

# Chemistry–A European Journal

Supporting Information

## Hydrogenation of CO<sub>2</sub> by a Bifunctional PC(*sp*<sup>3</sup>)P Iridium(III) Pincer Complex Equipped with Tertiary Amine as a Functional Group

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## 1. General Considerations.

All reactions were performed in Schlenk and Glovebox techniques under dry N<sub>2</sub> or Ar. All reagents used were purchased from the usual suppliers without further purifications. All reagents were weighed and handled under air. All catalytic reactions were carried out after purging the vessels from air; all solvents used were technical grade. Yields refer to isolated compounds with 95% or greater purity according to <sup>1</sup>H-NMR spectroscopy. <sup>1</sup>H-, <sup>13</sup>C-, <sup>31</sup>P-NMR spectra were recorded using Bruker 400 or 500 MHz instruments with chemical shifts reported in ppm relative to the residual deuterated solvent or the internal TMS standard. HRMS was recorded on a Bruker Maxis Impact QTOF with APCI solid probe by the MS department in the Faculty of Chemistry at Technion Institute of Technology, Haifa.

## 2. Synthetic methods.

### 2.1. 1,8-bis(diphenylphosphine)dibromoanthracene.

1,8-bis(diphenylphosphine)anthracene was prepared according to a previously published procedure. [20a]

### 2.2. (E)-1,4-di(piperidine-1-yl)but-2-ene-1,4-dione:

Piperidine (0.075 mol) was added to DCM (15 ml) and cooled down to  $-5^{\circ}\text{C}$  in a salt-ice bath. After 10 min, fumaryl chloride (0.0185 mol) was added dropwise in 10 min and left to heat to RT and stir overnight. The product was extracted using DCM and water. The organic phase was dried over  $\text{Na}_2\text{SO}_4$ . The drying agent was filtered, and the solvent was evaporated, receiving crude product. Recrystallization from hexane produced white product with 75% yield.  $^1\text{H}$ NMR ( $\text{CDCl}_3$ ),  $\delta$  (ppm): 1.52 (m, 8H), 1.6 (m, 4H), 3.48 (t, 4H,  $J = 5.2$  Hz), 3.57 (t, 4H,  $J = 5.2$  Hz), 7.33 (s, 2H).  $^{13}\text{C}$ NMR ( $\text{CDCl}_3$ ),  $\delta$  (ppm): 24.5, 25.5, 26.7, 43.3, 47.1, 131.2, 163.9.

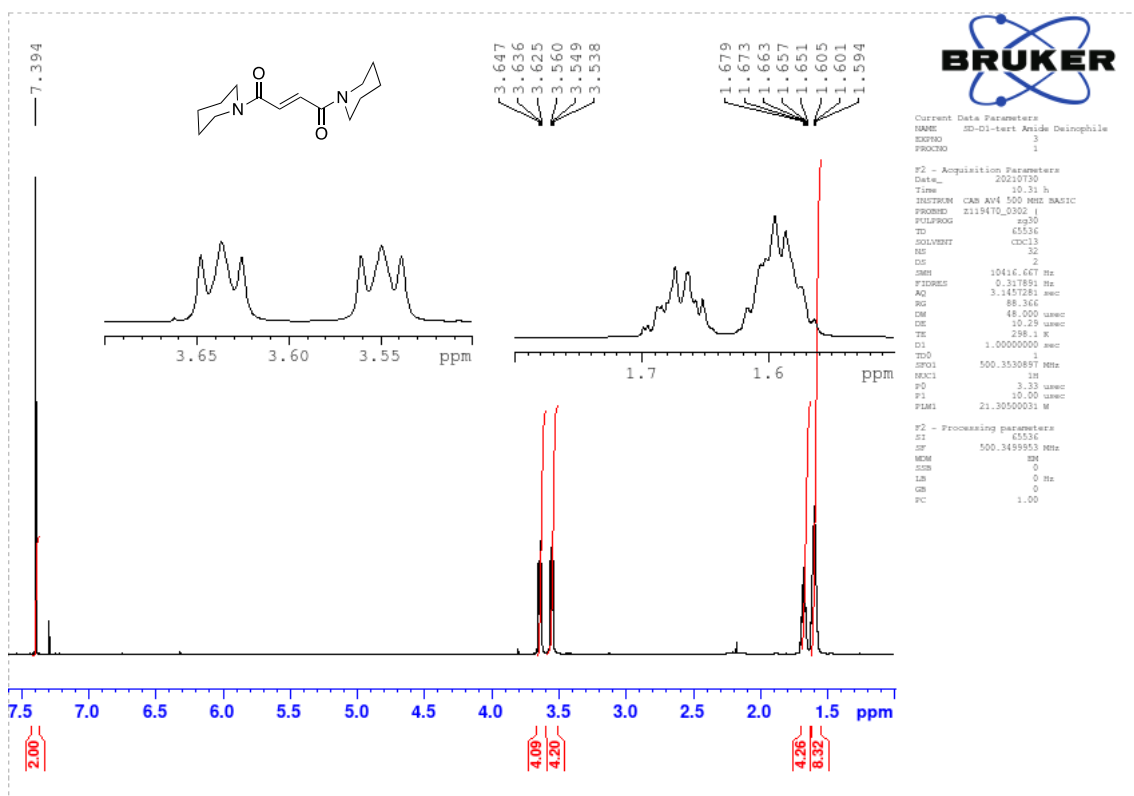
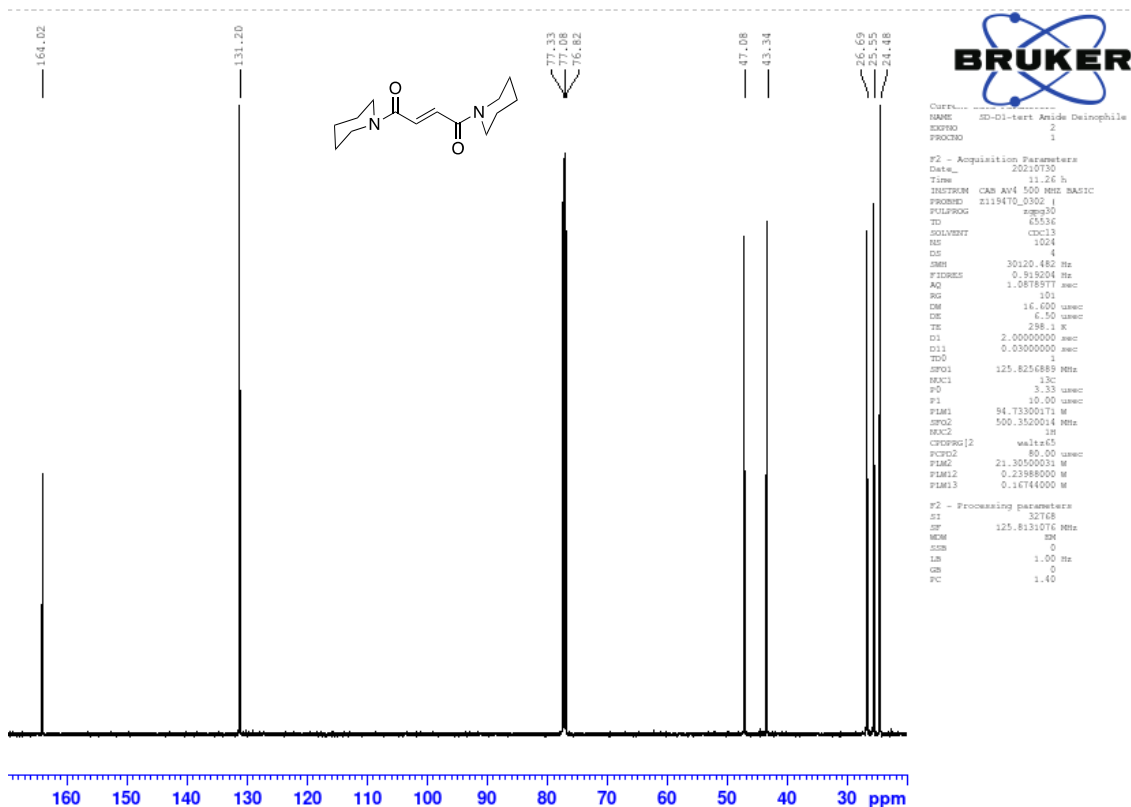


Figure S1:  $^1\text{H}$ NMR of (E)-1,4-di(piperidine-1-yl)but-2-ene-1,4-dione.



**Figure S2:**  $^{13}\text{C}$ NMR of (E)-1,4-di(piperidine-1-yl)but-2-ene-1,4-dione.

### 2.3. Compound 3:

1,8-bis(diphenylphosphine)anthracene and 6 eq. of (E)-1,4-di(piperidin-1-yl)but-2-ene-1,4-dione (**1**) were refluxed in dry Xylene (minimal amount) for 48h. The precipitated product was filtered and recrystallized from methanol as an off-white powder with 66% yield.  $^1\text{H}$ NMR ( $\text{CDCl}_3$ ),  $\delta$  (ppm): 1.02-1.07 (m, 1H), 1.11-1.15 (m, 2H), 1.25 (s, 1H), 1.34-1.4 (m, 2H), 1.47-1.54 (m, 2H), 1.66-1.72 (m, 2H), 2.87-2.91 (m, 1H), 2.95-3.00 (m, 1H), 3.21-3.27 (m, 2H), 3.58-3.62 (m, 3H), 3.74-3.76 (m, 1H), 4.02 (dd, 1H,  $J_1 = 4.95$  Hz,  $J_2 = 2.17$  Hz), 4.37 (s, 1H), 6.49 (dt, 1H,  $J_{1(\text{H-P})} = 5.6$  Hz,  $J_2 = 2.1$  Hz), 6.62 (ddd, 1H,  $J_1 = 7.76$  Hz,  $J_2 = 3.85$  Hz,  $J_3 = 1.11$  Hz), 6.92 (ddd, 1H,  $J_1 = 7.78$  Hz,  $J_2 = 3.65$  Hz,  $J_3 = 1.11$  Hz), 6.96-7.07 (m, 4H), 7.12-7.15 (m, 2H), 7.19-7.31 (m, 17H), 7.35-7.43 (m, 4H).  $^{31}\text{P}$ NMR ( $\text{CDCl}_3$ ),  $\delta$  (ppm): -19.97 (d, 1P,  $J = 14$  Hz), -21.15 (d, 1P,  $J = 14$  Hz).

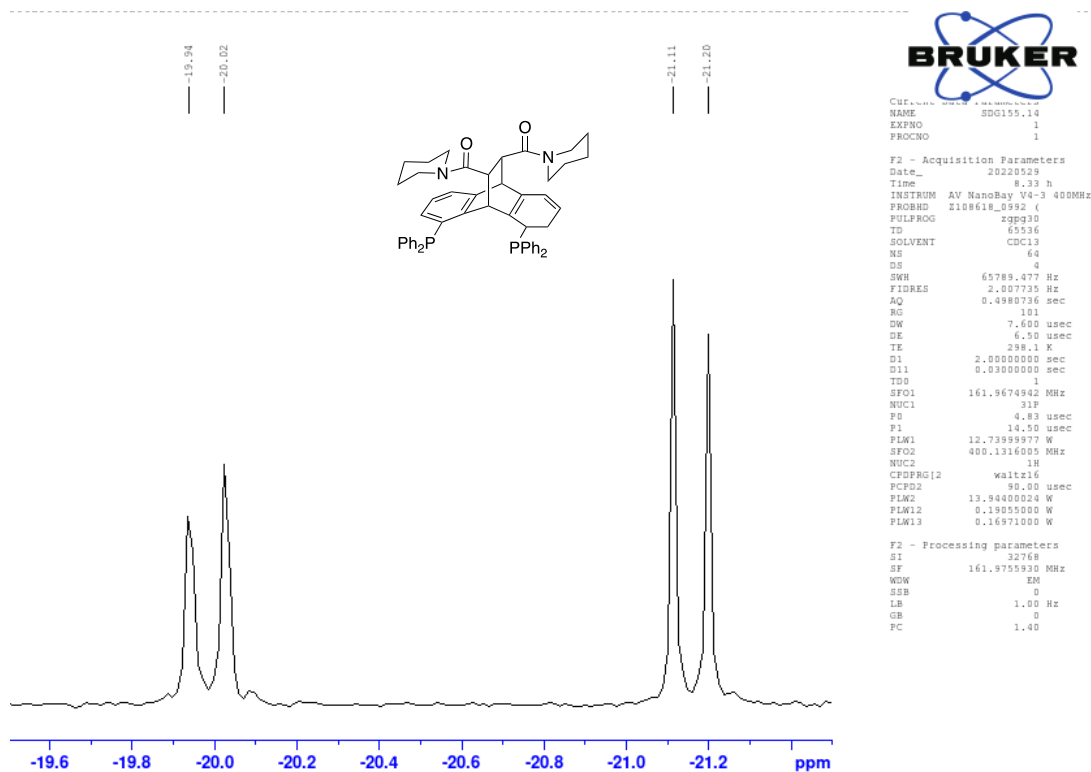


Figure S3:  $^{31}\text{P}$ NMR of ligand precursor 3.

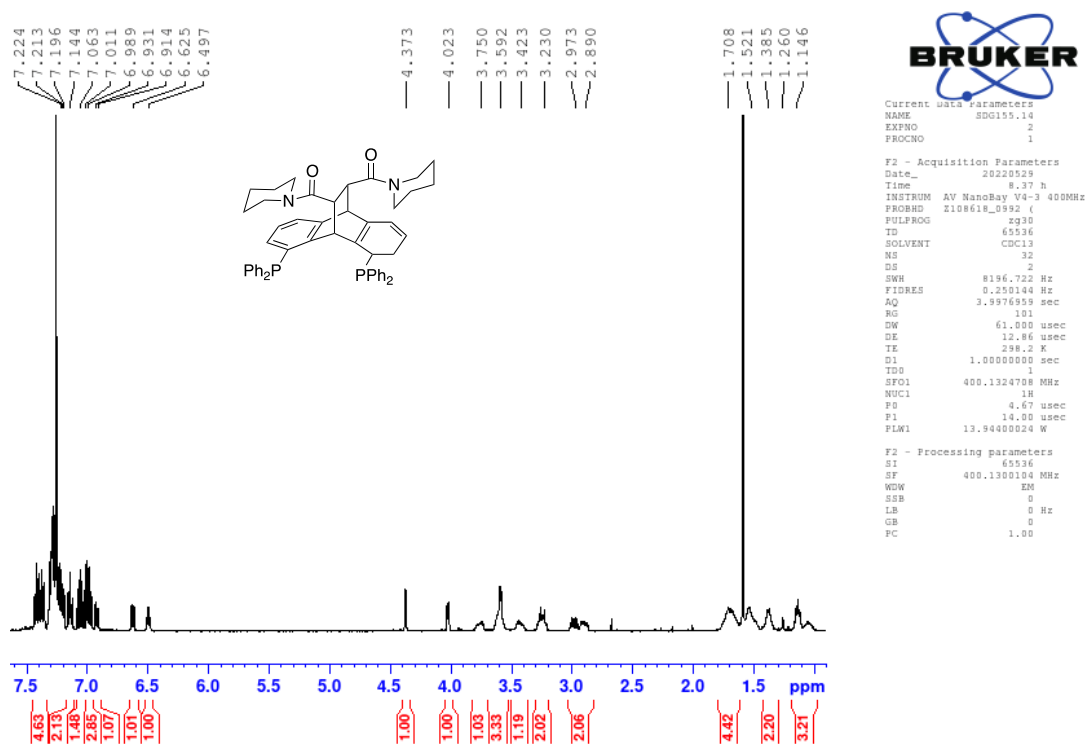


Figure S4:  $^1\text{H}$ NMR of ligand precursor 3.

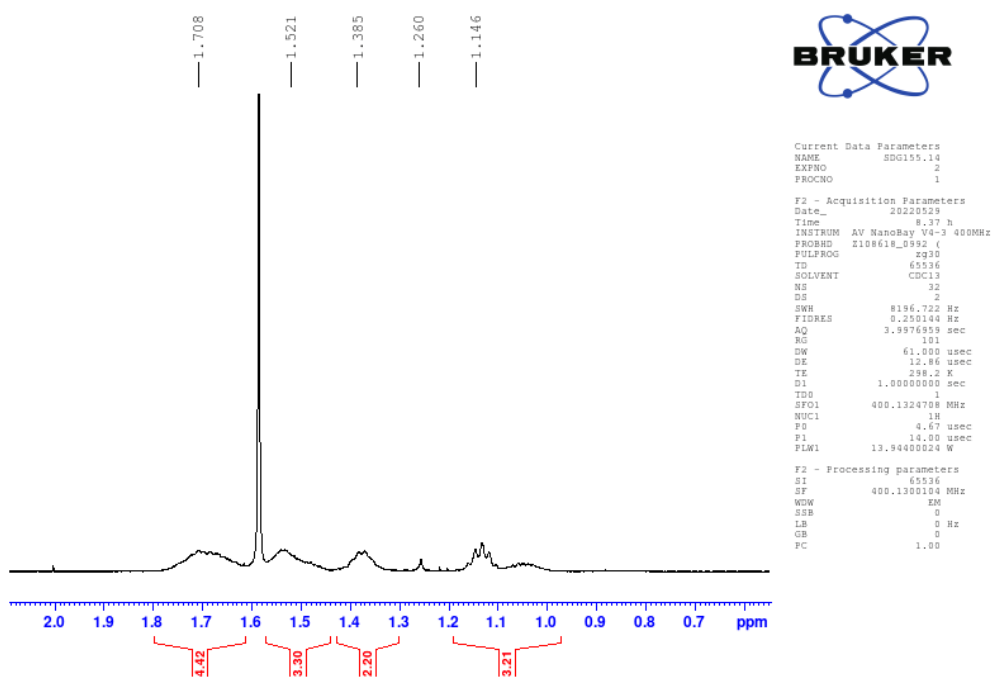


Figure S5: <sup>1</sup>H NMR of ligand precursor **3** – 1-1.8 ppm .

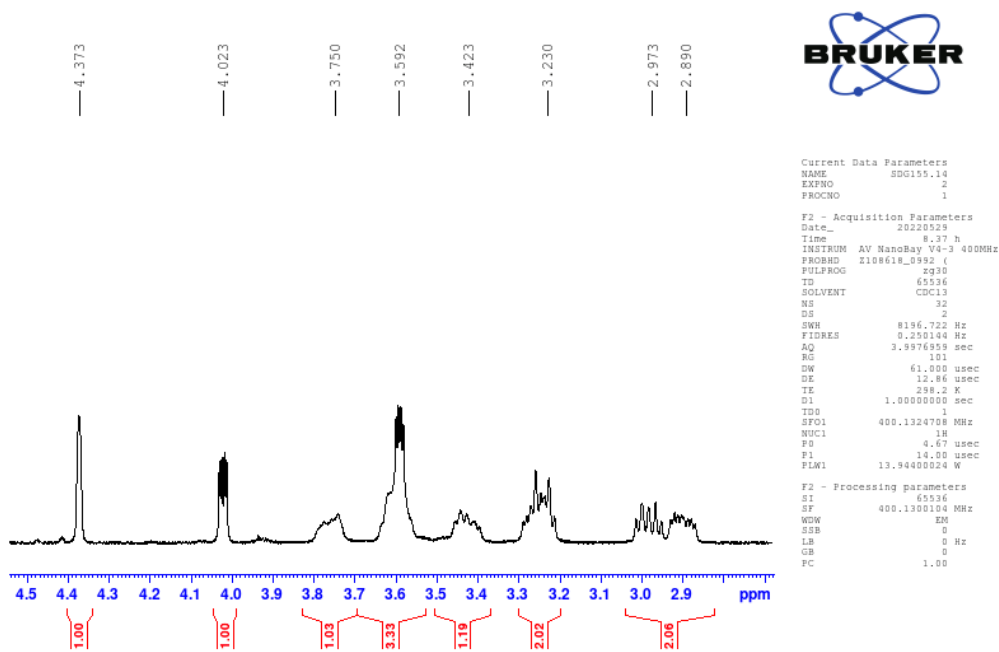
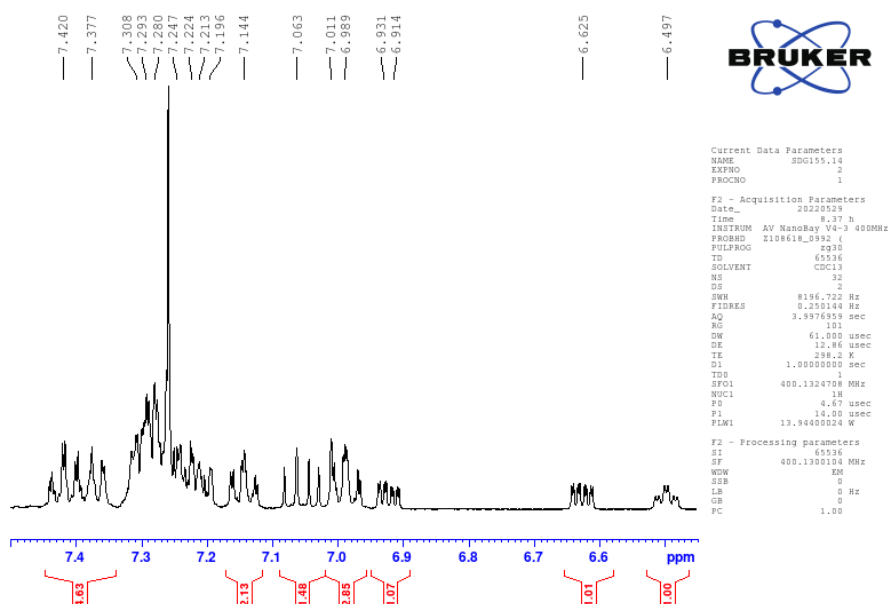


Figure S6: <sup>1</sup>H NMR of ligand precursor **3** – 2.8-4.4 ppm.



**Figure S7:**  $^1\text{H}$ NMR of ligand precursor **3** – 6.5-7.5ppm.

#### 2.4. Compound 4:

Dry THF was charged with precursor **2** and 6 eq. of  $\text{LiAlH}_4$  were added slowly and portion wise to the slurry and stirred for 48h at RT. The slurry was neutralized by a slow addition of a minimal amount water and the crude product was extracted with DCM three times. The organic phases were collected, dried over  $\text{Na}_2\text{SO}_4$ . The drying agent was filtered out and the solvent was evaporated to afford a white/pink sticky compound. The product was obtained with recrystallization from acetone as a white powder at 77% yield.  $^1\text{H}$ NMR ( $\text{CDCl}_3$ ),  $\delta$  (ppm): 1.01 (bs, 1H), 1.27 (m, 7H), 1.4 (m, 3H), 1.54-1.87 (m, 16H), 2.16 (s, 2H), 2.41 (s, 2H), 4.4 (s, 1H), 5.8 (dt, 1H,  $J_{1(\text{H-P})} = 4.7$  Hz,  $J_2 = 1.8$  Hz), 6.6 (ddd, 1H,  $J_1 = 7.7$  Hz,  $J_2 = 3.7$  Hz,  $J_3 = 1$  Hz), 6.81 (ddd, 1H,  $J_1 = 7.7$  Hz,  $J_2 = 3.7$  Hz,  $J_3 = 1$  Hz), 6.96 (t, 1H,  $J = 7.5$  Hz), 7 (t, 1H, 7.5 Hz), 7.07 (dt, 2H,  $J_1 = 7.6$  Hz,  $J_2 = 1.35$  Hz), 7.13 (dt, 2H,  $J_1 = 7.7$  Hz,  $J_2 = 1.4$  Hz), 7.18 (dt, 2H,  $J_1 = 7.6$  Hz,  $J_2 = 1.4$  Hz), 7.22-7.31 (m, 17H).  $^{31}\text{P}$ NMR ( $\text{CDCl}_3$ ),  $\delta$  (ppm): -17.72 (d, 1P,  $J = 16$  Hz) -19.86 (d, 1P,  $J = 16$  Hz). Calcd.  $m/z = 769.3762$  (monoprotonated) Found:  $m/z = 769.3835$  (monoprotonated).



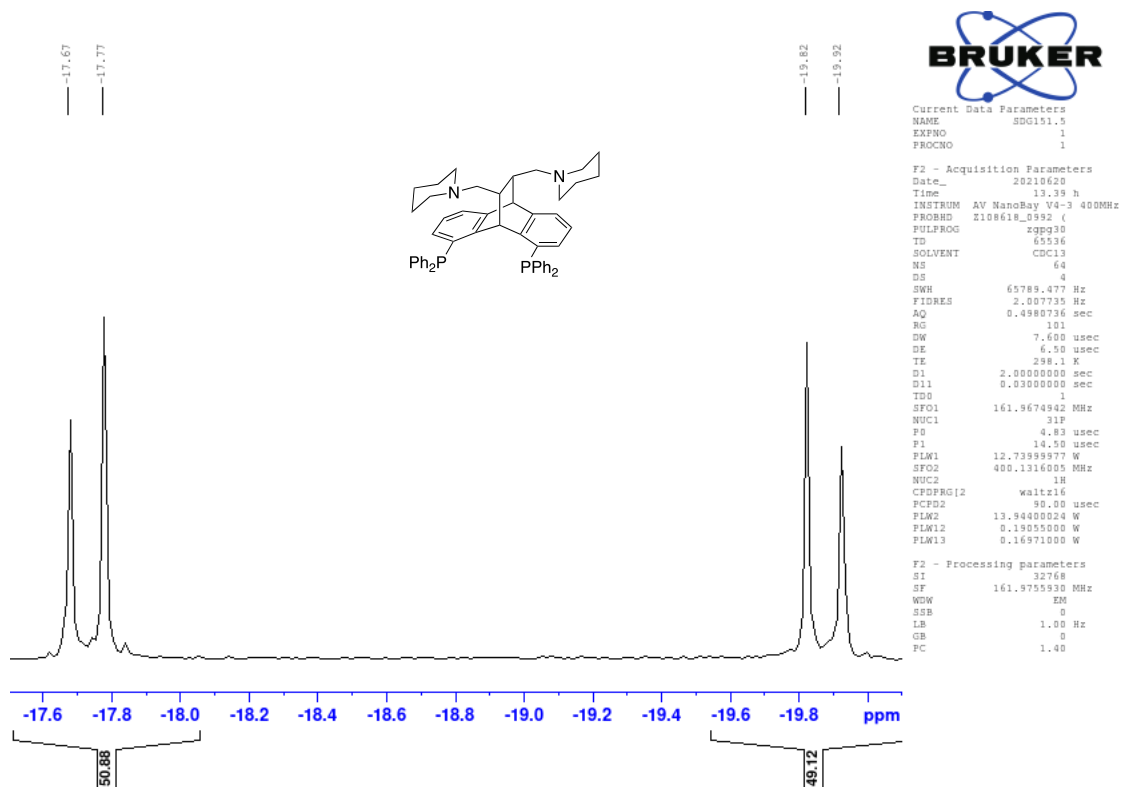


Figure S8: <sup>31</sup>P NMR of ligand 4.

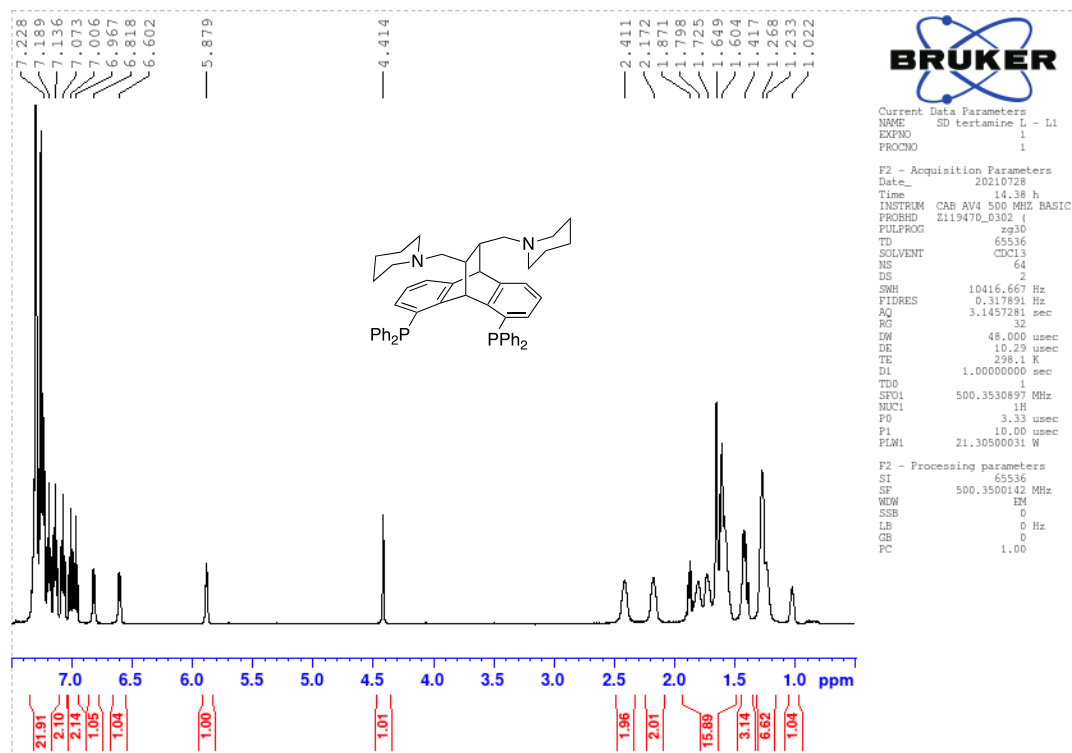


Figure S9: <sup>1</sup>H NMR of ligand 4.

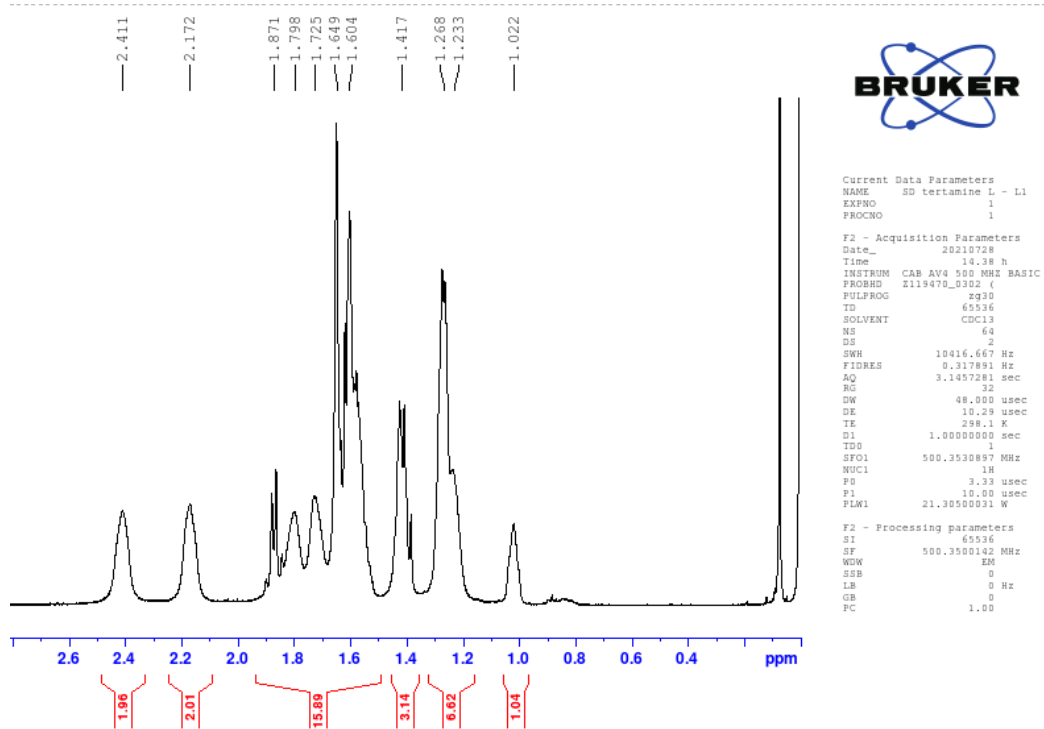


Figure S10:  $^1\text{H}$ NMR of ligand 4 – 0.8-2.6ppm.

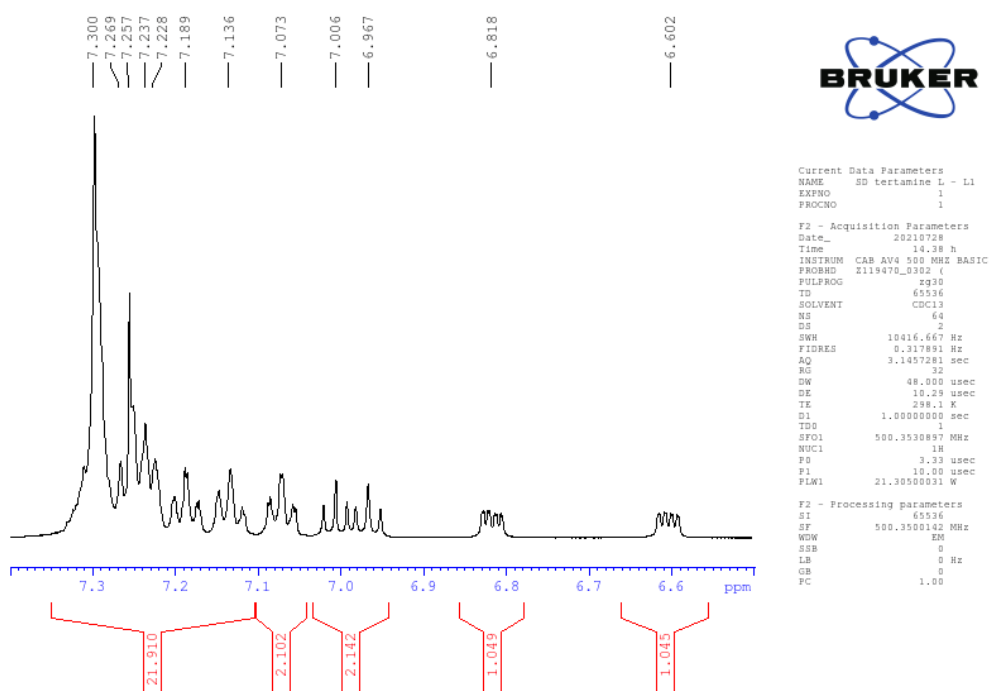
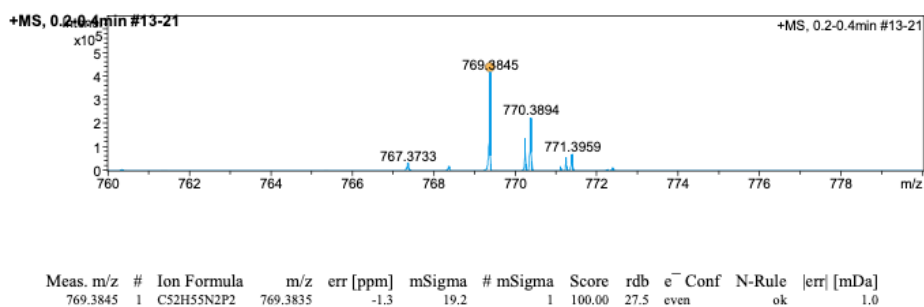


Figure S11:  $^1\text{H}$ NMR of ligand 4 – 6.6-7.3ppm.

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Acquisition Parameter			
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		Set Nebulizer	1.2 Bar
		Set Dry Heater	120 °C
		Set Dry Gas	1.5 l/min
		Set Divert Valve	Source
		Set APCI Heater	250 °C



**Figure S12:** HR-MS of ligand 4.

## 2.5. Complex 2.

The complex was synthesized according to an adapted procedure. [17a] Di tert-Amine ligand (3) (0.903 mmol) and 0.5 eq of  $[\text{IrCl}(\text{COE})_2]_2$  (0.451 mmol) were stirred in 1:1 mixture of IPA/ACN at RT for 8h. The solvents were evaporated, and the desired product was recrystallized from minimal amounts of cold methanol and diethyl ether.  $^1\text{H}$ NMR (THF- $d_8$ ),  $\delta$  (ppm): -9.87 (dd, 1H,  $J_1(\text{H-P}) = 32.8$  Hz,  $J_2(\text{H-P}) = 152$  Hz), 0.95-1.02 (m, 1H), 1.18-1.54 (m, 12H), 1.83-1.97 (m, 3H), 2.18-2.26 (m, 5H), 2.37 (s, 1H), 2.86-2.88 (m, 2H), 3.33-3.36 (m, 1H), 4.02 (t, 1H,  $J = 13.3$  Hz), 4.28 (s, 1H), 6.11 (dd, 2H,  $J_1 = 7.7$  Hz,  $J_2 = 11$  Hz), 6.31 (dt, 2H,  $J_1 = 2.3$  Hz,  $J_2 = 7.7$  Hz), 6.54-6.61 (m, 3H), 6.72 (tq, 1H,  $J_1 = 1.3$  Hz,  $J_2 = 7.5$  Hz), 6.87 (dt, 1H,  $J_1 = 3$  Hz,  $J_2 = 7.5$  Hz), 6.97 (dt, 1H,  $J_1 = 0.8$  Hz,  $J_2 = 7.5$  Hz), 7.03-7.13 (m, 4H), 7.16 (dt, 1H,  $J_1 = 1.7$  Hz,  $J_2 = 7.5$  Hz), 7.21-7.24 (m, 4H), 7.41-7.49 (m, 3H), 7.75 (bs, 2H), 8.19-8.25 (m, 2H).  $^{31}\text{P}$ NMR (THF- $d_8$ ),  $\delta$  (ppm): 3.8 (1P) 14.34 (1P).  $^{31}\text{P}$ NMR ( $\text{C}_2\text{D}_2\text{Cl}_4$ ) decoupled from aromatics,  $\delta$  (ppm): 4.76 (d, 1P,  $J = 70$  Hz) 14.94 (d 1P,  $J = 365$  Hz). Calcd for  $[\text{M}+\text{H}]^+$  996.3080, found 996.3061.

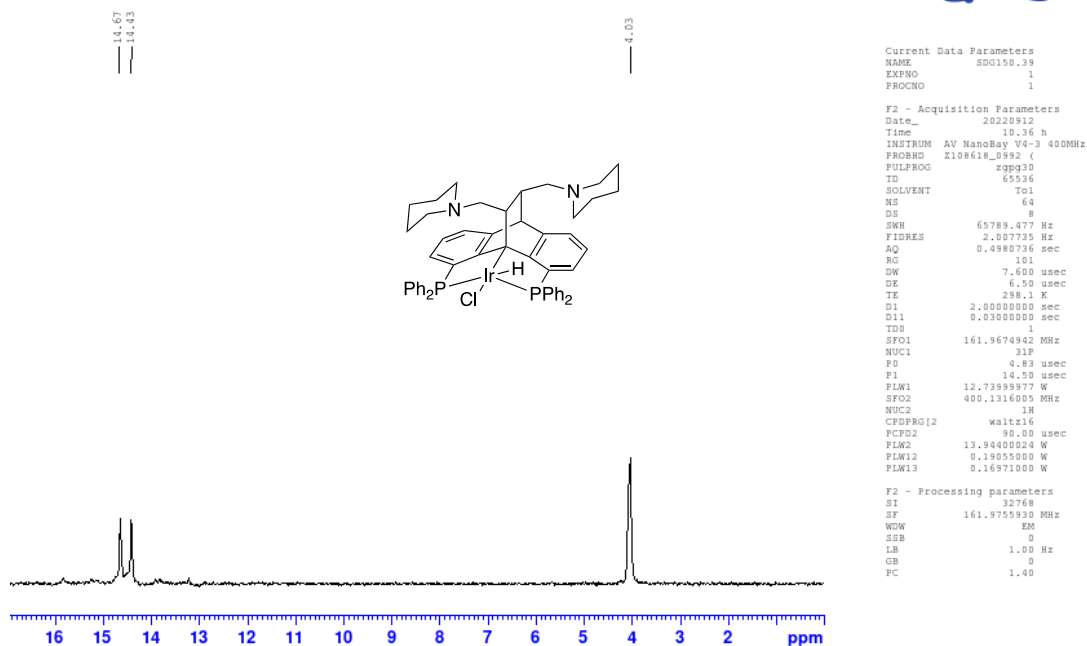


Figure S13:  $^{31}\text{P}$ NMR of iridium complex 2.

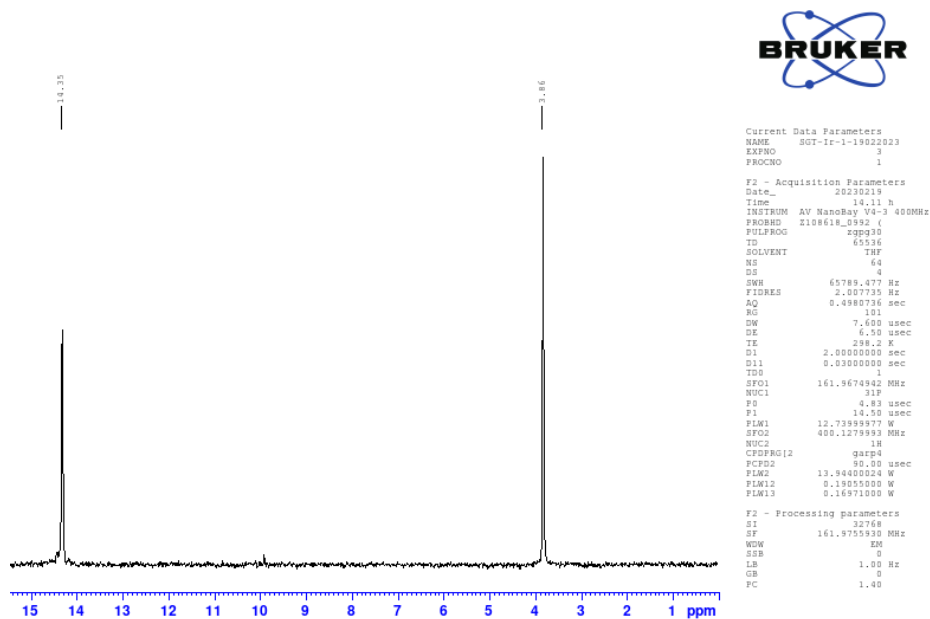
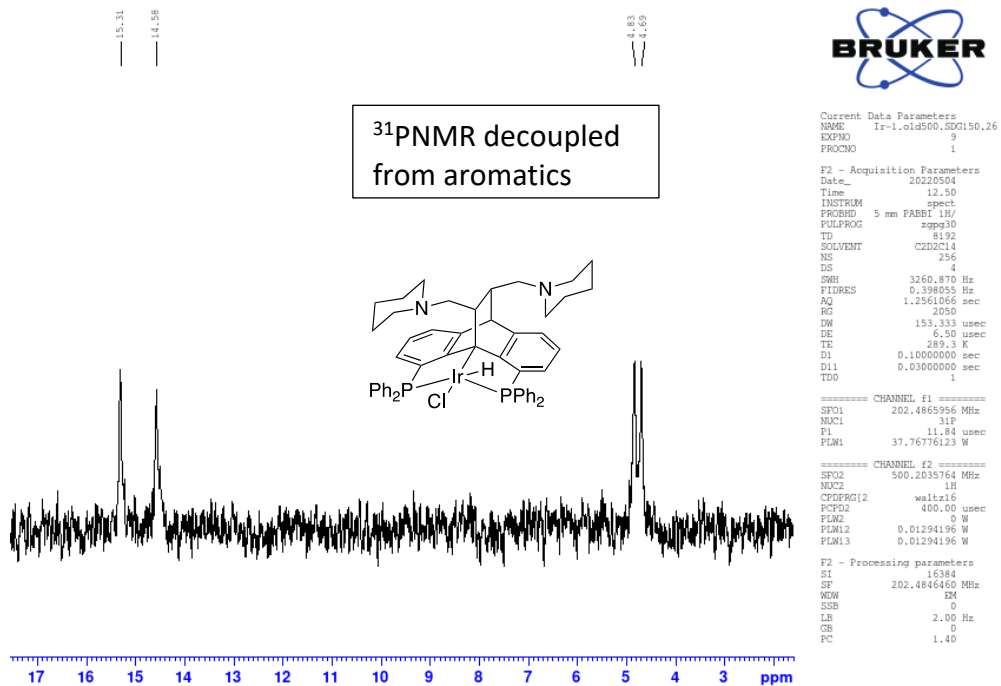
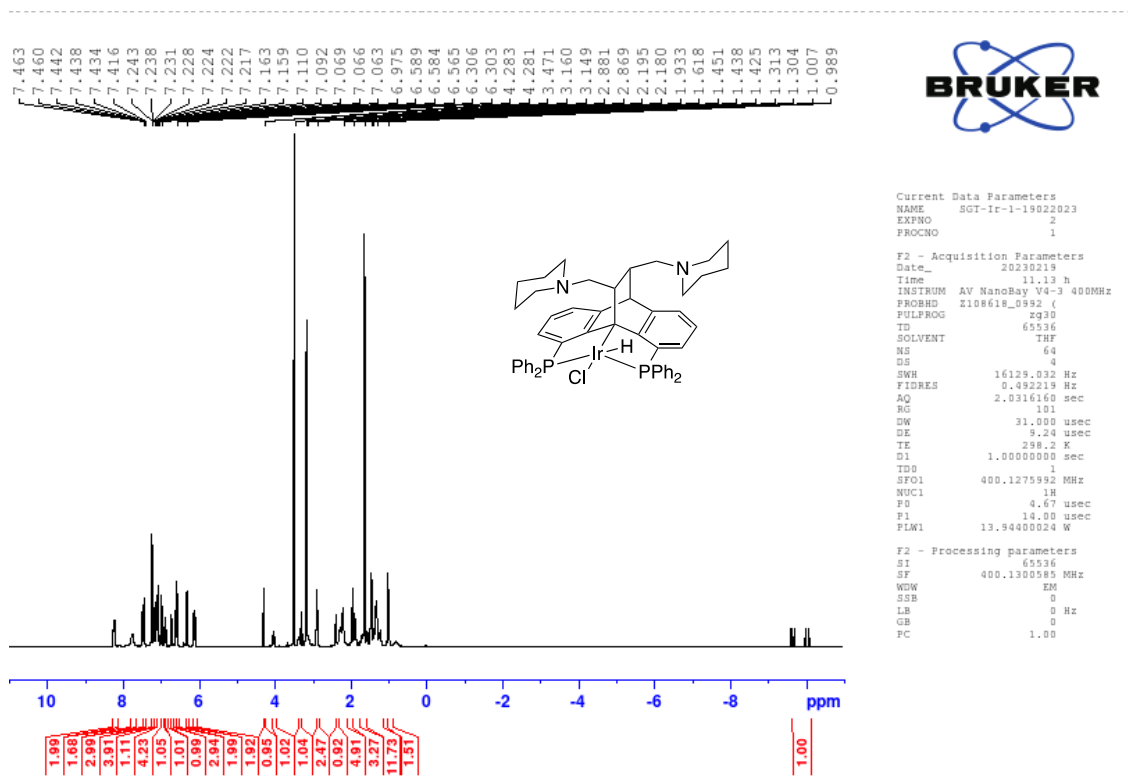


Figure S13:  $^{31}\text{P}$ NMR of complex 2 decoupled from hydrides.



**Figure S14:**  $^{31}\text{P}$ NMR of iridium complex **2** decoupled from aromatic protons.



**Figure S15:**  $^1\text{H}$ NMR of iridium complex **2**.

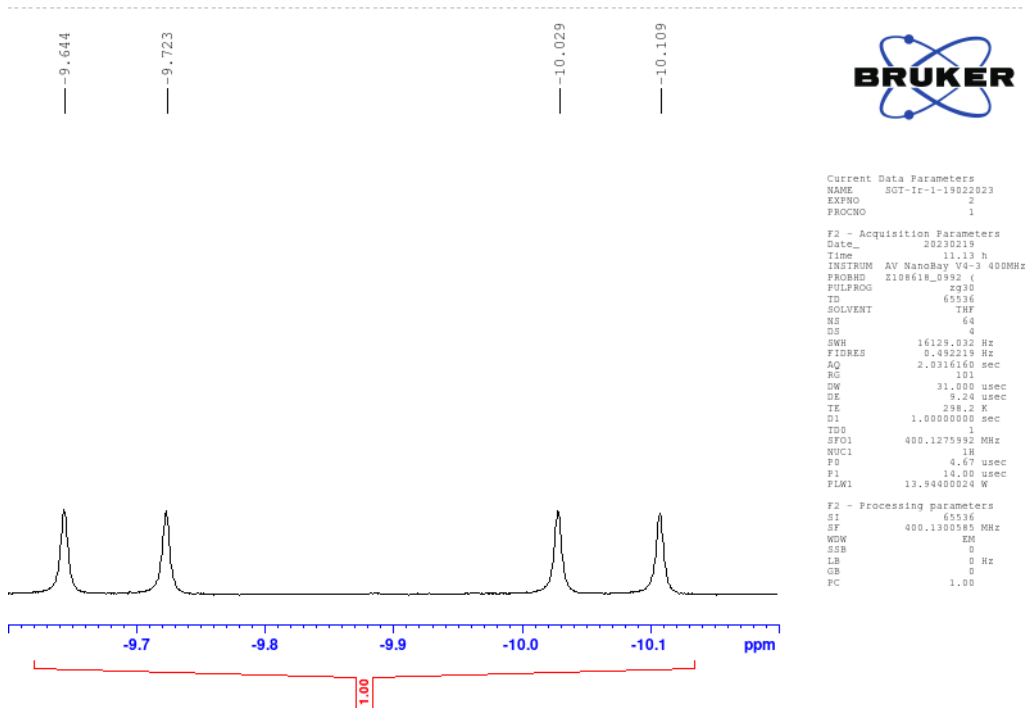


Figure S16: Hydride peak of complex 2.

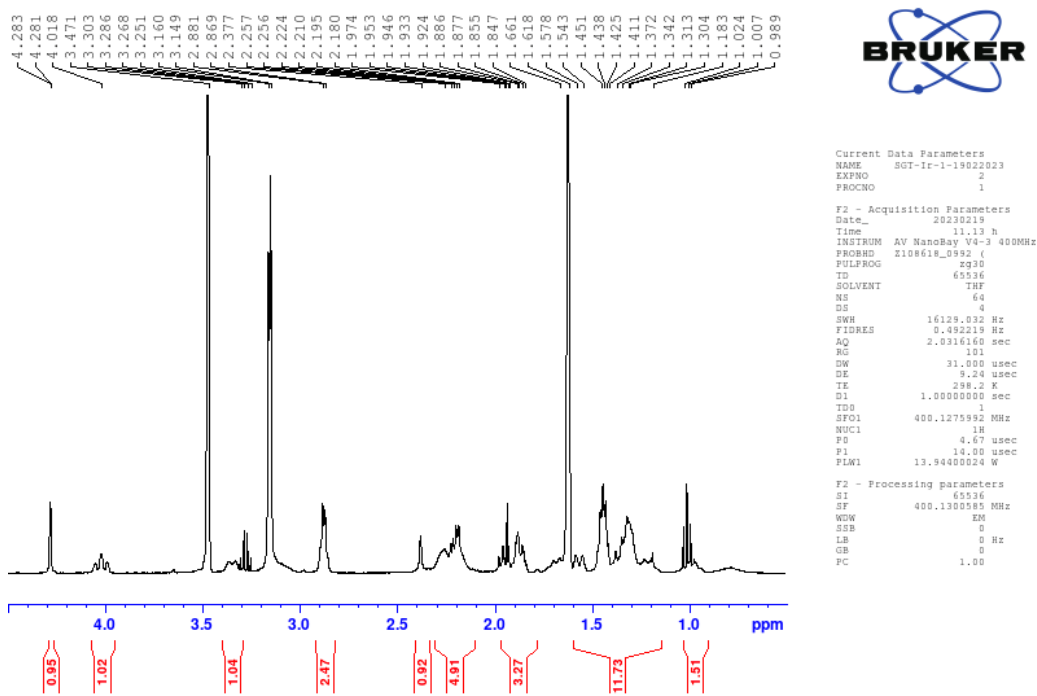
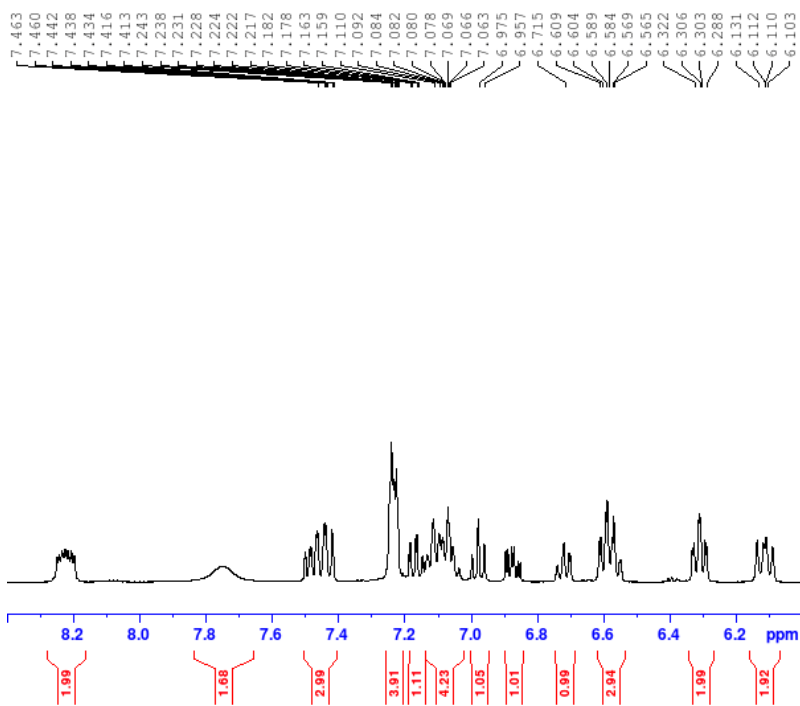


Figure S17: Aliphatic region of complex 2.



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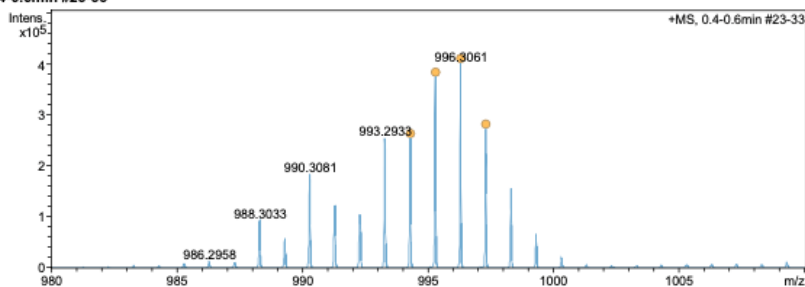
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Figure S18: Aromatic region of complex 2.

### Compound Spectrum SmartFormula Report

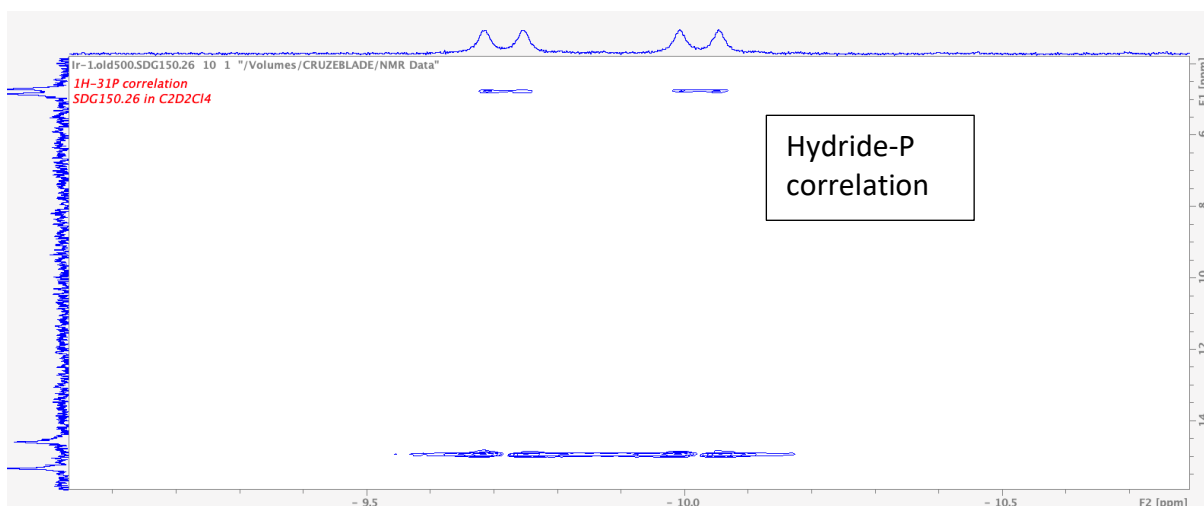
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Comment					
Acquisition Parameter					
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•MS, 0.4-0.6min #23-33

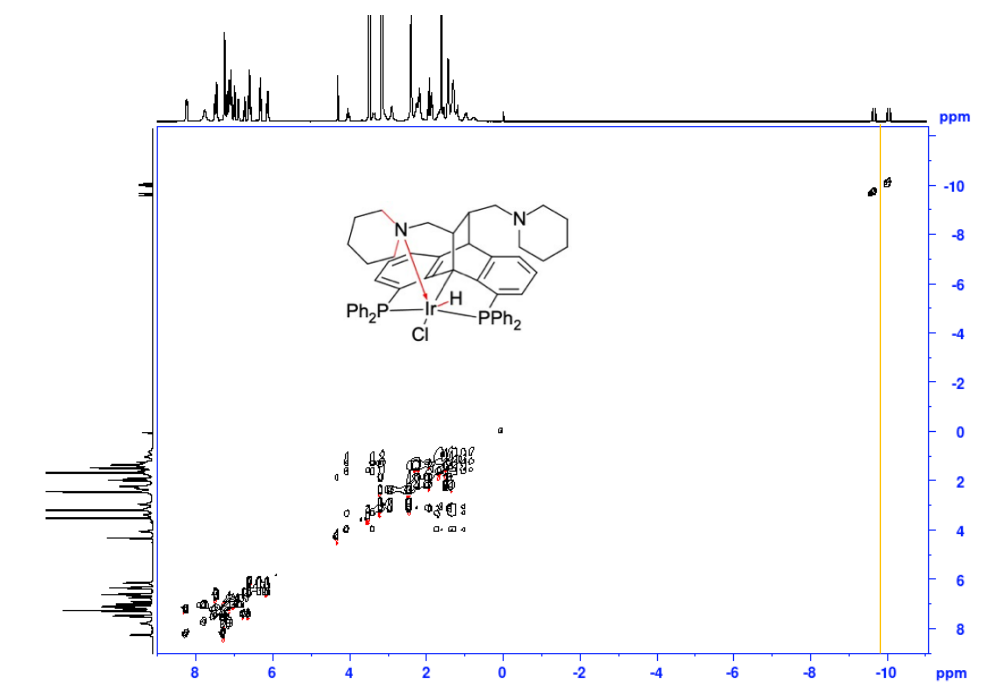


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	err  [mDa]
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	1	CS2H52ClIrN2P2	994.2929	-6.7	413.1	1	100.00	29.0	odd	ok	6.7
995.3012	1	CS2H53ClIrN2P2	995.3007	-0.9	270.7	1	100.00	28.5	even	ok	0.9
	1	CS2H53ClIrN2P2	995.3007	-0.9	270.7	1	100.00	28.5	even	ok	0.9
996.3061	1	CS2H53ClIrN2P2	995.3002	-3.4	270.7	1	100.00	28.5	even	ok	3.3
	2	CS2H55ClIrN2P2	997.3158	10.7	369.9	2	0.00	27.5	even	ok	10.7
	1	CS2H54ClIrN2P2	996.3086	2.0	264.6	1	100.00	28.0	odd	ok	2.0
	1	CS2H53ClIrN2P2	995.3002	-3.4	270.7	1	100.00	28.5	even	ok	3.3
	2	CS2H55ClIrN2P2	997.3158	10.7	369.9	2	0.00	27.5	even	ok	10.7
997.3085	1	CS2H55ClIrN2P2	997.3164	7.4	369.9	1	100.00	27.5	even	ok	7.4
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Figure S19: HRMS of iridium complex 2.

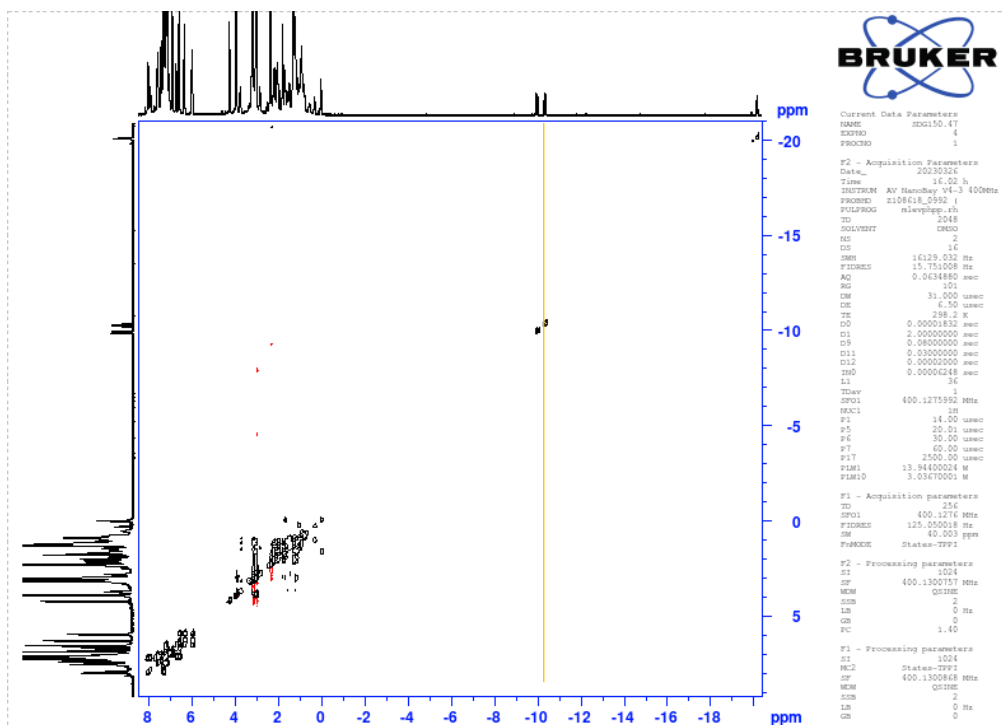


**Figure S20** P-Hydride correlation 2D NMR in iridium complex **2**.

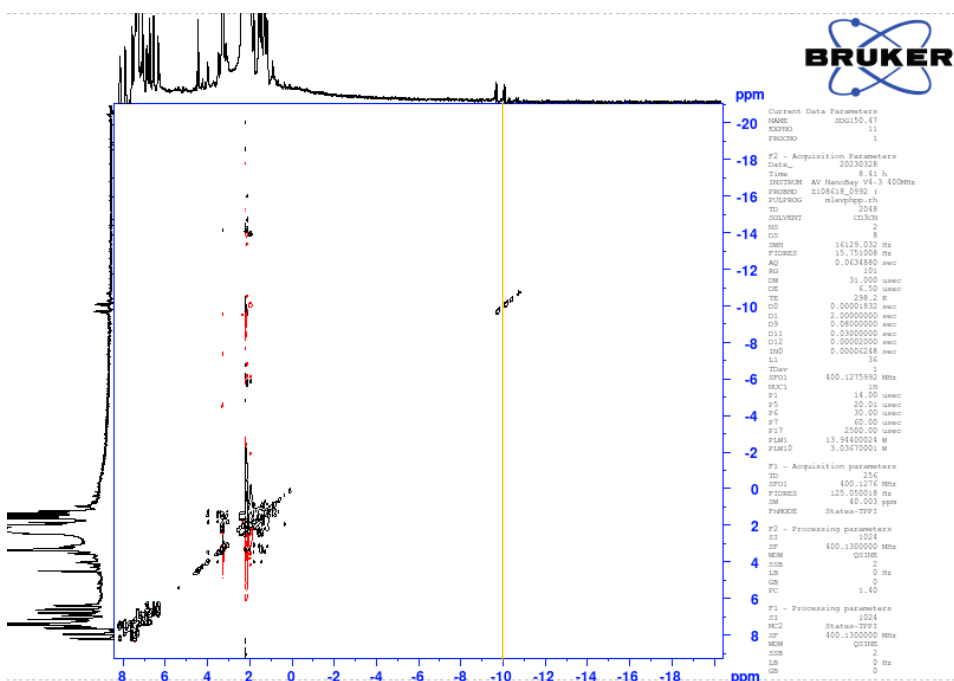


**Figure S21:** TOCSY of complex **2** in THF<sub>d8</sub>, no correlation between the hydride and aliphatic region of the complex.

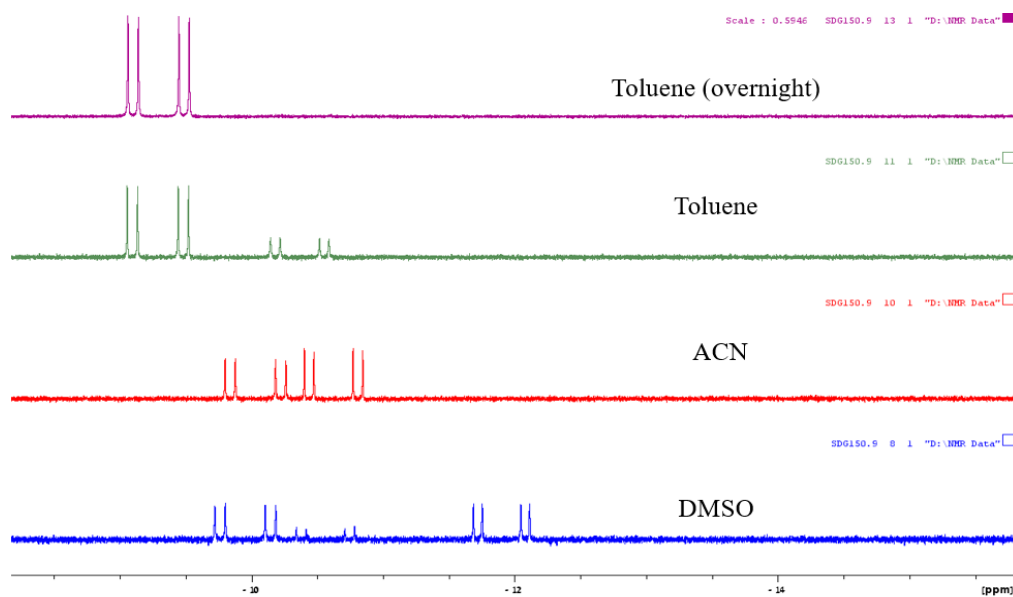




**Figure S22:** TOCSY of complex **2** in  $\text{DMSO-d}_6$ , no correlation between the hydride and aliphatic region of the complex. Formation of isomers is notable as DMSO is a coordinative solvent.

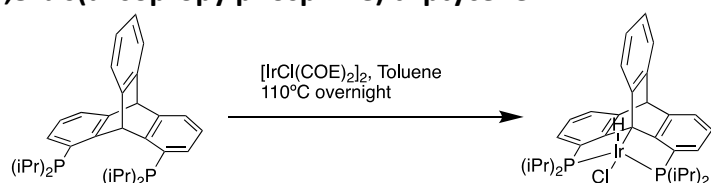


**Figure S23:** TOCSY of complex **2** in  $\text{MeCN-d}_3$ , no correlation between the hydride and aliphatic region of the complex. Formation of isomers is notable as MeCN is a coordinative solvent. Complex **2** is barely soluble in MeCN at RT.



**Figure S24:** Isomerization of complex **2** - hydride region of measured in coordinating solvents (DMSO and MeCN) and non-coordinative toluene.

## 2.6. 1,8-bis(diisopropylphosphine) triptycene

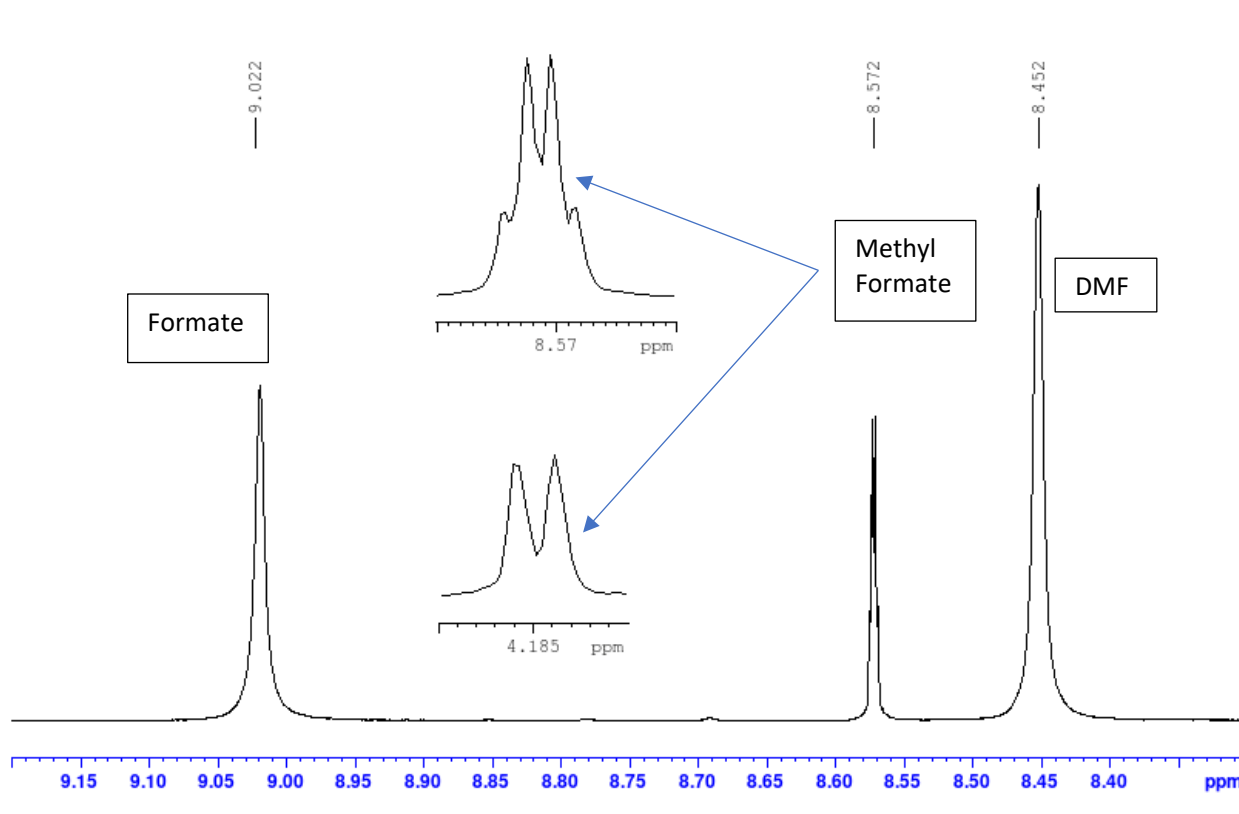


First 1,8-bis(diisopropylphosphine) triptycene was prepared according to previously published procedure. [39a] Complex **5** was prepared according to a previously published procedure. [39b]

### 3. Catalytic Hydrogenation Methods

#### 3.1. Hydrogenation of CO<sub>2</sub>

At catalyst load 0.001mol% DBU (1.886 mmol) and **2** ( $1.886 \times 10^{-5}$  mmol) at a ratio of 100000/1 respectively were charged in a parr bomb apparatus. The apparatus was pressured with CO<sub>2</sub> and H<sub>2</sub>. The parr bomb was set at the relevant temperature. At the end of the reaction, the parr bomb was cooled, the pressure was released, and the conversion was measured via NMR with DMF as standard (0.1 ml). <sup>1</sup>HNMR of formate (DMSO-d<sub>6</sub>),  $\delta$  (ppm): 9.022 (s, 1H). <sup>1</sup>HNMR of methyl formate (DMSO-d<sub>6</sub>),  $\delta$  (ppm): 8.572 (q<sup>4</sup>, 1H,  $J = 0.8$  Hz), 4.182 ppm (d, 3H,  $J = 0.8$  Hz).



**Figure S25:** <sup>1</sup>HNMR of formate anion, methyl formate and DMF in DMSO<sub>d6</sub> after hydrogenation of CO<sub>2</sub> by complex **2**.

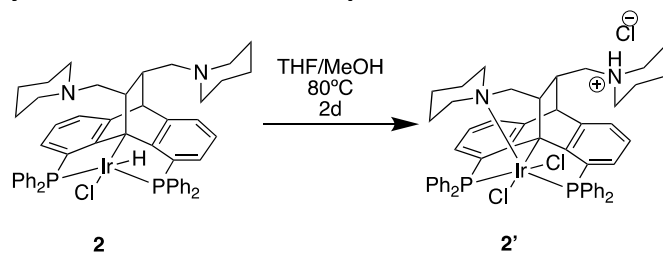
**Table S1:** Result summary of CO<sub>2</sub> hydrogenation.

Entry	Cat. (mol%)	Load	Time (h)	Temp. (°C)	P (CO <sub>2</sub> :H <sub>2</sub> bar)	Solv.	Base	Conv. (%) <sup>[a]</sup>	TON <sup>[c]</sup>
1	0.2		24	130	10:30	THF	DBU	19.5	97
2	0.2		24	130	10:30	THF	DBN	5	25
3	0.2		24	130	10:30	THF	NEt <sub>3</sub>	0	0
4	0.2		24	130	10:30	THF	iPr <sub>2</sub> NEt	0	0
5	0.2		24	130	10:30	MeCN	DBU	114.8	573
6	0.2		24	130	10:30	Tol	DBU	0	0
7	0.2		24	130	10:30	EtOH	DBU	54.8	275
8	0.2		24	130	10:30	MeOH	DBU	95.5	478
9	0.2		24	130	20:30	MeOH	DBU	94.5	468
10	0.02		1	130	10:30	MeOH	DBU	90.4	4551
11	0.02		1	90	20:30	MeOH	DBU	76	3780
12	0.02		1	110	20:30	MeOH	DBU	93	4633
13	0.02		1	130	20:30	MeOH	DBU	94	4681
14	0.02		1	110	10:40	MeOH	DBU	62.7	3138
15	0.02		1	110	15:35	MeOH	DBU	86.2	4315
16	0.02		1	110	20:30	MeOH	DBU	128.1	6222
17	0.02		1	110	25:25	MeOH	DBU	89.9	4504
18	0.02		1	110	30:20	MeOH	DBU	50.6	2535
19	0.001		72	110	20:30	MeCN	DBU	12.8	12827
20	0.001		72	130	20:30	MeCN	DBU	62	62080
21	0.001		72	110	10:40	MeOH	DBU	56.3	56201
22	0.001		72	110	20:30	MeOH	DBU	60.4	60499
23 <sup>[d]</sup>	0.02		1	110	20:30	MeOH	DBU	41.4%	2072

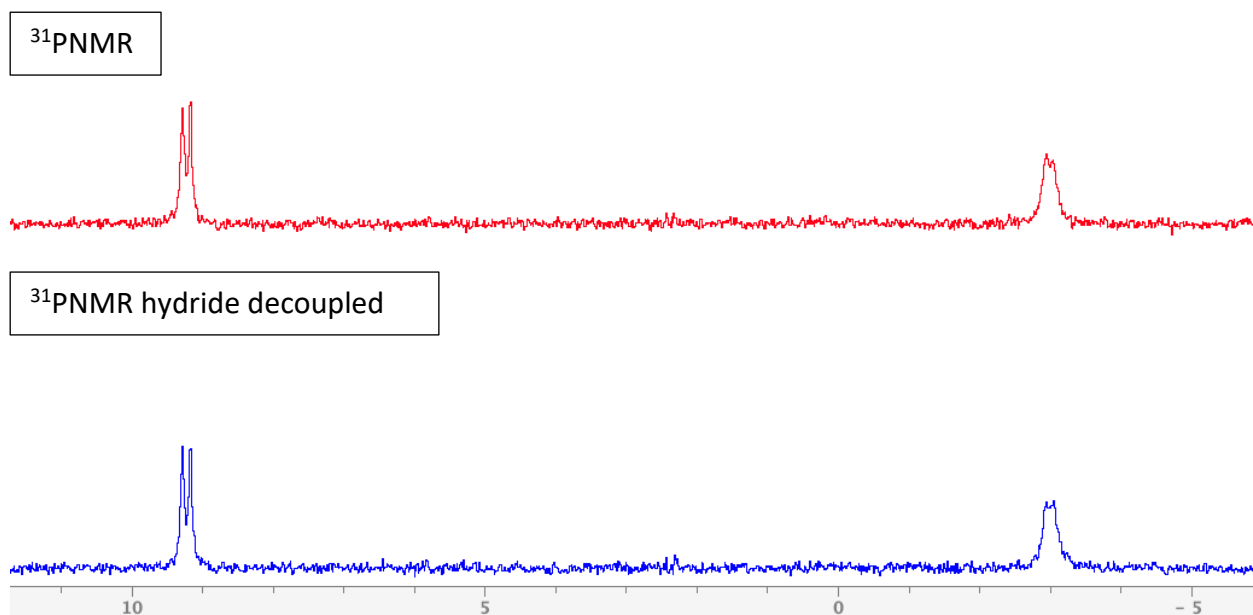
[a] **5** used as a catalyst [b] Conversion was calculated via NMR analysis with DMF as a standard. [c] Turnover number is calculated as  $\frac{\text{mol}(\text{substrate})}{\text{mol}(\text{catalysts})}$ .

## 4. Mechanistic Experiments

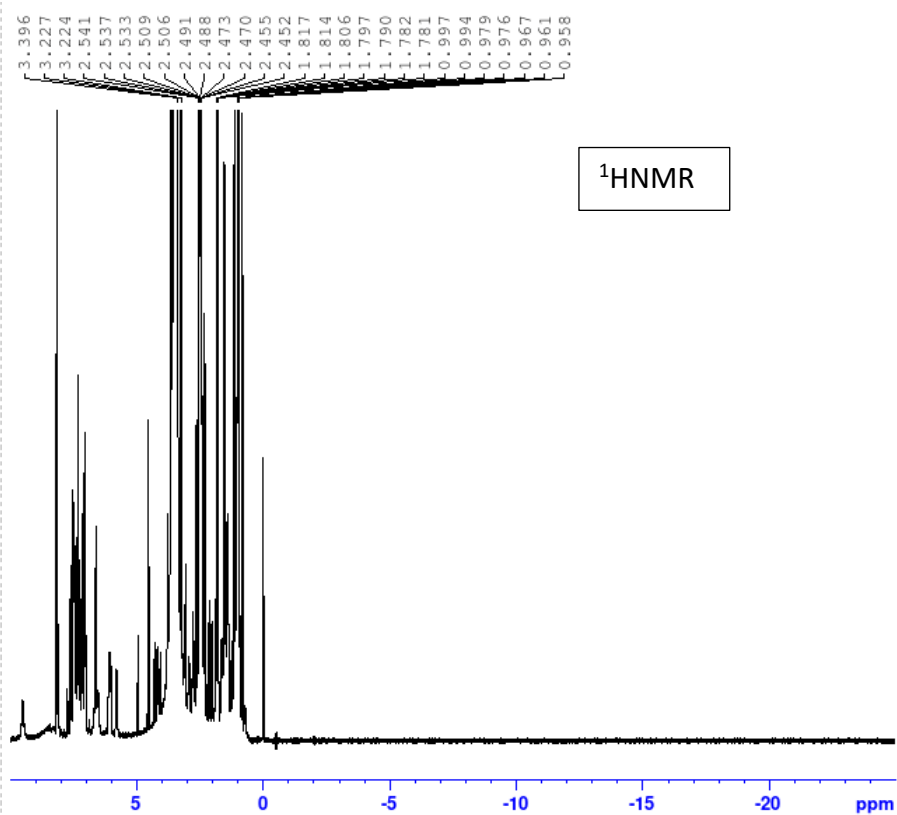
### 4.1. Hydride removal from complex 2.



Complex **2** was heated with 10 eq. of NH<sub>4</sub>Cl in a 2:1 solution of THF:MeOH. After 2 days at 80°C (in a pressure tube) the yellow precipitant formed was filtrated, dissolved in DCM and a few drops of triethylamine. The organic layer was washed with water 3 times, the organic layer then was dried using Na<sub>2</sub>SO<sub>4</sub> and the DCM was evaporated affording a yellow powder at 40% yield.



**Figure S26:** <sup>31</sup>P NMR (hydride coupled and decoupled) of complex **2'**.



```

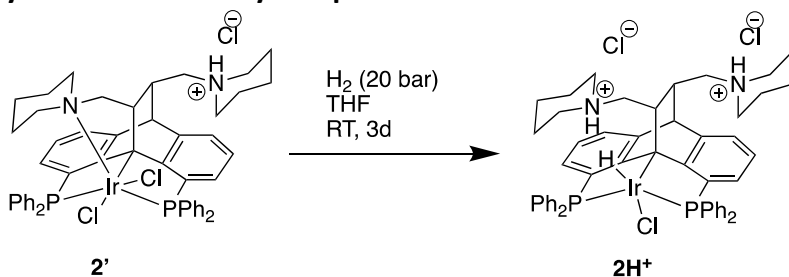
Current Data Parameters
NAME          SDMCat38.3
EXPNO         5
PROCNO        1

F2 - Acquisition Parameters
Date_         20220816
Time          13.20 h
INSTRUM       AV NanoBay V4-3 400MHz
PROBHD        X108618_0992 (
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            128
DS            4
SWH           16129.032 Hz
FIDRES        0.492219 Hz
AQ            2.0316160 sec
RG            65
DW            31.000 usec
DE            9.24 usec
TE            298.1 K
D1            1.00000000 sec
TD0           1
SFO1          400.1275992 MHz
NUC1           1H
PQ            4.67 usec
F1            14.00 usec
PLM1          13.94400020 W

F2 - Processing parameters
SI            65536
SF            400.1299886 MHz
WDW           EM
SSB           0
LB            0 Hz
GB            0
PC            1.00
  
```

Figure S27: <sup>1</sup>H NMR of complex 2' including hydride region.

## 4.2. Hydride activation by complex **2'** in THF



Complex **2'** was stirred at RT under 20 bars of hydrogen for 3 days in THF. THF was removed in a rotavapor to afford **2H<sup>+</sup>** as a white powder in a stoichiometric amount.

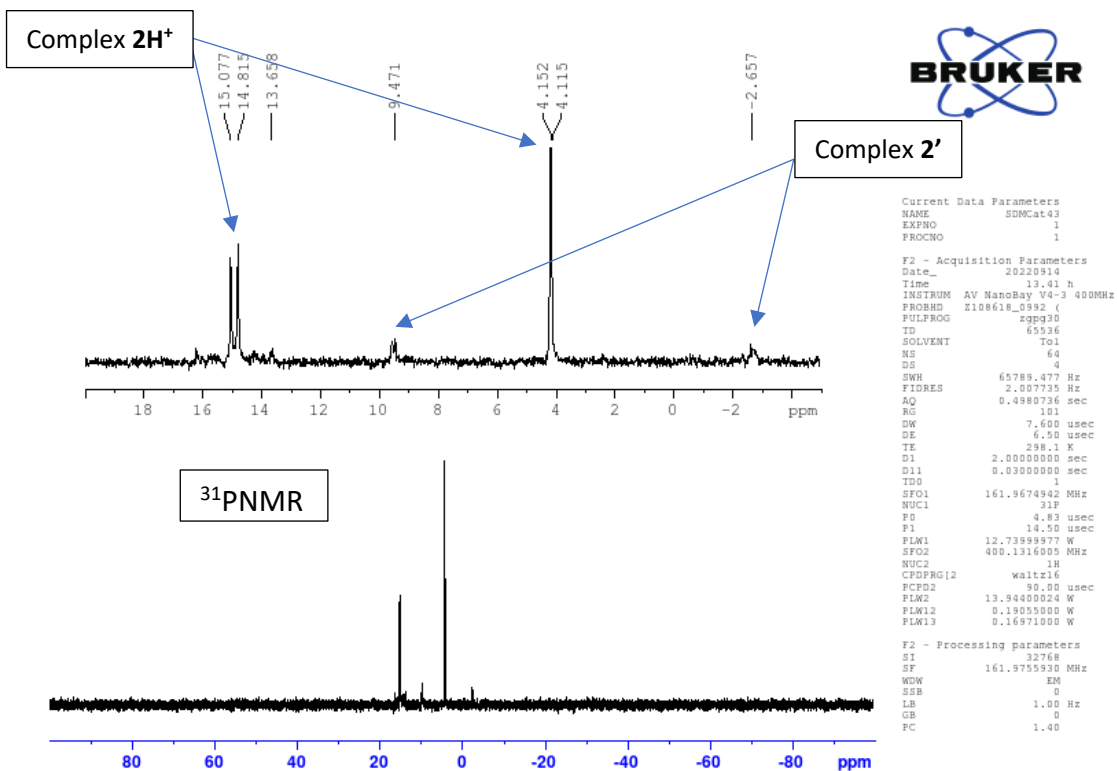


Figure S28: <sup>31</sup>P NMR of complex **2H<sup>+</sup>**.

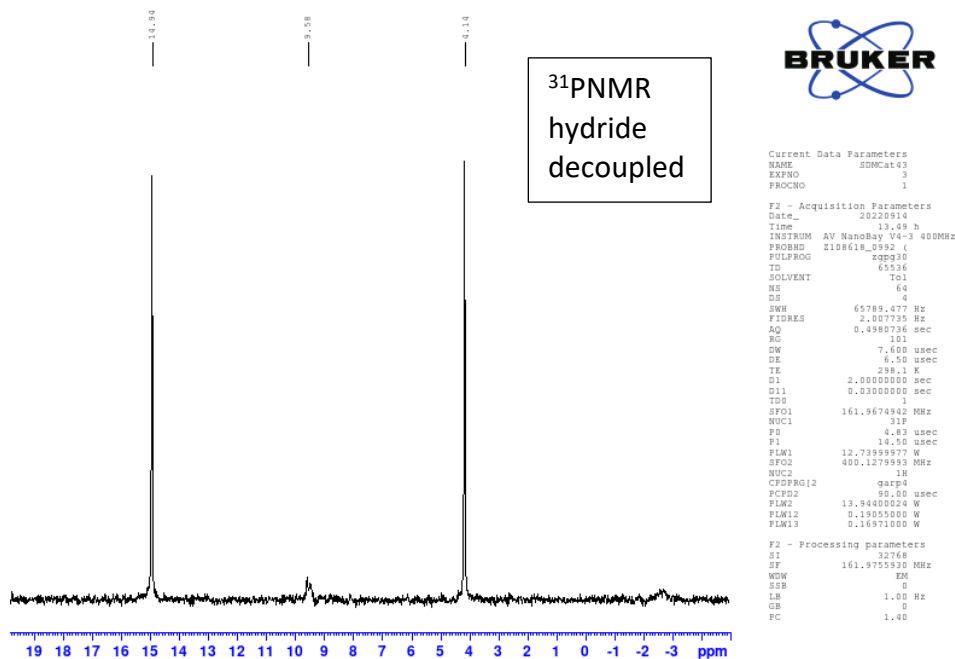


Figure S29: <sup>31</sup>P NMR (hydride decoupled) of complex 2H<sup>+</sup>.

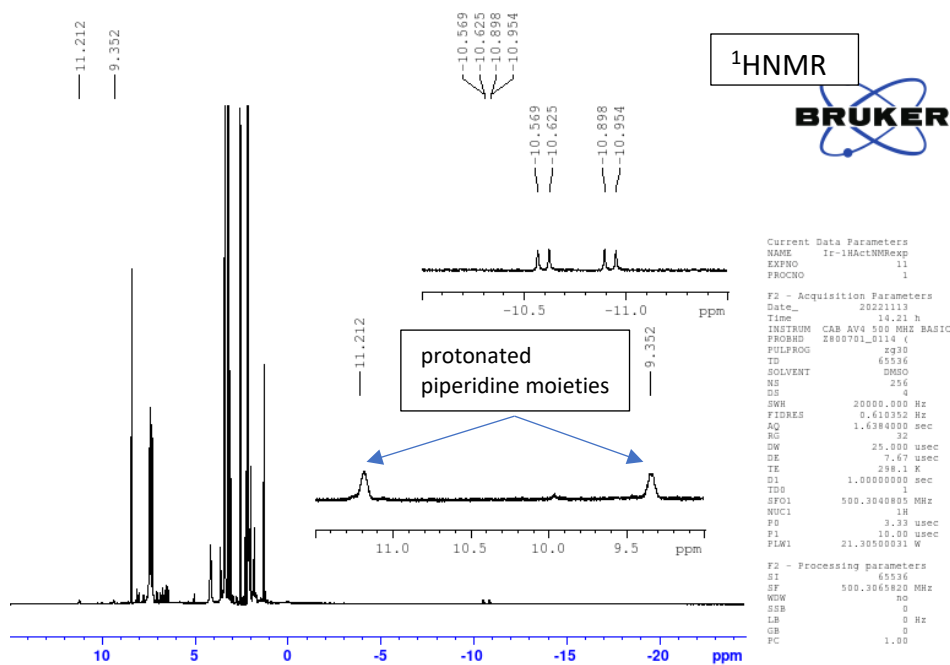
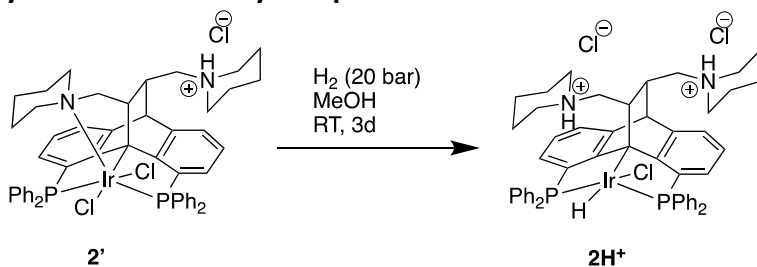


Figure S30: <sup>1</sup>H NMR of complex 2H<sup>+</sup>.



### 4.3. Hydride activation by complex **2'** in MeOH



Complex **2'** was stirred at RT under 20 bars of hydrogen for 4 days in methanol. Methanol was removed in a rotavapor and the **2H<sup>+</sup>** was obtained as white solid in a stoichiometric amount.

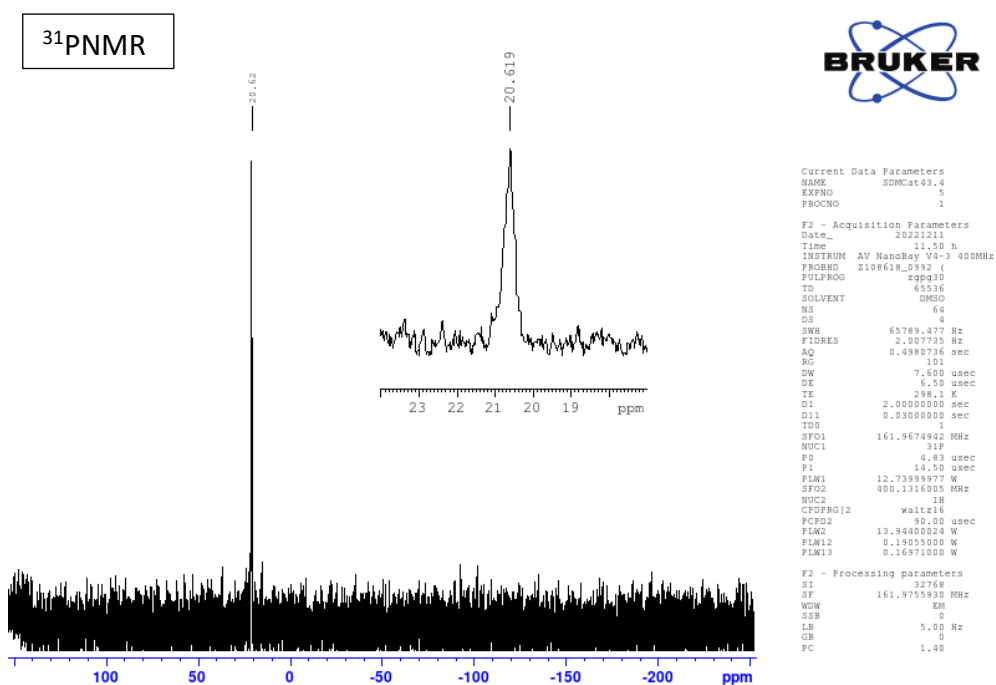
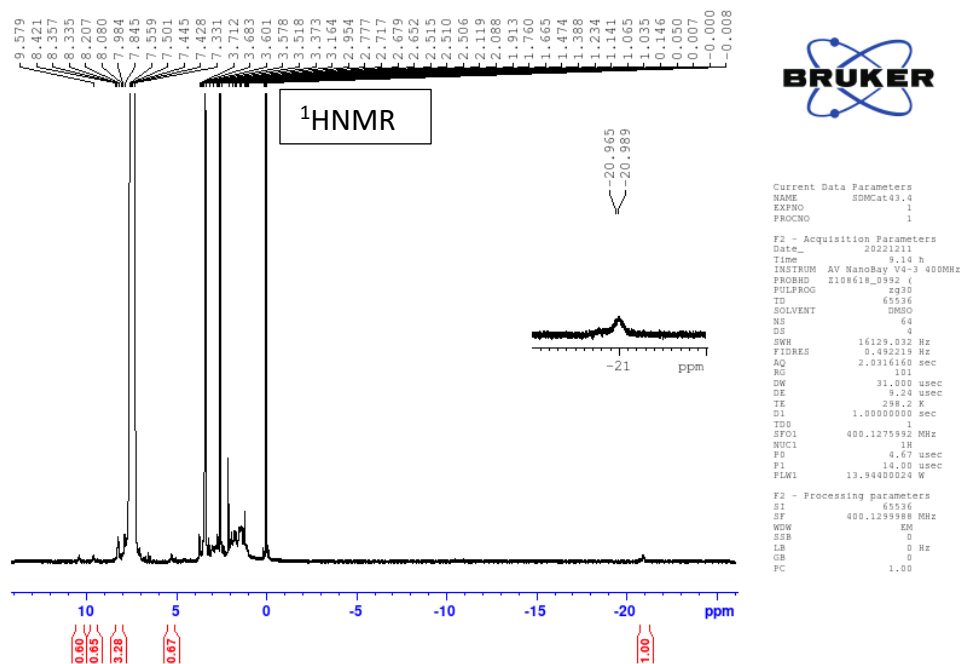


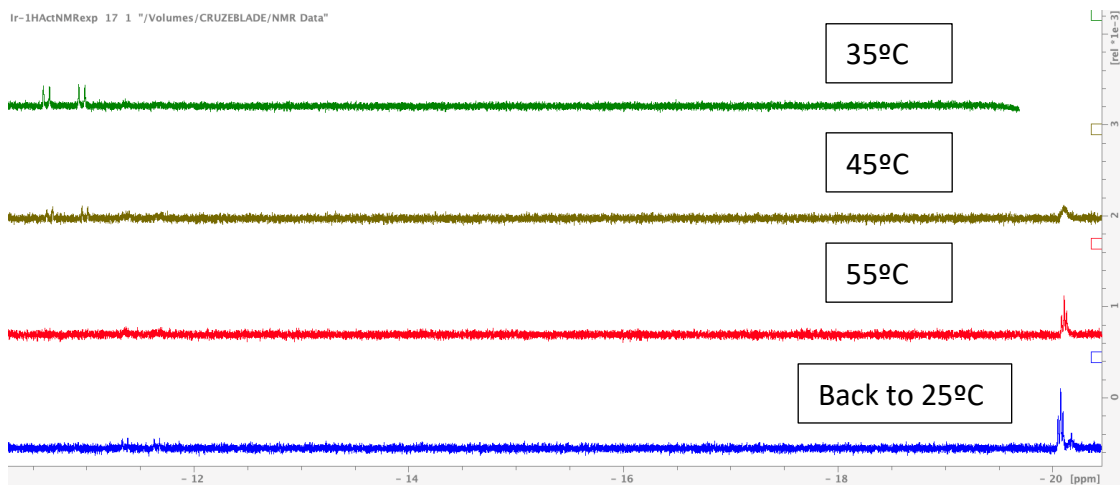
Figure S31: <sup>31</sup>P NMR of complex **2H<sup>+</sup>**.



**Figure S32:** <sup>1</sup>H NMR of complex **2H<sup>+</sup>**.

#### 4.4. Temperature Dependency in DMSO-d<sub>6</sub>.

Changes in the hydride peak were investigated in complex **4b** in DMSO-d<sub>6</sub> at different temperature from 35°C to 55°C.

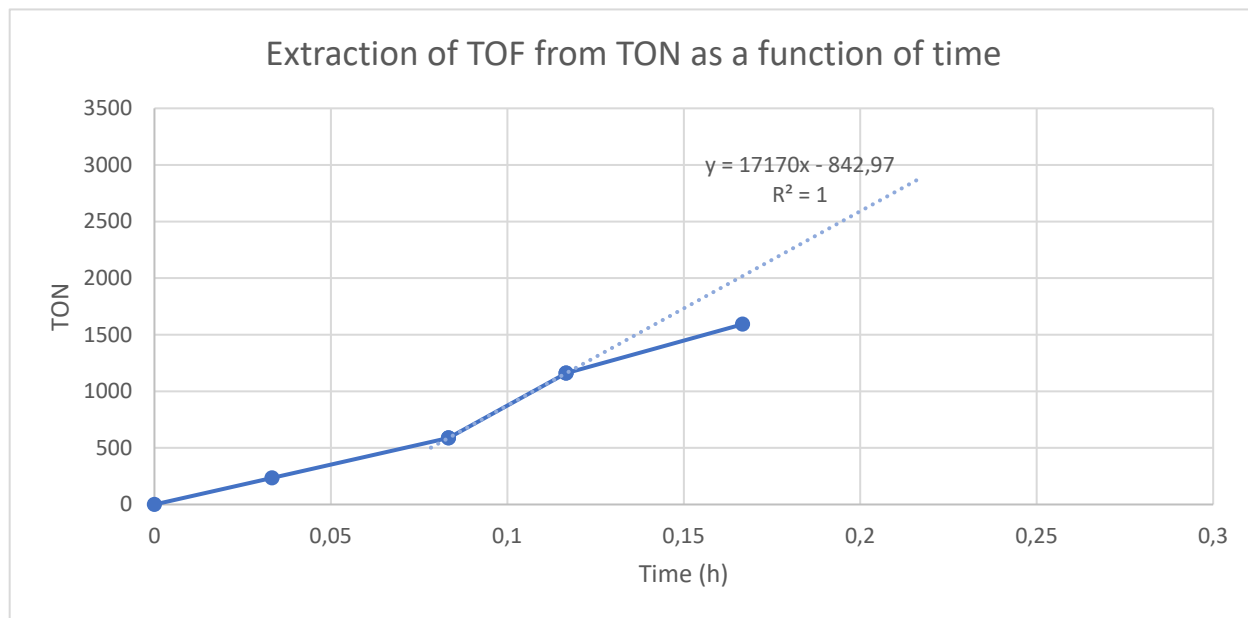


**Figure S33:** <sup>1</sup>H NMR (hydride region) of complex **2H<sup>+</sup>** in different temperatures.

#### 4.5. TOF measurement

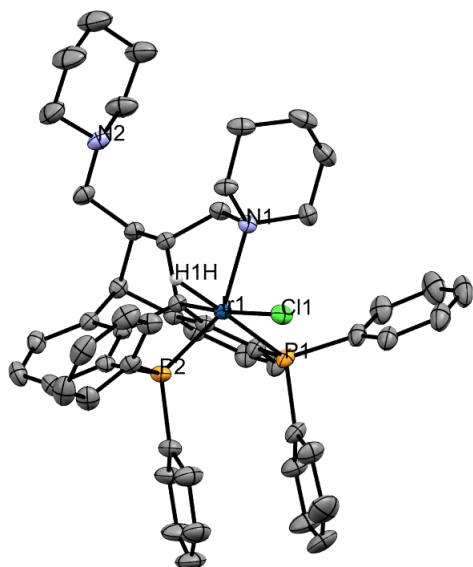
TOF was extracted as the initial rate of the reaction at optimized conditions (0.001mol% Ir-**1**, 20:30 bars CO<sub>2</sub>:H<sub>2</sub>, methanol, 110°C). The maximum rate was measured between 5 and 7 minutes. TOF is extracted from the slope of the trendline.

**Chart 1:** TON as a function of time in optimized conditions.



## 5. Crystal Structure Data

### 5.1. Complex 2

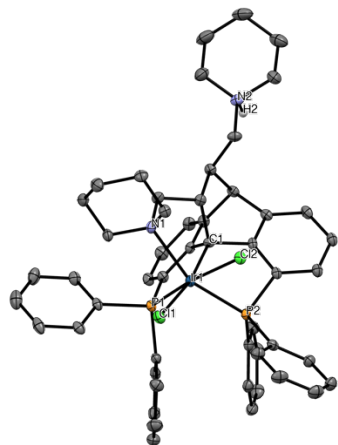


**Table 2 Crystal data and structure refinement for Stas2\_auto.**

Identification code	Stas2_auto
Empirical formula	C <sub>59</sub> H <sub>62</sub> ClIrN <sub>2</sub> P <sub>2</sub>
Formula weight	1088.69
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	12.81600(10)
b/Å	25.9297(3)
c/Å	14.8903(2)
α/°	90
β/°	93.5890(10)
γ/°	90
Volume/Å <sup>3</sup>	4938.57(10)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.464
μ/mm <sup>-1</sup>	2.864
F(000)	2216.0
Crystal size/mm <sup>3</sup>	0.204 × 0.164 × 0.079
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.17 to 64.792
Index ranges	-16 ≤ h ≤ 18, -37 ≤ k ≤ 38, -20 ≤ l ≤ 20

Reflections collected	86464
Independent reflections	15353 [ $R_{\text{int}} = 0.0318$ , $R_{\text{sigma}} = 0.0270$ ]
Data/restraints/parameters	15353/244/710
Goodness-of-fit on $F^2$	1.036
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0223$ , $wR_2 = 0.0482$
Final R indexes [all data]	$R_1 = 0.0325$ , $wR_2 = 0.0504$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.78/-0.32

## 5.2. Complex from ref. 32



**Table 3 Crystal data and structure refinement for Stas8.**

Identification code	Stas8
Empirical formula	C <sub>58</sub> H <sub>57</sub> Cl <sub>8</sub> F <sub>6</sub> IrN <sub>2</sub> O <sub>4</sub> P <sub>2</sub>
Formula weight	1497.79
Temperature/K	100.0(1)
Crystal system	monoclinic
Space group	I2/a
a/Å	35.1604(8)
b/Å	11.3069(2)
c/Å	33.2849(7)
α/°	90
β/°	117.196(3)
γ/°	90
Volume/Å <sup>3</sup>	11769.7(5)
Z	8
ρ <sub>calc</sub> /cm <sup>3</sup>	1.691
μ/mm <sup>-1</sup>	2.755
F(000)	5984.0
Crystal size/mm <sup>3</sup>	0.24 × 0.05 × 0.02
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	3.856 to 64.608
Index ranges	-46 ≤ h ≤ 46, -12 ≤ k ≤ 16, -43 ≤ l ≤ 46
Reflections collected	67742
Independent reflections	17503 [R <sub>int</sub> = 0.0422, R <sub>sigma</sub> = 0.0477]
Data/restraints/parameters	17503/0/735
Goodness-of-fit on F <sup>2</sup>	1.038

Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0374$ ,  $wR_2 = 0.0851$   
Final R indexes [all data]  $R_1 = 0.0560$ ,  $wR_2 = 0.0916$   
Largest diff. peak/hole /  $e \text{ \AA}^{-3}$  3.47/-1.01

## 6. Cartesian Coordinates

### H<sub>2</sub>

scf done: -1.173872

H	0.924203	-0.595409	0.000000
H	0.163602	-0.595409	-0.000000

### CO<sub>2</sub>

scf done: -188.363664

C	1.248207	-1.700143	-0.000000
O	2.409332	-1.700143	0.000000
O	0.087081	-1.700143	-0.000000

### DBU

scf done: -461.620960

N	1.642511	9.119862	9.956239
N	3.555228	7.769607	10.333890
C	1.705438	8.807802	8.542325
H	2.314028	9.570330	8.015536
H	0.692154	8.893720	8.112534
C	2.278554	7.424678	8.268565
H	1.587012	6.659728	8.662501
H	2.389614	7.238182	7.188782
C	3.625633	7.297587	8.955210
H	3.954728	6.245180	8.961050
H	4.395420	7.865252	8.397008
C	4.632877	7.350246	11.221747
H	5.105557	8.229790	11.694134
H	5.408805	6.907782	10.580148
C	4.230631	6.337894	12.295039
H	3.623044	5.545111	11.823437
H	5.147854	5.846595	12.662775
C	3.491158	6.946316	13.483539
H	4.187061	7.613651	14.025215
H	3.226142	6.144882	14.194631
C	2.234722	7.741611	13.134550
H	1.794538	8.119425	14.072680
H	1.471951	7.077911	12.689033
C	2.463517	8.941526	12.203182
H	1.625377	9.646076	12.290409
H	3.370294	9.487954	12.519465
C	2.545653	8.609102	10.730577

### [DBUH]<sup>+</sup>[HCOO]<sup>-</sup>

scf done: -651.202171

N	1.753871	8.960427	9.764917
H	1.007693	9.556425	10.110747
N	3.640631	7.735917	10.292797
C	1.763790	8.610465	8.353030
H	2.287521	9.393355	7.779780

H	0.725666	8.585315	7.996943
C	2.440283	7.264628	8.187066
H	1.790588	6.471532	8.592134
H	2.594605	7.060601	7.118558
C	3.772236	7.254719	8.909863
H	4.177031	6.233940	8.953144
H	4.514335	7.882485	8.387252
C	4.682497	7.323722	11.243438
H	5.133612	8.221429	11.696666
H	5.468709	6.853825	10.638991
C	4.206265	6.356892	12.323616
H	3.596818	5.565679	11.853311
H	5.099204	5.856777	12.733420
C	3.446557	7.020813	13.468232
H	4.135120	7.703528	13.998436
H	3.154466	6.251812	14.202578
C	2.205108	7.807011	13.056819
H	1.751437	8.245910	13.959544
H	1.442971	7.134584	12.626727
C	2.470010	8.961127	12.077228
H	1.634246	9.673606	12.108421
H	3.369554	9.521528	12.383964
C	2.642317	8.532246	10.650458
O	0.915052	8.613678	5.021555
O	2.515628	7.096391	4.558051
C	1.602373	7.899383	4.258368
H	1.371106	7.988048	3.152648

### 2

scf done: -3368.358713

Ir	-0.277949	-0.020903	-0.842382
H	0.479051	-1.277754	-1.493533
Cl	-1.308926	0.560203	-3.088094
P	-1.312842	1.788573	0.407690
P	-1.488958	-1.864715	-0.279722
N	1.652963	1.059368	-1.417577
N	5.320853	-0.977786	0.810191
C	0.743366	-0.372963	0.903833
C	0.434909	0.556251	2.067012
C	-0.519219	1.578342	2.049183
C	-0.719284	2.342233	3.216347
H	-1.438867	3.163962	3.226713
C	0.019713	2.071677	4.367294
H	-0.146520	2.669350	5.267939
C	0.976680	1.045843	4.379461
H	1.553812	0.843986	5.286961
C	1.182403	0.287455	3.231107
C	2.165153	-0.851739	3.050664
H	2.731805	-1.056377	3.969407



C	1.345036	-2.046072	2.600543	C	-1.564808	5.468772	-1.458459
C	1.250681	-3.307523	3.182826	H	-2.093610	5.868175	-2.328563
H	1.871193	-3.571619	4.044655	C	-1.746131	4.133497	-1.097501
C	0.332437	-4.237897	2.667257	H	-2.406646	3.508830	-1.702686
H	0.258226	-5.229675	3.122422	C	-3.150227	1.785296	0.595372
C	-0.513402	-3.906833	1.606427	C	-5.289278	1.728223	-0.559485
H	-1.249385	-4.636868	1.262203	H	-5.857557	1.596270	-1.484630
C	-0.413188	-2.638576	1.008794	C	-3.152700	-1.863076	0.519475
C	0.541078	-1.746411	1.487400	C	-5.573853	-1.875798	0.314767
C	2.272793	-0.260627	0.596275	H	-6.466035	-1.889672	-0.317467
H	2.520244	-1.110146	-0.060030	C	-4.309889	-1.867808	-0.275826
C	3.119518	-0.407600	1.889806	H	-4.227320	-1.876902	-1.366133
H	3.516613	0.577163	2.186487	C	-1.722518	-3.151052	-1.586902
C	2.496919	1.023976	-0.186411	C	-1.179223	-2.983030	-2.868003
H	2.206758	1.887787	0.432690	H	-0.671882	-2.047830	-3.114507
H	3.560829	1.147986	-0.439476	C	-1.316546	-3.984560	-3.833038
C	1.443494	2.451787	-1.893046	H	-0.893018	-3.834251	-4.830181
H	1.037874	3.031003	-1.057279	C	-1.994000	-5.166322	-3.530588
H	0.662866	2.396302	-2.667808	H	-2.098122	-5.950431	-4.285982
C	2.689809	3.134629	-2.450906	C	-2.549560	-5.338268	-2.260019
H	2.399550	4.144603	-2.785285	H	-3.091030	-6.256514	-2.015716
H	3.438009	3.276724	-1.651336	C	-2.422299	-4.336205	-1.297556
C	3.294824	2.329502	-3.594720	H	-2.884653	-4.481574	-0.318407
H	4.233001	2.787932	-3.949386	C	-3.898470	1.604403	-0.580289
H	2.597050	2.331955	-4.451934	H	-3.383755	1.360844	-1.516620
C	3.530172	0.894990	-3.136342	C	-5.952395	2.002874	0.638143
H	4.358824	0.863863	-2.408578	H	-7.041921	2.096265	0.655289
H	3.841712	0.254864	-3.978707	C	-5.217830	2.142111	1.817754
C	2.269962	0.276904	-2.534861	H	-5.730347	2.338456	2.763825
H	1.489226	0.191013	-3.305583	C	-3.824835	2.039317	1.798386
H	2.479403	-0.736452	-2.168972	H	-3.272490	2.159464	2.731756
C	4.286902	-1.388475	1.747846	C	-3.287807	-1.835652	1.915516
H	4.721495	-1.575919	2.757005	H	-2.401976	-1.823532	2.554897
H	3.884584	-2.356171	1.405252	C	-4.554793	-1.838904	2.503790
C	6.173448	0.072286	1.357225	H	-4.644052	-1.826294	3.593696
H	6.703169	-0.293925	2.269493	C	-5.700201	-1.866745	1.706285
H	5.544400	0.914908	1.683709	H	-6.691505	-1.878744	2.167824
C	7.204516	0.562811	0.347065				
H	7.842206	1.325581	0.824244				
H	6.684333	1.062033	-0.489450	<b>A</b>			
C	8.044922	-0.593121	-0.187791	scf done: -3556.709776			
H	8.682378	-0.986838	0.625346	Ir	-0.659376	-0.045090	-0.945749
H	8.727558	-0.247055	-0.981986	Cl	-2.180417	0.274948	-2.949673
C	7.137375	-1.708014	-0.700014	P	-1.608383	1.749175	0.386182
H	6.602031	-1.365275	-1.603360	P	-1.686398	-1.908014	-0.331845
H	7.726537	-2.592676	-0.993800	N	2.931029	1.770051	-1.178138
C	6.115299	-2.114105	0.354784	N	5.054559	-1.694941	0.665379
H	5.432023	-2.875075	-0.056521	C	0.593427	-0.319756	0.734001
H	6.646615	-2.596745	1.209902	C	0.313926	0.596334	1.921532
C	-1.080570	3.592208	0.015938	C	-0.650869	1.606603	1.944886
C	-0.215523	4.422552	0.745334	C	-0.809536	2.375309	3.114743
H	0.335878	4.030983	1.601999	H	-1.581838	3.146824	3.168925
C	-0.037115	5.760914	0.383372	C	0.009925	2.145360	4.218548
H	0.637620	6.390881	0.970075	H	-0.117387	2.748923	5.121552
C	-0.712287	6.290562	-0.716608	C	0.982759	1.134257	4.188845
H	-0.572827	7.337988	-0.998210	H	1.608073	0.950336	5.067816
				C	1.128157	0.350389	3.047916

C	2.053402	-0.838861	2.881761	C	-0.905040	5.970604	-1.455433
H	2.629406	-1.043365	3.794530	H	-0.757662	6.955754	-1.906987
C	1.172575	-1.996822	2.484364	C	-1.400485	4.913252	-2.221982
C	1.064043	-3.234221	3.113053	H	-1.637525	5.065127	-3.278894
H	1.676836	-3.462040	3.990276	C	-1.582215	3.653441	-1.648075
C	0.156701	-4.183431	2.621825	H	-1.936221	2.817005	-2.261352
H	0.076752	-5.161309	3.104725	C	-3.369662	1.900538	0.923754
C	-0.674151	-3.871987	1.546058	C	-5.644181	2.642748	0.483886
H	-1.412979	-4.600406	1.202683	H	-6.359712	3.140801	-0.176446
C	-0.568541	-2.616851	0.924597	C	-3.361953	-1.846166	0.423444
C	0.401712	-1.704922	1.346417	C	-5.717517	-1.364222	0.092131
C	2.151658	-0.075384	0.463730	H	-6.525351	-0.995302	-0.545779
H	2.426669	-0.662832	-0.425783	C	-4.407164	-1.365248	-0.383847
C	3.003291	-0.599635	1.667032	H	-4.185231	-0.991509	-1.388727
H	3.719196	0.178788	1.970114	C	-1.930846	-3.223159	-1.609708
C	2.431721	1.427398	0.200592	C	-1.240010	-3.202250	-2.829063
H	1.527407	2.028351	0.336007	H	-0.589853	-2.357243	-3.062550
H	3.177154	1.813607	0.904214	C	-1.391279	-4.243280	-3.747252
C	2.861378	3.265538	-1.423840	H	-0.848846	-4.208165	-4.696182
H	1.833935	3.575142	-1.198869	C	-2.234208	-5.318694	-3.460972
H	3.030177	3.392150	-2.504578	H	-2.351812	-6.132732	-4.181793
C	3.886754	4.063044	-0.639225	C	-2.933699	-5.344771	-2.252675
H	3.767025	5.116671	-0.938035	H	-3.601485	-6.179117	-2.020749
H	3.664264	4.022156	0.439966	C	-2.789601	-4.301913	-1.335703
C	5.300514	3.566121	-0.914624	H	-3.357651	-4.334215	-0.402831
H	6.029692	4.104950	-0.289149	C	-4.309963	2.529235	0.090724
H	5.565580	3.774832	-1.966354	H	-4.005520	2.945994	-0.871868
C	5.381833	2.066808	-0.655107	C	-6.062146	2.131262	1.714282
H	5.295619	1.864809	0.425204	H	-7.105628	2.229600	2.026183
H	6.360752	1.668576	-0.963855	C	-5.138577	1.489516	2.541063
C	4.329564	1.283881	-1.426151	H	-5.455178	1.079697	3.504161
H	4.493023	1.373351	-2.507670	C	-3.804142	1.366407	2.147137
H	4.361418	0.219417	-1.159283	H	-3.099442	0.859143	2.809584
C	3.788731	-1.886369	1.360211	C	-3.644034	-2.289022	1.722004
H	3.957094	-2.439748	2.312157	H	-2.843652	-2.647810	2.372542
H	3.160788	-2.545436	0.741370	C	-4.960410	-2.286978	2.193602
C	6.103438	-1.252005	1.580810	H	-5.171477	-2.643674	3.205628
H	6.249985	-2.008339	2.388762	C	-5.998814	-1.836235	1.378125
H	5.775536	-0.328168	2.083400	H	-7.028428	-1.843084	1.746349
C	7.434509	-1.015679	0.877646	C	1.906150	1.147579	-2.207752
H	8.188048	-0.722123	1.627284	O	0.742086	1.465620	-1.904396
H	7.333867	-0.166979	0.179737	O	2.385604	0.509245	-3.118982
C	7.880009	-2.257765	0.112325	H	0.193916	-1.184632	-1.706138
H	8.128520	-3.060463	0.830846				
H	8.799023	-2.055587	-0.462948				
C	6.758581	-2.733612	-0.806846	<b>B</b>			
H	6.604676	-1.998985	-1.617240	scf done: -3556.713965			
H	7.024085	-3.688035	-1.291093	Ir	0.534012	-0.083866	-0.854248
C	5.454546	-2.911981	-0.038776	Cl	2.384713	-0.459154	-2.568428
H	4.645324	-3.194914	-0.731521	P	1.388044	-1.658271	0.630324
H	5.568778	-3.761149	0.676237	P	1.396124	1.875341	0.042355
C	-1.288881	3.440309	-0.289967	N	-1.035338	-1.507524	-1.817054
C	-0.781726	4.504413	0.470386	N	-6.012219	0.380329	0.414315
H	-0.526689	4.364412	1.522484	C	-0.978435	0.123078	0.517100
C	-0.589779	5.760360	-0.111414	C	-0.966530	-0.871767	1.657654
H	-0.192190	6.579724	0.494182	C	0.035615	-1.813385	1.858654
				C	-0.009123	-2.624110	3.009667



P	1.490593	1.904379	0.138885	H	-8.683126	-0.141714	2.594314
N	-2.519338	-0.356468	-2.166748	H	-9.305708	-1.028773	1.198371
N	-5.545893	0.069845	1.365060	C	-7.887240	0.550625	0.710980
C	-0.612490	-0.101446	0.764658	H	-7.760091	0.167826	-0.320966
C	-0.352840	-1.302673	1.660118	H	-8.620986	1.376001	0.648910
C	0.734506	-2.170870	1.539328	C	-6.553916	1.109338	1.199510
C	0.945807	-3.182286	2.490409	H	-6.178928	1.864826	0.491523
H	1.809978	-3.847124	2.416532	H	-6.715995	1.649350	2.167676
C	0.057846	-3.320229	3.558909	C	1.959062	-3.165288	-0.957410
H	0.214223	-4.114118	4.294481	C	1.363889	-4.400560	-0.651110
C	-0.997814	-2.412035	3.724265	H	0.835278	-4.545715	0.292908
H	-1.649773	-2.487496	4.600118	C	1.437374	-5.466544	-1.557210
C	-1.184099	-1.393204	2.789153	H	0.959836	-6.417638	-1.310602
C	-2.168634	-0.252196	2.901813	C	2.099532	-5.307980	-2.775746
H	-2.781811	-0.323596	3.805407	H	2.156330	-6.140488	-3.477898
C	-1.353244	1.024614	2.848949	C	2.685879	-4.081060	-3.088657
C	-1.396055	2.092846	3.728882	H	3.191371	-3.941989	-4.053560
H	-2.068535	2.074403	4.596638	C	2.607549	-3.014578	-2.196591
C	-0.573662	3.217706	3.506442	H	3.020931	-2.037954	-2.468694
H	-0.623138	4.068939	4.196069	C	3.537933	-1.758042	1.025222
C	0.310324	3.248505	2.434583	C	5.901263	-2.328713	1.097580
H	0.938304	4.120268	2.270533	H	6.772487	-2.788052	0.617374
C	0.374779	2.149319	1.553421	C	3.216807	1.973527	0.770282
C	-0.488697	1.068697	1.737679	C	5.586278	1.633715	0.359033
C	-2.148567	-0.025680	0.379372	H	6.388659	1.293695	-0.306615
H	-2.304151	1.029480	0.100344	C	4.259674	1.535270	-0.068251
C	-3.051080	-0.295814	1.628036	H	4.021828	1.121818	-1.053660
H	-3.430146	-1.327232	1.558264	C	1.327210	3.441121	-0.865920
C	-2.620848	-0.906123	-0.780202	C	2.440095	4.180585	-1.294481
H	-2.081313	-1.861123	-0.789378	H	3.453048	3.870841	-1.030383
H	-3.684738	-1.141972	-0.620264	C	2.254928	5.335215	-2.061379
C	-3.147748	-1.324304	-3.123005	H	3.128769	5.907263	-2.394213
H	-2.714443	-2.310738	-2.913713	C	0.970645	5.763658	-2.402472
H	-2.822545	-1.011662	-4.120366	H	0.826985	6.668716	-3.000335
C	-4.668762	-1.353200	-3.056449	C	-0.139287	5.027381	-1.974287
H	-5.016886	-2.042324	-3.852199	H	-1.149706	5.352235	-2.231022
H	-5.019544	-1.787770	-2.108857	C	0.037408	3.871932	-1.214614
C	-5.266778	0.037103	-3.251845	H	-0.838792	3.301209	-0.886295
H	-6.361329	0.012346	-3.123179	C	4.674059	-2.334692	0.430050
H	-5.072945	0.382785	-4.283009	H	4.605790	-2.801342	-0.554842
C	-4.628236	1.014938	-2.263716	C	6.012957	-1.756058	2.360174
H	-4.941402	0.770095	-1.236910	H	6.972174	-1.764219	2.885069
H	-4.963439	2.045089	-2.461227	C	4.886450	-1.177868	2.956372
C	-3.110035	0.990737	-2.367508	H	4.964282	-0.722080	3.954520
H	-2.793424	1.292160	-3.379588	C	3.660920	-1.169803	2.290662
H	-2.641880	1.692440	-1.666789	H	2.793361	-0.706231	2.776927
C	-4.263558	0.652472	1.755042	C	3.531860	2.482288	2.038590
H	-4.318031	1.024966	2.804974	H	2.737872	2.810263	2.716735
H	-4.105533	1.549341	1.129571	C	4.856135	2.574751	2.456548
C	-6.000928	-0.954519	2.295506	H	5.081579	2.976835	3.448134
H	-6.158566	-0.512019	3.312562	C	5.894165	2.155308	1.611820
H	-5.220621	-1.717643	2.413404	H	6.934449	2.236491	1.940172
C	-7.298038	-1.610522	1.829064	C	-0.835951	-0.340355	-2.748069
H	-7.611127	-2.364308	2.571590	O	-0.306966	-1.354637	-2.322182
H	-7.109690	-2.148108	0.882786	O	-0.806138	0.221355	-3.839684
C	-8.390886	-0.567914	1.619377	H	-0.487564	0.817884	-1.790802

**TS\_2B**

scf done: -3556.6778368

Ir	0.955785	0.178130	0.893750
Cl	3.064016	0.553892	2.254486
P	1.703573	1.385253	-0.983808
P	1.487461	-1.966948	0.487362
N	-3.445478	2.334657	0.999324
N	-5.426008	-1.562788	-0.629795
C	-0.778362	-0.182469	-0.322661
C	-0.674288	0.378191	-1.736913
C	0.417004	1.087199	-2.245712
C	0.404911	1.508486	-3.588704
H	1.246409	2.058006	-4.012914
C	-0.694626	1.224778	-4.395766
H	-0.698457	1.556560	-5.437582
C	-1.784724	0.502087	-3.889555
H	-2.631387	0.260846	-4.539280
C	-1.772149	0.066233	-2.568197
C	-2.800897	-0.833915	-1.913104
H	-3.609945	-1.103116	-2.602739
C	-2.024369	-2.034365	-1.441211
C	-2.225018	-3.361628	-1.805559
H	-3.070795	-3.631607	-2.444550
C	-1.319328	-4.347686	-1.384373
H	-1.472135	-5.389838	-1.678145
C	-0.199545	-3.994258	-0.637867
H	0.542398	-4.751206	-0.369758
C	-0.019941	-2.654170	-0.250836
C	-0.944868	-1.677738	-0.609723
C	-2.157205	0.350789	0.239756
H	-2.265671	-0.079856	1.249167
C	-3.350242	-0.129293	-0.645695
H	-3.892937	0.767104	-0.980309
C	-2.215485	1.886429	0.354602
H	-1.307776	2.263264	0.852337
H	-2.203575	2.305003	-0.664176
C	-3.428547	2.315772	2.458381
H	-2.941479	1.389700	2.803403
H	-4.475605	2.260384	2.814463
C	-2.761411	3.540267	3.096567
H	-2.860165	3.480202	4.194249
H	-1.679428	3.528112	2.880506
C	-3.374948	4.835658	2.564993
H	-2.842126	5.713994	2.967452
H	-4.420002	4.917163	2.919198
C	-3.364195	4.845399	1.036441
H	-2.323808	4.910668	0.670598
H	-3.892076	5.732504	0.645286
C	-4.021138	3.573189	0.492111
H	-5.093652	3.590038	0.769278
H	-3.986719	3.556852	-0.609472
C	-4.322367	-1.014563	0.141703
H	-3.762150	-1.862857	0.568475
H	-4.689247	-0.423097	1.011183

C	-6.065838	-2.679612	0.054102
H	-6.536425	-2.348202	1.010826
H	-5.288837	-3.412148	0.327827
C	-7.123292	-3.345883	-0.818648
H	-7.598529	-4.165694	-0.254468
H	-6.626833	-3.804458	-1.692674
C	-8.163507	-2.334369	-1.292120
H	-8.755982	-1.988068	-0.425231
H	-8.876464	-2.803196	-1.991050
C	-7.474608	-1.137516	-1.941559
H	-7.005822	-1.449787	-2.891782
H	-8.204896	-0.349640	-2.190557
C	-6.400726	-0.555992	-1.028507
H	-5.881529	0.264554	-1.547222
H	-6.886294	-0.101187	-0.131722
C	1.587514	3.179412	-0.577407
C	0.684473	4.045292	-1.208881
H	0.008172	3.673338	-1.981601
C	0.648331	5.398623	-0.860002
H	-0.055224	6.066644	-1.364575
C	1.504708	5.895008	0.123876
H	1.474413	6.954191	0.394140
C	2.398170	5.032270	0.765481
H	3.066119	5.412949	1.543261
C	2.440351	3.681643	0.420754
H	3.127567	3.006696	0.940095
C	3.397185	1.278931	-1.683431
C	5.081379	1.998096	-3.278115
H	5.362804	2.605247	-4.142871
C	2.778453	-2.489494	-0.715172
C	4.826176	-3.620844	-1.357969
H	5.709813	-4.199396	-1.075097
C	3.915435	-3.232320	-0.371187
H	4.100491	-3.525968	0.662776
C	1.805506	-2.896343	2.041312
C	3.005601	-2.737569	2.754934
H	3.770038	-2.046862	2.397602
C	3.211618	-3.429618	3.948942
H	4.152311	-3.298800	4.490948
C	2.221226	-4.273350	4.456404
H	2.384890	-4.811225	5.394400
C	1.017353	-4.417935	3.765591
H	0.230040	-5.066522	4.159339
C	0.808644	-3.734178	2.566243
H	-0.143470	-3.854846	2.045585
C	3.776859	2.059732	-2.788783
H	3.066793	2.741098	-3.261699
C	6.027159	1.178520	-2.655926
H	7.051398	1.137300	-3.036978
C	5.665639	0.430456	-1.534947
H	6.407014	-0.192485	-1.027343
C	4.356589	0.478579	-1.049113
H	4.086134	-0.076048	-0.149482
C	2.562144	-2.154757	-2.062929
H	1.676474	-1.583038	-2.352667
C	3.467311	-2.553112	-3.044464

H	3.282752	-2.288887	-4.089142
C	4.605987	-3.283572	-2.693412
H	5.318209	-3.593973	-3.462815
C	0.010329	0.817188	3.095797
O	0.208722	1.759135	2.345360
O	-0.292183	0.468475	4.188966
H	0.147516	-0.471182	2.258603

## B.H2

scf done: -3557.887921

Ir	-0.660637	0.169416	-0.899824
Cl	-2.332523	0.349030	-2.798455
P	-1.820836	1.697982	0.370874
P	-1.514207	-1.914499	-0.225409
N	3.980104	1.759682	-0.244006
N	5.034658	-1.465554	0.947460
C	0.634260	-0.011445	0.800587
C	0.304240	1.006904	1.882296
C	-0.738696	1.930120	1.819616
C	-0.882858	2.889010	2.840344
H	-1.664643	3.650609	2.782116
C	-0.016192	2.869209	3.930900
H	-0.123560	3.616926	4.721455
C	0.971816	1.877553	4.040528
H	1.610792	1.838814	4.927814
C	1.126600	0.938998	3.025071
C	2.047883	-0.260696	3.024108
H	2.600507	-0.355502	3.968871
C	1.161758	-1.452759	2.755041
C	1.012296	-2.577742	3.557689
H	1.584420	-2.667808	4.485752
C	0.107630	-3.584290	3.188814
H	-0.019651	-4.464781	3.824341
C	-0.654508	-3.449128	2.033041
H	-1.395863	-4.210073	1.777130
C	-0.486941	-2.316844	1.213003
C	0.434905	-1.328340	1.552750
C	2.197578	0.160667	0.528575
H	2.458851	-0.551540	-0.268286
C	3.016729	-0.191619	1.807747
H	3.728090	0.627094	1.990970
C	2.569802	1.587330	0.062257
H	1.943445	1.877103	-0.800821
H	2.314225	2.291843	0.868901
C	4.368344	1.371055	-1.596070
H	3.876757	0.419286	-1.851181
H	5.455306	1.166128	-1.597929
C	4.066040	2.432600	-2.660065
H	4.450042	2.090785	-3.636598
H	2.973974	2.536819	-2.780509
C	4.673000	3.781877	-2.274979
H	4.389015	4.559941	-3.003935
H	5.776498	3.709288	-2.311812
C	4.246476	4.178925	-0.861931
H	3.163982	4.400652	-0.847029
H	4.760419	5.101474	-0.540764

C	4.554598	3.048063	0.124361
H	5.653706	2.927471	0.182533
H	4.218280	3.312036	1.140162
C	3.807259	-1.510165	1.722700
H	4.017495	-1.861361	2.760069
H	3.161104	-2.280401	1.274170
C	6.118444	-0.808091	1.666411
H	6.362558	-1.371010	2.600080
H	5.784560	0.190389	1.988103
C	7.377662	-0.681921	0.816695
H	8.174018	-0.209688	1.415829
H	7.171822	-0.004936	-0.030847
C	7.825483	-2.042402	0.289746
H	8.175128	-2.664473	1.134396
H	8.683106	-1.933958	-0.395253
C	6.662006	-2.744766	-0.404346
H	6.403267	-2.205969	-1.333075
H	6.938592	-3.771415	-0.697016
C	5.433452	-2.794027	0.496103
H	4.587696	-3.246645	-0.046904
H	5.644983	-3.464333	1.364064
C	-1.913233	3.366641	-0.416027
C	-0.771831	4.185039	-0.402916
H	0.142904	3.847708	0.090960
C	-0.792252	5.438325	-1.015139
H	0.103655	6.064682	-0.991571
C	-1.950824	5.890324	-1.651273
H	-1.966635	6.873235	-2.130045
C	-3.088262	5.082152	-1.669525
H	-4.000812	5.428066	-2.162674
C	-3.072326	3.827561	-1.055590
H	-3.976839	3.216866	-1.076504
C	-3.539190	1.407703	0.934984
C	-5.825168	0.849655	0.341012
H	-6.551362	0.518727	-0.406218
C	-3.232908	-2.193678	0.364440
C	-5.502085	-2.989960	0.031135
H	-6.263051	-3.411826	-0.631038
C	-4.226236	-2.725740	-0.470554
H	-4.012181	-2.956259	-1.515208
C	-1.256174	-3.229779	-1.488607
C	-1.816534	-3.086877	-2.768847
H	-2.366038	-2.176310	-3.022926
C	-1.638552	-4.082129	-3.729954
H	-2.081395	-3.957632	-4.722126
C	-0.888782	-5.222953	-3.433798
H	-0.747460	-6.000119	-4.190107
C	-0.310319	-5.358746	-2.171430
H	0.291697	-6.240041	-1.933548
C	-0.489373	-4.367865	-1.202860
H	-0.015145	-4.490197	-0.227604
C	-4.480491	0.970575	-0.012165
H	-4.154184	0.728636	-1.028482
C	-6.240174	1.143353	1.641984
H	-7.294391	1.048281	1.916564
C	-5.302410	1.546610	2.594166

H	-5.616409	1.762406	3.619083
C	-3.956995	1.680591	2.245417
H	-3.240892	1.996754	3.005279
C	-3.546216	-1.912139	1.704603
H	-2.790972	-1.490508	2.371533
C	-4.819120	-2.187806	2.203556
H	-5.043728	-1.978541	3.252699
C	-5.799554	-2.730897	1.369651
H	-6.795336	-2.951438	1.763923
C	1.325446	-0.715036	-3.035295
O	0.645399	-1.112703	-2.022236
O	1.347544	0.401750	-3.548789
H	1.958186	-1.532026	-3.462719
H	-0.137185	1.553072	-1.840600
H	0.366364	1.573583	-1.148993

### TS\_BC

scf done: -3557.9266318

Ir	-0.492339	0.163745	-0.818772
Cl	-2.243632	0.316997	-2.657703
P	-1.539565	1.745448	0.461536
P	-1.500173	-1.921205	-0.205772
N	2.268503	1.663824	-1.147475
N	5.266616	-1.093808	1.067829
C	0.734592	-0.156440	0.919375
C	0.395824	0.780853	2.069222
C	-0.608907	1.745253	2.031231
C	-0.886784	2.511123	3.179412
H	-1.706203	3.233847	3.182390
C	-0.131213	2.324678	4.334564
H	-0.343326	2.925426	5.223228
C	0.873095	1.345774	4.378389
H	1.436561	1.180272	5.301527
C	1.123036	0.561676	3.256641
C	2.077734	-0.605907	3.166645
H	2.595038	-0.790748	4.117966
C	1.256456	-1.789140	2.722632
C	1.172715	-3.017306	3.370751
H	1.765007	-3.200576	4.272036
C	0.322392	-4.012495	2.871660
H	0.265033	-4.984626	3.368664
C	-0.477784	-3.750910	1.763627
H	-1.164572	-4.518858	1.400085
C	-0.404348	-2.501627	1.117598
C	0.510056	-1.537611	1.552174
C	2.297067	-0.023642	0.710315
H	2.585619	-0.784083	-0.030598
C	3.084136	-0.303737	2.028440
H	3.611094	0.616972	2.326755
C	2.729130	1.354398	0.203973
H	2.337638	2.127616	0.884547
H	3.828971	1.412976	0.266941
C	2.079928	3.099793	-1.405271
H	1.490049	3.521944	-0.578452
H	1.458279	3.181158	-2.316362
C	3.374360	3.880438	-1.607654

H	3.121867	4.928265	-1.840075
H	3.950603	3.900198	-0.665528
C	4.213318	3.258254	-2.720999
H	5.182414	3.775721	-2.816448
H	3.689970	3.387552	-3.686027
C	4.419755	1.769907	-2.452539
H	5.084416	1.637465	-1.581574
H	4.925672	1.281239	-3.301715
C	3.091499	1.054425	-2.208490
H	2.490003	1.063405	-3.130462
H	3.263969	0.000088	-1.951693
C	4.119084	-1.426673	1.897814
H	4.446968	-1.734302	2.917820
H	3.627093	-2.309379	1.458959
C	6.219550	-0.239375	1.770111
H	6.620890	-0.765925	2.669103
H	5.696806	0.653869	2.146178
C	7.383007	0.183737	0.881013
H	8.085426	0.792597	1.474313
H	7.005374	0.834441	0.072930
C	8.086546	-1.029215	0.279375
H	8.603478	-1.586047	1.082662
H	8.865778	-0.715978	-0.435626
C	7.068796	-1.945040	-0.394964
H	6.654697	-1.445593	-1.288906
H	7.545637	-2.876764	-0.742050
C	5.924743	-2.290039	0.551094
H	5.174097	-2.902787	0.025913
H	6.317859	-2.919847	1.384655
C	-1.458833	3.446835	-0.254082
C	-1.105678	4.563195	0.518018
H	-0.838032	4.452451	1.569609
C	-1.073200	5.836996	-0.055146
H	-0.789376	6.696003	0.559165
C	-1.396286	6.012303	-1.401566
H	-1.371104	7.010554	-1.847346
C	-1.745379	4.904550	-2.176968
H	-1.994077	5.030541	-3.234475
C	-1.771939	3.628471	-1.611636
H	-2.031785	2.761664	-2.228589
C	-3.298773	1.635050	0.999675
C	-5.641108	2.216955	0.732361
H	-6.426976	2.720197	0.162399
C	-3.236222	-2.027187	0.403156
C	-5.587351	-1.581952	-0.021004
H	-6.361222	-1.117695	-0.638359
C	-4.245024	-1.425368	-0.368964
H	-3.970367	-0.824015	-1.241086
C	-1.473727	-3.233530	-1.506609
C	-2.448982	-3.254925	-2.515897
H	-3.229451	-2.493941	-2.548615
C	-2.424564	-4.239756	-3.505107
H	-3.193060	-4.238832	-4.283219
C	-1.428128	-5.217565	-3.503013
H	-1.413207	-5.990610	-4.276443
C	-0.448587	-5.197990	-2.508571

H	0.341044	-5.954633	-2.498866
C	-0.467098	-4.212055	-1.520055
H	0.317687	-4.209596	-0.761391
C	-4.322071	2.266902	0.277446
H	-4.097239	2.817025	-0.638497
C	-5.952926	1.541747	1.913635
H	-6.984411	1.515864	2.275586
C	-4.941637	0.896839	2.629514
H	-5.177382	0.360355	3.552478
C	-3.623961	0.934081	2.172018
H	-2.844832	0.424963	2.743711
C	-3.597072	-2.740776	1.555580
H	-2.835646	-3.192473	2.192613
C	-4.941812	-2.883874	1.905293
H	-5.205946	-3.446798	2.804899
C	-5.940956	-2.318974	1.111354
H	-6.993454	-2.442458	1.381330
C	0.998397	-1.297693	-3.160037
O	0.725506	-1.272469	-1.908203
O	0.790007	-0.439605	-4.013927
H	1.513215	-2.247540	-3.456727
H	0.128861	1.623460	-1.559940
H	0.873322	1.210905	-1.168085

**TS\_BC'**

scf done: -3557.8774559

Ir	-0.687064	0.162241	-0.907038
Cl	-2.343263	0.453331	-2.787489
P	-1.734059	1.730825	0.393091
P	-1.574956	-1.917052	-0.203915
N	3.332773	1.737374	-1.211208
N	5.069109	-1.578548	0.724607
C	0.653992	-0.061846	0.740244
C	0.396955	0.951254	1.844683
C	-0.612130	1.912513	1.821382
C	-0.689247	2.863606	2.856586
H	-1.445557	3.652223	2.832819
C	0.214853	2.803745	3.915357
H	0.158688	3.546031	4.716315
C	1.180424	1.785748	3.977115
H	1.856901	1.725735	4.834991
C	1.268572	0.852906	2.948310
C	2.168893	-0.362115	2.887762
H	2.767718	-0.479020	3.801275
C	1.254126	-1.537155	2.647558
C	1.127405	-2.669051	3.445093
H	1.741097	-2.777314	4.344307
C	0.190633	-3.657124	3.109643
H	0.079027	-4.542182	3.741842
C	-0.623994	-3.496148	1.993069
H	-1.391178	-4.241229	1.768140
C	-0.479573	-2.358955	1.175944
C	0.473954	-1.387041	1.482605
C	2.203163	0.136228	0.401059
H	2.434961	-0.517082	-0.453047
C	3.078455	-0.297535	1.621200

H	3.833551	0.481185	1.806914
C	2.505860	1.599909	-0.018897
H	1.561401	2.116506	-0.235174
H	2.928148	2.136975	0.855499
C	3.137621	2.991308	-1.932768
H	2.057691	3.169586	-2.057244
H	3.550477	2.861507	-2.951430
C	3.813164	4.206074	-1.287228
H	3.660321	5.095209	-1.923127
H	3.331670	4.429358	-0.318041
C	5.303215	3.939104	-1.074627
H	5.780058	4.775845	-0.535796
H	5.802874	3.879606	-2.060131
C	5.511985	2.621294	-0.327584
H	5.163822	2.729173	0.715585
H	6.585368	2.372164	-0.270242
C	4.756093	1.476494	-1.013552
H	5.208619	1.304994	-2.009286
H	4.872434	0.533115	-0.458098
C	3.806216	-1.644123	1.444286
H	3.963949	-2.102380	2.447196
H	3.145226	-2.337382	0.902454
C	6.154898	-1.111793	1.579729
H	6.297871	-1.813879	2.436192
H	5.872677	-0.142746	2.022018
C	7.473280	-0.974646	0.826479
H	8.259849	-0.664320	1.534313
H	7.385744	-0.168908	0.077042
C	7.849289	-2.279738	0.130995
H	8.091228	-3.044404	0.892125
H	8.756919	-2.148991	-0.481826
C	6.683170	-2.769767	-0.722759
H	6.525285	-2.076167	-1.567826
H	6.899828	-3.759635	-1.157673
C	5.400358	-2.853413	0.095639
H	4.559442	-3.150101	-0.552246
H	5.508381	-3.659178	0.860657
C	-1.827053	3.405440	-0.377855
C	-0.715114	4.259663	-0.306412
H	0.183610	3.952152	0.233486
C	-0.747174	5.515509	-0.914722
H	0.124358	6.171830	-0.843017
C	-1.886505	5.932625	-1.606083
H	-1.911145	6.917019	-2.081474
C	-2.994356	5.087083	-1.684213
H	-3.891795	5.404533	-2.222280
C	-2.967773	3.831705	-1.073218
H	-3.848754	3.191350	-1.142611
C	-3.445497	1.469175	1.000255
C	-5.746811	0.908116	0.470044
H	-6.490549	0.562977	-0.253214
C	-3.262181	-2.183147	0.486359
C	-5.557523	-2.951441	0.287954
H	-6.357946	-3.374063	-0.325503
C	-4.305728	-2.715095	-0.284691
H	-4.149568	-2.967270	-1.334918



C	-1.426541	-3.229248	-1.487873	H	-0.028086	-4.652363	3.658448
C	-2.033736	-3.031539	-2.739229	C	-0.691790	-3.553968	1.924714
H	-2.540882	-2.086019	-2.952513	H	-1.452207	-4.294769	1.664491
C	-1.956156	-4.018006	-3.722937	C	-0.537953	-2.396088	1.138508
H	-2.436042	-3.852050	-4.691639	C	0.406858	-1.427780	1.500593
C	-1.259431	-5.203957	-3.478651	C	2.176065	0.121813	0.534855
H	-1.197279	-5.974598	-4.252162	H	2.450475	-0.546128	-0.294940
C	-0.632034	-5.393893	-2.246770	C	3.009831	-0.298136	1.788791
H	-0.070028	-6.311353	-2.050989	H	3.718717	0.505951	2.036309
C	-0.711961	-4.412477	-1.255318	C	2.474038	1.583600	0.125491
H	-0.202975	-4.578343	-0.304162	H	1.555975	2.180971	0.142116
C	-4.409463	1.014560	0.084955	H	3.183455	2.057176	0.815380
H	-4.107398	0.750620	-0.933635	C	2.811158	3.094434	-1.840592
C	-6.132468	1.233541	1.772351	H	1.752833	3.346452	-1.692807
H	-7.180598	1.148344	2.072315	H	2.983840	2.985290	-2.922337
C	-5.172756	1.657565	2.693259	C	3.741521	4.142320	-1.257431
H	-5.463586	1.900468	3.718984	H	3.534523	5.095261	-1.769858
C	-3.834919	1.777872	2.311803	H	3.510278	4.306068	-0.190991
H	-3.102180	2.111658	3.048072	C	5.200744	3.730668	-1.428708
C	-3.501341	-1.875418	1.835966	H	5.868861	4.464662	-0.950620
H	-2.705495	-1.455838	2.455558	H	5.454693	3.722591	-2.503705
C	-4.750307	-2.121323	2.405847	C	5.429900	2.342042	-0.838459
H	-4.916613	-1.890067	3.461318	H	5.348816	2.386131	0.260761
C	-5.781564	-2.663526	1.634675	H	6.447994	1.984453	-1.057893
H	-6.758517	-2.860838	2.084433	C	4.457266	1.311813	-1.393041
C	1.051299	-0.486145	-3.121623	H	4.623863	1.156028	-2.469434
O	0.526971	-1.120350	-2.155668	H	4.568828	0.342839	-0.884412
O	0.924583	0.737446	-3.310099	C	3.805716	-1.599486	1.599961
H	1.660541	-1.089277	-3.825663	H	3.965447	-2.073996	2.594697
H	0.115635	1.660502	-1.327548	H	3.193066	-2.311626	1.026035
H	0.224473	1.105438	-2.074561	C	6.114038	-0.940490	1.809743
<b>C</b>				H	6.265554	-1.654441	2.654265
scf done: -3557.926632				H	5.768542	0.001836	2.264058
Ir	-0.621787	0.199963	-0.888669	C	7.446347	-0.719352	1.104453
Cl	-2.070261	0.585672	-2.927293	H	8.190835	-0.379996	1.843746
P	-1.655472	1.770994	0.324777	H	7.339637	0.094271	0.366268
P	-1.631083	-1.928649	-0.251954	C	7.913117	-1.991704	0.403761
N	3.024458	1.730962	-1.256643	H	8.168509	-2.753743	1.163024
N	5.079180	-1.442789	0.909864	H	8.832837	-1.805860	-0.175842
C	0.610530	-0.079747	0.800163	C	6.804791	-2.530081	-0.496973
C	0.332321	0.917700	1.917172	H	6.646801	-1.839707	-1.344589
C	-0.628008	1.926793	1.838959	H	7.088132	-3.503841	-0.929831
C	-0.722985	2.867194	2.880417	C	5.497082	-2.688084	0.269970
H	-1.447088	3.683417	2.833535	H	4.696246	-3.012671	-0.414251
C	0.116667	2.760349	3.989566	H	5.615050	-3.501041	1.025212
H	0.041871	3.495898	4.795423	C	-1.796995	3.471790	-0.392797
C	1.041750	1.710019	4.091593	C	-1.196208	3.790947	-1.617725
H	1.674114	1.621784	4.980230	H	-0.669897	3.010061	-2.169905
C	1.146108	0.782543	3.058253	C	-1.293744	5.083502	-2.139995
C	2.043618	-0.434257	3.003447	H	-0.823529	5.314630	-3.100039
H	2.604631	-0.579100	3.936975	C	-1.992486	6.072177	-1.445843
C	1.151746	-1.608866	2.684846	H	-2.067218	7.083837	-1.854660
C	1.014429	-2.764721	3.446786	C	-2.609412	5.759035	-0.231883
H	1.604089	-2.893286	4.359476	H	-3.171325	6.522973	0.312779
C	0.095138	-3.747544	3.056735	C	-2.521561	4.466380	0.286708
				H	-3.035680	4.236340	1.223110

C	-3.393760	1.512108	0.879000	H	1.634749	1.476633	5.127029
C	-5.680180	1.042107	0.212310	C	1.136334	0.726662	3.162402
H	-6.402492	0.787555	-0.568381	C	2.053072	-0.465662	3.058308
C	-3.316601	-2.238635	0.451083	H	2.616579	-0.635580	3.986027
C	-5.621631	-2.988786	0.237984	C	1.191321	-1.647912	2.687017
H	-6.418780	-3.409387	-0.381588	C	1.094442	-2.844869	3.389569
C	-4.361273	-2.767803	-0.322442	H	1.687658	-2.997522	4.296176
H	-4.197958	-3.028022	-1.370027	C	0.215253	-3.842247	2.946460
C	-1.506616	-3.253533	-1.532456	H	0.125488	-4.779533	3.502625
C	-2.089037	-3.004603	-2.787367	C	-0.569897	-3.626576	1.817572
H	-2.545679	-2.030036	-2.987459	H	-1.292982	-4.386296	1.509876
C	-2.045579	-3.972087	-3.792584	C	-0.459281	-2.424108	1.093250
H	-2.506336	-3.764252	-4.762714	C	0.435577	-1.434407	1.514416
C	-1.403097	-5.192315	-3.568386	C	2.184147	0.098203	0.571512
H	-1.365571	-5.948289	-4.357921	H	2.423240	-0.660474	-0.187461
C	-0.796584	-5.434454	-2.334804	C	3.013489	-0.239132	1.858141
H	-0.275746	-6.379258	-2.154448	H	3.624513	0.638245	2.118861
C	-0.847009	-4.472207	-1.322255	C	2.586247	1.483134	-0.010743
H	-0.355967	-4.680486	-0.369845	H	1.791862	2.211441	0.213261
C	-4.331406	1.182005	-0.114482	H	3.478859	1.843649	0.539685
H	-3.993178	1.032743	-1.146040	C	2.579827	2.785381	-2.103739
C	-6.107903	1.225757	1.530594	H	1.624067	3.200975	-1.747024
H	-7.166581	1.120468	1.783844	H	2.450618	2.596398	-3.187113
C	-5.177312	1.532845	2.523998	C	3.715863	3.797795	-1.922828
H	-5.502501	1.664665	3.559875	H	3.485126	4.716700	-2.489280
C	-3.823764	1.671226	2.202781	H	3.785500	4.094392	-0.860450
H	-3.109336	1.905556	2.994513	C	5.043321	3.193710	-2.381924
C	-3.572724	-1.918835	1.795303	H	5.880903	3.883602	-2.181650
H	-2.781000	-1.498724	2.420340	H	5.013477	3.051018	-3.478821
C	-4.830314	-2.148360	2.354857	C	5.279246	1.843591	-1.705466
H	-5.004649	-1.905478	3.406647	H	5.469404	1.999818	-0.628965
C	-5.859751	-2.687616	1.579478	H	6.180382	1.353541	-2.111979
H	-6.843592	-2.871068	2.020152	C	4.069874	0.917307	-1.884467
C	1.442605	-0.935793	-2.956251	H	3.981476	0.656982	-2.956708
O	0.553023	-1.195193	-2.095873	H	4.234004	-0.026735	-1.342623
O	2.002959	0.151757	-3.182238	C	3.946652	-1.452983	1.715882
H	1.744903	-1.816870	-3.573421	H	4.108071	-1.900887	2.724141
H	2.475879	1.086733	-1.893001	H	3.433898	-2.227902	1.124384
H	0.275910	1.444327	-1.349636	C	6.143419	-0.493865	1.991239
<b>C'</b>				H	6.315951	-1.107942	2.907833
scf done: -3557.903458				H	5.670457	0.440852	2.331052
Ir	-0.667416	0.288793	-0.774432	C	7.487735	-0.182694	1.343679
Cl	-2.137213	0.830937	-2.813721	H	8.138698	0.306860	2.087039
P	-1.736894	1.739829	0.537537	H	7.339258	0.543472	0.525853
P	-1.536696	-1.944943	-0.301596	C	8.142002	-1.447454	0.795902
N	2.805194	1.501350	-1.452401	H	8.433771	-2.102158	1.637967
N	5.232924	-1.188910	1.085088	H	9.070251	-1.204803	0.251970
C	0.615555	-0.055796	0.867790	C	7.163761	-2.193254	-0.107033
C	0.330607	0.895535	2.021817	H	6.989310	-1.610311	-1.028721
C	-0.673514	1.863781	2.013383	H	7.580022	-3.164894	-0.421308
C	-0.802422	2.750660	3.096996	C	5.833006	-2.428632	0.597313
H	-1.558973	3.539669	3.083108	H	5.121958	-2.911867	-0.092587
C	0.046643	2.622609	4.195646	H	5.991853	-3.146100	1.437818
H	-0.047791	3.315034	5.036784	C	-1.885785	3.466382	-0.101980
C	1.002475	1.596017	4.241951	C	-0.760509	4.305012	-0.050604
				H	0.172724	3.943971	0.389304

C	-0.821387	5.605679	-0.551423	H	0.139196	-6.174479	-2.435912
H	0.062303	6.247489	-0.497674	C	-0.576822	-4.367418	-1.500233
C	-2.005157	6.084981	-1.118425	H	-0.169658	-4.645872	-0.526357
H	-2.052270	7.103836	-1.512836	C	-4.370878	0.935050	0.110569
C	-3.127465	5.257891	-1.174053	H	-4.034052	0.765886	-0.916452
H	-4.059518	5.624572	-1.613028	C	-6.142473	0.926251	1.760059
C	-3.071227	3.957570	-0.665539	H	-7.190219	0.757763	2.024062
H	-3.964937	3.332434	-0.711758	C	-5.230773	1.333229	2.735760
C	-3.454580	1.371767	1.082340	H	-5.559637	1.480352	3.768309
C	-5.708612	0.723789	0.447837	C	-3.893547	1.558488	2.400624
H	-6.413706	0.393261	-0.319596	H	-3.197590	1.878124	3.178189
C	-3.219767	-2.399493	0.309718	C	-3.548119	-2.164859	1.655911
C	-5.463048	-3.266602	-0.046076	H	-2.809131	-1.731863	2.334639
H	-6.207950	-3.698689	-0.720285	C	-4.812352	-2.494390	2.145454
C	-4.195257	-2.945448	-0.537619	H	-5.045671	-2.316906	3.198901
H	-3.969791	-3.137827	-1.588994	C	-5.774203	-3.048868	1.296871
C	-1.259208	-3.154017	-1.667104	H	-6.763563	-3.310282	1.682430
C	-1.741281	-2.815201	-2.943426	C	1.105468	-0.580631	-3.210196
H	-2.231471	-1.849338	-3.100313	O	0.736548	-0.884422	-2.079743
C	-1.570756	-3.687999	-4.019554	O	0.531639	0.273012	-3.999734
H	-1.954344	-3.411709	-5.005852	H	1.990461	-1.065589	-3.658470
C	-0.900540	-4.900784	-3.841721	H	0.129044	1.644540	-1.065248
H	-0.761604	-5.581787	-4.686121	H	-0.344064	0.592393	-3.604843
C	-0.398321	-5.233278	-2.582313				