Supporting Information

Carbocyclic Pincer Carbene Complexes of Ruthenium: Syntheses and Reversible Hydrogenation

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Content

1 Experimental Section 2
2 Crystallographic Details 3
3 NMR Data 5
3.1 ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ spectra for compound **2** 5
3.2 ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ spectra for compound **3** 8
3.3 ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ spectra for compound **4** 11
3.4 ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ spectra for compound **5** 23
4 Quantum chemical calculations 26
5 References 28

1 Experimental Section

General procedure for the dehydrogenation of complex 4. Method A: BCH-P^{t}Bu$_2$-RuHCl **4** (0.033 mmol) was dissolved in toluene (15–20 mL) with or without an external chloride source (100 eq. NaCl, Et_4NCl or 10 eq. HCl×Et_2O). Subsequently the reaction mixture was heated under reflux for several days. Filtration, in case of excess of external chloride source, followed by evaporation of the solvent under reduced pressure and trituration with *n*-pentane (1 × 5 mL) results in the product mixture. Complex **2** was recovered in 49–79 % yield.

2 Crystallographic Details

Table 1S: Structure refinement table of compound **2**, **3**, **4**.

	2	**3**	**4**
Empirical formula	$C_{94}H_{146}Cl_6P_6Ru_3$ 3 × $C_{29}H_{47}Cl_2P_2Ru$ + 1 × C_7H_8	$C_{29}H_{47}ClP_2Ru$	$C_{29}H_{53}ClP_2Ru$
M [g·mol^{-1}]	1977.83	594.12	600.17
λ [Å]	0.71073	0.71073	0.71073
T [K]	100(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	*P*1	$P2_1/c$	*Cc*
Z	1	4	4
a [Å]	12.1104(2)	13.4968(5)	8.3945(2)
b [Å]	14.1717(3)	17.6039(6)	21.4072(5)
c [Å]	14.9865(3)	12.2964(5)	16.9249(4)
α [°]	67.4590(10)	90	90
β [°]	89.6070(10)	104.829(2)	95.5880(10)
γ [°]	88.4290(10)	90	90
V [Å^3]	2374.66(8)	2824.27(18)	3027.00(12)
D_c [g·cm^{-3}]	1.383	1.397	1.317
μ [mm^{-1}]	0.784	0.779	0.727
F(000)	1034	1248	1272
Crystal size [mm]	0.24 × 0.21 × 0.20	0.19 x 0.16 x 0.15	0.18 x 0.15 x 0.12
Θ range [°]	2.94 – 30.52	3.38 – 29.55	2.62 – 28.28
Limiting indices	−15 ≤ h ≤ 15 −18 ≤ k ≤ 18 −19 ≤ l ≤ 19	−18 ≤ h ≤ 17 −24 ≤ k ≤ 24 −17 ≤ l ≤ 17	−11 ≤ h ≤ 11 −28 ≤ k ≤ 28 −21 ≤ l ≤ 22
Reflections collected	69257	30789	25834
Independent	20132	7884	7213
R_{int}	0.0333	0.0254	0.0346
Completeness	99.5	99.4	99.2
Absorption correction	multi-scan	multi-scan	multi-scan
Max. , Min.	0.7461, 0.7213	0.7459, 0.7061	0.7457, 0.6920
Parameters/ restraints	1019/3	322/ 0	318/ 5
R_1, wR_2 [I>2σI]	0.0279, 0.0657	0.0247, 0.0593	0.0253, 0.0515
R_1, wR_2 (all data)	0.0297, 0.0667	0.0307, 0.0620	0.0289, 0.0526
GooF on F^2	1.037	1.033	1.008
Peak/ hole [e·Å^{-3}]	2.331, –0.754	0.806, –0.403	0.709, -0.351
Flack	0.010(8)		
CCDC	2036979	2036978	2036977

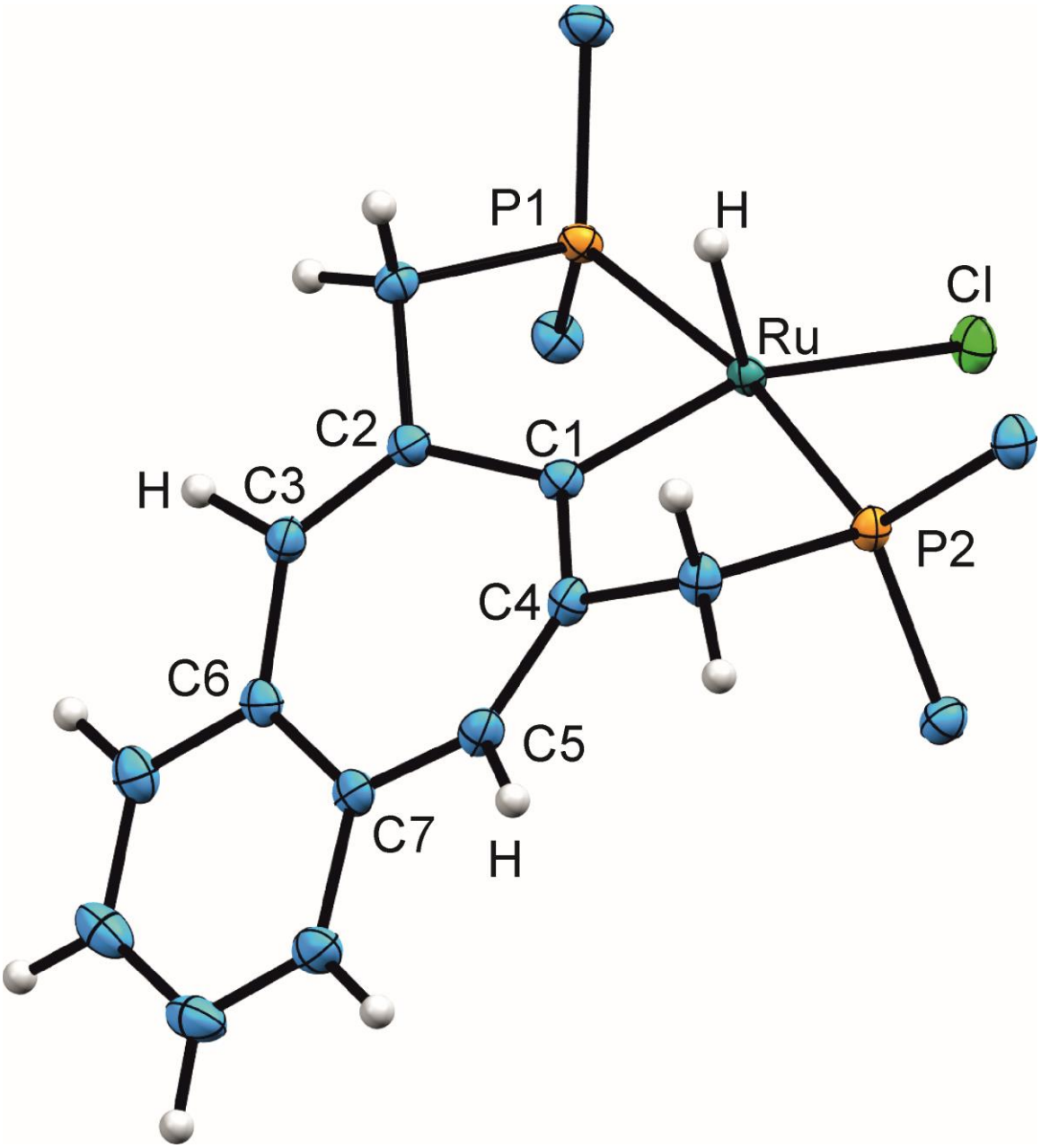
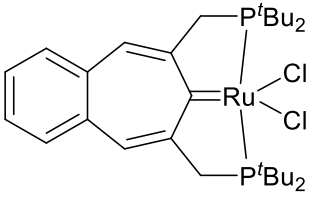


Figure S1. ORTEP (50% thermal ellipsoids) with selected atom labeling of **3**. ^{t}Bu groups were omitted for clarity. Selected interatomic distances [Å] and angles [deg]: H1-Ru 1.70(3), C–Ru 1.9286(15), P1–Ru 2.3311(4), P2–Ru 2.3267(4), Ru–Cl 2.4318(4), P2–Ru1–P1 169.183(14), H1–Ru–C 86.6(8), H1–Ru1–Cl 119.8(8), C–Ru–Cl 153.65(5), C1–C4 1.480(2), C1–C2 1.477(2), C2–C3 1.359(2), C4–C5 1.361(2), C5–C7 1.451(2), C3–C6 1.446(2), C6–C7 1.413(2).

3 NMR Data

3.1 ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ spectra for compound **2**



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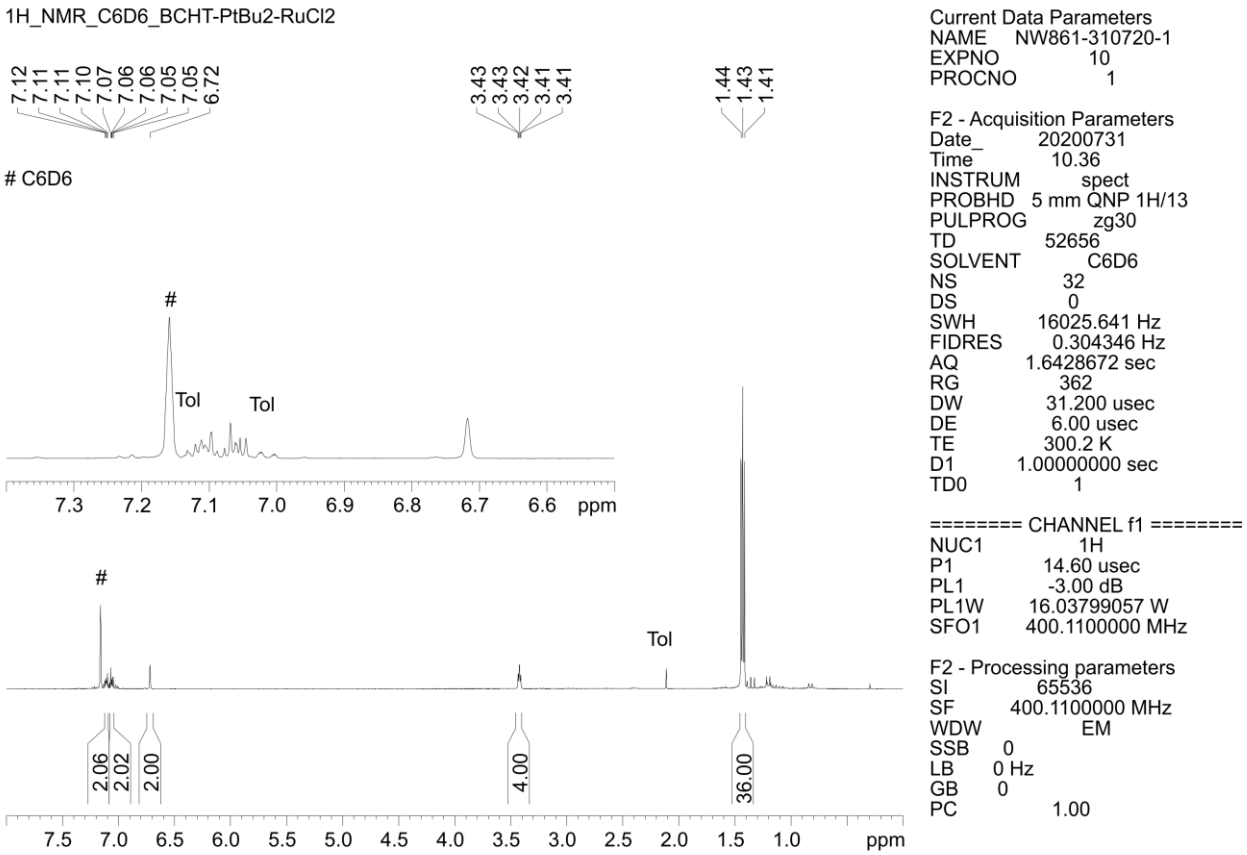


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D1          1.00000000 sec
TD0                 1

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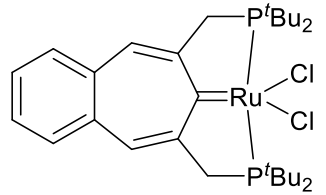
Figure S1. ^{1}H NMR spectrum of complex **2**.



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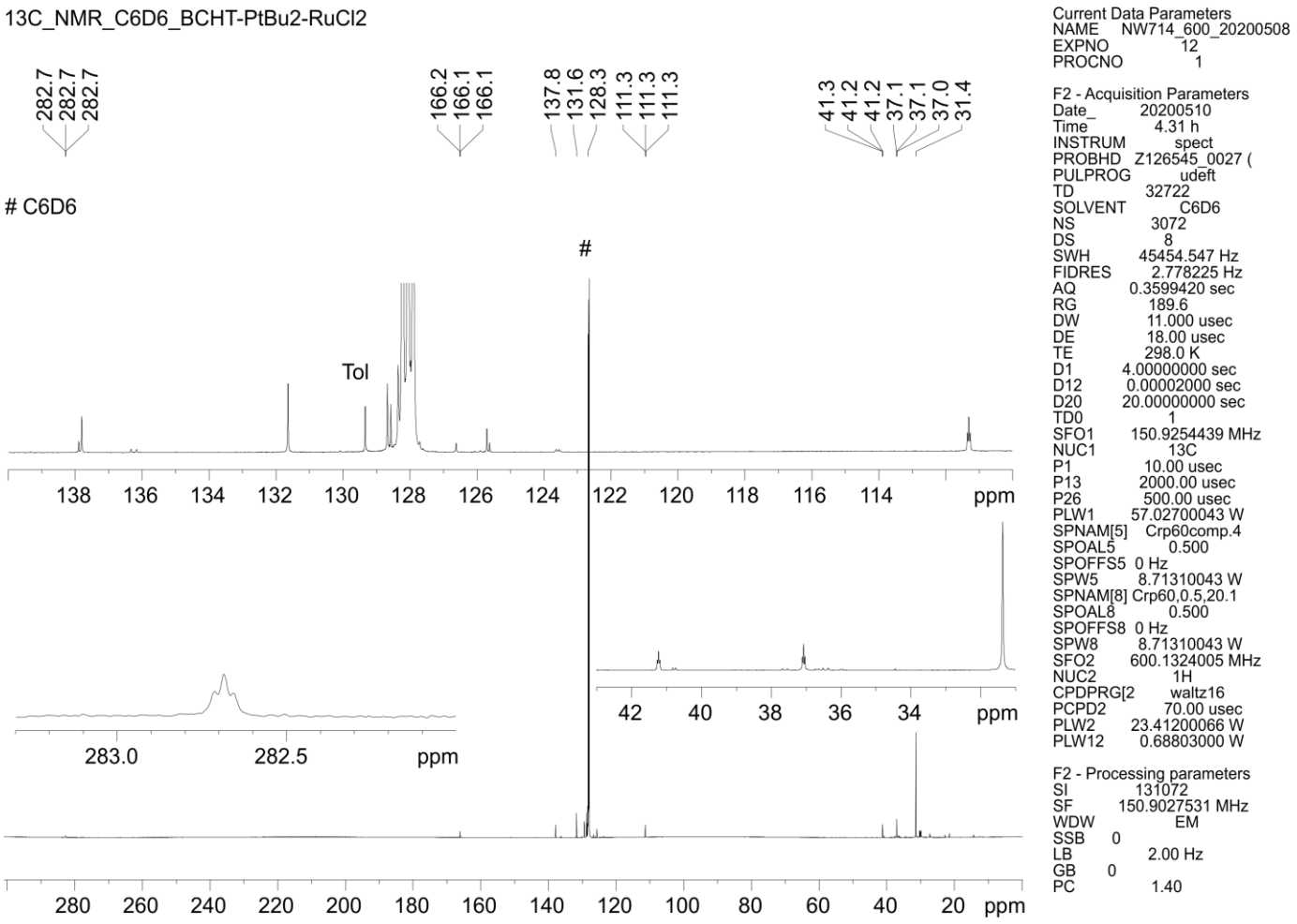

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D20 20.00000000 sec
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P13 2000.00 usec
P26 500.00 usec
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PLW12 0.68803000 W

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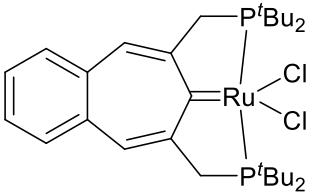
Figure S2. $^{13}C\{^1H\}$ NMR spectrum of complex **2**.



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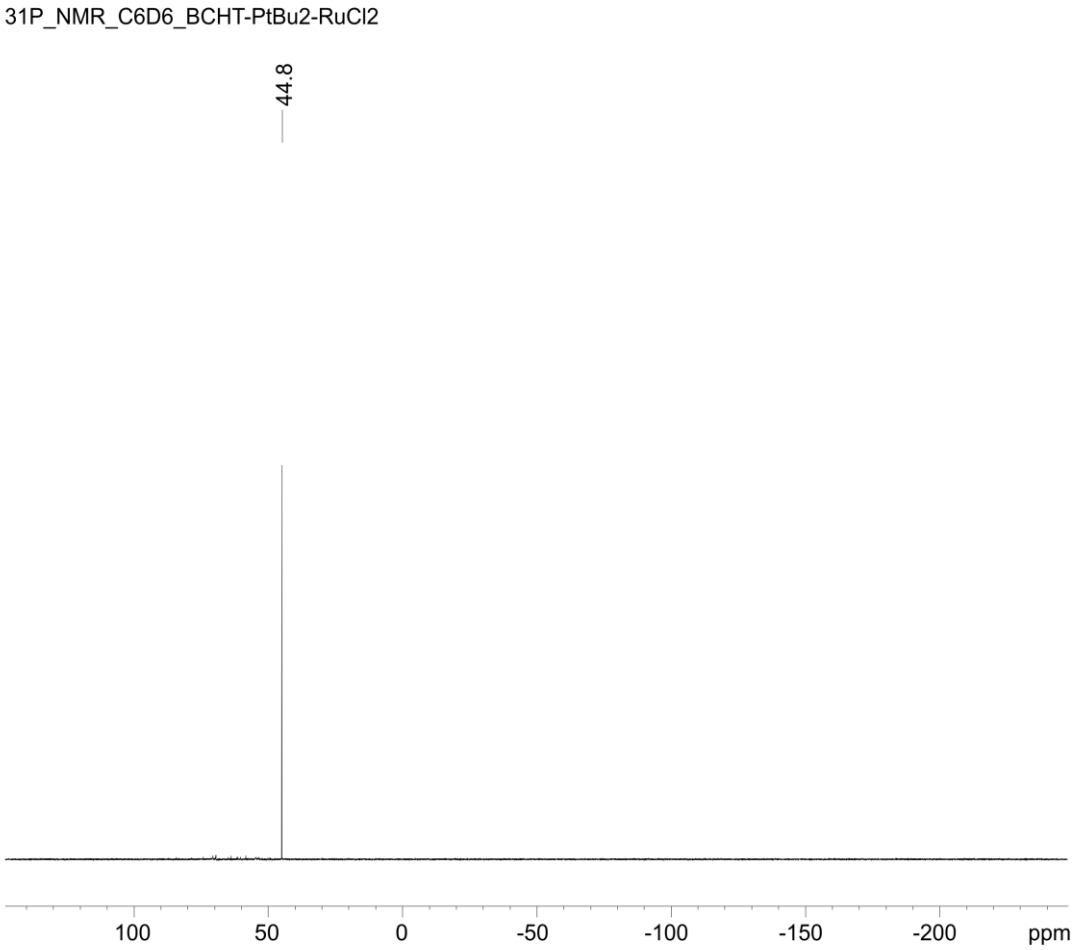


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TE               298.0 K
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D11          0.03000000 sec
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NUC1               31P
P1               12.00 usec
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NUC2               1H
CPDPRG[2         waltz16
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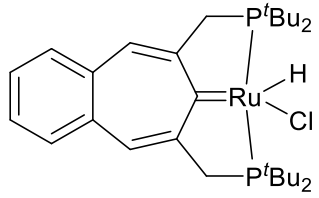
Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of complex **2**.



3

3.2 ^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H} spectra for compound **3**

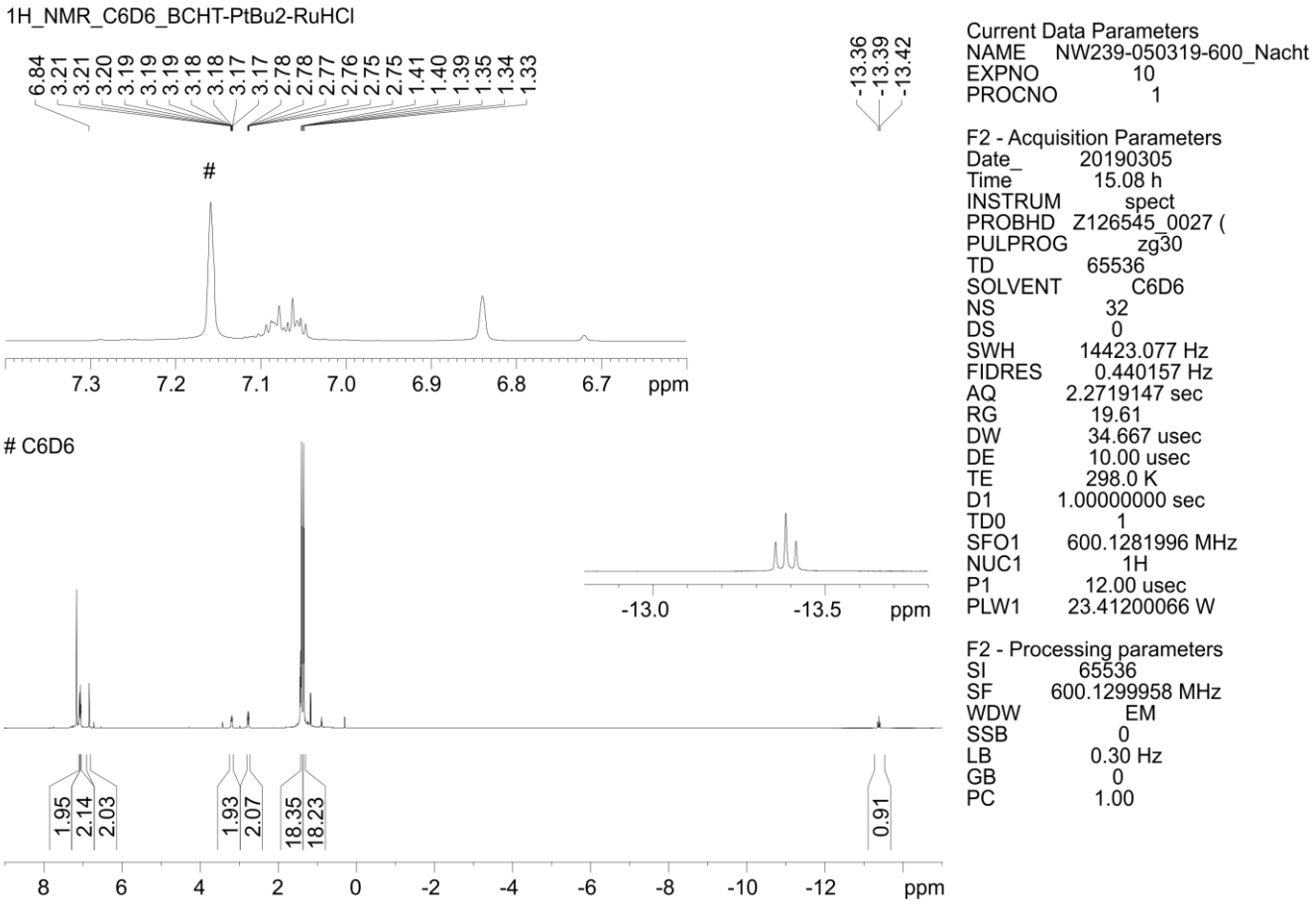
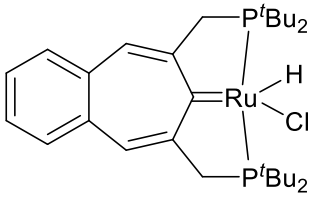


Figure S4. ^{1}H NMR spectrum of complex **3**.



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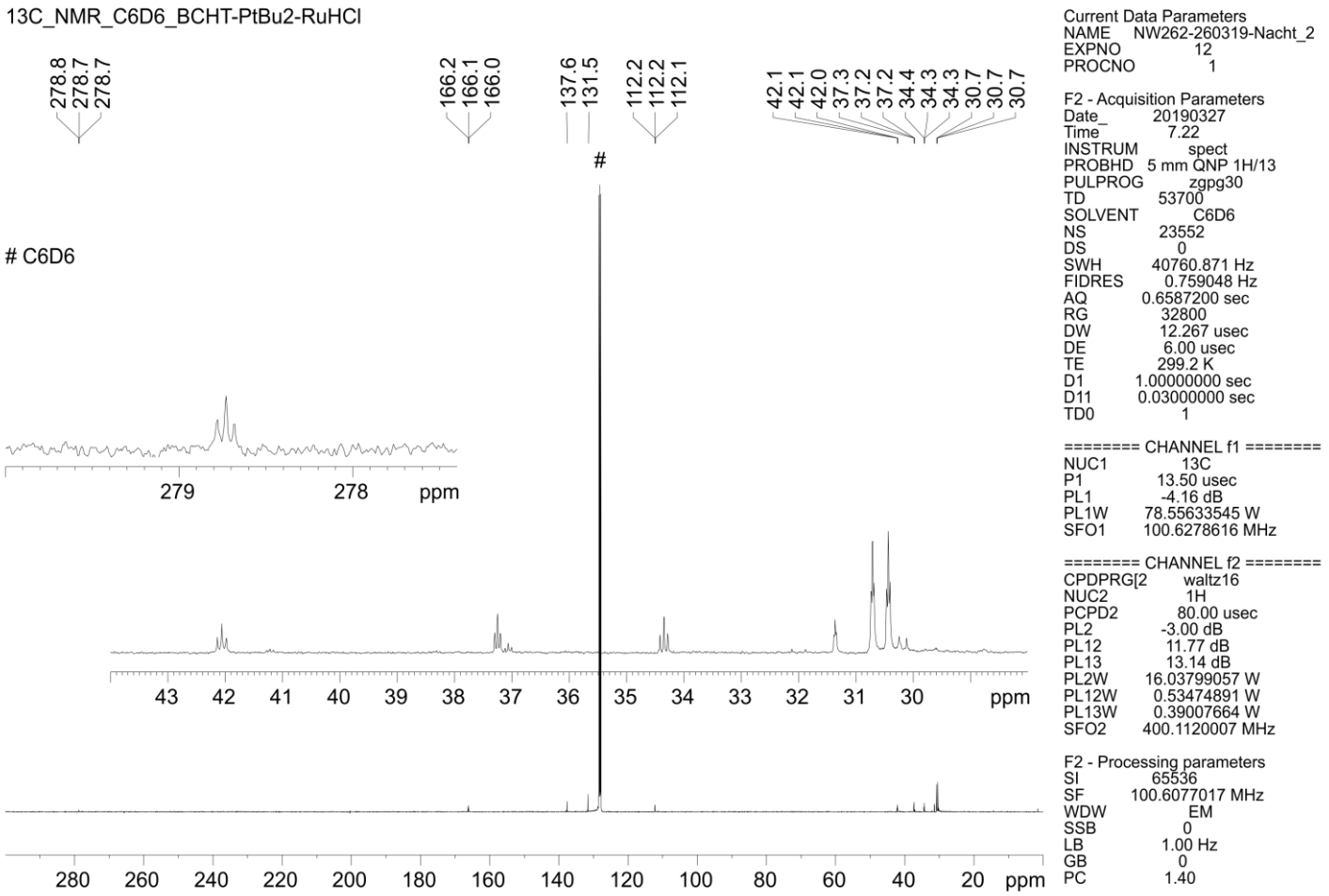

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D11 0.03000000 sec
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P1 13.50 usec
PL1 -4.16 dB
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======== CHANNEL f2 ========
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NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
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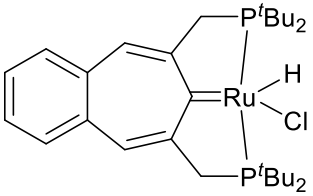
Figure S5. $^{13}C\{^1H\}$ NMR spectrum of complex **3**.



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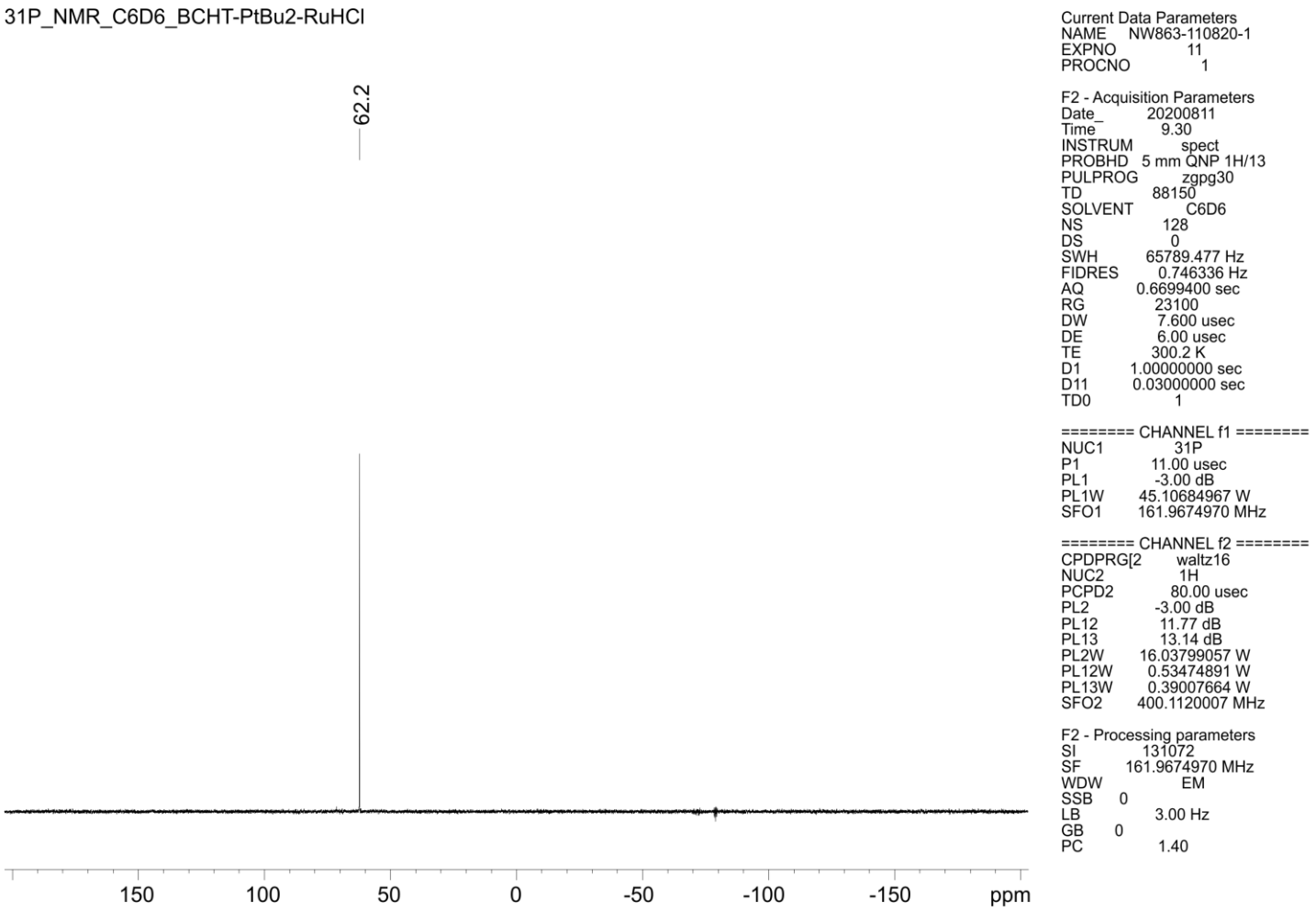

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DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
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P1 11.00 usec
PL1 -3.00 dB
PL1W 45.10684967 W
SFO1 161.9674970 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
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WDW EM
SSB 0
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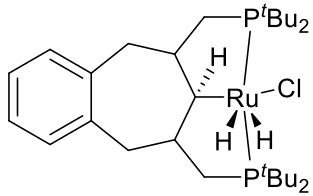
PC 1.40

Figure S6. $^{31}P\{^1H\}$ NMR spectrum of complex **3**.



4

3.3 ^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H} spectra for compound **4**

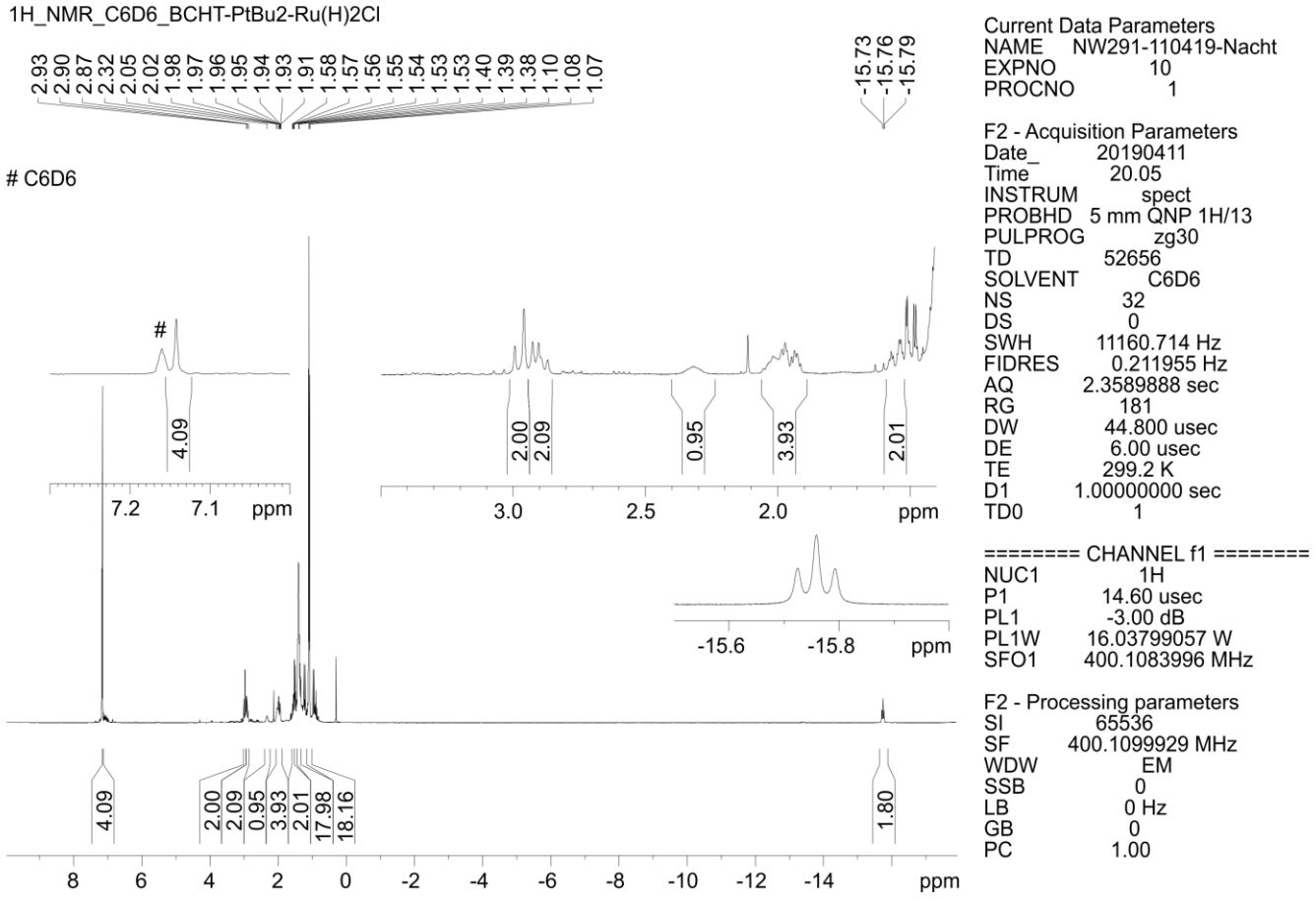
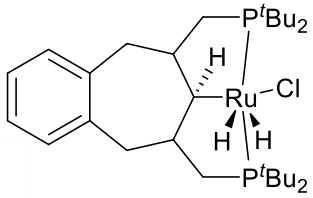


Figure S7. ^{1}H NMR spectrum of complex **4**.



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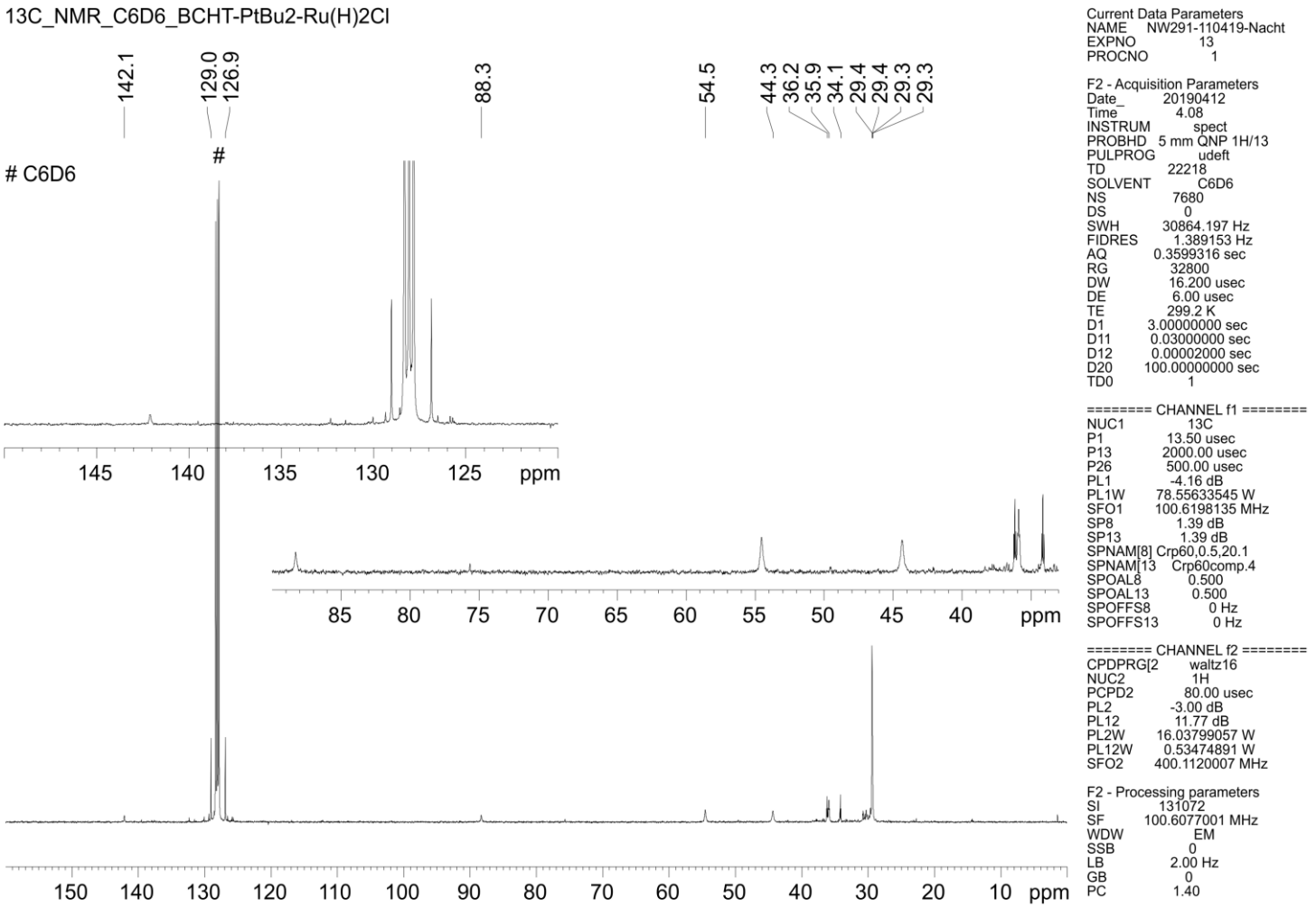
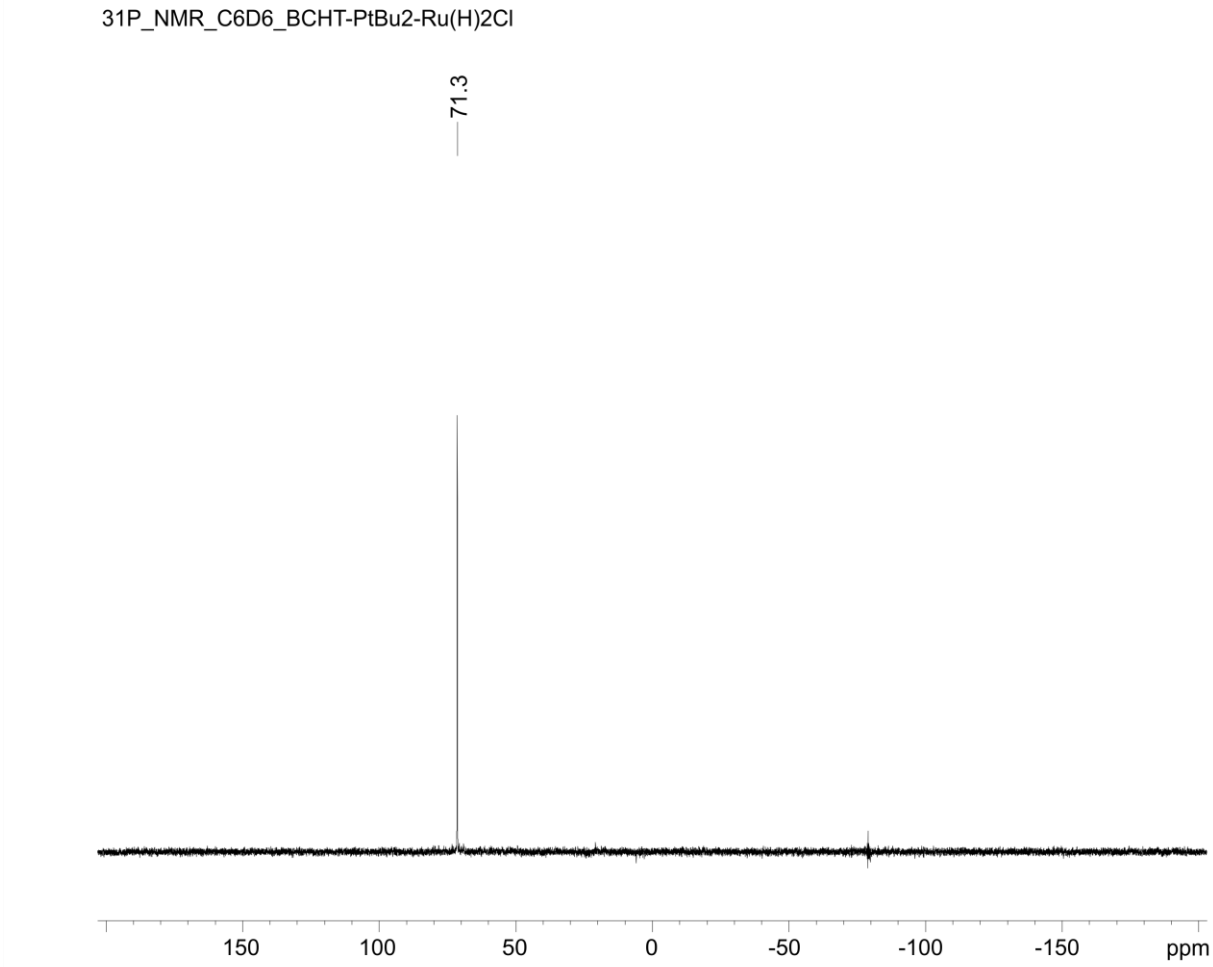


Figure S8. $^{13}C\{^1H\}$ NMR spectrum of complex **4**.



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FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 31P
P1 11.00 usec
PL1 -3.00 dB
PL1W 45.10684967 W
SFO1 161.9674970 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
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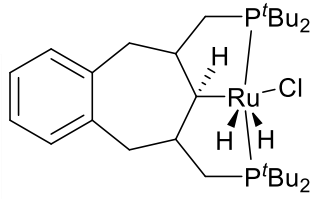
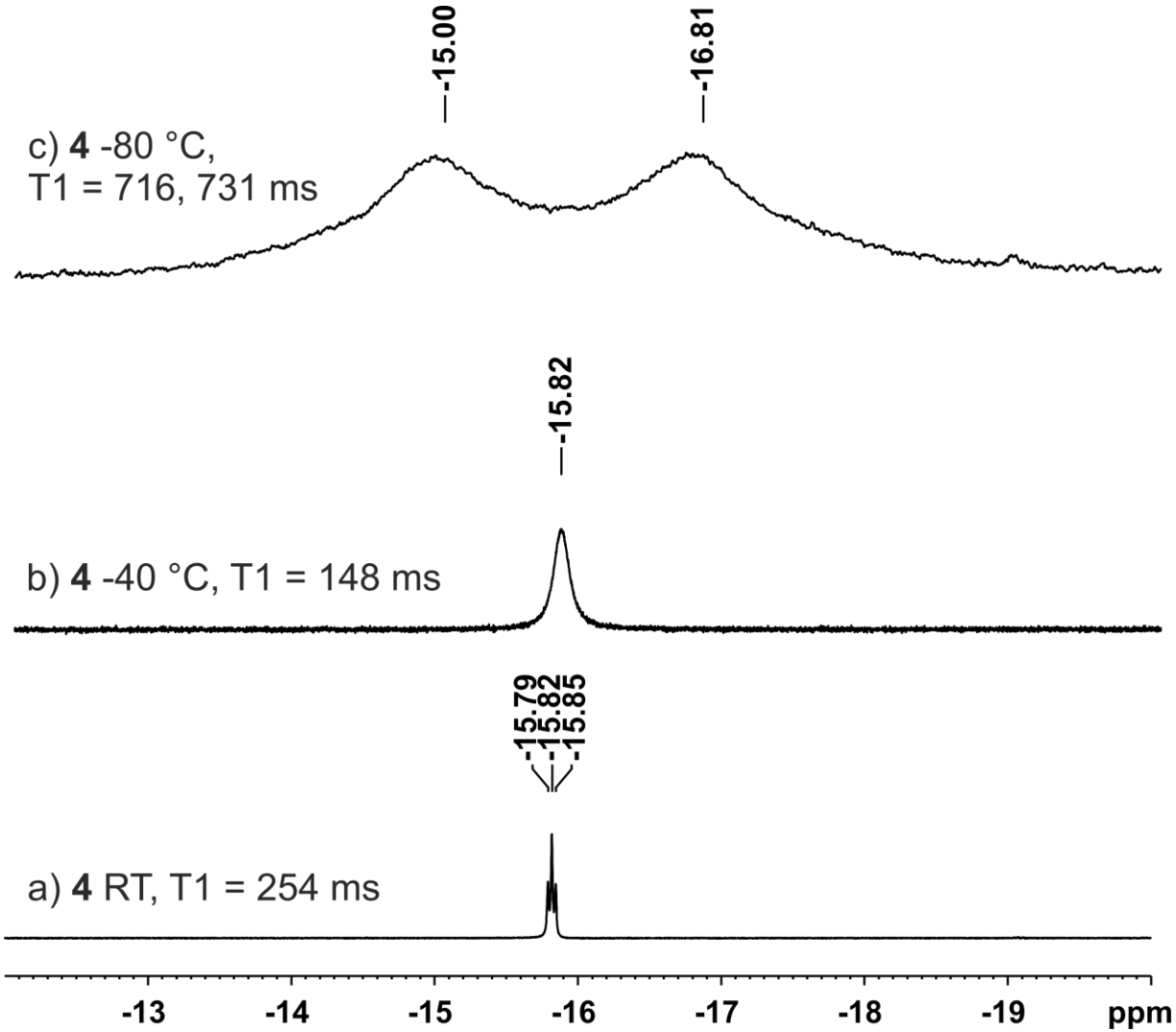


4

Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of complex **4**.



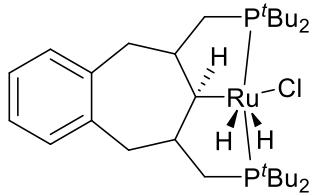


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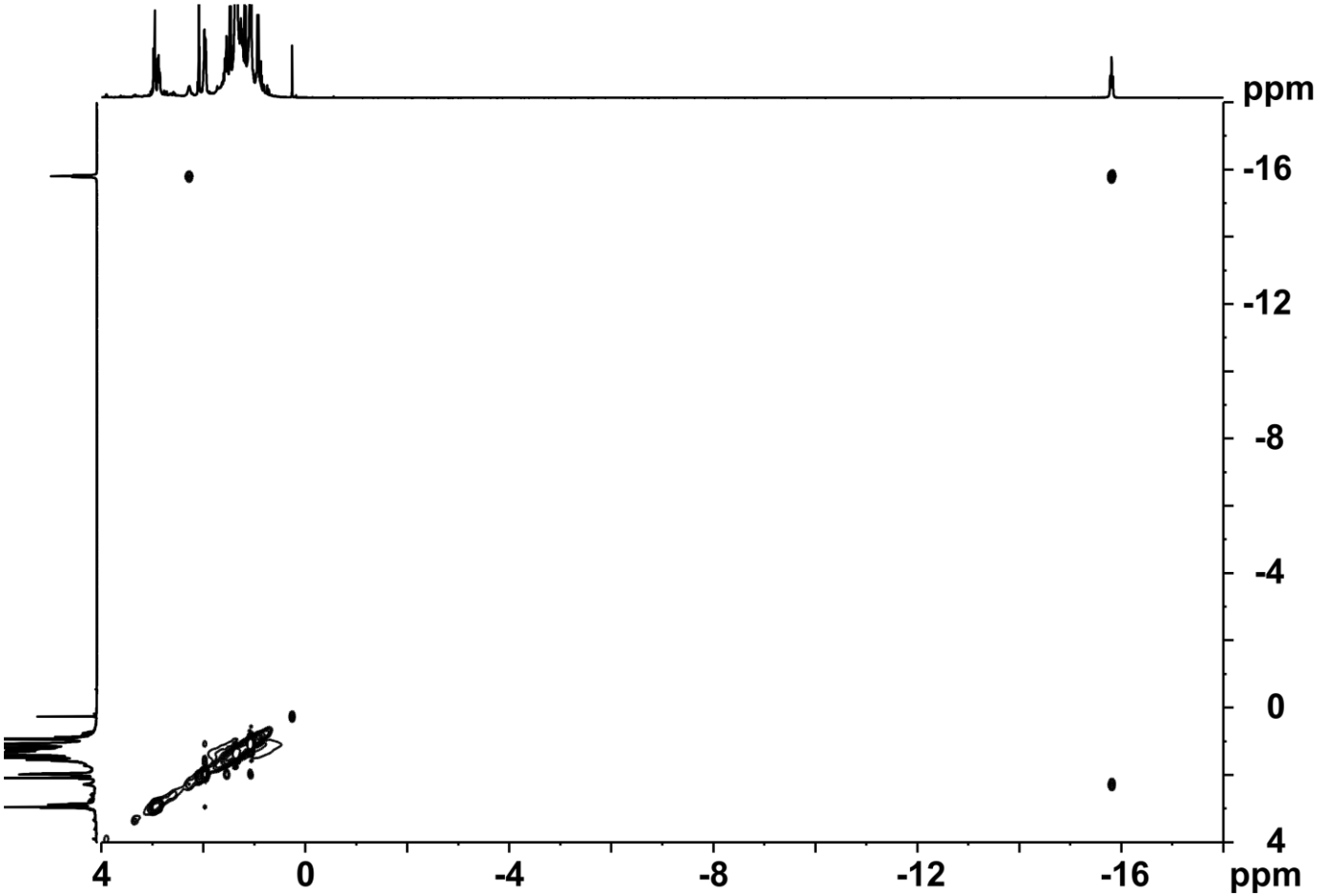
Figure S10. ^{1}H VT NMR and determination of relaxation times of the Ru-H units.



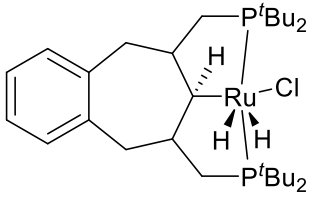


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Figure S11. ^{1}H NOESY of **4** showing the exchange of the protons of the CH and RuH units.

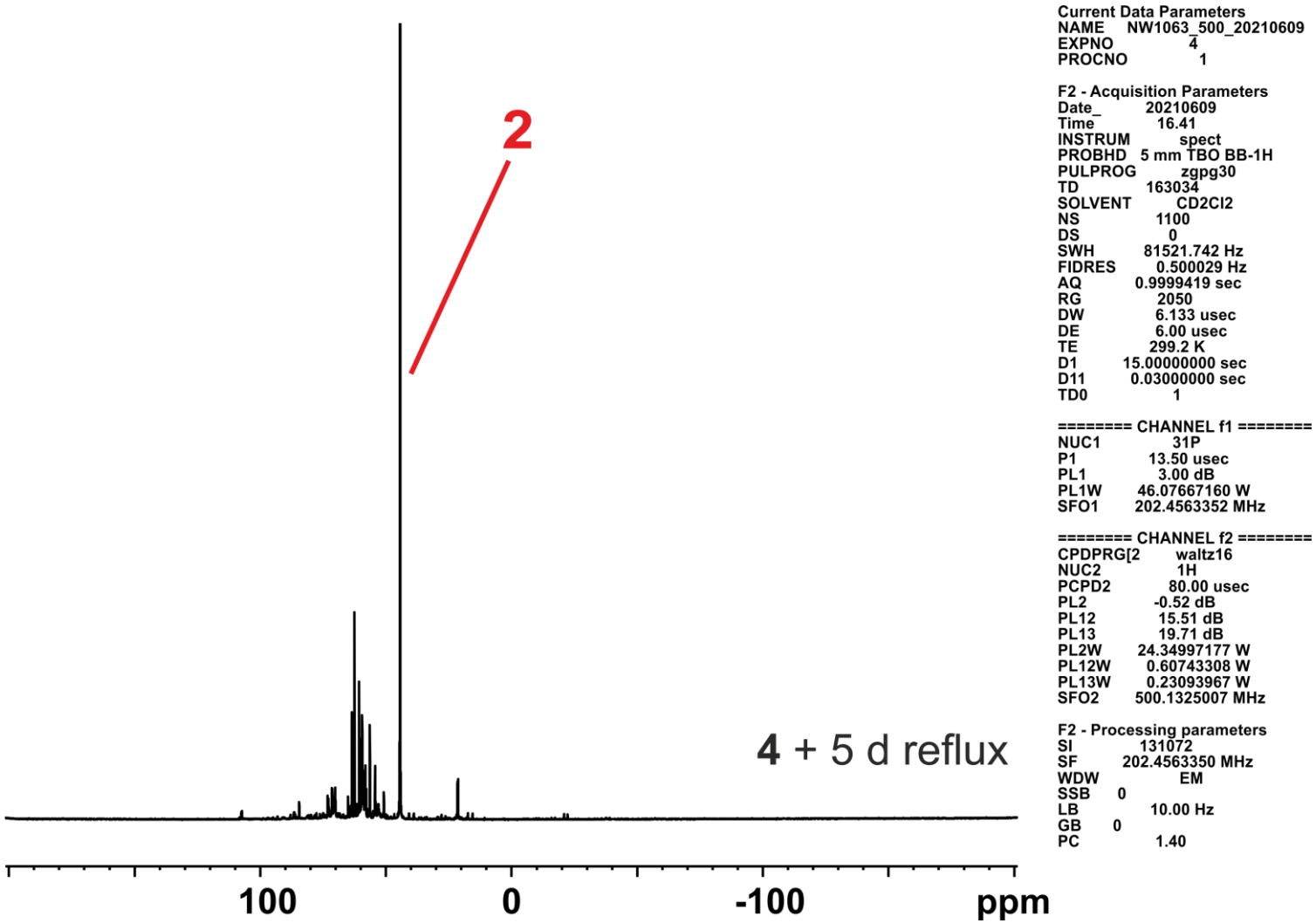


Figure S12. $^{31}P\{^{1}H\}$ NMR spectra of the dehydrogenation of **4** after 5 days under reflux in toluene. D1 was adjusted according to the longest spin lattice relaxation time.

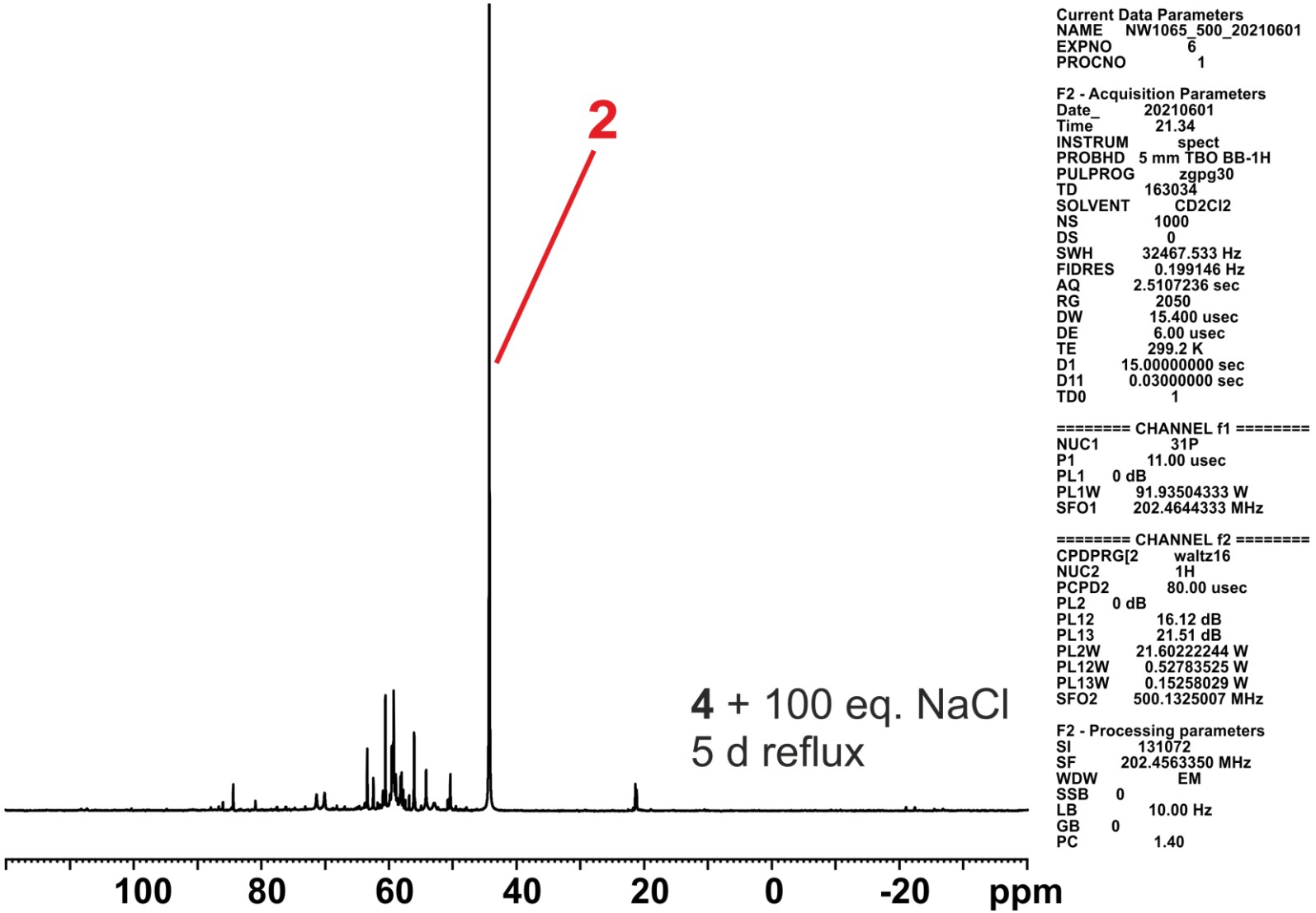


Figure S13. $^{31}P\{^{1}H\}$ NMR spectra of the dehydrogenation of **4** after 5 days under reflux in toluene. D1 was adjusted according to the longest spin lattice relaxation time.

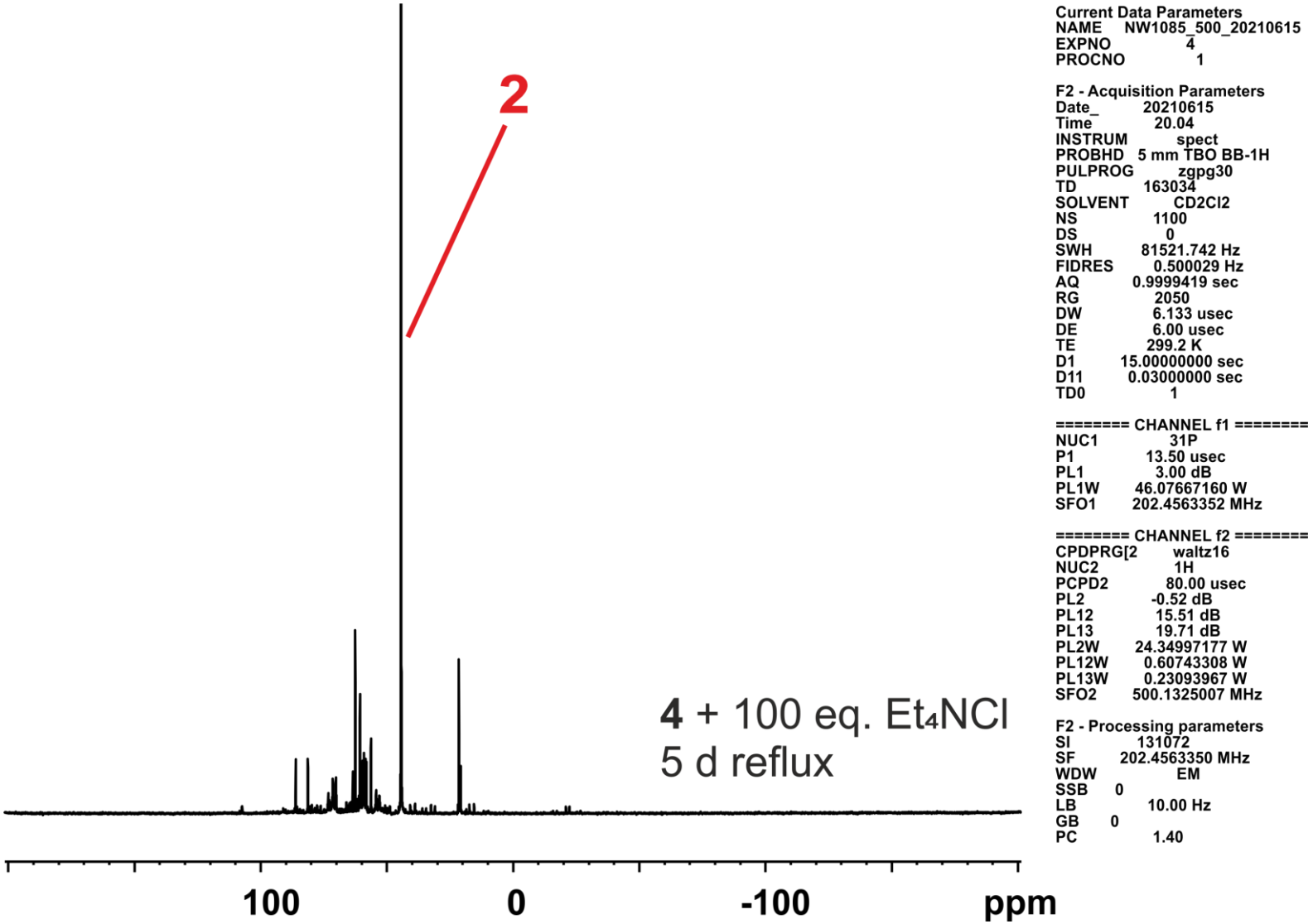


Figure S14. $^{31}P\{^{1}H\}$ NMR spectra of the dehydrogenation of **4** after 5 days under reflux in toluene. D1 was adjusted according to the longest spin lattice relaxation time.

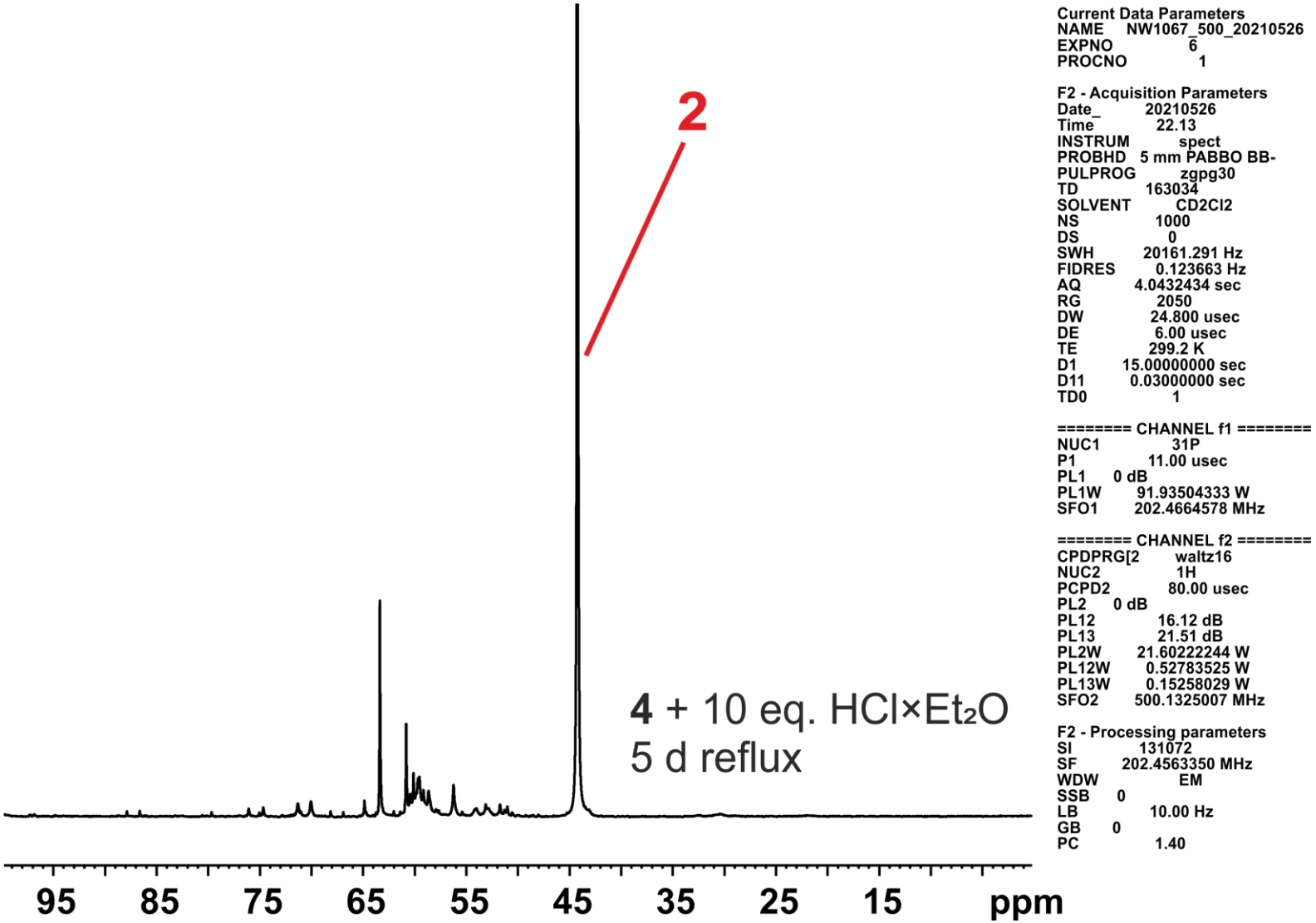


Figure S15. $^{31}P\{^{1}H\}$ NMR spectra of the dehydrogenation of **4** after 5 days under reflux in toluene. D1 was adjusted according to the longest spin lattice relaxation time.

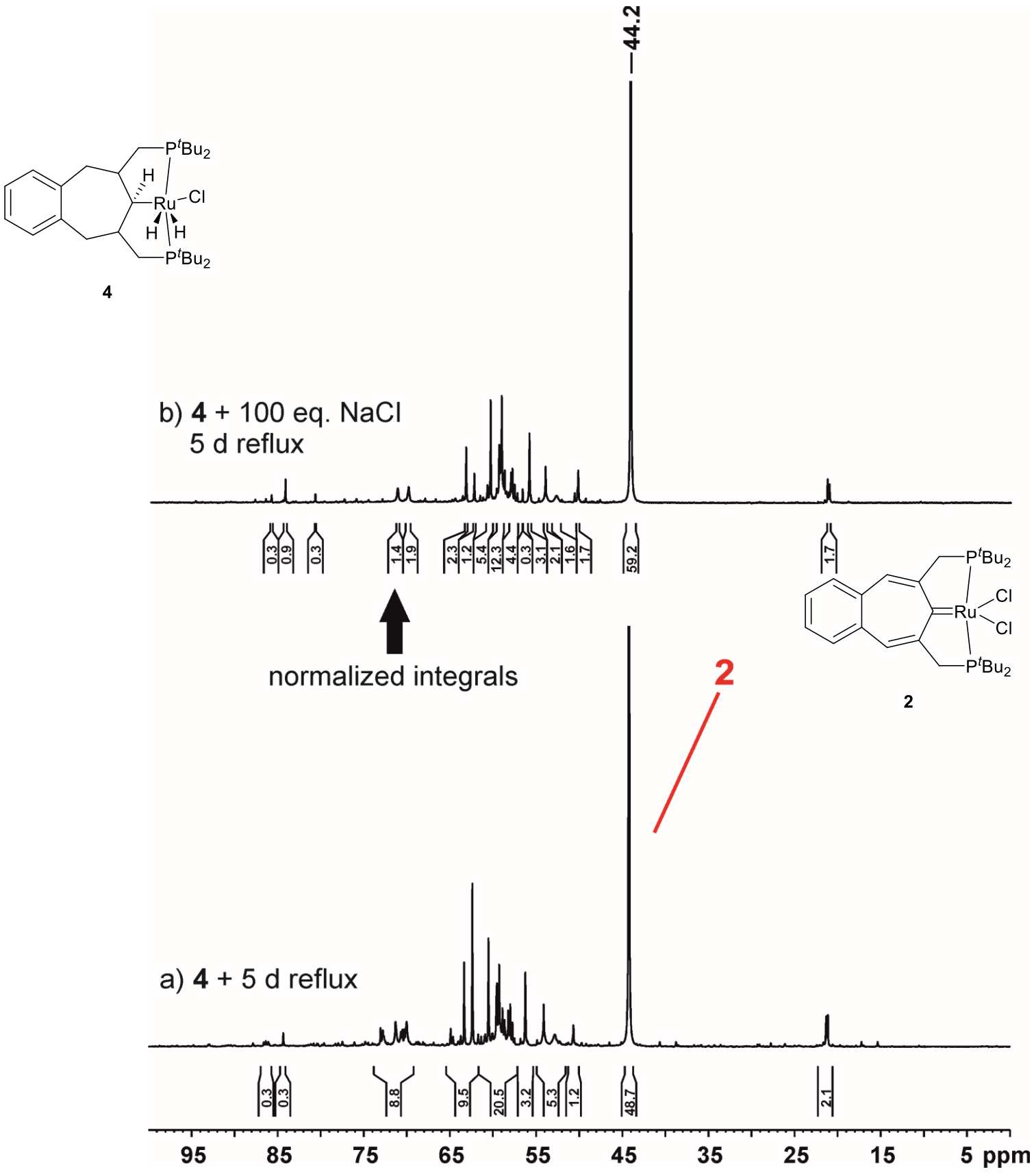


Figure S16. $^{31}P\{^1H\}$ NMR spectra of the dehydrogenation of **4** after 5 days under reflux in toluene. D1 was adjusted according to the longest spin lattice relaxation time.

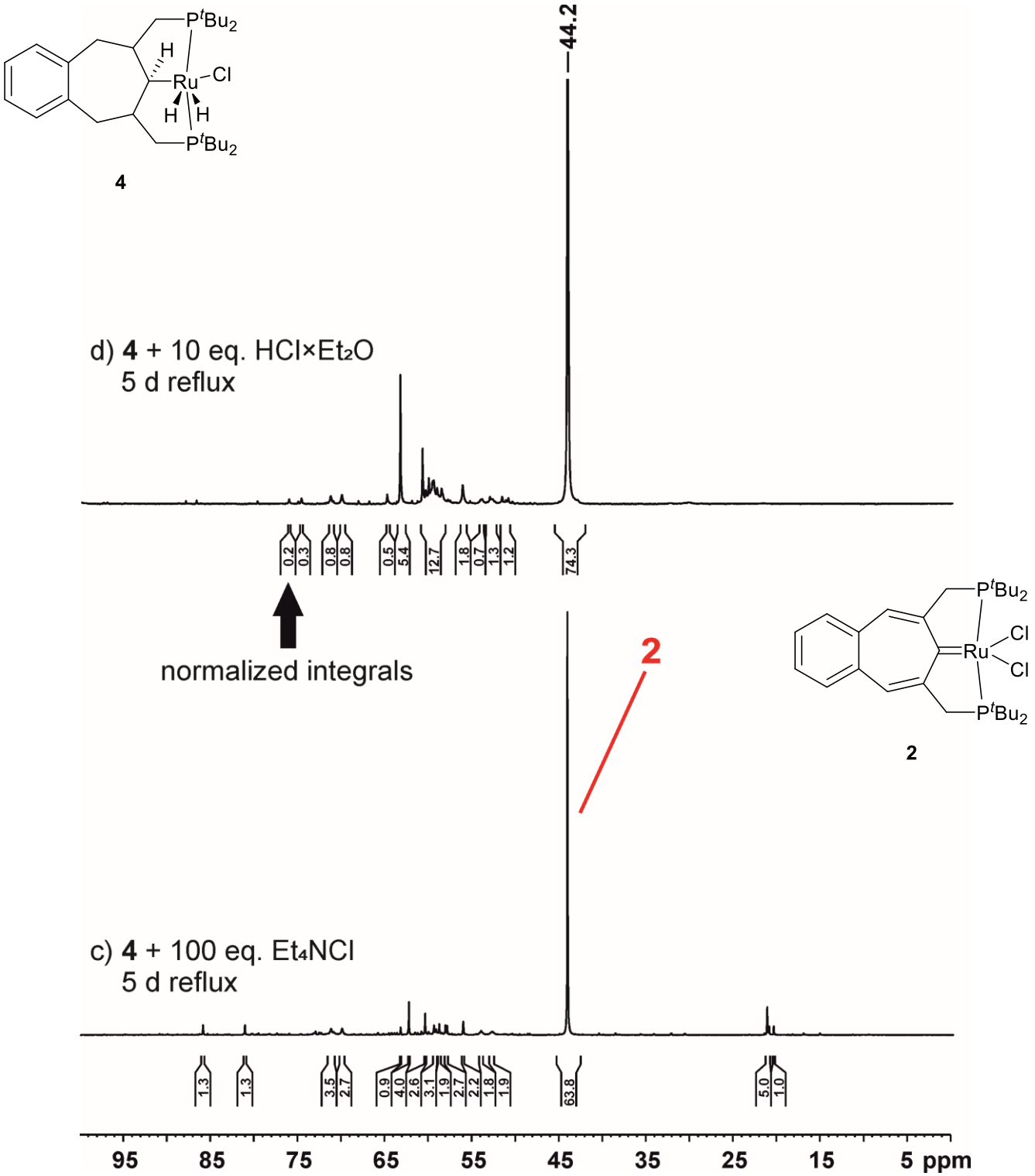


Figure S17. $^{31}P\{^1H\}$ NMR spectra of the dehydrogenation of **4** after 5 days under reflux in toluene. D1 was adjusted according to the longest spin lattice relaxation time.

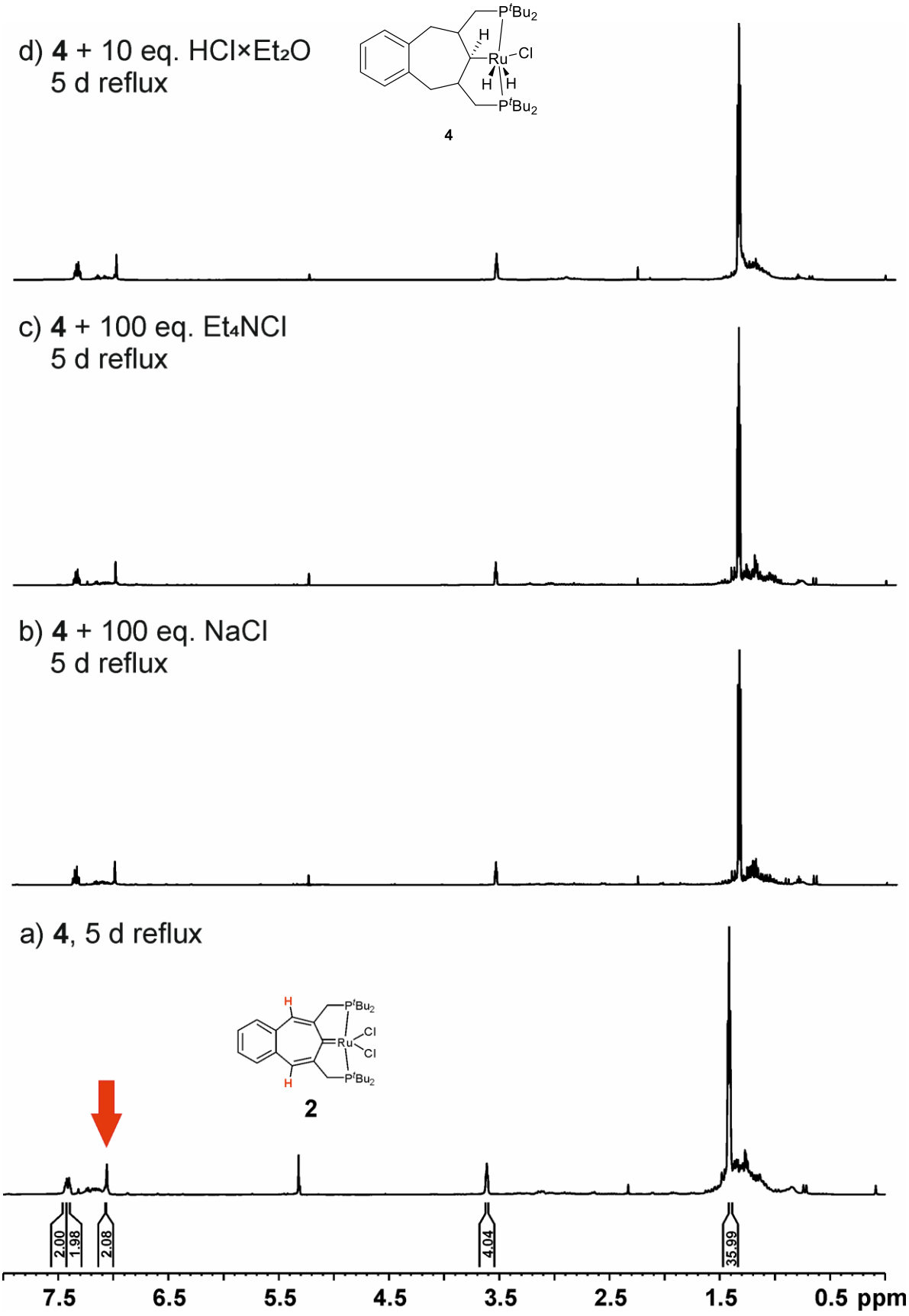
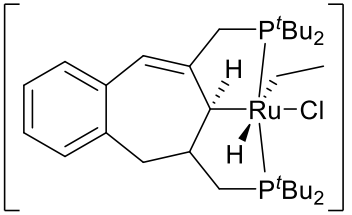


Figure S18. ^{1}H NMR spectra of the dehydrogenation of **4** after 5 days under reflux in toluene.

3.4 ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ spectra for compound **5**



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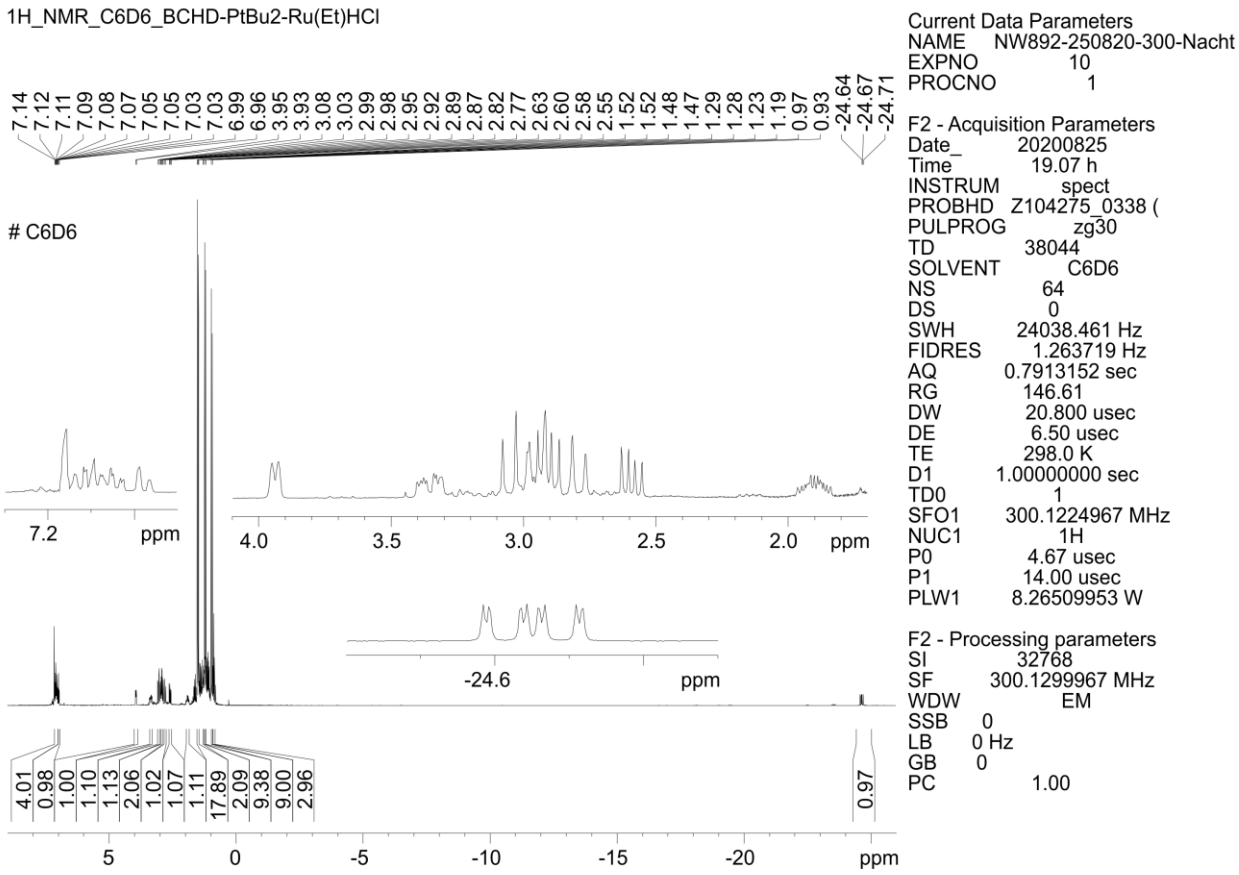
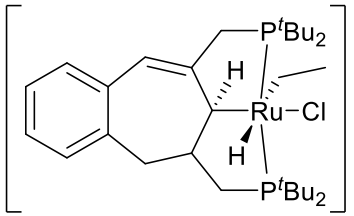


Figure S19. ^{1}H NMR spectrum of complex **5**.



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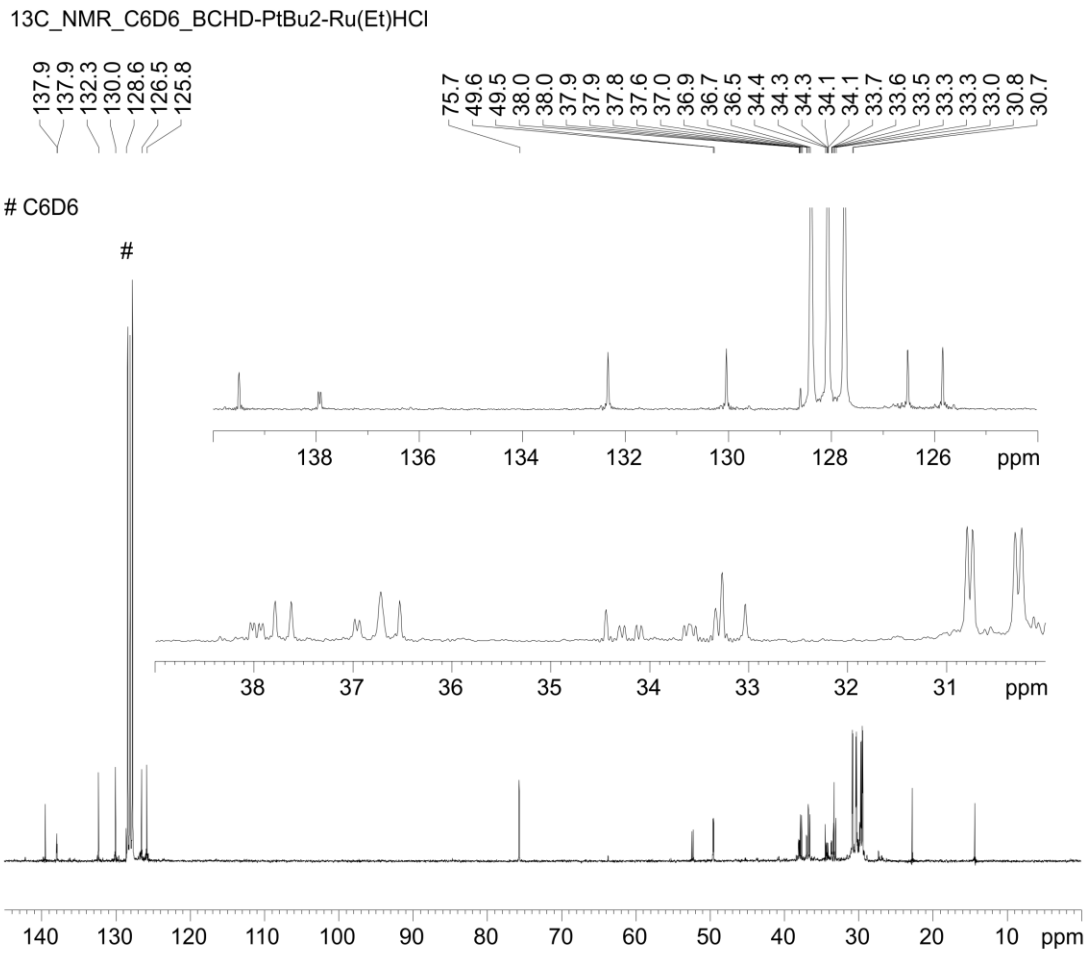

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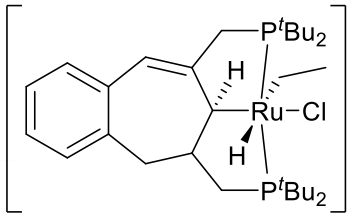
Figure S20. $^{13}C\{^1H\}$ NMR spectrum of complex **5**.



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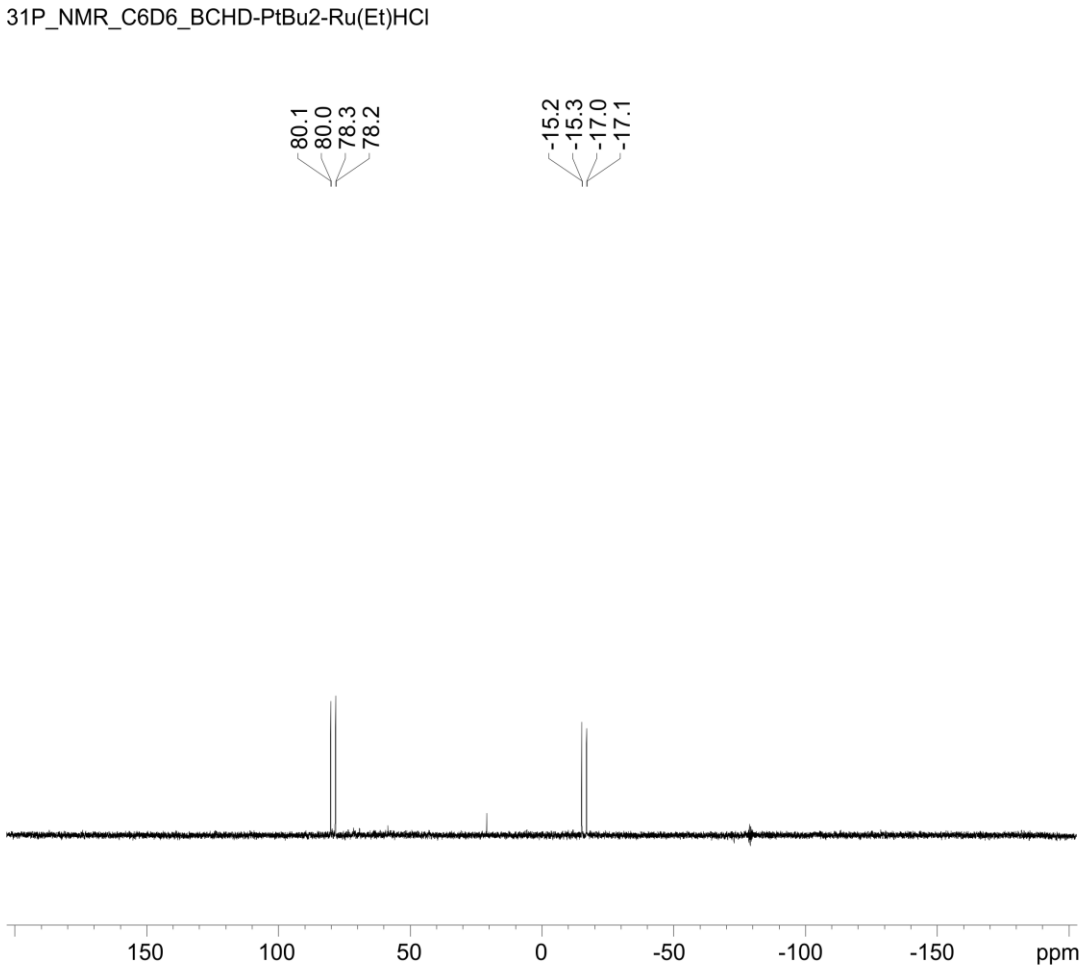

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PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
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SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure S21. $^{31}P\{^{1}H\}$ NMR spectrum of complex **5**.

4 Quantum chemical calculations

On the basis of the molecular structures of **2** determined in the solid state the structure was optimized using the programme Orca4.2[1] with BP86,[2] Grimme´s dispersion correction and Becke-Johnson damping (D3BJ)[3] making use of the resolution of identity (RI) approximation. The basis set chosen was def2-TZVP for Ru and def2-SVP for all other elements as implemented in ORCA4.2.[4] For all calculations *tight* convergence criteria for optimisations and *verytight* for SCF convergence were applied with *grid6* and *finalgrid7* gridsizes. Absence of imaginary frequencies on this level of theory confirmed local minima on the PES. The electronic structure of **2** was analysed sing NBO7.[5]

Ru-C bond
σ-type (1.88) 44.2 % Ru, 55.8 % C,
π-type (1.86) 67.5 % Ru, 32.5 % C
charges: Ru (-0.066), C19 (+0.029)
Wiberg index Ru-C 1.1967

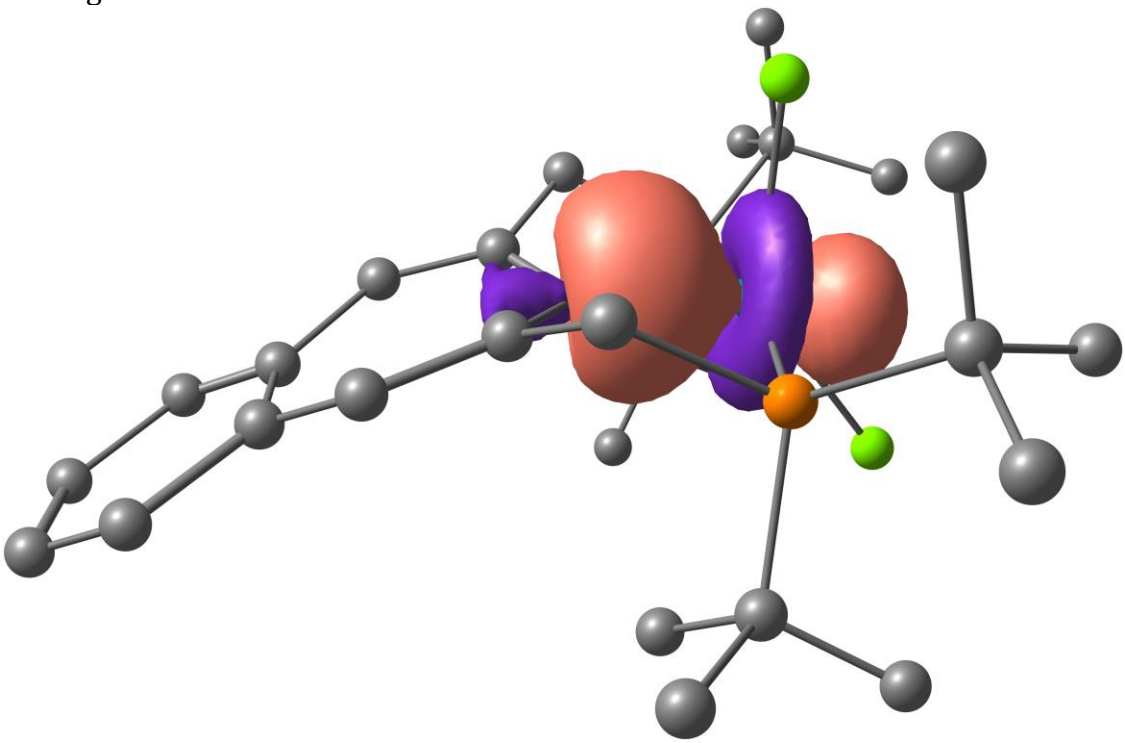

Figure S22. NBO of σ-type Ru-C interaction in **2**.

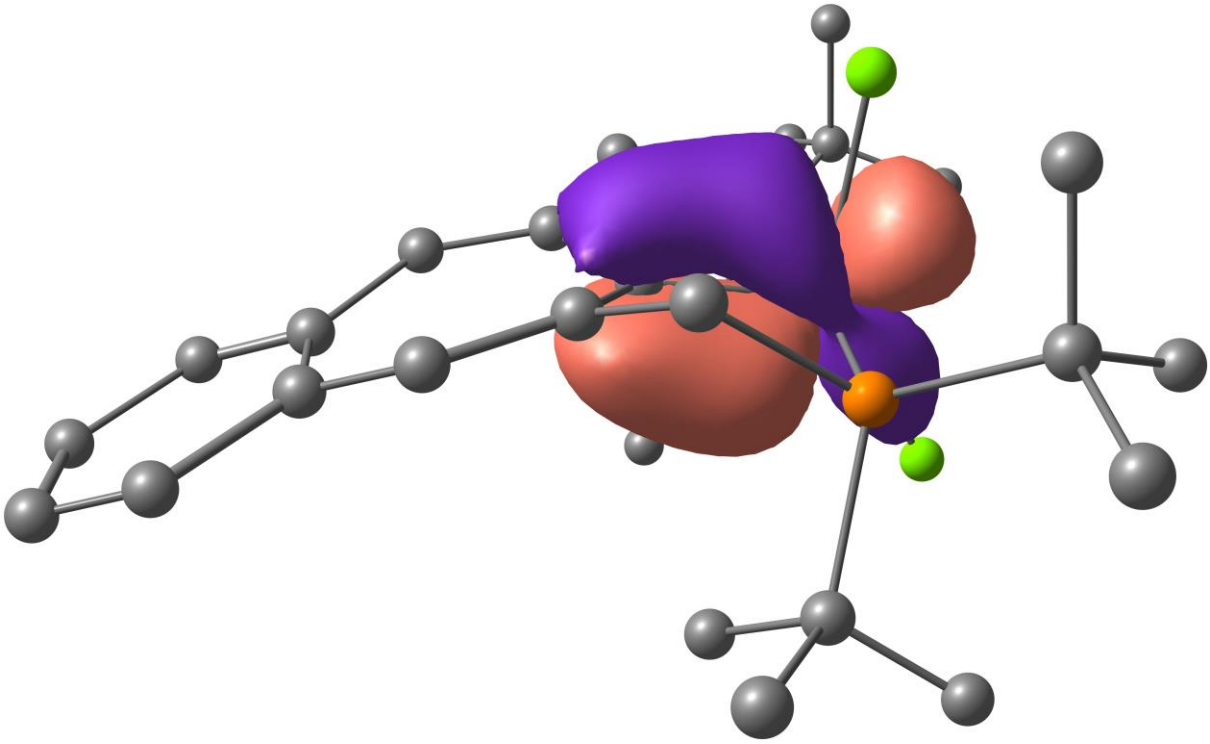

Figure S23. NBO of π-type Ru-C interaction in **2**

Table S2. Comparison of measured and calculated structural data of **2**.

	X-ray data	calculated
Ru-Cl1	2.3227(10)	2.352
Ru-Cl2	2.3754(11)	2.377
Ru-C1	1.909(4)	1.915
Ru-P1	2.3850(11)	2.366
Ru-P2	2.3900(11)	2.367
P2-Ru-P1	169.0(1)	168.3
Cl1-Ru-C1	93.7(1)	92.0
Cl1-Ru-Cl2	136.7(1)	138.5

Table S3 Coordinates of **2** obtained from calculations.

Ru	14.04417010482033	3.64480713732179	2.35305275534754
Cl	14.41843275843287	4.82889729092952	0.35562212835836
P	15.99305116840229	4.51022592831686	3.37932901255530
Cl	14.47690191417947	1.48770316548319	3.25209090436874
P	11.86937892676040	2.97915548510786	1.70105414259268
C	10.99638814715708	6.73162302094027	5.00561014098180
C	9.81746456601134	7.01182332349709	5.74941796894226
H	8.85318157310464	6.66947512245627	5.34215169037128
C	9.85287556005903	7.69262890486731	6.96670800957147
H	8.92128065731426	7.87935182415702	7.52180548386247
C	11.08757961114786	8.14970911873892	7.47156379342108
H	11.13048635583485	8.69720255605818	8.42512439852368
C	12.25622501697304	7.91465930399596	6.74659557298145

H	13.22032061949640	8.28628738754388	7.12780966422292
C	12.25278075563248	7.19674821060833	5.51932506426097
C	13.52082600806634	7.04110687883067	4.84386572274087
H	14.31501249649698	7.68147028333373	5.26555079390998
C	13.93943287891878	6.19190529954095	3.84113957168456
C	13.16071806899457	5.14347921923919	3.15453832032664
C	11.71917613185429	5.36861115903194	2.93426404101739
C	10.83175770457716	6.04493661481996	3.74475892725339
H	9.78004750455870	6.00130292744674	3.41216565240532
C	15.39582382293180	6.26638848277301	3.42991774274178
H	15.98694760030519	6.96452871562933	4.05269292577326
H	15.44509694190039	6.59389263047903	2.36988810493786
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H	11.60817655136617	5.16717478896560	0.80310692086770
H	10.05483485866230	4.76203629960864	1.63179353281245
C	17.68070165278165	4.49807571014344	2.47054769147180
C	16.23889777935290	4.03274066106565	5.22808933481245
C	18.90153637181388	4.87164443164237	3.32985166284371
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H	18.81889089560132	5.89940423582230	3.73667939882440
H	19.80501380834020	4.85000481156965	2.68272526708326
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H	17.83294095883426	2.29621523547756	2.69036602523547
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H	16.98098269872682	2.83875465483154	1.21621468552654
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H	14.33773351809626	2.93480435478009	5.37687920137305
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H	16.29262134493801	6.07004530421915	6.06627170315228
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C	17.03935407927609	2.71813159590807	5.32685645297901
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H	16.53999270077990	1.91434861921834	4.75216103956129
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