Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Solvent-Free Hydrogenation of Levulinic Acid to γ-Valerolactone using a Shvo Catalyst precursor: Optimization, Mechanistic Insights, and Life Cycle Assessment

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1. Experimental procedures

1.1. Materials and Methods

Levulinic acid (99% pure), triruthenium dodecacarbonyl (99% pure), tetraphenylcyclopentadienone (98% pure), and N-methyl-N-trimethylsilyl-trifluoro acetamide (≥98.5% pure) were purchased from Sigma Aldrich. The acetonitrile-appended Knölker-type catalyst (**Fe-2**) was used from the batch, that was synthesized in our earlier work.[27] All other chemicals were purchased from miscellaneous sources. Standard Schlenk techniques were applied for preparations involving inert atmosphere and/or vacuum. Unless otherwise stated, all commercial chemicals were used without further purification. Hydrogenation reactions were performed in a 5500 HP compact 100 ml autoclave from *Parr Instrument Company.* NMR spectra were recorded on a Bruker AVANCE-300 Ultra Shield spectrometer (300 MHz) at 298 K. GC measurements were performed by using a Shimadzu 2010 Plus gas chromatograph equipped with a Supelco SLB-5 column (length = 30 m, internal diameter = 0.32 mm, and film thickness = 0.50 μm), and with a flame ionization detector. GC method: 2 minutes isothermal at 60 °C; then 10°C min^{-1} to 300°C.

1.2. Catalyst synthesis

The spectroscopic analysis of all synthesized complexes is in accordance with reported data.[22,29,57,64,65]

$[Ph_4(\eta_4\text{-}C_4CO)]Ru^0(CO)_3$ (**Ru-1**).
In a dried 100 mL Schlenk a solution of 1.60 g (2.50 mmol) triruthenium dodecacarbonyl and 2.89 g (7.51 mmol) 2,3,4,5-tetraphenyl-cyclopentadienone in 60 mL dry toluene was refluxed at 110°C for 48 hours under a nitrogen atmosphere. The resulting yellow mixture was concentrated *in vacuo*, and purified by column chromatography on silica using dichloromethane first to elute unreacted ligand, then hexane/ethyl acetate (70:30) to obtain **Ru-1**. The product material was obtained as a pale yellow solid in 4.19 g yield (98%).

$\{[Ph_4(\eta_5\text{-}C_4CO)]_2H\}(Ru^{II})_2(CO)_4(m\text{-}H)$ (**Ru-2**).
In a dried 100 mL Schlenk a suspension of 213 mg (0.333 mmol) triruthenium dodecacarbonyl and 385 mg (1.00 mmol) 2,3,4,5-tetraphenyl-cyclopentadienone in 50 mL methanol was refluxed at 65°C for 48 hours under a nitrogen atmosphere. The resulting yellow-orange mixture was stored in the freezer at -20°C for 64 hours. Bright orange crystals were isolated by decantation, washing with 2x 3 mL cold methanol, and drying *in vacuo*. A yield of 276 mg (51%) was obtained.

$\{[Ph_4(\eta_4\text{-}C_4CO)]Ru^0(CO)_2\}_2$ (**Ru-3**).
In a dried 100 mL Schlenk a suspension of 213 mg (0.333 mmol) triruthenium dodecacarbonyl and 385 mg (1.00 mmol) 2,3,4,5-tetraphenyl-cyclopentadienone in 70 mL dry heptane was refluxed at 100°C for 72 hours under a nitrogen atmosphere. The resulting yellow-orange mixture was stored in the freezer at -20°C for 36 hours. Orange crystals were isolated by decantation, washing with 2x 3 mL cold methanol, and drying *in vacuo*. A yield of 340 mg (63%) was obtained.

1.3. Hydrogenation experiments

H_2-mediated hydrogenation:
A typical experiment was conducted by charging a 100 mL *Parr* autoclave with 50 g (431 mmol) of molten LA and a desired amount of catalyst. The reactor was sealed subsequently, and purged with 5x 2.5 bar N_2 and 3x 10 bar H_2. The H_2 pressure was increased to a value of approximately 10 bar below the target pressure and the reactor was heated to the desired reaction temperature in about 15 minutes (temperature overshoot not more than 5 °C). After the reaction temperature was reached, the H_2 pressure was adjusted to the desired value. The stirring speed was kept at 1000 rpm throughout all reactions. After 5 hours, the reaction was stopped by allowing the reactor to cool down to 40 °C within 1 - 1.5 hours. During cooling the supply of H_2 gas was discontinued, but the remaining H_2 pressure inside the reactor was not released. Samples were collected at various time intervals for GC-fid analysis.

FA-mediated transfer hydrogenation:
In a reflux setup under a N_2 atmosphere 23.2 g (200 mmol) LA and 109 mg (1.0 mmol) **Ru-2** were dissolved in 23.0 g formic acid (500 mmol). The reaction mixture was heated to 100°C for 6 hours, during which the CO_2 by-product was released *via* a needle-pierced septum on top of the reflux cooler.

IPA-mediated transfer hydrogenation:
A typical reaction was prepared by dissolving 23.2 g (200 mmol) LA and 114 mg (2.0 mmol) **Ru-1** in 30.0 g isopropyl alcohol (500 mmol) in a 100 mL *Parr* autoclave. The reactor was sealed, and purged with 5x 2.5 bar N_2. The system was then pressurized with 2.5 bar N_2, and the reactor was heated to the desired reaction temperature while stirring at 1000 rpm. The reactions were allowed to continue, until complete conversion was observed, based on GC-fid analysis of the collected samples.

1.4. GC analysis

GC samples were prepared by dissolving aliquots (11.6 mg) of the kinetic samples and the final reaction mixture in 1.00 mL of a 0.1 v% hexadecane (external standard) solution in dichloromethane. An excess of 50 μL of N-methyl-N-trimethylsilyl-trifluoro acetamide was added for derivatization of unreacted LA; complete derivatization was always confirmed by the absence of the signal for free LA in the GC-fid analyses. GVL concentrations were calibrated against hexadecane for quantification. Turn-over frequencies were calculated for the linear range in the kinetic plots.

1.5. Catalyst recycling

For catalyst recycling experiments no samples were collected during the reaction with exception of the final reaction mixture. The crude reaction mixture was subjected to vacuum distillation with a strict N_2 atmosphere regulation. First, the H_2O side product was distilled at 50°C and 40 mbar pressure. Next, GVL was distilled at 90 °C at 1 mbar pressure. A clear distillate was obtained, and the catalyst remained as a viscous orange residue. A fresh loading of 50 g LA was added to dissolve this residue for catalyst reuse.

1.6. Computational experiments

Calculations for all chemical geometries were performed by using the Gaussian 09 software package. Optimizations were performed at the level of DFT by means of the hybrid B3LYP[37] functional and the basis set LANL2DZ[38] was employed for all elements. All calculations were performed without freezing any atom. Frequency calculations were performed for all stationary points at the same level to identify the minima (zero imaginary frequencies) and transition states (TS, only one imaginary frequency) and to provide free energies at 298.15 K and 1 atm.

1.7. Life Cycle Assessment

Modelling of all the acquired data was performed using the Simapro V8 (PRé consultant, NL) software. Environmental impacts were calculated using the IMPACT 2002+ V2.14 method,[66] and climate change impacts were calculated using the IPCC GWP 100a mid-point method.[67] Secondary data for common chemicals were gathered from the ecoinvent v3.2 database (ecoinvent Centre, St-Gallen, Switzerland).

Data acquisition and processing:

The LCI described above is divided in the following data categories, in the order of importance:

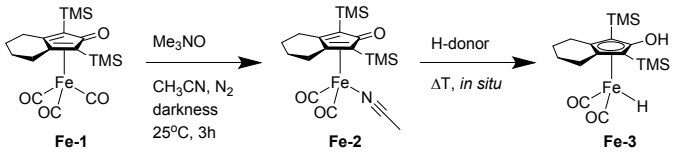
1. Primary data from laboratory-scale experiments, conducted in this work. This includes the syntheses of the Shvo catalyst precursors as in Section 2.1 (*i.e.* 'reactions a, b, and c' within the total retrosynthesis in Scheme 8), the (transfer) hydrogenation reactions described in Section 2.4 (Figure 7), and the applied GVL isolation / catalyst recycling methodology described in Section 2.3. The electricity consumptions of equipment used in this work were recorded in real-time using a *Voltcraft Energy Logger 4000* device, while those for all literature procedures were mimicked in our hands using comparable equipment and methodologies (See Supporting Information). Cooling water consumption was always set on 5 L, since we always applied a water circulation pump for that purpose.Gas consumptions were determined, based on the applied reaction system volumes in all reactions, in conjunction with the ideal gas law.

2. Secondary data were modelled on the basis of laboratory-scale synthesis, found in literature procedures (*i.e.* reactions d – l of the catalyst retrosynthesis in Scheme 8).

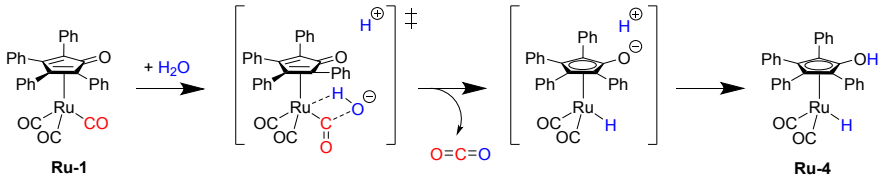
3. Secondary data from the ecoinvent v3.2 database (ecoinvent Centre, St-Gallen, Switzerland) was applied for modelling the use of common chemicals, such as solvents, gases, inorganic salts, acids and bases, and also the starting synthons for the ligand of the Shvo catalyst: benzaldehyde and benzyl chloride. These data were preferably obtained from the global market, otherwise from the European market. Similarly, the environmental impact for the electricity production is calculated as an average of the European energy grid mix with low voltage. The environmental impact for mining, purifying, and refining the ruthenium metal could only be obtained for the impact category of global warming potential (GWP).

4. Data from chemicals unavailable in the ecoinvent database were replaced by alternative chemicals with equivalent functions (*i.e.* potassium bicarbonate → ammonium bicarbonate; mesitylene → xylene).

5. Suppressed data, that are regarded as negligible conform a cut-off threshold of <0.1 wt% of the total chemical input of the corresponding chemical reaction (*i.e.* a Ir-Re plug-flow used for triethylamine synthesis, applied in reaction j[63c] of the catalyst retrosynthesis in Scheme 8).



Scheme S1.1: Pre-activation of Knölker's complex into the acetonitrile adduct, and *in situ* formation of Casey's catalyst.



Scheme S1.2: Proposed mechanism for the water-mediated activation of Ru-1.

2. Kinetic Studies of Hydrogenation Reactions

Table S2.1: **Numerical GC-yields of GVL obtained from temperature optimization experiments using 0.1% Ru-1 at 50 bar H_2 pressure.**

	GVL yields (%) [a]			
Time (min)	**T = 100°C**	**T = 120°C**	**T = 140°C**	**T = 160°C**
15	0.3	0.4	0.2	1.1
30	0.9	4.2	17.0	12.6
45	2.7	20.8	55.2	43.2
60	5.7	38.2	77.2	73.0
90	10.9	62.3	94.1	77.4
120	17.6	81.2	96.7	77.8
180	30.0	94.4	97.5	78.2
240	44.8	98.7	97.7	78.5
300	58.8	99.8	97.6	78.6
end	63.0	99.7	97.3	78.8
TOF[b] ($h^{-1} \cdot [Ru]^{-1}$)	144	598	1209	1204

[a] All GVL yields were determined by GC-fid analysis, and calibrated against hexadecane external standard.
[b] All TOF values were determined for the linear parts of the corresponding kinetic curves.

Table S2.2: **Numerical GC-yields of GVL obtained from pressure optimization experiments using 0.1% Ru-1 at 120°C.**

	GVL yields (%) [a]				
Time (min)	**P_{H2} = 20 bar**	**P_{H2} = 40 bar**	**P_{H2} = 50 bar**	**P_{H2} = 60 bar**	**P_{H2} = 100 bar**
15	0.0	0.2	0.4	0.2	0.1
30	1.3	4.7	4.2	5.1	8.9
45	5.5	13.4	20.8	17.8	24.2
60	10.5	24.6	38.2	34.9	40.6
90	27.5	50.7	62.3	62.1	65.9
120	48.0	70.6	81.2	80.2	81.8
180	75.2	88.1	94.4	94.3	92.4
240	90.7	97.0	98.7	98.0	98.8
300	97.1	99.0	99.8	99.4	99.5
end	97.7	99.1	99.7	99.6	99.6
TOF[b] ($h^{-1} \cdot [Ru]^{-1}$)	376	465	598	512	570

[a] All GVL yields were determined by GC-fid analysis, and calibrated against hexadecane external standard.
[b] All TOF values were determined for the linear parts of the corresponding kinetic curves.

Table S2.3: **Numerical GC-yields of GVL obtained from catalyst loading optimization experiments using Ru-1 at 120°C and 50 bar H_2 pressure.**

	GVL yields (%) [a]			
Time (min)	**0.2% Ru**	**0.1% Ru**	**0.05% Ru**	**0.02% Ru**
15	5.0	0.4	0.0	0.2
30	22.4	4.2	2.0	1.0
45	50.8	20.8	9.0	4.8
60	64.6	38.2	15.0	10.0
90	N/A	62.3	34.0	21.2
120	96.3	81.2	52.0	33.0
180	99.7	94.4	75.0	50.5
240	99.9	98.7	88.0	62.1
300	N/A	99.8	93.0	69.2
end	99.9	99.7	94.1	69.7
TOF[b] ($h^{-1} \cdot [Ru]^{-1}$)	414	598	740	1019

[a] All GVL yields were determined by GC-fid analysis, and calibrated against hexadecane external standard.
[b] All TOF values were determined for the linear parts of the corresponding kinetic curves.

Table S2.4: **Numerical GC-yields of GVL obtained from experiments regarding the retrospective catalyst screening using 0.1% [Ru] at 120°C and 50 bar H_2 pressure.**

	GVL yields (%) [a]		
Time (min)	**Ru-1**	**Ru-2**	**Ru-3**
15	0.4	6.8	5.7
30	4.2	26.1	23.9
45	20.8	46.6	41.3
60	38.2	59.2	56.4
90	62.3	78.3	75.2
120	81.2	90.4	88.9
180	94.4	98.0	97.8
240	98.7	99.5	99.1
300	99.8	99.7	99.8
end	99.7	99.6	99.1
TOF[b] ($h^{-1} \cdot [Ru]^{-1}$)	598	711	678

[a] All GVL yields were determined by GC-fid analysis, and calibrated against hexadecane external standard.
[b] All TOF values were determined for the linear parts of the corresponding kinetic curves.

Table S2.5: **Numerical GC-yields of GVL obtained from the experiment using 0.005% Ru-1 at 120°C and 50 bar H_2 pressure.**

Time (h)	GVL yields (%) [a]
1	2.4
2	8.9
3	17.6
4	24.8
6	33.9
8	39.6
10	42.7
24	44.5
28	45.2
32	45.7
TOF[b] ($h^{-1} \cdot [Ru]^{-1}$)	1517

[a] All GVL yields were determined by GC-fid analysis, and calibrated against hexadecane external standard.
[b] All TOF values were determined for the linear parts of the corresponding kinetic curves.

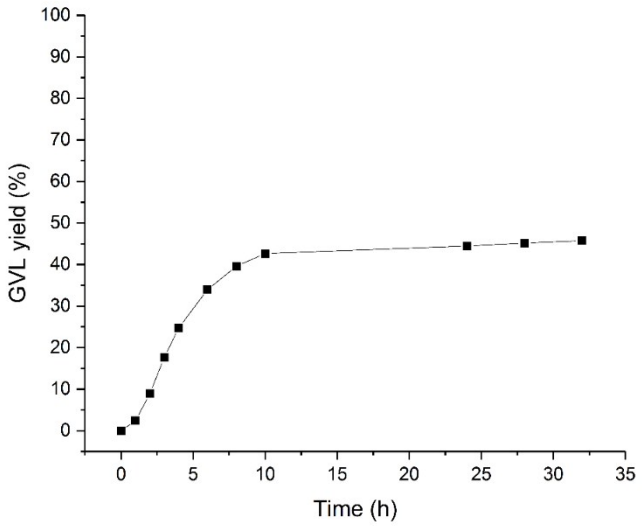


Figure S2.1: **Long-term LA hydrogenation experiment using 0.005% Ru-1 at 120°C and 50 bar H_2 pressure.**

Table S2.6: **Numerical GC-yields of GVL obtained from LA and EL hydrogenation experiments using 0.1% Ru-1.**

	GVL yields (%) [a]	
Time (min)	**LA**	**EL**
15	0.4	0.5
30	4.2	5.8
45	20.8	18.3
60	38.2	33.8
90	62.3	63.3
120	81.2	80.0
180	94.4	96.8
240	98.7	98.8
300	99.8	98.9
end	99.7	0.5
TOF[b] ($h^{-1} \cdot [Ru]^{-1}$)	598	580

[a] All GVL yields were determined by GC-fid analysis, and calibrated against hexadecane external standard.
[b] All TOF values were determined for the linear parts of the corresponding kinetic curves.

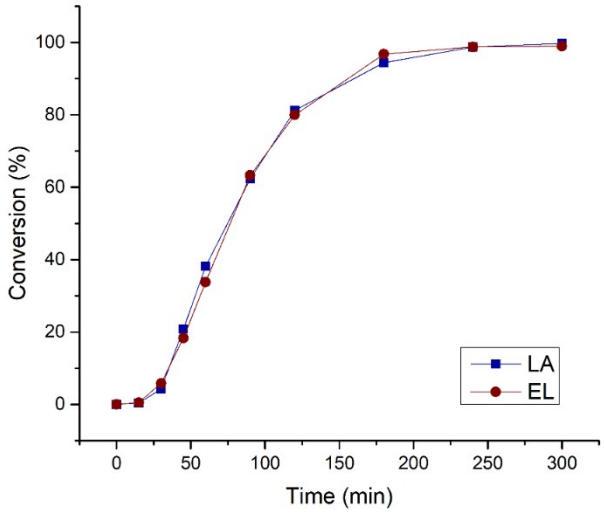


Figure S2.2: **Comparison of the kinetic reaction profiles for EL hydrogenation versus LA hydrogenation using 0.1% Ru-1 at 120°C and 50 bar H_2 pressure.**

Table S2.7: **Numerical GC-yields of GVL obtained from (transfer) hydrogenation experiments using 0.1% Ru-1.**

	GVL yields (%) [a]				
Time	**FA; 100°C** [c]	**IPA; 100°C**	**IPA ;120°C**	**H_2; 100°C**	**H_2; 120°C**
15 min	3.8	-	-	-	0.4
30 min	15.9	-	-	-	4.2
45 min	28.9	-	-	-	20.8
60 min	43.5	-	22.1	6.4	38.2
90 min	65.3	-	-	-	62.3
2 h	79.8	14.0	46.1	16.6	81.2
3 h	94.1	-	65.1	28.1	94.4
4 h	98.0	29.2	76.7	44.5	98.7
5 h	99.3	-	83.2	60.8	99.8
6 h	99.7	43.0	88.2	72.2	-
7 h	-	-	91.0	79.8	-
8 h	-	53.0	93.0	84.3	-
9 h	-	-	94.7	88.2	-
10 h	-	61.0	96.2	91.6	-
11 h	-	-	97.7	95.0	-
12 h	-	65.7	98.9	97.3	-
14 h	-	72.1	-	-	-
16 h	-	76.5	-	-	-
18 h	-	80.2	-	-	-
20 h	-	83.8	-	-	-
22 h	-	88.7	-	-	-
24 h	-	90.8	-	-	-
26 h	-	91.7	-	-	-
28 h	-	94.1	-	-	-
30 h	-	95.8	-	-	-
32 h	-	97.3	-	-	-
TOF[b] ($h^{-1} \cdot [Ru]^{-1}$)	400	81	257	144	598

[a] All GVL yields were determined by GC-fid analysis, and calibrated against hexadecane external standard.
[b] All TOF values were determined for the linear parts of the corresponding kinetic curves.
[c] **Ru-2** was used, because **Ru-1** could not be activated in this reaction.

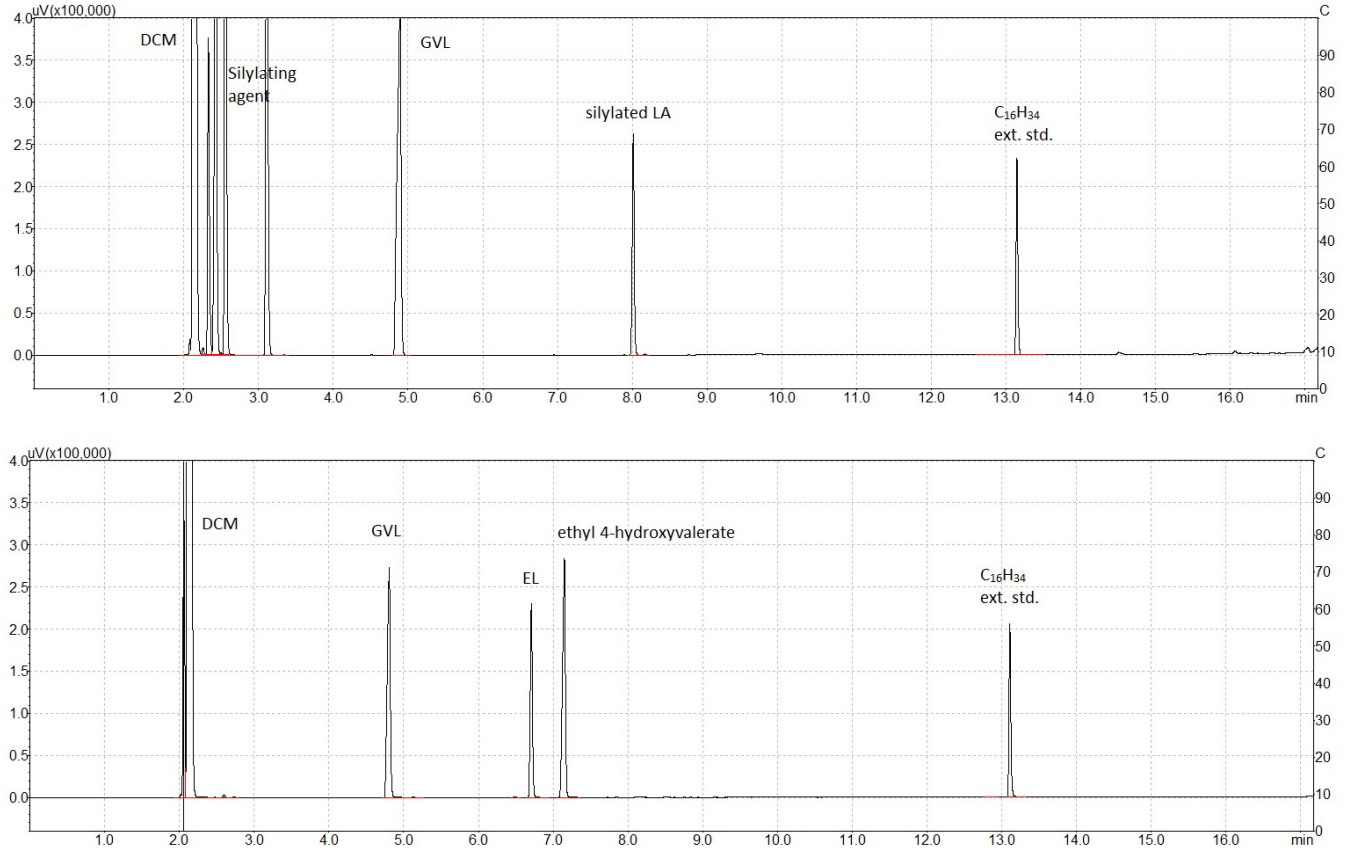


Figure S2.3: **Representative GC-chromatograms of LA hydrogenation (top) and EL hydrogenation (bottom).**

3. Catalyst recycling studies

Figure S3.1: Photograph of Ru-1.

Figure S3.2: Photograph of Ru-2.

Figure S3.3: Photograph of Ru-3.

Figure S3.4: Photograph of recycled catalyst.

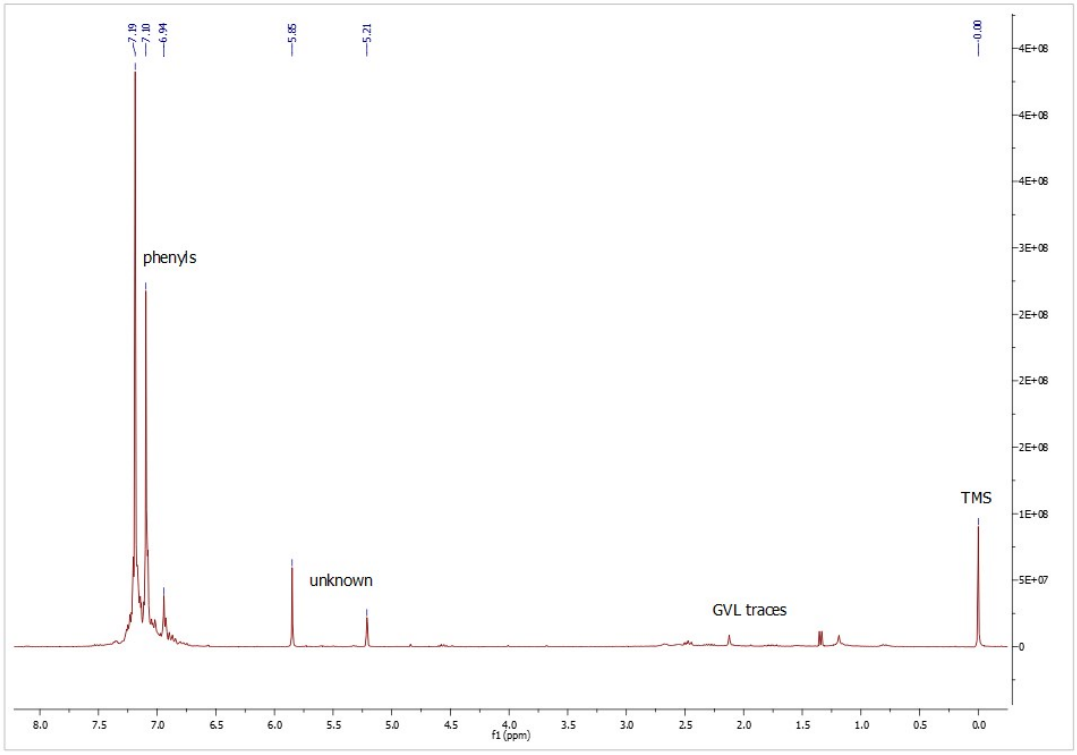


Figure S3.5: **^{1}H-NMR spectrum of the recycled Shvo catalyst from LA hydrogenation.**

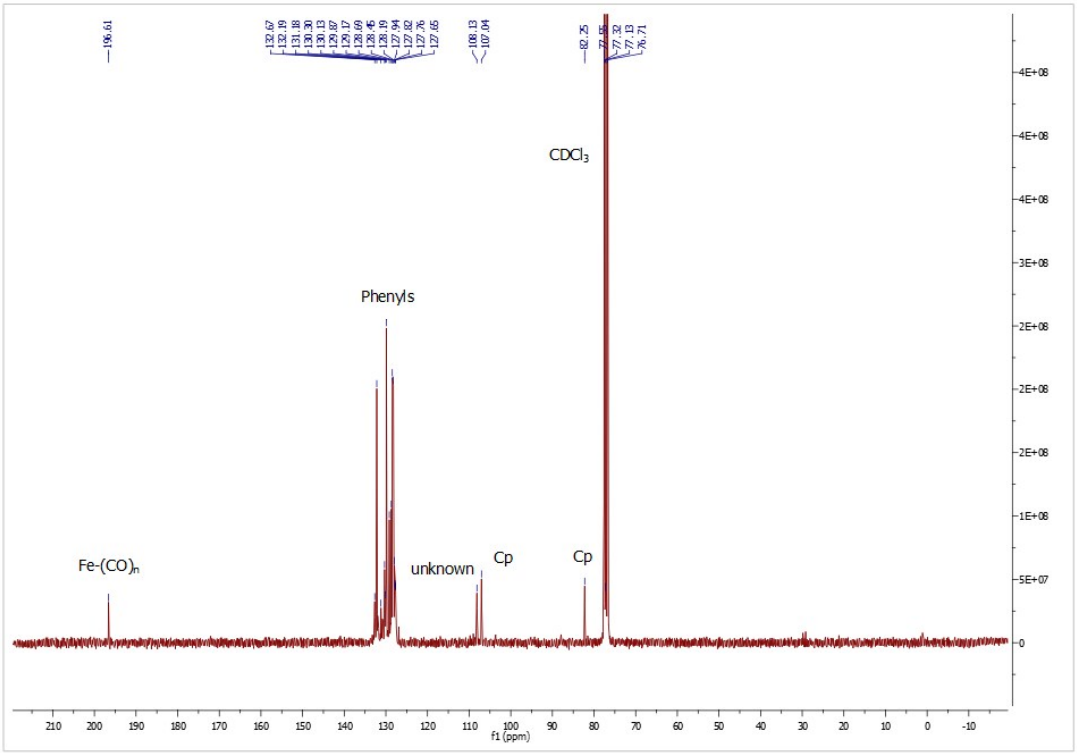


Figure S3.6: **^{13}C-NMR spectrum of the recycled Shvo catalyst from LA hydrogenation.**

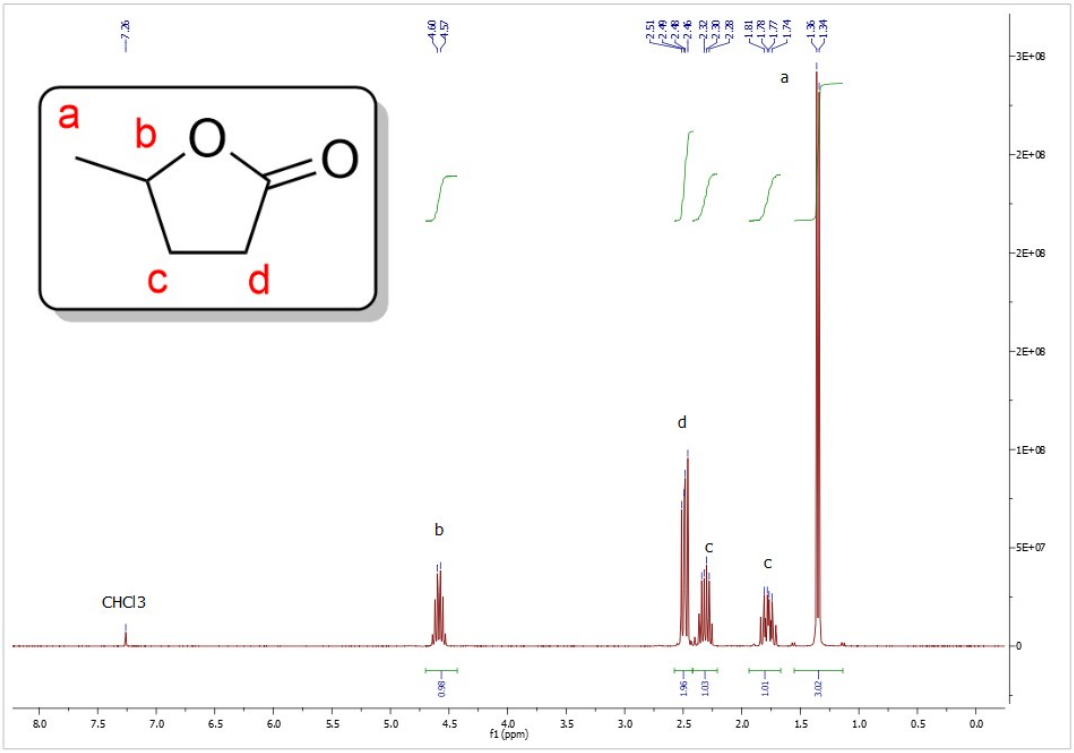


Figure S3.7: ^{1}H-NMR spectrum of isolated GVL product.

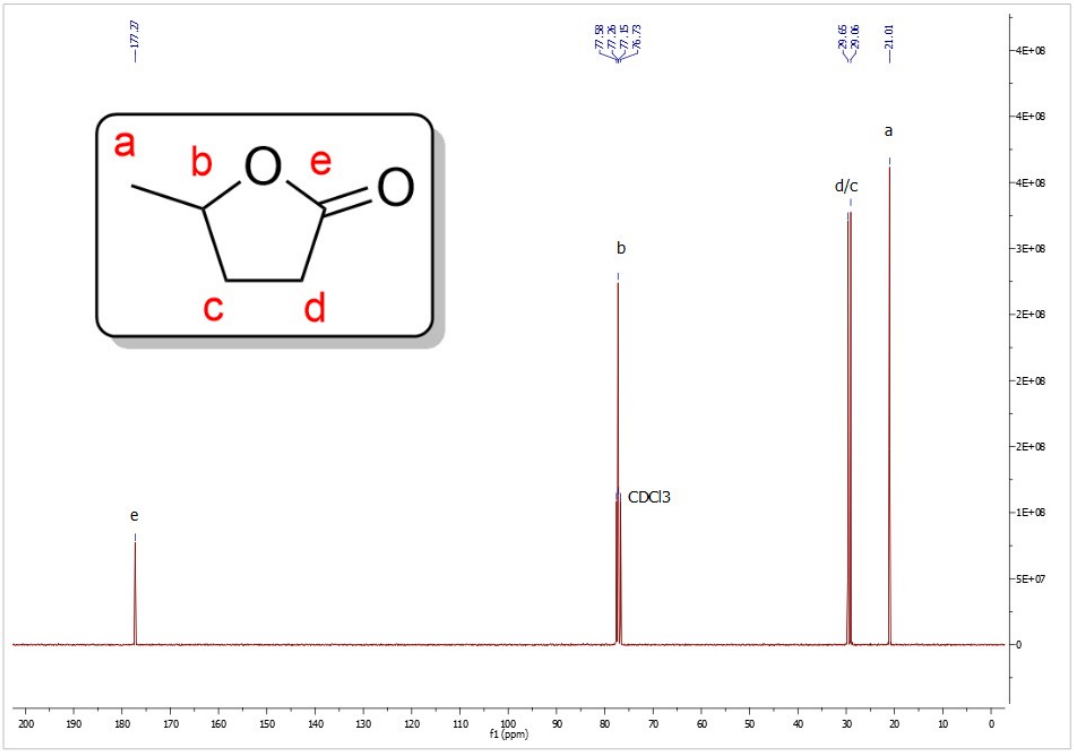


Figure S3.8: ^{13}C-NMR spectrum of isolated GVL product.

4. DFT calculations

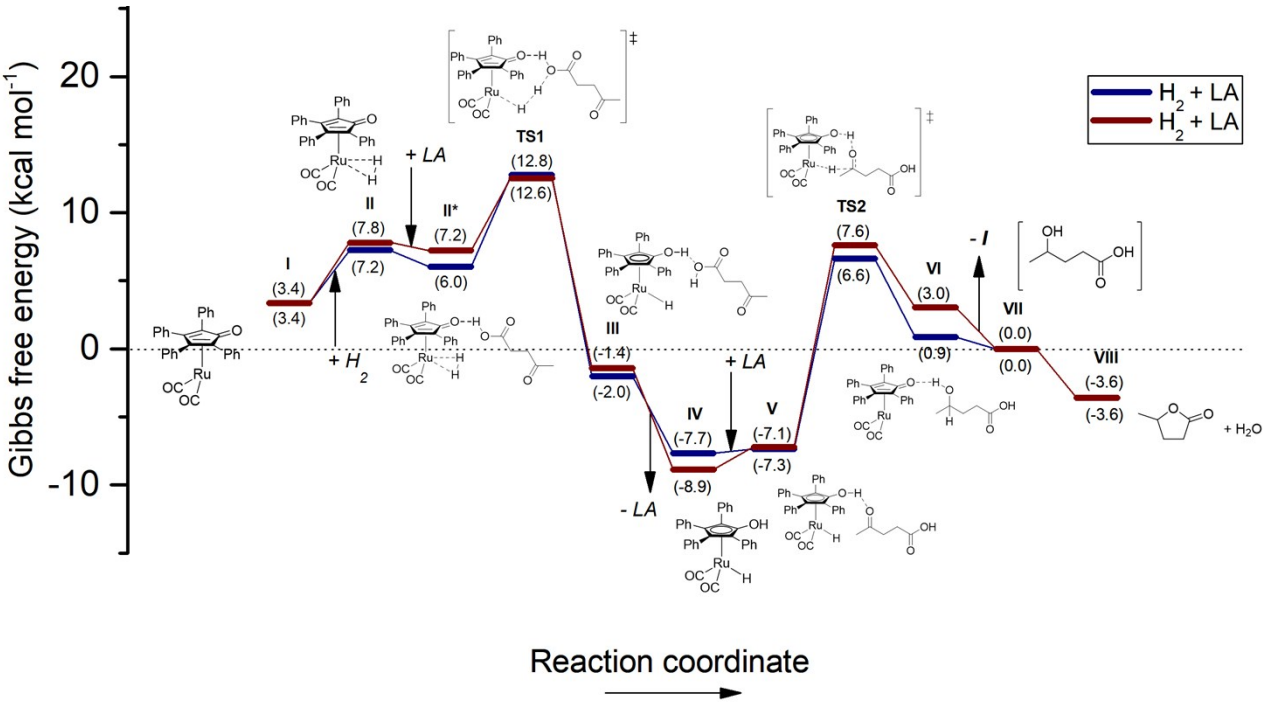


Figure S4.1: **Energetic reaction profile for the regeneration of the active Shvo catalyst species using H_2, followed by the Shvo-catalyzed hydrogenation of LA to GVL. The H_2 is heterolytically split via a concerted relay-mechanism employing one oxygen atom of the carboxylic acid functionality of LA as co-catalyst. The Gibbs free energy is normalized as such, that stage VII equals 0.0 kcal.mol^{-1}.**

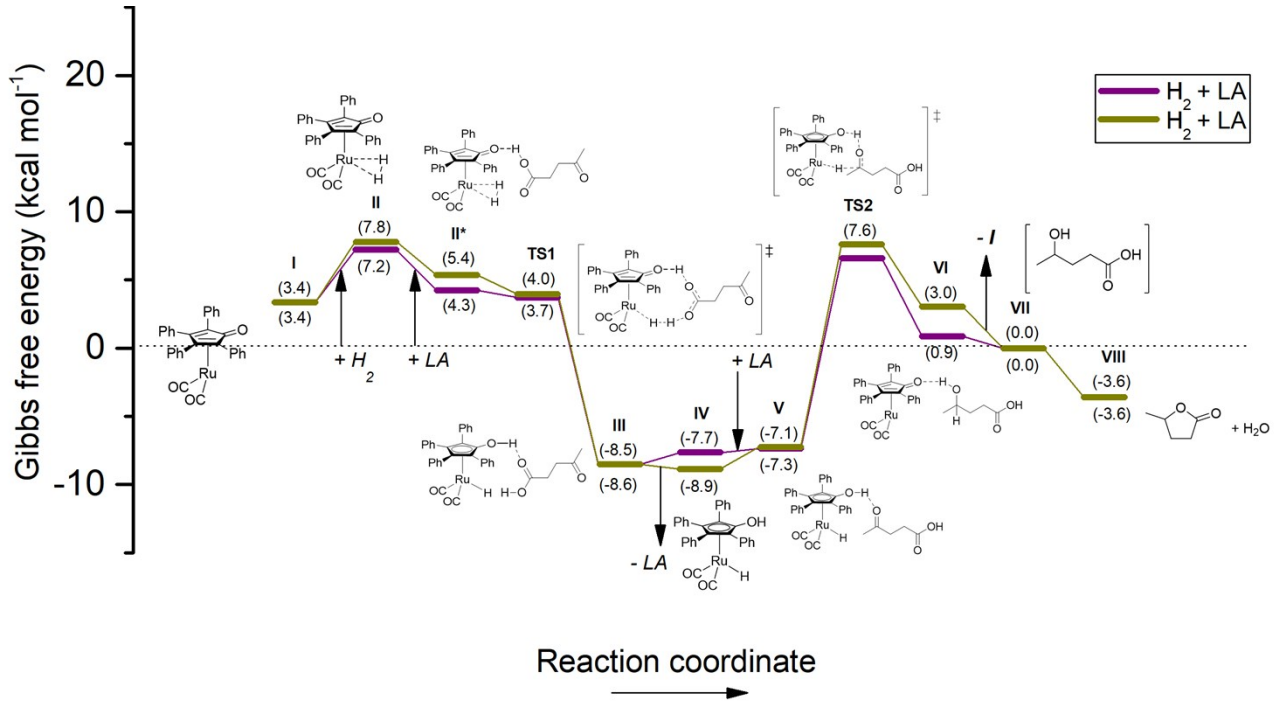
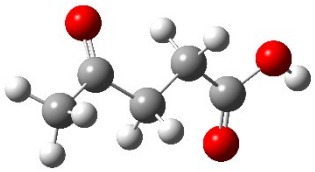


Figure S4.2: **Energetic reaction profile for the regeneration of the active Shvo catalyst species using H_2, followed by the Shvo-catalyzed hydrogenation of LA to GVL. The H_2 is heterolytically split via a concerted relay-mechanism employing the full carboxylic acid functionality of LA as co-catalyst. However, this mechanism is considered non-existent. The Gibbs free energy is normalized as such, that stage VII equals 0.0 kcal.mol^{-1}.**

Organic molecules

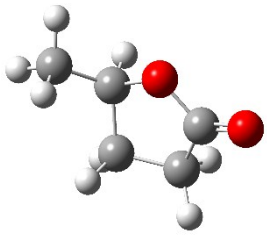
Levulinic acid: E_{Gibbs} = -420.887883 eH

C	-1.92052225	0.15451571	-0.05237017
O	-2.03281756	1.33441666	-0.44896381
C	-3.13687227	-0.71581141	0.21968004
H	-2.99263689	-1.73297385	-0.16572119
H	-3.29205070	-0.79834678	1.30542775
H	-4.02931821	-0.26932705	-0.22690274
C	-0.55459333	-0.49064274	0.17633123
H	-0.58007243	-1.07064234	1.10934437
H	-0.39249298	-1.23221778	-0.62081585
C	0.59541977	0.52573290	0.17954176
H	0.62683456	1.10549073	1.10868438
H	0.43991482	1.26331587	-0.61990427
C	1.94092674	-0.12811041	-0.03334327
O	2.15443812	-1.27542198	-0.45661845
O	2.98099825	0.73466317	0.28790650
H	3.85271936	0.31133415	0.11225605



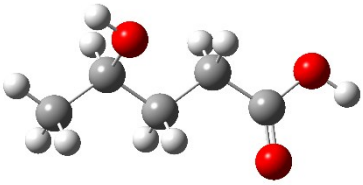
γ-Valerolactone: E_{Gibbs} = -345.663517 eH

C	-0.58147360	1.31984071	-0.14076055
C	0.94970348	1.23244172	0.03551059
C	1.24571092	-0.27145785	-0.00971503
C	-1.08672914	-0.03698242	0.41374362
H	-1.03033341	2.16562408	0.38914216
H	-0.83982927	1.40407223	-1.20336153
H	1.27677135	1.61592508	1.01115125
H	1.52639264	1.75085808	-0.73445967
H	-1.21753248	0.01331002	1.50333088
O	2.32768779	-0.83484253	-0.17413240
O	0.05323697	-0.97706441	0.17613544
C	-2.33150167	-0.61020654	-0.25281385
H	-2.57486133	-1.59432161	0.16191717
H	-3.18757466	0.05731991	-0.08740306
H	-2.17469094	-0.71934596	-1.33213017



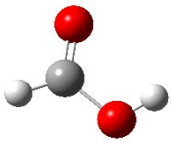
4-Hydroxyvaleric acid: E_{Gibbs} = -422.068977 eH

C	-3.03120887	0.83815027	0.15076305
H	-3.03524860	1.23558486	-0.87162499
H	-2.95204465	1.68038485	0.85041833
H	-3.99626763	0.34389070	0.33246029
C	-1.86008660	-0.13846542	0.33792621
H	-1.88899991	-0.55388316	1.36097581
C	-0.49702791	0.52202558	0.09434991
H	-0.38043258	1.37016591	0.78168115
H	-0.47615302	0.92696523	-0.92460672
C	0.66004929	-0.47385942	0.27707646
H	0.50803114	-1.34039340	-0.37845010
H	0.69451995	-0.87101198	1.30130732
C	2.00930385	0.12960588	-0.03222264
O	3.04231508	-0.75990883	0.25765061
H	3.91396533	-0.35923671	0.03493428
O	2.24198598	1.25924382	-0.48990112
O	-1.94091469	-1.25132404	-0.62667731
H	-2.82063960	-1.68129523	-0.58303074



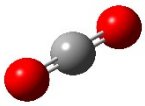
Formic acid: E_{Gibbs} = -189.712214 eH

C	-1.95955367	-0.16039051	0.00000000
H	-3.02955367	-0.16039051	0.00000000
O	-1.33251324	0.93065984	0.00000000
O	-1.24700772	-1.40022045	0.00000000
H	-0.40177568	-1.28406209	0.44010231



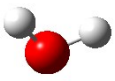
Carbon dioxide: E_{Gibbs} = -188.549993 eH

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.19325250
O	0.00000000	0.00000000	-1.19325250



Water: E_{Gibbs} = -76.411213 eH

O	-0.00000000	-0.00000000	0.11199599
H	0.00000000	-0.80040217	-0.44798395
H	0.00000000	0.80040217	-0.44798395

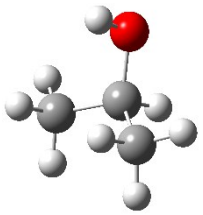


Dihydrogen: E_{Gibbs} = -1.175751 eH

H	0.00000000	0.00000000	0.37173909
H	0.00000000	0.00000000	-0.37173909

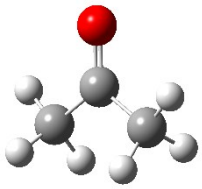
Isopropanol: **E_{Gibbs} = -194.254821 eH**

C	-0.00000063	0.02224860	-0.37734581
H	-0.00000483	0.07573127	-1.47165849
C	-1.28290463	-0.67742962	0.10294940
H	-2.16587240	-0.12076953	-0.23165849
H	-1.34490044	-1.69977094	-0.29302278
H	-1.30911055	-0.74045903	1.20104641
C	1.28290403	-0.67743101	0.10294535
H	1.34492189	-1.69975623	-0.29306287
H	2.16586799	-0.12074566	-0.23162991
H	1.30909414	-0.74050416	1.20104175
O	-0.00000440	1.44116692	0.01872196
H	0.00004684	1.51261106	0.99787504



Acetone: **E_{Gibbs} = -193.073432 eH**

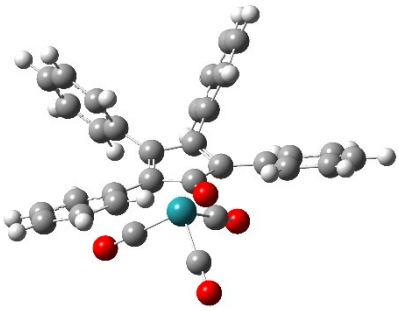
C	0.00000058	0.17526666	0.00000636
C	1.29764748	-0.62251624	0.00287877
H	1.27024555	-1.41359819	0.76358114
H	1.43159287	-1.11405543	-0.97150204
H	2.14805231	0.03969343	0.18548597
C	-1.29762753	-0.62254812	-0.00288777
H	-1.27013262	-1.41378902	-0.76341432
H	-1.43166987	-1.11386839	0.97159310
H	-2.14803096	0.03960909	-0.18570128
O	-0.00002256	1.42434933	-0.00000335



General Shvo Catalyst Structures

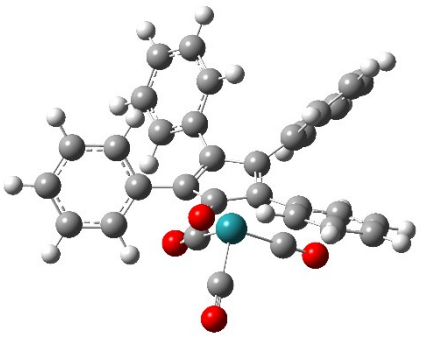
Ru-1 (mirror): E_{Gibbs} = -1625.706337 eH

C	0.00006593	-1.52997436	1.21356615
C	1.19196968	-0.76019423	0.69718083
C	0.72933665	0.59006193	0.37942332
C	-0.72933755	0.59000328	0.37936160
C	-1.19187854	-0.76031743	0.69719303
O	0.00017146	-2.61449076	1.84829161
C	-2.60517024	-1.17968706	0.89128291
C	-2.92951321	-2.19975423	1.82187726
C	-3.66365737	-0.57912752	0.16176349
C	-4.26607728	-2.59081857	2.01980013
H	-2.13328450	-2.68779061	2.37070104
C	-4.99418519	-0.97299840	0.36083061
H	-3.45275221	0.19679672	-0.56706867
C	-5.30580601	-1.98188678	1.29433141
H	-4.49053276	-3.37576242	2.73823849
H	-5.78579739	-0.49773940	-0.21351541
H	-6.33779245	-2.28918256	1.44655295
C	-1.56414503	1.82547909	0.38805141
C	-1.71652989	2.67530042	-0.72696832
C	-2.20025108	2.17471438	1.60296134
C	-2.48588567	3.84834972	-0.63407652
H	-1.24754858	2.41479879	-1.67153585
C	-2.96410359	3.34950494	1.69835435
H	-2.09880623	1.52373626	2.46765061
C	-3.11098083	4.19182387	0.57908010
H	-2.59771502	4.48819812	-1.50583636
H	-3.44565689	3.60329579	2.63942373
H	-3.70724455	5.09812436	0.65075549
C	1.56412934	1.82552638	0.38779430
C	2.20114679	2.17444774	1.60233776
C	1.71556801	2.67571538	-0.72707758
C	2.96493425	3.34928487	1.69750972
H	2.10044221	1.52316985	2.46688421
C	2.48486491	3.84882182	-0.63439582
H	1.24590923	2.41540025	-1.67135825
C	3.11084047	4.19198079	0.57838422
H	3.44720560	3.60285185	2.63827138
H	2.59594758	4.48895552	-1.50604164
H	3.70703955	5.09833562	0.64991574
C	2.60528257	-1.17950494	0.89127103
C	3.66364660	-0.57938882	0.16121259
C	2.92974338	-2.19900016	1.82243171
C	4.99420479	-0.97310756	0.36033945
H	3.45258391	0.19607038	-0.56807313
C	4.26634838	-2.58992117	2.02041878
H	2.13359307	-2.68674821	2.37162449
C	5.30595968	-1.98141252	1.29443523
H	5.78574606	-0.49821630	-0.21440714
H	4.49091626	-3.37443107	2.73929491
H	6.33797332	-2.28859495	1.44670339
Ru	-0.00005688	-0.77655079	-1.29815042
C	0.00047623	-2.69933517	-1.61995046
C	1.39179401	-0.36098412	-2.56165532
C	-1.39247164	-0.36133357	-2.56114576
O	-2.26343316	-0.12601043	-3.31692621
O	2.26246083	-0.12590907	-3.31786743
O	0.00084655	-3.85566994	-1.81413535



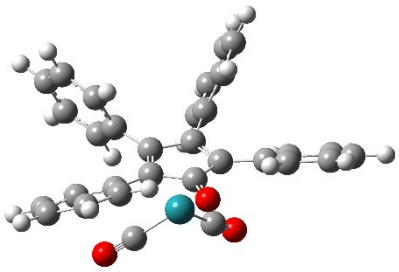
Ru-1 (propeller): E_{Gibbs} = -1625.704387 eH

C	0.04306659	-1.47982833	-1.24278382
C	-1.17044083	-0.72565861	-0.74609480
C	-0.72394878	0.62565420	-0.39989526
C	0.73412508	0.63822714	-0.36221808
C	1.20213245	-0.71692024	-0.65087902
O	0.09932806	-2.53890751	-1.90764885
C	2.60695974	-1.12085614	-0.93609633
C	3.20814341	-2.21848838	-0.28435990
C	3.33476371	-0.45530185	-1.95099796
C	4.50582412	-2.63752167	-0.62634163
H	2.65769436	-2.74769726	0.48886123
C	4.63216997	-0.87139706	-2.29415832
H	2.88324394	0.38259797	-2.47600937
C	5.22453425	-1.96394277	-1.63195556
H	4.95083585	-3.48629690	-0.11281756
H	5.17631523	-0.34827340	-3.07701259
H	6.22812507	-2.28717649	-1.89809869
C	1.59811804	1.85035835	-0.28109199
C	2.77673347	1.88060758	0.49864431
C	1.29050937	2.97731179	-1.08119844
C	3.61110401	3.00940827	0.49795694
H	3.05064244	1.02199241	1.10219829
C	2.12948819	4.10507008	-1.08778424
H	0.40184337	2.97265604	-1.70416948
C	3.29110831	4.12938648	-0.29384059
H	4.50946430	3.01201509	1.10988750
H	1.87521292	4.95921127	-1.71048692
H	3.93814336	5.00315656	-0.29456880
C	-1.58565993	1.83872896	-0.30157774
C	-1.52894653	2.71880268	0.80130369
C	-2.44156050	2.15447827	-1.38291993
C	-2.30912990	3.88653817	0.82556194
H	-0.87401255	2.48905327	1.63754432
C	-3.21975641	3.32464875	-1.36028840
H	-2.49926489	1.48568318	-2.23718243
C	-3.15765189	4.19562380	-0.25540902
H	-2.25601490	4.55067047	1.68453162
H	-3.87387502	3.55121378	-2.19854915
H	-3.76353699	5.09815884	-0.23494558
C	-2.57094435	-1.16702262	-0.98220343
C	-3.65264230	-0.67259023	-0.20942166
C	-2.85284145	-2.10898025	-2.00411372
C	-4.96761391	-1.09224891	-0.45542109
H	-3.47196093	0.04114011	0.58816287
C	-4.17392747	-2.52579020	-2.24945606
H	-2.03641903	-2.52007849	-2.58612608
C	-5.23805398	-2.02130133	-1.48047905
H	-5.77860815	-0.69999282	0.15351771
H	-4.36679927	-3.24948714	-3.03788552
H	-6.25771295	-2.34891739	-1.66900384
Ru	-0.02745167	-0.79282154	1.27513678
C	-0.10881877	-2.71755407	1.55797747
C	-1.43460159	-0.35570413	2.52115432
C	1.33163076	-0.44450255	2.59303763
O	2.17866632	-0.26532970	3.39074276
O	-2.30835547	-0.09892564	3.26569861
O	-0.16822388	-3.87569870	1.73848656



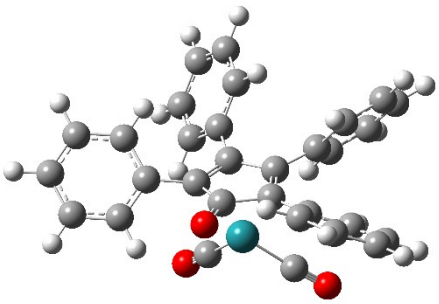
I (mirror): **E_{Gibbs} = -1512.375087 eH**

C	0.00009798	-1.83220739	-0.76545154
C	-1.20351217	-0.95807231	-0.53796122
C	-0.74220185	0.39434909	-0.39555211
C	0.74226812	0.39439823	-0.39558580
C	1.20364789	-0.95798113	-0.53799076
O	0.00017712	-3.08343517	-0.93712292
C	2.60334004	-1.43080924	-0.65738656
C	3.67426804	-0.75617357	-0.01695156
C	2.90300504	-2.57512544	-1.43937512
C	4.99616234	-1.20067550	-0.16265039
H	3.47676500	0.11334307	0.60179667
C	4.22956391	-3.01664634	-1.58508581
H	2.09741577	-3.12226255	-1.91423943
C	5.28337785	-2.33340218	-0.95048236
H	5.79941937	-0.66882444	0.34140051
H	4.43662532	-3.89638204	-2.18974890
H	6.30850815	-2.67893697	-1.06105724
C	1.56635430	1.62676590	-0.53520857
C	1.71527566	2.57778704	0.49540450
C	2.20008505	1.85954978	-1.77844954
C	2.48356046	3.73738913	0.29159309
H	1.24793924	2.40199377	1.45990686
C	2.96111450	3.02204255	-1.98488940
H	2.09926831	1.12869932	-2.57699842
C	3.10689165	3.96590874	-0.94954517
H	2.59555499	4.45646092	1.09918436
H	3.44151036	3.18781028	-2.94601573
H	3.70096754	4.86279446	-1.10701164
C	-1.56641796	1.62662674	-0.53526881
C	-2.19954421	1.85957279	-1.77878260
C	-1.71611806	2.57735194	0.49550761
C	-2.96073492	3.02194005	-1.98534944
H	-2.09814949	1.12893078	-2.57744914
C	-2.48455265	3.73683267	0.29155859
H	-1.24930210	2.40146931	1.46024984
C	-3.10727279	3.96552027	-0.94985734
H	-3.44065825	3.18781953	-2.94669235
H	-2.59713946	4.45568932	1.09925996
H	-3.70146286	4.86231498	-1.10741093
C	-2.60319923	-1.43090184	-0.65743702
C	-2.90288493	-2.57531201	-1.43926744
C	-3.67412754	-0.75613517	-0.01711854
C	-4.22946533	-3.01678552	-1.58497351
H	-2.09731123	-3.12255983	-1.91402464
C	-4.99603364	-1.20058742	-0.16281198
H	-3.47659514	0.11344032	0.60154247
C	-5.28327145	-2.33340546	-0.95051133
H	-4.43654217	-3.89659507	-2.18952320
H	-5.79928729	-0.66863441	0.34113566
H	-6.30841486	-2.67890258	-1.06108849
Ru	0.00006183	-0.70941463	1.44813430
C	-1.36940888	-0.30640819	2.70273839
C	1.36939916	-0.30582548	2.70272081
O	2.24106585	0.00285726	3.43823282
O	-2.24122172	0.00171428	3.43831509



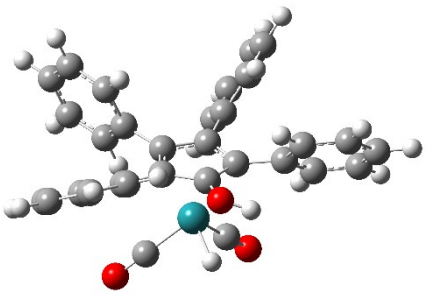
I (propeller): **E_{Gibbs} = -1512.374038 eH**

C	0.03315120	-1.76969708	-0.84851559
C	-1.18689722	-0.91658994	-0.62231324
C	-0.74636150	0.43503660	-0.43351530
C	0.73909826	0.45744175	-0.40696449
C	1.21929200	-0.88548832	-0.58061415
O	0.06248295	-3.01275877	-1.06302305
C	2.60869132	-1.36293713	-0.78138522
C	3.54203921	-0.62036064	-1.54431112
C	3.00534678	-2.62014247	-0.26490580
C	4.83970885	-1.11228319	-1.76523215
H	3.25422843	0.33292587	-1.97585170
C	4.30370008	-3.10887881	-0.48334414
H	2.29172064	-3.21707801	0.29456096
C	5.22907651	-2.35600027	-1.23202902
H	5.54198559	-0.52841368	-2.35558839
H	4.59000520	-4.07542072	-0.07612269
H	6.23388405	-2.73509668	-1.40296405
C	1.55135051	1.70587008	-0.43265719
C	2.61235456	1.93750330	0.47080627
C	1.29430605	2.66794051	-1.43861748
C	3.39219094	3.10178492	0.37638800
H	2.83378694	1.21171774	1.24562475
C	2.08009893	3.82906267	-1.53860229
H	0.48569182	2.50631839	-2.14550313
C	3.13117026	4.05281607	-0.62926037
H	4.20143394	3.26346349	1.08383863
H	1.86896743	4.55535440	-2.31947688
H	3.73626452	4.95320570	-0.70200211
C	-1.59218218	1.65869375	-0.43919843
C	-2.48891910	1.87006568	-1.51277395
C	-1.48796671	2.64247686	0.56875405
C	-3.26299791	3.04122417	-1.57537762
H	-2.58069000	1.11927411	-2.29300134
C	-2.26742681	3.80948006	0.50947137
H	-0.80436463	2.48771858	1.39894661
C	-3.15710628	4.01487934	-0.56297874
H	-3.94789597	3.18960224	-2.40653922
H	-2.18104743	4.55413276	1.29664267
H	-3.76067144	4.91814843	-0.60792063
C	-2.57225227	-1.42880550	-0.75203140
C	-3.65451288	-0.86262309	-0.03145034
C	-2.83951348	-2.51377828	-1.62476488
C	-4.95880395	-1.35341341	-0.18826786
H	-3.47996621	-0.04226339	0.65735484
C	-4.14850924	-3.00210377	-1.78126510
H	-2.02208894	-2.97945037	-2.16276732
C	-5.21487801	-2.42544245	-1.06686441
H	-5.77178023	-0.90607706	0.37832591
H	-4.33151778	-3.83505920	-2.45574555
H	-6.22613462	-2.80729194	-1.18551409
Ru	-0.00214604	-0.75576259	1.38630481
C	-1.37285014	-0.37979343	2.64921505
C	1.34949736	-0.47846950	2.68747792
O	2.21268632	-0.26569728	3.46684046
O	-2.23976384	-0.08116493	3.39456469



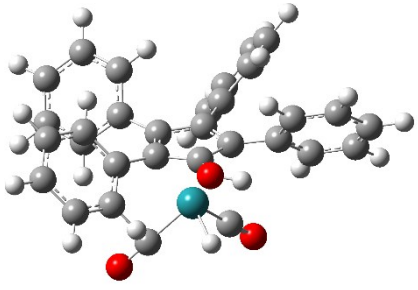
IV (mirror): E_{Gibbs} = -1513.568381 eH

C	-0.01212961	-1.74293026	-0.59609125
C	-1.19070751	-0.92236351	-0.45733016
C	-0.72704430	0.46973606	-0.38179141
C	0.71384304	0.46455655	-0.40316793
C	1.17345317	-0.93586862	-0.50686960
C	-2.57997837	-1.40959678	-0.66391446
C	-2.85605681	-2.26396442	-1.76161477
C	-3.65008234	-1.02912646	0.17786102
C	-4.16184417	-2.73052058	-2.00131016
H	-2.05769031	-2.53476196	-2.44900790
C	-4.95445273	-1.48676266	-0.06747662
H	-3.46125043	-0.37808559	1.02596182
C	-5.21700408	-2.34477647	-1.15422362
H	-4.35363186	-3.38360064	-2.84947801
H	-5.76293572	-1.18051594	0.59158617
H	-6.22680318	-2.70325678	-1.33778348
C	-1.60596061	1.66386451	-0.51491550
C	-2.39951159	1.79428289	-1.67945619
C	-1.65603184	2.68818464	0.45519402
C	-3.21527228	2.92234655	-1.87017208
H	-2.37389104	1.01370850	-2.43553609
C	-2.47216497	3.81688722	0.26641395
H	-1.06852777	2.59231397	1.36379252
C	-3.25421986	3.94012439	-0.89756414
H	-3.81761884	3.00596599	-2.77162348
H	-2.49984444	4.59336234	1.02690954
H	-3.88721691	4.81228964	-1.04271100
C	1.57333264	1.66803560	-0.58887812
C	2.12415220	1.90774682	-1.86965119
C	1.84359873	2.58708344	0.44714812
C	2.92131666	3.04015654	-2.10757168
H	1.92842042	1.20393576	-2.67512317
C	2.64172329	3.72094070	0.21155305
H	1.44186997	2.40494359	1.44064787
C	3.18294504	3.95266048	-1.06688084
H	3.33722387	3.20903230	-3.09801719
H	2.84197352	4.41634475	1.02311294
H	3.80199894	4.82788926	-1.24917205
C	2.56925897	-1.40435107	-0.70189977
C	2.83565800	-2.52503190	-1.52621201
C	3.66389182	-0.73674435	-0.10157126
C	4.15528913	-2.95637196	-1.74715271
H	2.01191344	-3.06280566	-1.98193899
C	4.98026105	-1.16911665	-0.32259762
H	3.48966475	0.11679707	0.54560890
C	5.23524956	-2.28143188	-1.14843022
H	4.33754792	-3.81989323	-2.38273398
H	5.80412434	-0.64301512	0.15343646
H	6.25557630	-2.61774890	-1.31685723
O	0.00820379	-3.11092298	-0.80780405
H	-0.85012037	-3.52417559	-0.57200391
Ru	0.00531503	-0.65440513	1.54495817
H	-0.14416302	-2.11082216	2.20380328
C	1.42403095	-0.44509374	2.76242945
C	-1.26055752	-0.13603939	2.82836935
O	2.32511996	-0.33002986	3.51910581
O	-2.07462311	0.17305656	3.63064992



IV (propeller): E_{Gibbs} = -1513.569245 eH

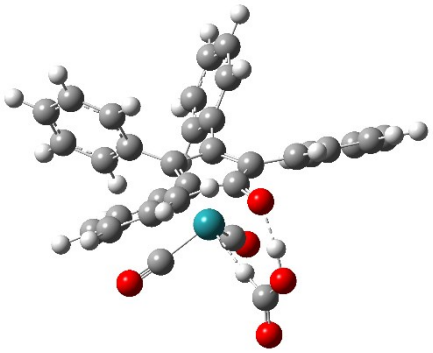
C	0.02865271	-1.68929918	-0.68457125
C	-1.16952564	-0.90217175	-0.52899696
C	-0.73612822	0.50014425	-0.41182633
C	0.70395581	0.52971588	-0.43106771
C	1.19113929	-0.85748090	-0.55913177
C	-2.54048974	-1.43085809	-0.76411682
C	-2.78522827	-2.20404801	-1.92778268
C	-3.61758895	-1.17983041	0.11581306
C	-4.06800157	-2.71783284	-2.19541504
H	-1.98219729	-2.37187222	-2.64267304
C	-4.89991106	-1.68263469	-0.15749270
H	-3.45140252	-0.59453251	1.01481148
C	-5.13104845	-2.45917204	-1.31057918
H	-4.23601508	-3.30789588	-3.09329787
H	-5.71494559	-1.47564497	0.53146652
H	-6.12321758	-2.85348436	-1.51562014
C	-1.64608725	1.67833705	-0.40482908
C	-2.62688419	1.80943115	-1.41595504
C	-1.53350995	2.70015749	0.56539101
C	-3.47042600	2.93402220	-1.45651221
H	-2.72664076	1.03599444	-2.17262679
C	-2.37416119	3.82421260	0.52457989
H	-0.79060071	2.60788514	1.35324414
C	-3.34763719	3.94687830	-0.48660535
H	-4.21886614	3.01711477	-2.24101057
H	-2.27361025	4.59834408	1.28128230
H	-4.00123430	4.81544472	-0.51559919
C	1.55416524	1.75109707	-0.49326465
C	1.26521984	2.74906625	-1.45446344
C	2.68079656	1.92715758	0.34210215
C	2.07421812	3.89320711	-1.57025310
H	0.40908565	2.62752540	-2.11193824
C	3.49112940	3.06863951	0.22591362
H	2.92502623	1.17410635	1.08514860
C	3.19131510	4.05909593	-0.72978495
H	1.83271911	4.64967371	-2.31317926
H	4.35154602	3.18439224	0.88033171
H	3.81711690	4.94405547	-0.81727150
C	2.58007525	-1.32177842	-0.81470917
C	3.39608484	-0.65420713	-1.75746966
C	3.08810355	-2.47469973	-0.17334448
C	4.69131417	-1.12202184	-2.04149169
H	3.01944292	0.22451614	-2.27245052
C	4.38083676	-2.94307445	-0.45866551
H	2.46667771	-2.99893042	0.54711653
C	5.19039701	-2.26717578	-1.39288152
H	5.30570223	-0.59497901	-2.76766968
H	4.75624057	-3.82908444	0.04763238
H	6.19294076	-2.62755272	-1.61130709
O	0.10566601	-3.03863797	-0.97115043
H	-0.76733448	-3.47653524	-0.87419454
Ru	0.01228489	-0.70468890	1.48451239
H	-0.12310076	-2.19110874	2.07567834
C	1.41376479	-0.52767466	2.72462724
C	-1.26980693	-0.24954446	2.77903543
O	2.30722265	-0.44242179	3.49511240
O	-2.09242252	0.02142621	3.58554661



Formic acid mediation with Shvo catalyst

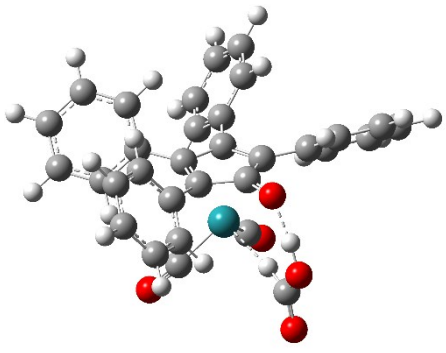
II-a (mirror): E_{Gibbs} = -1702.093161 eH

C	-0.00009242	-1.27270362	1.17225862
C	1.19919525	-0.46969453	0.81097612
C	0.73900121	0.83262564	0.38682038
C	-0.73892807	0.83268743	0.38685237
C	-1.19925628	-0.46953021	0.81121187
Ru	-0.00013587	-0.63830132	-1.18329022
C	-1.37326864	-0.43630958	-2.49330264
C	1.37257159	-0.43593902	-2.49362903
O	2.24083070	-0.25443761	-3.26918801
O	-2.24182511	-0.25500983	-3.26856416
O	-0.00010393	-2.49801656	1.55714256
C	-2.59622644	-0.90350949	1.05703961
C	-2.87599161	-1.81724653	2.10357366
C	-3.67738517	-0.40980273	0.28551017
C	-4.19712916	-2.21431474	2.37316501
H	-2.06088720	-2.22337269	2.69144161
C	-4.99437836	-0.80935899	0.55562221
H	-3.49309143	0.28339609	-0.52929737
C	-5.26278244	-1.71351211	1.60265540
H	-4.39099077	-2.91772256	3.17918103
H	-5.80809216	-0.42201609	-0.05232643
H	-6.28357300	-2.02631994	1.80826101
C	-1.57276718	2.06093120	0.27596363
C	-2.21776308	2.52579960	1.44635770
C	-1.71897351	2.79276195	-0.92063946
C	-2.98625662	3.70116734	1.41843381
H	-2.11931026	1.96532493	2.37265818
C	-2.49506600	3.96441425	-0.95048018
H	-1.24320629	2.43902777	-1.83063268
C	-3.12893523	4.42504034	0.21869949
H	-3.47498397	4.04667452	2.32590726
H	-2.60505543	4.51246908	-1.88276088
H	-3.72894953	5.33133336	0.19504651
C	1.57304728	2.06076481	0.27610156
C	2.21826027	2.52506705	1.44662631
C	1.71936094	2.79300036	-0.92022390
C	2.98704690	3.70024278	1.41908778
H	2.11970655	1.96430209	2.37274032
C	2.49577149	3.96446133	-0.94968845
H	1.24338776	2.43985714	-1.83032689
C	3.12985328	4.42450134	0.21959779
H	3.47589349	4.04531389	2.32666345
H	2.60582476	4.51282373	-1.88178034
H	3.73013242	5.33062601	0.19621730
C	2.59612757	-0.90384963	1.05665343
C	2.87596692	-1.81727855	2.10343166
C	3.67720094	-0.41053851	0.28474646
C	4.19710847	-2.21444745	2.37288518
H	2.06093492	-2.22310800	2.69159951
C	4.99418889	-0.81019130	0.55472293
H	3.49283320	0.28243676	-0.53023860
C	5.26267433	-1.71404098	1.60200226
H	4.39102975	-2.91760763	3.17910262
H	5.80783853	-0.42315094	-0.05350449
H	6.28346627	-2.02690984	1.80750986
C	-0.00010031	-3.86230497	-1.37555794
H	-0.00022931	-2.71348879	-1.37412643
O	0.00009055	-4.39242278	-0.14712831
H	0.00020601	-3.71925643	0.62656968
O	-0.00016160	-4.47120436	-2.44325928



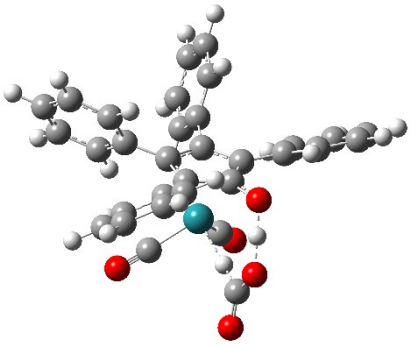
II-a (propeller): E_{Gibbs} = -1702.091137 eH

C	0.03169748	-1.23279968	-1.19011984
C	-1.18160658	-0.43227809	-0.85528121
C	-0.73792617	0.87057234	-0.42202731
C	0.74150025	0.87876378	-0.38721439
C	1.21298615	-0.42897331	-0.78835728
Ru	-0.02258749	-0.63382638	1.15601449
C	1.33544045	-0.53338587	2.49107247
C	-1.39533479	-0.38802420	2.45990046
O	-2.25700843	-0.17713298	3.23540053
O	2.19725230	-0.42715546	3.28789044
O	0.04932734	-2.44877015	-1.59349202
C	2.60504207	-0.84437339	-1.10183303
C	3.41286334	-0.03904547	-1.93968591
C	3.12070558	-2.07863599	-0.64699154
C	4.70587749	-0.45333544	-2.30135509
H	3.02825945	0.90497159	-2.31544649
C	4.41359272	-2.49364175	-1.00858561
H	2.51711306	-2.71762753	-0.00927976
C	5.21274173	-1.68195935	-1.83599340
H	5.31238045	0.17764716	-2.94657591
H	4.79228587	-3.44666946	-0.64827402
H	6.21289249	-2.00338740	-2.11628636
C	1.58520718	2.08821073	-0.19234506
C	1.28034019	3.27114668	-0.90834664
C	2.73723154	2.07087477	0.62717904
C	2.10254534	4.40590513	-0.80112308
H	0.40919739	3.30447753	-1.55506089
C	3.55201786	3.20777028	0.74232731
H	3.00095246	1.17155711	1.17319779
C	3.23912817	4.38143912	0.02852641
H	1.85378976	5.30391727	-1.36088140
H	4.42905558	3.17589214	1.38336873
H	3.87187926	5.26104825	0.11712881
C	-1.59548390	2.06902681	-0.21722486
C	-2.48400460	2.45736891	-1.24742888
C	-1.51038927	2.86171122	0.94847885
C	-3.26713799	3.61646489	-1.11343075
H	-2.56195535	1.85489742	-2.14826836
C	-2.29902705	4.01584864	1.08479984
H	-0.83330480	2.57005032	1.74663903
C	-3.17924702	4.39948233	0.05401313
H	-3.94540526	3.90263143	-1.91328723
H	-2.22737413	4.61167107	1.99100062
H	-3.78997362	5.29255652	0.16055408
C	-2.56550136	-0.89862124	-1.11903614
C	-2.81274330	-1.74877045	-2.22547384
C	-3.65943695	-0.51187615	-0.30634304
C	-4.11721141	-2.18576646	-2.51477273
H	-1.98516525	-2.07528782	-2.84534120
C	-4.95966222	-0.95152605	-0.59582009
H	-3.49896554	0.12845457	0.55549940
C	-5.19672176	-1.79023079	-1.70331787
H	-4.28649764	-2.83898776	-3.36712849
H	-5.78376123	-0.64748690	0.04463041
H	-6.20408111	-2.13480631	-1.92372080
C	-0.09682599	-3.87974239	1.29173272
H	-0.21156060	-2.74086387	1.30803154
O	0.07498877	-4.38096926	0.06042283
H	0.06651297	-3.69471028	-0.70296345
O	-0.13410593	-4.51611988	2.34381452



TS: II-a – III-a (mirror): E_{Gibbs} = -1702.092125 eH

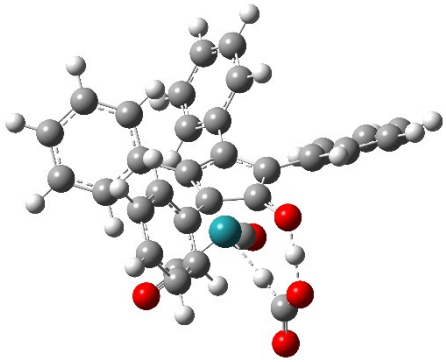
C	0.12448639	-1.29124581	-1.10196142
C	-1.16252816	-0.67414632	-0.79924245
C	-0.88666794	0.69527423	-0.36284529
C	0.56338388	0.91408372	-0.41253358
C	1.20104102	-0.32607159	-0.80586445
Ru	0.06188023	-0.66816424	1.19488865
C	1.27143727	-0.07949248	2.54628495
C	-1.36709436	-0.84059283	2.44330403
O	-2.28014514	-0.92138461	3.18227911
O	2.02873523	0.32783688	3.35083769
O	0.29937821	-2.54960656	-1.47212210
C	2.64036350	-0.56971285	-1.07395097
C	3.65606652	0.00843604	-0.27542709
C	3.01873843	-1.38034463	-2.17181387
C	5.01015177	-0.21143407	-0.56864650
H	3.39098583	0.62559687	0.57795071
C	4.37621285	-1.59866156	-2.46408791
H	2.25408648	-1.84642215	-2.78416094
C	5.37781787	-1.01611865	-1.66555503
H	5.77565666	0.23634326	0.05990990
H	4.64882564	-2.22735152	-3.30805803
H	6.42746899	-1.19133046	-1.88819022
C	1.22262041	2.24406808	-0.31956642
C	1.94354855	2.70867400	-1.44538007
C	1.11532709	3.07908678	0.81312670
C	2.53983952	3.98027546	-1.43635579
H	2.03550257	2.07586745	-2.32398883
C	1.71861851	4.34803695	0.82461353
H	0.57548193	2.73359927	1.68956656
C	2.43125171	4.80510585	-0.30002080
H	3.08899493	4.32314893	-2.30959081
H	1.63374185	4.97505729	1.70840593
H	2.89795601	5.78694327	-0.29028881
C	-1.89110621	1.79089565	-0.25017923
C	-2.47908986	2.27162794	-1.44332092
C	-2.26396047	2.37552853	0.97745835
C	-3.41606132	3.31795926	-1.40567790
H	-2.20549684	1.82357499	-2.39558808
C	-3.20502672	3.41975591	1.01646055
H	-1.83037332	2.00592212	1.90286235
C	-3.78287995	3.89639288	-0.17498698
H	-3.86000287	3.67712567	-2.33077693
H	-3.48563568	3.85557960	1.97202471
H	-4.51066897	4.70347944	-0.14563635
C	-2.48661134	-1.29263809	-1.05836840
C	-3.64553536	-0.90660699	-0.34162988
C	-2.61393714	-2.27922956	-2.06747782
C	-4.89213824	-1.48297619	-0.62794916
H	-3.57898800	-0.16136940	0.44428669
C	-3.86457433	-2.85298032	-2.35324355
H	-1.73340550	-2.60604445	-2.60835578
C	-5.01010353	-2.45883358	-1.63699545
H	-5.76776129	-1.17556470	-0.06165304
H	-3.94112514	-3.61025449	-3.12964685
H	-5.97617552	-2.90733433	-1.85561504
C	1.12552850	-3.52274023	1.44271040
H	0.56868041	-2.42078286	1.48602636
O	1.25048884	-3.94222063	0.23138592
H	0.81684130	-3.26683825	-0.71493679
O	1.43128878	-3.96937161	2.54825528



ν_{TS} = -602.07 cm^{-1}

TS: II-a – III-a (propeller): E_{Gibbs} = -1702.090104 eH

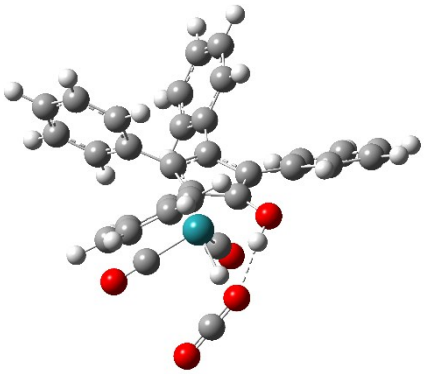
C	0.06232567	-1.24542537	-1.13933254
C	-1.17490827	-0.51345843	-0.84178816
C	-0.78674752	0.81936429	-0.40014890
C	0.67920275	0.89678203	-0.38443262
C	1.20819648	-0.39633621	-0.79579398
Ru	-0.00241142	-0.68586558	1.16151972
C	1.32818176	-0.44727347	2.50742011
C	-1.40418579	-0.53956798	2.44605799
O	-2.29026709	-0.41360499	3.21064444
O	2.16712128	-0.27155855	3.31475172
O	0.12457152	-2.49376837	-1.55996693
C	2.61451982	-0.73630073	-1.14104018
C	3.34715535	0.11681950	-2.00067508
C	3.21916114	-1.93420410	-0.69874350
C	4.65387261	-0.21478401	-2.39613252
H	2.89343988	1.03353462	-2.36660525
C	4.52611175	-2.26599067	-1.09511666
H	2.67732132	-2.61290576	-0.04731205
C	5.25035612	-1.40723187	-1.94325960
H	5.20141750	0.45239276	-3.05739478
H	4.97349154	-3.19242082	-0.74436442
H	6.26152324	-1.66457078	-2.24899945
C	1.47755530	2.13720278	-0.18800585
C	1.10852381	3.31882058	-0.87515510
C	2.64769643	2.15435786	0.60557689
C	1.88375393	4.48582845	-0.76287373
H	0.22342155	3.32642164	-1.50320099
C	3.41681656	3.32222061	0.72461302
H	2.96221940	1.25735399	1.12825137
C	3.03856539	4.49473713	0.04139989
H	1.58471097	5.38255406	-1.29963776
H	4.30875875	3.31566726	1.34558887
H	3.63539380	5.39875795	0.13362925
C	-1.70467805	1.97250220	-0.19293709
C	-2.59400397	2.33238728	-1.23273282
C	-1.67611237	2.75343946	0.98313846
C	-3.43225904	3.45236860	-1.09832466
H	-2.62964967	1.73833759	-2.14185213
C	-2.51793458	3.86967007	1.11912238
H	-0.99904219	2.48387816	1.78923103
C	-3.39827695	4.22523058	0.07854922
H	-4.11062440	3.71626427	-1.90574362
H	-2.48753404	4.45767340	2.03278230
H	-4.05034900	5.08861105	0.18490528
C	-2.53820569	-1.02860648	-1.12941296
C	-2.73694131	-1.87575189	-2.24697389
C	-3.65685539	-0.68446461	-0.33320056
C	-4.02104412	-2.35303156	-2.56263424
H	-1.88689312	-2.17165770	-2.85186064
C	-4.93712920	-1.16352983	-0.64938496
H	-3.53261518	-0.04654236	0.53643830
C	-5.12712524	-1.99952868	-1.76755870
H	-4.15368745	-3.00461607	-3.42273686
H	-5.78189699	-0.89160561	-0.02150828
H	-6.11875963	-2.37440826	-2.00899532
C	0.29298812	-3.72187857	1.36825064
H	0.02882024	-2.52249109	1.41072185
O	0.48849759	-4.12533750	0.15817592
H	0.33423803	-3.34073179	-0.79453900
O	0.32019481	-4.27043218	2.47083395



ν_{TS} = -583.23 cm^{-1}

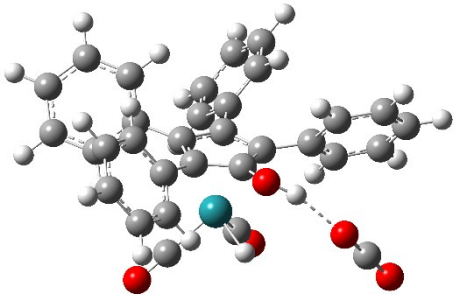
III-a (mirror): E_{Gibbs} = -1702.114414 eH

C	-0.24185119	1.28417129	-0.96051034
C	1.13177831	0.95737855	-0.67910118
C	1.16307621	-0.47985762	-0.34862955
C	-0.18708848	-0.98327360	-0.39266426
C	-1.08250431	0.12840930	-0.73960552
Ru	-0.08871034	0.59803257	1.33050545
C	-1.21988331	-0.16174104	2.62103999
C	1.18115789	1.08857204	2.63185289
O	1.98207367	1.41345066	3.43830421
O	-1.95232061	-0.63358698	3.42302900
O	-0.64775609	2.52020970	-1.41910518
C	-2.52246725	0.03785886	-1.09712193
C	-2.97208569	0.60360399	-2.31567712
C	-3.46103362	-0.63119248	-0.27788130
C	-4.32258345	0.51007060	-2.69725502
H	-2.26267335	1.10546261	-2.96832032
C	-4.80869543	-0.72968006	-0.66162364
H	-3.13751562	-1.07450791	0.65912108
C	-5.24816106	-0.15588531	-1.87143172
H	-4.64855863	0.95059829	-3.63659730
H	-5.51347357	-1.24932901	-0.01731517
H	-6.29228088	-0.22978464	-2.16553794
C	-0.58697145	-2.41744663	-0.35749968
C	-1.10138454	-3.00286024	-1.53867787
C	-0.44381971	-3.22536200	0.79084387
C	-1.45833846	-4.36147035	-1.56989640
H	-1.21834692	-2.39327725	-2.43117091
C	-0.80131178	-4.58468447	0.76167322
H	-0.06692669	-2.78618046	1.71026524
C	-1.30890419	-5.15915691	-0.41882756
H	-1.85135288	-4.79479698	-2.48653608
H	-0.68747133	-5.18972561	1.65778205
H	-1.58735734	-6.21007356	-0.44118495
C	2.38868935	-1.32439134	-0.27712664
C	3.13025616	-1.53480113	-1.46326586
C	2.82641445	-1.94188883	0.91361008
C	4.27771165	-2.34576054	-1.45755510
H	2.80774778	-1.05938045	-2.38646042
C	3.97498486	-2.75353468	0.92187086
H	2.27605147	-1.77233198	1.83539976
C	4.70462736	-2.95994188	-0.26395183
H	4.83653415	-2.49639845	-2.37816493
H	4.29886358	-3.21846174	1.84990479
H	5.59379543	-3.58591672	-0.25823511
C	2.30190958	1.84757027	-0.88781007
C	2.26360620	2.84855771	-1.88933044
C	3.48653334	1.70338833	-0.12588479
C	3.37872417	3.67212029	-2.12346393
H	1.35950231	2.98772448	-2.47086009
C	4.59799771	2.52704698	-0.36042610
H	3.54046633	0.95247820	0.65591270
C	4.55218611	3.51625622	-1.36239251
H	3.32832609	4.43541811	-2.89658908
H	5.49503762	2.40104380	0.24090719
H	5.41320179	4.15581084	-1.54199740
O	-3.01800530	3.30716930	-0.04826242
H	-1.53918175	2.77875717	-1.09294766
H	-0.79776941	1.98778612	1.72227187
C	-3.72865173	3.16646092	0.89994970
O	-4.44235034	3.03781164	1.84087578



III-a (propeller): E_{Gibbs} = -1702.113307 eH

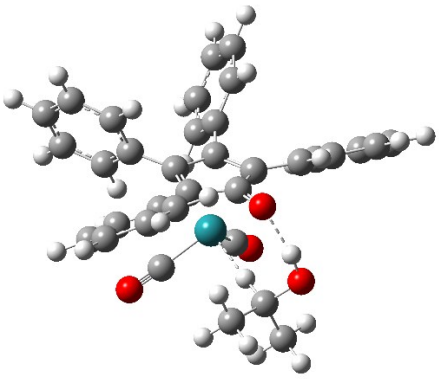
C	0.27366266	1.25694969	-0.91065139
C	1.06553009	0.06586472	-0.70451968
C	0.11863057	-1.02372892	-0.41562646
C	-1.21162262	-0.47112011	-0.38637689
C	-1.11244138	0.97463502	-0.65702496
Ru	0.06181646	0.54708986	1.34961032
C	-1.19072783	1.09366780	2.64298269
C	1.12221736	-0.30233119	2.64692688
O	1.81027898	-0.83102020	3.45207281
O	-1.97752767	1.46479668	3.44453147
O	0.70726046	2.48355709	-1.35899567
C	-2.21989248	1.93113135	-0.91909918
C	-3.29203762	1.56685441	-1.76656620
C	-2.19233356	3.23942930	-0.38474800
C	-4.31592800	2.48436609	-2.06124875
H	-3.32370837	0.57161232	-2.19996227
C	-3.21395818	4.15640948	-0.68009577
H	-1.36913333	3.53214019	0.26066694
C	-4.28286135	3.78248427	-1.51833335
H	-5.13350533	2.18601625	-2.71327158
H	-3.17810383	5.15739059	-0.25687917
H	-5.07572033	4.49161040	-1.74467924
C	-2.47970317	-1.24590125	-0.28721689
C	-2.68851753	-2.34672012	-1.15199657
C	-3.51329132	-0.88656387	0.60713503
C	-3.89344326	-3.07054406	-1.11817968
H	-1.90896199	-2.63399121	-1.85196972
C	-4.71874324	-1.60712895	0.64022353
H	-3.37510544	-0.04512170	1.27923171
C	-4.91499310	-2.70404207	-0.22146323
H	-4.03277743	-3.91515858	-1.78879783
H	-5.49982837	-1.31418946	1.33742871
H	-5.84706802	-3.26342733	-0.19325012
C	0.47675877	-2.46454275	-0.30155431
C	1.25380003	-3.07431970	-1.31434995
C	0.02223294	-3.26099677	0.77413972
C	1.56650754	-4.44408117	-1.25264491
H	1.60928797	-2.48051346	-2.15178157
C	0.33240913	-4.62910111	0.83564379
H	-0.56934180	-2.80357645	1.56271910
C	1.10711602	-5.22800619	-0.17752445
H	2.16614952	-4.89481059	-2.03989538
H	-0.02426843	-5.22382661	1.67292827
H	1.35105533	-6.28650951	-0.12741850
C	2.50805996	-0.04831254	-1.05228866
C	2.94205090	0.41493567	-2.31900986
C	3.46149614	-0.62094682	-0.18030503
C	4.29254837	0.31236350	-2.69925202
H	2.21965561	0.84597772	-3.00789515
C	4.81016263	-0.72805842	-0.56127270
H	3.14952663	-0.98188771	0.79502181
C	5.23345505	-0.25898362	-1.82112964
H	4.60659446	0.67302869	-3.67592369
H	5.52762012	-1.17282307	0.12374784
H	6.27763224	-0.34034180	-2.11303482
O	3.24603917	3.17730562	-0.20904464
H	1.64360883	2.67147220	-1.12551938
H	0.85400519	1.88254046	1.76669711
C	4.12828944	3.04755597	0.58317834
O	5.00968217	2.93100196	1.37174529



Isopropanol mediation with Shvo catalyst

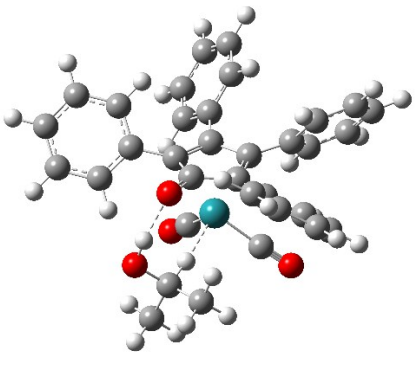
II-b (mirror): **E_{Gibbs} = -1706.628511 eH**

C	-0.02135582	-1.07227686	1.33386831
C	1.19718257	-0.34100424	0.87789314
C	0.77533816	0.94896144	0.37760140
C	-0.69693397	0.99201142	0.37383563
C	-1.19473008	-0.27069617	0.87793173
Ru	-0.01304129	-0.58527313	-1.10736544
C	-1.38023634	-0.42107277	-2.41681011
C	1.35377510	-0.48192035	-2.42668774
O	2.22137359	-0.36951398	-3.21965849
O	-2.24870066	-0.27349525	-3.20431389
O	-0.05725908	-2.23830347	1.85640998
C	-2.60776989	-0.63327837	1.14956413
C	-2.92515337	-1.47340274	2.24662115
C	-3.67061556	-0.14365439	0.34942267
C	-4.26147235	-1.80193276	2.53562677
H	-2.12527286	-1.87446598	2.85806310
C	-5.00258707	-0.47419829	0.63946123
H	-3.45971902	0.49425984	-0.50307817
C	-5.30746180	-1.30519826	1.73606887
H	-4.48242572	-2.44735081	3.38252528
H	-5.80023557	-0.08794213	0.00954390
H	-6.34019819	-1.56271402	1.95884532
C	-1.49294842	2.23868749	0.19734163
C	-2.08626973	2.80857703	1.34850566
C	-1.65271757	2.88859421	-1.04379910
C	-2.81836684	4.00392796	1.25764358
H	-1.97692950	2.31204812	2.30959176
C	-2.39062767	4.08172459	-1.13638481
H	-1.21537688	2.45381129	-1.93795374
C	-2.97409842	4.64569150	0.01352689
H	-3.26809071	4.42946430	2.15135811
H	-2.50999767	4.56611344	-2.10233703
H	-3.54502117	5.56820923	-0.05834261
C	1.64443054	2.14448183	0.19543025
C	2.31908492	2.64797908	1.33263955
C	1.79374344	2.81382655	-1.03692799
C	3.11934630	3.79835113	1.23757514
H	2.21881079	2.13538474	2.28604565
C	2.60029052	3.96110065	-1.13403274
H	1.29520316	2.42870114	-1.92171818
C	3.26382902	4.45992885	0.00256112
H	3.63097282	4.17294274	2.12070716
H	2.71092866	4.46053294	-2.09332181
H	3.88766653	5.34722995	-0.07295880
C	2.58553297	-0.79215731	1.14234914
C	2.85704032	-1.63599362	2.24774965
C	3.67008300	-0.38303869	0.32714667
C	4.17163738	-2.04415606	2.53261423
H	2.03866978	-1.98087889	2.86893854
C	4.98049024	-0.79346672	0.61191477
H	3.49308492	0.25300600	-0.53459542
C	5.24042109	-1.62608763	1.71871861
H	4.35739624	-2.69388821	3.38453739
H	5.79573550	-0.46989522	-0.03068158
H	6.25607933	-1.94777547	1.93659046
C	-0.13240332	-3.71155167	-1.05896790
H	-0.02593211	-2.55810907	-1.20494979
O	0.63810527	-4.11154415	0.07046354
H	0.37710761	-3.61485888	0.89716431
C	-1.63238691	-4.00163514	-0.88412098
H	-2.20421004	-3.66387606	-1.75753679
H	-1.77534050	-5.08329677	-0.76589414
H	-2.02990974	-3.50344690	0.00743486
C	0.49214278	-4.34490476	-2.30420757
H	0.40453224	-5.43639669	-2.23766151
H	-0.01494124	-4.00367922	-3.21488208
H	1.55567771	-4.09155829	-2.36460204



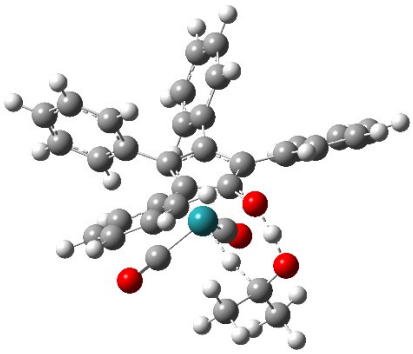
II-b (propeller): **E_{Gibbs} = -1706.627163 eH**

C	-0.06636160	-1.04165044	-1.33713134
C	-1.17951964	-0.13529333	-0.91453158
C	-0.59024012	1.08316585	-0.40935554
C	0.87510885	0.91674177	-0.37601301
C	1.19555438	-0.41105380	-0.85701207
Ru	-0.06815524	-0.57197961	1.08610263
C	1.28065393	-0.68816325	2.41948453
C	-1.40442696	-0.22306717	2.39243754
O	-2.24219517	0.04937070	3.17983976
O	2.14129139	-0.73026411	3.22721612
O	-0.18596929	-2.19714681	-1.86286986
C	2.53754762	-0.95894703	-1.18928068
C	3.47009696	-0.17618093	-1.91164000
C	2.87762255	-2.29203346	-0.86316272
C	4.71708215	-0.70713156	-2.28266735
H	3.21962521	0.84262498	-2.19256584
C	4.12604804	-2.82070876	-1.23437544
H	2.16847705	-2.92164363	-0.33318244
C	5.05276112	-2.03167317	-1.94234299
H	5.42049443	-0.09108482	-2.83808051
H	4.36963535	-3.84814875	-0.97508754
H	6.01766561	-2.44335277	-2.22925036
C	1.84856430	2.01470789	-0.11956138
C	1.70659485	3.23878465	-0.81631425
C	2.96004524	1.85030745	0.73735541
C	2.64745257	4.27058535	-0.65465364
H	0.86684424	3.38333875	-1.48926068
C	3.89559616	2.88365089	0.90531722
H	3.10076175	0.91633083	1.27024675
C	3.74435058	4.09962230	0.21049140
H	2.52171000	5.20249849	-1.20024985
H	4.74084693	2.73763322	1.57290641
H	4.47000415	4.89884770	0.34032712
C	-1.29981369	2.36442849	-0.14194812
C	-2.13359907	2.91017879	-1.14604941
C	-1.11942672	3.08311516	1.06040562
C	-2.77045426	4.14779698	-0.95046080
H	-2.28265915	2.36800306	-2.07575732
C	-1.76027732	4.31715588	1.25768768
H	-0.48246723	2.67213029	1.83883348
C	-2.58782002	4.85587855	0.25305044
H	-3.40857897	4.55350692	-1.73158279
H	-1.61546420	4.85463998	2.19138732
H	-3.08504923	5.81046102	0.40712124
C	-2.60873414	-0.40697269	-1.20961827
C	-2.95352223	-1.13550778	-2.37575573
C	-3.65345623	0.05128919	-0.36924492
C	-4.30062140	-1.38484192	-2.69351641
H	-2.16760098	-1.51296091	-3.02026599
C	-4.99658392	-0.19979192	-0.68781876
H	-3.42065015	0.60241196	0.53655656
C	-5.32905170	-0.91894182	-1.85343618
H	-4.54345739	-1.94505115	-3.59329859
H	-5.78088330	0.16024948	-0.02642615
H	-6.37018069	-1.11528776	-2.09828610
C	-0.61054974	-3.68562203	1.02424498
H	-0.40177559	-2.55535515	1.17765133
O	0.17117749	-4.15738968	-0.07797873
H	-0.02140359	-3.64744478	-0.91544739
C	-0.10965698	-4.38759691	2.28850308
H	-0.62753945	-4.00776312	3.17759375
H	-0.29542925	-5.46530548	2.20379551
H	0.96843483	-4.23614481	2.40882895
C	-2.11987466	-3.83525845	0.77633137
H	-2.36025516	-4.89926613	0.65637301
H	-2.69891259	-3.43556476	1.61820812
H	-2.42433103	-3.30959729	-0.13577430



TS: II-b – III-b (mirror): E_{Gibbs} = -1706.619494 eH

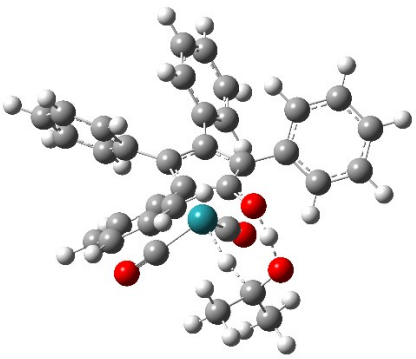
C	0.02226423	-1.05729551	-1.24991866
C	-1.18692188	-0.33044867	-0.86644902
C	-0.76421187	0.97613889	-0.36166342
C	0.68872264	1.02175943	-0.36639574
C	1.18747211	-0.25755850	-0.86884520
Ru	0.01503610	-0.61692805	1.12674685
C	1.37068172	-0.50667141	2.43601455
C	-1.35561249	-0.60514885	2.42757490
O	-2.23078246	-0.59397175	3.22251583
O	2.23761913	-0.43708595	3.23818806
O	0.07340478	-2.27414798	-1.78550187
C	2.59818387	-0.61684749	-1.16192818
C	2.90042399	-1.43360219	-2.28001845
C	3.66978046	-0.14216595	-0.36632953
C	4.23287820	-1.75634678	-2.59306503
H	2.09073391	-1.82118173	-2.88784993
C	4.99850565	-0.46594498	-0.68072780
H	3.46805637	0.47794514	0.50161956
C	5.28923369	-1.27463478	-1.79747631
H	4.44311474	-2.38383763	-3.45612945
H	5.80432537	-0.09075264	-0.05446379
H	6.31918107	-1.52592823	-2.03970502
C	1.49851447	2.25867060	-0.18363509
C	2.10374532	2.83270892	-1.32647269
C	1.66202169	2.89665568	1.06381906
C	2.85070527	4.01796218	-1.22203799
H	1.99041835	2.34729334	-2.29278132
C	2.41199019	4.08126783	1.17026374
H	1.21556729	2.45791130	1.95202271
C	3.00783320	4.64793470	0.02797414
H	3.30944391	4.44597594	-2.11010523
H	2.53150790	4.55665565	2.14077873
H	3.58887161	5.56335197	0.11016964
C	-1.64822695	2.15980044	-0.17040788
C	-2.31780588	2.68117920	-1.30246688
C	-1.81905101	2.80115398	1.07441307
C	-3.13363647	3.81933393	-1.19062939
H	-2.20020046	2.19185659	-2.26615508
C	-2.63806441	3.93834917	1.18836869
H	-1.32460682	2.40112231	1.95541969
C	-3.29688977	4.45363341	0.05637657
H	-3.64128106	4.20703803	-2.07053909
H	-2.76228011	4.41668773	2.15684192
H	-3.93105578	5.33252538	0.14439287
C	-2.57401246	-0.77126105	-1.16273777
C	-2.82709215	-1.58004808	-2.29759478
C	-3.67032732	-0.37924521	-0.35744520
C	-4.13732751	-1.97517915	-2.61869356
H	-1.99706496	-1.90694028	-2.91427238
C	-4.97751391	-0.77536600	-0.67887667
H	-3.50528163	0.23262870	0.52411926
C	-5.21978692	-1.57555089	-1.81288690
H	-4.30992871	-2.59824026	-3.49314216
H	-5.80370597	-0.46442672	-0.04398048
H	-6.23257540	-1.88545220	-2.05955504
C	0.12354150	-3.80916340	0.96789074
H	0.06079749	-2.30443556	1.27998174
O	-0.46862712	-3.96686801	-0.19846655
H	-0.19193938	-3.18551365	-1.10950596
C	1.64512824	-3.96643489	1.02022723
H	2.12346327	-3.43868122	0.18998123
H	2.05758127	-3.60826605	1.96798600
H	1.87399312	-5.03829188	0.91976044
C	-0.67860421	-4.27678181	2.17810010
H	-0.26184389	-3.89545831	3.11529618
H	-1.72351347	-3.97102040	2.08083121
H	-0.64552816	-5.37625850	2.20231470



ν_{TS} = -847.31 cm^{-1}

TS: II-b – III-b (propeller): E_{Gibbs} = -1706.617372 eH

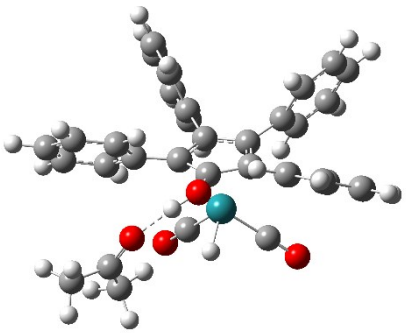
C	0.05088943	-1.03099026	-1.25488519
C	-1.19354922	-0.38056783	-0.86066645
C	-0.84968589	0.95555968	-0.36735838
C	0.59735543	1.09335355	-0.39685620
C	1.16926782	-0.15485584	-0.89715427
Ru	0.06167315	-0.61863018	1.10187012
C	1.38389814	-0.33174310	2.41913370
C	-1.29718685	-0.79967910	2.40222973
O	-2.16404795	-0.92105861	3.19715973
O	2.22710596	-0.14335152	3.22666436
O	0.16889953	-2.23413112	-1.81054469
C	2.59179014	-0.44309937	-1.21551834
C	2.91079485	-1.15770187	-2.39675611
C	3.65201337	-0.00857394	-0.38373308
C	4.25041084	-1.41866590	-2.73682047
H	2.10954923	-1.51709561	-3.03319564
C	4.98822295	-0.26922463	-0.72534371
H	3.43608294	0.53106285	0.53333173
C	5.29605300	-0.97538852	-1.90537716
H	4.47422047	-1.96883340	-3.64776076
H	5.78581078	0.07398511	-0.07085795
H	6.33139258	-1.17882036	-2.16853330
C	1.34365044	2.35354972	-0.12708108
C	2.17863024	2.88967944	-1.13539483
C	1.20000377	3.06381025	1.08535172
C	2.85208567	4.10720441	-0.93449656
H	2.29976191	2.35529476	-2.07375793
C	1.87388120	4.27974039	1.28703805
H	0.56325881	2.66073993	1.86850536
C	2.70311709	4.80760201	0.27803608
H	3.49130684	4.50401463	-1.71946145
H	1.75409440	4.81093608	2.22799219
H	3.22718983	5.74720836	0.43558793
C	-1.81621035	2.05800485	-0.09911869
C	-1.67665944	3.28362995	-0.79323475
C	-2.91400144	1.90102343	0.77662045
C	-2.60465845	4.32379190	-0.61055750
H	-0.84586116	3.42198340	-1.47882622
C	-3.84024059	2.94034596	0.96188699
H	-3.04928542	0.96759853	1.31311636
C	-3.69015696	4.15808791	0.27005326
H	-2.47888496	5.25764834	-1.15307872
H	-4.67595411	2.79857251	1.64252547
H	-4.40717913	4.96266397	0.41451825
C	-2.54342530	-0.89703200	-1.21258273
C	-3.45073766	-0.07852752	-1.92694506
C	-2.91958670	-2.22766837	-0.91713463
C	-4.70578738	-0.57249075	-2.32154801
H	-3.17413665	0.93970366	-2.18314104
C	-4.17468298	-2.72031468	-1.31327158
H	-2.23314362	-2.88185241	-0.38762337
C	-5.07548876	-1.89563411	-2.01404743
H	-5.38900489	0.07210629	-2.86960423
H	-4.44574048	-3.74669977	-1.07774177
H	-6.04670681	-2.27859477	-2.31876377
C	0.54063245	-3.75384643	0.93396726
H	0.34065435	-2.29173947	1.24439299
O	-0.09661887	-3.98166343	-0.20048158
H	0.05489661	-3.15444169	-1.14712506
C	2.07154316	-3.76625429	0.89998019
H	2.50131504	-3.36880068	1.82443265
H	2.39411097	-4.81173788	0.78270261
H	2.45144056	-3.19716902	0.04683072
C	-0.13183329	-4.30780512	2.18880179
H	0.02293651	-5.39676036	2.20319481
H	0.29784275	-3.88285447	3.10123210
H	-1.20838774	-4.11867266	2.16313770



ν_{TS} = -791.12 cm^{-1}

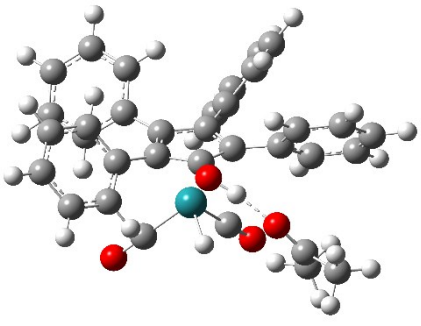
III-b (mirror): E_{Gibbs} = -1706.642328 eH

C	-0.46975093	-1.08176725	0.84980947
C	0.95552352	-1.15966196	0.61920942
C	1.42280700	0.21535513	0.36431526
C	0.27673517	1.08735177	0.35653091
C	-0.92141957	0.27417008	0.62163184
Ru	0.02510517	-0.39607238	-1.41949431
C	-0.88546874	0.61539023	-2.71010596
C	1.23012546	-1.07734608	-2.69388619
O	1.98587635	-1.52403814	-3.48689228
O	-1.49007687	1.24083800	-3.51647275
O	-1.21443652	-2.14988041	1.25299804
C	-2.27567665	0.80100197	0.93469641
C	-2.93080585	0.37971272	2.11730792
C	-2.91412497	1.76353589	0.11847619
C	-4.18734951	0.90317695	2.46982809
H	-2.45417900	-0.35205112	2.76349256
C	-4.16730125	2.28993895	0.47210857
H	-2.42961146	2.10325723	-0.79197907
C	-4.81271455	1.86131942	1.64933188
H	-4.67197923	0.56730923	3.38371200
H	-4.63667079	3.03398454	-0.16716745
H	-5.78151148	2.27193553	1.92447815
C	0.31087242	2.57738784	0.38656998
C	0.09125550	3.22533725	1.62523814
C	0.56688889	3.36813569	-0.75328426
C	0.13250306	4.62654590	1.72044301
H	-0.11087965	2.62850626	2.51150882
C	0.60817684	4.77104731	-0.66080093
H	0.72327364	2.88544427	-1.71420477
C	0.39222561	5.40609891	0.57636876
H	-0.03744940	5.10760736	2.68083066
H	0.80504183	5.36314427	-1.55134665
H	0.42270482	6.49079214	0.64833216
C	2.83967136	0.67240121	0.38821129
C	3.59278272	0.47981105	1.57051504
C	3.44889148	1.32929546	-0.70242391
C	4.91896204	0.93493335	1.65880255
H	3.13781964	-0.02851692	2.41684094
C	4.77632021	1.78504817	-0.61599916
H	2.88805515	1.46754951	-1.62286591
C	5.51712908	1.59081561	0.56504244
H	5.48312621	0.77687148	2.57494944
H	5.22977957	2.28527331	-1.46836487
H	6.54478733	1.94028865	0.63141043
C	1.80452707	-2.36166249	0.82496578
C	1.43643650	-3.34040907	1.78048115
C	3.00683603	-2.54982380	0.10069624
C	2.25139299	-4.46362053	2.00787720
H	0.50760017	-3.22691111	2.32711370
C	3.81843250	-3.67143493	0.32855726
H	3.30741497	-1.82315767	-0.64772598
C	3.44689448	-4.63618886	1.28576734
H	1.94902084	-5.20380082	2.74540033
H	4.73470304	-3.79512995	-0.24379649
H	4.07461522	-5.50708275	1.46010229
O	-3.75882752	-2.45510166	0.64763414
H	-2.18064580	-2.16150499	0.97788428
H	-0.91878981	-1.61093796	-1.89055295
C	-4.61860493	-2.38532101	-0.26279385
C	-4.26160642	-1.97021866	-1.67387819
H	-3.23963504	-1.58780569	-1.72603311
H	-4.34872799	-2.84017183	-2.34107368
H	-4.96411445	-1.21144050	-2.04116637
C	-6.06919033	-2.71296052	0.03457487
H	-6.64009617	-1.77533942	0.09870576
H	-6.51293916	-3.30904882	-0.77166969
H	-6.15388145	-3.24079591	0.98769057



III-b (propeller): E_{Gibbs} = -1706.641243 eH

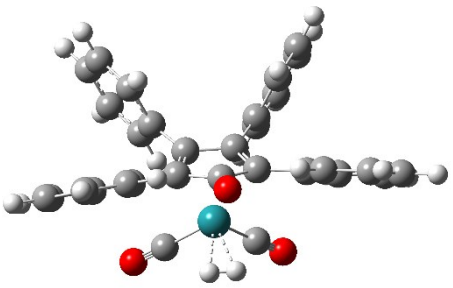
C	-0.47235894	-1.05592649	-0.84730137
C	-0.90432264	0.31125826	-0.64468738
C	0.31126225	1.11126421	-0.40486087
C	1.44428847	0.22297858	-0.39671288
C	0.94955130	-1.14650198	-0.61713993
Ru	0.01535258	-0.37393988	1.39837949
C	1.17110581	-1.11477839	2.68352475
C	-0.83041060	0.70662037	2.68096635
O	-1.39211703	1.38091405	3.47753417
O	1.89099124	-1.60848736	3.48285487
O	-1.20248622	-2.12805116	-1.25948439
C	1.75231000	-2.36859811	-0.88672692
C	1.42007014	-3.60538735	-0.28944788
C	2.82745662	-2.32654528	-1.80461317
C	2.14919644	-4.76714736	-0.59146376
H	0.58953754	-3.64993581	0.40915498
C	3.55939839	-3.48873326	-2.10603415
H	3.08840821	-1.38868446	-2.28643575
C	3.22484971	-4.71419940	-1.49983340
H	1.88060032	-5.70944675	-0.11973734
H	4.38496189	-3.43633159	-2.81208447
H	3.79150481	-5.61321375	-1.73146612
C	2.87698675	0.62770896	-0.34839586
C	3.81156996	-0.01900935	0.49242199
C	3.34219774	1.65063571	-1.20902344
C	5.16659754	0.34994251	0.48119293
H	3.48090246	-0.81081889	1.15739139
C	4.69825335	2.02210799	-1.22025804
H	2.64400051	2.15363013	-1.87155104
C	5.61776896	1.37438933	-0.37403050
H	5.86631108	-0.16000920	1.13879851
H	5.03337931	2.81274532	-1.88751146
H	6.66663028	1.66149808	-0.38061874
C	0.36320874	2.59868876	-0.34183854
C	-0.15831105	3.35865766	-1.41525843
C	0.96478327	3.28005983	0.73990450
C	-0.07793831	4.76246590	-1.40694663
H	-0.62289875	2.85145714	-2.25667908
C	1.04798651	4.68244622	0.74836369
H	1.36319169	2.70685939	1.57294833
C	0.52660685	5.43100664	-0.32512441
H	-0.48569075	5.32984711	-2.24029322
H	1.51396329	5.18818257	1.59053938
H	0.58758329	6.51674712	-0.31692090
C	-2.26243885	0.83584781	-0.94863288
C	-2.89977797	1.79930309	-0.13219864
C	-2.92806907	0.39971019	-2.12027625
C	-4.16105494	2.31345060	-0.47563568
H	-2.40800441	2.14940029	0.77036341
C	-4.19383160	0.90952998	-2.46173183
H	-2.45154144	-0.33240318	-2.76632878
C	-4.81747181	1.86926664	-1.64144394
H	-4.62805240	3.06005350	0.16239836
H	-4.68638484	0.56233789	-3.36706618
H	-5.79285805	2.26950995	-1.90826747
O	-3.73664518	-2.52251880	-0.64693684
H	-2.17229514	-2.14977791	-1.00227243
H	-1.00637451	-1.52489428	1.87037209
C	-4.65087919	-2.31869000	0.18752009
C	-4.43427872	-1.45245903	1.41039538
H	-3.38139052	-1.45258923	1.70716465
H	-4.70707856	-0.41720013	1.15736318
H	-5.06638808	-1.77037363	2.24643635
C	-6.02341026	-2.92700050	-0.02019619
H	-6.20187444	-3.69693943	0.74387499
H	-6.80307954	-2.16448890	0.10449942
H	-6.09588881	-3.38083705	-1.01137203



Dihydrogen mediation with Shvo catalyst

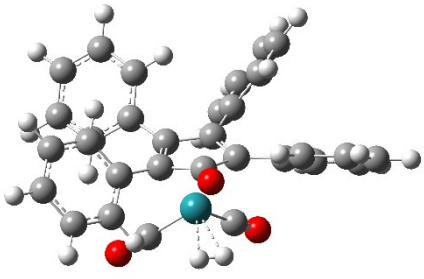
II-c (mirror): **E_{Gibbs} = -1513.544649 eH**

C	-0.00011672	-1.83476924	-0.86531409
C	-1.19427705	-0.99081947	-0.49710101
C	-0.73505627	0.38101880	-0.36668781
C	0.73506858	0.38094486	-0.36680144
C	1.19412695	-0.99091899	-0.49715048
Ru	-0.00007199	-0.69828720	1.47478685
C	1.37056484	-0.12949383	2.68437269
C	-1.37096139	-0.13056958	2.68460297
O	-2.23066987	0.24511714	3.39937036
O	2.23012779	0.24701174	3.39890694
O	-0.00016188	-3.02257034	-1.28026178
C	2.60556565	-1.44067951	-0.62468507
C	2.92959228	-2.57114208	-1.41707034
C	3.66265946	-0.75723021	0.02938609
C	4.26512259	-2.99022804	-1.55620294
H	2.13416691	-3.12259085	-1.90346947
C	4.99261321	-1.17866144	-0.11071108
H	3.44971170	0.10525515	0.65282549
C	5.30413661	-2.29888619	-0.90719473
H	4.48962898	-3.86007494	-2.16923539
H	5.78349351	-0.63749488	0.40321081
H	6.33544306	-2.62704374	-1.01379520
C	1.56658314	1.60532362	-0.54462807
C	2.20553365	1.78412470	-1.79451695
C	1.71296812	2.60148082	0.44256482
C	2.96821170	2.93563512	-2.04934202
H	2.10793468	1.01895272	-2.56051808
C	2.48141007	3.75145146	0.19035507
H	1.24125045	2.47191864	1.41209806
C	3.11004790	3.92489408	-1.05677394
H	3.45267981	3.05775233	-3.01494590
H	2.58961799	4.50589265	0.96561203
H	3.70508033	4.81384435	-1.25132635
C	-1.56635199	1.60552055	-0.54484105
C	-2.20433160	1.78462485	-1.79517835
C	-1.71341004	2.60147340	0.44245067
C	-2.96670312	2.93626745	-2.05034089
H	-2.10622942	1.01958444	-2.56124862
C	-2.48153313	3.75157975	0.18990273
H	-1.24254955	2.47150698	1.41233581
C	-3.10918117	3.92534155	-1.05768120
H	-3.45043214	3.05864351	-3.01628270
H	-2.59028874	4.50587057	0.96522968
H	-3.70396385	4.81439942	-1.25250926
C	-2.60576725	-1.44038135	-0.62468394
C	-2.92990456	-2.57101109	-1.41677903
C	-3.66281760	-0.75655352	0.02907562
C	-4.26549709	-2.98989599	-1.55594831
H	-2.13451829	-3.12273452	-1.90293333
C	-4.99282786	-1.17778266	-0.11106140
H	-3.44977539	0.10605262	0.65231861
C	-5.30446190	-2.29817620	-0.90726902
H	-4.49008558	-3.85988010	-2.16875640
H	-5.78367799	-0.63633394	0.40261033
H	-6.33581888	-2.62616467	-1.01390318
H	0.39779376	-2.51191367	2.03976790
H	-0.39669844	-2.51216373	2.03968451



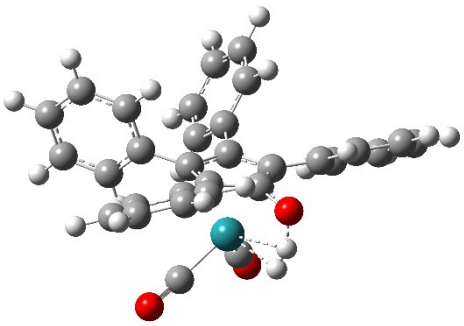
II-c (propeller): **E_{Gibbs} = -1513.542696 eH**

C	0.05460334	-1.78415432	-0.91365661
C	-1.16747201	-0.96819537	-0.56460561
C	-0.73986968	0.40868975	-0.40019244
C	0.73031613	0.44283387	-0.35966113
C	1.21458861	-0.92082292	-0.49509881
Ru	-0.01098785	-0.72044276	1.43995504
C	1.33951324	-0.25052653	2.70829272
C	-1.38367761	-0.12947128	2.64169176
O	-2.23676826	0.26717873	3.35268229
O	2.18636399	0.04925415	3.47331921
O	0.11140886	-2.95945496	-1.35023200
C	2.61585875	-1.36774446	-0.71736523
C	3.45479504	-0.69873853	-1.63999459
C	3.10628769	-2.53207846	-0.08445958
C	4.75275503	-1.17032583	-1.90329177
H	3.09231074	0.18286318	-2.16024868
C	4.40236705	-3.00593249	-0.34728231
H	2.46724840	-3.07159195	0.60979674
C	5.23445406	-2.32377781	-1.25597428
H	5.38240134	-0.64184534	-2.61531424
H	4.75979080	-3.90371624	0.15118676
H	6.23841555	-2.68839432	-1.46018052
C	1.55772459	1.68125323	-0.43777673
C	1.25474888	2.64693111	-1.42777958
C	2.68770633	1.89055775	0.38392701
C	2.05394077	3.79285865	-1.58284823
H	0.39943295	2.50115920	-2.08024557
C	3.48253471	3.03848028	0.23428435
H	2.95487313	1.15760243	1.13702933
C	3.16926065	3.99701572	-0.74897857
H	1.80389265	4.52211625	-2.34942214
H	4.34459924	3.18100199	0.88085442
H	3.78498032	4.88570228	-0.86424230
C	-1.60835608	1.61859283	-0.45983015
C	-2.48486280	1.77379675	-1.55944762
C	-1.53858516	2.64573690	0.50656065
C	-3.27182185	2.93125556	-1.68759749
H	-2.55095160	0.99056759	-2.30954604
C	-2.32883126	3.80009700	0.38115813
H	-0.86780511	2.53865660	1.35442479
C	-3.19861497	3.94878682	-0.71668683
H	-3.94145054	3.03445349	-2.53783687
H	-2.26659066	4.57875505	1.13712812
H	-3.81194003	4.84147408	-0.81223636
C	-2.56050403	-1.46587210	-0.71626270
C	-2.83495490	-2.53839748	-1.60207313
C	-3.64205634	-0.89735336	0.00357535
C	-4.14913948	-3.01188687	-1.76897455
H	-2.01772641	-3.00541664	-2.13891871
C	-4.95082603	-1.37235229	-0.16472201
H	-3.46518637	-0.08320413	0.69923723
C	-5.21399766	-2.43306784	-1.05491206
H	-4.33633633	-3.83599871	-2.45341598
H	-5.76225181	-0.92015546	0.40055890
H	-6.22856032	-2.80310768	-1.18287854
H	-0.50142630	-2.52408635	1.98265249
H	0.29039870	-2.57030723	1.94733147



TS: II-c – IV (mirror): E_{Gibbs} = -1513.497916 eH

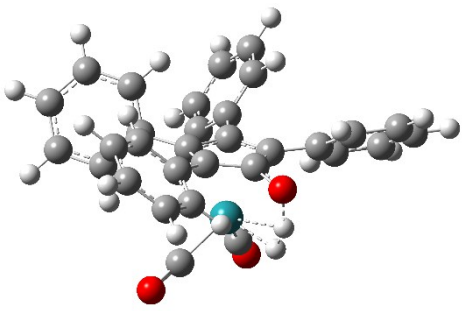
C	0.01599424	-1.75612594	-0.64251037
C	-1.20074081	-0.91175543	-0.50228988
C	-0.75820161	0.46607818	-0.38205224
C	0.70423725	0.48250383	-0.34169448
C	1.19062637	-0.89378136	-0.56730394
Ru	0.00224629	-0.76064261	1.44306929
C	1.49295701	-0.62032549	2.62758005
C	-1.22445069	-0.10277545	2.74566036
O	-2.01475486	0.30265950	3.52140420
O	2.43933607	-0.53322889	3.32444624
O	0.01818365	-3.09405601	-0.52527700
C	2.58312964	-1.35069899	-0.78223850
C	3.70352388	-0.62377829	-0.31036323
C	2.81102319	-2.54626838	-1.50923315
C	5.00884669	-1.07078968	-0.56819653
H	3.56355237	0.28558609	0.26437180
C	4.11865038	-2.98832304	-1.76831543
H	1.96193514	-3.13354715	-1.84161536
C	5.22539846	-2.25318480	-1.30198032
H	5.85450556	-0.49963272	-0.19280897
H	4.27226461	-3.90843419	-2.32707509
H	6.23745848	-2.59865853	-1.49933295
C	1.51921644	1.72502353	-0.45683018
C	1.85014235	2.53429088	0.64910947
C	1.96194167	2.11034462	-1.74368417
C	2.60751375	3.70689888	0.47738460
H	1.52547764	2.23813262	1.64328011
C	2.71663851	3.28280613	-1.91668198
H	1.71919062	1.48977948	-2.60301187
C	3.04249265	4.08610655	-0.80637849
H	2.85784715	4.31749134	1.34139353
H	3.05110477	3.56653517	-2.91152754
H	3.62976708	4.99124067	-0.94027663
C	-1.60695952	1.68059740	-0.50810706
C	-1.63407695	2.70685733	0.46023594
C	-2.37650349	1.83146974	-1.68626706
C	-2.41458799	3.85805873	0.25869955
H	-1.05792593	2.60102460	1.37473304
C	-3.15088441	2.98536338	-1.89029403
H	-2.36787288	1.04620731	-2.43747401
C	-3.17421900	4.00363090	-0.91754839
H	-2.43018919	4.63603976	1.01775491
H	-3.73615112	3.08644155	-2.80085090
H	-3.77847124	4.89414624	-1.07227131
C	-2.58422632	-1.41984077	-0.66282358
C	-2.81825646	-2.55183803	-1.48089317
C	-3.69001604	-0.79916923	-0.03292745
C	-4.12360008	-3.03480750	-1.67678046
H	-1.97628574	-3.06214901	-1.93597558
C	-4.99192659	-1.28485927	-0.22783461
H	-3.53633994	0.05826519	0.61572277
C	-5.21709120	-2.40410209	-1.05408000
H	-4.28389561	-3.90613442	-2.30721568
H	-5.82727494	-0.79596523	0.26755788
H	-6.22605815	-2.78191299	-1.20164278
H	-0.25972965	-2.95651153	0.85765275
H	-0.35341273	-2.58830434	1.74080756



ν_{TS} = -1947.41 cm^{-1}

TS: II-c – IV (propeller): E_{Gibbs} = -1513.497922 eH

C	0.03711959	-1.72112254	-0.73002365
C	-1.19148686	-0.89118211	-0.57171541
C	-0.76501949	0.48526988	-0.40458160
C	0.69630104	0.51589240	-0.35477385
C	1.19949017	-0.84921962	-0.62734861
Ru	-0.00763759	-0.82082266	1.38328476
C	1.47140222	-0.81047065	2.58628994
C	-1.20917817	-0.16864673	2.71239572
O	-1.98101233	0.23994968	3.50446756
O	2.40954405	-0.81788765	3.30103376
O	0.04594273	-3.06185457	-0.66639449
C	2.59671247	-1.27671074	-0.88860596
C	3.03469459	-2.57643102	-0.53070019
C	3.50216836	-0.42229155	-1.56394276
C	4.34165004	-2.99678664	-0.82353485
H	2.34161243	-3.25421938	-0.04596172
C	4.80965168	-0.84716391	-1.85627442
H	3.18834998	0.56706666	-1.87718293
C	5.23885583	-2.13426232	-1.48362854
H	4.65870331	-3.99706244	-0.53855339
H	5.48758617	-0.17470046	-2.37661431
H	6.25140537	-2.46173847	-1.70744505
C	1.50283672	1.77078803	-0.35802402
C	2.46772426	2.05991495	0.63046870
C	1.32546375	2.68755739	-1.42177218
C	3.24112304	3.23122890	0.55736173
H	2.61745089	1.37261310	1.45678594
C	2.09914489	3.85850424	-1.49681006
H	0.58577152	2.48194236	-2.19097727
C	3.06169209	4.13545802	-0.50698244
H	3.97941220	3.43552731	1.32863277
H	1.94907953	4.55064221	-2.32172018
H	3.65969976	5.04175598	-0.56264582
C	-1.63169617	1.69359376	-0.41649345
C	-1.54090741	2.69482761	0.57567224
C	-2.53144651	1.87726780	-1.49295672
C	-2.33460283	3.85083667	0.49830899
H	-0.85396161	2.56585554	1.40766057
C	-3.32101829	3.03717107	-1.57288117
H	-2.61271637	1.11513771	-2.26303165
C	-3.22767744	4.02787754	-0.57640418
H	-2.25729041	4.60875287	1.27367068
H	-4.00771528	3.16328537	-2.40621488
H	-3.84318133	4.92223274	-0.63490442
C	-2.56515201	-1.41995942	-0.75531812
C	-2.77557149	-2.49841775	-1.64859471
C	-3.68031952	-0.87753355	-0.07233615
C	-4.06900615	-3.00411054	-1.86610704
H	-1.92453988	-2.95087051	-2.14640122
C	-4.97021026	-1.38554833	-0.28947834
H	-3.54295169	-0.06433087	0.63431190
C	-5.17266736	-2.45005426	-1.19075904
H	-4.21159848	-3.83373855	-2.55431722
H	-5.81341521	-0.95758359	0.24723042
H	-6.17214261	-2.84571177	-1.35525307
H	-0.32596293	-2.98265805	0.70177607
H	-0.45376166	-2.64531974	1.59107165

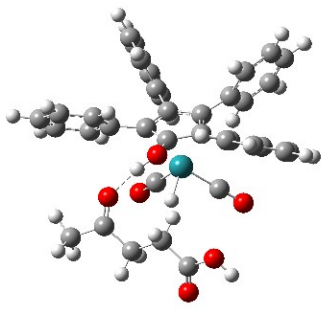


ν_{TS} = -1951.18 cm^{-1}

Levulinic acid Hydrogenation

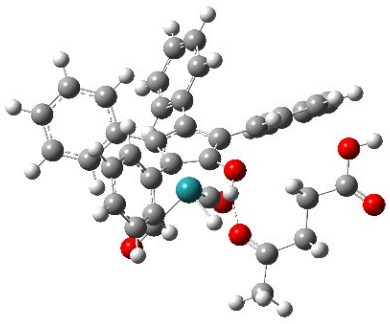
V (mirror): **E_{Gibbs} = -1934.455757 eH**

C	-0.42951328	0.07558445	1.20514420
C	0.19318554	-1.18749519	0.87898328
C	1.52490975	-0.87509588	0.33018778
C	1.66014249	0.55780889	0.26128775
C	0.42362765	1.16307342	0.77992419
Ru	-0.07786783	-0.05019385	-1.17426714
C	0.01015574	1.23569721	-2.53998734
C	-0.25297542	-1.46214248	-2.40485631
O	-0.37389710	-2.36088891	-3.16467966
O	0.04112495	2.06374941	-3.38720852
O	-1.63395850	0.16983823	1.84915347
C	0.22236904	2.60018990	1.10047155
C	-0.26328251	2.96694253	2.37845748
C	0.55619421	3.62616233	0.18682340
C	-0.41417872	4.31962442	2.72955481
H	-0.51908517	2.19405093	3.09802553
C	0.40890725	4.97769925	0.53807185
H	0.93122567	3.36873583	-0.79929318
C	-0.07881041	5.33258095	1.81150326
H	-0.78990091	4.58064774	3.71625871
H	0.67474358	5.75081142	-0.17895517
H	-0.19211827	6.37952220	2.08330375
C	2.92427902	1.30261837	-0.00032288
C	3.59948924	1.88229029	1.09970565
C	3.48669316	1.43932592	-1.28692218
C	4.80777113	2.57562148	0.91631462
H	3.17496768	1.78933030	2.09643182
C	4.69562936	2.13346693	-1.47316479
H	2.97089753	1.01309251	-2.14317075
C	5.36197875	2.70338673	-0.37228781
H	5.31340362	3.01445399	1.77324832
H	5.11164974	2.23039615	-2.47311254
H	6.29598988	3.24163186	-0.51553111
C	2.63670408	-1.84758797	0.14216920
C	3.11515325	-2.55241758	1.27195126
C	3.26041119	-2.06503993	-1.10507600
C	4.19187349	-3.44747013	1.15636124
H	2.64051098	-2.39852206	2.23780051
C	4.33769532	-2.96102879	-1.22275019
H	2.89076148	-1.54539862	-1.98497276
C	4.80938724	-3.65494441	-0.09259454
H	4.54599901	-3.98095514	2.03528120
H	4.80280082	-3.11832581	-2.19294826
H	5.64143255	-4.34921658	-0.18346091
C	-0.32483721	-2.53202698	1.24130341
C	-1.11464820	-2.70100657	2.40473279
C	-0.02283980	-3.67540150	0.46241167
C	-1.57822305	-3.97481309	2.77873566
H	-1.37419687	-1.83443533	3.00202497
C	-0.48602917	-4.94566038	0.83714831
H	0.57086102	-3.57419459	-0.44079107
C	-1.26619167	-5.10432219	1.99954123
H	-2.18579058	-4.08203177	3.67448538
H	-0.24299552	-5.80818651	0.22112941
H	-1.62712483	-6.08877883	2.28843689
O	-3.24104505	2.07350027	0.97707778
H	-2.20797070	0.94729079	1.57954812
H	-1.67293875	0.10399847	-1.33468903
C	-4.04660592	2.26038444	0.03378985
C	-4.72478839	1.11508777	-0.69692308
H	-4.26829207	1.04637277	-1.69645617
H	-5.77297008	1.38483410	-0.88456394
C	-4.37645936	3.66791133	-0.41851521
H	-4.43965384	3.72520832	-1.51172669
H	-5.36038101	3.95640766	-0.02058928
H	-3.62641054	4.36968719	-0.04578380
C	-4.62132078	-0.23918057	0.01860046
H	-3.57555761	-0.53846194	0.16064072
H	-5.05698343	-0.20143181	1.02483289
C	-5.31664313	-1.32983684	-0.76475037
O	-5.81075408	-1.22774786	-1.89905300
O	-5.34651058	-2.51981336	-0.05536052
H	-5.76162574	-3.23702293	-0.58723101



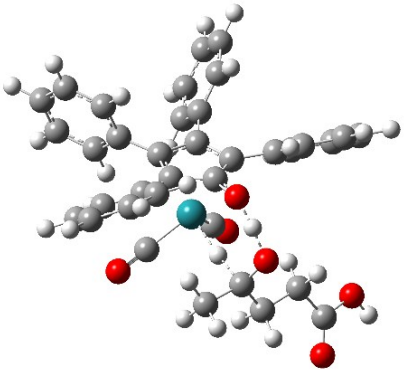
V (propeller): **E_{Gibbs} = -1934.454445 eH**

C	-0.53697812	0.14920663	0.52071681
C	0.06787037	-1.14764562	0.33925064
C	1.52761473	-0.94068436	0.35140109
C	1.78308329	0.47025513	0.47436085
C	0.48748644	1.16892651	0.52015000
Ru	0.62556996	0.13129820	-1.56549551
C	1.28770179	1.48068918	-2.68986595
C	0.79822927	-1.16653152	-2.91606729
O	0.88762536	-1.98990554	-3.76135140
O	1.67726685	2.35187448	-3.39165368
O	-1.87589143	0.31375859	0.74457780
C	0.25813197	2.59273570	0.88978817
C	0.78044567	3.08297779	2.11110713
C	-0.51026825	3.46185961	0.08512641
C	0.54376412	4.40823949	2.51258224
H	1.37228467	2.42481495	2.74165314
C	-0.75184328	4.78736179	0.48873808
H	-0.91028516	3.10495909	-0.85973920
C	-0.22502932	5.26721688	1.70233897
H	0.95696867	4.76903783	3.45160354
H	-1.34395824	5.44240988	-0.14587263
H	-0.40663069	6.29403298	2.01147926
C	3.10311704	1.11949216	0.70466107
C	3.98520186	0.58649595	1.67514834
C	3.48426643	2.30150977	0.02862664
C	5.21507520	1.20947449	1.95085944
H	3.70797132	-0.31336853	2.21575891
C	4.71186806	2.92533290	0.30413721
H	2.82412489	2.73352392	-0.71706987
C	5.58595541	2.38175008	1.26564469
H	5.87882231	0.78032857	2.69781499
H	4.98536023	3.83076118	-0.23212988
H	6.53798269	2.86320556	1.47640937
C	2.55321223	-2.01954128	0.39375123
C	2.48926813	-2.99605748	1.41550171
C	3.62157026	-2.07325411	-0.52891195
C	3.47074201	-3.99774795	1.51335461
H	1.67185828	-2.97044402	2.13130377
C	4.60436543	-3.07286232	-0.43104944
H	3.67515911	-1.33284102	-1.32291642
C	4.53386927	-4.04014729	0.59067618
H	3.40383933	-4.74176733	2.30366442
H	5.41848742	-3.09871477	-1.15130182
H	5.29225145	-4.81613633	0.66368351
C	-0.65597859	-2.44570368	0.37683229
C	-1.75516500	-2.61421333	1.25361992
C	-0.26285701	-3.54290532	-0.42582411
C	-2.43605478	-3.84274121	1.32545859
H	-2.07894428	-1.78362142	1.87110090
C	-0.94052971	-4.76998411	-0.35114836
H	0.57009968	-3.43789431	-1.11422147
C	-2.03248845	-4.92798508	0.52531242
H	-3.27935423	-3.94425213	2.00445579
H	-0.62130322	-5.59748829	-0.98018689
H	-2.55944977	-5.87794044	0.57923646
O	-3.48822073	2.11514394	-0.37939707
H	-2.30683075	1.14325443	0.39902984
H	-0.79169382	0.45148546	-2.25199800
C	-4.66160961	2.01474024	-0.81059332
C	-5.59062703	0.87942463	-0.41339045
H	-5.74359905	0.25105075	-1.30442958
H	-6.58338885	1.29823319	-0.19746947
C	-5.21686145	3.05193124	-1.76733630
H	-5.83488652	2.58600026	-2.54376255
H	-5.86287957	3.74719237	-1.21159640
H	-4.40414591	3.62212354	-2.22424255
C	-5.08931631	0.02065447	0.75683041
H	-4.11525737	-0.43346756	0.53926449
H	-4.93215297	0.62332700	1.66072919
C	-6.07044618	-1.08079000	1.08447472
O	-7.12345090	-1.34155364	0.48085555
O	-5.66214127	-1.81783759	2.18830201
H	-6.30774656	-2.53564766	2.38330970



TS: V – VI (mirror): E_{Gibbs} = -1934.433550 eH

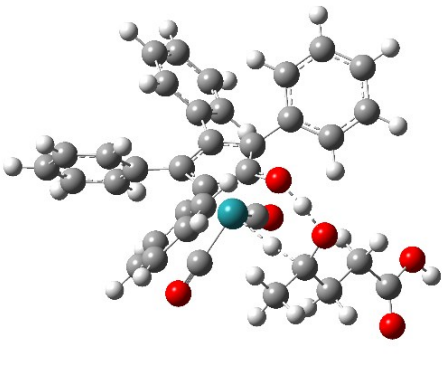
C	-0.10721224	-0.56432827	1.56374321
C	0.25779525	0.79674243	1.16720016
C	-0.84168223	1.31880465	0.35939551
C	-1.82833006	0.26366370	0.18872748
C	-1.35855608	-0.92532871	0.90247490
Ru	0.13350128	-0.41334566	-0.83274457
C	-0.52405981	-1.50606197	-2.22729922
C	1.21964423	0.57223168	-2.02205832
O	1.88948307	1.21414009	-2.75576351
O	-0.95557190	-2.19887650	-3.08250008
O	0.60782605	-1.37254570	2.34388117
C	-2.09743634	-2.19687187	1.11120811
C	-1.94606967	-2.90905350	2.32733312
C	-2.98165783	-2.71619756	0.13372116
C	-2.66284429	-4.09668440	2.55706644
H	-1.25838894	-2.53674748	3.07791942
C	-3.69567702	-3.90167690	0.36578257
H	-3.11243697	-2.19893263	-0.81154312
C	-3.54225109	-4.59955915	1.58003764
H	-2.53224577	-4.62720710	3.49738290
H	-4.36720655	-4.28142258	-0.40043287
H	-4.09535767	-5.51868174	1.75835243
C	-3.20497860	0.46989103	-0.34346841
C	-4.27443203	0.52795773	0.58075642
C	-3.48464988	0.63086528	-1.71655198
C	-5.59040319	0.74661973	0.13962305
H	-4.07322100	0.39834775	1.64141217
C	-4.80162517	0.84663327	-2.15983634
H	-2.67462971	0.57130298	-2.43839254
C	-5.85958746	0.90714536	-1.23361352
H	-6.40127652	0.78877416	0.86276576
H	-4.99912354	0.96362716	-3.22258676
H	-6.87828531	1.07287869	-1.57574014
C	-1.06034372	2.75150797	0.01675047
C	-1.18791240	3.67755385	1.07896638
C	-1.18437190	3.21791124	-1.30909453
C	-1.43740792	5.03529980	0.81923834
H	-1.08874045	3.33238856	2.10492943
C	-1.42929612	4.57740241	-1.57014283
H	-1.07350783	2.52236614	-2.13618953
C	-1.55873430	5.49153452	-0.50778074
H	-1.53292695	5.73341790	1.64726701
H	-1.51546591	4.92010747	-2.59831626
H	-1.74700311	6.54317683	-0.70995671
C	1.42333387	1.54995593	1.69645070
C	1.88845762	1.29041119	3.00881684
C	2.07428080	2.55105304	0.93603292
C	2.96677646	2.01679223	3.54351790
H	1.41361580	0.51415463	3.59899789
C	3.15161049	3.27381710	1.47067868
H	1.74374256	2.76534343	-0.07595164
C	3.60413103	3.01185471	2.77906288
H	3.31016205	1.80153752	4.55264646
H	3.64064179	4.03372896	0.86624850
H	4.44185718	3.56925030	3.19126090
C	2.37337054	-2.54145332	-0.01523033
H	1.41575448	-1.51476713	-0.61312447
O	2.56030251	-2.18311567	1.23977116
H	1.58230406	-1.81335626	1.92214399
C	1.53863581	-3.79673754	-0.27690726
H	1.30071653	-3.91198853	-1.33878680
H	2.12993407	-4.66605799	0.04680060
H	0.61302124	-3.78263466	0.30582146
C	3.55597170	-2.29749417	-0.96010213
H	4.22137513	-3.16878160	-0.85532398
H	3.21261226	-2.29539575	-2.00027869
C	4.34064475	-1.02308966	-0.62506522
H	3.77278544	-0.11752166	-0.86414280
H	4.53002736	-0.98016992	0.45543633
C	5.66627081	-0.96646859	-1.34618506
O	6.22389689	-1.89183519	-1.95840863
O	6.25098658	0.28950051	-1.24071764
H	7.12340058	0.30447153	-1.69745178



ν_{TS} = -801.37 cm^{-1}

TS: V – VI (propeller): E_{Gibbs} = -1934.430915 eH

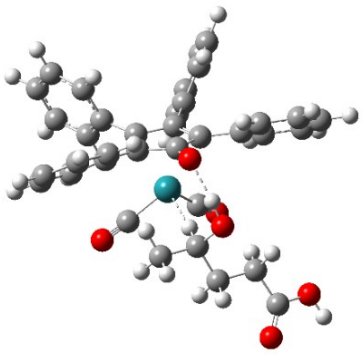
C	-0.04003016	-0.39553421	1.60632479
C	0.09745752	0.98861731	1.16252642
C	-1.05723905	1.29030042	0.31556194
C	-1.85772788	0.08243355	0.18861800
C	-1.20900006	-0.98351593	0.95131284
Ru	0.22822487	-0.33589368	-0.76977113
C	-0.28098838	-1.48184462	-2.18243268
C	1.28312773	0.71839406	-1.92949149
O	1.94005299	1.39250263	-2.64559409
O	-0.62051633	-2.20709063	-3.05170928
O	0.77307800	-1.03345260	2.44486313
C	-1.72384099	-2.35092441	1.22211810
C	-1.57262553	-2.91020841	2.51523848
C	-2.38764015	-3.11359724	0.23077879
C	-2.07943047	-4.18955998	2.80599074
H	-1.04790233	-2.34756931	3.27954617
C	-2.89249951	-4.38998777	0.52312859
H	-2.50975099	-2.71316665	-0.77091495
C	-2.74260049	-4.93573733	1.81370155
H	-1.95324101	-4.60136828	3.80448296
H	-3.39748419	-4.95816924	-0.25426803
H	-3.13198317	-5.92570678	2.03905519
C	-3.20030870	0.00738357	-0.45159429
C	-4.31190434	-0.38835513	0.32902756
C	-3.41070595	0.37270582	-1.79933394
C	-5.60304497	-0.41384658	-0.22607674
H	-4.16491675	-0.67450311	1.36706686
C	-4.70075890	0.34569583	-2.35501484
H	-2.56355138	0.67372695	-2.40988136
C	-5.80313139	-0.04659085	-1.57087774
H	-6.44649868	-0.72113187	0.38740933
H	-4.84404652	0.62784634	-3.39507042
H	-6.80117227	-0.06909334	-2.00177617
C	-1.45960799	2.64565418	-0.15667433
C	-2.75000947	3.13352162	0.15994804
C	-0.57040958	3.49487605	-0.85343470
C	-3.14057127	4.43069591	-0.21582772
H	-3.44655056	2.50231931	0.70349063
C	-0.96090211	4.78941366	-1.23246693
H	0.42855211	3.14915598	-1.09824423
C	-2.24872760	5.26435197	-0.91633464
H	-4.13638348	4.78637612	0.03714860
H	-0.26161077	5.42404659	-1.77088685
H	-2.55085516	6.26659763	-1.21041516
C	1.06549109	1.95012569	1.75405326
C	0.60824239	3.17808516	2.28945076
C	2.43770920	1.63064547	1.87077416
C	1.50191380	4.06857282	2.90847242
H	-0.44522383	3.43427212	2.23236369
C	3.33056990	2.52203280	2.48928437
H	2.80674274	0.68409639	1.48884169
C	2.86882557	3.74684475	3.00811388
H	1.13090303	5.00709977	3.31353670
H	4.38301159	2.26008463	2.56678033
H	3.56137249	4.43618481	3.48535072
C	2.56977423	-2.27674942	0.16122709
H	1.58598334	-1.34129864	-0.49844856
O	2.77665341	-1.78474421	1.37044664
H	1.75878451	-1.43890636	2.05233577
C	1.77802046	-3.58188856	0.05461974
H	1.51338078	-3.81192827	-0.98220208
H	2.41451621	-4.39127254	0.44171510
H	0.87030873	-3.54811807	0.66290462
C	3.72040430	-2.11392049	-0.84072004
H	4.38841275	-2.97543084	-0.68513751
H	3.34225748	-2.20218745	-1.86477987
C	4.51711220	-0.81831945	-0.65070064
H	3.92235931	0.06671400	-0.90492609
H	4.79719356	-0.70289927	0.40385639
C	5.77727261	-0.79670824	-1.48407640
O	6.23997784	-1.72563972	-2.16459627
O	6.41610878	0.43442682	-1.40079727
H	7.23936443	0.43716083	-1.94119277



ν_{TS} = -786.47 cm^{-1}

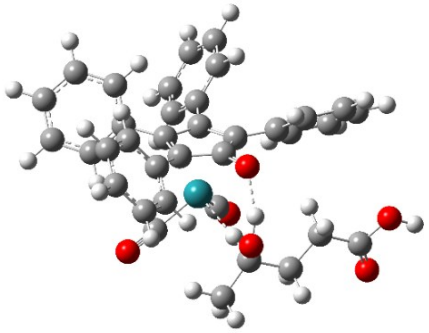
VI (mirror): E_{Gibbs} = -1934.442693 eH

C	-0.10713141	-0.46366169	1.70462796
C	0.10641831	0.93015260	1.21000989
C	-1.00256303	1.26391108	0.34620160
C	-1.83233702	0.06002429	0.16055484
C	-1.24971238	-1.02235279	0.92670815
Ru	0.20085899	-0.32427181	-0.76176698
C	-0.29561064	-1.47308131	-2.19251893
C	1.18030826	0.81466459	-1.92723815
O	1.73932045	1.57207677	-2.64058224
O	-0.66188985	-2.17590287	-3.06802847
O	0.64676588	-1.10692266	2.51111886
C	-1.81306811	-2.37981321	1.13021553
C	-1.63359796	-3.04393966	2.36998044
C	-2.55688539	-3.03666381	0.11804280
C	-2.18733434	-4.31798193	2.58746760
H	-1.05293031	-2.56692176	3.15093921
C	-3.10670081	-4.30819757	0.33742850
H	-2.70526090	-2.55761767	-0.84442957
C	-2.92603075	-4.95768104	1.57490567
H	-2.03803037	-4.80955554	3.54591510
H	-3.67078809	-4.79278497	-0.45572204
H	-3.35011649	-5.94463211	1.74366923
C	-3.20183381	0.07773990	-0.42636659
C	-4.29797646	-0.00812257	0.46397362
C	-3.45478196	0.20718698	-1.80742881
C	-5.61613597	0.04080467	-0.01895252
H	-4.11564289	-0.11699500	1.53031551
C	-4.77400206	0.24954572	-2.29206214
H	-2.62340123	0.25877346	-2.50451090
C	-5.85977648	0.16949982	-1.40024143
H	-6.44791482	-0.02558935	0.67800075
H	-4.95114776	0.34239742	-3.36065040
H	-6.87987268	0.20231631	-1.77496172
C	-1.42713671	2.63604160	-0.04663754
C	-1.75032454	3.54569706	0.98807467
C	-1.56499914	3.05241918	-1.38721876
C	-2.20509618	4.83968490	0.68580285
H	-1.64100397	3.23899947	2.02523897
C	-2.01268069	4.35009408	-1.68975010
H	-1.30688445	2.37184789	-2.19321363
C	-2.33741367	5.24794759	-0.65567853
H	-2.44961423	5.52651065	1.49227071
H	-2.10504124	4.65767387	-2.72832070
H	-2.68354506	6.25152671	-0.89043869
C	1.15141359	1.84650713	1.72897014
C	1.67717957	1.65842260	3.03146460
C	1.63647128	2.93338242	0.95881513
C	2.64697794	2.53605947	3.54685478
H	1.33675734	0.82023508	3.62809864
C	2.60590596	3.80551546	1.47429942
H	1.26196518	3.09845988	-0.04657772
C	3.11686763	3.61340147	2.77358201
H	3.03848733	2.37242593	4.54799690
H	2.96733354	4.62815805	0.86222651
H	3.87206243	4.28734982	3.17090203
C	2.58551498	-2.19527250	0.11774275
H	1.83014725	-1.42379182	-0.31794048
O	2.98907192	-1.76791099	1.41771113
H	2.20969271	-1.63251215	2.02822638
C	1.88732789	-3.56390084	0.13836004
H	1.57582896	-3.86340839	-0.87036916
H	2.58470963	-4.31612577	0.52763854
H	1.00363490	-3.54952318	0.78582902
C	3.81629718	-2.15765875	-0.80060278
H	4.50423599	-2.94705465	-0.47201064
H	3.51114818	-2.40541801	-1.82539131
C	4.54213937	-0.80442115	-0.76166881
H	3.92158100	0.00789755	-1.16130816
H	4.75750658	-0.53439486	0.27991129
C	5.84066201	-0.82209096	-1.53188917
O	6.40501828	-1.80837411	-2.03145328
O	6.39174514	0.45265174	-1.62994750
H	7.24592654	0.42159273	-2.11910686



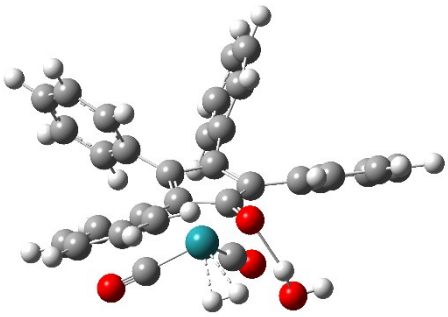
VI (propeller): E_{Gibbs} = -1934.438175 eH

C	0.18098275	-0.61823363	1.38546287
C	0.42560118	0.78954538	0.94892408
C	-0.80673708	1.30131972	0.39612625
C	-1.80076868	0.20911031	0.37239964
C	-1.18268032	-0.98440605	0.90272596
Ru	-0.06373094	-0.31970947	-1.03489889
C	-0.98174482	-1.28330837	-2.39396563
C	0.78226067	0.78539207	-2.33105773
O	1.26811443	1.52331238	-3.11410292
O	-1.59381069	-1.86352997	-3.22024176
O	1.03149787	-1.40414022	1.92189525
C	-1.84123277	-2.26805230	1.26132365
C	-3.08867114	-2.26679640	1.93183151
C	-1.20345388	-3.50643429	1.01795442
C	-3.69045429	-3.47218587	2.33035966
H	-3.58446773	-1.32640261	2.15353448
C	-1.80835211	-4.71109798	1.41628194
H	-0.23122426	-3.53642800	0.53534390
C	-3.05497844	-4.70168292	2.07041282
H	-4.64782931	-3.45046741	2.84572798
H	-1.30114585	-5.65280552	1.22133989
H	-3.51999591	-5.63508327	2.37897193
C	-3.24565798	0.38532009	0.05675103
C	-3.96829523	1.42461200	0.69043250
C	-3.94214668	-0.49917819	-0.79765642
C	-5.34818120	1.57714427	0.47009539
H	-3.45666394	2.10869196	1.36055217
C	-5.31839587	-0.34124099	-1.02513987
H	-3.41446835	-1.31337725	-1.28232002
C	-6.02889666	0.69776258	-0.39256534
H	-5.88605452	2.38014287	0.96777720
H	-5.83379695	-1.02910704	-1.69037867
H	-7.09502244	0.81834217	-0.56849346
C	-1.11156663	2.72548548	0.08812936
C	-0.88200367	3.70531448	1.08239123
C	-1.67586201	3.12169931	-1.14417341
C	-1.21332286	5.05078906	0.84795453
H	-0.44509399	3.41511532	2.03395190
C	-2.00001896	4.46766560	-1.38078917
H	-1.85406301	2.37721640	-1.91520330
C	-1.77202382	5.43805237	-0.38549165
H	-1.03122110	5.79218388	1.62195405
H	-2.42740582	4.75734091	-2.33733982
H	-2.02278203	6.47988903	-0.56934636
C	1.66288876	1.54406121	1.26999727
C	2.35801712	1.26173014	2.47238034
C	2.16743381	2.56089592	0.42225506
C	3.51429963	1.98287565	2.81748854
H	2.00140252	0.46985011	3.12167138
C	3.32132604	3.27994724	0.76959605
H	1.66297312	2.79254366	-0.51060521
C	4.00097628	2.99582293	1.97083167
H	4.03760712	1.74583520	3.74024869
H	3.69178533	4.05381923	0.10184466
H	4.89823624	3.54923935	2.23697694
C	2.24819047	-2.56630139	-0.99679364
H	1.53138371	-1.66998700	-1.05938867
O	2.07045031	-3.22642708	0.26674039
H	1.85957492	-2.60358877	1.02103842
C	1.85394776	-3.55328492	-2.10116786
H	1.97891461	-3.10421598	-3.09440120
H	2.49304324	-4.44189607	-2.03521875
H	0.81402780	-3.87552917	-1.98319712
C	3.68292724	-2.02867495	-1.19220728
H	4.34048973	-2.89558374	-1.34634793
H	3.72685562	-1.43141402	-2.11182787
C	4.20933258	-1.20569242	-0.00527910
H	3.56342357	-0.34154242	0.20518292
H	4.22879716	-1.80125343	0.91367401
C	5.60091583	-0.67195011	-0.25979895
O	6.18028448	-0.58287286	-1.35390378
O	6.21336817	-0.25124858	0.91698281
H	7.10571558	0.11878855	0.72475037



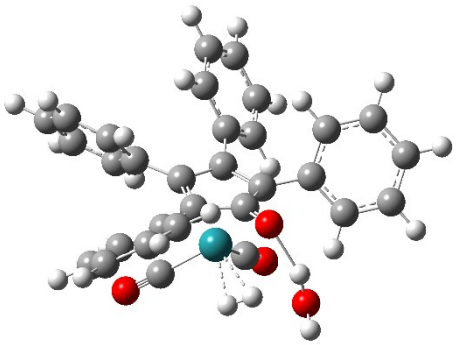
II-d (mirror): E_{Gibbs} = -1589.955769 eH

C	-0.05262194	-1.64905409	-0.90724560
C	-1.18382718	-0.73868648	-0.56494758
C	-0.63490618	0.59762798	-0.35513537
C	0.82794059	0.49945514	-0.38037813
C	1.19409579	-0.89272816	-0.56794821
Ru	-0.00653155	-0.62200009	1.42255632
C	1.35422717	-0.10589607	2.66527546
C	-1.39534646	-0.12538587	2.63181845
O	-2.27433857	0.20295164	3.34670745
O	2.21006073	0.23426890	3.40120284
O	-0.13344402	-2.86972002	-1.26421310
C	2.56725331	-1.44233200	-0.70706354
C	2.80959693	-2.54548238	-1.56325963
C	3.66519268	-0.88522719	-0.00368816
C	4.10880021	-3.06174343	-1.71691113
H	1.97843722	-3.00366850	-2.08570332
C	4.95921802	-1.40302185	-0.15813034
H	3.51199126	-0.04796260	0.67014286
C	5.19052454	-2.49511829	-1.01847443
H	4.27161196	-3.91007718	-2.37758669
H	5.78398904	-0.95998162	0.39490207
H	6.19353566	-2.89881889	-1.13515532
C	1.74038208	1.67143189	-0.48929340
C	2.47698430	1.82093832	-1.68851118
C	1.86158951	2.65920433	0.51041155
C	3.31065423	2.93447914	-1.88154367
H	2.39788069	1.06389075	-2.46430573
C	2.70099450	3.77039799	0.32024654
H	1.31456911	2.55286453	1.44231006
C	3.42706425	3.91464948	-0.87678203
H	3.86992378	3.03367577	-2.80853882
H	2.78824213	4.51789974	1.10474884
H	4.07700427	4.77388725	-1.02307808
C	-1.39112737	1.87690399	-0.47877097
C	-1.91959793	2.20462483	-1.74964202
C	-1.58121915	2.77787885	0.58868984
C	-2.61638378	3.40851499	-1.94559726
H	-1.78738292	1.51451985	-2.57946343
C	-2.28282154	3.98112324	0.39507565
H	-1.19349622	2.53353975	1.57351619
C	-2.80122941	4.30263946	-0.87304539
H	-3.01600239	3.64574172	-2.92852769
H	-2.42468065	4.66114354	1.23138616
H	-3.34446751	5.23239391	-1.02334572
C	-2.61593062	-1.07735861	-0.77083986
C	-2.98343724	-2.08273360	-1.70128523
C	-3.65005246	-0.40093894	-0.07696267
C	-4.33651118	-2.39417646	-1.92781564
H	-2.20981115	-2.61695247	-2.24058589
C	-4.99895785	-0.71329675	-0.30409455
H	-3.40519263	0.37282523	0.64335859
C	-5.35248457	-1.71398499	-1.23081334
H	-4.59386323	-3.16656166	-2.64902154
H	-5.77192237	-0.17911266	0.24308802
H	-6.39791619	-1.95710670	-1.40487561
H	0.27309774	-2.32742092	2.16279556
H	-0.38187038	-2.59388577	1.76715491
H	-0.99793067	-3.84058097	-0.01027001
O	-1.38684426	-3.97639073	0.89298604
H	-2.36020920	-3.91735304	0.85108193



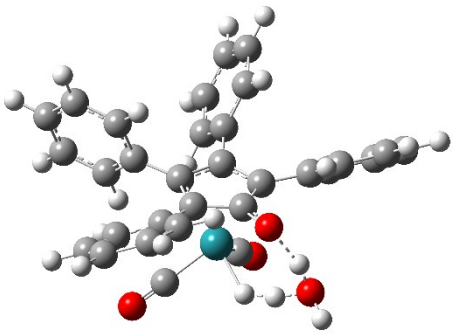
II-d (propeller): E_{Gibbs} = -1589.954702 eH

C	-0.07924988	-1.58518866	-0.96359760
C	-1.20071314	-0.68962526	-0.56577680
C	-0.65426320	0.64800158	-0.34987645
C	0.80936141	0.55185666	-0.39318306
C	1.17373876	-0.83275650	-0.62682746
Ru	0.00624195	-0.65159609	1.38488799
C	1.34194660	-0.09457317	2.64071462
C	-1.39561702	-0.28626194	2.62541020
O	-2.28455077	-0.05195431	3.36399390
O	2.17323703	0.28186918	3.38773223
O	-0.16712742	-2.78742442	-1.36887422
C	2.53792157	-1.39202234	-0.81211132
C	2.76565304	-2.36060084	-1.82111094
C	3.63463239	-0.98126751	-0.01470363
C	4.05255524	-2.88830079	-2.03091301
H	1.93287439	-2.70612540	-2.42275559
C	4.91716887	-1.50974993	-0.22513136
H	3.48933066	-0.24894506	0.77367020
C	5.13484889	-2.46679010	-1.23666213
H	4.20595180	-3.63013866	-2.81123686
H	5.74282005	-1.17996322	0.40091198
H	6.12848956	-2.87841056	-1.39756715
C	1.73647531	1.71761465	-0.36935931
C	2.67050986	1.87196516	-1.42061318
C	1.66745495	2.71173075	0.63169542
C	3.51417038	2.99535124	-1.46736545
H	2.73607127	1.11637629	-2.19832387
C	2.51413569	3.83086483	0.58796699
H	0.95257218	2.60625813	1.44296307
C	3.44138227	3.97865968	-0.46211454
H	4.22654729	3.09849199	-2.28214011
H	2.45111892	4.58319477	1.37005806
H	4.09809091	4.84460706	-0.49491241
C	-1.43372838	1.91837632	-0.38446208
C	-1.08035008	2.91569385	-1.32529568
C	-2.56988753	2.13094986	0.42764154
C	-1.83518918	4.09567639	-1.44034952
H	-0.22048967	2.76780873	-1.97163157
C	-3.32099362	3.31249673	0.31769115
H	-2.87603555	1.37476450	1.14200759
C	-2.95682018	4.30235436	-0.61553168
H	-1.54690876	4.84882804	-2.16957252
H	-4.18954438	3.45630370	0.95525540
H	-3.53908572	5.21668078	-0.70048659
C	-2.62513794	-1.03222384	-0.83468929
C	-3.34096147	-0.32623990	-1.83115313
C	-3.26431831	-2.10208850	-0.16937486
C	-4.66680355	-0.67134333	-2.14378148
H	-2.86028196	0.48869717	-2.36562033
C	-4.59116917	-2.44646421	-0.48335677
H	-2.72688497	-2.67488280	0.58068057
C	-5.29979185	-1.73242127	-1.46816994
H	-5.20110914	-0.11657036	-2.91168357
H	-5.06676976	-3.27285239	0.03948741
H	-6.32637550	-1.99997387	-1.70803919
H	0.39730671	-2.35340644	2.10788078
H	-0.18687660	-2.67632868	1.66295130
H	-0.78761554	-3.91316715	-0.21020870
O	-0.97627745	-4.24581341	0.71023334
H	-0.65185707	-5.15647889	0.83490284



TS II-d – IV (mirror): E_{Gibbs} = -1589.946446 eH

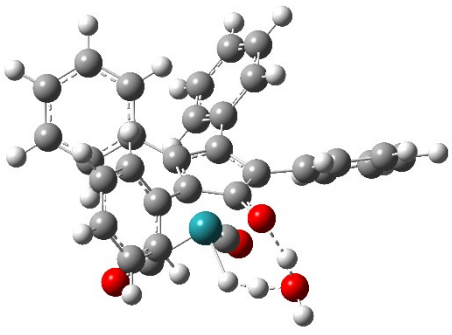
Ru	0.00864744	-0.66079155	1.40323117
C	-0.06081344	-1.61492298	-0.75076398
C	-1.20580520	-0.71460237	-0.54437707
C	1.17429955	-0.85061929	-0.57577479
C	0.78675477	0.54839473	-0.35334027
C	-0.66867101	0.63005443	-0.36729415
C	1.46668268	-0.42595070	2.60676592
C	-1.26640168	-0.03897832	2.67590726
O	2.38974319	-0.28134323	3.32655895
O	-2.07363952	0.36346132	3.43725948
H	-0.09825776	-2.27024126	2.06111213
H	-0.71177168	-2.96402788	1.80840491
O	-1.26756726	-3.90599994	1.03420844
O	-0.13095160	-2.94848735	-1.05592061
H	-0.92584416	-3.61797431	0.08406806
H	-1.14648579	-4.84494134	1.26275645
C	2.54460120	-1.37604134	-0.79959317
C	2.73906029	-2.49574868	-1.64650313
C	3.68337356	-0.77383805	-0.20950720
C	4.03222048	-2.98472267	-1.90157759
H	1.87220486	-2.98367592	-2.07673416
C	4.97252346	-1.26627506	-0.46398857
H	3.56858499	0.07698177	0.45424741
C	5.15632674	-2.37429088	-1.31432081
H	4.15947428	-3.84468986	-2.55537499
H	5.83056208	-0.78902011	0.00351406
H	6.15571229	-2.75623565	-1.50998102
C	1.68845934	1.73157769	-0.44691473
C	2.22596906	2.05007588	-1.71603066
C	2.00771860	2.55466364	0.65245323
C	3.05962656	3.16903229	-1.87922952
H	1.99381855	1.41773412	-2.56958149
C	2.84451838	3.67339331	0.49126714
H	1.61281413	2.31281794	1.63540682
C	3.37234482	3.98617012	-0.77527463
H	3.46545304	3.40003999	-2.86113649
H	3.08371602	4.29455065	1.35100762
H	4.02031630	4.85033246	-0.90035151
C	-1.44686913	1.89642282	-0.44957290
C	-2.17836898	2.14832942	-1.63457461
C	-1.44857102	2.87192766	0.57005234
C	-2.88966132	3.34896214	-1.79487362
H	-2.19035724	1.40311090	-2.42548205
C	-2.16474498	4.07107237	0.41214567
H	-0.90343583	2.68992163	1.49156924
C	-2.88641912	4.31615429	-0.77111646
H	-3.44643707	3.52626486	-2.71174421
H	-2.16012479	4.80852305	1.21092577
H	-3.44112992	5.24344251	-0.89244823
C	-2.62645913	-1.08598316	-0.76497222
C	-2.95062723	-2.03991886	-1.76000185
C	-3.67966229	-0.48506541	-0.03608380
C	-4.29122382	-2.37330381	-2.02178483
H	-2.15003800	-2.52275526	-2.30992355
C	-5.01740644	-0.81977936	-0.29760154
H	-3.45729678	0.24269264	0.73874707
C	-5.33138755	-1.76571901	-1.29343402
H	-4.52160421	-3.10750336	-2.79049863
H	-5.81141465	-0.34759731	0.27595789
H	-6.36794735	-2.02679398	-1.49399508



ν_{TS} = -909.06 cm^{-1}

TS II-d – IV (propeller): E_{Gibbs} = -1589.944108 eH

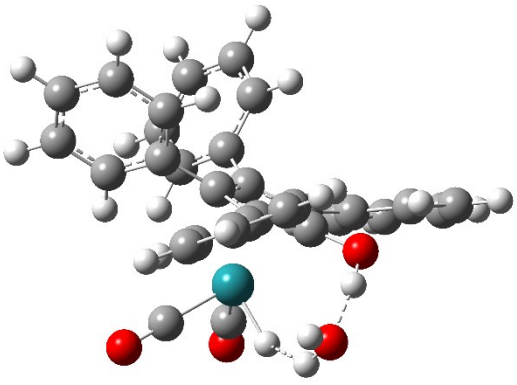
Ru	-0.00691412	-0.68162299	1.36836982
C	-0.01101529	-1.57089031	-0.81430595
C	-1.17736911	-0.70013328	-0.60141129
C	1.19933024	-0.78302774	-0.58862592
C	0.78639283	0.60591070	-0.36825656
C	-0.67059892	0.65450971	-0.38310602
C	1.39273970	-0.43527564	2.63529346
C	-1.33695380	-0.13575715	2.61968541
O	2.27811393	-0.29539887	3.40296461
O	-2.17465928	0.22187059	3.36963213
H	-0.08031437	-2.31279876	1.97536444
H	-0.66948013	-3.01515017	1.69043227
O	-1.18466230	-3.94791636	0.87794546
O	-0.03819700	-2.89590893	-1.16074595
H	-0.83422849	-3.62162745	-0.05652330
H	-1.04135965	-4.88972668	1.08034000
C	2.56626940	-1.29199103	-0.86700160
C	3.40785928	-0.61854361	-1.78320759
C	3.02587745	-2.49596841	-0.28751430
C	4.67998891	-1.12808602	-2.09762420
H	3.06715293	0.29706678	-2.25778816
C	4.29603619	-3.00647661	-0.60145761
H	2.38307398	-3.02944082	0.40623597
C	5.13153644	-2.32312778	-1.50674365
H	5.31282411	-0.59546680	-2.80371542
H	4.63301245	-3.93334441	-0.14319663
H	6.11584217	-2.71696943	-1.74918254
C	1.68889908	1.79186437	-0.37028837
C	1.44026643	2.84410740	-1.28396758
C	2.83432606	1.87126881	0.45312835
C	2.30801857	3.94713266	-1.36426340
H	0.57276131	2.79827114	-1.93533367
C	3.69924917	2.97503022	0.37707275
H	3.05685290	1.07113390	1.15089574
C	3.44013661	4.01983762	-0.53116906
H	2.09889734	4.74477473	-2.07291249
H	4.57283545	3.01688078	1.02267542
H	4.10998032	4.87438998	-0.58935986
C	-1.48756501	1.89927163	-0.34886239
C	-2.38087903	2.16339460	-1.41341430
C	-1.35761668	2.85484224	0.68312658
C	-3.12473138	3.35586413	-1.44359412
H	-2.49395065	1.43797149	-2.21416210
C	-2.10274047	4.04503103	0.65449905
H	-0.67519508	2.66323416	1.50682447
C	-2.98982854	4.30167074	-0.40921644
H	-3.80829972	3.54183341	-2.26838141
H	-1.99306603	4.76720364	1.45967703
H	-3.56889552	5.22177471	-0.42948986
C	-2.58268946	-1.10996767	-0.85811532
C	-2.85442977	-2.00274783	-1.92330734
C	-3.66732173	-0.61599019	-0.09651824
C	-4.17593102	-2.37816322	-2.22292879
H	-2.02788398	-2.40762644	-2.49759816
C	-4.98620994	-0.99268299	-0.39585853
H	-3.48561372	0.06065810	0.73316448
C	-5.24845028	-1.87533161	-1.46227283
H	-4.36574832	-3.06405980	-3.04541362
H	-5.80520015	-0.60293928	0.20394485
H	-6.27011428	-2.16925148	-1.69178471



ν_{TS} = -917.19 cm^{-1}

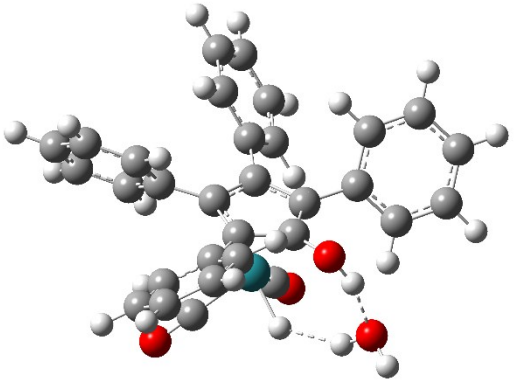
III-d (mirror): E_{Gibbs} = -1589.986747 eH

C	0.07985883	-1.59330498	-0.72207562
C	-1.16872961	-0.88333682	-0.57260395
C	-0.83121061	0.54040680	-0.39026520
C	0.60543173	0.66748394	-0.37838143
C	1.18622505	-0.67323072	-0.53934218
C	-2.52304885	-1.45740881	-0.77747266
C	-2.70302551	-2.55508036	-1.65475941
C	-3.66322827	-0.91694856	-0.13459432
C	-3.98413077	-3.08623124	-1.88553482
H	-1.83935027	-2.99814098	-2.13676273
C	-4.94065891	-1.44946705	-0.36543397
H	-3.55520410	-0.08471178	0.55364246
C	-5.11025117	-2.53697756	-1.24470354
H	-4.09990583	-3.93032903	-2.56157663
H	-5.80036718	-1.02044248	0.14364480
H	-6.10034866	-2.95073475	-1.42153036
C	-1.78665467	1.67854148	-0.49941988
C	-2.39427984	1.92745740	-1.75247664
C	-2.09234938	2.53044648	0.58285656
C	-3.28065996	3.00504332	-1.91807492
H	-2.17334661	1.27341404	-2.59257290
C	-2.98003642	3.60894381	0.41963927
H	-1.64686344	2.33716949	1.55527427
C	-3.57674280	3.85159931	-0.83180174
H	-3.73927256	3.18210417	-2.88801277
H	-3.20627934	4.25283486	1.26614435
H	-4.26450160	4.68432931	-0.95843720
C	1.36699792	1.94439835	-0.47029854
C	2.07150955	2.22248640	-1.66587315
C	1.38877686	2.90319224	0.56533726
C	2.77525948	3.42870469	-1.82103205
H	2.06461266	1.49381913	-2.47257807
C	2.09339190	4.11017695	0.41216324
H	0.86604112	2.69928331	1.49558724
C	2.78888416	4.37901145	-0.78160808
H	3.31000193	3.62558310	-2.74716744
H	2.10100883	4.83450205	1.22296335
H	3.33527421	5.31174581	-0.89955387
C	2.61767759	-0.99468366	-0.77729337
C	2.97339942	-1.85283548	-1.84798532
C	3.65335407	-0.43878510	0.01022426
C	4.32222957	-2.15192894	-2.11379235
H	2.19384629	-2.28074805	-2.47167564
C	5.00064858	-0.73252411	-0.25906137
H	3.40593137	0.22418253	0.83375677
C	5.34354492	-1.59433392	-1.31997467
H	4.57369746	-2.81155043	-2.94105063
H	5.77946171	-0.29105588	0.35783297
H	6.38625519	-1.82281930	-1.52643489
O	0.16860957	-2.92611993	-1.01298648
H	0.89695091	-3.40099290	-0.48828191
Ru	-0.00293566	-0.60803090	1.47740633
H	0.21287486	-2.08902166	2.09078244
C	1.25224409	-0.04763016	2.75663527
C	-1.42343991	-0.51480095	2.71285234
O	2.06341805	0.28915863	3.55185064
O	-2.32207380	-0.47287666	3.47940533
H	1.60125414	-3.57557901	1.49629714
O	1.91472278	-3.90324892	0.62792521
H	2.86406317	-3.71509208	0.49917906



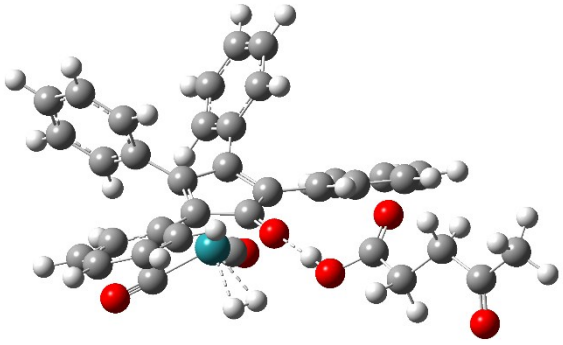
III-d (propeller): E_{Gibbs} = -1589.982221 eH

C	-0.07669027	-1.52929601	-0.81222775
C	-1.20063241	-0.64415464	-0.59479358
C	-0.65008841	0.70338440	-0.37968993
C	0.78985155	0.60929167	-0.40053317
C	1.15960046	-0.79605047	-0.63557169
C	-2.61516383	-0.98027610	-0.91541199
C	-3.31516653	-2.01489773	-0.25725101
C	-3.26536569	-0.28224123	-1.96157232
C	-4.62992021	-2.34382574	-0.63292841
H	-2.83728522	-2.56594700	0.54670925
C	-4.57972487	-0.60829154	-2.33505395
H	-2.73983911	0.51251078	-2.48369153
C	-5.26932063	-1.64186190	-1.67172842
H	-5.15231530	-3.14309613	-0.11259389
H	-5.06221925	-0.05922587	-3.14023695
H	-6.28740546	-1.89402903	-1.95912732
C	-1.45407501	1.95718668	-0.35379211
C	-2.59620830	2.09775995	0.46729725
C	-1.11596289	3.02143436	-1.22375231
C	-3.36991509	3.26918929	0.43061957
H	-2.88260035	1.29288823	1.13704274
C	-1.88949712	4.19481414	-1.26111712
H	-0.25046323	2.93045787	-1.87316992
C	-3.01963565	4.32585733	-0.43233617
H	-4.24218004	3.35611314	1.07373662
H	-1.61001569	5.00105740	-1.93516771
H	-3.61753054	5.23376006	-0.45888956
C	1.73271461	1.76125088	-0.35012981
C	1.71148160	2.69663735	0.70851307
C	2.64101013	1.96260925	-1.41584220
C	2.57284233	3.80621343	0.70289592
H	1.02121553	2.55077715	1.53534433
C	3.50387019	3.07272425	-1.42202864
H	2.67182928	1.25201577	-2.23729235
C	3.47346163	4.00008725	-0.36275534
H	2.54348536	4.51367730	1.52793959
H	4.19704299	3.21015362	-2.24847423
H	4.14277835	4.85710193	-0.36554575
C	2.51899086	-1.34420601	-0.88536440
C	2.71576579	-2.27095568	-1.93795474
C	3.64002669	-0.94794448	-0.11828093
C	3.99773240	-2.77789442	-2.21667667
H	1.86346890	-2.60089641	-2.52175958
C	4.91906943	-1.45451620	-0.39753713
H	3.51596583	-0.24655366	0.70123969
C	5.10623801	-2.37268217	-1.44971722
H	4.12808640	-3.48869154	-3.02956273
H	5.76529744	-1.13744616	0.20723105
H	6.09689070	-2.76690005	-1.66417042
O	-0.13209510	-2.83168729	-1.22531995
H	-0.61935537	-3.45738638	-0.60263073
Ru	0.01546085	-0.68320337	1.41547316
H	0.08506567	-2.20100377	1.97858460
C	1.38199187	-0.36555267	2.67261809
C	-1.33524723	-0.40884458	2.69781957
O	2.24983262	-0.17708839	3.45264370
O	-2.19981731	-0.25710443	3.49136664
H	-0.66785286	-3.70999045	1.47564123
O	-1.01666250	-4.27485435	0.74834587
H	-0.84460368	-5.22221477	0.89743580



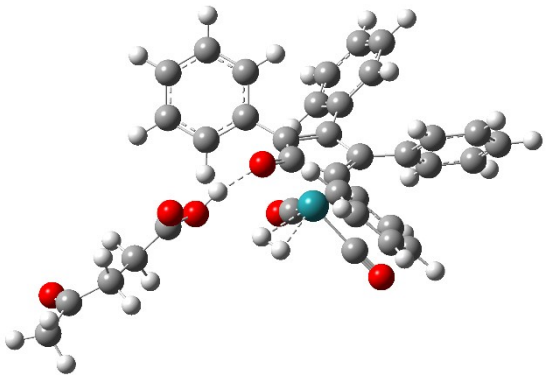
II-e (mirror): E_{Gibbs} = -1934.434530 eH

C	-0.36862917	-0.41633757	-0.00455219
C	0.19204958	0.97539779	0.03090928
C	1.57988819	0.89754318	-0.37957224
C	1.97687619	-0.51649726	-0.41653473
C	0.81542908	-1.32797875	-0.06640577
Ru	1.49096443	-0.00244263	1.71146606
C	2.74097528	-1.16368176	2.57806004
C	2.18431119	1.52010445	2.64941571
O	2.62580943	2.46989798	3.18923601
O	3.52328078	-1.88925872	3.07829466
O	-1.57979038	-0.75134124	0.11711968
C	0.73136867	-2.81158707	-0.12533289
C	-0.47065542	-3.44699696	-0.52609821
C	1.84531356	-3.62922431	0.19195643
C	-0.54916419	-4.84869647	-0.60962631
H	-1.34139316	-2.84732192	-0.75963086
C	1.76455495	-5.02666439	0.10765218
H	2.78056166	-3.17724479	0.50554426
C	0.56491500	-5.64719275	-0.29404877
H	-1.48344308	-5.31271108	-0.91644459
H	2.63357205	-5.63003063	0.35870537
H	0.50087057	-6.73096892	-0.35496685
C	3.22045144	-1.01599658	-1.07110826
C	4.49731002	-0.95397778	-0.47725923
C	3.09885348	-1.55307478	-2.37434081
C	5.63128055	-1.41762620	-1.16738867
H	4.60519731	-0.55672659	0.52800046
C	4.23186480	-2.01072004	-3.06712826
H	2.11809918	-1.61518131	-2.83958778
C	5.50382392	-1.94500971	-2.46583485
H	6.60766480	-1.36783014	-0.69189429
H	4.12204683	-2.41957485	-4.06846732
H	6.38048615	-2.30328109	-2.99979732
C	2.38772385	2.01343260	-0.94391411
C	3.66458634	2.36965253	-0.46074661
C	1.86072017	2.70882871	-2.05806572
C	4.39872962	3.39944699	-1.07329887
H	4.07821596	1.85528290	0.40145141
C	2.59828252	3.73214235	-2.67552234
H	0.87542553	2.44979721	-2.43601268
C	3.87078112	4.08299813	-2.18467557
H	5.37734273	3.66697431	-0.68287790
H	2.17905738	4.25615510	-3.53070853
H	4.43922005	4.87981665	-2.65797580
C	-0.63088716	2.20888733	0.13624162
C	-1.97644428	2.20875368	-0.30398057
C	-0.09222821	3.41310665	0.65654968
C	-2.75655375	3.37690760	-0.22373352
H	-2.43622572	1.31122425	-0.69655648
C	-0.87066442	4.57679356	0.73246014
H	0.93613804	3.44522161	1.00378888
C	-2.21073523	4.56557160	0.29274632
H	-3.78872313	3.33698210	-0.56045316
H	-0.43640907	5.48765930	1.13781064
H	-2.81600543	5.46679337	0.35827395
H	0.16749885	-0.71803134	2.92333524
H	0.02049986	0.06307490	2.96735131
H	-3.17982766	-1.03876793	0.28720586
O	-4.13751149	-1.32239361	0.39465347
C	-5.05387695	-0.49485521	-0.18098242
O	-4.74293058	0.52984428	-0.82716177
C	-6.47635603	-0.95346491	0.08190570
H	-6.50550258	-2.04763959	0.04511955
H	-6.73595345	-0.68464583	1.11514722
C	-7.48600061	-0.31710032	-0.88268089
H	-7.44400103	-0.78737674	-1.87534086
H	-7.21244963	0.73617101	-1.05114420
C	-8.92399935	-0.35308482	-0.37252808
C	-10.01226147	-0.04022585	-1.38919137
H	-10.15980677	-0.91036521	-2.04554579
H	-10.95521468	0.17702450	-0.88007569
H	-9.72690729	0.80433846	-2.02908700
O	-9.20039144	-0.61659669	0.81788936



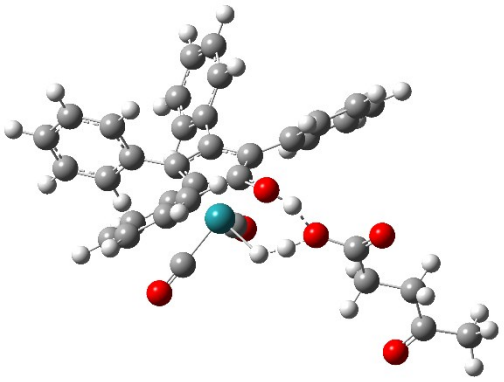
II-e (propeller): E_{Gibbs} = -1934.431549 eH

C	0.15602157	-0.21376152	-1.08017165
C	-0.81884625	-1.26764048	-0.65236106
C	-2.06600077	-0.60038588	-0.31669572
C	-1.83456523	0.84990091	-0.31388029
C	-0.43464940	1.08434117	-0.64026587
Ru	-0.57432803	-0.08418253	1.33576591
C	-0.62689296	1.34191005	2.61121706
C	-1.24069802	-1.32455830	2.63847134
O	-1.68550760	-2.09070769	3.41489997
O	-0.66995843	2.23579924	3.37759512
O	1.30137936	-0.39301146	-1.59395825
C	0.20471416	2.38860409	-0.96477981
C	-0.40585135	3.26718065	-1.89131049
C	1.46489605	2.73652385	-0.43058087
C	0.22127129	4.47001957	-2.25835159
H	-1.36470525	3.00776294	-2.33130698
C	2.09295276	3.93896634	-0.79836523
H	1.96298856	2.06552935	0.26317651
C	1.47242591	4.81323536	-1.71082638
H	-0.26245343	5.13324291	-2.97156760
H	3.06377502	4.18776471	-0.37732466
H	1.95815181	5.74367277	-1.99505465
C	-2.89852668	1.89157010	-0.24819203
C	-2.76282336	3.05930481	0.53579831
C	-4.04648186	1.75586666	-1.06567021
C	-3.75343498	4.05403844	0.51990214
H	-1.88329539	3.19913330	1.15474154
C	-5.03475124	2.75506000	-1.08764908
H	-4.16562367	0.87604715	-1.69017719
C	-4.89583137	3.90675519	-0.29074024
H	-3.63098127	4.94175733	1.13494035
H	-5.90786795	2.63248326	-1.72361373
H	-5.66208623	4.67794011	-0.30316300
C	-3.40356405	-1.24469473	-0.19142712
C	-4.26521393	-0.98972026	0.89774950
C	-3.85266031	-2.08606810	-1.23645839
C	-5.54535925	-1.56549517	0.94575276
H	-3.93275306	-0.34257788	1.70477911
C	-5.13611919	-2.65686766	-1.19118067
H	-3.19998511	-2.29280537	-2.08003347
C	-5.98730227	-2.40064195	-0.09894257
H	-6.19423894	-1.36321770	1.79401459
H	-5.46625355	-3.30166308	-2.00175542
H	-6.97797315	-2.84691120	-0.06096277
C	-0.59689333	-2.72443833	-0.84936256
C	0.25972948	-3.17249330	-1.88570006
C	-1.22633416	-3.69462133	-0.02989959
C	0.46545553	-4.54750364	-2.09986017
H	0.77481195	-2.44729315	-2.50456189
C	-1.01885488	-5.06484412	-0.24575422
H	-1.87839828	-3.38331510	0.78031115
C	-0.17183089	-5.50057747	-1.28471723
H	1.12928673	-4.86890057	-2.89866919
H	-1.51145465	-5.79003669	0.39744994
H	-0.00775616	-6.56285439	-1.44935592
H	1.34806429	-0.11444928	1.60656681
H	1.14513614	-0.87521385	1.71850570
H	2.79120621	-0.10694817	-1.01221526
O	3.54461086	0.06644184	-0.35832029
C	4.78665643	-0.34157576	-0.76727120
O	4.99537088	-0.90913299	-1.85608494
C	5.85514411	0.00920927	0.25352416
H	6.01909841	1.09466081	0.22050428
H	5.46849144	-0.20019136	1.25727678
C	7.17796568	-0.72101812	-0.01087912
H	7.38992245	-0.71253575	-1.09115298
H	7.10774148	-1.78508039	0.25613594
C	8.36989780	-0.10127146	0.71195807
C	9.65030201	-0.92328127	0.73841201
H	9.84365612	-1.38864184	-0.23627912
H	10.49737048	-0.29570251	1.02866014
H	9.54752483	-1.73612618	1.47221763
O	8.30727380	1.02465302	1.25277612



TS II-e – IV (mirror): E_{Gibbs} = -1934.423721 eH

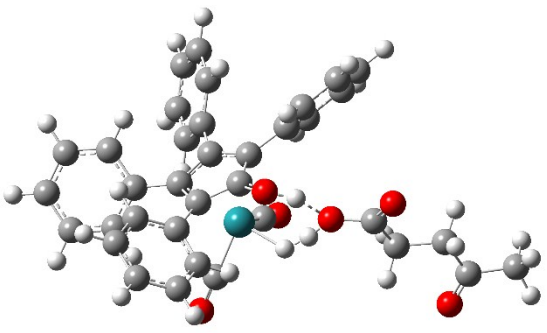
Ru	-0.16436391	-0.39182676	-1.00766812
C	-0.20468903	-0.65296628	1.36728375
C	-0.09270389	0.76289144	1.00717358
C	-1.42792412	-1.19732931	0.82003695
C	-2.12413056	-0.08799301	0.14391356
C	-1.32408101	1.11703775	0.30867469
C	-0.68361038	-1.67230263	-2.31477781
C	0.44612929	0.83235580	-2.31998760
O	-1.02518075	-2.47610512	-3.10505910
O	0.82315770	1.61652343	-3.11676522
H	1.39661328	-1.16475267	-1.03003322
H	2.11844832	-1.03932953	-0.40969189
O	2.78137505	-1.11349371	0.75247336
O	0.69289830	-1.37494738	2.07123074
H	1.67467412	-1.25484316	1.74153414
C	-1.94458385	-2.56853757	1.05628465
C	-1.57353534	-3.26902819	2.23083374
C	-2.83317015	-3.19578280	0.14905937
C	-2.08503736	-4.55224688	2.48995668
H	-0.87391671	-2.81649555	2.92369901
C	-3.33930253	-4.47802087	0.40920396
H	-3.12737681	-2.69020315	-0.76485657
C	-2.97037806	-5.16388087	1.58300169
H	-1.78652112	-5.07385333	3.39607803
H	-4.01526425	-4.94268238	-0.30434486
H	-3.36124754	-6.15872437	1.78279511
C	-3.55059999	-0.09595132	-0.29020389
C	-4.54829517	-0.11797962	0.71215780
C	-3.94682671	-0.06370480	-1.64313247
C	-5.91009377	-0.10392438	0.36606008
H	-4.25588132	-0.14959704	1.75906113
C	-5.30925862	-0.05173029	-1.99131613
H	-3.19020841	-0.06054442	-2.42352394
C	-6.29607217	-0.07026169	-0.98802607
H	-6.66526855	-0.12144964	1.14800842
H	-5.59684815	-0.03087979	-3.03959471
H	-7.34970312	-0.06236587	-1.25621824
C	-1.79892813	2.50020762	0.03223636
C	-1.88542119	3.40542738	1.11660783
C	-2.22156457	2.92744195	-1.24487763
C	-2.38461276	4.70448789	0.92581290
H	-1.56331017	3.09212134	2.10588951
C	-2.71591094	4.22863184	-1.43688600
H	-2.15370959	2.24982997	-2.09066015
C	-2.80123719	5.12241594	-0.35278851
H	-2.44461115	5.38693528	1.76992297
H	-3.03060027	4.54265469	-2.42886163
H	-3.18269433	6.12954638	-0.50202371
C	0.95425066	1.69122979	1.50708490
C	1.46162713	1.53090035	2.81854274
C	1.44009177	2.76045733	0.71899637
C	2.42596319	2.41821867	3.32671918
H	1.11184334	0.70927826	3.43581462
C	2.40003288	3.64843703	1.22864141
H	1.07287412	2.89956468	-0.29371648
C	2.89900201	3.48166310	2.53589455
H	2.81232198	2.27175777	4.33209317
H	2.76121291	4.46402780	0.60688315
H	3.64829055	4.16521204	2.92775638
C	4.14006241	-1.08412594	0.86830030
O	4.69039903	-1.16789197	1.98204094
C	4.89248637	-0.95363089	-0.45317975
H	4.72058560	-1.85916133	-1.05027636
H	4.45835305	-0.12767909	-1.03171018
C	6.39770468	-0.74426673	-0.24766966
H	6.77509267	-1.47256797	0.48584280
H	6.60253210	0.23775976	0.20151336
C	7.21087617	-0.88906400	-1.52967947
C	8.67045148	-0.46386643	-1.46094182
H	9.13965205	-0.80092225	-0.52821737
H	9.21993337	-0.85731618	-2.32051906
H	8.73227701	0.63413237	-1.47801253
O	6.71037647	-1.33287671	-2.58658258



ν_{TS} = -923.83 cm^{-1}

TS II-e – IV (propeller): E_{Gibbs} = -1934.422924 eH

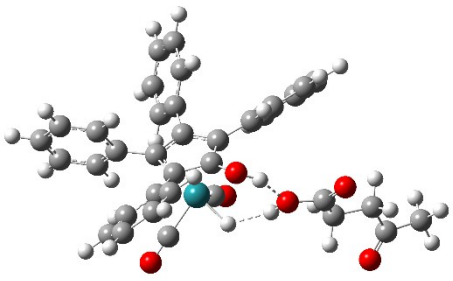
Ru	-0.17426621	0.38525420	0.99496352
C	-0.23196240	0.66048975	-1.36309431
C	-0.10867841	-0.75657099	-1.02075337
C	-1.45532826	1.18639827	-0.80237208
C	-2.16152643	0.06280326	-0.16745516
C	-1.34235778	-1.12866464	-0.32662406
C	-0.69545002	1.61931514	2.34287561
C	0.48356396	-0.85200847	2.27515533
O	-1.02822654	2.40212173	3.15856664
O	0.88654841	-1.64430871	3.04993267
H	1.37124313	1.18887364	1.00765816
H	2.09268171	1.07547586	0.38454706
O	2.74890831	1.15851829	-0.78081592
O	0.63287244	1.40883700	-2.07692453
H	1.62001747	1.29106780	-1.78473243
C	-1.97061206	2.55460899	-1.06843564
C	-3.27558277	2.73571063	-1.58289516
C	-1.14850399	3.68978425	-0.88529996
C	-3.74961751	4.02215991	-1.89405741
H	-3.91673343	1.87560709	-1.75082454
C	-1.62240688	4.97441443	-1.19594377
H	-0.13876892	3.56344130	-0.50621154
C	-2.92671289	5.14720073	-1.69963515
H	-4.75542355	4.14311203	-2.28905553
H	-0.97663421	5.83627900	-1.04783446
H	-3.29364386	6.14231305	-1.93943186
C	-3.57269342	0.08426174	0.31105341
C	-4.50519370	-0.81501204	-0.25933640
C	-4.03299792	1.01764174	1.26634192
C	-5.85809449	-0.78462692	0.12082589
H	-4.17442082	-1.53486057	-1.00233244
C	-5.38426087	1.04720492	1.64868821
H	-3.34040716	1.72459692	1.71157675
C	-6.30392151	0.14552604	1.07871780
H	-6.55841814	-1.48432223	-0.32860064
H	-5.71668965	1.77204178	2.38739231
H	-7.34952468	0.16828976	1.37585614
C	-1.76534509	-2.51516190	0.01443219
C	-1.75526623	-3.50368399	-0.99748590
C	-2.23869158	-2.86106066	1.29951817
C	-2.20717021	-4.80710083	-0.72760592
H	-1.39636208	-3.25431825	-1.99200388
C	-2.68686065	-4.16419284	1.57002636
H	-2.25497790	-2.11072482	2.08543252
C	-2.67349461	-5.14356104	0.55759820
H	-2.19130422	-5.55523846	-1.51624078
H	-3.04299135	-4.41394776	2.56619437
H	-3.01841448	-6.15297481	0.76784908
C	0.94914205	-1.66421877	-1.53844682
C	1.41486603	-1.49869364	-2.86470937
C	1.48902190	-2.71129926	-0.75644152
C	2.39120632	-2.36073241	-3.39339296
H	1.02258522	-0.69289338	-3.47771377
C	2.46056959	-3.57462991	-1.28669594
H	1.15386098	-2.85366245	0.26672485
C	2.91764995	-3.40334766	-2.60858571
H	2.74533756	-2.21040450	-4.40996925
H	2.86326315	-4.37398055	-0.66934494
H	3.67627588	-4.06693259	-3.01644101
C	4.10701274	1.09660814	-0.89269866
O	4.66287615	1.17120811	-2.00433250
C	4.85370289	0.94665952	0.43051504
H	4.70400854	1.85625362	1.02750066
H	4.39820497	0.13161923	1.00815803
C	6.35394648	0.70081785	0.22864937
H	6.74488946	1.40552579	-0.52076500
H	6.53814366	-0.29456795	-0.19939695
C	7.17184496	0.85760757	1.50637367
C	8.61873515	0.38987675	1.44937313
H	8.64969736	-0.70874236	1.49159252
H	9.09746249	0.69206711	0.50952716
H	9.17876253	0.78765172	2.30008874
O	6.68512116	1.34550213	2.55024008



ν_{TS} = -915.82 cm^{-1}

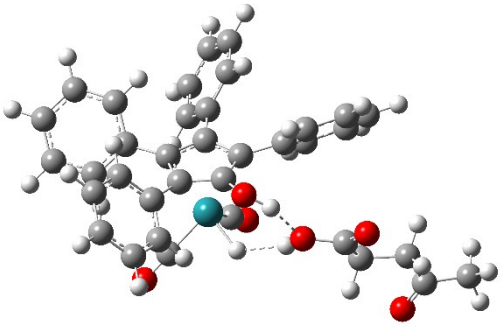
III-e (mirror): E_{Gibbs} = -1934.447285 eH

C	0.35689339	0.89483829	1.26277377
C	-0.02443373	-0.48199260	1.01187143
C	1.12951439	-1.13000708	0.37169715
C	2.15838184	-0.13568915	0.17912202
C	1.66605949	1.14801579	0.70994666
C	-1.22678782	-1.15993469	1.56408122
C	-1.67825320	-0.83475541	2.86626746
C	-1.91744094	-2.16104221	0.84151580
C	-2.79082423	-1.48779421	3.42496287
H	-1.15940020	-0.07341361	3.44113437
C	-3.02352735	-2.81916508	1.40315645
H	-1.58792444	-2.42932361	-0.15788459
C	-3.46880082	-2.48385060	2.69758381
H	-3.12751205	-1.21633736	4.42228333
H	-3.53429356	-3.59190672	0.83336650
H	-4.32746527	-2.99083803	3.13116190
C	1.30622139	-2.60096191	0.21659506
C	1.30547723	-3.40281250	1.38260039
C	1.51080278	-3.22378849	-1.03301384
C	1.50650151	-4.79081750	1.29887570
H	1.14734068	-2.93741008	2.35217634
C	1.70974330	-4.61289617	-1.11873933
H	1.50137121	-2.62369540	-1.93849099
C	1.70944809	-5.40236810	0.04647738
H	1.50325804	-5.39136217	2.20530687
H	1.86168179	-5.07518763	-2.09098509
H	1.86200694	-6.47694701	-0.01971641
C	3.56812519	-0.42795589	-0.20470406
C	3.95189897	-0.77951029	-1.51598510
C	4.56037118	-0.37537673	0.80249898
C	5.29331594	-1.07618319	-1.81648860
H	3.20330835	-0.80558880	-2.30348276
C	5.90083397	-0.67264984	0.50451224
H	4.27964759	-0.09816882	1.81572808
C	6.27301306	-1.02581381	-0.80729279
H	5.57083755	-1.34163687	-2.83371377
H	6.65080164	-0.62679218	1.29048505
H	7.31069054	-1.25338236	-1.03928461
C	2.43873229	2.40902863	0.84771594
C	2.24722373	3.23821353	1.97991279
C	3.39734649	2.79910456	-0.11858220
C	2.99846573	4.41569963	2.14089548
H	1.50172610	2.96799576	2.71865017
C	4.14445242	3.97557367	0.04311764
H	3.55608130	2.18967940	-1.00274243
C	3.95110862	4.79115821	1.17548605
H	2.83510777	5.03945147	3.01662186
H	4.87113539	4.25786649	-0.71478824
H	4.52873652	5.70422345	1.29897528
O	-0.36126868	1.83668273	1.95165617
H	-1.33589451	1.84461180	1.72667388
Ru	0.30074820	0.46711683	-1.10839832
H	-0.88476066	1.56673314	-1.26934483
C	1.08373718	1.42055783	-2.53736960
C	-0.71170800	-0.61215115	-2.26791311
O	1.57593305	2.03238554	-3.41909620
O	-1.36694068	-1.29739171	-2.97693239
H	-2.26994431	1.63902113	-0.22948054
O	-2.66507437	1.82393732	0.66164163
C	-4.04532571	1.62911345	0.79692378
O	-4.56708798	1.82814910	1.89350312
C	-4.75202543	1.20487777	-0.48043715
H	-4.18490664	0.39652169	-0.96097711
H	-4.74171147	2.04474516	-1.18993239
C	-6.20309721	0.77388731	-0.22623910
H	-6.24757111	-0.22010663	0.23838534
H	-6.66971274	1.45585185	0.50060771
C	-7.05367571	0.78434699	-1.49571682
C	-8.40204664	0.08860915	-1.41766927
H	-9.02795686	0.38049729	-2.26508944
H	-8.25382796	-1.00072818	-1.44967788
H	-8.91479331	0.31866463	-0.47518869
O	-6.66147446	1.34383361	-2.54225798



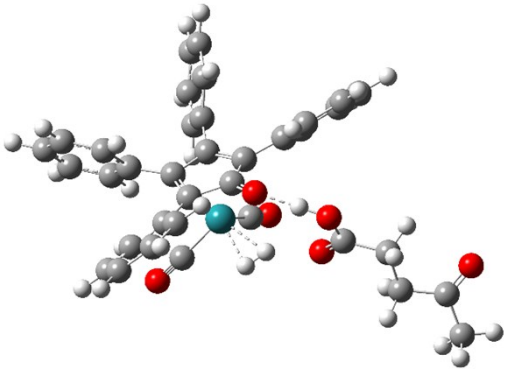
III-e (propeller): E_{Gibbs} = -1934.445291 eH

C	0.36992043	-0.95156047	-1.18858589
C	-0.04926609	0.42267562	-0.98243432
C	1.11236940	1.13693832	-0.42812411
C	2.18410631	0.18906492	-0.23998653
C	1.70531940	-1.13214387	-0.67951150
C	-1.30264224	1.02267715	-1.51370157
C	-1.74453083	0.67076935	-2.81225342
C	-2.05826970	1.96318910	-0.77550218
C	-2.91010823	1.24140899	-3.35363480
H	-1.17693956	-0.04763288	-3.39689229
C	-3.21726626	2.54072224	-1.32029190
H	-1.73841634	2.24808805	0.22250098
C	-3.65135516	2.18052345	-2.61198492
H	-3.23825813	0.95039744	-4.34822921
H	-3.77649956	3.27075588	-0.73970518
H	-4.54969435	2.62538041	-3.03331118
C	1.21336302	2.61157820	-0.24406473
C	0.92852973	3.46736930	-1.33398218
C	1.64141624	3.18470541	0.97427354
C	1.06842253	4.86063714	-1.20678041
H	0.60153302	3.04396371	-2.27976605
C	1.78143795	4.57641998	1.10225093
H	1.86237093	2.53796939	1.81932442
C	1.49510009	5.42156004	0.01216629
H	0.84388987	5.50338682	-2.05459929
H	2.10911306	4.99881450	2.04885914
H	1.60024830	6.49921342	0.11212896
C	3.58652384	0.52031816	0.13909668
C	4.28290946	-0.18747901	1.14460012
C	4.27249778	1.53672695	-0.56768889
C	5.62231962	0.11465165	1.44085353
H	3.78079105	-0.97522627	1.69774160
C	5.61291027	1.84064038	-0.27179689
H	3.75880254	2.08687795	-1.35086862
C	6.29460121	1.13148361	0.73517585
H	6.13761560	-0.44154716	2.21998190
H	6.12080109	2.62659530	-0.82563213
H	7.33086251	1.36627107	0.96619376
C	2.50053578	-2.37601461	-0.85350717
C	3.77266626	-2.32791321	-1.46971688
C	1.97850892	-3.63312195	-0.47287852
C	4.50792363	-3.50640295	-1.68753572
H	4.18515357	-1.37421947	-1.78538590
C	2.71229005	-4.81027263	-0.69082983
H	0.99794711	-3.68458594	-0.00846883
C	3.98251698	-4.75243747	-1.29755868
H	5.48500580	-3.45022108	-2.16152123
H	2.29564654	-5.76806160	-0.38888572
H	4.55187071	-5.66376891	-1.46468188
O	-0.30912994	-1.95128149	-1.82970081
H	-1.28502425	-1.97353571	-1.62023426
Ru	0.37323627	-0.44396666	1.14512735
H	-0.83790207	-1.50402544	1.36740908
C	1.18964041	-1.38742339	2.56002118
C	-0.55415057	0.68137888	2.33499281
O	1.69757273	-2.00214933	3.43162235
O	-1.14927242	1.39761322	3.06461834
H	-2.25791431	-1.64314622	0.32854340
O	-2.63269324	-1.92882789	-0.54354850
C	-4.00930620	-1.74705864	-0.73108227
O	-4.50754653	-2.07683262	-1.80684813
C	-4.74103300	-1.16312327	0.46636004
H	-4.19485654	-0.28262540	0.83006429
H	-4.72454914	-1.89194077	1.28911274
C	-6.19458645	-0.80041039	0.13403122
H	-6.24466974	0.10447831	-0.48652793
H	-6.64569301	-1.59617738	-0.47762945
C	-7.05921969	-0.61463390	1.37965244
C	-8.42551243	0.01720299	1.17166658
H	-9.05712093	-0.15101076	2.04795622
H	-8.30884197	1.10124956	1.02709119
H	-8.91519300	-0.37950325	0.27354660
O	-6.66442673	-0.97071656	2.51086102



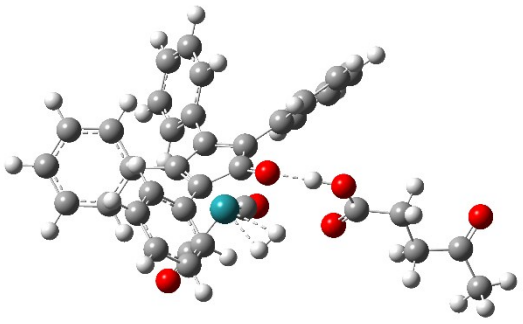
II-f (mirror): E_{Gibbs} = -1934.437291 eH

C	0.00784884	-0.63555987	1.28235661
C	-0.03242400	0.77831056	0.83142138
C	-1.36141429	1.03340670	0.27856735
C	-2.09052855	-0.23656004	0.23671738
C	-1.20741752	-1.28931084	0.70994843
Ru	-0.32538864	-0.29284029	-1.20589318
C	-1.23221005	-1.20488722	-2.62255441
C	0.33602067	1.04522837	-2.39793636
O	0.73329420	1.89599514	-3.10965405
O	-1.82300896	-1.76516471	-3.47495804
O	0.94202428	-1.22184236	1.92624690
C	-1.55246932	-2.72272256	0.89583291
C	-1.02789140	-3.44517954	1.99616644
C	-2.41868345	-3.39853418	0.00021824
C	-1.37066210	-4.79455767	2.19630996
H	-0.34286867	-2.95363003	2.67640181
C	-2.75798213	-4.74431798	0.20159742
H	-2.82859461	-2.87594380	-0.85866474
C	-2.23679482	-5.45173018	1.30350988
H	-0.95594268	-5.33054160	3.04679119
H	-3.42289131	-5.24120257	-0.50073390
H	-2.49758863	-6.49606926	1.45805811
C	-3.55926273	-0.35343927	0.02161623
C	-4.34667289	-0.81873491	1.10172632
C	-4.20339815	0.03117952	-1.17312275
C	-5.74449426	-0.89289853	0.98754757
H	-3.86318160	-1.12247518	2.02640402
C	-5.60150454	-0.05027487	-1.29013406
H	-3.61403237	0.37924445	-2.01596101
C	-6.37844660	-0.50991923	-0.21036580
H	-6.33453134	-1.25162534	1.82721208
H	-6.08054992	0.24320348	-2.22079142
H	-7.46007315	-0.57233444	-0.30133498
C	-1.99408186	2.37718654	0.14580357
C	-2.24683321	3.10164017	1.33447287
C	-2.36853320	2.94564052	-1.08884210
C	-2.86543916	4.36182532	1.28608936
H	-1.95287824	2.67958116	2.29236566
C	-2.98392897	4.20906148	-1.13891571
H	-2.16775316	2.40915137	-2.01198982
C	-3.23682458	4.92119637	0.04801669
H	-3.05183420	4.90621593	2.20852376
H	-3.26047549	4.63469741	-2.10032915
H	-3.71083183	5.89893904	0.00962781
C	0.95509150	1.81421648	1.23275729
C	1.64270598	1.69161337	2.46522275
C	1.20335067	2.95905339	0.43763101
C	2.54846292	2.68208149	2.88447944
H	1.47155958	0.82431885	3.09297582
C	2.10656167	3.94699941	0.85713260
H	0.69231817	3.08313249	-0.51166797
C	2.78711126	3.81380972	2.08367866
H	3.06922309	2.56405385	3.83157704
H	2.28287984	4.81529738	0.22698958
H	3.49252205	4.57619977	2.40534168
H	1.00938743	-1.55294282	-1.55202184
H	1.50512638	-1.05508810	-1.15341207
H	2.47370593	-1.17978580	1.86427341
O	3.50016568	-1.18352674	1.81871067
C	4.01802468	-0.99242617	0.58919735
O	3.31664727	-0.88742917	-0.45047701
C	5.53168738	-0.89164248	0.59616262
H	5.80131388	0.11758158	0.93672894
H	5.92383053	-1.57544760	1.35622068
C	6.15110501	-1.14915008	-0.78393363
H	5.55075448	-0.64002320	-1.55354681
H	6.11419183	-2.21605694	-1.04635637
C	7.58971893	-0.65352679	-0.90520645
C	8.37680415	-1.14424465	-2.11146394
H	7.76586378	-1.11437671	-3.02259576
H	9.27891430	-0.54126762	-2.24583790
H	8.67362252	-2.19137836	-1.95326548
O	8.09791980	0.12028676	-0.06510760



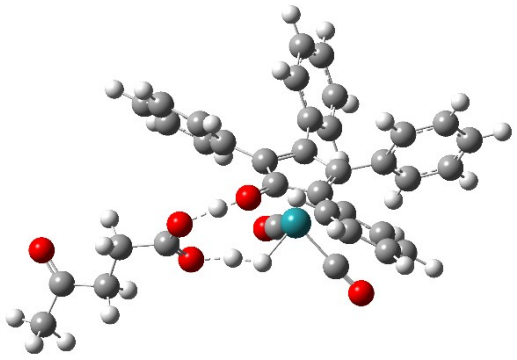
II-f (propeller): E_{Gibbs} = -1934.434477 eH

C	0.01279149	-0.68055846	-1.24112024
C	0.02480683	0.75024938	-0.83547375
C	1.35974852	1.05618672	-0.32581951
C	2.12212681	-0.19354657	-0.24817061
C	1.24772550	-1.28012077	-0.66074170
Ru	0.36667969	-0.26421113	1.22108900
C	1.26417599	-1.15562548	2.65650844
C	-0.23424207	1.11254603	2.40418122
O	-0.58475710	1.98687679	3.11170727
O	1.83206765	-1.70367852	3.53220748
O	-0.89829086	-1.32006372	-1.85965902
C	1.61882393	-2.69617915	-0.92414822
C	2.75078637	-3.00494865	-1.71451781
C	0.80125162	-3.75510812	-0.47093551
C	3.06549306	-4.33891874	-2.02644621
H	3.37993730	-2.20375965	-2.09220062
C	1.11388240	-5.08913386	-0.78288279
H	-0.08225203	-3.53230065	0.12147503
C	2.24994262	-5.38742609	-1.55991686
H	3.93993908	-4.55735124	-2.63488440
H	0.47273504	-5.89086755	-0.42465873
H	2.49265184	-6.41947154	-1.80183254
C	3.58667030	-0.30100966	0.00504469
C	4.47140147	0.57490927	-0.66908952
C	4.13568200	-1.30875471	0.83051124
C	5.86289376	0.45227857	-0.51168343
H	4.07645984	1.34684842	-1.32157438
C	5.52469224	-1.42667266	0.99389233
C	6.39654181	-0.54573830	0.32464103
H	6.52466234	1.13446809	-1.03945905
H	5.92389001	-2.20536973	1.63862175
H	7.47248071	-0.63787277	0.45110694
C	1.92671700	2.42161216	-0.13598665
C	1.87418071	3.33969737	-1.21087153
C	2.56504092	2.81103551	1.06179096
C	2.45240383	4.61526495	-1.08957897
H	1.38112544	3.05800696	-2.13710444
C	3.14077439	4.08637862	1.18399554
H	2.60639191	2.11571964	1.89582957
C	3.08807251	4.99429582	0.10835546
H	2.40109165	5.31007805	-1.92418613
H	3.62448345	4.37092926	2.11498982
H	3.53011484	5.98301562	0.20429230
C	-1.01604643	1.73102766	-1.24409387
C	-1.65970064	1.57716888	-2.49657109
C	-1.36739960	2.84183774	-0.44078770
C	-2.62203388	2.50682375	-2.92927563
H	-1.41190594	0.73107480	-3.12856528
C	-2.32722100	3.76952513	-0.87343249
H	-0.89430578	2.98662192	0.52513938
C	-2.96200465	3.60696650	-2.12092022
H	-3.10807332	2.36512723	-3.89140744
H	-2.58360781	4.61265876	-0.23662645
H	-3.71141444	4.32174520	-2.45221143
H	-0.99602200	-1.47466653	1.63380537
H	-1.48281153	-1.00124655	1.19853599
H	-2.42640700	-1.29631515	-1.84613987
O	-3.45476794	-1.29798458	-1.81036170
C	-3.98186266	-1.06225415	-0.59373029
O	-3.28960801	-0.93173414	0.44987788
C	-5.49418787	-0.94289162	-0.61805815
H	-5.74616271	0.06288622	-0.98175755
H	-5.88783108	-1.63731871	-1.36753528
C	-6.13117302	-1.16084514	0.76094648
H	-5.51968733	-0.65901908	1.52670807
H	-6.13059722	-2.22430536	1.03942075
C	-7.55390495	-0.61722807	0.86592954
C	-8.36597051	-1.07097342	2.07007462
H	-7.76102366	-1.05384606	2.98551930
H	-9.24827298	-0.43693570	2.19252606
H	-8.69668693	-2.10883411	1.91813585
O	-8.02971727	0.16579434	0.01550225
H	3.48250764	-2.00731400	1.34221534



TS II-f – IV (mirror): E_{Gibbs} = -1934.438146 eH

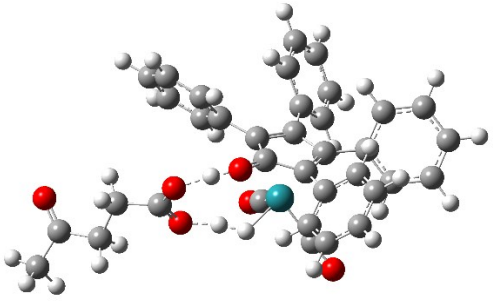
C	-0.19457230	-0.82861615	-1.25243635
C	-1.50763065	-1.19160571	-0.74139642
C	-2.11189472	0.03571676	-0.19878582
C	-1.14720592	1.11467888	-0.32997110
C	0.07362750	0.56957513	-0.92467561
Ru	-0.31772425	-0.44869652	1.13848040
C	0.47573944	0.73663546	2.39350248
C	-1.19052153	-1.44383070	2.49970639
O	-1.74951239	-2.07370644	3.32418368
O	0.95842987	1.49529297	3.15651806
O	0.62422770	-1.67597741	-1.87979981
C	1.24512512	1.34698234	-1.40712082
C	1.70135185	1.15723117	-2.73363556
C	1.89459653	2.30662573	-0.59822153
C	2.77711780	1.90993920	-3.23517413
H	1.22210251	0.41739442	-3.36821846
C	2.96872518	3.05908692	-1.09953953
H	1.56780266	2.46205641	0.42558271
C	3.41624848	2.86406110	-2.42115228
H	3.11903044	1.74569196	-4.25405585
H	3.45895175	3.78879136	-0.46008179
H	4.25343502	3.44082429	-2.80641907
C	-1.44199621	2.56330028	-0.15442386
C	-1.36651411	3.40184047	-1.29188424
C	-1.83635946	3.12585686	1.07819380
C	-1.68345274	4.76699844	-1.19702502
H	-1.05963701	2.98467926	-2.24715888
C	-2.14939727	4.49244996	1.17467440
H	-1.88346960	2.50047551	1.96487300
C	-2.07672122	5.31868009	0.03753126
H	-1.62022739	5.39674967	-2.08098107
H	-2.44504207	4.90944379	2.13409036
H	-2.31780780	6.37623061	0.11252038
C	-3.55919538	0.22922183	0.10077842
C	-4.46779452	0.18563066	-0.98277944
C	-4.05855137	0.47695507	1.39607271
C	-5.84182102	0.38994385	-0.77322263
H	-4.09676399	-0.01332080	-1.98530008
C	-5.43407259	0.67895456	1.60784804
H	-3.37516761	0.49759300	2.24065176
C	-6.33093119	0.63792124	0.52418808
H	-6.52699030	0.35246570	-1.61656191
H	-5.80189729	0.86407938	2.61405615
H	-7.39472817	0.79219484	0.68761142
C	-2.18052324	-2.49913607	-0.95005363
C	-1.83130442	-3.30543160	-2.06161365
C	-3.19610286	-2.96096262	-0.07715054
C	-2.48589399	-4.52764513	-2.29405470
H	-1.03840295	-2.98273865	-2.72581675
C	-3.84598606	-4.18219115	-0.31042216
H	-3.48033097	-2.37272008	0.78945684
C	-3.49649843	-4.97339436	-1.42235681
H	-2.20137139	-5.13162869	-3.15245578
H	-4.61958199	-4.51738661	0.37614659
H	-3.99899854	-5.92103425	-1.60129705
H	1.67520201	-1.61102308	-1.66591048
O	3.02001304	-1.59490600	-1.36125890
C	3.67716797	-1.28895581	-0.30789659
O	3.15208929	-1.11569238	0.88652871
C	5.17677914	-1.06066492	-0.42798443
H	5.53671525	-1.63776876	-1.28534191
H	5.32882485	-0.00331327	-0.68595012
C	5.96228478	-1.38429355	0.85200861
H	6.01516710	-2.46867183	1.02592471
H	5.42768992	-0.97237049	1.72064247
C	7.37633878	-0.80886107	0.85479515
C	8.32031681	-1.33542091	1.92568853
H	8.66122427	-2.34369968	1.64860162
H	9.19365400	-0.68361224	2.01505032
H	7.81312830	-1.41927972	2.89515257
O	7.74268687	0.05494135	0.02848826
H	0.95794553	-1.59136510	1.33634914
H	1.84306618	-1.29936414	1.10635529



ν_{TS} = -893.49 cm^{-1}

TS II-f – IV (propeller): E_{Gibbs} = -1934.436684 eH

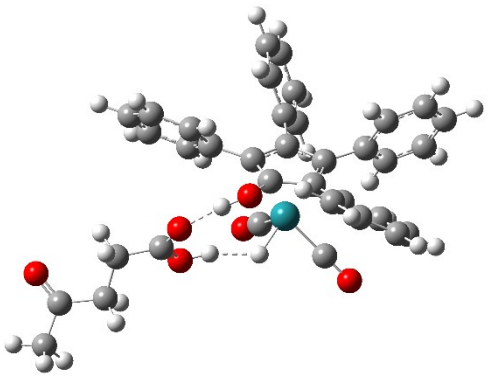
C	-0.22247882	-0.83581866	-1.24233281
C	-1.53916830	-1.17461988	-0.72936627
C	-2.14582453	0.06664009	-0.22927874
C	-1.16273037	1.12890465	-0.35503930
C	0.05992538	0.56264476	-0.93468806
Ru	-0.33397633	-0.44175342	1.12669374
C	0.48078120	0.74895263	2.36565553
C	-1.19168122	-1.40639268	2.51763564
O	-1.72909160	-2.02555037	3.36509563
O	0.97260069	1.51175870	3.11767632
O	0.56617380	-1.71204739	-1.86676276
C	1.24794760	1.30885745	-1.42971515
C	1.65653729	1.12745759	-2.77296111
C	1.96368393	2.21913150	-0.62051785
C	2.75011276	1.84222520	-3.29142198
H	1.12619901	0.42236910	-3.40695418
C	3.05561129	2.93425558	-1.13886549
H	1.67488008	2.36600362	0.41569862
C	3.45475796	2.74906332	-2.47722899
H	3.05503024	1.68460587	-4.32298553
H	3.59716116	3.62660295	-0.49928300
H	4.30576727	3.29625839	-2.87512296
C	-1.41108589	2.57521440	-0.10110202
C	-1.15693181	3.51191100	-1.13010547
C	-1.94935446	3.03678702	1.12090226
C	-1.43686499	4.87648513	-0.93977763
H	-0.74316429	3.17557117	-2.07636305
C	-2.22634474	4.39993865	1.31203439
H	-2.14684017	2.32748221	1.92024888
C	-1.97173187	5.32676947	0.28204096
H	-1.23388389	5.58318209	-1.74062984
H	-2.63544441	4.73752991	2.26091261
H	-2.18315088	6.38283284	0.43110788
C	-3.58401616	0.25624885	0.11235569
C	-4.32667296	1.24221064	-0.58053598
C	-4.25592889	-0.55843093	1.05060028
C	-5.70020398	1.41262786	-0.33526919
H	-3.83234052	1.87210947	-1.31428147
C	-5.62776390	-0.38682489	1.29888365
H	-3.71326839	-1.33032765	1.58614089
C	-6.35715944	0.60033796	0.60812656
H	-6.25234747	2.17609989	-0.87776503
H	-6.12408961	-1.02268455	2.02755450
H	-7.41883405	0.73310935	0.80147782
C	-2.20504969	-2.47961995	-0.98082048
C	-3.47208935	-2.52889348	-1.60731639
C	-1.55566304	-3.69524293	-0.66723853
C	-4.07954134	-3.76309550	-1.89830039
H	-3.98002923	-1.60747301	-1.87599241
C	-2.16162146	-4.92791531	-0.95885607
H	-0.57540254	-3.67053930	-0.20039252
C	-3.42858032	-4.96791058	-1.57375164
H	-5.05454513	-3.78194740	-2.37940464
H	-1.64760755	-5.85288395	-0.70930122
H	-3.89855099	-5.92245107	-1.79853339
H	1.61246064	-1.64926944	-1.68302975
O	2.97943688	-1.62886989	-1.36029115
C	3.64570521	-1.30833184	-0.31890035
O	3.13163642	-1.13305523	0.88256439
C	5.14110980	-1.06114937	-0.45535053
H	5.50085804	-1.64318261	-1.30955112
H	5.27451082	-0.00479024	-0.72742303
C	5.94496904	-1.35679232	0.82005310
H	6.02622717	-2.43815518	1.00124473
H	5.40736999	-0.95160748	1.69010673
C	7.34401373	-0.74571085	0.80803685
C	8.31364711	-1.25065299	1.86633517
H	8.67485445	-2.25030391	1.58374959
H	9.17223053	-0.57829117	1.94589208
H	7.82063150	-1.34757085	2.84192204
O	7.67845534	0.13000734	-0.01928957
H	0.93089012	-1.59877194	1.30999095
H	1.81980592	-1.30987162	1.09098046



ν_{TS} = -876.72 cm^{-1}

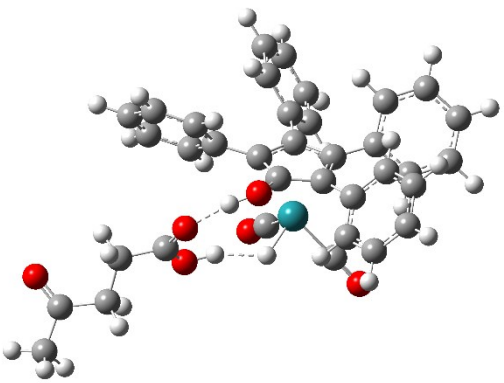
III-f (mirror): E_{Gibbs} = -1934.457692 eH

C	-0.21393275	0.79375639	1.21998554
C	-1.52033913	1.20104883	0.75471164
C	-2.18003975	-0.00670932	0.22436312
C	-1.24973580	-1.10691213	0.31510029
C	0.00360389	-0.60282978	0.89387194
Ru	-0.36533911	0.45088419	-1.16691070
C	0.43054124	-0.67931179	-2.44499417
C	-1.14051308	1.53714400	-2.50154307
O	-1.62516104	2.23331116	-3.32330662
O	0.93016674	-1.39961843	-3.24033325
O	0.63594414	1.62234252	1.88637995
C	1.14834199	-1.42691060	1.36461187
C	1.60363762	-1.28335428	2.69774318
C	1.77012656	-2.39054942	0.53860548
C	2.65284723	-2.08070055	3.18743915
H	1.13723683	-0.54948494	3.34925180
C	2.81587763	-3.19000020	1.02858308
H	1.43894613	-2.51431439	-0.48828042
C	3.26441704	-3.03799566	2.35563311
H	2.99148968	-1.95375541	4.21291632
H	3.28048004	-3.92584910	0.37693039
H	4.07695481	-3.65378149	2.73348669
C	-1.57898190	-2.54689650	0.12469969
C	-1.57971494	-3.39111899	1.26042461
C	-1.92240877	-3.09816447	-1.12804659
C	-1.92067502	-4.74908441	1.14464588
H	-1.31348759	-2.98225840	2.23173701
C	-2.26214216	-4.45715431	-1.24601809
H	-1.90880350	-2.46742912	-2.01237711
C	-2.26458862	-5.28827830	-0.11018394
H	-1.91627377	-5.38299265	2.02808928
H	-2.51978194	-4.86415985	-2.22069511
H	-2.52622389	-6.33979570	-0.20111397
C	-3.63558830	-0.14002437	-0.06481261
C	-4.54456793	-0.01910622	1.01261871
C	-4.14418225	-0.40642620	-1.35357094
C	-5.92631025	-0.16639576	0.80508130
H	-4.16632817	0.19458314	2.00933256
C	-5.52701247	-0.55286829	-1.56353760
H	-3.45916153	-0.48240480	-2.19387373
C	-6.42366236	-0.43507280	-0.48512260
H	-6.61101116	-0.06935578	1.64419770
H	-5.90086789	-0.75404695	-2.56454109
H	-7.49318773	-0.54567368	-0.64733031
C	-2.14805250	2.52861023	0.97893036
C	-1.78806891	3.30414218	2.10838371
C	-3.13449894	3.03875235	0.10016619
C	-2.40318684	4.54489242	2.35167640
H	-1.01858227	2.94225609	2.78029104
C	-3.74568363	4.27786523	0.34401159
H	-3.42319058	2.47326700	-0.78025739
C	-3.38528315	5.03905161	1.47330039
H	-2.11127114	5.12488809	3.22420016
H	-4.49718623	4.65029281	-0.34795951
H	-3.85767955	6.00049323	1.66088940
H	1.61619019	1.48039489	1.69865386
O	3.16710449	1.37894989	1.28716712
C	3.90031823	1.05504395	0.32650337
O	3.41703559	0.82849486	-0.92641314
C	5.39035699	0.84213896	0.45135168
H	5.71974152	1.32144996	1.37733199
H	5.56347611	-0.23530716	0.58141726
C	6.19914547	1.33392598	-0.76266617
H	6.18434010	2.43081331	-0.83545791
H	5.74028868	0.96492440	-1.69082612
C	7.65057500	0.85528684	-0.73150845
C	8.59978912	1.49890705	-1.72913223
H	8.85657402	2.51273816	-1.38893515
H	9.51998576	0.91382605	-1.80713531
H	8.13253868	1.59645626	-2.71710298
O	8.03429285	-0.02270244	0.07043670
H	0.89839864	1.45684942	-1.33266397
H	2.42380324	0.92404169	-1.01538534



III-f (propeller): E_{Gibbs} = -1934.456565 eH

C	-0.23049027	-0.79837369	-1.20451627
C	-1.54129735	-1.19077383	-0.74488925
C	-2.21193714	0.02644397	-0.25577502
C	-1.27502401	1.12008619	-0.34944900
C	-0.01163867	0.60270328	-0.90124978
Ru	-0.38364107	-0.44070205	1.15705180
C	0.38994775	0.71348589	2.43083515
C	-1.13692522	-1.52708908	2.50231742
O	-1.59816537	-2.23279449	3.33029786
O	0.87293758	1.45014924	3.22035942
O	0.59656222	-1.65014551	-1.86708326
C	1.15010470	1.40159709	-1.37807252
C	1.57164573	1.26301344	-2.72296023
C	1.82676563	2.32462952	-0.54948398
C	2.64125567	2.02687656	-3.22211853
H	1.06353521	0.55781105	-3.37529930
C	2.89277494	3.09142308	-1.04892815
H	1.52185157	2.44364845	0.48593610
C	3.30705480	2.94513820	-2.38773445
H	2.95400496	1.90358513	-4.25618247
H	3.39948079	3.79699986	-0.39517587
H	4.13530826	3.53512758	-2.77258693
C	-1.57507648	2.55453962	-0.08305841
C	-1.35108889	3.51201257	-1.10008841
C	-2.12916995	2.98558638	1.14328218
C	-1.67492756	4.86485197	-0.89508427
H	-0.92702267	3.19924190	-2.05013352
C	-2.45278738	4.33661996	1.34883747
H	-2.30152187	2.26092631	1.93470443
C	-2.22732047	5.28347143	0.33030241
H	-1.49458128	5.58696058	-1.68779326
H	-2.87508974	4.64936542	2.30057101
H	-2.47492733	6.33008985	0.49058945
C	-3.65833081	0.14388173	0.08271196
C	-4.44874724	1.10475674	-0.59206466
C	-4.28856911	-0.71302350	1.01299088
C	-5.82719292	1.21081826	-0.33684377
H	-3.98561954	1.76598294	-1.31874823
C	-5.66592890	-0.60879489	1.26838152
H	-3.70504614	-1.46251906	1.53830259
C	-6.44267294	0.35481121	0.59591219
H	-6.41579900	1.95759918	-0.86430271
H	-6.12956935	-1.27686151	1.98994401
H	-7.50841052	0.43655709	0.79575144
C	-2.15171100	-2.51763738	-1.02194071
C	-3.40117233	-2.60674031	-1.67862470
C	-1.46850491	-3.71233706	-0.69992441
C	-3.95710926	-3.85916688	-1.99405837
H	-3.93520935	-1.70090595	-1.94970450
C	-2.02258656	-4.96319375	-1.01615458
H	-0.50395735	-3.65481386	-0.20397175
C	-3.27159586	-5.04297264	-1.66336008
H	-4.91937333	-3.90844679	-2.49825478
H	-1.48354729	-5.87176790	-0.75868414
H	-3.70193895	-6.01168559	-1.90652012
H	1.57930475	-1.49865209	-1.71691831
O	3.14890643	-1.38789011	-1.29607720
C	3.88528673	-1.03771342	-0.34777185
O	3.40621950	-0.78156963	0.90240286
C	5.37438346	-0.82254534	-0.48129984
H	5.70325405	-1.32085942	-1.39741066
H	5.54327170	0.25244626	-0.63469967
C	6.18777969	-1.28455514	0.74147213
H	6.18554958	-2.38011993	0.83305222
H	5.72365590	-0.90475229	1.66265932
C	7.63361354	-0.78949140	0.70501481
C	8.58914192	-1.40920082	1.71176191
H	8.85945492	-2.42358713	1.38390707
H	9.50171412	-0.81162830	1.78448577
H	8.12132118	-1.50107929	2.70001701
O	8.00781023	0.08302887	-0.10728665
H	0.89454540	-1.42737612	1.32930724
H	2.41370715	-0.87545075	0.99576247



5. Life Cycle Assessment

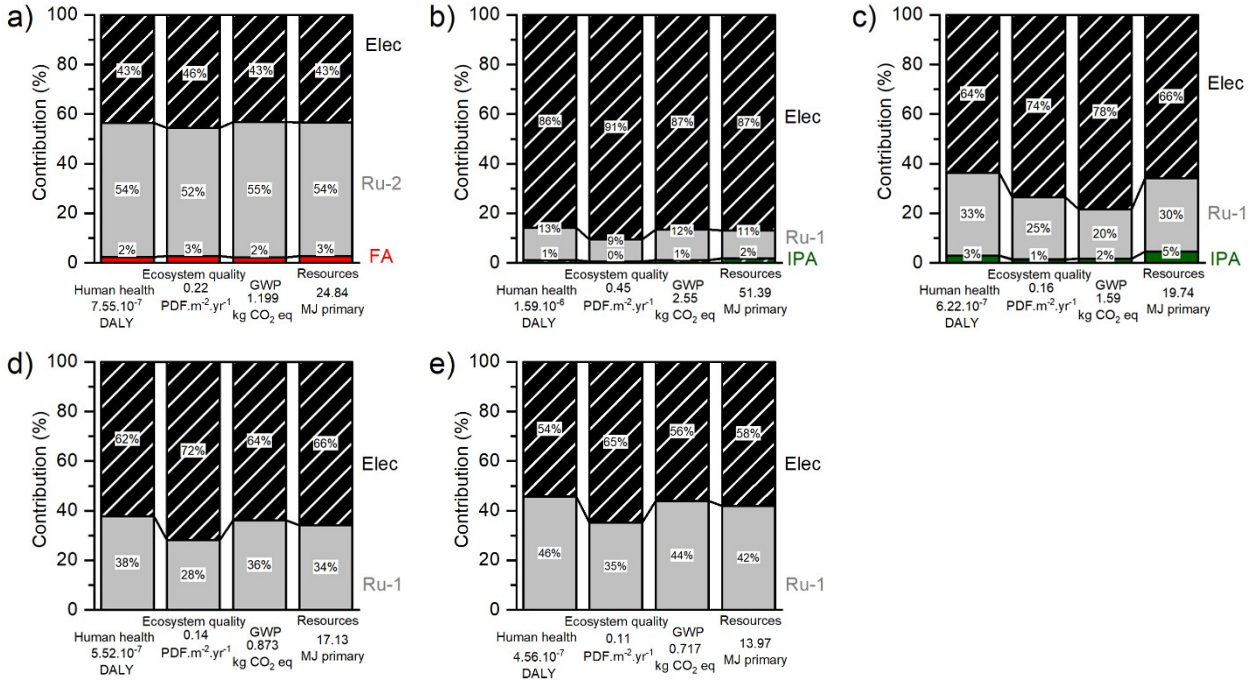


Figure S5.1: **Magnitude of contribution to four environmental impact categories for:**
a) transfer hydrogenation using 0.1% Ru-2 and 2.5 eq. FA at 100°C for 6 hours in a reflux setup.
b) transfer hydrogenation using 0.1% Ru-1 and 2.5 eq. IPA at 100°C for 32 hours in an autoclave.
c) transfer hydrogenation using 0.1% Ru-1 and 2.5 eq. IPA at 120°C for 12 hours in an autoclave.
d) hydrogenation using 0.1% Ru-1 and 50 bar H_2 at 100°C for 12 hours in an autoclave.
e) hydrogenation using 0.1% Ru-1 and 50 bar H_2 at 120°C for 5 hours in an autoclave.
The total values for each impact category are indicated below the x-axis.
The relative contributions of formic acid (FA), isopropyl alcohol (IPA), the applied Shvo catalyst precursors (Ru-1; Ru-2), and the electric consumption (elec) are indicated along the y-axis.

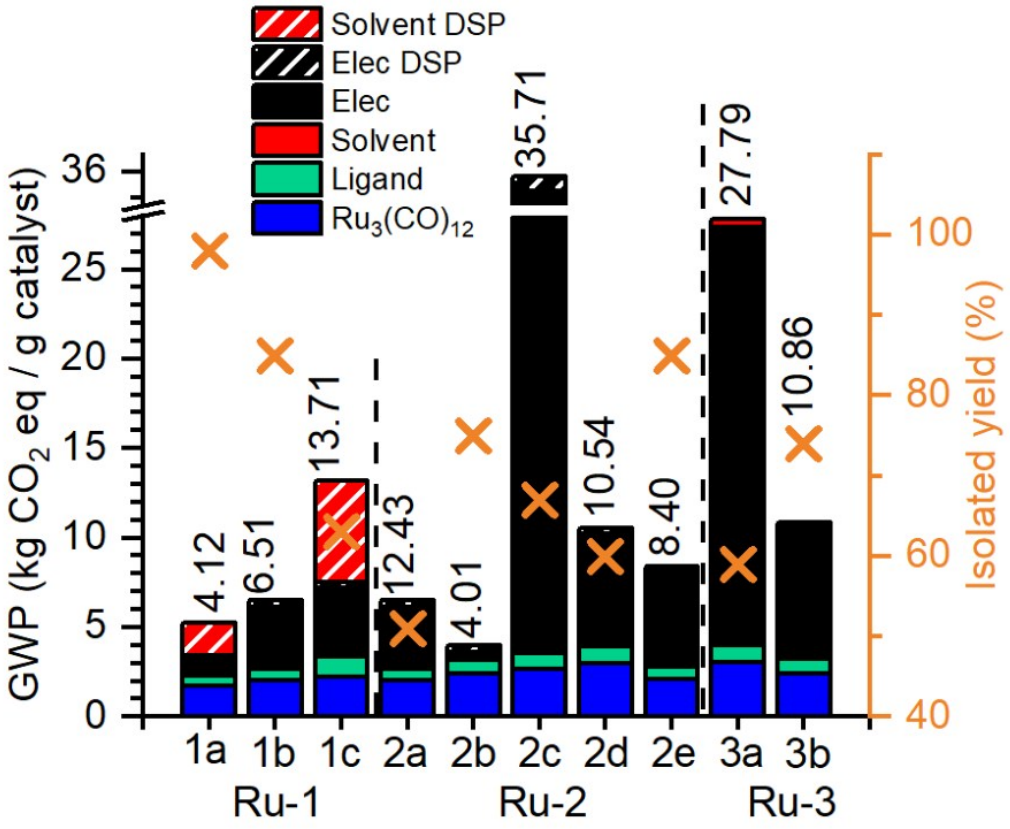


Figure S5.2: **Contribution distribution to the GWP for various reported synthetic procedures of the Shvo catalyst precursors in conjunction with their isolated yields.**

1a: **This work.**

1b: **M. I. Bruce, J. R. Knight, J. Organomet. Chem., 1968, 12, 411.**

1c: **B. A. Persson, A. L. E. Larsson, M. Le Ray, J-E. Bäckvall, J. Am. Chem. Soc., 1999, 121, 1645.**

2a: **This work.**

2b: **C. Cesari, L. Sambri, S. Zacchini, V. Zanotti, R. Mazzoni, Organometallics, 2014, 33, 2814. (microwave procedure)**

2c: **C. Cesari, L. Sambri, S. Zacchini, V. Zanotti, R. Mazzoni, Organometallics, 2014, 33, 2814. (oil bath procedure)**

2d: **B. L. Conley, M. K. Pennington-Boggio, E. Boz, T. J. Williams, *Chem. Rev.*, 2010, 110, 19.**

2e: **Fábos, L. T. Mika, I. T. Horvath, *Organometallics* 2014, *33*, 181.**

3a: **This work.**

3b: **M. J. Mays, M. J. Morris, P. R. Raithby, Y. Shvo, D. Czarkie, Organometallics, 1989, 8, 1162.**

Each synthetic procedure of the Shvo catalyst precursors is indicated below the x-axis.

The contributions of the applied chemicals, the electric consumptions (elec), and the down-stream processing (DSP) are accumulated along the y-axis.

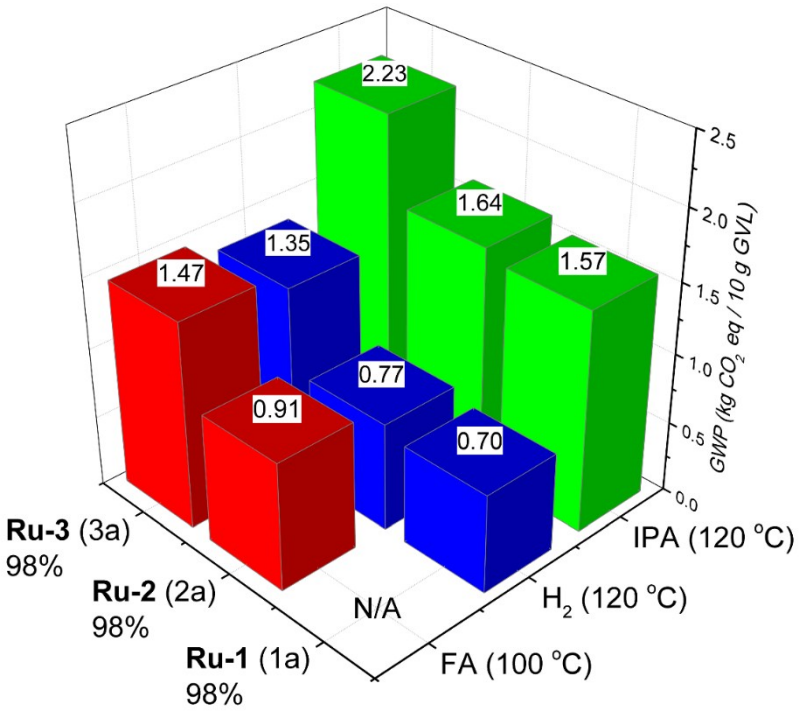


Figure S5.3: Combinatorial comparison of GWP for the LA hydrogenations with three different H-donors under their optimal conditions and the three Shvo catalyst precursors normalized to 98% isolated yield. (N/A = not applicable)

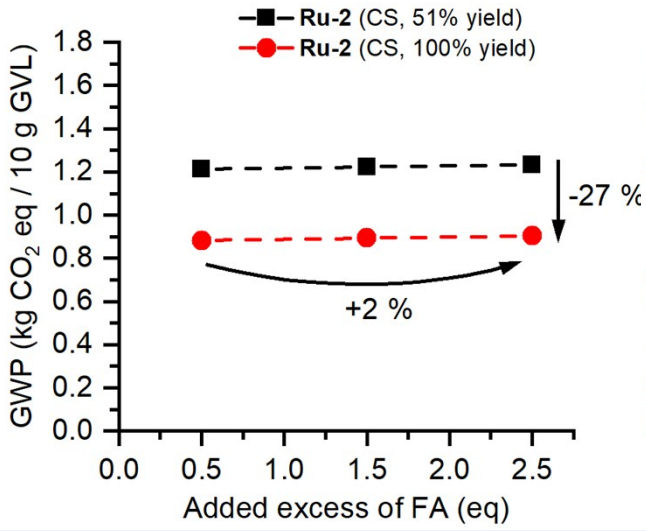


Figure S5.4: The effect of applying an excess FA on the GWP of the FA-mediated transfer hydrogenation of LA.

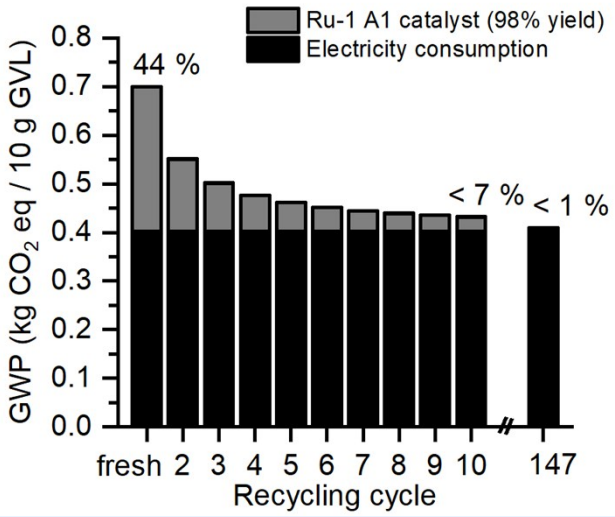


Figure S5.5: The hypothetical effect of recycling Ru-1 from the H_2-mediated LA hydrogenation on the corresponding GWP.

Table S5.1: List of equipment used for electric consumption recording.

Reaction description	Device description	Brand, model	Recorded energy for isothermal averages
General	Heating plate for oil bath	Heidolph, MR Hei-Tec	5.5 W; (20°C) 93.4 W; (50°C) 120.8W; (65°C) 152.2 W; (80°C) 170.4 W; (90°C) 192.8 W; (100°C) 219.4 W; (110°C) 294.7 W; (135°C) 379.4 W; (165°C)
General	Water circulation pump	Julabo, EH v.2	108.8 W
General	Vacuum pump	Vacuubrand RZ-6	288.8 W
General	Rotavaporator	KNF Lab, RC900	907.2 W; (40°C)
Hydrogenation	Autoclave	Parr 5500 compact	197.8 W; (100°C) 208.4 W; (120°C)
GVL distillation procedure	Membrane pump	Vacuubrand, PC3001 VARIO Pro	4.9 W
Retrosynthesis step e	Inorganic tube oven	Nabertherm RT 50-250/11	101.8 W; (390°C)
Retrosynthesis steps b(2), g	Microwave	Biotage Initiator+	153.5 W; (70°C) 168.8 W; (110°C)
Retrosynthesis step i	Ultrasonic bath	Branson 3800	63.5 W
*Copper sulfate synthesis	Drying oven	Memmert, UF55	8.5 W; (100°C)
*Triethylamine synthesis	Fixed bed reactor	Parr 5400	413.7 W