Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Materials for

A Practical and Concise Homogeneous Nickel Catalyst for Efficient Solvent-free Synthesis of γ-Valerolactone

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1. Literature overview

Table S1 Homogenous catalyzed conversion of LA into GVL

Year	Catalyst	S/C[a]	Additive	Reaction Conditions				Yield of GVL	Ref
				Solvent	H_2 (bar)	T (°C)	Time (h)		
1982	$[RuCl_2(PPh_3)_3]$	180	–	Toluene	12	180	24	99	[1]
1982	$[RuH_2(PPh_3)_4]$	180	–	Toluene	12	180	24	58	[1]
1990	$Ru(COOCH_3)_2$/S-BINAP	1000	–	Ethanol	100	25	110	96	[2]
2001	Ru/SEGPHOS[a]	1000	–	Ethanol	50	50	20	>99	[3]
2004	[Ru-tetraMe-BITIOP]$(OTf)_2$ [b]	500	–	Ethanol	100	45	76	>99	[4]
2004	[Ru-tetraMe-BITIOP]$(OTf)_2$ [b]	500	1-bromo butane	Ethanol	100	45	43	>99	[4]
2005	$[Ru(Me\text{-}allyl)_2(COD)]$/S-BINAP	200	HCl	Ethanol	60	60	5	96	[5]
2005	$[Ru(Me\text{-}allyl)_2(COD)]$/S-BINAP[b]	200	HCl	Ethanol	60	60	5	95	[5]
2008	$RuCl_3$/(R-BINAP)][b]	200	HCl	Methanol	60	65	6	96	[6]
2008	$[Ru(acac)_3]/PBu_3$	1660	NH_4PF_6	–	100	135	8	>99	[7]
2008	$[Ru(acac)_3]$/TPPTS	600	–	Water	69	140	12	95	[7]
2009	$RuCl_3/PPh_3$[c]	1000	1.0 eq. FA 10mol% pyridine	Water	–	150	12	93	[8]
2010	$[Ru(acac)_3]/P\textit{n}Oct_3$	1000	1mol% NH_4PF_6	–	100	160	18	99	[9]
2010	$[Ru(acac)_3]$/DPPB	1000	1mol% NH_4PF_6	–	100	160	18	89	[9]
2010	$[Ru(acac)_3]$/triphos	1000	1mol% p-TsOH	–	100	160	18	58	[9]
2011	$[RuH_2(CO)(triphos)]$	1000	–	–	100	160	18	22	[10]
2011	$RuCl_3$/TPPTS	1000	–	DCM/Water	45	90	1.33	>99	[11]
2012	$[Ir(COE)_2Cl_2]_2$/PNP*t*Bu	1000	1.2 eq. KOH	Ethanol	50	100	15	96	[12]
2012	$[IrH_3(PNPtBu)]$	10000	1.2 eq. KOH	Ethanol	50	100	24	98	[12]
2012	$[IrH_3(PNPtBu)]$	100000	1.2 eq. KOH	Ethanol	100	100	48	71	[12]
2012	$[Ru(acac)_3]$/*n*Bu-DPPDS	6370	–	–	100	140	1.8	>99	[13]
2013	$[Cp^*Ir(Bipy\text{-}OMe)]SO_4$	10000	–	Water	10	120	4	98	[14]
2013	$[Cp^*Ir(Bipy\text{-}OMe)]SO_4$ [c]	1000	1.2 eq. FA	Water	–	25	24	94	[14]
2014	$[Ru(acac)_3]$/tertaphos	100000	0.002 mol% $Sc(OTf)_3$	–	80	140	22	73	[15]
2014	$[Ru(acac)_3]$/DPPB	12740	–	–	100	140	1.8	>99	[16]
2014	$Fe(OTf)_2$/tetraphos[c,d]	20	2.0 eq. FA	Dioxane	–	140	24	98	[17]
2014	Shov's catalyst[c]	2400	1.5 eq. FA	–	–	100	8	>99	[18]
2015	$[RuH_2(CO)(triphos)]$	200	–	THF	65	150	25	85	[19]
2015	$[RuH_2(CO)(N\text{-}triphos)]$	200	NH_4PF_6	THF	65	150	25	95	[19]
2015	$[RuH_2(PPh_3)(N\text{-}triphos)]$	200	p-TsOH	THF	65	150	25	77	[19]
2015	$[Pd(DTBPE)Cl_2]$	1000	–	Water	5	80	5	>99	[20]
2015	$[Pd(DTBPE)Cl_2]$[c]	1000	2.1 eq. FA 10mol% NEt_3	Water	–	100	5	>99	[20]
2015	Casey's catalyst[c,e]	100	5 mol% $NaHCO_3$	*i*-PrOH	–	100	19	95	[21]
2015	$[Fe_3(CO)_{12}]$[c]	25	2.1 eq. FA 4 eq. ImN	Water	–	180	15	92	[22]
2016	$[RuCl_2(p\text{-}cymene)(i\text{Pr}_2\text{-}imy)]$	1000	–	Water	12	130	2.66	96	[23]
2016	$[RuCl_2(p\text{-}cymene)(i\text{Pr}_2\text{-}imy)]$	1000	–	–	12	130	2.66	5	[23]
2017	$[Cp^*Ir(dpa)]SO_4$	1000	–	Water	5	110	16	100	[24]
2017	$[Cp^*Ir(dpa)]SO_4$	10000	–	Water	5	110	72	99	[24]
2017	$[Cp^*Ir(dpa)]SO_4$ [c]	2000	–	Water	–	110	24	100	[24]
2017	[(mbdpa)(p-cymene)RuCl]Cl [c]	2000	2 eq. FA 1 eq. Et_3N	–	–	150	16	99	[25]
2017	NHC-Ir	2000	1 eq. KOH	*i*-PrOH	50	100	4	>99	[26]

2017	NHC-Ir	10000	1 eq. KOH	*i*-PrOH	50	100	24	>99	[26]
2017	[Ru(p-cymene)Cl(N_2-COOH)]Cl [c]	1000	2 eq. FA 0.1 eq. Et_3N	–	–	150	12	98	[27]
2018	$RuCl_3$•3H_2O/Taurine	2000	–	Water	40	140	1	99.9	[28]
2018	$RuCl_3$•3H_2O/BPhDS	3000	–	Water	80	140	1	99.9	[28]
2018	Iron pinicer complex	2000	KOH	Methanol	50	100	12	95	[29]
2018	Shov's catalyst	1000	–	Toluene	60	100	7	98	[30]
2018	Knölker-type catalysts	1000	–	EtOH	60	100	20	57	[30]
2019	[Co($BF4)_2$]•4H_2O /Tetraphos	40	–	DMI	1	100	24	99	[31]
2019	Shov's catalyst	1000	–	–	50	120	5	>99	[32]
now	[Ni($OAc)_2$]•3H_2O /triphos	100	–	–	1	150	20	98	This work
now	[Ni($OAc)_2$]•3H_2O /DCyPE	100	–	–	1	150	20	88	This work
now	[Ni($OAc)_2$]•3H_2O /DCyPP	100	–	–	1	150	20	90	This work
now	[Ni($OAc)_2$]•3H_2O /DIPAMP	100	–	–	1	150	20	90	This work
now	[Ni($OAc)_2$]•3H_2O /Me-BPE	100	–	–	1	150	20	93	This work
now	[Ni($OAc)_2$]•3H_2O /triphos [c]	100	2 eq. FA	–	–	150	20	94	This work
now	[Ni($OAc)_2$]•3H_2O /triphos	1000	–	–	15	150	20	96	This work
now	[Ni($OAc)_2$]•3H_2O /triphos	10000	–	–	30	150	20	94	This work
now	[Ni($OAc)_2$]/DPPP	1000	–	–	15	150	20	94	This work

[a] Substrate/catalyst based on moles of metal [b] Conversion of Ethyl levulinate into GVL. [c] Conditions for Transfer hydrogenation catalysis using formic acid as hydrogen source. [d] Conversion of Methyl levulinate into GVL. [e] Conditions for transfer hydrogenation catalysis using isopropanol as hydrogen source;

2. General information

The air and moisture sensitive operations were carried out using standard vacuum line, Schlenk or handled in a nitrogen-filled glovebox. All commercially available compounds and chemicals were purchased from sigma, Alfa-aesar, Adamas-beta, Energy Chemical, TCI and Aladdin, and used as received directly. Glassware was dried well before use. Solvents such as Tetrahydrofuran (THF), Ethanol were purchased “anhydrous” form.

Gas chromatographic **(GC)** analysis was performed on a Shimadzu GC-2014 series GC system facilitated with a flame-ionization detector. **EPR** spectra of in-situ formed catalysts was recorded on a JEOL JES-FA200 spectrometer at 20K using liquid Nitrogen as a coolant.

Ambient pressure X-ray photoelectron spectroscopy (**AP-XPS**) was measured using horizontal linear polarized X-ray beam. The incident and emission angles were kept among 0^{o}-68^{o}. Highly purified hydrogen gas was introduced into an ambient-pressure gas cell within limit of 5×10^{-10} Torr. During hydrogen exposure, the temperature of sample was raised from room temperature to 150^{o}C, and the Ni_{2P} core-level spectra were measured at the photon energies of 800 eV to 900 eV.

3. Experimental procedures

a. Hydrogenation of levulinic acid (LA) to γ-Valerolactone (GVL)

Method a: atmospheric H_2 Pressure hydrogenation reactions

The hydrogenation of LA to GVL at 1atm H_2 was carried out by adding 5 mmol LA, 1mol% Ni salt and 1mol% triphos in a 10 mL Schlenk reaction tube with H_2 filled balloon at 150°C for 20 h. During reaction, calculated amount of reaction mixture was transferred to sampling tubes and diluted by using N,N-Dimethylacetamide (DMA) as solvent. N-methyl pyrrolidone (NMP) was used as internal standard, and analyzed by gas chromatography (see Figure S1 for details)

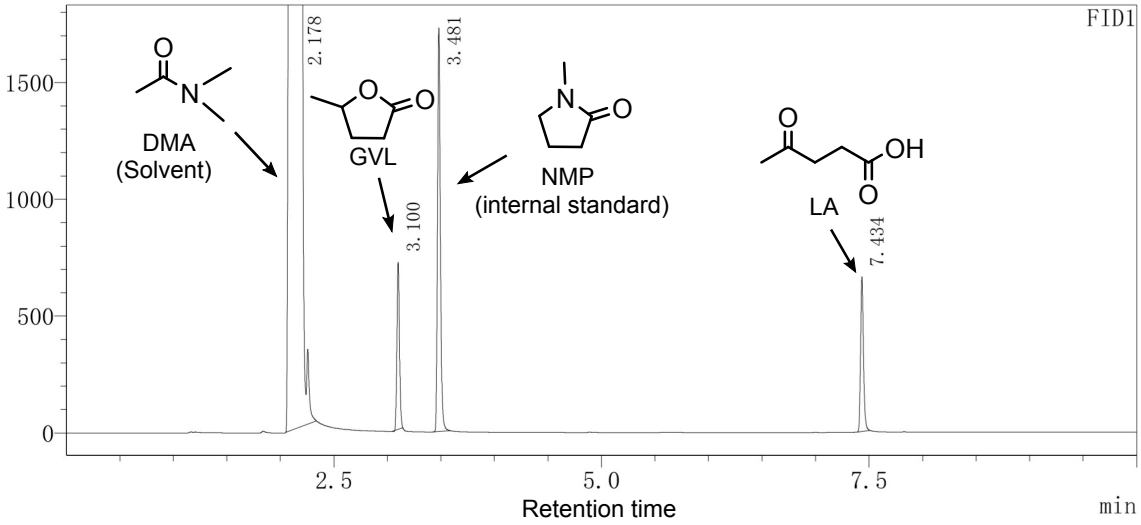


Figure S1. Conversion of LA and yield of GVL were determined via GC instrument, equipped with FID detector. DB-FFAP column (internal diameter: 0.32 mm; film: 0.25 mm; carrier gas: N_2) was used with N-methyl pyrrolidone (NMP) as internal standard. The column temperature was 120°C(1min) and raised to 225°C(1min) with 7°C min^{-1}. The detector temperature was 250°C; H_2 flow: 30 $mLmin^{-1}$; airflow: 300 $mLmin^{-1}$ .The resulting GC chromatogram of reaction contents are shown in figure.

Method b: hydrogenation of LA at low catalyst quantity

For selected hydrogenation experiments, 10 mmol of LA and desired amount of catalyst ($Ni(OAc)_2.4H_2O$ and phosphine ligand) were loaded in a 50 mL Zr alloy reactor, flushed and filled with hydrogen and stirred at 700 rpm. The temperature of autoclave was elevated to the 150°C in 30 min and maintain for 20h, then cooled down in water to room temperature. After the reaction a known amount of reaction mixture was taken from the reactor and diluted with N,N-Dimethylacetamide(DMA). Then N-methyl

pyrrolidone (NMP) was added as internal standard and analyzed by gas chromatography. For *S/C* 10,000 and 100,000 reactions, stock solution of LA and catalysts was prepared and then further diluted to required concentration by LA. **For *kilogram scale* conversion, please see section 6 for detail.**

b. Hydrolysis of carbohydrate biomass

9 g Carbohydrate: cellulose, glucose, sucrose, fructose or starch was loaded in a 100 mL stainless steel reactor and 50 mL 0.8 M HCl solution was added. The reactor flushed and filled with nitrogen and heated to 220 °C under vigorous stirring for 1 h. The reaction mixture from reactor was then transferred to 200 mL flask, neutralized with NaOH (pH=2) and filtered by using pressure-equalizing dropping funnel. Then the filtrate was concentrated via rotary evaporator, and LA was distilled under reduced pressure. Finally, the concentrated LA subjected to the typical hydrogenation reactions.

c. Catalyst Recycle test

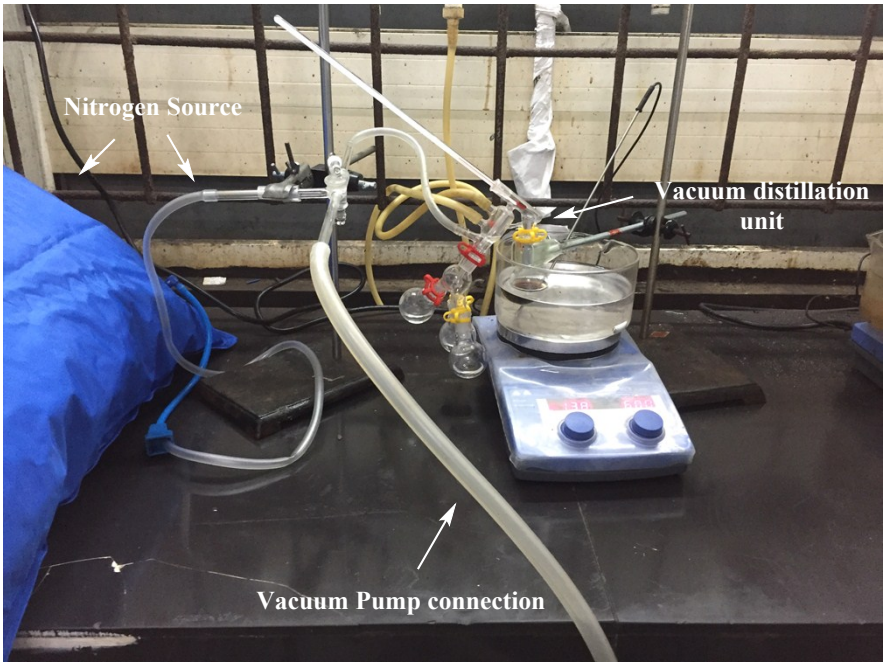
Reuse of catalyst in open air

10 mol LA, 0.01 mmol Ni(OAc)2•4H_2O, and 0.01mmol triphos or DPPP were added in a 50 ml reactor. Then the reactor was flushed and filled with H_2 up to 15 atm and allowed for 20h at 150°C. After completing reaction, the reaction mixture was transferred to vacuum distillation unit and the product was removed from catalyst via reduced pressure distillation. Then the catalyst was transferred back to reactor and reloaded with 10 mol LA and then system was subjected to the next run. After completion of each run, the products were analyzed as above-mentioned.

Reuse of catalyst under Nitrogen atmosphere

All the post-treatment process was carried under nitrogen atmosphere carefully. 10 mol LA, 0.01 mmol Ni(OAc)2•4H_2O, and 0.01mmol triphos or DPPP were added in a 50 ml reactor. Then the reactor was flushed and filled with H_2 up to 15 atm and allowed for 20h at 150°C. Upon completion of the reaction, the reactor was cooled to room temperature, and carefully moved to inert atmosphere inside the glovebox. After transferring reaction mixture to vacuum distillation unit, it was then taken out from glovebox under nitrogen atmosphere and connected to vacuum pump. Reaction product

was removed by reduced pressure distillation. Remaining catalyst was transferred back to reactor inside glovebox, reloaded with 10 mol LA and then system was subjected to the next run. After completion of each run, the products were analyzed as above-mentioned.

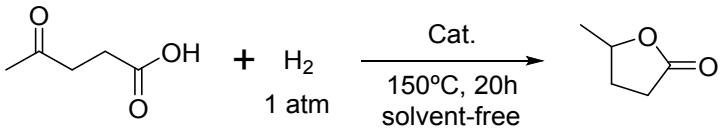


d. Preparation of samples for XPS and EPR analysis

Fresh samples of In-situ [$Ni(OAc)_2$]/triphos and [$Ni(OAc)_2$]/DPPP) catalysts was prepared by dissolving 0.5 mmol of $Ni(OAc)_2$. In 15 ml anhydrous ethanol in a 100ml Schlenk flask equipped with distillation tube under nitrogen atmosphere. 0.5 mmol solution of ligand in 20ml THF was then added to the flask by a syringe and allowed for stirring at 80^oC for 3h. After completing reaction, solvent was evaporated via rotary evaporator at room temperature. The resulting powder further dried in a vacuum oven at 60^oC for overnight and sent for EPR and XPS analysis

4. Screening of Ni salts, ligands, reaction conditions

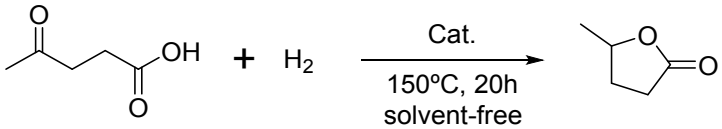
Table S2. Screening of Ni salts for conversion of LA to GVL

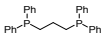
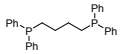
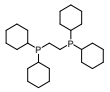
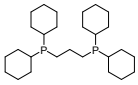
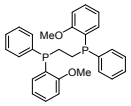
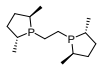
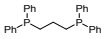
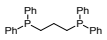


entry	Ni^{2+}	Ligand	Yield
1	1mol% $Ni(acac)_2$	1mol% triphos	94%
2	**1mol% $Ni(OAc)_2$**	**1mol% triphos**	**98%**
3	1mol% $Ni(OTf)_2$	1mol% triphos	89%
4	1mol% $Ni(SO_4)_2$	1mol% triphos	84%
5	1mol% $Ni(BF_4)_2$	1mol% triphos	91%
6	1mol% $Ni(ClO_4)_2$	1mol% triphos	16%
7	1mol% $NiCl_2$	1mol% triphos	41%
8	1mol% $NiBr_2$	1mol% triphos	8%
9	1mol% NiI_2	1mol% triphos	2%
10	1mol% $Ni(HCOO)_2$	1mol% triphos	82%

All reaction was carried out in solvent free conditions. Reaction conditions: 5mmol LA, 1atm H_2, 1mol% Ni-catalysts, 1mol% triphos, 150°C, 20h.

Table S3. Screening of ligands for conversion of LA to GVL



entry	Ni^{2+}	Ligand	H_2 (atm)	Yield
1	1mol% $Ni(OAc)_2•4H_2O$	1mol% DPPM 	1	5%
2	1mol% $Ni(OAc)_2•4H_2O$	1mol% DPPE 	1	30%
3	1mol% $Ni(OAc)_2•4H_2O$	1mol% DPPP 	1	37%
4	1mol% $Ni(OAc)_2•4H_2O$	1mol% DPPB 	1	8%
5	1mol% $Ni(OAc)_2•4H_2O$	2mol% PPh_3 	1	trace
6	1mol% $Ni(OAc)_2•4H_2O$	1mol% DCyPE 	1	88%
7	1mol% $Ni(OAc)_2•4H_2O$	1mol% DCyPP 	1	90%
8	1mol% $Ni(OAc)_2•4H_2O$	1mol% DIPAMP 	1	90%
9	1mol% $Ni(OAc)_2•4H_2O$	1mol% (R,R)-Me-BPE 	1	93%
10	1mol% $Ni(OAc)_2•4H_2O$	1mol% triphos 	1	98%
11	0.1mol% $Ni(OAc)_2•4H_2O$	0.1mol% triphos 	15	97%
12	0.01mol% $Ni(OAc)_2•4H_2O$	0.01mol% triphos 	30	94%
13	0.1mol% $Ni(OAc)_2•4H_2O$	0.1mol% DPPP 	15	94%
14	0.01mol% $Ni(OAc)_2•4H_2O$	0.01mol% DPPP 	30	48%

All reaction was carried out in solvent free conditions. Reaction conditions: 5mmol LA, 1atm H_2, 1mol% Ni-catalysts, 1mol% triphos, 150°C, 20h.

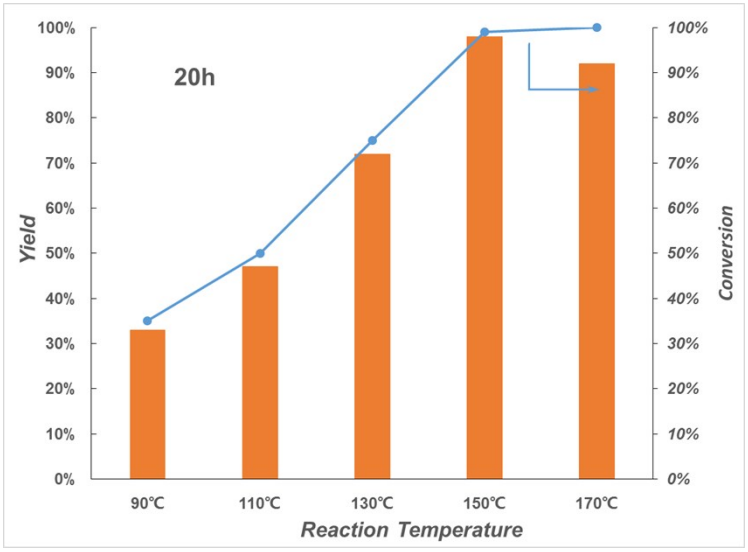


Figure S2 Tthe effect of reaction temperatures on GVL yield.

Reaction conditions: LA (5 mmol), $Ni(OAc)_2 \cdot 4H_2O$ (0.05 mmol), triphos (0.05mmol), H_2 (1 atm), 20h.

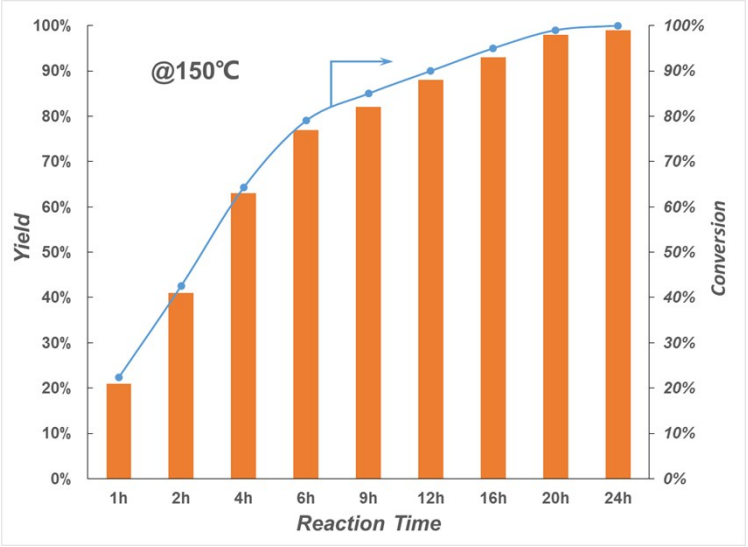
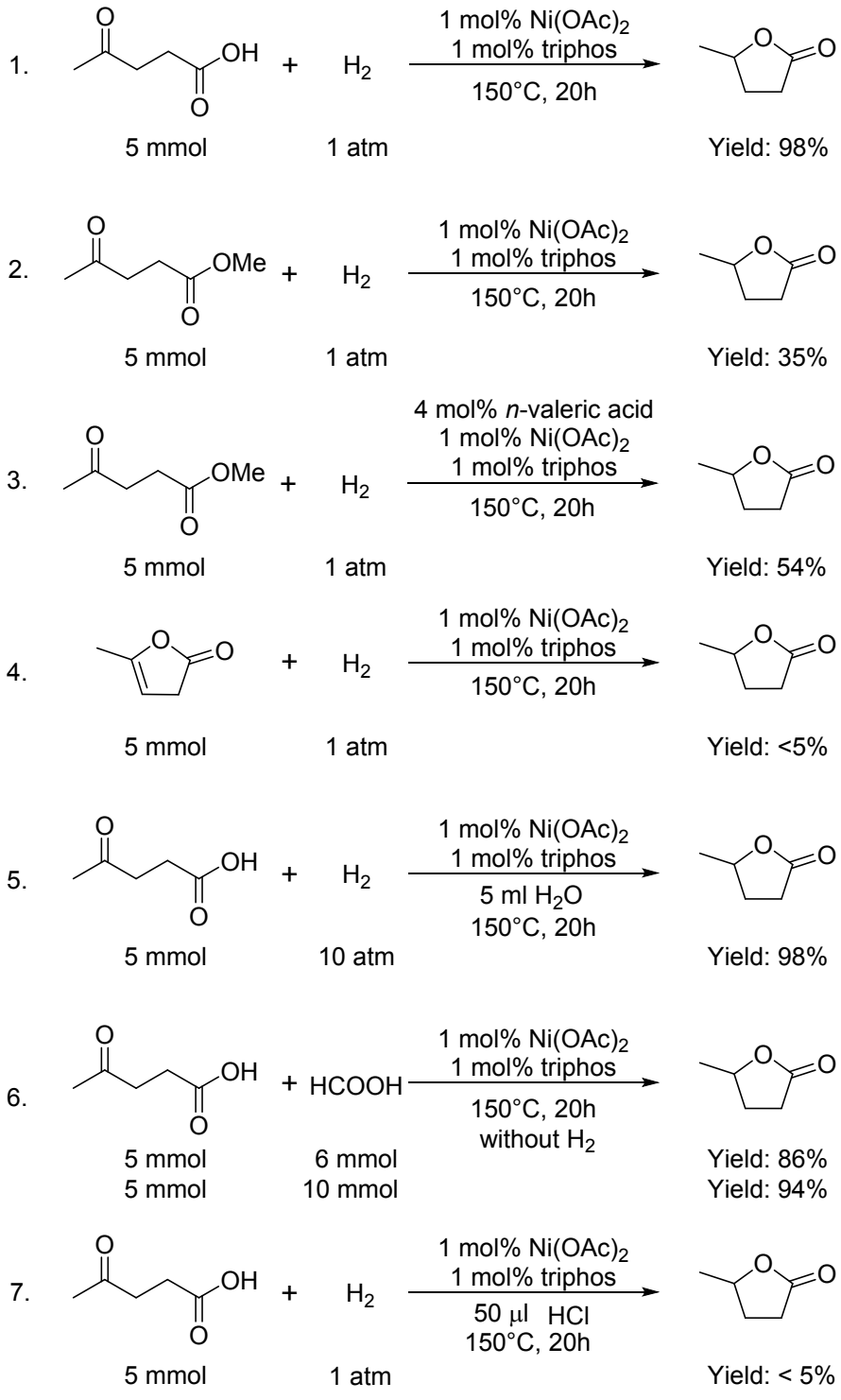
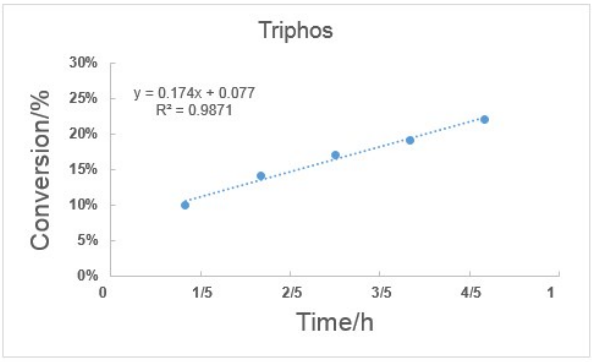


Figure S3 Tthe effect of reaction time on GVL yield.

Reaction conditions: LA (5 mmol), $Ni(OAc)_2 \cdot 4H_2O$ (0.05 mmol), triphos (0.05mmol), H_2 (1 atm), 150°C.



Scheme S1. Study for influence of substrate, H_2O, formic acid and HCl.



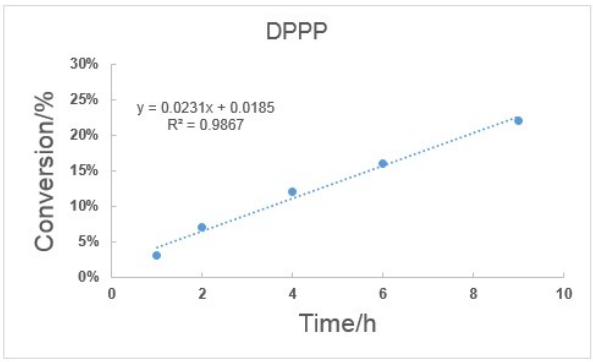


Figure S4 The conversions of LA with different ligands at the beginning of the reaction.

Reaction conditions: LA, 1 mol% $Ni(OAc)_2 \cdot 4H_2O$, 1 mol% triphos (0.05mmol) or DPPP, H_2 (1 atm), 150°C.

From the results of Figure S4, the initial reaction rate is 0.174 mol/h (for Triphos) and 0.0231 mol/h (for DPPP), respectively. According to Eyring equation ($k = \frac{k_B T}{h} e^{-\Delta G^{\neq}/RT}$), the activation energy of the reaction is 33.4 kcal/mol (Triphos) and 35.1 kcal/mol (DPPP), respectively. And the reaction activation energy calculated by DFT is 34.8 kcal/mol (Triphos) and 37.4 kcal/mol (DPPP), respectively.

5. EPR analysis

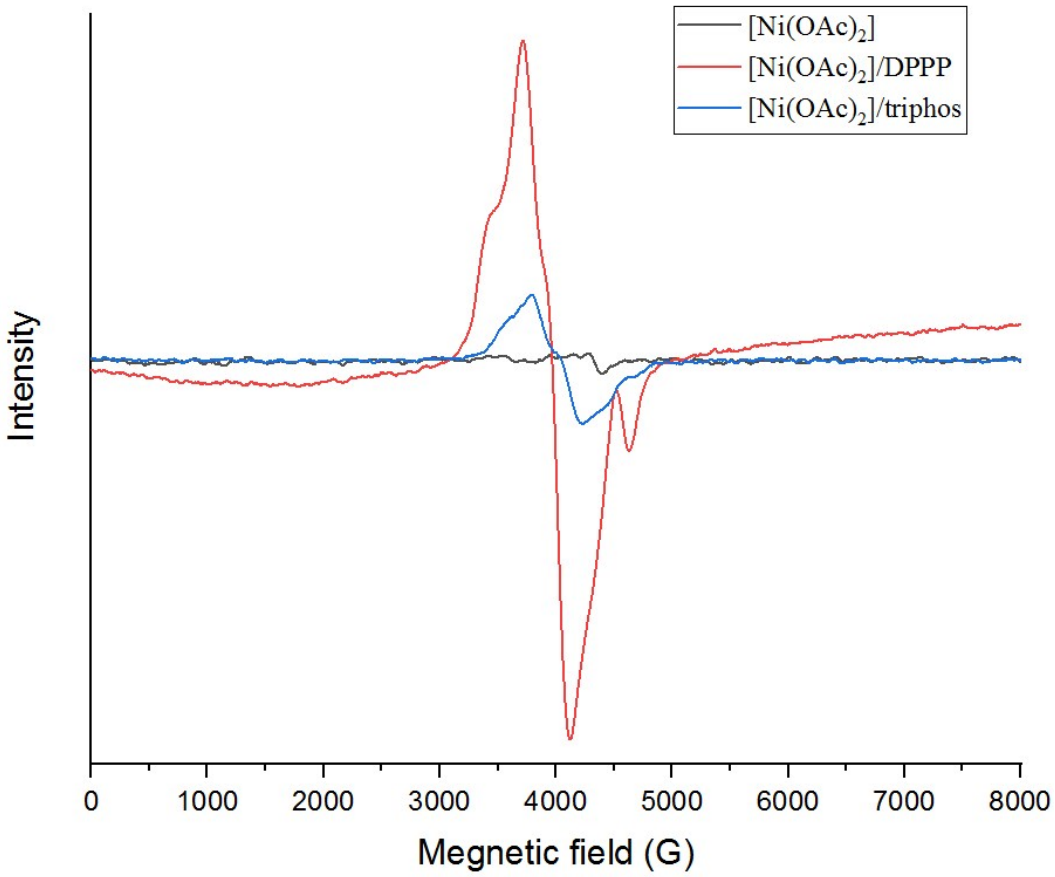
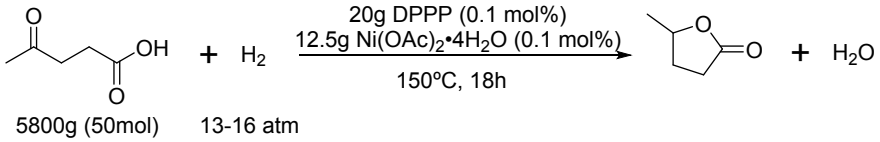


Figure. S5. EPR spectra Nickel catalysts [$Ni(OAc)_2$]/ triphos, $Ni(OAc)_2$]/ DPPP and $Ni(OAc)_2$.

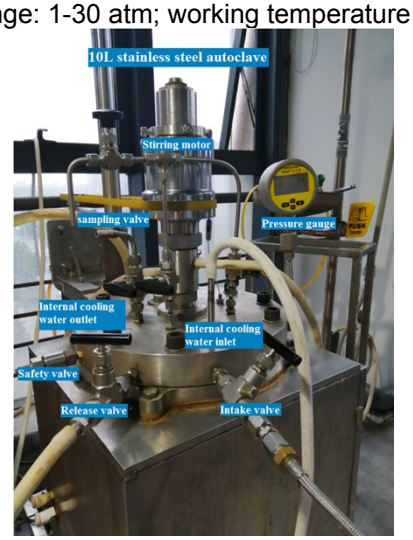
6. Kilogram scale preparation of γ-valerolactone under solvent-free condition

Reaction equation:



5800g (50mol) 13-16 atm

Reaction equipment: 10L stainless steel mechanical stirring autoclave with sampling valve (working pressure range: 1-30 atm; working temperature range: r.t-350 °C)



Input form: Levulinic acid (Industrial products, Purity ≥99%): 5.8kg (50 mol)

DPPP (Industrial products, Purity ≥99%): 20g (0.05 mol, 0.1 mol%)

$Ni(OAc)_2•4H_2O$ (Purity ≥98%): 12.5g (0.05 mol, 0.1 mol%)

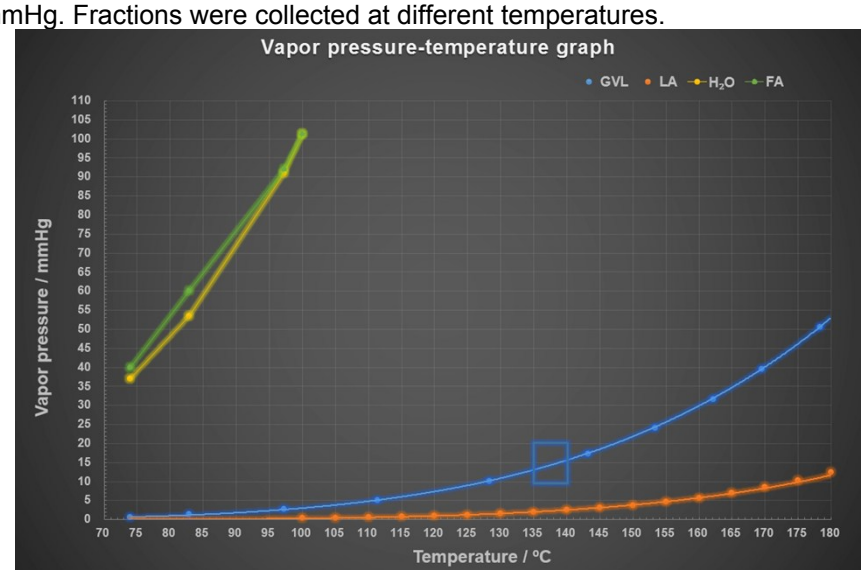
H_2 (Purity ≥99.9%): 13-16 atm

Reaction conditions: Reaction temperature: room temperature $\xrightarrow{1h}$ 150°C $\xrightarrow{18h}$ 150°C
Stirring rate: 550 rpm
Hydrogen pressure: 13-16 atm

Operation process: The weighed levulinic acid (5800 g), 1,3-bis(diphenylphosphaneyl)propane (DPPP, 20 g) and $Ni(OAc)_2•4H_2O$ (12.5 g) were put into the autoclave in turn. Seal the autoclave, turn on mechanical stirring, and control the speed to 550 rpm. After replacing the air in the autoclave 5 times with nitrogen, 15 atm of hydrogen was charged. Turn on heat according to the set heating program. During the reaction, the pressure of the reaction system was adjusted to be maintained in the range of 13-16 atm through the intake valve. After the reaction took about 18 hours, the rate of hydrogen consumption was significantly reduced. A small amount of the reaction solution was taken out through the sampling valve for GC analysis. GC analysis showed that the conversion of raw materials was about 95%. The heating was stopped, and the internal cooling water was passed to cool down the reaction system. When the reaction system reached room temperature, the residual hydrogen in the kettle was carefully released. 5935 g of the reaction

solution was taken out through a bottom valve of the autoclave.

Post-processing: The reaction solution was distilled under reduced pressure with a water pump, and the vacuum degree was controlled within the range of 15 ± 5 mmHg. Fractions were collected at different temperatures.



The fraction composition table is as follows:

Fraction composition table:

Fractions	Weight	Water	GVL	LA	Others
front cut fraction (≤ 135 °C)	1057g	758g (71.7%)	296.7g (28.1%)	n.d.	2.3g (0.2%)
main fraction (135 - 140 °C)	**4137g**	**45.5g (1.1%)**	**4058g (98.1%)**	**24.8g (0.6%)**	**8.7g (0.2%)**
distillation residue	653.5g	1.4g (0.21%)	359.4g (55.0%)	247.7g (37.9%)	45.0g (6.9%)
sum	5847.5g	804.9g (13.8%)	4714g (80.6%)	272.5g (4.7%)	56g (0.9%)

Vacuum distillation loss: 5935g – 5847.5g = 87.5g
Conversion of LA: (1 - 272.5g / 5800g) × 100% = 95.3%
Yield of GVL: 4714g / 5000g = 94.3%
Isolated yield of GVL: 4058g / 5000g = 81.2% (purity: >98%)
By adding anhydrous sodium carbonate to remove residual water and LA, the purity of the main fraction can be further improved to more than 99.5%.

Catalyst cost:

raw material	Supplier	unit price	dosage	cost
DPPP (CAS No. 6737-42-4)	Puyang Huicheng Electronic Material Co., Ltd	100$/kg	20g	2.00$
$Ni(OAc)_2•4H_2O$ (CAS No. 6018-89-9)	Sinopharm Chemical Reagent Co., Ltd	8$/kg	12.5g	0.10$

Catalyst cost: (2.00$ + 0.10$) / 4058g GVL = 0.52$/kg GVL

According to the results of the catalyst cycle test, the cost of the catalyst can be further reduced to 0.1 $ / kg GVL.

7. Computational Details

All calculations were carried out with Gaussian 16 package. [33] Geometry optimizations were performed using B3LYP [34] functional, and a mixed basis set in which SDD [35] was used for Ni and 6-31G(d) was for the other atoms was employed. Frequency analyses were conducted at the same level of theory to obtain the thermal correction and confirm the stationary points to be minima or transition states. For single-point energy calculations, M06 [36] functional was applied with Grimme's empirical dispersion-correction [37] (known as Grimme-D3), combining the mixed basis set in which SDD was employed for Ni and 6-311+G(d,p) was for the others. Solvation effect of levulinic acid was introduced using SMD [38] model throughout the calculations, including geometry optimizations, thermal correction calculations and single-point energy calculations. Since levulinic acid is not in the pre-defined solvents list, the dielectric constant (eps= 19.081) and the square of the index of refraction (epsinf = 2.070721) were used and other parameters were taken from pentanoic acid. The relative Gibbs energies (in kcal mol^{-1}) are reported in this study.

Cartesian coordinates and energies of the species

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$LNi(OAc)_2$ (**L=triphos**), total electronic energy = -3237.0200927, thermal corrections to Gibbs free energy = 0.691895

H	-7.01055400	-1.67175200	-4.50030400
H	-6.30437500	0.64043400	-3.91460600
C	-6.40235400	-1.49564100	-3.61726700
C	-6.00361100	-0.19576400	-3.28902200
H	-6.32446900	-3.57675000	-3.05389500
C	-6.01740200	-2.56428800	-2.80625600
C	-5.22074500	0.03216500	-2.15647200
H	-4.93234200	1.05053400	-1.91025600
H	-4.42249000	2.03089700	4.16964700
H	-6.86156600	2.39198600	3.80466800
H	2.03106500	-4.90263800	4.83694600
H	3.58185100	-5.08705900	2.89580900
C	-5.23151500	-2.33313900	-1.67334500
C	-4.91642800	1.59669500	3.30444700
C	-6.28422200	1.79957300	3.10021100

C	-4.81943700	-1.03474400	-1.33301500
H	-3.11820200	0.67540600	2.59387700
C	1.87294800	-4.29362000	3.95132400
C	-4.17718500	0.83155900	2.40188800
C	2.74344600	-4.39671800	2.86189000
H	-4.93018500	-3.17072100	-1.04909600
C	-6.90196300	1.22874000	1.98636000
H	-7.96582900	1.37515900	1.81802600
H	0.11433500	-3.31843600	4.73153000
C	0.79909800	-3.40485000	3.89237000
C	-4.78228800	0.26760200	1.26297200
H	-2.83814600	1.03201000	-1.14887100
C	-6.15947800	0.46993500	1.07682100
C	2.53996100	-3.61521300	1.72470600
H	3.22645600	-3.70292400	0.88836000
H	-0.49749100	-0.49820800	1.15244700
H	-6.65987200	0.03921300	0.21571200
H	-2.05292700	-1.97930200	-1.87479200
P	-3.76589100	-0.84523800	0.17880500
C	0.59102600	-2.62269400	2.75223400
C	-2.42576600	0.36935100	-0.37935900
C	1.45660400	-2.72054800	1.65146500
H	-0.25541800	-1.94507900	2.73640800
H	-2.20794100	0.99980700	0.48722600
H	-1.93246000	-0.54632100	-2.90747100
C	-0.47611100	-1.10047800	0.23556800
C	-1.41072600	-1.13365100	-2.14325900
H	-1.12108800	-1.96574300	0.42082600
C	-1.09836900	-0.25426700	-0.91260900
H	-0.49881400	-1.53719800	-2.59096900
P	1.29649500	-1.67912300	0.13417000
Ni	2.86993400	0.22322400	0.10687400
H	-0.06648600	-4.28953300	-0.32422400
H	-0.07834400	2.27897700	4.53449000
H	1.16803200	1.36199600	2.59737700
C	-0.33156200	2.60228700	3.52862100
C	0.36696000	2.07741300	2.43582200

C	-0.18338500	0.90898800	-1.42189500
C	0.59311300	-4.10404500	-1.16755700
H	-0.81156700	1.65275500	-1.92456600
C	1.37431400	-2.93568300	-1.21071600
H	-1.87877200	3.95649000	4.17762400
C	-1.34047000	3.54522200	3.32819400
H	0.49065900	0.50519900	-2.18733600
P	1.00846700	1.78123800	-0.27300100
C	0.05270700	2.49049000	1.13112400
H	0.05402200	-5.93618100	-2.15821600
C	0.66340800	-5.03761200	-2.20038800
C	-1.65359100	3.96824700	2.03132400
C	-0.96121200	3.44668400	0.93962200
C	2.23476200	-2.72528700	-2.29939800
H	-2.43533600	4.70566600	1.87233600
H	2.84312700	-1.82686600	-2.34158900
H	-1.20568200	3.78964200	-0.06185400
C	1.51896500	-4.81925400	-3.28589400
C	1.48393400	3.27301000	-1.24732900
C	2.30335200	-3.66617900	-3.33244400
H	2.00423600	4.41197900	0.51829900
H	1.10393400	2.43178700	-3.20976400
H	1.57420700	-5.54914600	-4.08889800
C	1.97073400	4.40359800	-0.56733900
C	1.46034400	3.29037800	-2.65116100
H	2.97316600	-3.49570000	-4.17090500
C	2.40575200	5.52576000	-1.27201100
C	1.89671400	4.41688900	-3.35508700
H	2.77283700	6.39180300	-0.72821100
H	1.86220800	4.41507700	-4.44111500
C	2.36882000	5.53712600	-2.66932300
H	2.70578300	6.41214800	-3.21792100
O	4.37286000	1.65997700	-0.46187900
O	3.40205400	0.33834900	-1.92984700
C	4.26399900	1.24256100	-1.65251500
C	5.11444500	1.82586200	-2.75797700
H	5.38468700	1.05279100	-3.48239000

H	6.01502000	2.29128100	-2.35145300
H	4.53300100	2.59250900	-3.28360500
C	4.96795500	-1.00172900	3.24744500
H	4.94122800	-0.24023000	4.03054600
H	4.51678500	-1.91956400	3.64284400
C	4.17992500	-0.55620600	2.03659500
O	3.20341200	0.25537400	2.17642400
O	4.46096600	-1.00833000	0.88477100
H	6.00233500	-1.22371700	2.97330000

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HA, total electronic energy = -420.9287321, thermal corrections to Gibbs free energy = 0.091207

C	-3.11251000	0.76687300	0.03142000
H	-3.05990700	1.49296500	-0.78846300
H	-4.04134500	0.19701800	-0.03919000
H	-3.10727600	1.34100400	0.96628600
C	-0.54768300	0.48146400	-0.00112500
H	-0.47435800	1.13732600	-0.87880200
H	-0.48587900	1.15634300	0.86248200
C	0.59578700	-0.52703800	0.01463600
H	0.53326300	-1.20389700	-0.84523600
H	0.53815600	-1.17437700	0.89727300
C	1.95612100	0.13130800	-0.00117200
C	-1.92219100	-0.17049900	-0.00846900
O	2.94804200	-0.78600400	0.03328900
H	3.79285900	-0.29576600	0.01832700
O	2.17212700	1.32665100	-0.04098500
O	-2.05925200	-1.38355600	-0.04285500

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$LNi(A)_2$ or I1, total electronic energy = -3620.8056409, thermal corrections to Gibbs free energy = 0.807266

H	8.00043100	1.31023200	4.43598600
H	7.18814900	2.90129400	2.70489900
C	7.38247200	0.95388300	3.61634800
C	6.92411500	1.84886700	2.64400600
H	7.39811500	-1.09894600	4.27966200
C	7.04450400	-0.39741000	3.52900600

C	6.12862700	1.39341300	1.59178000
H	5.79301600	2.10118900	0.83859300
H	5.20023800	-0.33328400	-4.77811300
H	7.62729900	0.23349200	-4.73565900
H	-0.91206600	-6.85168400	-1.27469600
H	-2.39869000	-6.02159100	0.54357300
C	6.24609100	-0.85056900	2.47459200
C	5.72102300	-0.22746000	-3.83010200
C	7.08190200	0.09038100	-3.80690000
C	5.77430600	0.03615600	1.49352500
H	3.96891500	-0.67890400	-2.68503400
C	-0.77279300	-5.85416800	-0.86766000
C	5.02280600	-0.41582000	-2.63691100
C	-1.60748700	-5.38778700	0.15259700
H	5.98182800	-1.90350300	2.41540500
C	7.73436600	0.21578700	-2.57940900
H	8.79351400	0.45813600	-2.54703000
H	0.89762700	-5.38340400	-2.14831900
C	0.24074900	-5.03043900	-1.35810300
C	5.66252600	-0.27151100	-1.39149000
H	3.68929700	1.58980300	0.26516200
C	7.03287100	0.03628000	-1.38366400
C	-1.42859700	-4.10704800	0.67513100
H	-2.08698000	-3.75692200	1.46414100
H	1.41286400	-1.06291000	-0.69911600
H	7.55985800	0.14291500	-0.44111900
H	3.08633800	-0.53151000	2.57403700
P	4.70875600	-0.66751200	0.15149600
C	0.42400800	-3.74708200	-0.83428400
C	3.30663800	0.59542800	0.00766000
C	-0.40620500	-3.26974400	0.19201600
H	1.22360000	-3.13364700	-1.23446800
H	3.03974000	0.63215600	-1.05236600
H	2.89186900	1.22685700	2.63565500
C	1.44485100	-1.05402800	0.39739700
C	2.39840800	0.29077600	2.35032100
H	2.14475000	-1.84346900	0.69036700

C	2.02415300	0.31696500	0.85232300
H	1.51524400	0.16759400	2.98266500
P	-0.28045500	-1.56653900	0.89541900
Ni	-1.98048000	-0.02707400	-0.00719700
H	1.26658700	-3.45222200	2.60498600
H	0.67985500	-0.77647600	-4.99786600
H	-0.45215100	-0.45564400	-2.81600300
C	0.94535100	0.07132500	-4.37250100
C	0.31168500	0.24638600	-3.13748700
C	1.04677000	1.52545100	0.66014500
C	0.61999900	-2.86736500	3.25351300
H	1.63616700	2.44779500	0.61277000
C	-0.23711400	-1.89555900	2.70761600
H	2.39345400	0.85400600	-5.76508900
C	1.90558800	0.98757000	-4.80353000
H	0.41730300	1.60533300	1.55479800
P	-0.22629400	1.53423100	-0.71059900
C	0.64273000	1.34004000	-2.32133200
H	1.30919800	-3.84779400	5.04023800
C	0.64174600	-3.09575100	4.62856900
C	2.23436600	2.08511200	-3.99968700
C	1.60643300	2.26246300	-2.76773300
C	-1.07907500	-1.16582700	3.56107300
H	2.97817100	2.80258900	-4.33449000
H	-1.74384500	-0.41237200	3.14969800
H	1.86248500	3.12316300	-2.15623000
C	-0.19620100	-2.36113400	5.47469900
C	-0.77622700	3.29381900	-0.74256800
C	-1.05519200	-1.40017300	4.94002600
H	-1.41321700	3.18552200	-2.80873400
H	-0.29417400	3.75201800	1.32152200
H	-0.17964100	-2.54211900	6.54593400
C	-1.35407800	3.80495100	-1.91843200
C	-0.72114400	4.11682600	0.39371400
H	-1.71122500	-0.83115900	5.59314600
C	-1.84724200	5.10888500	-1.96049700
C	-1.21591700	5.42358300	0.34879400

H	-2.28335700	5.48827500	-2.88048400
H	-1.15653900	6.04848000	1.23565200
C	-1.77811500	5.92437500	-0.82672000
H	-2.15798600	6.94161000	-0.86109700
C	-7.84411800	-4.17988000	-1.54085600
H	-8.35156500	-3.38818100	-2.10707000
H	-8.25728400	-5.14810700	-1.83190800
H	-8.04289900	-3.99037300	-0.47985300
C	-5.59504300	-2.94453100	-1.27192800
H	-6.16405200	-2.02914100	-1.48343400
H	-5.59449500	-3.03640600	-0.17720000
C	-4.16029700	-2.83696000	-1.78724900
H	-4.13963000	-2.63162200	-2.86152400
H	-3.65035400	-3.79821000	-1.64495800
C	-3.34075000	-1.77939800	-1.07295300
C	-6.35696400	-4.13519600	-1.83266200
O	-2.42976800	-1.15363800	-1.71328600
O	-3.52833700	-1.53139100	0.15694500
O	-5.80388100	-5.01063900	-2.48055100
C	-6.67901800	5.64436900	0.70217200
H	-7.13573600	5.18670800	-0.18304000
H	-7.44306400	6.15361000	1.29355200
H	-5.95117600	6.38150000	0.33998900
C	-4.99305700	3.69491200	0.81723800
H	-5.56210500	3.10188800	0.08861000
H	-4.31981600	4.31847500	0.21413200
C	-4.20307600	2.77606000	1.74571100
H	-4.89221200	2.22182200	2.39598100
H	-3.56023400	3.35271400	2.41831500
C	-3.34260000	1.75698700	1.02250000
C	-5.97258800	4.60091900	1.54599400
O	-2.38938500	1.19021800	1.66151600
O	-3.56517400	1.44072200	-0.18229700
O	-6.18285200	4.49760700	2.74509300

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HOAc, total electronic energy = -229.0379932, thermal corrections to Gibbs free energy = 0.034586

O	-0.77901500	1.04340900	-0.00007000
O	-0.64425100	-1.20418200	0.00004500
C	-0.09211700	-0.12215300	-0.00033500
C	1.39658800	0.11100700	-0.00009100
H	1.68479000	0.68332600	0.88781800
H	1.68373000	0.70029600	-0.87699600
H	1.91949300	-0.84551800	-0.00897600
H	-1.72871000	0.81495700	0.00090500

2

H_2, total electronic energy = -1.1706913, thermal corrections to Gibbs free energy = -0.001354

H	0.00000000	0.00000000	0.37151500
H	0.00000000	0.00000000	-0.37151500

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TS1, total electronic energy = -3621.9546636, thermal corrections to Gibbs free energy = 0.82016

H	8.44531600	0.10118800	4.22736600
H	7.65313500	1.99007700	2.81585900
C	7.76004500	-0.08421400	3.40473900
C	7.31302200	0.97818400	2.61224200
H	7.66791600	-2.21274300	3.74435500
C	7.32392700	-1.38208300	3.13413400
C	6.43146100	0.74234800	1.55646900
H	6.10588600	1.57831200	0.94321400
H	5.06896500	0.09138700	-4.93137800
H	7.53267700	0.46817100	-4.95173200
H	-1.24069800	-6.59950300	-2.00876500
H	-2.52588100	-5.97020600	0.03005000
C	6.43941600	-1.61506600	2.07677600
C	5.64240300	0.01036800	-4.01180700
C	7.02385500	0.22206100	-4.02378400
C	5.97819400	-0.55871600	1.27514900
H	3.91784500	-0.48557300	-2.84315700
C	-1.03368200	-5.66232700	-1.49985900
C	4.99079600	-0.31076300	-2.82056500
C	-1.75546000	-5.30846600	-0.35628100
H	6.09937900	-2.62775500	1.87460000

C	7.74377300	0.10839300	-2.83335500
H	8.81920800	0.26653900	-2.82918100
H	0.52516800	-5.07048500	-2.86836600
C	-0.04447400	-4.80446600	-1.98219600
C	5.70033200	-0.40836600	-1.60904200
H	3.94151100	1.28705300	0.45403400
C	7.08971200	-0.20402900	-1.63812800
C	-1.48836300	-4.10601700	0.29876700
H	-2.05643300	-3.84657500	1.18683700
H	1.48051100	-1.01928700	-0.84270000
H	7.66919400	-0.28322600	-0.72413000
H	3.29620100	-1.19531200	2.37131200
P	4.79735600	-0.97665300	-0.08980300
C	0.22549900	-3.59905900	-1.32777900
C	3.48181000	0.37753100	0.05036400
C	-0.48899200	-3.23632200	-0.17458300
H	1.00138400	-2.95410500	-1.72611200
H	3.17715900	0.61316100	-0.97275900
H	3.24708000	0.53051000	2.76128700
C	1.51854200	-1.19237700	0.24023000
C	2.66586400	-0.30000700	2.34467400
H	2.14192600	-2.08012600	0.38807700
C	2.22158200	0.02956700	0.90201100
H	1.80963700	-0.47600700	3.00020200
P	-0.24995000	-1.61463000	0.67270100
Ni	-1.79594800	0.07623000	-0.17222300
H	1.06503500	-3.76800300	2.27216100
H	1.34704800	0.64750700	-5.02003900
H	0.10295400	0.32458000	-2.90172500
C	1.52515800	1.31683500	-4.18293600
C	0.82517600	1.13117400	-2.98615800
C	1.32206200	1.30450400	1.00319200
C	0.47121100	-3.16004000	2.94911800
H	1.96954300	2.17021200	1.18307100
C	-0.27378200	-2.07452700	2.45496700
H	2.98047900	2.51166400	-5.23370000
C	2.43975500	2.36392800	-4.30307700

H	0.68571400	1.20349700	1.89164600
P	0.08537600	1.72264500	-0.33792900
C	1.03636700	1.99082700	-1.89692800
H	1.03083800	-4.30821700	4.68034000
C	0.45024300	-3.46852400	4.30841300
C	2.65496800	3.22828500	-3.22400800
C	1.95743000	3.04572300	-2.03084800
C	-1.04772800	-1.31187900	3.34383600
H	3.36390600	4.04661200	-3.31436000
H	-1.63325700	-0.47646000	2.97128300
H	2.12438200	3.73080800	-1.20446300
C	-0.31739800	-2.69970400	5.19032400
C	-0.41970000	3.44088800	0.10762400
C	-1.06546900	-1.62541000	4.70707800
H	-1.23458900	3.80748200	-1.86332300
H	0.24688100	3.41845900	2.17128600
H	-0.33314300	-2.94242800	6.24929200
C	-1.08211900	4.21033100	-0.86606200
C	-0.24755300	3.98502100	1.38989200
H	-1.66775000	-1.03006000	5.38787900
C	-1.54113200	5.49348200	-0.57113700
C	-0.71103200	5.27093800	1.68489000
H	-2.04402400	6.07410800	-1.33961900
H	-0.56245000	5.67701000	2.68169000
C	-1.35638400	6.02936000	0.70711900
H	-1.71399600	7.02889300	0.93785800
H	-1.61202900	-0.45678400	-1.79552100
C	-8.46738200	-3.43524300	-2.64109100
H	-8.13990500	-3.22812500	-3.66634700
H	-9.11300300	-4.31597400	-2.62550000
H	-9.04212600	-2.56191500	-2.30691600
C	-6.17697200	-2.59513700	-1.80128200
H	-5.70993600	-2.67948200	-2.79163700
H	-6.63486900	-1.59704800	-1.77935800
C	-5.12043100	-2.74463200	-0.70530900
H	-4.74261300	-3.77502500	-0.70713400
H	-5.54860900	-2.56702100	0.28454900

C	-3.92485400	-1.82735800	-0.88456900
C	-7.27966800	-3.64057100	-1.72203700
O	-3.46524100	-1.68835800	-2.07994800
H	-2.45119800	-0.99738200	-1.95806600
O	-3.41748900	-1.27130200	0.12295200
O	-7.21149400	-4.59416300	-0.96229400
C	-7.49434600	4.67279900	0.51407100
H	-8.20004000	3.85266200	0.69800300
H	-7.91616600	5.60290600	0.90109800
H	-7.36521200	4.74420600	-0.57207700
C	-5.37411800	3.20814900	0.63420400
H	-6.04487800	2.34641400	0.51602300
H	-5.07087100	3.47462000	-0.38728200
C	-4.14764900	2.84389500	1.46757700
H	-4.43653600	2.48966800	2.46231700
H	-3.53302500	3.73780000	1.63334800
C	-3.25593000	1.79690200	0.82604300
C	-6.17438100	4.37179900	1.19746800
O	-2.44836500	1.13518800	1.55839000
O	-3.27947900	1.59858800	-0.42752600
O	-5.77923900	5.03211100	2.14626700

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I2, total electronic energy = -3621.960082, thermal corrections to Gibbs free energy = 0.823723

H	7.72757100	-0.69335600	5.09769700
H	7.15229900	1.40131100	3.88551500
C	7.17085100	-0.73926300	4.16568600
C	6.84565000	0.43866300	3.48507300
H	7.02932900	-2.89200400	4.16495800
C	6.77905400	-1.97254300	3.64279100
C	6.12889500	0.38177300	2.28902600
H	5.89716100	1.30659200	1.76757000
H	5.73364500	0.69130600	-4.36357600
H	8.17112400	1.02914600	-3.96746300
H	-0.98985200	-6.06234300	-3.53403800
H	-2.50625100	-5.79772900	-1.57568800
C	6.05959500	-2.02625000	2.44525800

C	6.16505900	0.47350700	-3.39019000
C	7.53194300	0.66342000	-3.16855900
C	5.72137800	-0.85263200	1.75279200
H	4.28919000	-0.15481500	-2.56956600
C	-0.84865500	-5.23798000	-2.84076200
C	5.34615100	-0.00116000	-2.36512300
C	-1.69998400	-5.08851800	-1.74231500
H	5.75242600	-2.98988300	2.04637200
C	8.06834000	0.37298100	-1.91308600
H	9.13044100	0.51232100	-1.72832700
H	0.85497600	-4.42933200	-3.88791900
C	0.18484800	-4.32164100	-3.03941700
C	5.86913800	-0.27853500	-1.08821900
H	3.83358400	1.14360600	0.92834300
C	7.24629500	-0.09367100	-0.88324300
C	-1.51678500	-4.03122600	-0.85054900
H	-2.18404300	-3.93193000	0.00034500
H	1.55977200	-0.85038400	-1.04893800
H	7.68442400	-0.30902900	0.08584800
H	2.89617000	-1.59012100	2.32592000
P	4.75144800	-1.03734200	0.18508100
C	0.36941200	-3.26066500	-2.14820200
C	3.43534100	0.31554800	0.33072900
C	-0.47526800	-3.10400800	-1.03743400
H	1.18139500	-2.56475800	-2.32994400
H	3.28796800	0.70611400	-0.67962500
H	2.80939600	0.05732300	2.96804200
C	1.45595000	-1.20338800	-0.01535300
C	2.28636300	-0.68053200	2.34893700
H	2.05975900	-2.11354900	0.06163300
C	2.06067700	-0.12034100	0.92683300
H	1.34190600	-0.92570600	2.84058000
P	-0.35192200	-1.66322200	0.11036100
Ni	-1.77380400	0.18727500	-0.62710300
H	0.78129400	-4.09888400	1.42511400
H	1.88907600	1.32116400	-4.93611500
H	0.37835200	0.78360200	-3.03951600

C	1.99668000	1.84993500	-3.99300600
C	1.14797100	1.54158700	-2.92440800
C	1.16541900	1.15144900	1.09464500
C	0.10900100	-3.61724000	2.12986500
H	1.78685900	1.96519900	1.48564800
C	-0.57990200	-2.44757700	1.76262900
H	3.62569100	3.08379300	-4.68154400
C	2.96939800	2.84026300	-3.85064400
H	0.41274900	0.93853700	1.86395200
P	0.11988900	1.78831600	-0.32316700
C	1.26868300	2.21951500	-1.70146100
H	0.47094600	-5.07519400	3.67030000
C	-0.06803400	-4.17234500	3.39644000
C	3.09486800	3.52467300	-2.63639800
C	2.25046300	3.21876100	-1.57014000
C	-1.45644900	-1.85129700	2.68292800
H	3.84927500	4.29820900	-2.52243500
H	-1.99643100	-0.95014700	2.40737600
H	2.35071200	3.76458000	-0.63614700
C	-0.93803700	-3.56888700	4.31126200
C	-0.39932300	3.45229500	0.28543600
C	-1.63105300	-2.41188400	3.95279400
H	-0.73689200	4.20689400	-1.71513900
H	-0.21281900	3.03485100	2.40485900
H	-1.07541500	-4.00337000	5.29767500
C	-0.79831400	4.42210600	-0.65219200
C	-0.49800900	3.76121500	1.65171900
H	-2.31166100	-1.94337300	4.65858100
C	-1.26314100	5.66978700	-0.23567700
C	-0.96436000	5.01170800	2.06750700
H	-1.55707000	6.40790400	-0.97698000
H	-1.02443300	5.23380000	3.12948500
C	-1.34617800	5.97031000	1.12740700
H	-1.70441000	6.94317500	1.45230700
H	-1.48803900	-0.09905800	-2.23148900
C	-8.08391600	-3.57575800	0.64142000
H	-8.67655100	-2.65209700	0.63553900

H	-8.75621400	-4.43416800	0.58034800
H	-7.53565000	-3.59660100	1.59033400
C	-6.00771400	-2.54799300	-0.49452200
H	-6.43500800	-1.56613400	-0.25271500
H	-5.35797600	-2.79531900	0.35549800
C	-5.19741600	-2.49357900	-1.78605000
H	-5.81021100	-2.16016600	-2.62976400
H	-4.84628500	-3.49759600	-2.05611200
C	-3.97985500	-1.60312900	-1.70158400
C	-7.12932700	-3.57548200	-0.53535900
O	-3.44711100	-1.30740700	-2.86781900
H	-2.58787700	-0.75570800	-2.66630800
O	-3.50946800	-1.20444100	-0.62669700
O	-7.25155500	-4.35867700	-1.46430100
C	-6.51825200	5.72685200	0.63962900
H	-6.74050100	5.56652000	-0.42170200
H	-7.40853900	6.09352200	1.15522300
H	-5.73233800	6.49131200	0.68844200
C	-4.89871800	3.72008000	0.57350700
H	-5.28106400	3.38530400	-0.40031800
H	-4.10858000	4.44454000	0.33508400
C	-4.33769900	2.53566600	1.35636600
H	-5.15607300	1.86903400	1.65788800
H	-3.86634900	2.86723800	2.28695000
C	-3.33038100	1.70011000	0.58475200
C	-6.02570900	4.44747700	1.28853900
O	-2.54694700	0.92971200	1.23121500
O	-3.28095400	1.74072100	-0.68186500
O	-6.51213000	4.02921200	2.32849600

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I3, total electronic energy = -3201.000217, thermal corrections to Gibbs free energy = 0.708284

H	-7.11395500	0.84684100	4.96265600
H	-5.99272000	-1.29325400	4.37059200
C	-6.57088300	0.75787100	4.02572600
C	-5.93871000	-0.44472800	3.69372400
H	-6.99162200	2.77906700	3.39938400

C	-6.50210200	1.84181800	3.14911400
C	-5.23875600	-0.56027700	2.49179700
H	-4.76572400	-1.50707400	2.24596100
H	-4.74259700	-2.50820000	-3.92564200
H	-6.96705200	-3.41055600	-3.25647500
H	0.32271700	6.11933200	-4.61260600
H	2.32455000	5.92698200	-3.14313700
C	-5.79832000	1.72384000	1.94701500
C	-5.20609400	-2.18676200	-2.99668100
C	-6.45428800	-2.69265800	-2.62223300
C	-5.15489000	0.52453700	1.60104000
H	-3.59086600	-0.86654100	-2.50706400
C	0.36214400	5.35601800	-3.84058900
C	-4.55219900	-1.26006100	-2.18439600
C	1.48594000	5.24797600	-3.01577100
H	-5.74294800	2.57434200	1.27201200
C	-7.03843100	-2.26168400	-1.43019700
H	-8.01084500	-2.64382100	-1.13016000
H	-1.58553600	4.55297200	-4.30295900
C	-0.70760600	4.47696500	-3.66729500
C	-5.11911400	-0.83309000	-0.96869200
H	-2.83961400	-1.16535100	1.21052700
C	-6.37822500	-1.34099100	-0.61096200
C	1.53604800	4.26775500	-2.02523100
H	2.41490400	4.19807700	-1.38921700
H	-1.27160500	0.89229200	-1.29614400
H	-6.84926100	-1.02316300	0.31337500
H	-2.61622300	1.94711900	1.89831600
P	-4.23702500	0.48838700	-0.00784200
C	-0.66045500	3.49364900	-2.67436900
C	-2.64044900	-0.43352200	0.41904300
C	0.45984300	3.38109900	-1.83671600
H	-1.50532900	2.82248000	-2.56313800
H	-2.38422500	-1.00884300	-0.47524400
H	-2.09088000	0.59415900	2.91044400
C	-1.09024700	1.41309300	-0.34818400
C	-1.78570400	1.26135300	2.09634600

H	-1.78807400	2.25575200	-0.31761200
C	-1.42351800	0.44699700	0.83307800
H	-0.93794300	1.85750900	2.44425500
P	0.64751000	2.05609300	-0.56940300
Ni	1.91701300	0.19970900	-1.45060600
H	-0.47497000	4.49656700	0.76709900
H	-1.46432400	-3.64001600	-3.80083900
H	-0.07053300	-1.87293300	-2.74467600
C	-1.28158300	-3.66337500	-2.73004200
C	-0.49440900	-2.66950800	-2.13980200
C	-0.24849600	-0.48977300	1.25976600
C	0.36763400	4.14440600	1.35593100
H	-0.64083400	-1.22451100	1.97253400
C	1.08695200	3.00683400	0.94843900
H	-2.43712000	-5.45496200	-2.40632900
C	-1.82599300	-4.68266700	-1.94753400
H	0.47941600	0.11723600	1.81207800
P	0.80095400	-1.37304000	-0.00817800
C	-0.24693800	-2.68984400	-0.75916900
H	0.16631500	5.70671700	2.82184700
C	0.73023000	4.83034100	2.51441100
C	-1.57934700	-4.71246100	-0.57058600
C	-0.79209100	-3.72519200	0.02046800
C	2.18466400	2.58122500	1.71308300
H	-1.99732200	-5.50719000	0.04113200
H	2.76461300	1.72142500	1.38956600
H	-0.59518700	-3.76734200	1.08834300
C	1.81858500	4.39256400	3.27760500
C	1.96692400	-2.34994800	1.03944800
C	2.54549500	3.27155700	2.87494800
H	2.71018600	-3.42210300	-0.68725500
H	1.49202300	-1.46972900	2.96517100
H	2.10008700	4.92972200	4.17912600
C	2.79363700	-3.28332500	0.38653900
C	2.10972700	-2.17868400	2.42508000
H	3.39766900	2.93508700	3.45906500
C	3.72746700	-4.03139600	1.10266900

C	3.05050200	-2.92665000	3.14011200
H	4.35233600	-4.75161800	0.58174800
H	3.14293700	-2.78328600	4.21318100
C	3.85975000	-3.85470200	2.48392100
H	4.58689900	-4.43760600	3.04225300
H	0.95865500	0.18046800	-2.73209500
C	8.31348000	-1.10121200	1.94915800
H	7.98737300	-2.05185000	2.39005000
H	9.40500800	-1.06954800	1.93154400
H	7.92645100	-0.30239700	2.59224700
C	6.25645300	-0.81326100	0.41907700
H	5.76730200	-1.57113900	1.04574200
H	5.98754700	0.15185500	0.86930700
C	5.74746700	-0.87909300	-1.02045100
H	5.89247100	-1.87557900	-1.44712000
H	6.33304600	-0.18997000	-1.64304000
C	4.28580600	-0.49632700	-1.16714200
C	7.76314600	-0.97739800	0.54158200
O	3.57695900	-1.04579300	-2.06630300
O	3.77528900	0.39661300	-0.41293600
O	8.49382600	-1.00566500	-0.43688100

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TS2, total electronic energy = -3621.944535, thermal corrections to Gibbs free energy = 0.829542

H	-6.57077500	-2.83881400	5.27580500
H	-5.84279700	-4.07365100	3.24268100
C	-6.19178600	-2.29463700	4.41503200
C	-5.78058200	-2.98906900	3.27257400
H	-6.43380800	-0.35488400	5.32772500
C	-6.11482500	-0.90138900	4.44439400
C	-5.29158500	-2.29189500	2.16702300
H	-4.98957000	-2.84742100	1.28323500
H	-5.92579900	0.16007700	-3.99258600
H	-8.17228100	-0.84491800	-3.59781700
H	-0.37627100	7.32629400	-1.12671600
H	1.80450500	6.50575100	-0.24438900
C	-5.62308000	-0.20577500	3.33578700

C	-6.22790500	-0.12723100	-2.98894700
C	-7.48768800	-0.69086700	-2.76825700
C	-5.20189800	-0.88866800	2.18366900
H	-4.38399700	0.52978000	-2.12003300
C	-0.27376900	6.29750600	-0.79232400
C	-5.35155400	0.07483100	-1.92222700
C	0.94938100	5.83688200	-0.29507800
H	-5.56065000	0.87918200	3.36730500
C	-7.85962200	-1.04813300	-1.47119400
H	-8.83798100	-1.48368800	-1.28484800
H	-2.31676700	5.77227600	-1.24370200
C	-1.36105700	5.42623000	-0.85918300
C	-5.70485900	-0.29925500	-0.61229200
H	-3.14438400	-1.88735000	0.45883100
C	-6.97826700	-0.85414900	-0.40368800
C	1.08565900	4.51602900	0.13198000
H	2.04937900	4.16769500	0.49149700
H	-1.62312100	1.22032500	-0.62141400
H	-7.28744300	-1.14281500	0.59559600
H	-2.51140000	0.18326700	2.81957700
P	-4.55149800	0.12826500	0.77805200
C	-1.23198700	4.10200100	-0.42694500
C	-3.00386900	-0.82183600	0.24336300
C	-0.00920100	3.63197000	0.07670600
H	-2.09715600	3.45100300	-0.48757300
H	-2.94897200	-0.73071200	-0.84489500
H	-2.00332900	-1.50795000	2.69278200
C	-1.41735400	1.12611300	0.45237200
C	-1.74339800	-0.48146700	2.40975800
H	-2.15880500	1.74847200	0.96382900
C	-1.65424800	-0.35409200	0.87251600
H	-0.79463300	-0.22789300	2.88961900
P	0.27162300	1.89843000	0.65096000
Ni	1.94976900	0.81570800	-0.77499800
H	-1.10044600	3.55717700	2.71821300
H	-2.13143100	1.11344700	-4.83032000
H	-0.46636300	1.00894600	-2.99429800

C	-1.97985100	0.18221600	-4.29159500
C	-1.04558800	0.12648000	-3.25233500
C	-0.53098200	-1.34413200	0.41772200
C	-0.31560500	2.99085100	3.21230300
H	-0.94075900	-2.36028700	0.43445400
C	0.50833200	2.12952800	2.46795800
H	-3.42468300	-0.91842100	-5.45432400
C	-2.70395600	-0.95830600	-4.64237400
H	0.27211100	-1.31983000	1.16380800
P	0.40870500	-1.09098000	-1.18375300
C	-0.83060600	-1.07014100	-2.54998300
H	-0.77278700	3.80246800	5.15236800
C	-0.12868400	3.13427400	4.58717100
C	-2.49572100	-2.15607400	-3.94995300
C	-1.56643400	-2.21301400	-2.91177400
C	1.52937800	1.42544100	3.12406800
H	-3.05655700	-3.04632300	-4.22057500
H	2.17341200	0.76281900	2.55532400
H	-1.40804400	-3.15121200	-2.38799100
C	0.88685900	2.42349800	5.23503000
C	1.24056800	-2.72428300	-1.40893900
C	1.71478800	1.57132800	4.50225700
H	1.49615100	-2.43882000	-3.53927300
H	1.19187500	-3.33955100	0.67003000
H	1.03309800	2.53843800	6.30557600
C	1.69534700	-3.08540100	-2.69016100
C	1.51731300	-3.58566400	-0.33449700
H	2.50926200	1.02175700	4.99988600
C	2.39276900	-4.27624100	-2.89267700
C	2.21591800	-4.77933100	-0.53942300
H	2.72848300	-4.53791800	-3.89239700
H	2.40825600	-5.43727600	0.30381900
C	2.65597200	-5.12891200	-1.81709400
H	3.19722900	-6.05753900	-1.97473100
H	1.57207200	1.69279200	-2.09309100
C	2.42470500	0.78819400	-4.33637800
H	3.12719000	0.41659700	-5.09711700

H	1.64230300	0.04175400	-4.19943600
H	1.98756800	1.72011100	-4.70275700
C	4.03504900	2.27042700	-3.00649100
H	4.66120300	2.22410000	-3.91310200
H	3.37313900	3.12963700	-3.15321400
C	4.95482600	2.46676300	-1.79638400
H	5.67863000	3.25052700	-2.03484400
H	5.52336100	1.54482600	-1.62237700
C	4.25486300	2.86347700	-0.48629100
C	3.21147300	0.99513700	-3.06111800
O	4.60641200	3.90849200	0.08412000
O	3.36076500	2.05754500	-0.01825100
O	3.49426400	-0.01183000	-2.35224900
C	6.74641000	-4.89995200	2.60869900
H	7.47938500	-4.79157300	1.80089800
H	7.24782100	-5.21704900	3.52546100
H	6.03857000	-5.67773400	2.29542300
C	5.38146500	-2.94717000	1.61699300
H	6.19001400	-2.69261200	0.92004400
H	4.76821000	-3.69425700	1.09529700
C	4.55598100	-1.70345800	1.96342700
H	5.19169800	-0.98179200	2.49217000
H	3.73080600	-1.95220200	2.63364200
C	3.98196500	-1.00235400	0.75637400
C	6.00707200	-3.59836900	2.84281700
O	2.80627800	-0.62335200	0.71238000
H	4.39621400	-0.37043000	-1.00344400
O	4.84578600	-0.81763400	-0.22422800
O	5.91678300	-3.09667300	3.95186200

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I4, total electronic energy = -3622.000327, thermal corrections to Gibbs free energy = 0.837763

H	-6.47948400	4.61282300	-3.77096100
H	-5.69268000	5.05458100	-1.45293700
C	-6.12011100	3.79450200	-3.15302200
C	-5.67583800	4.04319900	-1.85023500
H	-6.44556600	2.29129300	-4.66586000

C	-6.10093500	2.49245700	-3.65521100
C	-5.21160900	2.99390400	-1.05592200
H	-4.88290100	3.20455900	-0.04180600
H	-5.92282500	-1.46378400	3.87688700
H	-8.09393400	-0.24124000	3.94443800
H	-0.86465900	-7.30260000	-1.07267300
H	1.42676900	-6.42000300	-1.48920900
C	-5.63398200	1.44345100	-2.85770000
C	-6.20980300	-0.81253900	3.05547600
C	-7.42782100	-0.12771600	3.09359400
C	-5.18054500	1.67754100	-1.54957600
H	-4.42472500	-1.22781900	1.94654900
C	-0.68721700	-6.23093300	-1.09966400
C	-5.35798200	-0.66984600	1.95983800
C	0.59744600	-5.73463400	-1.33520300
H	-5.61627500	0.43238900	-3.25695000
C	-7.78284200	0.69746900	2.02539000
H	-8.72939500	1.23167800	2.04021300
H	-2.74508800	-5.71213200	-0.71044700
C	-1.74117000	-5.33964300	-0.89530400
C	-5.69269400	0.17634700	0.88585300
H	-3.10050000	1.94530500	0.41626900
C	-6.92483100	0.84821400	0.93190200
C	0.82961300	-4.35873800	-1.36666900
H	1.83657200	-3.98159000	-1.51300500
H	-1.68307500	-1.38987800	0.23323800
H	-7.21956300	1.49842400	0.11472600
H	-2.49406400	0.94139100	-2.53544300
P	-4.56589400	0.21788100	-0.58920900
C	-1.51639000	-3.96039900	-0.93131500
C	-2.98857500	0.87156700	0.22656600
C	-0.22804500	-3.45046300	-1.16943700
H	-2.36065900	-3.29903400	-0.77501700
H	-2.93311500	0.38766600	1.20666600
H	-1.89838900	2.42064100	-1.76628900
C	-1.47747000	-0.89825100	-0.72541400
C	-1.69985300	1.35128900	-1.90213100

H	-2.25280100	-1.23888900	-1.41862700
C	-1.64713600	0.63402200	-0.53613600
H	-0.75575100	1.24878100	-2.44454100
P	0.15443700	-1.63790600	-1.26018500
Ni	2.10653800	-0.94670900	0.19263400
H	-1.27896300	-2.70495300	-3.65303100
H	-1.30629700	-3.61382000	3.84911800
H	0.14705500	-2.42528900	2.24004500
C	-1.36465700	-2.53218300	3.76868300
C	-0.54510000	-1.85860700	2.85807600
C	-0.50854300	1.32080700	0.29077000
C	-0.54368700	-1.98281100	-3.99671300
H	-0.91888600	2.21507700	0.77129100
C	0.29092000	-1.33025300	-3.07418200
H	-2.88203100	-2.33461700	5.28728500
C	-2.24776000	-1.81337000	4.57584700
H	0.26809500	1.66358300	-0.40299200
P	0.51105700	0.37296000	1.53883100
C	-0.60585900	-0.46079800	2.74141200
H	-1.07876800	-2.22916300	-6.06639500
C	-0.42817700	-1.71834200	-5.36179500
C	-2.30985400	-0.41917200	4.47405800
C	-1.49320600	0.25386200	3.56567100
C	1.24802800	-0.41536800	-3.54225600
H	-2.99283500	0.14323600	5.10420700
H	1.89386200	0.09627800	-2.83430800
H	-1.54133100	1.33734300	3.50410200
C	0.52382500	-0.80317200	-5.82138100
C	1.27287700	1.71780100	2.54296300
C	1.35954200	-0.15353300	-4.91096000
H	1.66336600	0.40454700	4.21858400
H	1.06919900	3.29816900	1.07080200
H	0.61454600	-0.60125500	-6.88514900
C	1.77646300	1.40793600	3.81896800
C	1.43698300	3.02367500	2.05352400
H	2.10305400	0.55612900	-5.26365300
C	2.41364800	2.38105000	4.58813200

C	2.07667800	3.99684500	2.82658000
H	2.78970000	2.12422900	5.57459800
H	2.18656600	5.00408000	2.43412800
C	2.56579100	3.68001400	4.09447900
H	3.06100200	4.43807000	4.69469700
H	3.97195900	-2.72694800	1.87848200
C	4.89438400	-1.67764800	3.51273000
H	5.40543300	-0.72812800	3.71133500
H	4.00125700	-1.72827200	4.14392100
H	5.56606200	-2.49500600	3.79958600
C	5.74326300	-1.75972500	1.12003800
H	6.38414800	-0.91210500	1.39834500
H	6.32085700	-2.66998000	1.32467100
C	5.43868300	-1.67075400	-0.39052700
H	6.36586100	-1.85090300	-0.94355800
H	5.09168500	-0.66317600	-0.62745000
C	4.39984300	-2.70048100	-0.84011900
C	4.51447800	-1.78871500	2.03741200
O	4.76675200	-3.79934800	-1.27434000
O	3.14462100	-2.37009000	-0.72479700
O	3.55684600	-0.75099900	1.71494700
C	5.81313300	6.11291000	-1.38115200
H	6.79745700	5.71861600	-1.10159500
H	5.92656000	6.85903900	-2.17055600
H	5.39529100	6.58890300	-0.48545500
C	4.69290600	3.84444400	-0.87275700
H	5.67155300	3.40020100	-0.64855400
H	4.35053400	4.26299600	0.08344400
C	3.72582500	2.77820200	-1.37724200
H	4.05852900	2.39704500	-2.35102900
H	2.73267000	3.20351600	-1.55647600
C	3.57171800	1.57952000	-0.44288000
C	4.90517500	4.99106800	-1.84834700
O	2.61300700	0.77801400	-0.74889400
H	4.00307000	0.09310200	1.39010900
O	4.36371500	1.43411400	0.51853800
O	4.37725700	5.01289500	-2.95012500

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I5, total electronic energy = -422.1300191, thermal corrections to Gibbs free energy = 0.11664

H	-1.86661600	-0.54498700	1.34452300
C	-2.99759600	0.85618800	0.16003600
H	-3.00025900	1.27914700	-0.85117800
H	-3.96513100	0.36827800	0.33009000
H	-2.90517600	1.67643500	0.88126800
C	-0.48773600	0.49412200	0.05912600
H	-0.46554000	0.87814300	-0.96802800
H	-0.36995000	1.35767400	0.72369100
C	0.66989000	-0.48298700	0.26794000
H	0.54591300	-1.36501900	-0.37113600
H	0.68857100	-0.86303700	1.29786800
C	2.02264800	0.12151900	-0.02709500
C	-1.85251000	-0.14508700	0.31678100
O	3.02459800	-0.74741400	0.24211000
H	3.86159700	-0.29433300	0.02225100
O	2.23054100	1.23951000	-0.45657400
O	-1.98394500	-1.22663600	-0.61619600
H	-2.82113500	-1.67850900	-0.42479100

34

I6, total electronic energy = -843.0783332, thermal corrections to Gibbs free energy = 0.23067

H	1.28348800	1.69783900	0.73580500
C	2.59481300	3.18987200	-0.09540300
H	2.74394900	3.74510600	0.83795400
H	3.51990700	3.24659900	-0.68134500
H	1.79835200	3.67882100	-0.66611200
C	3.30731100	1.02368400	1.01793000
H	4.27977200	1.12284700	0.52081400
H	3.39247800	1.51381300	1.99517400
C	2.99796300	-0.46788800	1.24403700
H	1.99959300	-0.60161200	1.67044100
H	3.72094800	-0.88261100	1.95744500
C	3.08735400	-1.31171000	-0.00420900
C	2.23270700	1.73159700	0.18102900

O	4.30362000	-1.28791200	-0.56228500
H	4.27873300	-1.86228300	-1.35258200
O	2.19683000	-2.02355300	-0.45938000
O	2.07147500	1.04280200	-1.06409500
H	1.19349700	0.61140100	-1.05003700
C	-5.59884300	1.47279500	-0.06423700
H	-5.36706600	1.97544600	-1.01037400
H	-6.66676200	1.25045400	-0.01339500
H	-5.33567500	2.17080800	0.74051500
C	-3.29022300	0.32190000	-0.12216100
H	-3.11403200	0.63460200	-1.16009300
H	-2.91934700	1.15315800	0.49137900
C	-2.53374300	-0.96637100	0.18260300
H	-2.95634100	-1.80365800	-0.38592500
H	-2.63841200	-1.25030300	1.23555000
C	-1.05858400	-0.88596500	-0.14207400
C	-4.79278500	0.19760200	0.08084700
O	-0.39110000	-1.95283300	0.28768500
H	0.57080900	-1.90333400	0.01588000
O	-0.54207800	0.05117100	-0.74214100
O	-5.32121000	-0.87094800	0.34630900

34

TS3, total electronic energy = -843.0427473, thermal corrections to Gibbs free energy = 0.231201

H	1.10296400	1.74923400	0.58748200
C	2.53987900	2.81918500	-0.62317800
H	2.65396600	3.66960400	0.05866500
H	3.50235600	2.63497600	-1.11227000
H	1.80384800	3.08839300	-1.38732500
C	3.07429900	1.13174700	1.24978700
H	4.10593700	1.35123600	0.95394300
H	2.87785500	1.64655600	2.19403700
C	2.86973900	-0.37975800	1.35782900
H	1.91402600	-0.62111500	1.83295300
H	3.66982900	-0.88360800	1.90756400
C	2.83983500	-0.90590500	-0.06627100
C	2.09655600	1.59013400	0.15323400

O	4.04860900	-0.85045500	-0.65563100
H	3.99379800	-1.33132000	-1.50237500
O	2.13689700	-1.96482400	-0.40830500
O	1.97421000	0.45148200	-0.75394400
H	0.91052300	0.17931800	-0.82114100
C	-5.39494600	1.53788600	0.22168000
H	-4.98041600	2.34085300	-0.39859800
H	-6.45268000	1.39497500	-0.00995200
H	-5.29626100	1.85861600	1.26680000
C	-3.11673700	0.33532900	0.07796000
H	-2.78313800	0.91342400	-0.79427200
H	-2.83577600	0.94271300	0.94892700
C	-2.41740600	-1.02241100	0.09895400
H	-2.80778500	-1.64191500	-0.71918500
H	-2.63328100	-1.56834600	1.02173000
C	-0.90567900	-0.94675100	-0.07224900
C	-4.63331800	0.24275700	0.01653300
O	-0.21030700	-1.84201700	0.49024800
H	1.17294600	-1.93733100	0.00971800
O	-0.44306600	-0.00517700	-0.79754900
O	-5.21034800	-0.81395100	-0.19011500

18

I7, total electronic energy = -422.1138283, thermal corrections to Gibbs free energy = 0.120638

H	2.65437100	-1.71063300	-0.32042800
C	2.45766400	-0.75682000	0.18071000
H	3.37551000	-0.15826500	0.14742900
H	2.21106900	-0.95876900	1.22906500
C	1.31944300	-0.00981400	-0.49748800
C	0.91954400	1.31931700	0.17064600
O	0.11933800	-0.82828500	-0.48279800
C	-0.58757900	1.37977400	-0.09078100
H	1.11516000	1.27434600	1.24796800
H	1.47254200	2.16788000	-0.24201600
H	-1.14553300	2.00215100	0.61222600
H	-0.79987300	1.72412400	-1.10891800
C	-0.98821800	-0.09544700	0.02105900

O	-2.12769800	-0.48941200	-0.69601300
O	-1.23182900	-0.38479500	1.36540300
H	-1.39290900	-1.34342900	1.41860500
H	1.57019400	0.16401800	-1.55321300
H	-1.86413900	-0.56354400	-1.62833400

34

TS4, total electronic energy = -843.038402, thermal corrections to Gibbs free energy = 0.230478

H	-5.20095100	-0.55085100	0.60593400
C	-5.16625200	1.48178600	-0.12375600
H	-5.79116500	1.88913200	0.67862400
H	-4.43203300	2.24072800	-0.41342100
H	-5.80994900	1.26549600	-0.98219600
C	-3.47433600	0.42311500	1.52540900
H	-3.10562300	1.45284900	1.53631300
H	-3.93873800	0.21147700	2.49133700
C	-2.33733200	-0.54577300	1.18086800
H	-2.54725100	-1.56329400	1.53083700
H	-1.35585300	-0.24804600	1.55159800
C	-2.41125200	-0.57773100	-0.33693700
C	-4.46831300	0.22619800	0.36443700
O	-1.57091900	0.95172300	-0.69410900
H	-1.67050300	1.04770800	-1.65987200
O	-1.79249500	-1.46596700	-1.07720100
O	-3.66716700	-0.33876200	-0.73623300
H	-0.49257600	0.76870300	-0.49558500
C	6.05302800	1.25233000	-0.46025000
H	5.63725500	2.25404300	-0.61816200
H	6.97168800	1.31679400	0.12693100
H	6.28871700	0.84454600	-1.45175300
C	3.64000100	0.34826600	-0.33812500
H	3.19910300	1.33280800	-0.13133400
H	3.70110100	0.28402400	-1.43290500
C	2.74550100	-0.75050700	0.23468700
H	2.81038200	-0.72835600	1.33034800
H	3.08594100	-1.74237500	-0.07472300
C	1.27481500	-0.60408800	-0.13819400

C	5.05012200	0.34935600	0.23109300
O	0.61455800	-1.66226300	-0.33414700
H	-0.80248000	-1.56799500	-0.75326300
O	0.80747700	0.58344900	-0.18752100
O	5.36067500	-0.33381900	1.19494800

3

H2O, total electronic energy = -76.4253027, thermal corrections to Gibbs free energy = 0.003422

O	0.00000000	0.00000000	0.12041100
H	0.00000000	0.75999800	-0.48164300
H	0.00000000	-0.75999800	-0.48164300

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I8, total electronic energy = -345.6998812, thermal corrections to Gibbs free energy = 0.096492

H	-2.54985400	-1.58908000	0.17391400
C	-2.30309900	-0.60791400	-0.24374900
H	-3.15089600	0.06298800	-0.06701300
H	-2.16088900	-0.71084500	-1.32490100
C	-1.05792900	-0.03578600	0.40638400
C	-0.56838600	1.31230800	-0.14948100
O	0.05994100	-0.95179100	0.17520900
C	0.94853800	1.22329900	0.04132800
H	-0.81614600	1.38646100	-1.21456700
H	-1.03005300	2.15666500	0.36805100
H	1.54232800	1.74645100	-0.71142400
H	1.26253200	1.59014700	1.02698300
C	1.21866100	-0.27331200	-0.01004200
O	2.27302600	-0.84528200	-0.17666200
H	-1.18746500	0.02223100	1.49394200

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$LNi(OAc)_2$ (**L=DPPP**), total electronic energy = -2354.632832, thermal corrections to Gibbs free energy = 0.480178

H	-6.55603100	2.64912500	0.82466500
H	-6.43666700	0.17362100	1.06126300
C	-5.64947900	2.11714200	0.55014900
C	-5.58237700	0.72796500	0.68248900
H	-4.58681600	3.89868100	-0.04592300
C	-4.54419700	2.81834800	0.06240700
C	-4.41975500	0.04283800	0.32566700
H	-4.38511700	-1.03751300	0.42941600
H	-0.70780400	1.68861700	-1.68799200
C	-3.37791200	2.13595700	-0.29218400
C	-3.30512500	0.73782300	-0.17265200
H	-2.52793900	2.70206200	-0.65919800
C	-1.09940600	0.73626600	-2.06330200
H	-1.92804600	0.98035200	-2.73672200
C	-0.00005900	0.00068800	-2.86005300
P	-1.74232400	-0.15796800	-0.55753000
Ni	0.00015700	-0.00081200	1.19167200
H	-3.47901100	-0.99628000	-2.83353600
H	1.97804500	5.11312500	-0.48967600
H	1.24260100	2.89154100	0.33237100
C	2.30264800	4.21295900	-1.00437200
C	1.89113400	2.96089800	-0.53584300
C	1.09949900	-0.73517500	-2.06378100
C	-3.13914000	-1.89232200	-2.32109800
H	1.92810100	-0.97877800	-2.73742300
C	-2.30684800	-1.78970100	-1.19187800
H	3.44281600	5.27986400	-2.49123200
C	3.12538200	4.30641300	-2.12764600
H	0.70807800	-1.68780000	-1.68895400
P	1.74238900	0.15838900	-0.55759200
C	2.30638100	1.79066700	-1.19105200
H	-4.18511100	-3.21092700	-3.66196200
C	-3.54365800	-3.14257700	-2.78771800
C	3.54283200	3.14472100	-2.78616400

C	3.13865600	1.89410500	-2.32021400
C	-1.89193000	-2.96039300	-0.53728400
H	4.18427100	3.21372000	-3.66036600
H	-1.24339700	-2.89168500	0.33098500
H	3.47879400	0.99843300	-2.83311400
C	-3.12652200	-4.30473300	-2.12982000
C	3.30545400	-0.73719200	-0.17333900
C	-2.30377600	-4.21209300	-1.00648200
H	4.38538600	1.03807300	0.42908000
H	2.52833800	-2.70134200	-0.66031600
H	-3.44420700	-5.27790400	-2.49393500
C	4.42009300	-0.04224600	0.32502100
C	3.37833900	-2.13528400	-0.29328400
H	-1.97939800	-5.11261800	-0.49227300
C	5.58279800	-0.72739300	0.68152500
C	4.54472300	-2.81769000	0.06097400
H	6.43709100	-0.17309800	1.06036400
H	4.58740800	-3.89798900	-0.04766900
C	5.64999900	-2.11653200	0.54878600
H	6.55662700	-2.64850900	0.82305800
O	1.44455600	-0.38884900	2.74268600
O	0.45471500	-2.00474200	1.62312300
C	1.25614800	-1.62637000	2.54499200
C	1.99709900	-2.66159300	3.36043100
H	1.35892200	-3.52902000	3.54961800
H	2.34449400	-2.23780900	4.30523400
H	2.86875400	-3.00296400	2.78953900
C	-1.99654600	2.65868500	3.36242200
H	-1.35747500	3.52501500	3.55366800
H	-2.86707900	3.00208000	2.79104200
C	-1.25591700	1.62382100	2.54621100
O	-0.45413100	2.00273400	1.62485600
O	-1.44470000	0.38621300	2.74293200
H	-2.34552500	2.23391600	4.30619600
H	-0.47121700	-0.73957500	-3.51628600
H	0.47097900	0.74115300	-3.51614200

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I1', total electronic energy = -2738.418438, thermal corrections to Gibbs free energy = 0.596178

H	7.12797600	0.00465600	0.17677800
H	6.18967000	0.03081400	-2.12906800
C	6.09438600	-0.28175200	0.00415800
C	5.56772500	-0.26725700	-1.28946500
H	5.68433300	-0.68109100	2.08529400
C	5.28402800	-0.66613200	1.07530600
C	4.24086000	-0.63959500	-1.51323600
H	3.84837400	-0.62890200	-2.52542600
H	1.35250200	-2.50013000	1.41598200
C	3.95491800	-1.03482000	0.85552500
C	3.41990200	-1.03452300	-0.44412700
H	3.33952200	-1.31704900	1.70368300
C	1.37822800	-2.91429600	0.40163000
H	2.24558000	-3.58157300	0.35765800
C	0.09523300	-3.73272300	0.14122200
P	1.64576700	-1.44709200	-0.71973000
Ni	0.04584500	0.31174900	-0.03264600
H	2.95477700	-3.79313600	-2.02019900
H	0.11839100	-1.14429300	5.51004900
H	-0.03137700	-0.41920200	3.14322700
C	-0.51204000	-1.69387700	4.81645800
C	-0.59873900	-1.28055400	3.48302000
C	-1.20077400	-2.95870700	-0.18249800
C	2.33248400	-3.29913800	-2.76153700
H	-2.05582700	-3.63740900	-0.09360700
C	1.60230400	-2.14636500	-2.42005500
H	-1.16107800	-3.12783200	6.29003000
C	-1.23079800	-2.80702000	5.25430400
H	-1.17602100	-2.61673100	-1.22360100
P	-1.49619400	-1.41948000	0.82880400
C	-1.41195300	-1.98136500	2.57801800
H	2.83977200	-4.70578200	-4.30885900
C	2.27338400	-3.81370000	-4.05629000
C	-2.04361700	-3.51010400	4.35853500

C	-2.13651600	-3.09933400	3.02916600
C	0.81743700	-1.51733000	-3.39964900
H	-2.60588500	-4.37620100	4.69635800
H	0.24216600	-0.63276300	-3.14378500
H	-2.78047800	-3.64656200	2.34596200
C	1.48924900	-3.18102300	-5.02689400
C	-3.28343400	-1.06952600	0.55479600
C	0.76487500	-2.03445300	-4.69812500
H	-3.64048900	-0.38074500	2.57444200
H	-3.27916600	-1.65154800	-1.53334900
H	1.44565300	-3.58268300	-6.03549800
C	-4.06942100	-0.53391400	1.58872300
C	-3.86489300	-1.25361500	-0.71109000
H	0.15582500	-1.53980900	-5.44973900
C	-5.40716200	-0.20329200	1.36538200
C	-5.20457700	-0.92490800	-0.93076000
H	-6.00205100	0.20344300	2.17855600
H	-5.64071900	-1.08225600	-1.91338500
C	-5.97994500	-0.39974100	0.10583200
H	-7.02269500	-0.14765900	-0.06563700
C	4.33556700	6.20715500	0.97405400
H	3.52748100	6.81961400	1.39403300
H	5.29755500	6.62218400	1.28251500
H	4.23886800	6.25700400	-0.11663000
C	3.00094800	3.99926700	0.94795500
H	2.10232900	4.62140800	1.05719200
H	3.12954200	3.87030800	-0.13513600
C	2.81790200	2.63927700	1.61865600
H	2.55945300	2.74940500	2.67632100
H	3.76590300	2.08692400	1.59344100
C	1.77079000	1.76632300	0.95356200
C	4.19972600	4.77894500	1.46493200
O	1.17506400	0.87140500	1.64550500
O	1.50401900	1.88700600	-0.27949700
O	5.01323700	4.28402300	2.23009100
C	-5.88822300	4.59365500	-1.04086200
H	-5.52344800	5.06361000	-0.12008300

H	-6.41573300	5.33064100	-1.65026400
H	-6.58895300	3.80465600	-0.73971100
C	-3.81622200	3.05712000	-1.05983900
H	-3.31579300	3.64894200	-0.28175900
H	-4.42719600	2.32541700	-0.51459300
C	-2.78135100	2.35991000	-1.94020700
H	-2.24255600	3.10585100	-2.53903200
H	-3.26197200	1.68961700	-2.65924600
C	-1.74723700	1.56727500	-1.16260100
C	-4.74211400	3.98706300	-1.82726800
O	-1.12078200	0.62014400	-1.75042100
O	-1.47714600	1.84449300	0.04359600
O	-4.57537100	4.23590200	-3.01169500
H	-0.07379600	-4.35597800	1.02646500
H	0.27457800	-4.42088700	-0.69239700

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I2', total electronic energy = -2739.572577, thermal corrections to Gibbs free energy = 0.611454

H	-6.26833400	-2.67430100	-2.12998600
H	-6.13845600	-1.03946900	-0.25631100
C	-5.32946300	-2.51738000	-1.60649200
C	-5.25598300	-1.59847500	-0.55547400
H	-4.23719100	-3.95057500	-2.79261100
C	-4.18988300	-3.23264900	-1.97838100
C	-4.05061800	-1.39766000	0.11856500
H	-4.00932300	-0.68379300	0.93620300
H	-0.02190200	-3.39321200	-0.59607100
C	-2.98150500	-3.03358100	-1.30500600
C	-2.89838900	-2.11758300	-0.24369900
H	-2.10889400	-3.60040400	-1.61382500
C	-0.34614300	-3.34215200	0.44972100
H	-1.00944300	-4.19730900	0.62008900
C	0.88027900	-3.46293100	1.37985800
P	-1.30110500	-1.74897900	0.59485600
Ni	-0.00108300	0.00141500	-0.53159500
H	-2.76344800	-3.57507900	2.45480200

H	2.39830800	-3.55714600	-4.43650100
H	1.51173800	-1.89276200	-2.82044200
C	2.79148700	-3.52406100	-3.42410100
C	2.29491400	-2.58187200	-2.51778000
C	1.79396300	-2.22705500	1.52985400
C	-2.45923000	-2.69578100	3.01641400
H	2.73946800	-2.53371300	1.99031900
C	-1.76055700	-1.65587000	2.37746000
H	4.17056700	-5.15307900	-3.73157800
C	3.78648700	-4.41907000	-3.02850000
H	1.33024500	-1.50564100	2.21204800
P	2.11628200	-1.26809300	-0.04026100
C	2.79358200	-2.52413500	-1.20724200
H	-3.31568100	-3.41468800	4.85529300
C	-2.77659100	-2.60486900	4.37135100
C	4.29058400	-4.36944600	-1.72441000
C	3.80074400	-3.42679800	-0.82068800
C	-1.39057100	-0.52290600	3.11952800
H	5.06661600	-5.06328400	-1.41303600
H	-0.84729600	0.28404400	2.63623200
H	4.21047600	-3.39104600	0.18517000
C	-2.40390700	-1.47273200	5.10415400
C	3.59456000	-0.25284500	0.38960000
C	-1.71319800	-0.43446100	4.47782500
H	4.49214000	-0.41207600	-1.57254300
H	2.97604400	0.15079200	2.42653600
H	-2.65380300	-1.40274800	6.15928500
C	4.57198800	0.02428600	-0.58126800
C	3.72488100	0.32936000	1.66207100
H	-1.42416500	0.44726300	5.04335400
C	5.65851000	0.84865700	-0.28285500
C	4.81551400	1.14954300	1.95992700
H	6.40782800	1.04536400	-1.04485200
H	4.90515500	1.58228200	2.95266100
C	5.78621100	1.41158200	0.98987600
H	6.63548700	2.04743200	1.22405100
H	-0.25187800	-0.69516700	-2.01150200

C	-5.34758500	5.18943700	-0.19371200
H	-4.72703900	5.98641700	-0.62290400
H	-6.39074900	5.51232300	-0.18428000
H	-4.99554400	5.02889400	0.83180500
C	-3.84020700	3.24373900	-0.96536600
H	-3.05453800	3.99822500	-1.10098100
H	-3.70157600	2.86278000	0.05528000
C	-3.69900200	2.11023600	-1.97747700
H	-3.71235400	2.48485100	-3.00548200
H	-4.55507500	1.42798200	-1.89668300
C	-2.45291800	1.27871100	-1.78421000
C	-5.19780100	3.92883300	-1.02065400
O	-2.09286400	0.58895000	-2.84568000
H	-1.27670900	0.01325600	-2.55860900
O	-1.83901200	1.22684900	-0.70912300
O	-6.11673900	3.48404300	-1.69063400
C	4.34143700	5.98205800	-0.51635500
H	4.26704300	5.83746700	-1.60036600
H	4.47043400	7.04265400	-0.28966400
H	5.22958300	5.43077100	-0.18191000
C	2.69628600	4.02490600	-0.17941200
H	2.37869000	4.03208800	-1.23100400
H	3.58401300	3.37913200	-0.15168600
C	1.58111400	3.46304200	0.70020900
H	0.74259900	4.17139400	0.72468800
H	1.91415900	3.35082000	1.73612900
C	1.03747700	2.12795400	0.22094400
C	3.11223800	5.44005500	0.18754900
O	0.53442900	1.32118200	1.06932600
O	1.05335500	1.82706600	-1.01200900
O	2.49406700	6.10825100	1.00255900
H	0.53946200	-3.73823000	2.38443400
H	1.47786400	-4.30531900	1.01371200

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I3’, total electronic energy = -2318.612901, thermal corrections to Gibbs free energy = 0.499050

H	6.86465900	-1.52356700	-3.09781800
H	5.52536200	-3.35934600	-2.08026500
C	6.00469400	-1.29193400	-2.47569600
C	5.25267600	-2.32230900	-1.90468300
H	6.22377100	0.84470000	-2.68079000
C	5.64479500	0.03668200	-2.24201000
C	4.14953200	-2.02556400	-1.10336500
H	3.57861300	-2.83717800	-0.66082300
H	2.45967200	2.04670000	0.07535500
C	4.53968700	0.33714300	-1.44162400
C	3.78264200	-0.69113600	-0.85656000
H	4.27635600	1.37700600	-1.27663100
C	2.59087200	1.32736900	0.89147900
H	3.63555300	1.39801700	1.21366300
C	1.67193600	1.70674500	2.07516600
P	2.26194800	-0.33554600	0.11838800
Ni	0.29358200	0.04757100	-1.26215100
H	4.24885300	-0.83604600	2.30398700
H	0.84470900	5.63721200	-2.16296400
H	0.59895700	3.19288300	-1.77760700
C	0.32540500	5.27842500	-1.27853300
C	0.18706100	3.90319500	-1.06615500
C	0.17840800	1.32264600	1.99080500
C	3.43035200	-1.54131500	2.42136200
H	-0.36706400	1.85633700	2.77724500
C	2.35476500	-1.53419200	1.51550300
H	-0.09676300	7.25417800	-0.52510700
C	-0.20378100	6.18565200	-0.35963200
H	0.06218200	0.25160600	2.19237800
P	-0.63667600	1.61132000	0.34162100
C	-0.48379800	3.42633500	0.06964400
H	4.29572200	-2.45291100	4.16848400
C	3.46132600	-2.45742900	3.47253400
C	-0.87648900	5.71816700	0.77471200
C	-1.01819100	4.34749500	0.98806300
C	1.31622700	-2.46524100	1.67798800
H	-1.29245800	6.42166000	1.49066200

H	0.48185500	-2.46693200	0.98200400
H	-1.55339200	3.99607700	1.86625900
C	2.42220000	-3.38129200	3.62818900
C	-2.43093800	1.37469000	0.68026300
C	1.35347500	-3.38557000	2.73065500
H	-3.00723800	2.37159800	-1.15272500
H	-2.22242500	0.30815800	2.55656800
H	2.44927400	-4.09536700	4.44669600
C	-3.35605000	1.83815600	-0.27269000
C	-2.90860600	0.68402200	1.80486800
H	0.54672500	-4.10412500	2.84694100
C	-4.72325800	1.62750000	-0.09747200
C	-4.27988500	0.47124300	1.97672500
H	-5.42396600	1.99795300	-0.84056400
H	-4.63302800	-0.05895200	2.85696000
C	-5.18997300	0.94212100	1.02862100
H	-6.25521000	0.77860000	1.16556700
H	1.15452300	1.01579600	-2.20056900
C	-5.44301800	-4.32185300	0.20034700
H	-6.08269900	-3.50658600	0.56194600
H	-6.06949800	-5.17032900	-0.08326700
H	-4.78555600	-4.60329900	1.03104400
C	-3.56706200	-2.80108300	-0.70728700
H	-3.99476600	-2.01900600	-0.06579900
H	-2.79012600	-3.28111400	-0.09683500
C	-2.94278500	-2.20250300	-1.96718700
H	-3.67205000	-1.61247200	-2.52975600
H	-2.62500000	-3.01422100	-2.63458500
C	-1.72790200	-1.33509000	-1.69060900
C	-4.63697900	-3.84343900	-0.99161300
O	-1.46521500	-0.35600500	-2.45513900
O	-0.95515700	-1.60222100	-0.71166500
O	-4.83673800	-4.27706700	-2.11598100
H	2.06476800	1.24984300	2.99027200
H	1.75317300	2.79103700	2.21160600

I4’, total electronic energy = -2739.614490, thermal corrections to Gibbs free energy = 0.626061

H	-6.75112500	-2.42633300	2.46427900
H	-4.95961100	-4.05710800	1.88847800
C	-5.90029200	-2.11409700	1.86525900
C	-4.89456100	-3.02936600	1.54184100
H	-6.58111900	-0.07720100	1.66063800
C	-5.80458200	-0.79640500	1.41484000
C	-3.80260600	-2.62931300	0.77182600
H	-3.03014700	-3.35262100	0.52580800
H	-2.91068300	1.47416500	-1.01472400
C	-4.71229700	-0.39318700	0.64201400
C	-3.70125700	-1.30732600	0.30599500
H	-4.66037900	0.63761300	0.30559300
C	-2.83213300	0.61582700	-1.69222200
H	-3.84607100	0.40064300	-2.04619700
C	-1.94780700	0.98875900	-2.90086600
P	-2.20851400	-0.79816700	-0.64379900
Ni	-0.28655300	0.15296800	0.76610500
H	-3.99869800	-2.10042300	-2.63765900
H	-2.28839600	5.37253600	1.12888400
H	-1.27285500	3.12230500	0.99220700
C	-1.77202300	5.06926700	0.22259700
C	-1.19854100	3.79685100	0.14371600
C	-0.41769800	0.98245700	-2.70081800
C	-3.02832800	-2.58657500	-2.69228400
H	0.05753200	1.49433900	-3.54438100
C	-1.98268400	-2.17866000	-1.84448300
H	-2.12577800	6.93364800	-0.80020100
C	-1.67918500	5.94513900	-0.86003500
H	-0.05046100	-0.05008900	-2.71164100
P	0.19804000	1.70165800	-1.09700100
C	-0.52532800	3.39018500	-1.01886400
H	-3.64725800	-3.93139600	-4.25383100
C	-2.83352800	-3.62504500	-3.60226900
C	-1.00841300	5.55038600	-2.02229000
C	-0.43283600	4.28251700	-2.10163600

C	-0.74337200	-2.83299500	-1.92025900
H	-0.93290200	6.23058300	-2.86596600
H	0.06722600	-2.52040000	-1.26784200
H	0.09389700	3.99173800	-3.00648800
C	-1.59497300	-4.27208500	-3.67335800
C	1.98670700	1.98584000	-1.42273000
C	-0.55394500	-3.87652500	-2.83264400
H	2.10478200	3.74847300	-0.17451100
H	2.23784400	0.26374500	-2.71783100
H	-1.44614100	-5.08259200	-4.38156300
C	2.65498200	3.05437200	-0.80223700
C	2.72363400	1.10242200	-2.22938900
H	0.40822000	-4.37904500	-2.88275200
C	4.02482800	3.24054800	-0.99335500
C	4.09446000	1.29240100	-2.41891700
H	4.52495400	4.07602800	-0.51131900
H	4.64791100	0.60443200	-3.05202700
C	4.74865400	2.36096700	-1.80239900
H	5.81450200	2.50821300	-1.95207300
H	-0.22148600	1.90184400	3.40313900
C	1.64130000	2.94866800	3.63971800
H	2.71775900	2.77146400	3.52947100
H	1.35284200	3.76010900	2.96371400
H	1.45179400	3.27334500	4.66937400
C	1.19335600	0.52618200	4.27106100
H	2.28382300	0.40653000	4.32073300
H	0.85998400	0.81823400	5.27454600
C	0.55880400	-0.82941400	3.89356500
H	0.68045900	-1.52012900	4.73420300
H	1.07851300	-1.24785100	3.02938300
C	-0.93495900	-0.67655900	3.59561600
C	0.84892700	1.68187700	3.32266000
O	-1.75273500	-0.71690300	4.52152900
O	-1.27288300	-0.47185100	2.35263700
O	1.04812000	1.32902400	1.93336900
C	6.50753600	-4.22892100	0.88498700
H	6.08331200	-4.96423600	1.58076300

H	7.23790000	-4.72492900	0.24201000
H	7.00214200	-3.46317000	1.49346800
C	4.42769600	-2.70733600	0.77705100
H	4.13101300	-3.18517100	1.72053800
H	4.98271100	-1.80770500	1.07563600
C	3.20790900	-2.31276500	-0.05157300
H	2.56358200	-3.17625600	-0.24224300
H	3.53710500	-1.95598300	-1.03613100
C	2.37211300	-1.19877300	0.57606200
C	5.39647800	-3.62448400	0.04839800
O	1.13460500	-1.18022000	0.22973800
H	1.87966200	0.76792300	1.80793300
O	2.92579800	-0.37721400	1.34668500
O	5.29373200	-3.86092300	-1.14593700
H	-2.16507000	0.30096300	-3.72557700
H	-2.26002000	1.98399300	-3.23639100

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TS1', total electronic energy = -2739.565816, thermal corrections to Gibbs free energy = 0.609933

H	-6.25686100	-2.85094900	-1.36526700
H	-5.89382100	-1.60561200	0.76015500
C	-5.25071000	-2.70818400	-0.98130100
C	-5.04671200	-2.00797700	0.21140100
H	-4.30311900	-3.77167900	-2.60158100
C	-4.15479100	-3.22402100	-1.67496600
C	-3.75481200	-1.82515600	0.70612800
H	-3.61117300	-1.28120400	1.63509500
H	0.17565100	-3.24540900	-1.06784800
C	-2.85978000	-3.04339300	-1.18156100
C	-2.64477200	-2.34665900	0.01859400
H	-2.02408000	-3.45341200	-1.73965100
C	0.06206100	-3.42531300	0.00743800
H	-0.49562000	-4.36192900	0.11586700
C	1.45393800	-3.58899500	0.65480000
P	-0.95001500	-1.99917400	0.64723600
Ni	-0.00729600	0.09474200	-0.21540500

H	-1.91801300	-4.29543500	2.28533300
H	1.73922600	-2.32760400	-5.23805100
H	1.10939300	-1.12243800	-3.16506700
C	2.32246200	-2.47024200	-4.33256400
C	1.96857100	-1.78672500	-3.16506300
C	2.29085200	-2.31315700	0.89305300
C	-1.57844400	-3.51791200	2.96447300
H	3.32868900	-2.59851500	1.09646800
C	-1.08064500	-2.30395800	2.45811200
H	3.69311900	-3.86636800	-5.23890000
C	3.41942100	-3.33284700	-4.33285800
H	1.92617000	-1.79325400	1.78632800
P	2.22456900	-1.03663200	-0.46704500
C	2.71284400	-1.95683900	-1.98751300
H	-2.03579700	-4.67324200	4.72137100
C	-1.65051100	-3.73139400	4.34058200
C	4.16850100	-3.50875200	-3.16453300
C	3.82088000	-2.82319300	-2.00084500
C	-0.66157400	-1.30785300	3.35419700
H	5.02481300	-4.17748600	-3.16131900
H	-0.27199600	-0.36809200	2.97387600
H	4.41965800	-2.95887800	-1.10428900
C	-1.23044200	-2.73420900	5.22755100
C	3.69585800	0.01979800	-0.12582700
C	-0.73817200	-1.52541600	4.73384100
H	4.08252000	0.43684000	-2.21357400
H	3.58489000	-0.15065500	2.03158100
H	-1.28931000	-2.90160100	6.29950200
C	4.38111400	0.63395200	-1.18799000
C	4.10441100	0.29488100	1.18979500
H	-0.41331700	-0.74791600	5.41983200
C	5.45498500	1.49033800	-0.94102700
C	5.18245400	1.14949900	1.43400800
H	5.97624400	1.95187100	-1.77527000
H	5.49082000	1.34367400	2.45768500
C	5.86083400	1.74956900	0.37071700
H	6.69888500	2.41368900	0.56258400

H	-0.49572500	-0.29104900	-1.81801100
C	-6.16209900	4.60955400	-2.49487000
H	-5.92297000	4.33275600	-3.52810300
H	-7.22950100	4.82122500	-2.40254600
H	-5.59364600	5.52083300	-2.26894800
C	-4.35238100	2.95606800	-1.68990800
H	-4.30892500	2.43180900	-2.65395300
H	-3.65068500	3.79568000	-1.78392700
C	-3.94144400	2.01318000	-0.55845600
H	-4.71307000	1.24286900	-0.43211700
H	-3.87040400	2.54369600	0.39471800
C	-2.62944800	1.29149100	-0.80541100
C	-5.76055700	3.51043300	-1.53135100
O	-2.39097700	0.89608600	-2.00778700
H	-1.33960600	0.25136000	-1.93617500
O	-1.85383200	1.07849500	0.16161400
O	-6.52716700	3.09139500	-0.67803600
C	1.79415000	7.16837500	0.60168200
H	0.80296100	7.44367400	0.98435400
H	2.51911900	7.92629000	0.90637200
H	1.71759900	7.14159500	-0.49140600
C	1.39417000	4.61950900	0.64666600
H	0.32449700	4.86384700	0.69844800
H	1.60986500	4.50377000	-0.42419100
C	1.70181200	3.31866300	1.38583900
H	1.38880600	3.37476700	2.43290200
H	2.78640500	3.15241100	1.40096600
C	1.06526100	2.09311300	0.75672800
C	2.19142800	5.81209800	1.15131100
O	0.79220900	1.08607700	1.49002800
O	0.83396400	2.04800600	-0.49091800
O	3.10434500	5.68832000	1.95349700
H	1.33979800	-4.08726300	1.62413700
H	2.02389500	-4.27535900	0.01870400

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TS2’, total electronic energy = -2739.555471, thermal corrections to Gibbs free energy =

0.620754

H	-7.01472100	-1.78592800	1.85856600
H	-4.96356400	-3.11856500	2.32885400
C	-6.08648100	-1.56206700	1.33992500
C	-4.93553500	-2.31157500	1.60152300
H	-6.92207900	0.07112700	0.20445600
C	-6.03463300	-0.52038400	0.41299100
C	-3.74094600	-2.02422100	0.94069600
H	-2.84680600	-2.59228400	1.17894400
H	-2.66572400	1.60781800	-1.33552200
C	-4.84174600	-0.23277400	-0.25786100
C	-3.68289300	-0.98448900	-0.00642500
H	-4.83178300	0.58129100	-0.97456400
C	-2.42557400	0.75489900	-1.98027000
H	-3.32222600	0.53862400	-2.57135900
C	-1.28825000	1.13818200	-2.95199200
P	-2.06409600	-0.66072400	-0.82742400
Ni	-0.35225100	0.02744100	0.81975400
H	-3.95380100	-2.16113200	-2.57810200
H	-3.08854100	5.17760200	0.64519800
H	-1.89281800	3.00642900	0.75768200
C	-2.24014300	4.99388200	-0.00818300
C	-1.56626700	3.77041000	0.05743700
C	0.15860500	1.17612100	-2.41257200
C	-2.96668600	-2.59679200	-2.70675700
H	0.78285000	1.73137700	-3.12132500
C	-1.87547700	-2.09745000	-1.97459300
H	-2.34347000	6.92646900	-0.95887200
C	-1.82136100	5.97503000	-0.90786100
H	0.56399000	0.16015200	-2.35602400
P	0.37596000	1.87843600	-0.69531100
C	-0.46626800	3.51720300	-0.77651900
H	-3.64833900	-4.03684200	-4.15339100
C	-2.79650500	-3.65950800	-3.59408300
C	-0.72604400	5.73260000	-1.74367300
C	-0.05207000	4.51320200	-1.67879100
C	-0.61375700	-2.68787300	-2.14469800

H	-0.39669200	6.49412100	-2.44517600
H	0.23535500	-2.31672700	-1.57916500
H	0.80285300	4.34049500	-2.32678300
C	-1.53472600	-4.23969100	-3.76016600
C	2.16404700	2.32472300	-0.64453500
C	-0.44599100	-3.75292500	-3.03530300
H	1.88270600	3.90542500	0.80760600
H	2.81800700	0.82452400	-2.06480600
H	-1.40433100	-5.06964300	-4.44925700
C	2.60298900	3.34111200	0.22223700
C	3.12176000	1.61933800	-1.39202800
H	0.53546900	-4.20334100	-3.15670600
C	3.95955100	3.64902600	0.33117700
C	4.47978400	1.93105200	-1.28299300
H	4.27763800	4.44223200	1.00217600
H	5.20441800	1.38272000	-1.87898900
C	4.90331600	2.94499900	-0.42146200
H	5.95916300	3.18693700	-0.33882900
H	-1.41279900	0.86935000	1.72561500
C	-0.39290800	2.51732000	3.38705400
H	0.21980000	2.88496800	4.22348700
H	-0.15539900	3.11107900	2.50408800
H	-1.44472500	2.64784000	3.65251700
C	-0.65930200	0.08991700	4.16530800
H	-0.38785400	0.49959300	5.15241100
H	-1.74935300	0.16846400	4.10663600
C	-0.19287100	-1.36858000	4.10936500
H	-0.49304100	-1.86480800	5.03619400
H	0.90385800	-1.39410200	4.07636900
C	-0.72648000	-2.21274200	2.93999500
C	-0.03779500	1.06221800	3.17621100
O	-1.25425200	-3.30761800	3.19111600
O	-0.55120500	-1.76301900	1.74203500
O	1.02607200	0.78462800	2.54987900
C	7.28860500	-2.79549700	-0.13122700
H	7.50704200	-2.62063700	0.92870300
H	7.88897300	-3.62918700	-0.50122000

H	7.56666100	-1.88081900	-0.66961900
C	4.84147000	-2.07159500	0.25223300
H	4.98878700	-2.05181500	1.33941600
H	5.12118800	-1.06964100	-0.10034200
C	3.38140000	-2.38648400	-0.08964700
H	3.13801500	-3.39939700	0.25588700
H	3.21667000	-2.37052600	-1.16880300
C	2.39130400	-1.44222500	0.54733300
C	5.81531700	-3.08430100	-0.33471900
O	1.44697500	-0.95448700	-0.08405000
H	1.93231900	-0.55670900	2.18091900
O	2.61325800	-1.20487800	1.82622100
O	5.42750300	-4.07430100	-0.93417000
H	-1.29568900	0.44280300	-3.79926800
H	-1.53834500	2.12366500	-3.36073400

References

[1] K. Osakada, T. Ikariya and S. Yoshikawa, *J. Organomet. Chem.* **1982**, *231*, 79-90.

[2] T. Ohkuma, M. Kitamura and R. Noyori, *Tetrahedron Lett.* **1990**, *31*, 5509-5512.

[3] T. Saito, T. Yokozawa, T. Ishizaki, T. Moroi, N. Sayo, T. Miura and H. Kumobayashi, *J. Organomet. Chem.***2001**, *343*, 264-267.

[4] T. Benincori, S. Rizzo, T. Pilati, A. Ponti, M. Sada, E. Pagliarini, S. Ratti, C. Giuseppe, L. De Ferra and F. Sannicolo, *Tetrahedron-asymmetry* **2004**, *15*, 2289-2297.

[5] E. V. Starodubtseva, O. V. Turova, M. G. Vinogradov, L. S. Gorshkova and V. A. Ferapontov, *Russ.Chem. Bull.* **2005**, *54*, 2374-2378.

[6] E. V. Starodubtseva, O. V. Turova, M. G. Vinogradov, L. S. Gorshkova, V. A. Ferapontov and M. I. Struchkova, *Tetrahedron* **2008**, *64*, 11713-11717.

[7] H. Mehdi, V. Fábos, R. Tuba, A. Bodor, L. T. Mika and I. T. Horváth, *Top. in Catal.* **2008**, *48*, 49-54.

[8] L. Deng, J. Li, D. Lai, Y. Fu and Q. Guo, *Angew. Chem. Int. Ed.* **2009**, *48*, 6529-6532.

[9] F. M. A. Geilen, B. Engendahl, A. Harwardt, W. Marquardt, J. Klankermayer and W. Leitner, *Angew. Chem. Int. Ed.* **2010**, *49*, 5510-5514.

[10] F. M. A. Geilen, B. Engendahl, M. Holscher, J. Klankermayer and W. Leitner, *J. Am Chem.Soc.* **2011**, *133*, 14349-14358.

[11] M. Chalid, A. Broekhuis and H. Heeres, *J Mol Catal A chem.* **2011**, *341*, 14-21.

[12] W. Li, J. Xie, H. Lin and Q. Zhou, *Green Chem.* **2012**, *14*, 2388-2390.

[13] J. M. Tukacs, D. Király, A. Strádi, G. Novodarszki, Z. Eke, G. Dibó, T. Kégl and L. T. Mika, *Green Chem.* **2012**, *14*.

[14] J. Deng, Y. Wang, T. Pan, Q. Xu, Q. Guo and Y. Fu, *Chemsuschem* **2013**, *6*, 1163-1167.

[15] A. D. Chowdhury, R. Jackstell and M. Beller, *Chemcatchem* **2014**, *6*, 3360-3365.

[16] J. M. Tukacs, M. Novak, G. Dibo and L. T. Mika, *Catal. Sci. Technol.* **2014**, *4*, 2908-2912.

[17] M. Fu, R. Shang, Z. Huang and Y. Fu, *Synlett* **2014**, *25*, 2748-2752.

[18] V. Fabos, L. T. Mika and I. T. Horvath, *Organometallics* **2014**, *33*, 181-187.

[19] A. Phanopoulos, A. J. P. White, N. J. Long and P. W. Miller, *ACS Catal.***2015**, 2500-2512.

[20] C. Ortizcervantes, M. Floresalamo and J. J. Garcia, *ACS Catal.* **2015**, *5*, 1424-1431.

[21] N. Dai, R. Shang, M. Fu and Y. Fu, *Chin. J. Chem.* **2015**, *33*, 405-408.

[22] G. Metzker and A. C. B. Burtoloso, *Chem. commun.* **2015**, *51*, 14199-14202.

[23] B. Y. Tay, C. Wang, P. H. Phua, L. P. Stubbs, H. V. Huynh, *Dalton Trans.* **2016**, *45*, 3558-3563.

[24] S. Wang, H. Huang, V. Dorcet, T. Roisnel, C. Bruneau, C. Fischmeister, *Organometallics* **2017**, *36*, 3152-3162.

[25] S. Wang, H. Huang, V. Dorcet, T. Roisnel, C. Bruneau, C. Fischmeister, *Organometallics* **2017**, *36*, 708-713.

[26] Y. Liu, Z. Sun, C. Huang, T. Tu, *Chem. Asian J.* **2017**, *12*, 355-360.

[27] N. K. Oklu, B. C. E. Makhubela, *Inorg. Chim. Acta* **2018**, *482*, 460-468.

[28] C. Moustania, E. Anagnostopouloua, K. Krommydaa, C. Panopouloua, K. G. Koukoulakisb, E. B. Bakeasb, G. Papadogianakis, *Appl. Catal. B: Environ.* **2018**, *238*, 82-92.

[29] Y. Yi, H. Liu, L. P. Xiao, B. Wang and G. Song, *ChemSusChem* **2018**, *11*, 1474-1478.

[30] C. A. M. R. van Slagmaat, S. M. A. D. Wildeman, *Eur. J. Inorg. Chem.* **2018**, 694-702.

[31] Z. Liu, Z. Yang, P. Wang, X. Yu, Y. Wu, H. Wang and Z. Liu, *ACS Sustainable Chem. Eng.* **2019**, *7*, 18236-18241.

[32] C. A. M. R. van Slagmaat, M. A. F. Delgove, J. Stouten, L. Morick, Y. van der Meer, K. V. Bernaerts, S. M. A. De Wildeman, *Green Chem.* **2020**, *22*, 2443-2458.

[33] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[34] (a) A. D. Becke, *Phys. Rev. A*, **1988**, *38*, 3098; (b) C. Lee, W. Yang, and R. G. Parr, *Phys. Rev. B*, **1988**, *37*, 785.

[35] M. Dolg, U. Wedig, H. Stoll, H. Preuss, *J. Chem. Phys.* **1987**, *86*, 866.

[36] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215.
[37] S. Grimme, J. Anthony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.
[38] A. V. Marenich, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B*. **2009**, *113*, 6378.