C	-3.361432	-2.278864	3.500834
H	-4.434661	-2.218672	3.697033

H	-3.218906	-2.750013	2.527107
H	-2.910243	-2.926903	4.259095
O	-2.786767	1.247738	2.519186
O	-4.296851	-0.295442	1.838492
C	-1.760780	-2.114031	-1.576580
H	-2.801027	-2.120365	-1.246860
H	-1.592153	-3.056252	-2.111194
C	-1.576547	-0.971751	-2.606613
H	-0.695494	-1.181077	-3.223667
H	-2.439449	-1.024508	-3.279874
Rh	-3.413550	2.618920	1.109890
Rh	-5.023797	0.947487	0.314856
O	-4.107528	3.896487	-0.377856
O	-5.579063	2.340939	-1.122601
C	-5.007852	3.481570	-1.178311
C	-5.420270	4.384902	-2.310837
H	-5.173066	5.423909	-2.088540
H	-4.877050	4.077535	-3.211551
H	-6.489274	4.281690	-2.508939
O	-4.873098	3.302218	2.419366
O	-6.349291	1.731486	1.708407
C	-6.005262	2.717800	2.445000
C	-7.034727	3.202462	3.432202
H	-6.713630	4.129538	3.908184
H	-7.991043	3.351628	2.923694
H	-7.181920	2.433592	4.197895
C	-1.416224	0.495097	-2.117182
C	-1.772038	1.426676	-3.306242
H	-2.810254	1.281865	-3.622296
H	-1.634911	2.478146	-3.034365
H	-1.119101	1.203522	-4.156474
C	0.031175	0.796172	-1.678041
H	0.167318	1.864711	-1.493732
H	0.309570	0.257766	-0.770335
H	0.721078	0.499856	-2.474361
C	-2.399970	0.888096	-1.011585
O	-2.051771	1.837499	-0.235133
O	-3.535975	0.308496	-0.990877
C	5.875061	-1.788991	1.372881
H	5.706967	-1.400360	2.381817
H	5.974872	-0.947428	0.681721
C	7.055292	-2.705382	1.306604
H	6.994269	-3.569936	1.966130
C	8.431180	-2.118533	1.123667
C	7.796394	-2.925872	0.003111
H	7.445816	-2.301693	-0.816371
H	8.456579	-1.044877	0.937240
C	8.221243	-4.328018	-0.442131
H	7.813755	-4.477802	-1.447304
H	7.746833	-5.085060	0.191505
C	9.743549	-4.643682	-0.489235
H	10.077310	-5.002027	0.487969
H	9.902548	-5.470395	-1.188821
C	10.613100	-3.498372	-0.896810

C	9.606279	-2.606560	1.944400
H	9.566431	-3.693569	2.051840
H	9.541175	-2.196729	2.959314
C	10.960021	-2.163178	1.351940
H	11.063086	-1.080095	1.478912
H	11.776246	-2.616165	1.927932
C	11.123814	-2.481234	-0.105083
N	16.995264	2.132863	-1.011104
C	15.990692	3.250608	-1.118147
C	16.764548	4.574791	-0.865504
O	17.945310	4.448435	-0.424876
C	14.859646	3.080016	-0.091319
C	14.045351	1.825229	-0.306160
C	13.128036	1.746289	-1.365882
C	14.216373	0.706179	0.518902
C	12.386097	0.590241	-1.586192
C	13.494080	-0.467516	0.298016
C	12.573672	-0.515771	-0.749638
O	16.128862	5.629967	-1.094040
N	11.821723	-1.703712	-0.988534
H	15.586223	3.244298	-2.130620
H	14.229851	3.968459	-0.187108
H	15.291340	3.086799	0.915398
H	12.985737	2.606072	-2.014479
H	14.924211	0.750045	1.342125
H	11.662565	0.537304	-2.392007
H	13.648207	-1.336180	0.928089
H	16.653951	1.321283	-0.489287
H	17.803607	2.580866	-0.530116
H	17.305806	1.812936	-1.931332
N	11.742988	-2.207065	-2.249882
N	11.008655	-3.288370	-2.186127
C	-6.506352	-0.482205	-0.326623
C	-6.020572	-1.843265	0.026525
O	-5.201028	-2.521163	-0.585025
O	-6.512439	-2.233581	1.230352
C	-6.121899	-3.552653	1.675029
H	-6.493778	-3.639560	2.695176
H	-6.588609	-4.308674	1.037600
H	-5.039276	-3.672409	1.652144
C	-7.926708	-0.212716	-0.261626
C	-8.902651	-1.241468	-0.181832
C	-8.411803	1.121716	-0.352754
C	-10.262431	-0.971416	-0.156146
H	-8.585831	-2.277019	-0.143420
C	-9.762771	1.404943	-0.328697
H	-7.701942	1.930481	-0.455059
C	-10.702161	0.359623	-0.247694
H	-10.968452	-1.790457	-0.107217
H	-10.124755	2.424761	-0.408969
O	-12.005102	0.732921	-0.286937
C	-13.006170	-0.291689	-0.376091
H	-13.957520	0.232616	-0.470343
H	-12.840485	-0.918791	-1.259017

H	-13.019363	-0.913249	0.525502
C	-11.050721	-1.366401	-3.616950
C	-10.380989	-2.588788	-3.486364
C	-9.003778	-2.606369	-3.297077
C	-8.265942	-1.401236	-3.228986
C	-8.955150	-0.178372	-3.395409
C	-10.331924	-0.164772	-3.579596
H	-12.127062	-1.349632	-3.759363
H	-10.936739	-3.520587	-3.522657
H	-8.481227	-3.551111	-3.174803
H	-8.409530	0.757799	-3.368488
H	-10.853225	0.781247	-3.686516
C	-6.858433	-1.466991	-2.911118
H	-6.429205	-2.464653	-2.869040
C	-6.071481	-0.416163	-2.513546
H	-6.402288	0.610026	-2.612410
H	-5.007130	-0.564112	-2.395245

TS III-IVc

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.508587
Thermal and entropic correction, BS1 (a.u.)	1.083847
Electronic Energy, BS2 (a.u.)	-3934.953131
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-231.1i

Molecular Geometry in Cartesian Coordinates

C	0.484971	-2.854727	1.032276
C	-0.138529	-2.494392	2.219954
C	-1.463331	-2.036473	2.190413
C	-2.100276	-1.956162	0.945206
C	-1.469501	-2.331173	-0.250176
C	-0.152002	-2.799414	-0.199495
H	0.411858	-2.560894	3.153472
H	0.381988	-3.091450	-1.097837
O	1.812764	-3.327967	1.071195
C	2.772462	-2.386530	1.251198
O	2.582236	-1.188291	1.342131
O	3.944275	-3.010764	1.306992
H	-3.113408	-1.589172	0.880630
C	-2.097463	-1.628789	3.513807
H	-1.452648	-0.865846	3.962831
H	-2.058480	-2.488954	4.193779
C	-3.557352	-1.101276	3.539102

C	-3.849934	-0.575874	4.965071
H	-3.155859	0.222067	5.243057
H	-4.871245	-0.185820	5.029257
H	-3.750674	-1.390798	5.689048
C	-3.681108	0.104634	2.597438
C	-4.568853	-2.209015	3.205234
H	-5.593441	-1.831346	3.257675
H	-4.419682	-2.633459	2.211298
H	-4.465263	-3.017146	3.936370
O	-2.790035	1.008068	2.711047
O	-4.654364	0.133108	1.772461
C	-2.209439	-2.210317	-1.564187
H	-3.263090	-2.030539	-1.350571
H	-2.161671	-3.170456	-2.091669
C	-1.714672	-1.126884	-2.555269
H	-0.846558	-1.507493	-3.103436
H	-2.511620	-1.006238	-3.297255
Rh	-2.738979	2.577116	1.357173
Rh	-4.745994	1.613843	0.306401
O	-2.749293	4.061139	-0.081388
O	-4.609975	3.193531	-1.045246
C	-3.648997	4.034273	-0.982675
C	-3.583570	5.054892	-2.087488
H	-2.878945	5.851249	-1.845543
H	-3.256482	4.550278	-3.003298
H	-4.576950	5.471597	-2.270867
O	-3.998681	3.718991	2.558466
O	-5.847007	2.809350	1.608533
C	-5.260029	3.594991	2.429117
C	-6.153535	4.416029	3.320845
H	-5.587876	5.200989	3.823937
H	-6.964846	4.851292	2.731898
H	-6.601852	3.757536	4.072523
C	-1.307769	0.278124	-2.018720
C	-1.562268	1.320727	-3.141284
H	-2.620566	1.347017	-3.418705
H	-1.263219	2.324222	-2.818505
H	-0.977070	1.056757	-4.028288
C	0.184495	0.324313	-1.638955
H	0.491043	1.341858	-1.383506
H	0.416296	-0.322419	-0.790599
H	0.784559	-0.006525	-2.492483
C	-2.175632	0.765415	-0.858203
O	-1.604635	1.428424	0.067782
O	-3.434825	0.566448	-0.944706
C	5.097876	-2.154221	1.600843
H	4.920161	-1.678759	2.570314
H	5.159922	-1.378384	0.832822
C	6.314601	-3.023445	1.610178
H	6.294190	-3.826200	2.345595
C	7.659165	-2.388568	1.365731
C	7.065363	-3.323728	0.327368
H	6.683212	-2.798053	-0.545392
H	7.629324	-1.335625	1.085070

C	7.565008	-4.736377	0.015321
H	7.132234	-5.019328	-0.949743
H	7.164774	-5.447713	0.745517
C	9.104299	-4.959473	-0.060111
H	9.486690	-5.221576	0.929801
H	9.297841	-5.823954	-0.702786
C	9.888351	-3.795818	-0.575430
C	8.866396	-2.742568	2.208389
H	8.890928	-3.817652	2.404717
H	8.790331	-2.254805	3.187353
C	10.182685	-2.270963	1.556231
H	10.224533	-1.177641	1.603371
H	11.034300	-2.633626	2.144844
C	10.339684	-2.686468	0.123016
N	15.787493	2.342702	-1.104906
C	14.695672	3.347803	-1.363817
C	15.336436	4.754935	-1.204450
O	16.497813	4.778253	-0.698600
C	13.531969	3.176920	-0.372350
C	12.845618	1.835104	-0.477589
C	11.944588	1.575031	-1.522144
C	13.122515	0.812425	0.439127
C	11.319145	0.337507	-1.637691
C	12.521272	-0.441633	0.322259
C	11.610629	-0.669171	-0.710441
O	14.622773	5.722121	-1.557102
N	10.966448	-1.934805	-0.834047
H	14.344550	3.208758	-2.386597
H	12.831028	3.986279	-0.592607
H	13.909258	3.333380	0.644102
H	11.718413	2.357233	-2.241391
H	13.816450	0.994740	1.255326
H	10.604187	0.147063	-2.430166
H	12.760866	-1.233223	1.023249
H	15.494267	1.556331	-0.519052
H	16.527936	2.910339	-0.640576
H	16.169584	1.965416	-1.975193
N	10.902569	-2.541692	-2.050050
N	10.248533	-3.662994	-1.885070
C	-6.547761	0.759825	-0.517991
C	-7.644876	1.732314	-0.294495
O	-8.391712	1.654056	0.681601
O	-7.664130	2.793983	-1.122565
C	-8.564870	3.861519	-0.752596
H	-8.468991	4.606788	-1.541485
H	-9.593553	3.497974	-0.698237
H	-8.269911	4.286163	0.210471
C	-6.865098	-0.644551	-0.394323
C	-8.188406	-1.155350	-0.403020
C	-5.812982	-1.593490	-0.327801
C	-8.450066	-2.514916	-0.317960
H	-9.025476	-0.471744	-0.478199
C	-6.054243	-2.949381	-0.251939
H	-4.798494	-1.228553	-0.346664

C	-7.379160	-3.424455	-0.263035
H	-9.474870	-2.862392	-0.337701
H	-5.238186	-3.663596	-0.215167
O	-7.521921	-4.772731	-0.240147
C	-8.839677	-5.323534	-0.383263
H	-8.707125	-6.405728	-0.394320
H	-9.481233	-5.042722	0.458623
H	-9.296206	-4.997342	-1.324388
C	-8.774896	-3.281716	-3.776522
C	-9.625313	-2.170513	-3.806175
C	-9.098703	-0.891760	-3.659324
C	-7.710747	-0.696567	-3.473938
C	-6.863968	-1.827850	-3.479476
C	-7.394052	-3.103928	-3.623448
H	-9.183512	-4.282028	-3.884621
H	-10.694843	-2.306484	-3.933492
H	-9.756439	-0.026940	-3.661841
H	-5.793232	-1.703861	-3.362965
H	-6.735779	-3.966961	-3.606994
C	-7.225843	0.640907	-3.211684
H	-7.951613	1.441365	-3.331254
C	-5.996547	0.962046	-2.698877
H	-5.200856	0.231539	-2.622879
H	-5.697102	1.998292	-2.627297

TS III-IVd

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.509967
Thermal and entropic correction, BS1 (a.u.)	1.083842
Electronic Energy, BS2 (a.u.)	-3934.953912
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-209.4i

Molecular Geometry in Cartesian Coordinates

C	0.628156	-2.822150	-1.717370
C	-0.325104	-3.771541	-1.378021
C	-1.668340	-3.383612	-1.248520
C	-1.984849	-2.036215	-1.460789
C	-1.015655	-1.080453	-1.801450
C	0.313418	-1.488298	-1.947972
H	-0.018848	-4.798998	-1.207011
H	1.099923	-0.783724	-2.198894

O	1.967791	-3.241994	-1.859296
C	2.792624	-2.943932	-0.824727
O	2.458564	-2.407898	0.214968
O	4.017463	-3.342547	-1.151413
H	-3.003235	-1.688784	-1.355800
C	-2.671470	-4.450631	-0.833375
H	-2.353219	-4.836506	0.141384
H	-2.587364	-5.294070	-1.529612
C	-4.179040	-4.093098	-0.736979
C	-4.918958	-5.311542	-0.136061
H	-4.522605	-5.567627	0.850219
H	-5.989273	-5.102188	-0.037059
H	-4.800277	-6.178580	-0.793540
C	-4.364404	-2.934991	0.253831
C	-4.777585	-3.783120	-2.117482
H	-5.850172	-3.588753	-2.044300
H	-4.312178	-2.919403	-2.595006
H	-4.632149	-4.649937	-2.769800
O	-3.810216	-3.069907	1.393299
O	-5.049163	-1.924574	-0.112583
C	-1.418226	0.368245	-1.964376
H	-2.508736	0.423084	-1.989763
H	-1.060940	0.739473	-2.932556
C	-0.897330	1.349472	-0.884226
H	0.147891	1.599156	-1.096591
H	-1.466063	2.275944	-1.016033
Rh	-3.861789	-1.491423	2.727617
Rh	-5.131933	-0.201830	1.074342
O	-3.913160	0.200795	3.945197
O	-5.098049	1.382316	2.412829
C	-4.462524	1.267674	3.516695
C	-4.327530	2.517424	4.344801
H	-4.070832	2.276466	5.377122
H	-3.524275	3.124114	3.911051
H	-5.249853	3.101218	4.307728
O	-5.699946	-2.168673	3.460781
O	-6.869202	-0.939737	1.953776
C	-6.784677	-1.774883	2.918567
C	-8.079135	-2.359019	3.419778
H	-7.966234	-2.737372	4.436770
H	-8.875190	-1.612840	3.377105
H	-8.358402	-3.191887	2.764669
C	-0.950866	0.936923	0.618810
C	-1.067873	2.230717	1.469556
H	-1.977196	2.786314	1.220841
H	-1.084602	1.995956	2.539189
H	-0.205538	2.876334	1.272434
C	0.318206	0.180063	1.049294
H	0.332283	0.026171	2.131507
H	0.397276	-0.794639	0.568291
H	1.202536	0.765304	0.778406
C	-2.201184	0.133928	0.977288
O	-2.110899	-0.735120	1.906985
O	-3.281154	0.454158	0.381968

C	5.049828	-3.062082	-0.144862
H	4.768674	-3.574459	0.779474
H	5.056289	-1.983772	0.036137
C	6.359946	-3.537915	-0.686261
H	6.465486	-4.619378	-0.756846
C	7.616079	-2.777022	-0.339836
C	7.079866	-2.747840	-1.761302
H	6.601573	-1.801558	-2.005648
H	7.451842	-1.848650	0.207432
C	7.688196	-3.446725	-2.983074
H	7.349735	-2.893404	-3.865390
H	7.275379	-4.456639	-3.083281
C	9.234141	-3.561136	-3.064863
H	9.580936	-4.410809	-2.472029
H	9.504748	-3.779582	-4.103017
C	9.960155	-2.329183	-2.630619
C	8.883072	-3.487975	0.085398
H	9.024641	-4.401811	-0.496394
H	8.786130	-3.804606	1.130668
C	10.124617	-2.578083	-0.008105
H	10.038391	-1.785675	0.743673
H	11.018586	-3.154714	0.259934
C	10.318248	-1.935852	-1.349976
N	15.378667	2.891321	1.173571
C	14.252934	3.817518	1.549676
C	14.866791	4.933290	2.443227
O	16.129683	5.026029	2.404794
C	13.092455	3.055371	2.193268
C	12.480234	2.044118	1.251047
C	11.585053	2.460236	0.253607
C	12.838497	0.691230	1.308733
C	11.052068	1.552120	-0.655896
C	12.324925	-0.229093	0.393932
C	11.428259	0.206545	-0.583543
O	14.057572	5.650790	3.076372
N	10.896008	-0.708967	-1.539170
H	13.920506	4.288698	0.620255
H	12.355313	3.805551	2.487380
H	13.450937	2.567091	3.106597
H	11.295687	3.506040	0.196799
H	13.534378	0.352083	2.071394
H	10.347684	1.872497	-1.415320
H	12.627709	-1.269628	0.431933
H	15.434869	2.090333	1.810118
H	16.231126	3.469861	1.307841
H	15.304670	2.535010	0.218665
N	10.892958	-0.366418	-2.855843
N	10.324825	-1.348159	-3.506726
C	-6.070813	0.902725	-0.514082
C	-6.748932	-0.079765	-1.397985
O	-6.210077	-0.532776	-2.408087
O	-7.916492	-0.563192	-0.935018
C	-8.508521	-1.635449	-1.699865
H	-9.470772	-1.827880	-1.227267

H	-8.651188	-1.333777	-2.739955
H	-7.880780	-2.527868	-1.655013
C	-5.441516	2.043686	-1.135797
C	-5.657839	2.401634	-2.492115
C	-4.595023	2.897364	-0.374398
C	-5.035862	3.495523	-3.074550
H	-6.322077	1.803244	-3.102861
C	-3.977834	3.995299	-0.938480
H	-4.437970	2.680775	0.673000
C	-4.196731	4.308796	-2.293953
H	-5.232691	3.729937	-4.112691
H	-3.337969	4.643947	-0.349364
O	-3.573815	5.423029	-2.748842
C	-3.832072	5.849764	-4.094892
H	-3.262513	6.770291	-4.225269
H	-3.491220	5.101933	-4.818500
H	-4.899024	6.051345	-4.241611
C	-7.701311	5.825675	-2.681200
C	-8.513102	4.805039	-3.188697
C	-8.787650	3.686344	-2.408751
C	-8.250601	3.559401	-1.107473
C	-7.458531	4.613087	-0.600510
C	-7.185364	5.729167	-1.382779
H	-7.479695	6.697601	-3.289471
H	-8.920240	4.880208	-4.192311
H	-9.402249	2.882538	-2.804756
H	-7.055300	4.551415	0.403927
H	-6.562119	6.525542	-0.988082
C	-8.472358	2.324088	-0.384590
H	-9.199504	1.645945	-0.823547
C	-7.756781	1.879902	0.693922
H	-7.062158	2.518550	1.226051
H	-8.054520	0.971318	1.200043

TS III-IVe

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.508844
Thermal and entropic correction, BS1 (a.u.)	1.082722
Electronic Energy, BS2 (a.u.)	-3934.953115
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-228.9i

Molecular Geometry in Cartesian Coordinates

C	-0.485765	-2.640551	-1.500015
C	0.233617	-2.233879	-2.616429
C	1.538334	-1.745104	-2.453321
C	2.057164	-1.685484	-1.153638
C	1.331372	-2.111649	-0.031616
C	0.035809	-2.605999	-0.214209
H	-0.225907	-2.290529	-3.598502
H	-0.568911	-2.935250	0.624529
O	-1.792075	-3.145149	-1.665262
C	-2.766124	-2.219654	-1.851704
O	-2.595207	-1.017633	-1.928291
O	-3.923729	-2.867112	-1.928594
H	3.051415	-1.299547	-0.986957
C	2.279272	-1.274180	-3.697449
H	1.719304	-0.429699	-4.114218
H	2.223203	-2.069439	-4.450624
C	3.771611	-0.857194	-3.594336
C	4.210134	-0.312341	-4.974659
H	3.594536	0.538689	-5.279032
H	5.256519	0.009740	-4.945148
H	4.116376	-1.097451	-5.731560
C	3.912949	0.308436	-2.603451
C	4.667120	-2.048670	-3.222906
H	5.718199	-1.750724	-3.182350
H	4.405323	-2.485745	-2.258480
H	4.562535	-2.826170	-3.986505
O	3.112934	1.286939	-2.763381
O	4.808540	0.231509	-1.697830
C	1.940720	-2.009993	1.348328
H	3.015801	-1.867313	1.242906
H	1.805358	-2.964139	1.871200
C	1.386221	-0.902557	2.279180
H	0.454181	-1.249770	2.737848
H	2.107391	-0.803897	3.098053
Rh	3.083548	2.820578	-1.371405
Rh	4.871410	1.641331	-0.155599
O	3.095567	4.261500	0.117455
O	4.765602	3.196316	1.224204

C	3.912412	4.138310	1.086963
C	3.884903	5.173690	2.180374
H	3.201815	5.987258	1.934604
H	3.564839	4.696043	3.111950
H	4.893067	5.566621	2.338391
O	4.566456	3.834653	-2.417592
O	6.211969	2.749631	-1.293599
C	5.789050	3.574009	-2.173261
C	6.836920	4.259536	-3.011294
H	6.495630	5.249808	-3.318417
H	7.779094	4.331343	-2.465051
H	7.004641	3.658539	-3.912095
C	1.083483	0.511377	1.703116
C	1.194569	1.533933	2.866317
H	2.204132	1.535224	3.289483
H	0.961925	2.546778	2.520850
H	0.487596	1.268992	3.659384
C	-0.338324	0.589566	1.113511
H	-0.592826	1.617393	0.843104
H	-0.453022	-0.033738	0.224625
H	-1.059803	0.248383	1.862552
C	2.117738	0.996473	0.685832
O	1.709301	1.763016	-0.246362
O	3.337695	0.683211	0.893211
C	-5.099780	-2.038684	-2.213523
H	-5.003565	-1.671230	-3.239920
H	-5.099775	-1.185136	-1.530478
C	-6.309861	-2.896053	-2.020863
H	-6.371288	-3.757663	-2.684225
C	-7.624879	-2.246140	-1.674601
C	-6.899611	-3.092509	-0.638563
H	-6.422223	-2.486416	0.128829
H	-7.575713	-1.174522	-1.480656
C	-7.317714	-4.478336	-0.134532
H	-6.886153	-4.595725	0.865063
H	-6.860586	-5.257568	-0.754420
C	-8.834553	-4.790011	-0.031839
H	-9.223340	-5.083747	-1.009633
H	-8.960267	-5.658355	0.623005
C	-9.661858	-3.665418	0.502482
C	-8.903368	-2.660799	-2.371970
H	-8.921918	-3.742902	-2.521551
H	-8.928511	-2.214877	-3.373276
C	-10.168265	-2.191454	-1.626276
H	-10.226883	-1.098631	-1.679559
H	-11.056455	-2.568558	-2.147919
C	-10.216018	-2.595205	-0.182577
N	-15.918330	1.997765	1.524001
C	-14.896589	3.106447	1.583605
C	-15.687101	4.443804	1.507877
O	-16.946010	4.335144	1.405907
C	-13.863102	2.993894	0.454081
C	-13.047873	1.723089	0.518599
C	-12.052182	1.566115	1.495548

C	-13.293408	0.663570	-0.363582
C	-11.312285	0.390814	1.583303
C	-12.573392	-0.528476	-0.275918
C	-11.578129	-0.656001	0.693811
O	-15.000763	5.490469	1.550017
N	-10.830812	-1.865896	0.799011
H	-14.400924	3.042485	2.553775
H	-13.217771	3.870936	0.548157
H	-14.381544	3.067563	-0.508386
H	-11.846766	2.378922	2.186700
H	-14.062285	0.765424	-1.124594
H	-10.530220	0.279016	2.325926
H	-12.791063	-1.351356	-0.947402
H	-15.792855	1.374849	0.721998
H	-16.817784	2.524959	1.435534
H	-15.927779	1.427345	2.371524
N	-10.661260	-2.447405	2.017324
N	-9.953172	-3.531131	1.829509
C	6.471284	0.610271	0.852294
C	7.608511	1.565158	0.931475
O	7.742840	2.495900	1.719785
O	8.453344	1.388695	-0.115906
C	9.435410	2.429528	-0.317867
H	9.954438	2.163118	-1.238092
H	8.947504	3.400972	-0.424348
H	10.138087	2.458380	0.518406
C	6.736511	-0.797424	0.675422
C	8.016363	-1.384898	0.852017
C	5.663780	-1.677865	0.379110
C	8.225325	-2.747772	0.700495
H	8.860720	-0.758567	1.115137
C	5.852017	-3.035601	0.230846
H	4.675464	-1.259915	0.275600
C	7.136361	-3.586037	0.402373
H	9.216621	-3.155546	0.851903
H	5.020126	-3.697466	0.013786
O	7.219352	-4.933411	0.281518
C	8.467495	-5.572911	0.586991
H	8.286486	-6.641911	0.471572
H	9.254190	-5.257857	-0.106383
H	8.770085	-5.357797	1.617768
C	7.940532	-3.766362	4.095595
C	8.839087	-2.721710	4.341828
C	8.417851	-1.402776	4.214641
C	7.089748	-1.099383	3.835968
C	6.187106	-2.166519	3.625712
C	6.613207	-3.483176	3.748907
H	8.268655	-4.797574	4.185406
H	9.865869	-2.939983	4.618507
H	9.116475	-0.587752	4.382134
H	5.156922	-1.959587	3.358081
H	5.916812	-4.295434	3.565789
C	6.736160	0.281285	3.597004
H	7.486455	1.018155	3.871268

C	5.623930	0.720305	2.927031
H	4.798695	0.059296	2.694619
H	5.411703	1.779607	2.882438

TS III-IVf

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.508647
Thermal and entropic correction, BS1 (a.u.)	1.081143
Electronic Energy, BS2 (a.u.)	-3934.952230
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-236.2i

Molecular Geometry in Cartesian Coordinates

C	0.623160	-2.794837	-1.666584
C	-0.302733	-3.752972	-1.279413
C	-1.650776	-3.388189	-1.131990
C	-1.999089	-2.054208	-1.374123
C	-1.056766	-1.089229	-1.761098
C	0.276552	-1.474434	-1.927268
H	0.028131	-4.768890	-1.086848
H	1.043494	-0.761628	-2.213363
O	1.966201	-3.197039	-1.824912
C	2.821096	-2.802860	-0.849131
O	2.517854	-2.181576	0.151875
O	4.039097	-3.218791	-1.181599
H	-3.021874	-1.724578	-1.255640
C	-2.623930	-4.459269	-0.661733
H	-2.306016	-4.775989	0.337795
H	-2.505323	-5.339368	-1.305362
C	-4.143776	-4.146332	-0.603538
C	-4.852068	-5.369876	0.026110
H	-4.450500	-5.591823	1.018419
H	-5.927736	-5.187255	0.119335
H	-4.709288	-6.248461	-0.610897
C	-4.387160	-2.962429	0.345910
C	-4.727211	-3.904957	-2.002106
H	-5.812951	-3.804615	-1.952592
H	-4.325485	-3.009728	-2.479594
H	-4.495599	-4.764198	-2.639629
O	-3.852570	-3.056859	1.499024
O	-5.090922	-1.977745	-0.057681
C	-1.489989	0.347749	-1.942371
H	-2.581268	0.379477	-1.973163
H	-1.134630	0.718487	-2.911297

C	-0.995836	1.347011	-0.866120
H	0.044019	1.619519	-1.076890
H	-1.585956	2.258829	-1.004499
Rh	-3.940418	-1.456164	2.800497
Rh	-5.213283	-0.223677	1.100339
O	-4.019832	0.253925	3.987388
O	-5.179307	1.391654	2.403933
C	-4.562025	1.308246	3.520525
C	-4.442749	2.580753	4.315798
H	-4.200771	2.369084	5.358018
H	-3.635236	3.178246	3.877259
H	-5.366529	3.159509	4.248768
O	-5.775042	-2.141514	3.530306
O	-6.946287	-0.967525	1.980709
C	-6.859035	-1.778595	2.965597
C	-8.150325	-2.370277	3.466151
H	-8.039343	-2.738515	4.486996
H	-8.952357	-1.631072	3.412911
H	-8.420007	-3.210513	2.816480
C	-1.043058	0.943439	0.638720
C	-1.156780	2.244456	1.478947
H	-2.067270	2.798228	1.229112
H	-1.169937	2.018680	2.550413
H	-0.295386	2.888688	1.273204
C	0.226857	0.187602	1.070975
H	0.254797	0.062954	2.156613
H	0.289582	-0.800811	0.616333
H	1.112931	0.755990	0.771844
C	-2.290315	0.142192	1.011603
O	-2.197113	-0.690768	1.973636
O	-3.367964	0.425466	0.394615
C	5.092510	-2.879634	-0.216682
H	4.827953	-3.334253	0.742408
H	5.107746	-1.792580	-0.100086
C	6.391125	-3.394217	-0.749516
H	6.471660	-4.479056	-0.799336
C	7.660942	-2.658459	-0.401126
C	7.140412	-2.637948	-1.828825
H	6.686944	-1.684365	-2.091469
H	7.514308	-1.718460	0.131070
C	7.748445	-3.366535	-3.033150
H	7.434911	-2.817151	-3.927027
H	7.313840	-4.367980	-3.126173
C	9.292223	-3.518326	-3.092060
H	9.610038	-4.368560	-2.483999
H	9.571359	-3.756816	-4.123496
C	10.044691	-2.299913	-2.663826
C	8.903147	-3.396573	0.049750
H	9.026941	-4.321864	-0.517638
H	8.783548	-3.696244	1.097658
C	10.169766	-2.522135	-0.037752
H	10.094638	-1.719169	0.703810
H	11.044204	-3.119286	0.248997
C	10.399107	-1.901236	-1.383986

N	15.560846	2.835433	1.246428
C	14.437432	3.774090	1.602143
C	15.034015	4.843389	2.562511
O	16.297245	4.842511	2.664312
C	13.236809	3.023834	2.186647
C	12.634733	2.032394	1.217321
C	11.798823	2.472522	0.179698
C	12.929946	0.666178	1.305192
C	11.257164	1.574767	-0.735132
C	12.410573	-0.244114	0.384092
C	11.566420	0.214236	-0.628949
O	14.214152	5.613184	3.114360
N	11.017212	-0.694888	-1.581119
H	14.148996	4.279840	0.676940
H	12.504500	3.785690	2.463107
H	13.549865	2.517338	3.106576
H	11.558955	3.529030	0.097574
H	13.579553	0.307606	2.099016
H	10.594836	1.915032	-1.522993
H	12.666746	-1.295564	0.448316
H	15.520303	1.966371	1.786522
H	16.411825	3.362439	1.534461
H	15.580166	2.592174	0.254251
N	11.040756	-0.369977	-2.902015
N	10.450373	-1.342026	-3.547535
C	-6.206450	0.866764	-0.475442
C	-7.036237	-0.107032	-1.235084
O	-8.127504	-0.558797	-0.901736
O	-6.376747	-0.574750	-2.324510
C	-7.082390	-1.559398	-3.113016
H	-6.360688	-1.922729	-3.842951
H	-7.439522	-2.378991	-2.488361
H	-7.929484	-1.088075	-3.618746
C	-5.578112	1.964894	-1.172114
C	-5.869891	2.296057	-2.521749
C	-4.660896	2.813781	-0.490076
C	-5.246640	3.348194	-3.175508
H	-6.597020	1.710480	-3.070527
C	-4.037530	3.867571	-1.126561
H	-4.455975	2.630268	0.555190
C	-4.327206	4.147851	-2.475610
H	-5.503840	3.563520	-4.204623
H	-3.341958	4.510694	-0.597692
O	-3.690639	5.221251	-3.004919
C	-4.044497	5.636542	-4.332669
H	-3.445586	6.525129	-4.533576
H	-3.805515	4.860651	-5.067307
H	-5.109541	5.887621	-4.388442
C	-7.741504	5.821917	-2.622318
C	-8.641059	4.845662	-3.066603
C	-8.920927	3.745813	-2.263432
C	-8.302676	3.593429	-1.000263
C	-7.423263	4.605624	-0.554684
C	-7.144441	5.702480	-1.361190

H	-7.515451	6.678327	-3.250615
H	-9.111496	4.940692	-4.040364
H	-9.602593	2.974694	-2.611660
H	-6.955332	4.525210	0.419810
H	-6.452557	6.464264	-1.015911
C	-8.529269	2.370541	-0.263742
H	-9.298319	1.715497	-0.663948
C	-7.766907	1.899339	0.774297
H	-7.037462	2.521327	1.277075
H	-8.078280	1.007065	1.301380

TS III-IVg

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.509214
Thermal and entropic correction, BS1 (a.u.)	1.082142
Electronic Energy, BS2 (a.u.)	-3934.954110
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-213.1i

Molecular Geometry in Cartesian Coordinates

C	-1.030949	-2.084642	-0.456797
C	-0.343428	-1.975136	-1.661215
C	0.984183	-1.525396	-1.655655
C	1.565451	-1.213063	-0.420369
C	0.872743	-1.335520	0.790828
C	-0.454223	-1.778263	0.769346
H	-0.841482	-2.242326	-2.588067
H	-1.031650	-1.888696	1.681544
O	-2.339645	-2.604787	-0.441578
C	-3.308163	-1.888432	-1.064050
O	-3.168039	-0.796590	-1.580386
O	-4.429846	-2.597632	-0.992450
H	2.591353	-0.880190	-0.366954
C	1.701028	-1.364622	-2.987406
H	1.324597	-0.453523	-3.467469
H	1.405932	-2.193574	-3.640894
C	3.253675	-1.304485	-3.001923
C	3.713956	-1.153439	-4.470734
H	3.272425	-0.268426	-4.936904
H	4.804408	-1.065739	-4.525114
H	3.414245	-2.035204	-5.045811
C	3.725788	-0.042417	-2.265625
C	3.873310	-2.580064	-2.411211
H	4.964951	-2.550435	-2.467847

H	3.597076	-2.730166	-1.365573
H	3.522883	-3.445972	-2.982131
O	3.225675	1.067701	-2.641682
O	4.583856	-0.177436	-1.332396
C	1.578089	-0.980423	2.078085
H	2.653163	-1.049954	1.907328
H	1.330522	-1.725059	2.843675
C	1.270651	0.408558	2.689574
H	0.304035	0.369596	3.204639
H	2.023702	0.569379	3.468811
Rh	3.712274	2.803079	-1.611475
Rh	5.150915	1.436792	-0.155346
O	4.265652	4.452522	-0.470822
O	5.561360	3.186001	0.891583
C	5.041522	4.295526	0.528065
C	5.343795	5.495870	1.385331
H	5.172400	6.420436	0.831955
H	4.676492	5.476185	2.254532
H	6.373092	5.454633	1.748114
O	5.357171	3.083765	-2.849674
O	6.693474	1.849749	-1.494332
C	6.471985	2.551268	-2.540286
C	7.646074	2.766968	-3.458716
H	7.339757	3.276683	-4.372662
H	8.399022	3.369231	-2.940281
H	8.102409	1.803557	-3.702168
C	1.215483	1.666812	1.778542
C	1.399525	2.910235	2.687406
H	2.377047	2.896440	3.180397
H	1.313481	3.835181	2.108387
H	0.625463	2.915203	3.461863
C	-0.144000	1.783699	1.059945
H	-0.229652	2.741267	0.540882
H	-0.294912	0.986157	0.330161
H	-0.949553	1.724907	1.798576
C	2.361497	1.750972	0.763960
O	2.152536	2.432031	-0.293459
O	3.471015	1.201543	1.070664
C	-5.611215	-1.987108	-1.610518
H	-5.406375	-1.865354	-2.678279
H	-5.763239	-1.000739	-1.163701
C	-6.766116	-2.898891	-1.341861
H	-6.704325	-3.871872	-1.827068
C	-8.154497	-2.328917	-1.196528
C	-7.435693	-2.895463	0.017690
H	-7.069265	-2.114973	0.681437
H	-8.211514	-1.240462	-1.204944
C	-7.757955	-4.202432	0.751060
H	-7.388603	-4.089479	1.775745
H	-7.188066	-5.029653	0.313669
C	-9.242289	-4.646903	0.832444
H	-9.534486	-5.151263	-0.091498
H	-9.332815	-5.390708	1.630731
C	-10.202712	-3.535032	1.106248

C	-9.343720	-2.985315	-1.866536
H	-9.256454	-4.073447	-1.817318
H	-9.345854	-2.727741	-2.932353
C	-10.689641	-2.515898	-1.278506
H	-10.837198	-1.460446	-1.533051
H	-11.506946	-3.062017	-1.765467
C	-10.798180	-2.660341	0.210495
N	-16.963953	1.570706	0.688426
C	-16.055925	2.774962	0.685235
C	-16.954417	4.008082	0.380539
O	-18.198415	3.774990	0.303876
C	-14.905231	2.620616	-0.315648
C	-13.997570	1.455033	0.003112
C	-13.063846	1.545878	1.047150
C	-14.098539	0.249394	-0.702379
C	-12.243563	0.469560	1.371340
C	-13.296802	-0.845022	-0.376843
C	-12.366188	-0.726843	0.656597
O	-16.363633	5.104947	0.253680
N	-11.539577	-1.833223	1.011042
H	-15.661515	2.880531	1.698192
H	-14.350483	3.561620	-0.288155
H	-15.324865	2.514308	-1.322328
H	-12.971014	2.474443	1.603545
H	-14.817818	0.159672	-1.512021
H	-11.510047	0.547223	2.165950
H	-13.401839	-1.781963	-0.912055
H	-16.804006	0.953240	-0.111956
H	-17.912990	2.001601	0.607138
H	-16.883057	1.015158	1.542055
N	-11.405606	-2.174200	2.321197
N	-10.595344	-3.199676	2.369936
C	6.322367	0.118114	1.080710
C	5.702387	0.117844	2.431055
O	4.910437	-0.753692	2.790105
O	5.928782	1.220339	3.168830
C	5.166415	1.334049	4.389557
H	5.522885	2.246507	4.866597
H	4.100228	1.416602	4.164659
H	5.343681	0.472658	5.037713
C	6.880472	-1.121612	0.592803
C	7.128111	-2.239696	1.431426
C	7.273272	-1.241346	-0.769193
C	7.686152	-3.414019	0.949866
H	6.875522	-2.183522	2.482841
C	7.838858	-2.400900	-1.259626
H	7.135407	-0.396529	-1.429780
C	8.061608	-3.495096	-0.401596
H	7.863156	-4.238541	1.628377
H	8.147958	-2.480962	-2.296613
O	8.662556	-4.571655	-0.964277
C	9.011702	-5.677931	-0.119203
H	9.509077	-6.399554	-0.767727
H	9.697999	-5.360083	0.673557

H	8.120062	-6.136629	0.320674
C	11.072514	-2.823843	1.853820
C	10.557654	-2.460049	3.103276
C	9.836407	-1.278189	3.237459
C	9.609667	-0.436881	2.124229
C	10.163112	-0.804873	0.877573
C	10.880168	-1.988062	0.746378
H	11.630233	-3.749137	1.744058
H	10.711201	-3.103151	3.964302
H	9.418379	-1.000547	4.201195
H	10.020823	-0.166380	0.013102
H	11.284642	-2.269516	-0.220855
C	8.758121	0.721402	2.292033
H	8.483172	0.961601	3.315731
C	8.165290	1.437712	1.286921
H	8.441455	1.304204	0.248164
H	7.611062	2.335967	1.522001

TS III-IVh

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.509539
Thermal and entropic correction, BS1 (a.u.)	1.082279
Electronic Energy, BS2 (a.u.)	-3934.954398
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-216.2i

Molecular Geometry in Cartesian Coordinates

C	-0.824371	-2.552097	-0.181209
C	0.007789	-2.788906	-1.266182
C	1.362732	-2.432773	-1.187052
C	1.813481	-1.835742	-0.002839
C	0.967860	-1.605641	1.093543
C	-0.376552	-1.979030	1.001848
H	-0.402246	-3.244908	-2.162221
H	-1.068768	-1.819173	1.822207
O	-2.172346	-2.956071	-0.272546
C	-3.040399	-2.023026	-0.734420
O	-2.754782	-0.880965	-1.041856
O	-4.242667	-2.585102	-0.787376
H	2.846458	-1.533297	0.098822
C	2.230036	-2.697079	-2.410083
H	1.794402	-2.140559	-3.247288
H	2.135921	-3.757229	-2.675591
C	3.746832	-2.376305	-2.360199

C	4.324494	-2.568320	-3.782448
H	3.827146	-1.914143	-4.503726
H	5.397143	-2.347342	-3.794422
H	4.185692	-3.605695	-4.102851
C	3.943315	-0.897785	-2.005754
C	4.499465	-3.304346	-1.391909
H	5.568922	-3.075436	-1.384178
H	4.131613	-3.230581	-0.366495
H	4.374640	-4.340619	-1.721582
O	3.268169	-0.045534	-2.668414
O	4.768419	-0.617528	-1.075141
C	1.530027	-0.974402	2.346935
H	2.617245	-1.030601	2.288866
H	1.236777	-1.579268	3.213211
C	1.124018	0.487351	2.662890
H	0.141523	0.492711	3.146676
H	1.835062	0.843080	3.416279
Rh	3.344868	1.966035	-2.133470
Rh	4.967880	1.329356	-0.395524
O	3.458253	3.923764	-1.446272
O	4.940460	3.344420	0.172049
C	4.170835	4.175501	-0.419679
C	4.071487	5.550729	0.185734
H	3.766675	6.283525	-0.563041
H	3.308016	5.515648	0.971968
H	5.019106	5.841108	0.642971
O	4.943023	2.258898	-3.434381
O	6.439744	1.721378	-1.817338
C	6.128176	2.072704	-3.007129
C	7.275519	2.270096	-3.962595
H	6.922355	2.619650	-4.933197
H	7.981768	2.991294	-3.541561
H	7.805482	1.320070	-4.083770
C	1.043525	1.533767	1.513208
C	1.295944	2.941127	2.120523
H	2.293967	3.004366	2.565577
H	1.208441	3.718438	1.353645
H	0.554369	3.143787	2.900322
C	-0.345967	1.527363	0.847872
H	-0.437659	2.341355	0.124308
H	-0.554123	0.588466	0.331099
H	-1.114254	1.668437	1.614789
C	2.145710	1.379381	0.465178
O	1.846872	1.639792	-0.745798
O	3.318990	1.096613	0.882760
C	-5.321365	-1.731600	-1.297326
H	-5.018047	-1.355611	-2.278730
H	-5.440800	-0.885966	-0.613928
C	-6.554857	-2.574449	-1.361447
H	-6.503594	-3.400396	-2.069574
C	-7.912352	-1.936671	-1.208765
C	-7.368544	-2.841587	-0.112094
H	-7.028051	-2.273592	0.751392
H	-7.901757	-0.878766	-0.946570

C	-7.840192	-4.253242	0.256709
H	-7.686145	-4.369290	1.334832
H	-7.196250	-4.998757	-0.223680
C	-9.310334	-4.636416	-0.042930
H	-9.441520	-4.838064	-1.108347
H	-9.528242	-5.574945	0.477473
C	-10.304626	-3.609887	0.396093
C	-9.039828	-2.295647	-2.154975
H	-9.006951	-3.358972	-2.403241
H	-8.891967	-1.759363	-3.100003
C	-10.429819	-1.906252	-1.618965
H	-10.492782	-0.814333	-1.546757
H	-11.192626	-2.205586	-2.348059
C	-10.758624	-2.485098	-0.275111
N	-16.884908	1.610155	0.723412
C	-16.016838	2.795992	1.055104
C	-16.924985	4.055631	0.971018
O	-18.169269	3.827487	0.901139
C	-14.782342	2.862435	0.151303
C	-13.920451	1.624629	0.250683
C	-13.127089	1.398404	1.385938
C	-13.934796	0.657175	-0.761648
C	-12.358424	0.244140	1.504684
C	-13.180663	-0.511193	-0.651247
C	-12.389221	-0.709080	0.481438
O	-16.343140	5.164640	1.008875
N	-11.615742	-1.899981	0.617348
H	-15.711688	2.671366	2.097398
H	-14.224838	3.750890	0.457629
H	-15.107664	3.018530	-0.883231
H	-13.105926	2.139497	2.180116
H	-14.550656	0.813211	-1.642903
H	-11.733295	0.077751	2.374808
H	-13.216243	-1.264662	-1.430109
H	-16.796840	1.338844	-0.260454
H	-17.851209	1.962451	0.874070
H	-16.680465	0.791291	1.299461
N	-11.682603	-2.615850	1.771665
N	-10.886018	-3.643575	1.631524
C	6.485998	0.824041	1.030879
C	6.463416	1.896440	2.053306
O	7.215818	2.870040	1.988823
O	5.453160	1.830352	2.940015
C	5.217814	3.018692	3.725824
H	4.383727	2.770226	4.381125
H	6.100082	3.273164	4.318050
H	4.953441	3.855383	3.074415
C	7.756863	0.248179	0.664324
C	8.923149	0.397132	1.459036
C	7.868993	-0.564590	-0.498157
C	10.130442	-0.190238	1.113208
H	8.876638	0.987350	2.366681
C	9.063392	-1.159044	-0.850980
H	6.992399	-0.729290	-1.109221

C	10.201962	-0.991318	-0.039522
H	10.992014	-0.058122	1.755031
H	9.139175	-1.790676	-1.730014
O	11.311665	-1.658971	-0.438470
C	12.466605	-1.637207	0.413659
H	13.205584	-2.273145	-0.074395
H	12.866330	-0.622781	0.513941
H	12.225807	-2.042114	1.402824
C	9.937675	-3.249034	2.958359
C	9.644624	-2.389113	4.022872
C	8.422006	-1.727164	4.061872
C	7.467755	-1.906862	3.034648
C	7.767252	-2.804600	1.985201
C	8.991367	-3.461151	1.947567
H	10.894326	-3.761414	2.921137
H	10.373400	-2.229978	4.811663
H	8.197591	-1.043526	4.876003
H	7.042758	-2.977425	1.196720
H	9.218781	-4.133294	1.126042
C	6.262116	-1.106387	3.055395
H	6.101954	-0.511722	3.951616
C	5.404054	-0.926921	2.005883
H	5.457206	-1.531012	1.108750
H	4.498408	-0.358017	2.147341

Intermediate IV

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3933.575937
Thermal and entropic correction, BS1 (a.u.)	1.085809
Electronic Energy, BS2 (a.u.)	-3935.022176
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	-0.964066	-2.029819	1.513110
C	-0.004688	-3.012060	1.308904
C	1.346762	-2.646090	1.206079
C	1.662989	-1.286208	1.295370
C	0.690300	-0.298103	1.506001
C	-0.647365	-0.681146	1.635295
H	-0.313200	-4.049844	1.228136
H	-1.433813	0.049690	1.792622
O	-2.305099	-2.446818	1.638879
C	-3.145362	-2.098977	0.632266

O	-2.840297	-1.473166	-0.365194
O	-4.352155	-2.566229	0.935348
H	2.686518	-0.952539	1.199626
C	2.366005	-3.748605	0.961252
H	2.124533	-4.214729	-0.000365
H	2.217017	-4.529287	1.717031
C	3.881277	-3.406103	0.961568
C	4.652175	-4.688264	0.564117
H	4.332780	-5.053587	-0.415791
H	5.729025	-4.498971	0.528472
H	4.467547	-5.473893	1.303446
C	4.166307	-2.362962	-0.126610
C	4.356876	-2.944758	2.348338
H	5.428731	-2.733531	2.346987
H	3.837918	-2.048593	2.693094
H	4.167509	-3.743337	3.072453
O	3.705377	-2.623343	-1.290979
O	4.825170	-1.311707	0.167999
C	1.117809	1.149883	1.561385
H	2.204476	1.178471	1.653774
H	0.715012	1.617855	2.467188
C	0.707152	2.043855	0.365920
H	-0.340160	2.344574	0.476797
H	1.301204	2.959777	0.455026
Rh	3.815694	-1.189963	-2.772539
Rh	5.004185	0.224509	-1.254441
O	3.936990	0.353891	-4.169608
O	5.065312	1.680711	-2.720797
C	4.483196	1.460631	-3.838007
C	4.396412	2.605974	-4.807819
H	4.269611	2.242055	-5.828412
H	3.520107	3.207314	-4.538092
H	5.282067	3.239917	-4.734622
O	5.648370	-1.977709	-3.383241
O	6.774395	-0.607435	-1.974332
C	6.725304	-1.527842	-2.856587
C	8.023603	-2.133742	-3.317392
H	8.187075	-1.874966	-4.368504
H	8.855833	-1.771724	-2.714060
H	7.959321	-3.223203	-3.249714
C	0.851492	1.487954	-1.081267
C	1.028034	2.688981	-2.049530
H	1.924882	3.265641	-1.803413
H	1.109370	2.345177	-3.086280
H	0.159686	3.351969	-1.974937
C	-0.392047	0.687773	-1.511553
H	-0.349861	0.443296	-2.576109
H	-0.492090	-0.243266	-0.954194
H	-1.290316	1.287688	-1.336562
C	2.118177	0.658480	-1.279164
O	2.060665	-0.317763	-2.102788
O	3.181592	1.045779	-0.690568
C	-5.403709	-2.260572	-0.043139
H	-5.063871	-2.603611	-1.024113

H	-5.528185	-1.174242	-0.071510
C	-6.654874	-2.949273	0.399296
H	-6.633329	-4.035433	0.322910
C	-7.990394	-2.303189	0.125174
C	-7.471286	-2.400062	1.551699
H	-7.109662	-1.442975	1.922153
H	-7.936798	-1.296081	-0.288600
C	-7.989301	-3.313370	2.669950
H	-7.816014	-2.788884	3.615636
H	-7.385819	-4.227115	2.715084
C	-9.480435	-3.734063	2.641512
H	-9.639016	-4.520164	1.900075
H	-9.725970	-4.173322	3.613958
C	-10.420235	-2.600792	2.382086
C	-9.145936	-3.102395	-0.439808
H	-9.165986	-4.107362	-0.012476
H	-8.992807	-3.234008	-1.517548
C	-10.504254	-2.401463	-0.249612
H	-10.515934	-1.479331	-0.841819
H	-11.299056	-3.035384	-0.661684
C	-10.824062	-2.054073	1.173519
N	-16.546353	2.472165	-0.463651
C	-15.537979	3.529071	-0.828554
C	-16.308070	4.642942	-1.594098
O	-17.570455	4.593215	-1.500474
C	-14.360457	2.933920	-1.604189
C	-13.612432	1.888031	-0.809598
C	-12.814859	2.267536	0.281205
C	-13.734125	0.525814	-1.109718
C	-12.150113	1.316611	1.048446
C	-13.083400	-0.441240	-0.341630
C	-12.290146	-0.039374	0.734030
O	-15.609087	5.493053	-2.193200
N	-11.621996	-1.005057	1.544009
H	-15.189293	3.957530	0.115100
H	-13.704977	3.770735	-1.857822
H	-14.731120	2.510714	-2.544414
H	-12.707179	3.320902	0.524796
H	-14.351404	0.213885	-1.947456
H	-11.522238	1.612041	1.881475
H	-13.202170	-1.495046	-0.567698
H	-16.555885	1.709367	-1.146998
H	-17.457030	2.969326	-0.520325
H	-16.387462	2.068866	0.461376
N	-11.704057	-0.908998	2.898307
N	-10.975166	-1.873651	3.396056
C	8.674371	1.103127	0.556545
C	8.822981	-0.351614	0.239089
O	9.741527	-0.813889	-0.428813
O	7.888884	-1.118995	0.820058
C	7.991380	-2.541199	0.588044
H	7.302750	-3.000735	1.293172
H	7.698671	-2.774626	-0.437663
H	9.010155	-2.887561	0.772041

C	7.346976	1.615788	1.030236
C	6.831129	1.245960	2.278097
C	6.606840	2.522524	0.254291
C	5.612224	1.743196	2.742905
H	7.396524	0.566685	2.907759
C	5.388672	3.028931	0.702012
H	6.985151	2.836914	-0.712880
C	4.884988	2.642421	1.950799
H	5.250985	1.438615	3.717292
H	4.815044	3.718140	0.090979
O	3.684334	3.197020	2.311788
C	3.203652	2.949968	3.637832
H	2.270658	3.507796	3.724658
H	3.006070	1.885845	3.803855
H	3.917040	3.313158	4.386474
C	9.688023	4.231789	4.661781
C	10.336148	2.996004	4.735280
C	10.434114	2.188625	3.601115
C	9.890414	2.598187	2.372605
C	9.246412	3.844888	2.310039
C	9.144518	4.651295	3.444535
H	9.608236	4.861878	5.542789
H	10.765001	2.659320	5.674833
H	10.934680	1.225889	3.665239
H	8.812908	4.187480	1.376537
H	8.640180	5.610944	3.375219
C	9.985112	1.670094	1.212580
H	10.759126	0.914752	1.315686
C	9.614556	2.019974	-0.192474
H	9.257262	3.023311	-0.396221
H	10.203557	1.573972	-0.986389

R,S Cyclopropane (3)

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-922.457095
Thermal and entropic correction, BS1 (a.u.)	0.271159
Electronic Energy, BS2 (a.u.)	-922.799117
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	-1.961329	0.138437	1.706188
C	-1.414310	-0.559961	0.476233
C	-1.870833	0.939836	0.448661

H	-2.806828	1.082986	-0.082211
H	-2.947681	-0.151749	2.049806
H	-1.246867	0.339615	2.497585
C	0.777384	-1.334502	1.481217
H	0.277360	-1.475913	2.434740
C	2.138211	-1.606904	1.379006
H	2.705336	-1.957586	2.235502
C	2.800295	-1.428249	0.156099
C	2.085749	-0.979022	-0.962836
H	2.574198	-0.831743	-1.918201
C	0.722715	-0.706760	-0.838853
H	0.175439	-0.343913	-1.703839
C	-0.878712	2.025491	0.209595
C	0.234834	2.248639	1.035951
H	0.401045	1.622905	1.906074
C	1.145376	3.265342	0.744841
H	2.000631	3.420578	1.396387
C	0.960894	4.081270	-0.374846
H	1.669755	4.873307	-0.597838
C	-0.144494	3.870902	-1.203103
H	-0.300846	4.499360	-2.075218
C	-1.052781	2.851612	-0.912736
H	-1.909260	2.690099	-1.562259
C	0.048058	-0.876234	0.375808
C	-2.307698	-1.497755	-0.269812
O	-1.913947	-2.376410	-1.025913
O	-3.617211	-1.273059	-0.042055
C	-4.539230	-2.109441	-0.773761
H	-4.370500	-3.162434	-0.536488
H	-5.532616	-1.800957	-0.449444
H	-4.424556	-1.952413	-1.849136
O	4.142158	-1.713309	0.157006
C	4.863452	-1.554334	-1.068205
H	4.479133	-2.222470	-1.847750
H	4.825273	-0.518270	-1.424501
H	5.897503	-1.819383	-0.842197

Intermediate III' 1-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3700.288158
Thermal and entropic correction, BS1 (a.u.)	0.976856
Electronic Energy, BS2 (a.u.)	-3701.665897
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	0.431613	-2.420023	0.439340
C	-0.105380	-2.037724	1.664448
C	-1.463204	-1.701512	1.746900
C	-2.232766	-1.783148	0.579041
C	-1.690843	-2.184119	-0.649857
C	-0.331323	-2.509163	-0.718142
H	0.531122	-1.998814	2.542362
H	0.132707	-2.818338	-1.649093
O	1.779790	-2.815772	0.350033
C	2.727230	-1.931932	0.752116
O	2.533344	-0.779766	1.087846
O	3.900398	-2.555952	0.700285
H	-3.286513	-1.545148	0.597110
C	-1.995006	-1.226911	3.091245
H	-1.573693	-0.233709	3.284882
H	-1.590221	-1.881087	3.872339
C	-3.528779	-1.147912	3.316702
C	-3.775028	-0.601032	4.742410
H	-3.310573	0.379535	4.877481
H	-4.848176	-0.506238	4.938966
H	-3.353269	-1.289578	5.481358
C	-4.134463	-0.123555	2.345942
C	-4.187047	-2.530241	3.189246
H	-5.260930	-2.473523	3.385838
H	-4.046354	-2.968956	2.200403
H	-3.740353	-3.206101	3.925501
O	-3.604033	1.032237	2.323493
O	-5.127006	-0.491061	1.630694
C	-2.586172	-2.235273	-1.866147
H	-3.620852	-2.273524	-1.524879
H	-2.400713	-3.166565	-2.414123
C	-2.459205	-1.076711	-2.886629
H	-1.597597	-1.258130	-3.538592
H	-3.346777	-1.138710	-3.526040
Rh	-4.239228	2.428891	0.926586
Rh	-5.856237	0.758099	0.143324
O	-4.941869	3.695722	-0.573008
O	-6.431529	2.145241	-1.290119

C	-5.830510	3.275522	-1.377031
C	-6.208407	4.138491	-2.549276
H	-5.892474	5.170010	-2.389486
H	-5.703755	3.744724	-3.438719
H	-7.285376	4.090825	-2.724553
O	-5.697674	3.101748	2.244864
O	-7.179245	1.533560	1.540169
C	-6.829907	2.522498	2.275567
C	-7.859126	3.011072	3.259934
H	-7.500761	3.891895	3.793332
H	-8.787074	3.247014	2.731151
H	-8.077648	2.211331	3.974465
C	-2.313607	0.385882	-2.381486
C	-2.749956	1.327828	-3.536462
H	-3.795602	1.154518	-3.807653
H	-2.631051	2.377890	-3.250609
H	-2.127202	1.139154	-4.417227
C	-0.856624	0.715129	-2.000070
H	-0.736993	1.783027	-1.801227
H	-0.528397	0.166248	-1.115667
H	-0.195447	0.449374	-2.830807
C	-3.257207	0.735573	-1.228181
O	-2.892854	1.667362	-0.439665
O	-4.384560	0.138868	-1.184110
C	5.046687	-1.774367	1.175141
H	4.854997	-1.505730	2.218438
H	5.114469	-0.858652	0.581050
C	6.266653	-2.625990	1.023858
H	6.235511	-3.564796	1.575548
C	7.620073	-1.967423	0.949220
C	7.041242	-2.659513	-0.277358
H	6.678806	-1.945442	-1.014184
H	7.604033	-0.879276	0.885606
C	7.510953	-3.976741	-0.906139
H	7.294813	-3.912331	-1.977836
H	6.908330	-4.809053	-0.525218
C	9.002108	-4.370987	-0.756512
H	9.186903	-4.778091	0.240067
H	9.209015	-5.181647	-1.462885
C	9.962842	-3.255748	-1.020313
C	8.772971	-2.491007	1.780236
H	8.748390	-3.582508	1.822896
H	8.650573	-2.144478	2.813422
C	10.146925	-1.995703	1.291682
H	10.212634	-0.913180	1.449204
H	10.931674	-2.440073	1.916151
C	10.428712	-2.279375	-0.153289
N	16.508344	1.921325	-0.195424
C	15.669605	3.136849	-0.492270
C	16.573126	4.378943	-0.246351
O	17.813096	4.139481	-0.148212
C	14.371294	3.134115	0.318940
C	13.509188	1.928400	0.022555
C	12.702429	1.894184	-1.124970

C	13.545950	0.797947	0.849065
C	11.943236	0.769560	-1.435625
C	12.806209	-0.343675	0.540980
C	12.001799	-0.350483	-0.600150
O	15.994426	5.489605	-0.204853
N	11.243368	-1.509748	-0.939531
H	15.442923	3.098696	-1.561380
H	13.847800	4.059259	0.067617
H	14.619484	3.174147	1.385585
H	12.660678	2.762887	-1.776206
H	14.168869	0.803735	1.739574
H	11.307088	0.752837	-2.313387
H	12.865331	-1.222451	1.173104
H	16.382835	1.606042	0.771134
H	17.484874	2.258889	-0.294805
H	16.307012	1.133298	-0.814252
N	11.276291	-1.981000	-2.215275
N	10.499087	-3.031907	-2.256144
C	-7.207974	-0.617012	-0.509760
C	-6.571709	-1.908056	-0.824437
O	-6.103070	-2.150433	-1.937605
O	-6.485123	-2.735597	0.222175
C	-5.731728	-3.960602	0.027948
H	-5.837188	-4.510996	0.961175
H	-6.148061	-4.532723	-0.803555
H	-4.682230	-3.728244	-0.161763
C	-8.585899	-0.470835	-0.765821
C	-9.392831	-1.579216	-1.175251
C	-9.232690	0.801648	-0.636843
C	-10.740610	-1.446353	-1.427073
H	-8.938255	-2.558768	-1.287621
C	-10.574052	0.944464	-0.892415
H	-8.644036	1.659212	-0.342036
C	-11.345227	-0.175812	-1.284487
H	-11.320927	-2.307988	-1.731060
H	-11.070343	1.904644	-0.801621
O	-12.644043	0.066894	-1.499300
C	-13.511935	-1.016173	-1.889240
H	-14.502999	-0.573534	-1.983760
H	-13.199173	-1.435024	-2.850016
H	-13.522893	-1.795761	-1.122039
O	-6.390342	0.325775	-3.523996
H	-6.183156	-0.495608	-3.043222
H	-6.354980	1.004423	-2.826713

TS III-IV' 1-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3700.268337
Thermal and entropic correction, BS1 (a.u.)	0.978645
Electronic Energy, BS2 (a.u.)	-3701.642525
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-224.8i

Molecular Geometry in Cartesian Coordinates

C	0.417875	-2.323028	0.260747
C	-0.113592	-1.986327	1.501981
C	-1.481993	-1.704067	1.612655
C	-2.267137	-1.789869	0.455963
C	-1.732024	-2.145424	-0.789098
C	-0.361875	-2.417796	-0.886072
H	0.534150	-1.940278	2.371289
H	0.097638	-2.690292	-1.830714
O	1.778458	-2.667947	0.140521
C	2.703849	-1.768539	0.561081
O	2.477458	-0.635841	0.939595
O	3.897077	-2.350737	0.472247
H	-3.328735	-1.591432	0.495565
C	-2.012187	-1.279852	2.974259
H	-1.598475	-0.289957	3.197685
H	-1.597801	-1.955019	3.732309
C	-3.545774	-1.221840	3.207322
C	-3.790507	-0.686806	4.638347
H	-3.336983	0.298290	4.777156
H	-4.863666	-0.605969	4.841202
H	-3.356908	-1.374982	5.370889
C	-4.171833	-0.198502	2.247319
C	-4.189936	-2.608986	3.080480
H	-5.257027	-2.562987	3.311037
H	-4.076007	-3.032333	2.080657
H	-3.716353	-3.290938	3.793906
O	-3.634352	0.955211	2.229008
O	-5.179095	-0.553024	1.545851
C	-2.649146	-2.207095	-1.990451
H	-3.679165	-2.258260	-1.629877
H	-2.462870	-3.137663	-2.539604
C	-2.541875	-1.052413	-3.017714
H	-1.678794	-1.227734	-3.669176
H	-3.428029	-1.131517	-3.657514
Rh	-4.287414	2.388202	0.888734
Rh	-5.912977	0.742386	0.078319
O	-5.026079	3.715778	-0.524043
O	-6.470337	2.163905	-1.330632

C	-5.937302	3.325360	-1.323955
C	-6.427926	4.289405	-2.371794
H	-6.029247	5.290028	-2.200949
H	-6.106821	3.933857	-3.356728
H	-7.521061	4.313275	-2.366677
O	-5.724625	3.003202	2.259415
O	-7.238235	1.496676	1.485399
C	-6.867419	2.441426	2.266452
C	-7.882465	2.904134	3.278754
H	-7.501321	3.746463	3.856823
H	-8.804442	3.192322	2.765346
H	-8.122229	2.075012	3.951763
C	-2.412716	0.418538	-2.526939
C	-2.884757	1.342653	-3.681548
H	-3.934266	1.156242	-3.931272
H	-2.772048	2.397345	-3.410663
H	-2.279466	1.150221	-4.573441
C	-0.955570	0.777281	-2.174433
H	-0.853895	1.847587	-1.978333
H	-0.601312	0.235116	-1.296096
H	-0.305616	0.523500	-3.017512
C	-3.335690	0.754322	-1.355977
O	-2.971700	1.665495	-0.550656
O	-4.463589	0.147689	-1.292571
C	5.022523	-1.548928	0.967603
H	4.818481	-1.305623	2.014719
H	5.068403	-0.620556	0.391308
C	6.268715	-2.361889	0.809234
H	6.256031	-3.316069	1.334866
C	7.608983	-1.668186	0.782525
C	7.066554	-2.334653	-0.476501
H	6.694975	-1.600547	-1.189109
H	7.568885	-0.579383	0.747938
C	7.563347	-3.612721	-1.161964
H	7.539055	-3.430195	-2.242007
H	6.852832	-4.426817	-0.975937
C	8.978289	-4.132824	-0.821952
H	9.011277	-4.520336	0.198535
H	9.187007	-4.982870	-1.480077
C	10.060513	-3.118118	-1.021094
C	8.735812	-2.184098	1.656450
H	8.698668	-3.273437	1.727943
H	8.575513	-1.810951	2.675123
C	10.137705	-1.723180	1.222291
H	10.198529	-0.630318	1.291495
H	10.871173	-2.111928	1.939107
C	10.527472	-2.131729	-0.165844
N	17.074684	1.607366	-0.083495
C	16.266808	2.849320	-0.359807
C	17.200819	4.061460	-0.073047
O	18.425072	3.779877	0.095477
C	14.964911	2.875689	0.445699
C	14.032059	1.733331	0.110934
C	13.321932	1.725512	-1.099825

C	13.880709	0.647333	0.982154
C	12.473965	0.671509	-1.427470
C	13.045950	-0.423809	0.661352
C	12.339194	-0.403378	-0.542054
O	16.659730	5.191072	-0.066246
N	11.492234	-1.495020	-0.900503
H	16.046099	2.845273	-1.430314
H	14.492043	3.835992	0.224867
H	15.207365	2.868638	1.514265
H	13.426238	2.560181	-1.787513
H	14.428697	0.631984	1.920166
H	11.914128	0.675905	-2.355990
H	12.958940	-1.271174	1.331676
H	16.846985	1.194671	0.825335
H	18.053551	1.964421	-0.048795
H	16.961443	0.886620	-0.798968
N	11.607976	-2.049002	-2.136995
N	10.740820	-3.024418	-2.203132
C	-7.295120	-0.669728	-0.722672
C	-6.956142	-2.050552	-0.281945
O	-6.204373	-2.845581	-0.846844
O	-7.548078	-2.315132	0.894024
C	-7.322626	-3.637241	1.443569
H	-7.809109	-3.629854	2.417654
H	-7.780717	-4.388164	0.795154
H	-6.256184	-3.835621	1.548290
C	-8.704672	-0.413143	-0.999751
C	-9.592171	-1.467175	-1.318841
C	-9.238290	0.896873	-0.948420
C	-10.940823	-1.245170	-1.561748
H	-9.217236	-2.484802	-1.383579
C	-10.580418	1.133517	-1.187448
H	-8.585427	1.724825	-0.711799
C	-11.444062	0.066386	-1.493277
H	-11.588021	-2.080057	-1.799708
H	-10.990139	2.137248	-1.137762
O	-12.741834	0.401491	-1.704633
C	-13.687079	-0.645018	-1.972708
H	-14.651657	-0.149244	-2.086400
H	-13.437478	-1.175083	-2.897936
H	-13.734803	-1.354287	-1.139747
O	-6.558618	-0.878132	-2.544076
H	-6.335613	-1.830532	-2.468558
H	-5.685790	-0.440568	-2.391463

Intermediate IV' 1-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3700.296004
Thermal and entropic correction, BS1 (a.u.)	0.984102
Electronic Energy, BS2 (a.u.)	-3701.673539
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	-0.391034	-2.845845	-0.206196
C	0.071656	-2.543225	-1.483031
C	1.422849	-2.218005	-1.667291
C	2.262159	-2.232039	-0.546223
C	1.795337	-2.556157	0.734419
C	0.442824	-2.869473	0.905142
H	-0.614521	-2.553814	-2.322865
H	0.036711	-3.117478	1.880462
O	-1.730046	-3.226327	0.002419
C	-2.712199	-2.398847	-0.434502
O	-2.555853	-1.310683	-0.953111
O	-3.873197	-2.998335	-0.183967
H	3.312755	-1.998899	-0.643291
C	1.872144	-1.828329	-3.068362
H	1.406933	-0.865694	-3.310281
H	1.451918	-2.550051	-3.778709
C	3.388794	-1.715616	-3.380192
C	3.541667	-1.239626	-4.843857
H	3.039643	-0.281811	-5.004703
H	4.599650	-1.124029	-5.102059
H	3.104068	-1.978984	-5.522055
C	4.015131	-0.630072	-2.495472
C	4.104371	-3.066065	-3.218425
H	5.162310	-2.981812	-3.482146
H	4.041786	-3.454141	-2.200018
H	3.641910	-3.797313	-3.888977
O	3.461601	0.520887	-2.511186
O	5.040589	-0.934608	-1.804464
C	2.759573	-2.535820	1.897495
H	3.774697	-2.581262	1.497053
H	2.621273	-3.441785	2.498966
C	2.656664	-1.332764	2.869671
H	1.833353	-1.507008	3.570945
H	3.574517	-1.343879	3.467918
Rh	4.149857	1.997890	-1.226911
Rh	5.813640	0.424729	-0.443208
O	4.903357	3.394013	0.109023
O	6.464133	1.921360	0.832934

C	5.895374	3.059435	0.844947
C	6.420429	4.066774	1.833623
H	6.004809	3.831855	2.819646
H	7.508256	3.992815	1.901755
H	6.122042	5.078957	1.557048
O	5.519482	2.607963	-2.660644
O	7.081615	1.136815	-1.920134
C	6.670562	2.057390	-2.706165
C	7.631967	2.516484	-3.769830
H	7.211109	3.337196	-4.351068
H	8.566829	2.833882	-3.298962
H	7.862330	1.676302	-4.432309
C	2.444722	0.104554	2.313719
C	2.913916	1.104074	3.405113
H	3.975869	0.967973	3.633352
H	2.755630	2.137826	3.081921
H	2.340262	0.938575	4.322844
C	0.963946	0.387915	1.992620
H	0.811191	1.446105	1.765854
H	0.608670	-0.196297	1.142173
H	0.348972	0.135288	2.861835
C	3.318515	0.417412	1.101637
O	2.894003	1.284312	0.269652
O	4.463002	-0.146594	1.027452
C	-5.055976	-2.321658	-0.724165
H	-4.965404	-2.325554	-1.814999
H	-5.060374	-1.286043	-0.373819
C	-6.265073	-3.066237	-0.252975
H	-6.275171	-4.125804	-0.504378
C	-7.601991	-2.373722	-0.304099
C	-6.962309	-2.688117	1.038923
H	-6.547226	-1.803658	1.518156
H	-7.568391	-1.318110	-0.574412
C	-7.435954	-3.748200	2.038247
H	-7.039215	-3.459870	3.017255
H	-6.983914	-4.717845	1.802778
C	-8.966224	-3.972578	2.192809
H	-9.316700	-4.675973	1.433558
H	-9.144600	-4.452293	3.160566
C	-9.797108	-2.731853	2.116943
C	-8.824380	-3.084681	-0.845572
H	-8.839956	-4.123857	-0.508193
H	-8.769633	-3.119798	-1.940138
C	-10.136264	-2.367349	-0.472385
H	-10.183887	-1.416030	-1.013321
H	-10.988935	-2.960423	-0.825412
C	-10.285006	-2.083670	0.992445
N	-16.015527	2.430184	-0.391990
C	-15.052679	3.588093	-0.411161
C	-15.818728	4.808081	-0.998608
O	-17.078729	4.693010	-1.037201
C	-13.765658	3.232332	-1.159200
C	-12.997577	2.114032	-0.492763
C	-12.108992	2.391339	0.556724

C	-13.198926	0.778082	-0.863869
C	-11.424853	1.369181	1.208563
C	-12.538357	-0.258975	-0.205420
C	-11.643765	0.042364	0.824062
O	-15.120044	5.792216	-1.337131
N	-10.948334	-1.000963	1.504485
H	-14.826880	3.813144	0.635157
H	-13.166741	4.144888	-1.192442
H	-14.018907	2.966222	-2.192096
H	-11.941512	3.422131	0.856190
H	-13.885830	0.541821	-1.672065
H	-10.721994	1.589207	2.004028
H	-12.724120	-1.290283	-0.483012
H	-15.958475	1.887060	-1.259204
H	-16.952304	2.871707	-0.359911
H	-15.861071	1.794823	0.393717
N	-10.870318	-0.980311	2.862870
N	-10.172134	-2.026136	3.223535
C	7.337592	-1.453077	1.156837
C	7.485173	-2.112928	-0.032860
O	6.619559	-3.079100	-0.425045
O	8.533499	-1.936384	-0.855432
C	8.281073	-2.083807	-2.275288
H	9.200756	-1.762232	-2.763718
H	8.073143	-3.126238	-2.525564
H	7.449033	-1.446186	-2.581058
C	8.177850	-0.399645	1.740446
C	7.844484	0.103491	3.009855
C	9.241157	0.228769	1.052836
C	8.485105	1.218525	3.554695
H	7.039678	-0.358008	3.570579
C	9.881880	1.338300	1.586283
H	9.542528	-0.131490	0.078304
C	9.492336	1.860723	2.829023
H	8.175409	1.583425	4.526468
H	10.681941	1.829011	1.040106
O	10.151008	2.996371	3.236882
C	9.716010	3.618562	4.448681
H	10.327679	4.515171	4.560718
H	8.658602	3.904399	4.393056
H	9.870935	2.964047	5.314452
O	6.294226	-1.960740	1.949824
H	5.902880	-3.095392	0.236572
H	5.543671	-1.330356	1.894782

Intermediate III' 2-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3776.739023
Thermal and entropic correction, BS1 (a.u.)	1.004958
Electronic Energy, BS2 (a.u.)	-3778.153354
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	0.539262	-2.229409	0.220610
C	0.024662	-1.968023	1.486100
C	-1.347554	-1.726680	1.636392
C	-2.155162	-1.778859	0.492212
C	-1.635028	-2.060391	-0.778727
C	-0.259902	-2.284259	-0.914311
H	0.687539	-1.950659	2.344838
H	0.185963	-2.503494	-1.879114
O	1.900494	-2.548173	0.058209
C	2.824830	-1.666096	0.514241
O	2.598291	-0.555110	0.952425
O	4.017305	-2.240011	0.383116
H	-3.220899	-1.613034	0.563430
C	-1.851605	-1.386959	3.032150
H	-1.440012	-0.408385	3.303946
H	-1.414825	-2.101733	3.739591
C	-3.378684	-1.357579	3.304669
C	-3.597586	-0.899485	4.766315
H	-3.157948	0.085755	4.943719
H	-4.666797	-0.850031	4.997890
H	-3.133315	-1.615703	5.451549
C	-4.032696	-0.294141	2.411958
C	-4.011405	-2.742790	3.116866
H	-5.079660	-2.716511	3.343859
H	-3.888341	-3.120612	2.100391
H	-3.533221	-3.450522	3.801378
O	-3.503064	0.861897	2.424174
O	-5.058856	-0.626945	1.725861
C	-2.561529	-2.118047	-1.973149
H	-3.590489	-2.185412	-1.613745
H	-2.365107	-3.039677	-2.533882
C	-2.457246	-0.952024	-2.983400
H	-1.539484	-1.068118	-3.569189
H	-3.283691	-1.080999	-3.687365
Rh	-4.155173	2.313647	1.102897
Rh	-5.828880	0.693976	0.320190
O	-4.856982	3.653016	-0.317388
O	-6.387462	2.155123	-1.053479

C	-5.770065	3.277707	-1.115381
C	-6.165311	4.189997	-2.243860
H	-5.675644	5.159470	-2.151063
H	-5.872469	3.717737	-3.187348
H	-7.251388	4.314464	-2.257862
O	-5.548275	2.964047	2.500427
O	-7.089824	1.467086	1.771793
C	-6.691847	2.410238	2.542218
C	-7.680422	2.880179	3.576100
H	-7.275850	3.714660	4.149340
H	-8.607481	3.182932	3.080705
H	-7.918543	2.050800	4.249140
C	-2.454336	0.515806	-2.454664
C	-3.130850	1.431230	-3.512360
H	-4.182208	1.163785	-3.658519
H	-3.082985	2.481094	-3.203455
H	-2.610717	1.329845	-4.470369
C	-1.011024	0.999132	-2.218497
H	-0.985974	2.052604	-1.930736
H	-0.516913	0.416065	-1.437249
H	-0.437601	0.884370	-3.143358
C	-3.296306	0.733289	-1.196317
O	-2.879873	1.583166	-0.349939
O	-4.418190	0.117925	-1.114886
C	5.148078	-1.469007	0.909939
H	4.924675	-1.218283	1.951095
H	5.235918	-0.543321	0.333724
C	6.369167	-2.323213	0.783445
H	6.315859	-3.267159	1.324700
C	7.731865	-1.678817	0.757766
C	7.180000	-2.350404	-0.494254
H	6.843738	-1.619381	-1.227060
H	7.731814	-0.590112	0.702909
C	7.639051	-3.662462	-1.141801
H	7.572859	-3.525247	-2.226634
H	6.932204	-4.462934	-0.894104
C	9.064294	-4.178253	-0.834081
H	9.120726	-4.564038	0.186050
H	9.262396	-5.027888	-1.495893
C	10.135082	-3.156387	-1.050932
C	8.836371	-2.221447	1.642342
H	8.771663	-3.309703	1.711486
H	8.680720	-1.844761	2.660406
C	10.247616	-1.790495	1.208445
H	10.335495	-0.701427	1.300666
H	10.978975	-2.212855	1.908325
C	10.610242	-2.176064	-0.193524
N	17.010397	1.631022	-0.091440
C	16.230862	2.882069	-0.399307
C	17.179452	4.085708	-0.133264
O	18.407619	3.798345	-0.019938
C	14.918826	2.932781	0.386803
C	14.001844	1.775483	0.062960
C	13.265781	1.763735	-1.131885

C	13.907885	0.670885	0.918957
C	12.447299	0.686699	-1.459415
C	13.102962	-0.422314	0.597973
C	12.370125	-0.406064	-0.589838
O	16.643008	5.217644	-0.094637
N	11.546792	-1.516193	-0.942742
H	16.023228	2.856141	-1.472678
H	14.446709	3.885059	0.134112
H	15.146334	2.952152	1.458575
H	13.326099	2.613000	-1.806803
H	14.476247	0.659309	1.844918
H	11.865708	0.687108	-2.374504
H	13.056518	-1.282496	1.256184
H	16.860988	1.323846	0.874422
H	18.002509	1.921320	-0.180380
H	16.780869	0.851867	-0.711771
N	11.639421	-2.050656	-2.189522
N	10.784147	-3.037813	-2.247649
C	-7.265889	-0.653104	-0.230861
C	-6.882325	-2.071152	-0.058594
O	-6.277927	-2.741376	-0.895905
O	-7.237689	-2.545387	1.140848
C	-6.894858	-3.930576	1.411021
H	-7.163610	-4.095535	2.452809
H	-7.475922	-4.585172	0.757389
H	-5.828396	-4.097036	1.257547
C	-8.577776	-0.406945	-0.686665
C	-9.425688	-1.465539	-1.145257
C	-9.113196	0.922057	-0.720447
C	-10.694120	-1.227513	-1.626313
H	-9.056250	-2.486261	-1.145102
C	-10.386395	1.164995	-1.171474
H	-8.501000	1.740174	-0.369805
C	-11.188015	0.097641	-1.641504
H	-11.300360	-2.050218	-1.982940
H	-10.800760	2.167270	-1.187061
O	-12.405111	0.441770	-2.078386
C	-13.297822	-0.575479	-2.575446
H	-14.204584	-0.046095	-2.866380
H	-12.866070	-1.077528	-3.446026
H	-13.526817	-1.304438	-1.792944
O	-5.744134	-1.231287	-3.166300
H	-6.102163	-1.889431	-2.539726
H	-5.168273	-0.712057	-2.569045
O	-7.169217	1.104616	-3.540160
H	-6.957102	1.511186	-2.680314
H	-6.752167	0.219977	-3.462504

TS III-IV' 2-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3776.720384
Thermal and entropic correction, BS1 (a.u.)	1.002144
Electronic Energy, BS2 (a.u.)	-3778.131622
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-241.0i

Molecular Geometry in Cartesian Coordinates

C	0.531970	-2.383423	0.348830
C	0.026639	-2.026101	1.595205
C	-1.332705	-1.709647	1.722530
C	-2.136926	-1.787840	0.578853
C	-1.628609	-2.166699	-0.670327
C	-0.266532	-2.468704	-0.785774
H	0.687404	-1.989467	2.454920
H	0.172274	-2.759558	-1.734749
O	1.881332	-2.761386	0.208574
C	2.836515	-1.892102	0.625483
O	2.647282	-0.760618	1.027086
O	4.012234	-2.502766	0.502404
H	-3.192573	-1.564317	0.632309
C	-1.833149	-1.254929	3.084863
H	-1.407579	-0.264200	3.281112
H	-1.410894	-1.918481	3.848674
C	-3.361787	-1.178540	3.344572
C	-3.573203	-0.625148	4.773819
H	-3.093758	0.349641	4.897171
H	-4.641099	-0.515948	4.990632
H	-3.146167	-1.317405	5.506366
C	-3.994237	-0.159624	2.384888
C	-4.025043	-2.559168	3.244973
H	-5.072961	-2.502585	3.548457
H	-3.985306	-2.974119	2.235893
H	-3.514161	-3.252473	3.920617
O	-3.451188	0.990469	2.348975
O	-5.011201	-0.514102	1.697778
C	-2.564333	-2.222163	-1.856863
H	-3.588424	-2.265078	-1.478481
H	-2.396122	-3.155988	-2.405978
C	-2.459336	-1.071861	-2.890024
H	-1.612305	-1.265279	-3.557142
H	-3.358779	-1.138975	-3.512281
Rh	-4.113541	2.416484	1.011441
Rh	-5.750019	0.766428	0.226301
O	-4.844083	3.758071	-0.385951
O	-6.300655	2.214036	-1.173526

C	-5.757743	3.375377	-1.180313
C	-6.245073	4.330859	-2.235745
H	-5.834844	5.328845	-2.078979
H	-5.932595	3.958654	-3.217233
H	-7.337812	4.364234	-2.225084
O	-5.547371	3.032014	2.387074
O	-7.074113	1.532359	1.623401
C	-6.694318	2.479027	2.398676
C	-7.703378	2.953818	3.411029
H	-7.317065	3.800257	3.979389
H	-8.627044	3.239676	2.899623
H	-7.941591	2.131022	4.092337
C	-2.294680	0.400592	-2.412423
C	-2.788932	1.322456	-3.560614
H	-3.851333	1.159075	-3.768673
H	-2.641176	2.376923	-3.306032
H	-2.220110	1.106388	-4.470995
C	-0.825417	0.739779	-2.097041
H	-0.705276	1.808211	-1.900864
H	-0.457418	0.190579	-1.228519
H	-0.199640	0.479310	-2.956222
C	-3.183955	0.759018	-1.225000
O	-2.809488	1.684928	-0.442156
O	-4.309765	0.154533	-1.129309
C	5.165816	-1.742450	0.996495
H	4.990168	-1.526398	2.054786
H	5.221865	-0.798414	0.447123
C	6.388167	-2.578670	0.785243
H	6.362613	-3.551848	1.274156
C	7.740196	-1.911034	0.757788
C	7.163218	-2.518722	-0.514390
H	6.795137	-1.753662	-1.195436
H	7.720727	-0.821085	0.767873
C	7.631520	-3.782201	-1.245726
H	7.487101	-3.603043	-2.316692
H	6.977722	-4.623707	-0.988793
C	9.094909	-4.247355	-1.051745
H	9.222117	-4.706566	-0.068986
H	9.295622	-5.034659	-1.786011
C	10.112308	-3.165726	-1.234301
C	8.884338	-2.485335	1.568908
H	8.848093	-3.577302	1.561859
H	8.752973	-2.186870	2.615920
C	10.271172	-1.986501	1.124354
H	10.340342	-0.907746	1.307216
H	11.036046	-2.449500	1.759819
C	10.590960	-2.242199	-0.317705
N	16.919093	1.828368	-0.334184
C	16.033947	3.047952	-0.381175
C	16.930760	4.266474	-0.017315
O	18.169909	4.022039	0.091096
C	14.814783	2.901536	0.534317
C	13.914572	1.751396	0.142967
C	13.125703	1.829306	-1.015598

C	13.876492	0.574711	0.901265
C	12.311596	0.768749	-1.401585
C	13.076737	-0.503041	0.519201
C	12.291428	-0.397640	-0.629720
O	16.345250	5.366273	0.111734
N	11.475499	-1.491959	-1.044918
H	15.712510	3.163761	-1.418831
H	14.275277	3.850214	0.475202
H	15.159027	2.783417	1.567764
H	13.142313	2.735223	-1.615146
H	14.485497	0.494716	1.797439
H	11.690783	0.836499	-2.287964
H	13.074296	-1.418540	1.099906
H	16.736939	1.247913	0.489452
H	17.876144	2.238053	-0.255255
H	16.830982	1.240275	-1.165238
N	11.534583	-1.921270	-2.334238
N	10.707801	-2.928571	-2.440820
C	-7.111886	-0.730700	-0.489151
C	-6.909062	-2.025321	0.223788
O	-6.179371	-2.957108	-0.114139
O	-7.618892	-2.024939	1.362875
C	-7.576296	-3.237666	2.155747
H	-8.041874	-2.978621	3.105452
H	-8.147962	-4.021335	1.652211
H	-6.548891	-3.566140	2.307979
C	-8.467718	-0.507910	-0.980156
C	-9.306594	-1.593910	-1.323047
C	-8.999735	0.796469	-1.107550
C	-10.605147	-1.405457	-1.773640
H	-8.927245	-2.609388	-1.246005
C	-10.298814	0.999125	-1.539719
H	-8.383335	1.647866	-0.855700
C	-11.111125	-0.096985	-1.880661
H	-11.213183	-2.263470	-2.031201
H	-10.711212	1.999259	-1.625927
O	-12.365366	0.207147	-2.298893
C	-13.238486	-0.862292	-2.691942
H	-14.171393	-0.384551	-2.992789
H	-12.822598	-1.418919	-3.538289
H	-13.429439	-1.544152	-1.856613
O	-6.180017	-1.325031	-2.142306
H	-6.000944	-2.247174	-1.859742
H	-5.320081	-0.852795	-1.988541
O	-6.643310	1.051362	-3.705163
H	-6.548291	1.493482	-2.839553
H	-6.626749	0.113525	-3.460657

Intermediate IV' 2-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3776.730508
Thermal and entropic correction, BS1 (a.u.)	1.007472
Electronic Energy, BS2 (a.u.)	-3778.142222
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	0.591670	-2.713918	0.369834
C	0.099262	-2.350140	1.619156
C	-1.246019	-1.977447	1.748211
C	-2.048525	-2.004304	0.600845
C	-1.552419	-2.393188	-0.650501
C	-0.206881	-2.756480	-0.766124
H	0.760786	-2.351026	2.479021
H	0.221169	-3.053515	-1.717998
O	1.928150	-3.131784	0.223495
C	2.906989	-2.274486	0.607888
O	2.745131	-1.145025	1.026843
O	4.070353	-2.894532	0.430109
H	-3.092380	-1.729176	0.654618
C	-1.731711	-1.520584	3.115404
H	-1.304849	-0.529514	3.308262
H	-1.300989	-2.185100	3.873378
C	-3.257912	-1.444536	3.393071
C	-3.452118	-0.947884	4.845306
H	-2.964953	0.018035	5.003394
H	-4.517277	-0.840220	5.076013
H	-3.023568	-1.671861	5.545572
C	-3.894088	-0.385140	2.480398
C	-3.929356	-2.817541	3.243316
H	-4.982057	-2.767957	3.533567
H	-3.878238	-3.201978	2.223177
H	-3.428994	-3.533693	3.902981
O	-3.360609	0.771776	2.492713
O	-4.907295	-0.718190	1.779454
C	-2.476512	-2.374446	-1.844870
H	-3.499167	-2.446613	-1.471262
H	-2.305380	-3.269883	-2.452768
C	-2.364888	-1.155247	-2.798841
H	-1.537710	-1.325283	-3.496440
H	-3.278877	-1.149261	-3.404216
Rh	-4.041496	2.239148	1.194857
Rh	-5.667119	0.609809	0.369496
O	-4.812608	3.598031	-0.172638
O	-6.311481	2.085077	-0.952054

C	-5.756577	3.242112	-0.945667
C	-6.260679	4.228494	-1.963746
H	-5.853097	5.222948	-1.780410
H	-5.954968	3.887423	-2.958450
H	-7.353216	4.256556	-1.942900
O	-5.458897	2.819220	2.597329
O	-6.971673	1.307556	1.828292
C	-6.594823	2.241126	2.618330
C	-7.595010	2.678823	3.656290
H	-7.195744	3.486665	4.269976
H	-8.511149	3.009335	3.157899
H	-7.852787	1.825947	4.291558
C	-2.143111	0.272125	-2.228022
C	-2.477027	1.285442	-3.356149
H	-3.524325	1.214680	-3.660328
H	-2.281482	2.310001	-3.024149
H	-1.844395	1.079970	-4.225796
C	-0.682315	0.510204	-1.791396
H	-0.512650	1.568979	-1.580750
H	-0.412881	-0.058999	-0.901192
H	-0.010341	0.214325	-2.602689
C	-3.092416	0.626162	-1.086852
O	-2.737720	1.530214	-0.274931
O	-4.241564	0.048432	-1.039454
C	5.247107	-2.155523	0.897925
H	5.118760	-1.975577	1.969841
H	5.284320	-1.192774	0.380655
C	6.454672	-2.987968	0.605052
H	6.435488	-3.985457	1.041901
C	7.802072	-2.314958	0.574416
C	7.196241	-2.855137	-0.710919
H	6.811903	-2.065720	-1.353805
H	7.779530	-1.227852	0.652963
C	7.680863	-4.082932	-1.487762
H	7.300421	-3.980989	-2.509432
H	7.220705	-4.991206	-1.083802
C	9.213587	-4.331116	-1.571052
H	9.544843	-4.894908	-0.695423
H	9.412183	-4.968127	-2.438839
C	10.046397	-3.095063	-1.686938
C	8.997456	-2.934407	1.267178
H	9.005521	-4.016476	1.114765
H	8.912665	-2.779227	2.349291
C	10.331050	-2.307543	0.813543
H	10.385080	-1.281001	1.191789
H	11.164048	-2.847604	1.280038
C	10.514938	-2.271544	-0.674743
N	16.238300	2.453378	-0.066494
C	15.261493	3.600090	-0.094985
C	16.024601	4.856801	0.413997
O	17.284097	4.742887	0.477227
C	13.995303	3.282437	0.705108
C	13.246802	2.079221	0.179100
C	12.369298	2.202820	-0.908519

C	13.442375	0.810699	0.740806
C	11.685368	1.097881	-1.408396
C	12.780513	-0.309388	0.238437
C	11.891776	-0.157840	-0.828178
O	15.324022	5.861140	0.680923
N	11.192136	-1.288380	-1.344697
H	15.010760	3.762792	-1.146797
H	13.370570	4.177140	0.658081
H	14.270149	3.128963	1.754918
H	12.206367	3.178963	-1.356811
H	14.123453	0.694253	1.579668
H	10.989552	1.201821	-2.233308
H	12.958699	-1.289566	0.665966
H	16.172498	1.928009	0.810756
H	17.168705	2.912291	-0.091162
H	16.110709	1.798339	-0.840472
N	11.140905	-1.490805	-2.688999
N	10.445652	-2.581375	-2.887037
C	-6.955274	-0.957497	-0.618874
C	-7.078628	-2.023839	0.382887
O	-6.339462	-3.023375	0.357300
O	-7.997893	-1.812458	1.327177
C	-8.112470	-2.833774	2.347323
H	-8.922797	-2.503520	2.995532
H	-8.355483	-3.797069	1.893694
H	-7.180969	-2.910936	2.911499
C	-8.183222	-0.420647	-1.271674
C	-8.458220	-0.606454	-2.632385
C	-9.098826	0.338132	-0.514153
C	-9.600136	-0.062957	-3.230392
H	-7.775026	-1.178039	-3.248432
C	-10.241076	0.872002	-1.094637
H	-8.901182	0.523625	0.534367
C	-10.499129	0.680907	-2.460615
H	-9.770720	-0.230171	-4.287172
H	-10.941827	1.455460	-0.505217
O	-11.648260	1.262386	-2.939108
C	-11.950864	1.098141	-4.326331
H	-12.887824	1.631798	-4.493982
H	-11.168981	1.530619	-4.961899
H	-12.085777	0.040989	-4.584047
O	-6.040390	-1.574893	-1.649332
H	-5.822353	-2.461227	-1.233152
H	-5.178317	-1.030127	-1.645455
O	-5.994349	1.159349	-3.625981
H	-6.169833	1.390724	-2.695094
H	-5.661655	0.253588	-3.572290

Intermediate III' 3-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3853.184205
Thermal and entropic correction, BS1 (a.u.)	1.023619
Electronic Energy, BS2 (a.u.)	-3854.635920
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

Rh	4.512239	-0.587571	-2.669134
Rh	5.610316	0.199421	-0.636414
O	4.725178	1.327312	-3.452385
O	5.696309	2.072635	-1.548313
C	5.211811	2.246396	-2.723788
C	5.203455	3.657893	-3.242199
H	4.435714	4.216402	-2.696086
H	6.166102	4.136977	-3.048298
H	4.977104	3.677715	-4.308435
O	6.393459	-1.140974	-3.376628
O	7.412674	-0.375763	-1.501941
C	7.423920	-0.913363	-2.665891
C	8.774271	-1.274438	-3.224013
H	8.671678	-1.904691	-4.107905
H	9.298761	-0.352680	-3.497775
H	9.369345	-1.784115	-2.462348
C	6.510649	0.769132	1.115060
C	6.154635	-0.120758	2.243315
O	5.063912	-0.151258	2.807607
O	7.159680	-0.957035	2.543901
C	6.934037	-1.864875	3.654237
H	7.767234	-2.565346	3.629924
H	6.936703	-1.298769	4.588830
H	5.986950	-2.390370	3.538742
C	7.407910	1.819713	1.391895
C	7.751759	2.180633	2.733968
C	8.016301	2.568743	0.333534
C	8.615365	3.216945	3.010335
H	7.301351	1.645022	3.564131
C	8.902444	3.582859	0.599006
H	7.780624	2.311109	-0.689810
C	9.205918	3.925945	1.937902
H	8.838648	3.475848	4.037305
H	9.381189	4.141486	-0.197895
O	10.069768	4.936499	2.091005
C	10.449868	5.352447	3.418382
H	11.151906	6.172860	3.273581
H	9.577570	5.704082	3.976740

H	10.938422	4.533587	3.954202
O	3.971203	2.883096	1.907822
H	3.898093	2.536024	2.824576
H	3.853850	2.106373	1.328443
O	3.720598	1.699759	4.384730
H	2.795562	1.419065	4.326476
H	4.209887	0.956578	3.983982
C	-0.487038	-2.804965	0.846430
C	0.490866	-3.666819	0.370596
C	1.842208	-3.295184	0.460757
C	2.144091	-2.046761	1.018934
C	1.149543	-1.178261	1.494430
C	-0.188040	-1.575712	1.422486
H	0.198903	-4.616498	-0.067040
H	-0.987668	-0.935063	1.779680
O	-1.826593	-3.237007	0.782506
C	-2.656739	-2.545167	-0.037492
O	-2.334897	-1.629478	-0.770534
O	-3.875057	-3.056305	0.104821
H	3.169632	-1.714206	1.098376
C	2.874115	-4.262399	-0.102504
H	2.670934	-4.373383	-1.173385
H	2.696766	-5.250787	0.338533
C	4.386782	-3.959876	0.068957
C	5.178761	-5.029005	-0.720952
H	4.897856	-5.029391	-1.777587
H	6.255473	-4.843387	-0.647695
H	4.974920	-6.021248	-0.306337
C	4.711058	-2.608214	-0.578311
C	4.814370	-4.012154	1.542379
H	5.891226	-3.853473	1.639160
H	4.305285	-3.262472	2.150769
H	4.576077	-5.000000	1.948906
O	4.295066	-2.432245	-1.768392
O	5.367336	-1.746060	0.098658
C	1.531068	0.177390	2.043221
H	2.610025	0.203817	2.198734
H	1.068079	0.314723	3.028894
C	1.114738	1.391968	1.181012
H	0.036502	1.551888	1.285368
H	1.599186	2.264490	1.626172
C	1.406042	1.373330	-0.352509
C	1.649002	2.832980	-0.827969
H	2.523294	3.274083	-0.341057
H	1.801672	2.868151	-1.912104
H	0.772896	3.443523	-0.585421
C	0.211197	0.791153	-1.131809
H	0.358320	0.889125	-2.210131
H	0.051348	-0.263468	-0.902555
H	-0.697472	1.337757	-0.861881
C	2.691805	0.641836	-0.740135
O	2.711028	0.027141	-1.851989
O	3.712430	0.778647	0.024872
C	-4.918395	-2.436993	-0.720830

H	-4.645899	-2.582041	-1.770294
H	-4.935332	-1.365457	-0.503325
C	-6.214587	-3.092610	-0.366191
H	-6.280521	-4.148249	-0.626010
C	-7.501644	-2.315261	-0.482538
C	-6.957835	-2.686211	0.889651
H	-6.512396	-1.831940	1.395656
H	-7.385369	-1.259276	-0.726563
C	-7.520092	-3.726405	1.865799
H	-7.285596	-3.374091	2.875963
H	-6.988562	-4.677180	1.745533
C	-9.039177	-4.026124	1.821665
H	-9.274174	-4.670132	0.971438
H	-9.297828	-4.595803	2.720379
C	-9.898458	-2.803469	1.772407
C	-8.720919	-2.935175	-1.133305
H	-8.796302	-3.994274	-0.876004
H	-8.598497	-2.896338	-2.222364
C	-10.029290	-2.196440	-0.794295
H	-9.994434	-1.192461	-1.232603
H	-10.867918	-2.709811	-1.280472
C	-10.300987	-2.059494	0.674052
N	-15.925967	2.778927	-0.034255
C	-14.926904	3.852522	-0.379460
C	-15.729251	5.025522	-1.013114
O	-16.988401	4.953995	-0.890956
C	-13.807772	3.315751	-1.276160
C	-13.050315	2.169443	-0.644686
C	-12.193363	2.394983	0.443965
C	-13.224114	0.856942	-1.100500
C	-11.517025	1.342665	1.053963
C	-12.563257	-0.210108	-0.491406
C	-11.706019	0.039695	0.581198
O	-15.054480	5.933041	-1.552405
N	-11.029206	-1.039153	1.223971
H	-14.513008	4.205143	0.568655
H	-13.141226	4.158784	-1.473840
H	-14.237217	3.005536	-2.235066
H	-12.048579	3.407411	0.810739
H	-13.891450	0.663508	-1.935582
H	-10.843490	1.520366	1.884841
H	-12.722726	-1.225441	-0.836735
H	-15.950592	2.039162	-0.741679
H	-16.836874	3.281931	-0.053214
H	-15.749918	2.344750	0.873438
N	-11.070398	-1.143920	2.579292
N	-10.383209	-2.208867	2.902264
O	5.284243	4.375232	0.047814
H	4.857734	3.950468	0.820285
H	5.508446	3.608194	-0.508616

TS III-IV' 3-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3853.171944
Thermal and entropic correction, BS1 (a.u.)	1.025201
Electronic Energy, BS2 (a.u.)	-3854.619011
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-229.6i

Molecular Geometry in Cartesian Coordinates

Rh	4.145153	0.270710	-2.696483
Rh	5.452889	0.415974	-0.622926
O	4.355955	2.323475	-2.916448
O	5.473049	2.478723	-0.953078
C	4.919206	2.987597	-1.991220
C	4.913731	4.489182	-2.084736
H	4.117097	4.867421	-1.433946
H	5.862227	4.897302	-1.729095
H	4.718795	4.812182	-3.107898
O	5.929954	-0.040620	-3.713673
O	7.154619	0.134808	-1.806690
C	7.030743	-0.038127	-3.069535
C	8.300834	-0.219340	-3.858443
H	8.110614	-0.804497	-4.759769
H	8.669369	0.768197	-4.157713
H	9.067572	-0.700010	-3.248273
C	6.500105	0.513720	1.235855
C	6.431908	-0.806567	1.921483
O	5.517967	-1.283649	2.588378
O	7.534803	-1.515078	1.601097
C	7.646021	-2.840941	2.174685
H	8.472035	-3.316094	1.647345
H	7.872432	-2.758019	3.240800
H	6.726198	-3.406403	2.035356
C	7.653092	1.344132	1.530610
C	8.325370	1.253380	2.772585
C	8.139346	2.281582	0.587757
C	9.426077	2.042198	3.069311
H	7.964914	0.559050	3.526441
C	9.245432	3.064548	0.864024
H	7.641302	2.380245	-0.366645
C	9.896751	2.954641	2.106205
H	9.910266	1.947130	4.032956
H	9.627233	3.773660	0.136762
O	10.965746	3.768738	2.282556
C	11.691721	3.699362	3.519501
H	12.497679	4.428103	3.428668
H	11.051871	3.964379	4.367649

H	12.115251	2.701039	3.671628
O	5.108057	1.494334	2.383911
H	4.932654	1.081543	3.274811
H	4.327823	1.272932	1.822480
O	4.518610	0.230526	4.671587
H	3.550161	0.214823	4.643723
H	4.779338	-0.556610	4.156344
C	-0.506973	-2.829453	0.705242
C	0.353343	-3.522002	-0.134671
C	1.721691	-3.208098	-0.132457
C	2.158580	-2.187685	0.721431
C	1.281023	-1.486565	1.563389
C	-0.074862	-1.827076	1.564503
H	-0.045065	-4.294035	-0.785831
H	-0.789023	-1.308501	2.196073
O	-1.869114	-3.194600	0.700860
C	-2.702057	-2.382542	0.003897
O	-2.373271	-1.378498	-0.599516
O	-3.927160	-2.888190	0.098297
H	3.201546	-1.905816	0.749423
C	2.616015	-3.968081	-1.102018
H	2.268923	-3.736502	-2.115266
H	2.438996	-5.041549	-0.964267
C	4.154163	-3.758906	-1.065815
C	4.765805	-4.549991	-2.246899
H	4.343888	-4.226694	-3.202225
H	5.851522	-4.410810	-2.281623
H	4.562966	-5.618322	-2.121544
C	4.473346	-2.278904	-1.315926
C	4.771514	-4.271023	0.242433
H	5.861616	-4.207528	0.198826
H	4.432646	-3.710862	1.115705
H	4.498632	-5.321641	0.382962
O	3.938706	-1.754827	-2.346431
O	5.240836	-1.668036	-0.497835
C	1.807816	-0.361794	2.424882
H	2.895773	-0.435753	2.460050
H	1.453972	-0.496703	3.454678
C	1.410926	1.077310	2.000798
H	0.399898	1.292142	2.362354
H	2.079066	1.749648	2.550382
C	1.420715	1.478936	0.493947
C	1.679983	3.009426	0.406426
H	2.653877	3.272747	0.831796
H	1.652012	3.350259	-0.633882
H	0.902371	3.542519	0.963267
C	0.082856	1.154594	-0.194666
H	0.062511	1.552995	-1.212258
H	-0.098883	0.080624	-0.245981
H	-0.737309	1.611841	0.367092
C	2.580946	0.871539	-0.282953
O	2.448600	0.644826	-1.524317
O	3.675697	0.713518	0.362920
C	-4.969227	-2.166774	-0.641227

H	-4.651994	-2.095884	-1.685517
H	-5.049774	-1.158271	-0.225783
C	-6.241463	-2.936174	-0.483018
H	-6.228850	-3.930703	-0.926608
C	-7.560502	-2.209093	-0.549626
C	-7.082084	-2.793904	0.769677
H	-6.722834	-2.029688	1.455921
H	-7.487884	-1.122662	-0.600886
C	-7.657198	-4.021892	1.484050
H	-7.400521	-3.921464	2.543850
H	-7.151216	-4.929054	1.135704
C	-9.185877	-4.275276	1.389351
H	-9.420988	-4.795595	0.457607
H	-9.469634	-4.954219	2.199917
C	-10.028763	-3.044655	1.484288
C	-8.717281	-2.760344	-1.356202
H	-8.771375	-3.846639	-1.252148
H	-8.542477	-2.563238	-2.420568
C	-10.063310	-2.108614	-0.982576
H	-10.047488	-1.059286	-1.296997
H	-10.867439	-2.585179	-1.556642
C	-10.388597	-2.157855	0.480911
N	-16.018426	2.670500	-0.125430
C	-15.030111	3.805898	-0.063545
C	-15.773286	5.080146	-0.557645
O	-17.032889	4.980183	-0.641211
C	-13.758146	3.487328	-0.853715
C	-13.044818	2.253157	-0.350921
C	-12.262484	2.305484	0.812801
C	-13.185753	1.024609	-1.008528
C	-11.621776	1.169018	1.298050
C	-12.563931	-0.126786	-0.525309
C	-11.775215	-0.047130	0.623899
O	-15.059343	6.082548	-0.795033
N	-11.129974	-1.211806	1.136259
H	-14.790235	3.946507	0.993905
H	-13.115753	4.366781	-0.769508
H	-14.018087	3.370313	-1.911747
H	-12.142527	3.250353	1.335567
H	-13.794025	0.964034	-1.906896
H	-11.002109	1.216525	2.186449
H	-12.702104	-1.076781	-1.029024
H	-15.941970	2.156645	-1.008604
H	-16.944048	3.139790	-0.110941
H	-15.912611	2.003179	0.641306
N	-11.218616	-1.495263	2.463645
N	-10.548816	-2.600460	2.665984
O	5.265067	4.056547	1.359636
H	5.232825	3.282008	1.951255
H	5.378116	3.615504	0.497125

Intermediate IV' 3-water

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-3853.187381
Thermal and entropic correction, BS1 (a.u.)	1.028739
Electronic Energy, BS2 (a.u.)	-3854.632898
Number of Imaginary Frequencies	1
Imaginary frequencies (cm^{-1})	-2.1i

Molecular Geometry in Cartesian Coordinates

Rh	4.151133	0.363689	-2.628982
Rh	5.423504	0.370677	-0.545925
O	4.456534	2.419305	-2.747966
O	5.590916	2.439958	-0.786485
C	5.078851	3.014833	-1.813817
C	5.220629	4.511058	-1.881113
H	4.591988	4.956073	-1.102546
H	6.255969	4.794469	-1.675173
H	4.911499	4.890269	-2.855461
O	5.924305	0.039024	-3.650414
O	7.127366	0.070233	-1.723875
C	7.016392	-0.034681	-2.992611
C	8.286574	-0.220960	-3.780120
H	8.095909	-0.806981	-4.681053
H	8.653318	0.766043	-4.084010
H	9.052974	-0.700442	-3.169101
C	6.334573	0.501041	1.567997
C	6.643344	-0.908135	1.820216
O	5.893074	-1.731947	2.366688
O	7.846653	-1.272682	1.323267
C	8.199694	-2.665264	1.457338
H	9.212599	-2.744842	1.063306
H	8.176926	-2.971360	2.505755
H	7.519882	-3.290310	0.875383
C	7.419307	1.520332	1.727057
C	7.422637	2.421241	2.802231
C	8.474233	1.615360	0.798363
C	8.425396	3.382502	2.956882
H	6.633020	2.381354	3.544089
C	9.483813	2.558669	0.946324
H	8.496177	0.949141	-0.054495
C	9.466284	3.453941	2.025824
H	8.383501	4.056239	3.803993
H	10.292871	2.622094	0.224817
O	10.504267	4.352887	2.081397
C	10.555903	5.239924	3.201521
H	11.459189	5.837571	3.068973
H	9.683975	5.904246	3.229471

H	10.622394	4.687347	4.146183
O	5.167527	0.907192	2.384071
H	5.012928	0.408534	3.318336
H	4.341949	0.841672	1.808714
O	4.823314	-0.376703	4.464875
H	3.865103	-0.473454	4.587025
H	5.104230	-1.190638	3.993096
C	-0.497059	-3.123082	0.751826
C	0.340865	-3.717636	-0.181836
C	1.693615	-3.346906	-0.228013
C	2.135323	-2.371803	0.674163
C	1.282696	-1.775365	1.613173
C	-0.056396	-2.173686	1.664658
H	-0.065660	-4.451497	-0.871054
H	-0.756884	-1.727878	2.363466
O	-1.854534	-3.508379	0.776527
C	-2.684814	-2.747237	0.019974
O	-2.348124	-1.792389	-0.654835
O	-3.915200	-3.232052	0.149266
H	3.163941	-2.041320	0.664646
C	2.571548	-3.982726	-1.294749
H	2.209841	-3.638503	-2.270433
H	2.403134	-5.066071	-1.279373
C	4.108182	-3.762743	-1.247519
C	4.724079	-4.458203	-2.485038
H	4.286452	-4.078579	-3.412258
H	5.806440	-4.294990	-2.519193
H	4.543608	-5.536532	-2.432604
C	4.415502	-2.264075	-1.387358
C	4.727550	-4.369591	0.019746
H	5.818207	-4.313557	-0.018743
H	4.396336	-3.873376	0.933126
H	4.447451	-5.425855	0.083386
O	3.883942	-1.670408	-2.382727
O	5.167598	-1.706043	-0.521110
C	1.816413	-0.668572	2.489892
H	2.906807	-0.726716	2.485436
H	1.500784	-0.831563	3.527494
C	1.373541	0.768897	2.105551
H	0.373777	0.953280	2.513107
H	2.048871	1.452189	2.632834
C	1.302882	1.203396	0.611789
C	1.308733	2.756239	0.583560
H	2.230927	3.158940	1.013335
H	1.212373	3.126059	-0.442053
H	0.460254	3.130966	1.165311
C	0.024695	0.705143	-0.092940
H	-0.099163	1.200257	-1.059600
H	0.039933	-0.370367	-0.265088
H	-0.848432	0.939323	0.523292
C	2.530868	0.794995	-0.192458
O	2.436898	0.684506	-1.450615
O	3.636249	0.648056	0.445107
C	-4.943826	-2.535594	-0.633594

H	-4.670688	-2.618024	-1.689672
H	-4.936632	-1.480418	-0.347334
C	-6.259470	-3.178193	-0.332184
H	-6.346522	-4.217052	-0.647441
C	-7.520370	-2.358331	-0.444179
C	-7.026408	-2.811301	0.921766
H	-6.571327	-1.996471	1.481343
H	-7.366079	-1.295956	-0.633275
C	-7.648854	-3.879523	1.828883
H	-7.434927	-3.583916	2.861518
H	-7.142468	-4.839579	1.677565
C	-9.174472	-4.130499	1.727513
H	-9.403559	-4.726123	0.841177
H	-9.474228	-4.734874	2.590068
C	-9.995696	-2.880998	1.715994
C	-8.738166	-2.907354	-1.157432
H	-8.853787	-3.974178	-0.953518
H	-8.583333	-2.820732	-2.239571
C	-10.031250	-2.142974	-0.818013
H	-9.953351	-1.121880	-1.208467
H	-10.872040	-2.606154	-1.348807
C	-10.338678	-2.066825	0.647596
N	-15.793713	2.835666	-0.436619
C	-14.787948	3.955182	-0.370022
C	-15.492071	5.229354	-0.918575
O	-16.752857	5.158273	-1.011411
C	-13.495572	3.587682	-1.102766
C	-12.822460	2.367557	-0.516693
C	-12.025058	2.477344	0.632411
C	-13.026272	1.097573	-1.071911
C	-11.430677	1.355506	1.203070
C	-12.451992	-0.038480	-0.501603
C	-11.647052	0.097553	0.631078
O	-14.750498	6.204985	-1.181652
N	-11.046041	-1.049329	1.230125
H	-14.582821	4.119437	0.691563
H	-12.842588	4.460506	-1.034758
H	-13.723510	3.427439	-2.162805
H	-11.857772	3.454739	1.076398
H	-13.646891	0.992724	-1.957825
H	-10.798608	1.446147	2.079265
H	-12.636058	-1.018685	-0.926651
H	-15.716530	2.320120	-1.319002
H	-16.712825	3.315697	-0.431596
H	-15.703216	2.167203	0.331200
N	-11.131673	-1.223477	2.576379
N	-10.492834	-2.328267	2.861617
O	4.692902	3.764231	1.552722
H	4.729285	3.051605	2.205857
H	5.066215	3.336716	0.758991

H2O

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-76.430550
Thermal and entropic correction, BS1 (a.u.)	0.003490
Electronic Energy, BS2 (a.u.)	-76.475784
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

O	0.000000	0.000000	0.120477
H	0.000000	0.756452	-0.481907
H	0.000000	-0.756452	-0.481907

Styrene (2)

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-309.663901
Thermal and entropic correction, BS1 (a.u.)	0.102849
Electronic Energy, BS2 (a.u.)	-309.775529
Number of Imaginary Frequencies	0
Imaginary frequencies (cm^{-1})	None

Molecular Geometry in Cartesian Coordinates

C	2.264409	0.266598	-0.000002
C	1.783705	-1.044455	0.000001
C	0.408766	-1.285702	0.000002
C	-0.515565	-0.225150	0.000002
C	-0.014877	1.091814	0.000002
C	1.356949	1.332680	-0.000001
H	3.333391	0.458467	-0.000004
H	2.477555	-1.880326	0.000004
H	0.041176	-2.308842	0.000001
H	-0.701765	1.932708	0.000006
H	1.722078	2.355858	-0.000004
C	-1.956037	-0.536019	-0.000003
H	-2.190806	-1.600175	-0.000005
C	-2.970764	0.339077	-0.000001

H	-2.820835	1.415465	0.000006
H	-4.000312	-0.006213	0.000000

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