

Electronic Supporting Information

Cycloaddition of carbon dioxide to epoxides by highly active constrained aluminum chloride complexes

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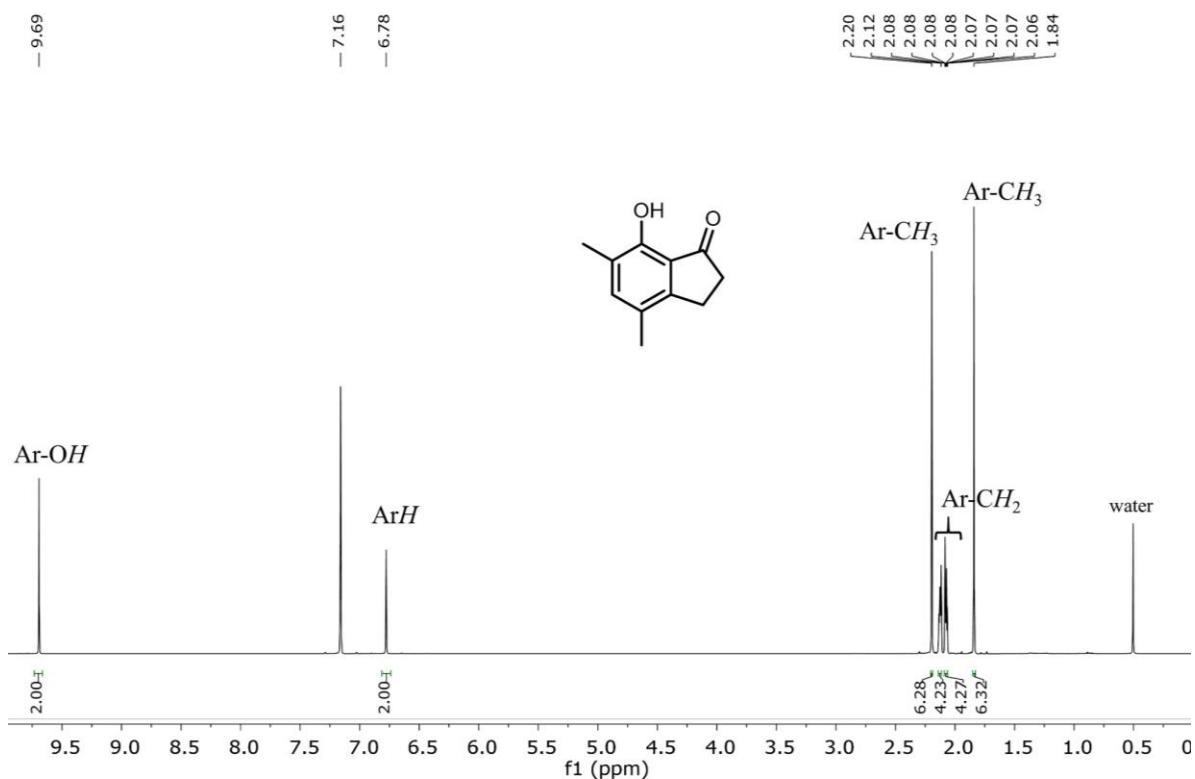


Figure S1 ¹H NMR spectrum (600 MHz, C₆D₆, 30 °C) of 4,6-Dimethyl-7-hydroxy-1-indanone.

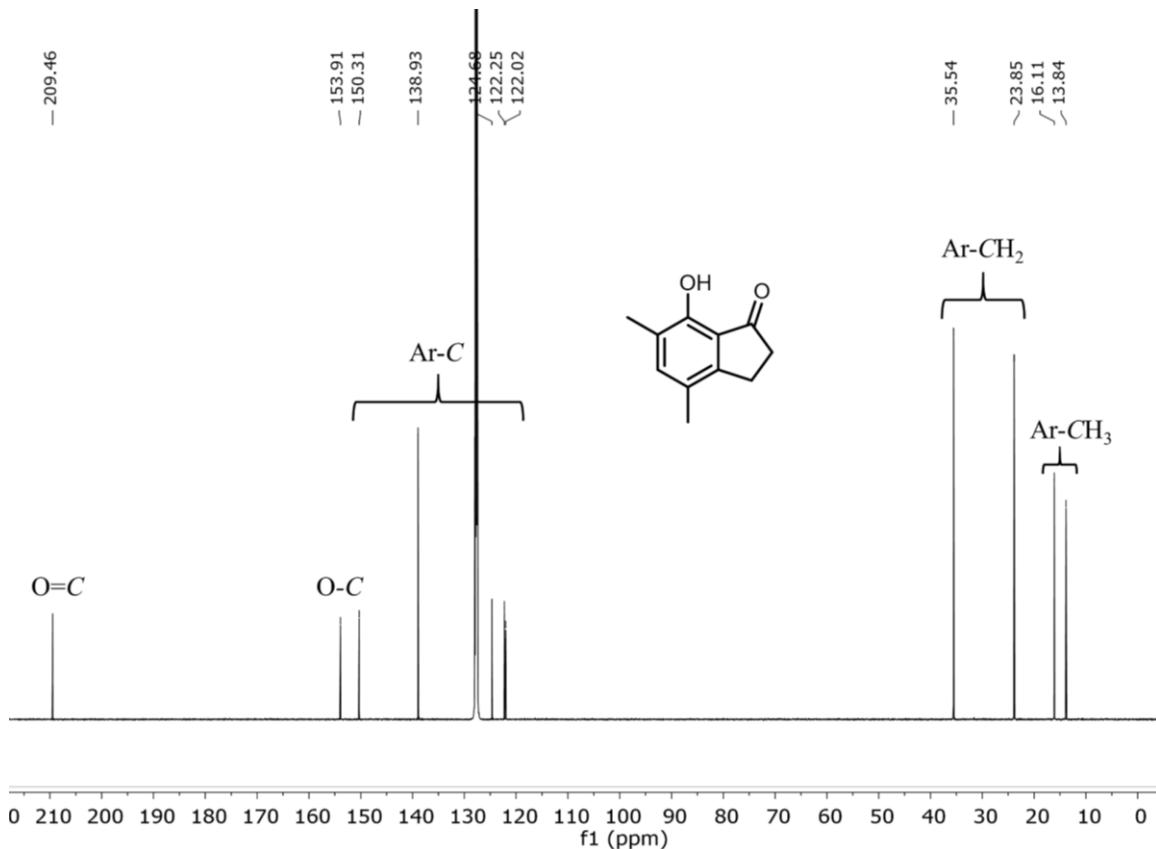


Figure S2 ¹³C{¹H} NMR spectrum (150 MHz, C₆D₆, 30 °C) of 4,6-Dimethyl-7-hydroxy-1-indanone.

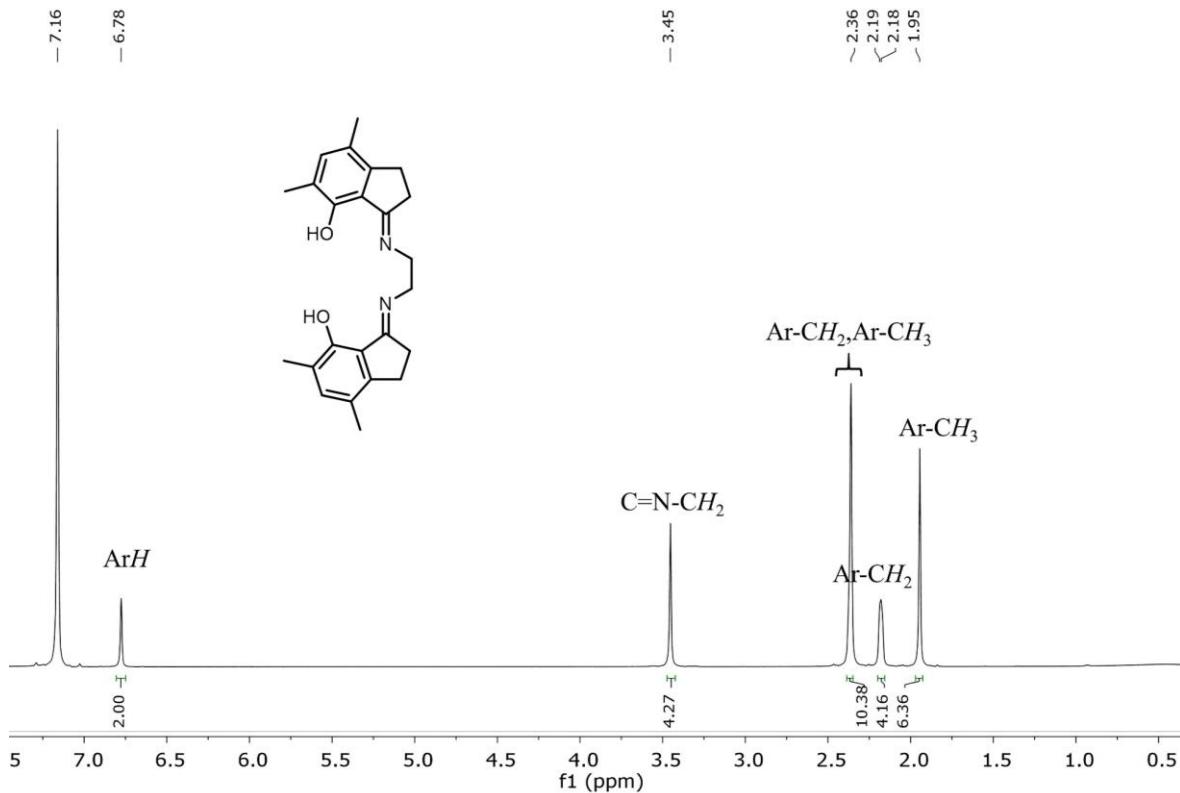


Figure S3 ^1H NMR spectrum (600 MHz, C_6D_6 , 30 °C) of ligand **1b**.

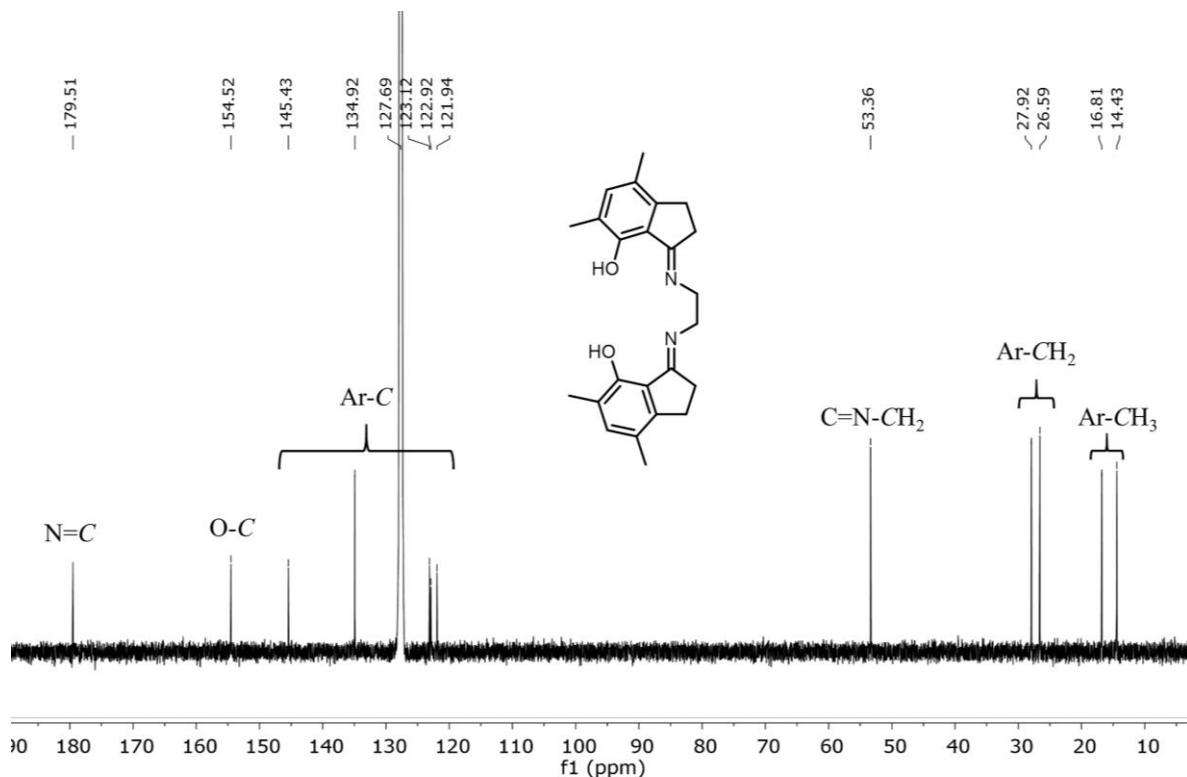


Figure S4 $^{13}\text{C}\{\text{H}\}$ NMR spectrum (150 MHz, C_6D_6 , 30 °C) of ligand **1b**.

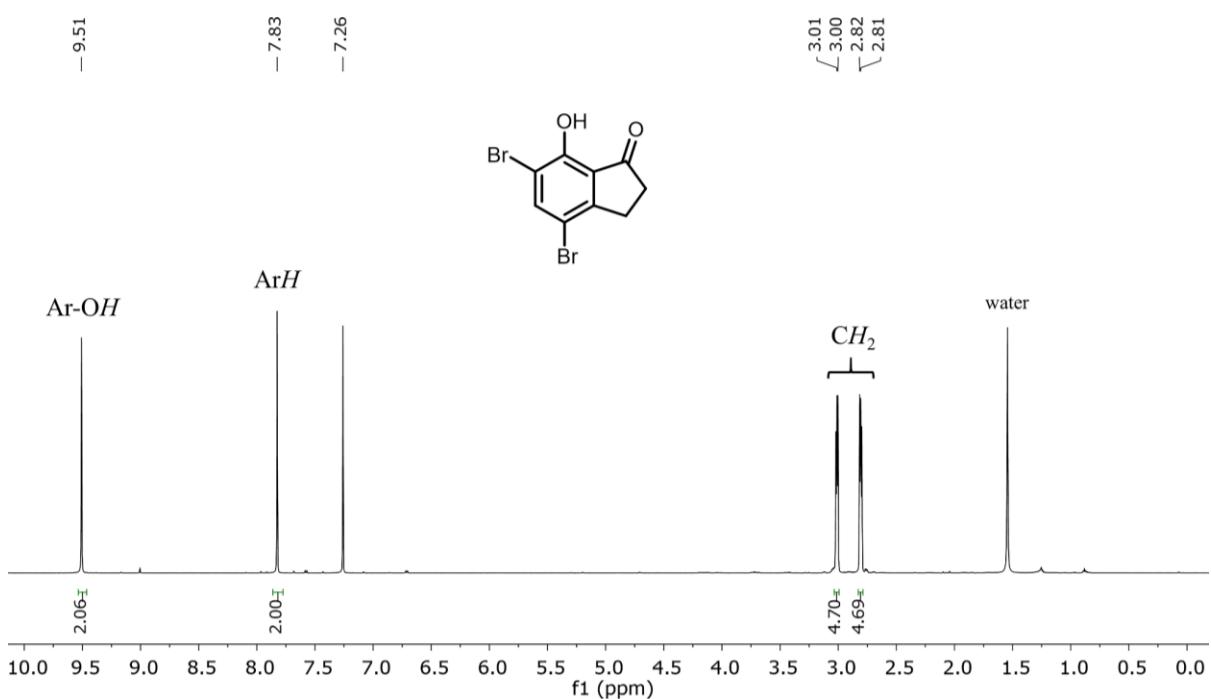


Figure S5 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of 4,6-Dibromo-7-hydroxy-1-indanone.

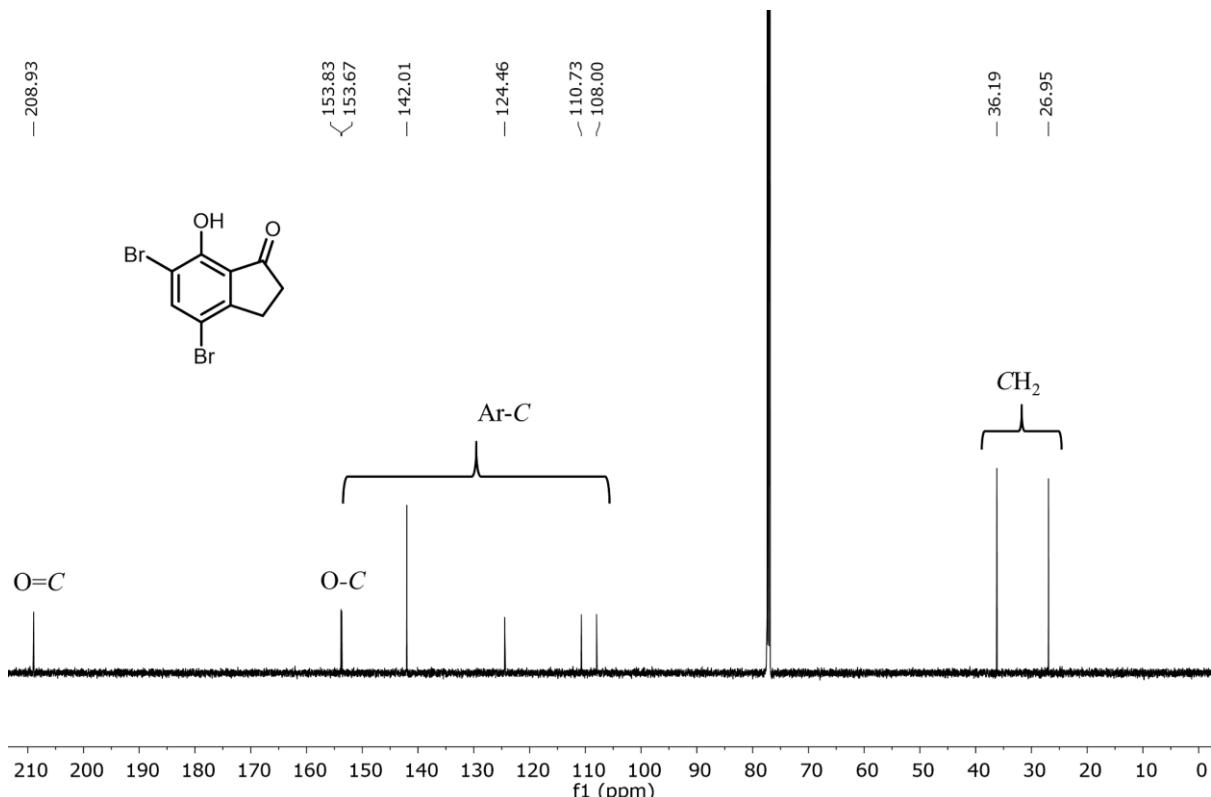


Figure S6 ¹³C{¹H} NMR spectrum (150 MHz, CDCl₃, 30 °C) of 4,6-Dibromo-7-hydroxy-1-indanone.

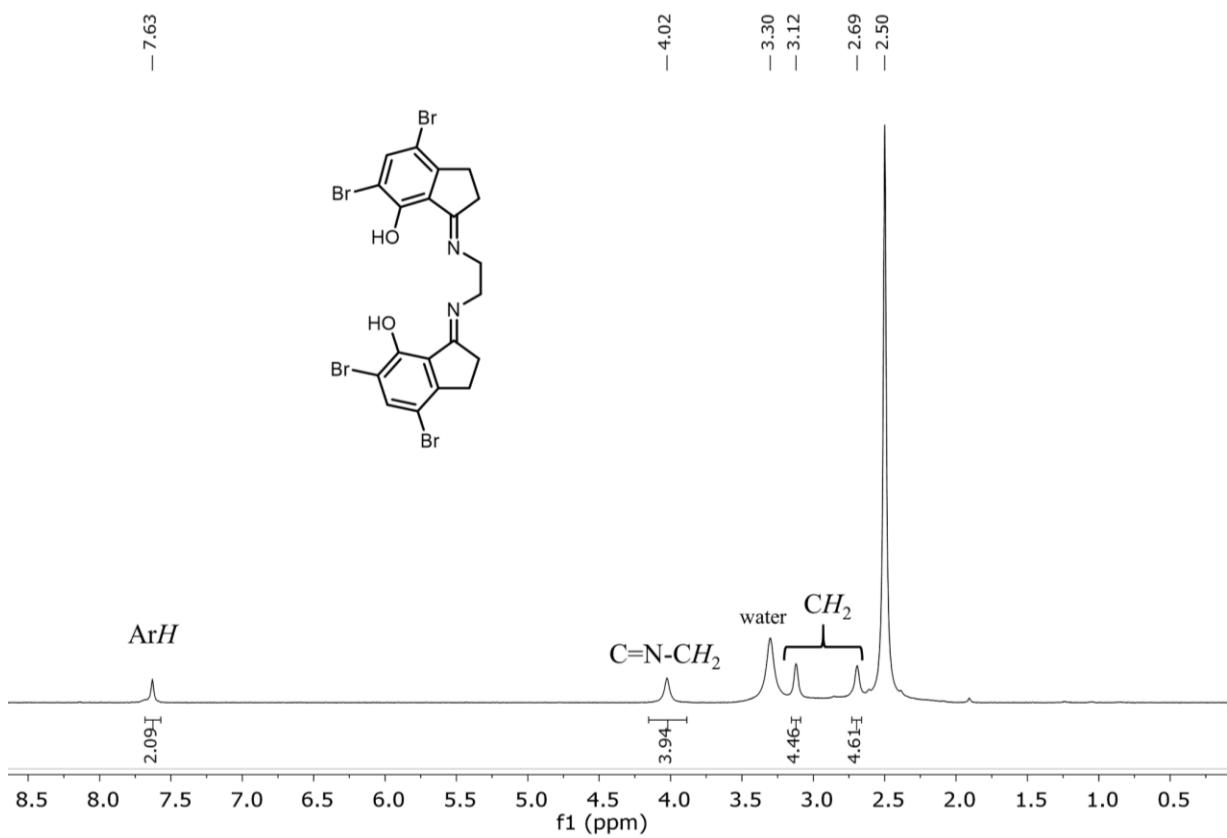


Figure S7 ^1H NMR spectrum (600 MHz, DMSO- d_6 , 30 °C) of ligand **1d**.

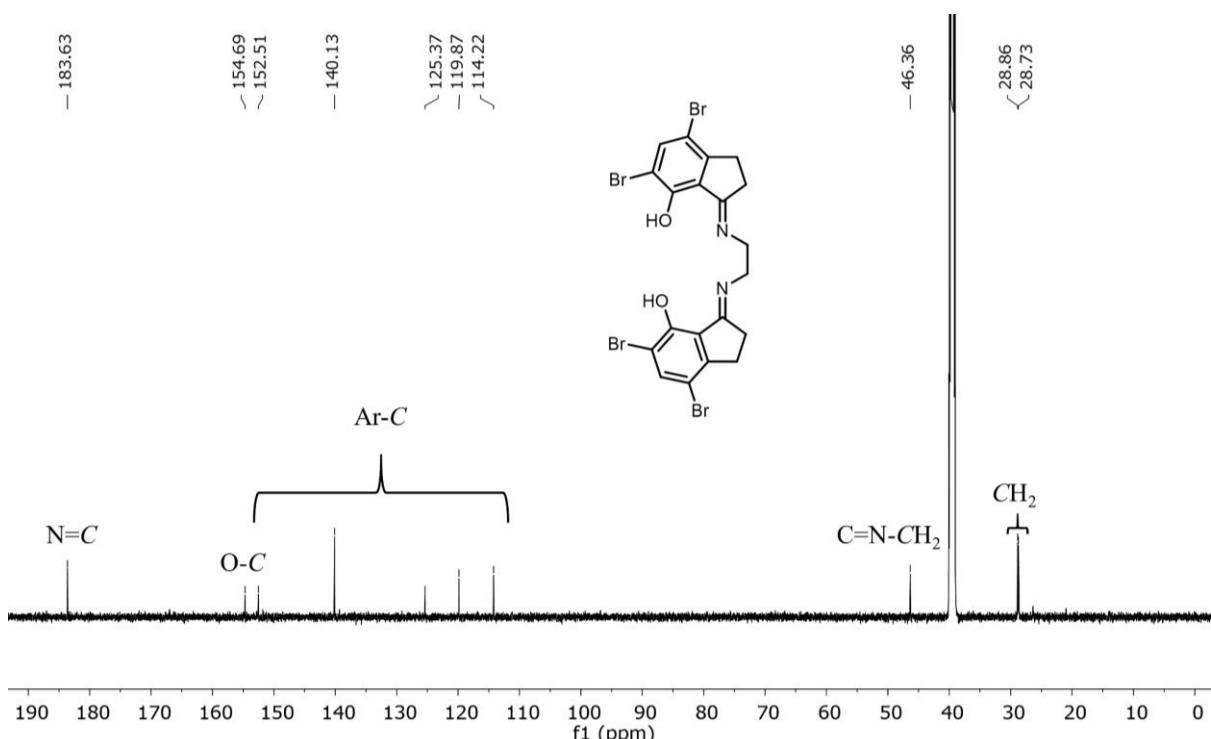


Figure S8 $^{13}\text{C}\{\text{H}\}$ NMR spectrum (150 MHz, DMSO- d_6 , 30 °C) of ligand **1d**.

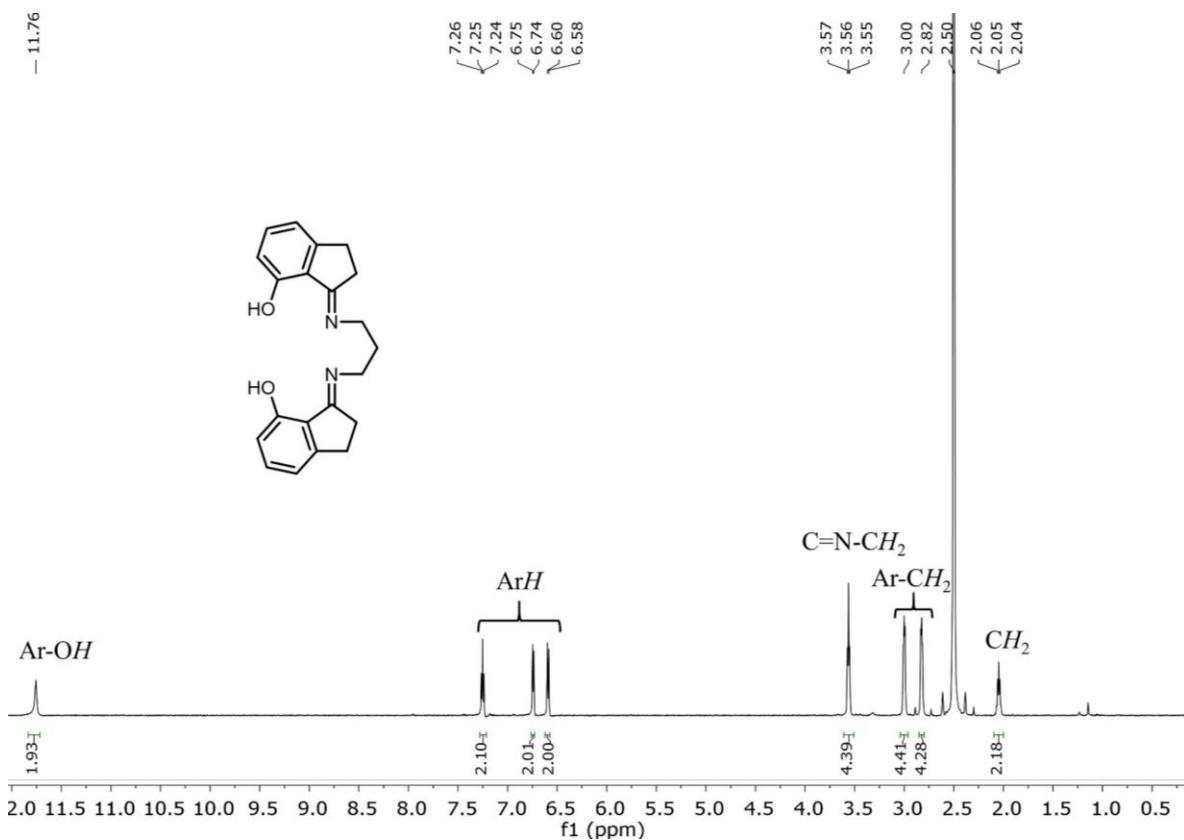


Figure S9 ^1H NMR spectrum (600 MHz, DMSO- d_6 , 30 °C) of ligand **1e**.

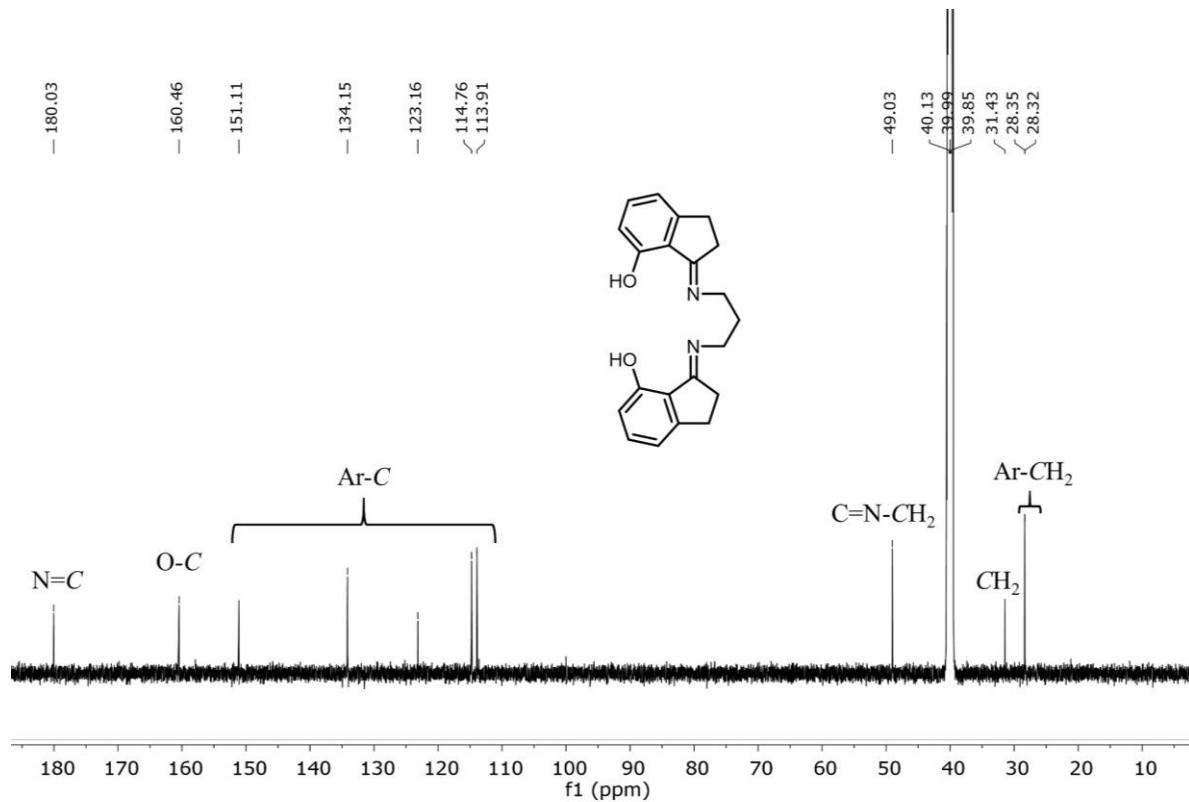


Figure S10 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (150 MHz, DMSO- d_6 , 30 °C) of ligand **1e**.

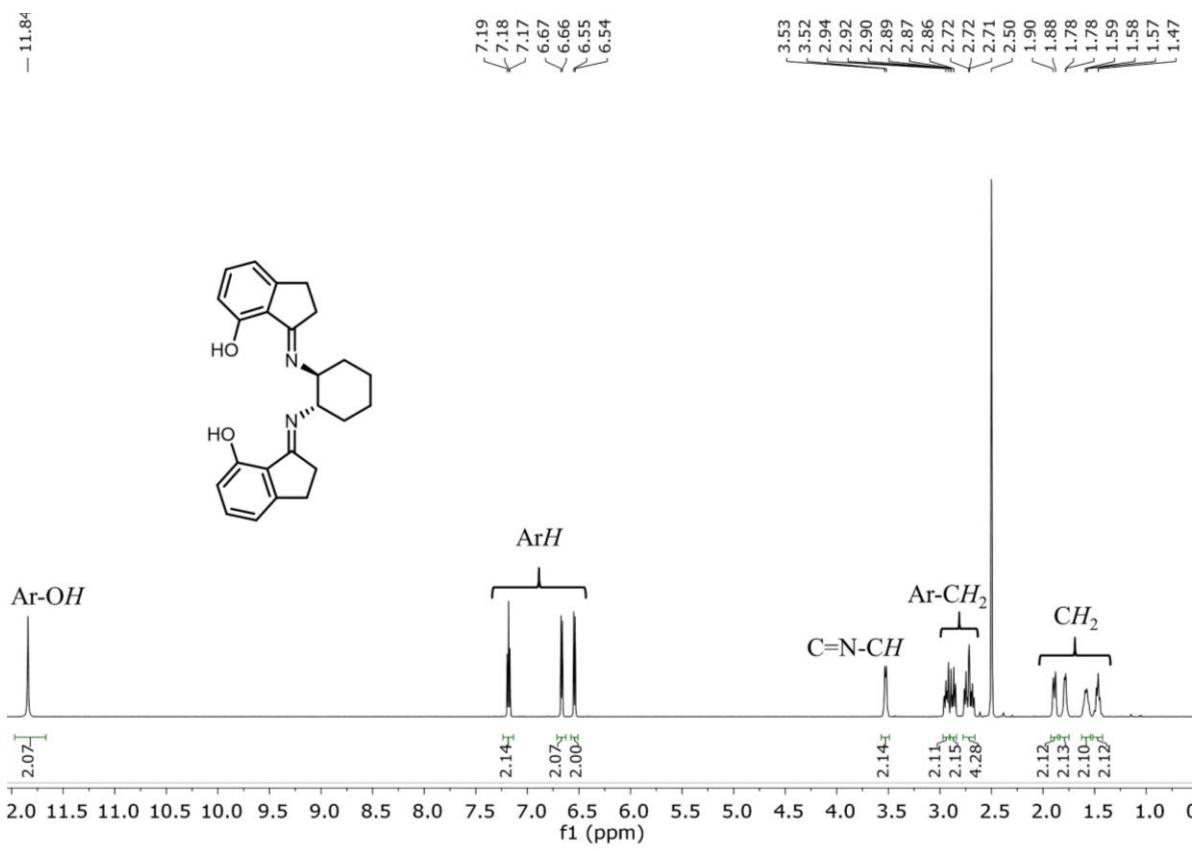


Figure S11 ^1H NMR spectrum (600 MHz, DMSO- d_6 , 30 °C) of ligand **1f**.

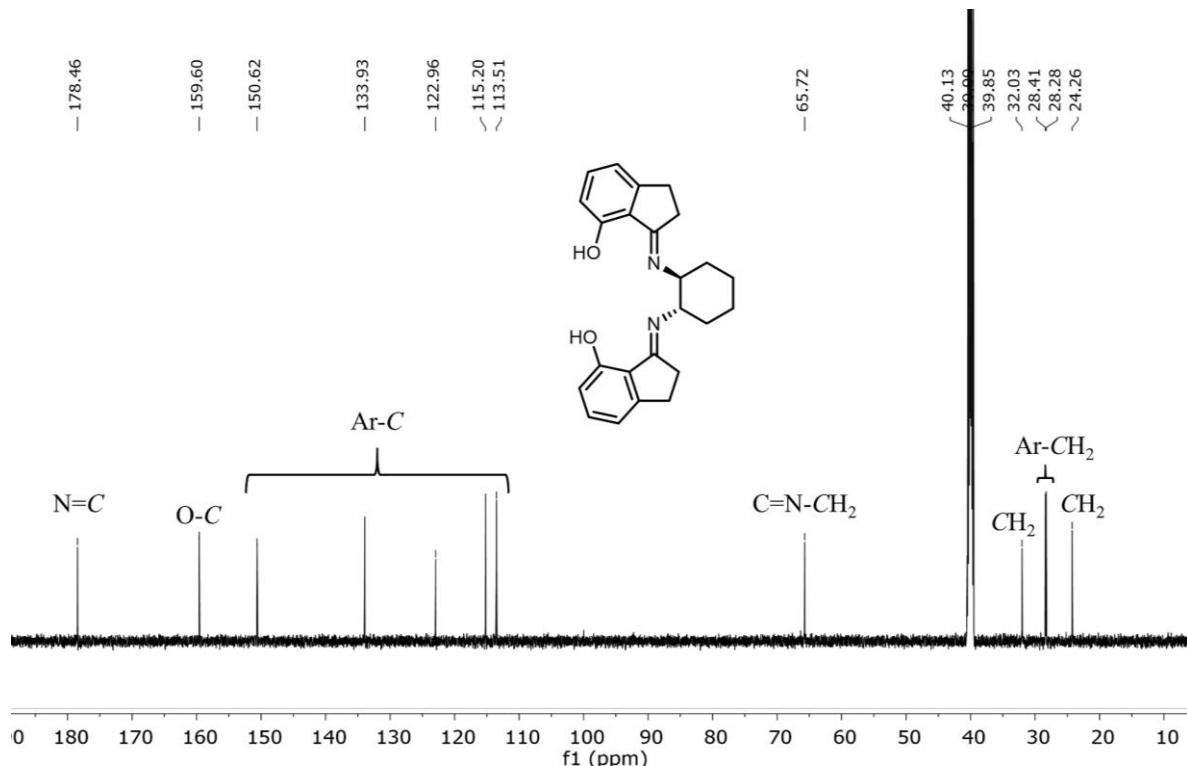


Figure S12 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (150 MHz, DMSO- d_6 , 30 °C) of ligand **1f**.

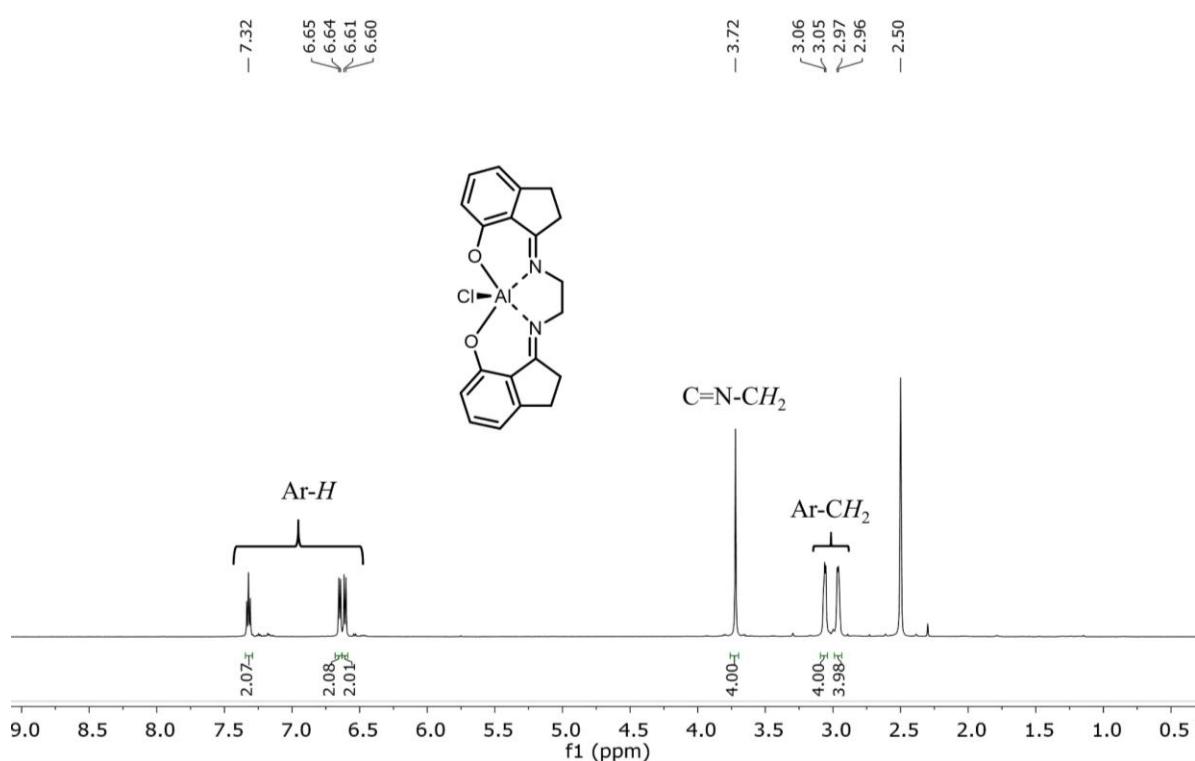


Figure S13 ^1H NMR spectrum (600 MHz, DMSO- d_6 , 30 °C) of complex **2a**.

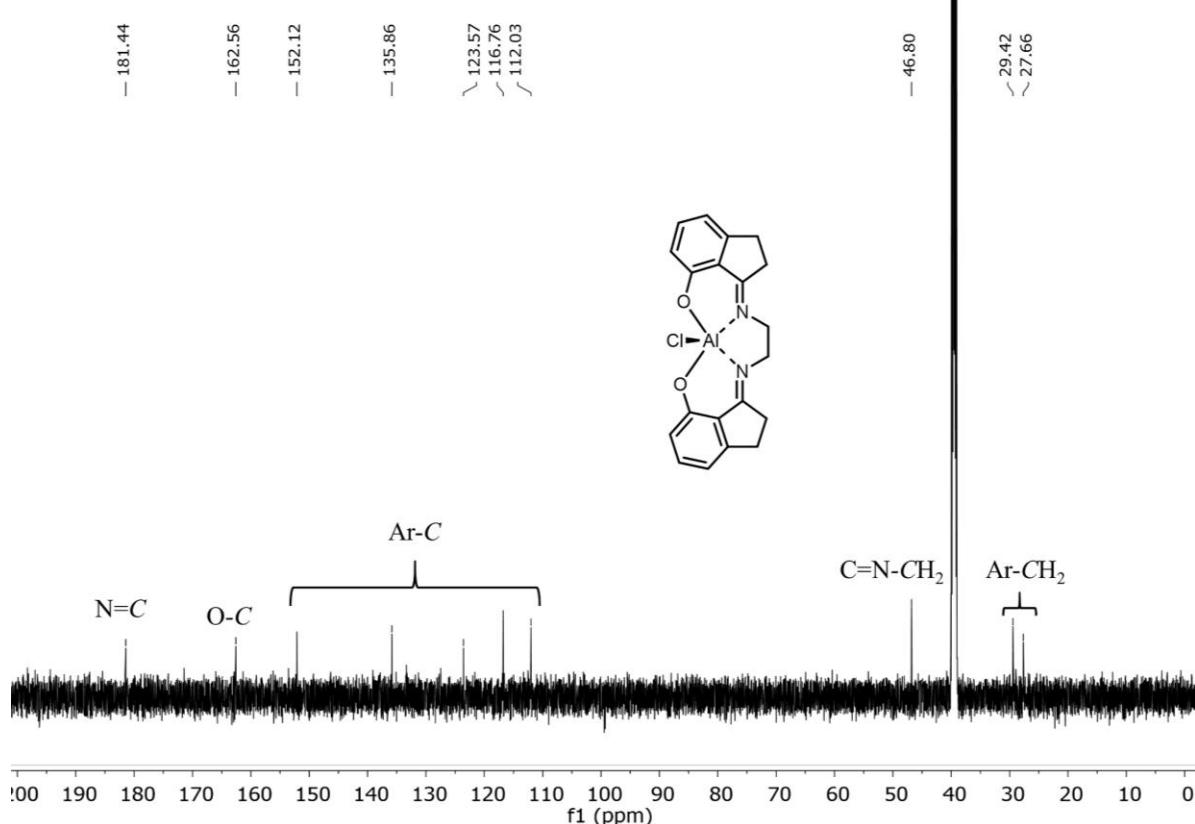


Figure S14 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (150 MHz, DMSO- d_6 , 30 °C) of complex **2a**.

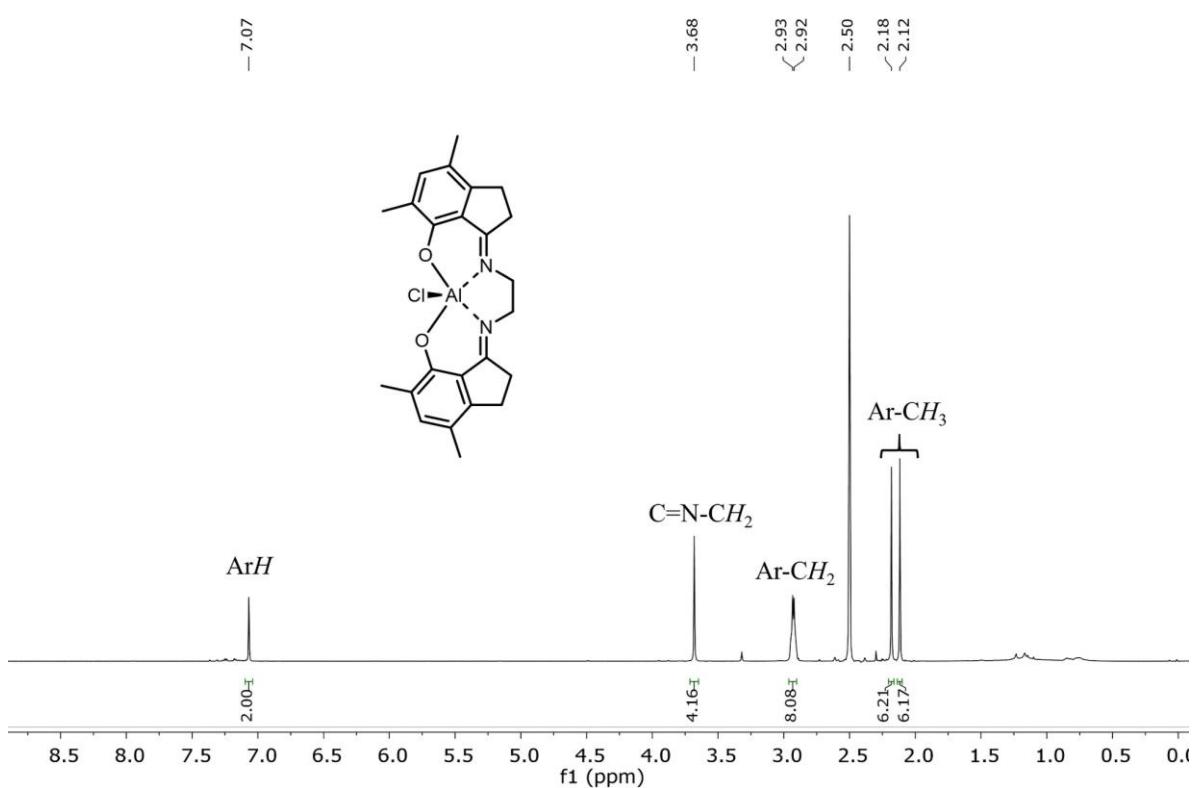


Figure S15 ^1H NMR spectrum (600 MHz, DMSO- d_6 , 30 °C) of complex **2b**.

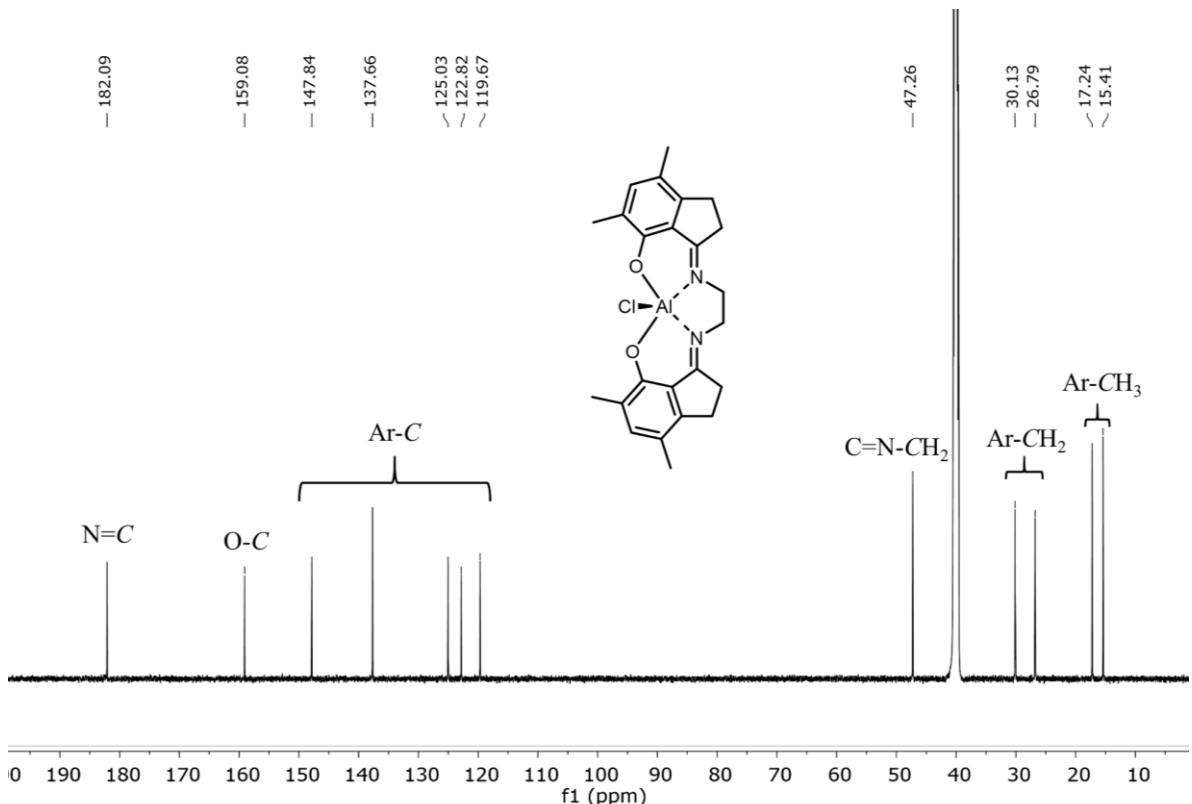


Figure S16 $^{13}\text{C}\{\text{H}\}$ NMR spectrum (150 MHz, DMSO- d_6 , 30 °C) of complex **2b**.

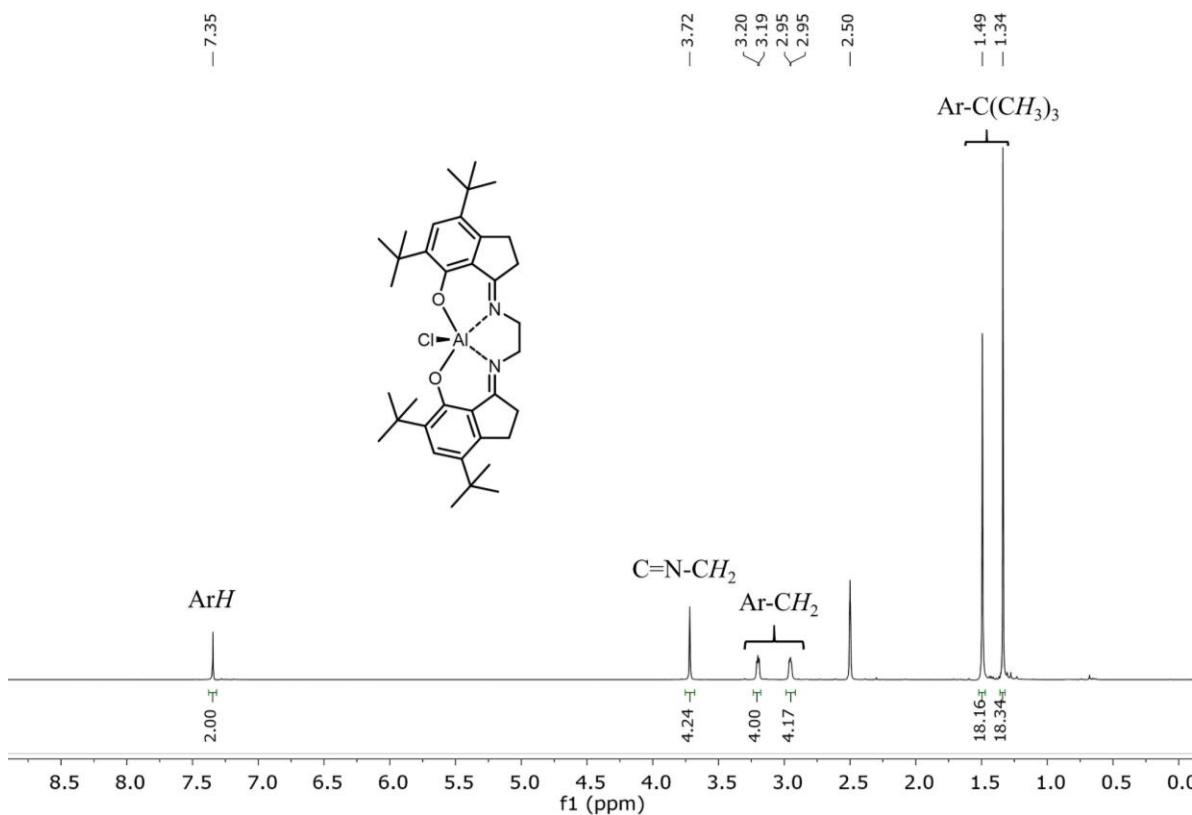


Figure S17 ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2c**.

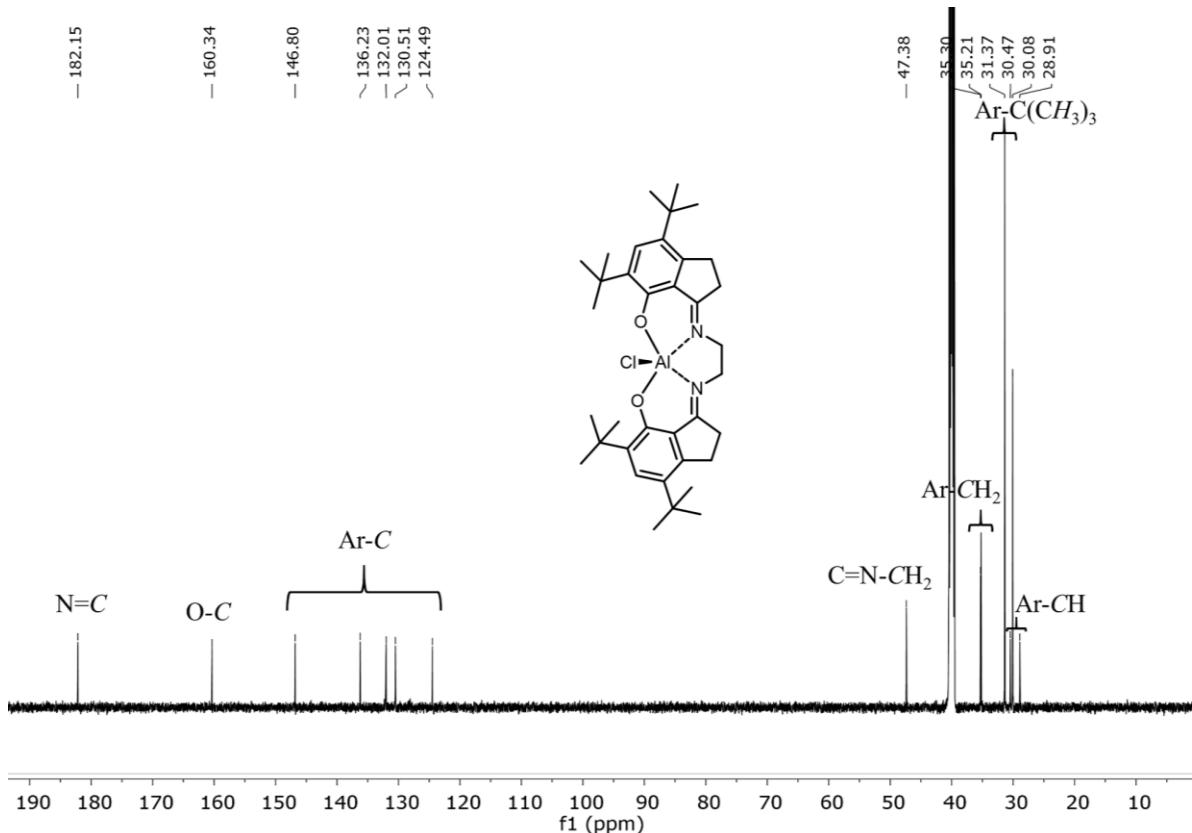


Figure S18 $^{13}\text{C}\{\text{H}\}$ NMR spectrum (150 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2c**.

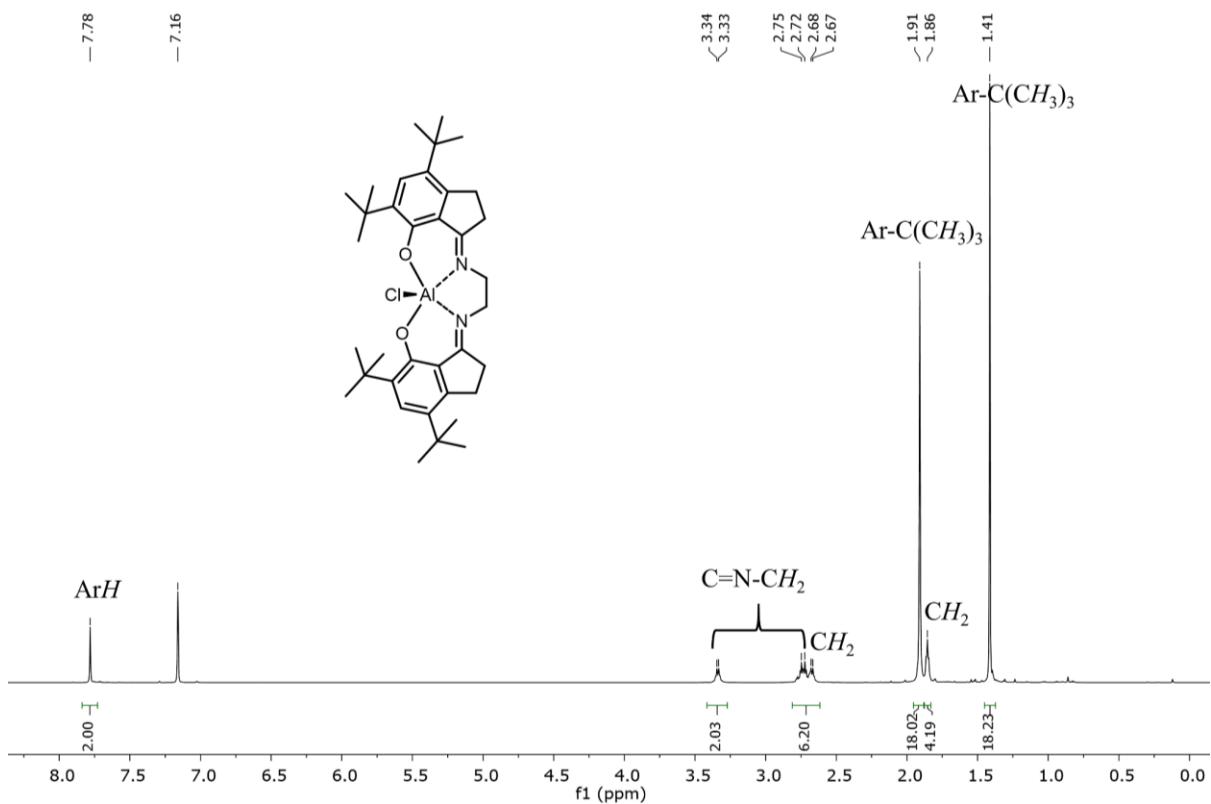


Figure S19 ^1H NMR spectrum (600 MHz, C₆D₆, 30 °C) of complex **2c**.

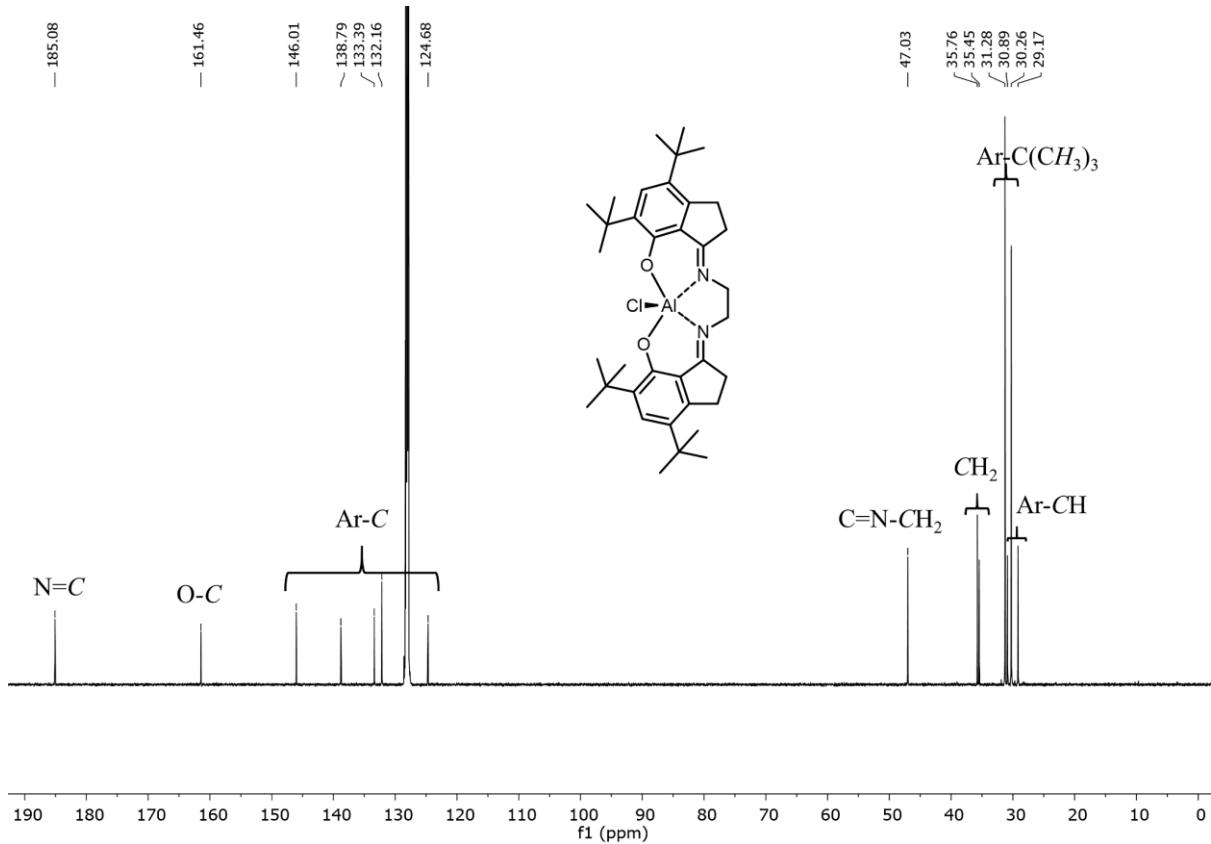


Figure S20 $^{13}\text{C}\{\text{H}\}$ NMR spectrum (150 MHz, C₆D₆, 30 °C) of complex **2c**.

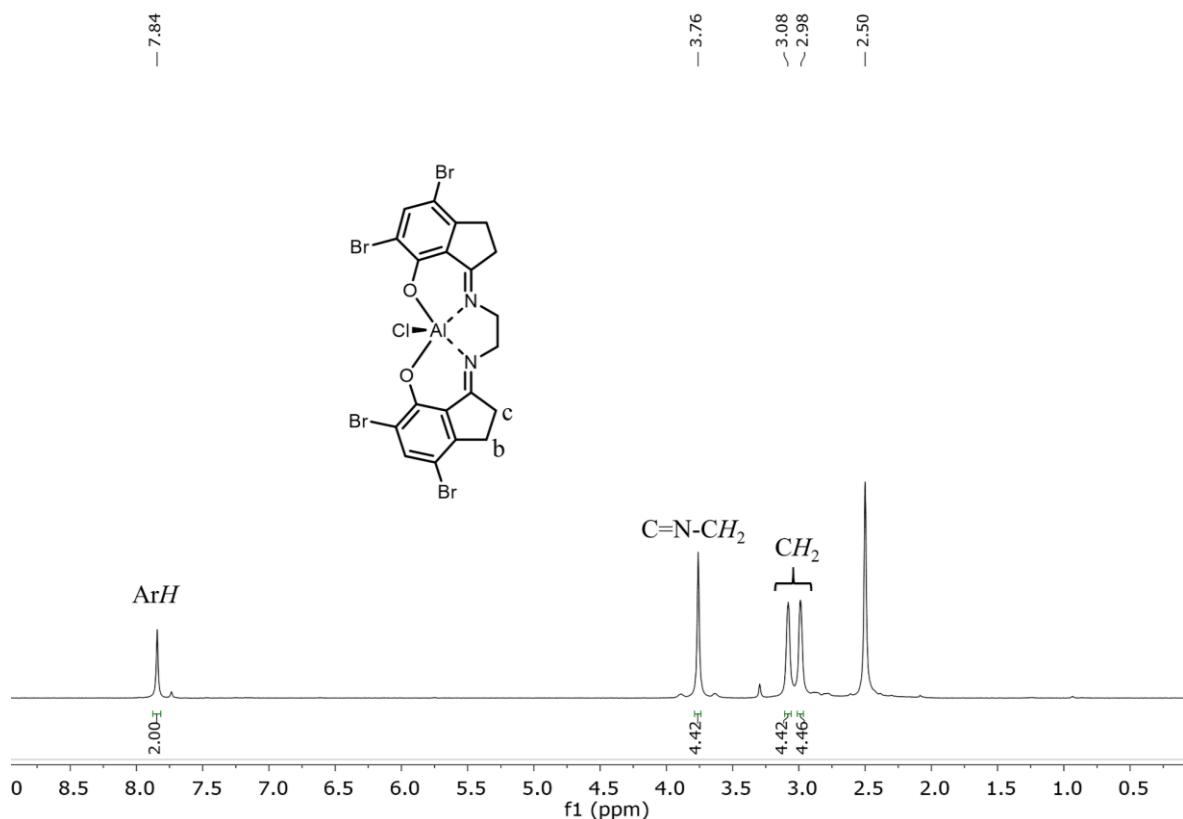


Figure S21 ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2d**

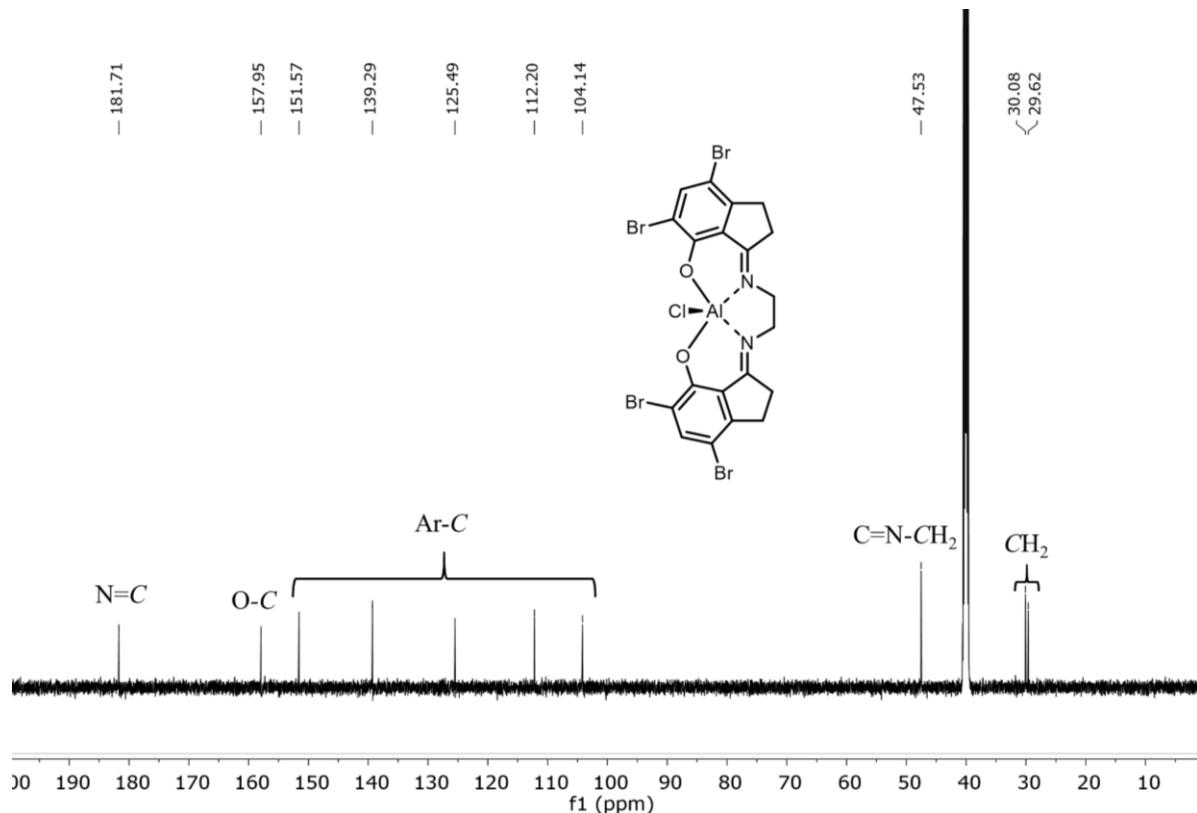


Figure S22 $^{13}\text{C}\{\text{H}\}$ NMR spectrum (150 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2d**.

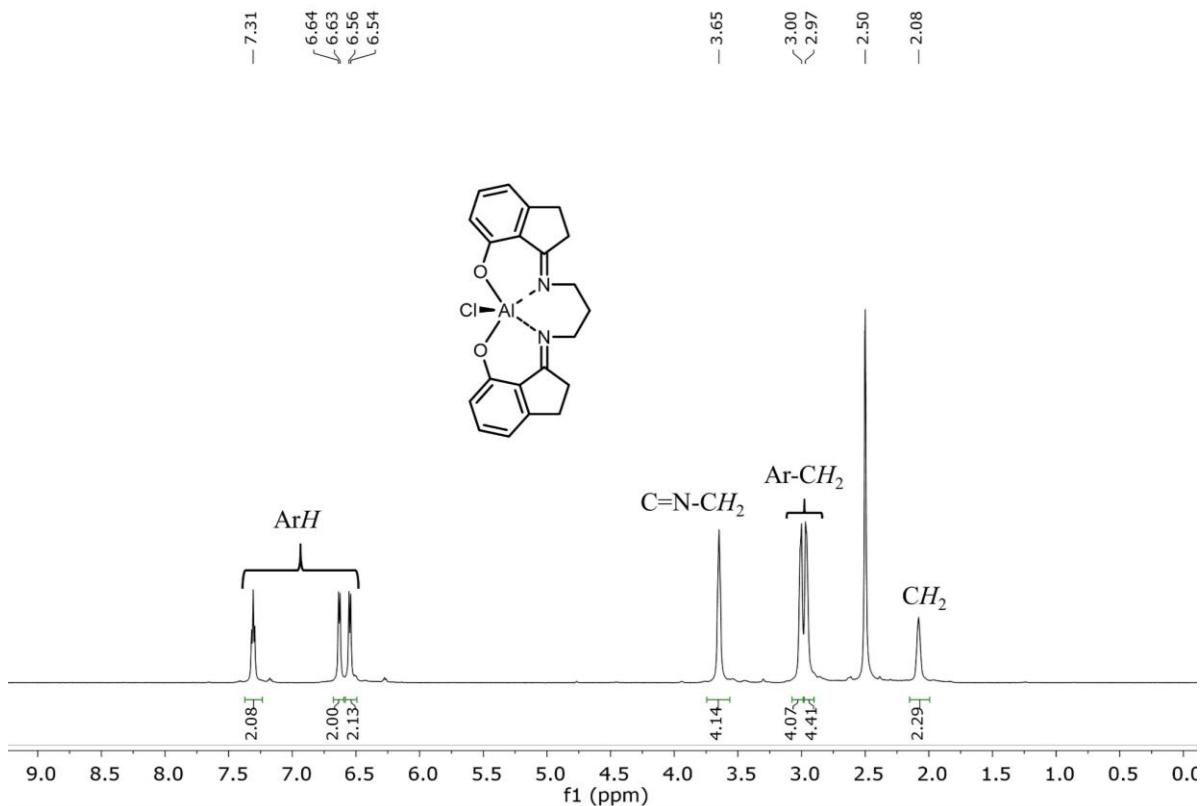


Figure S23 ^1H NMR spectrum (600 MHz, DMSO-*d*₆, 30 °C) of complex **2e**.

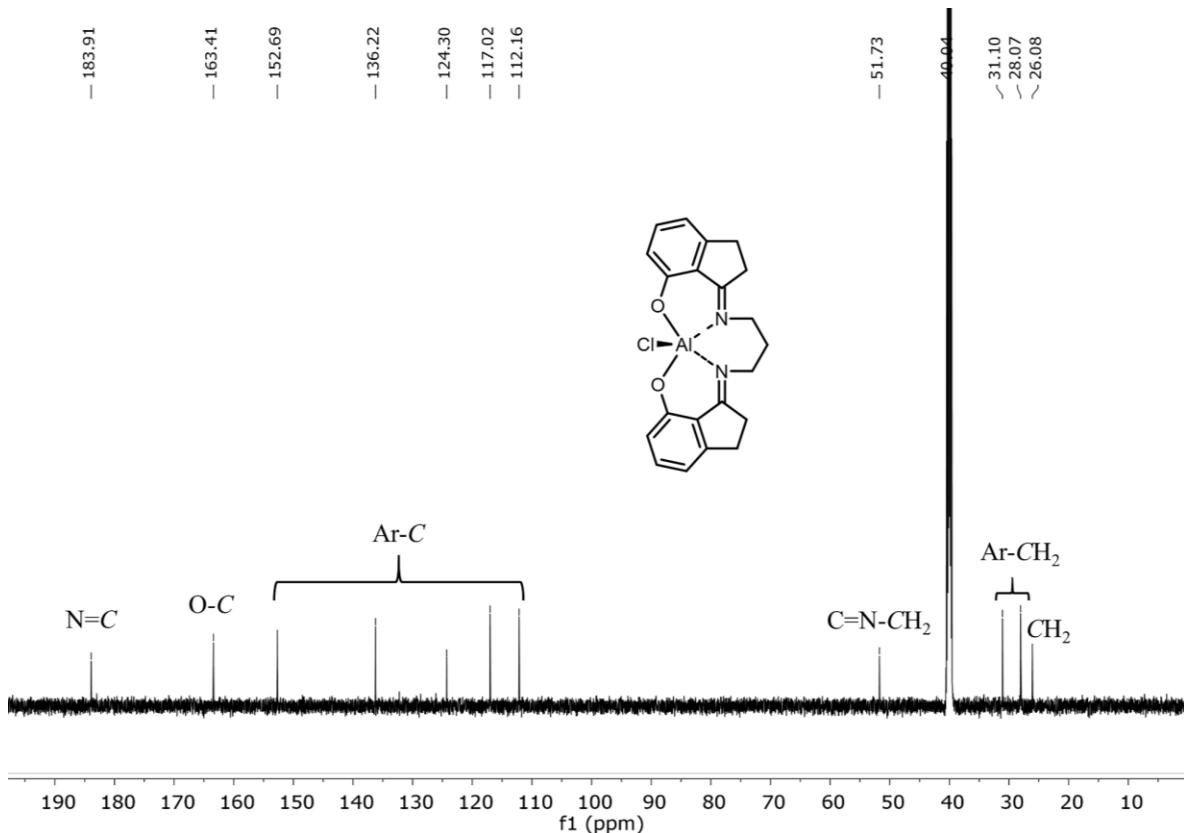


Figure S24 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (150 MHz, DMSO-*d*₆, 30 °C) of complex **2e**.

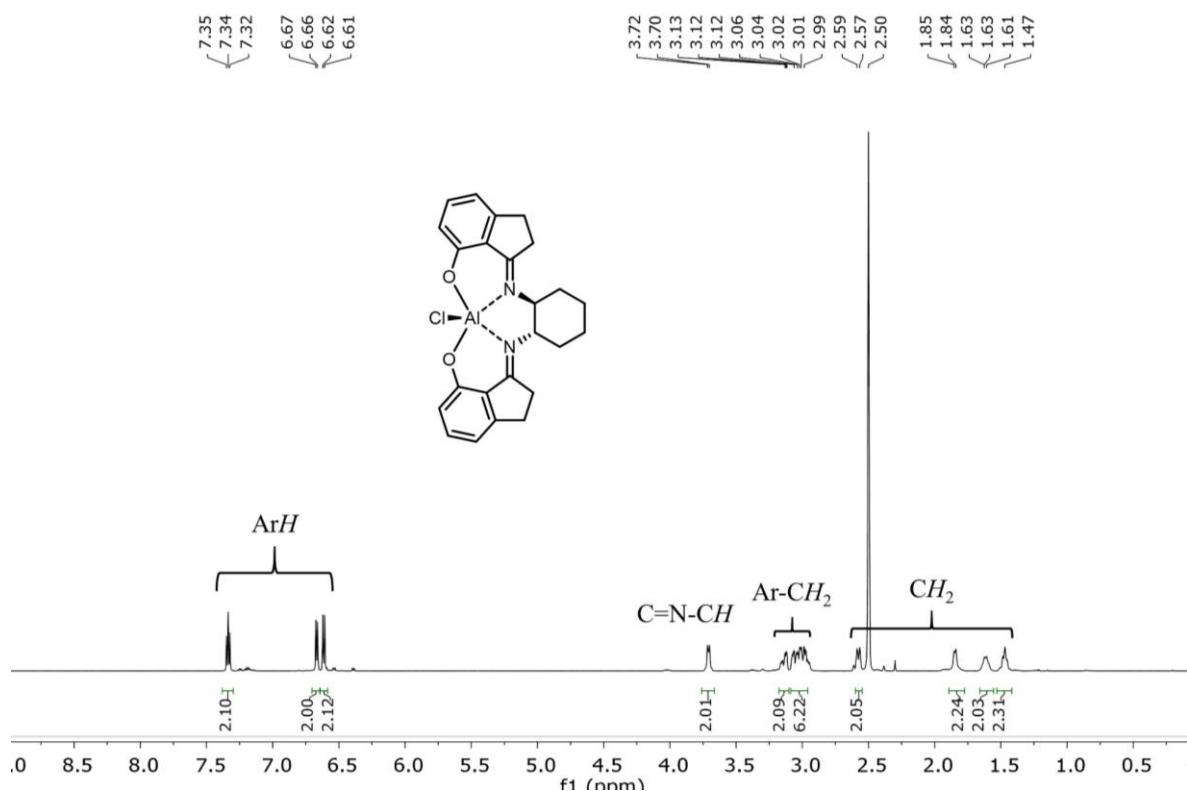


Figure S25 ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2f**.

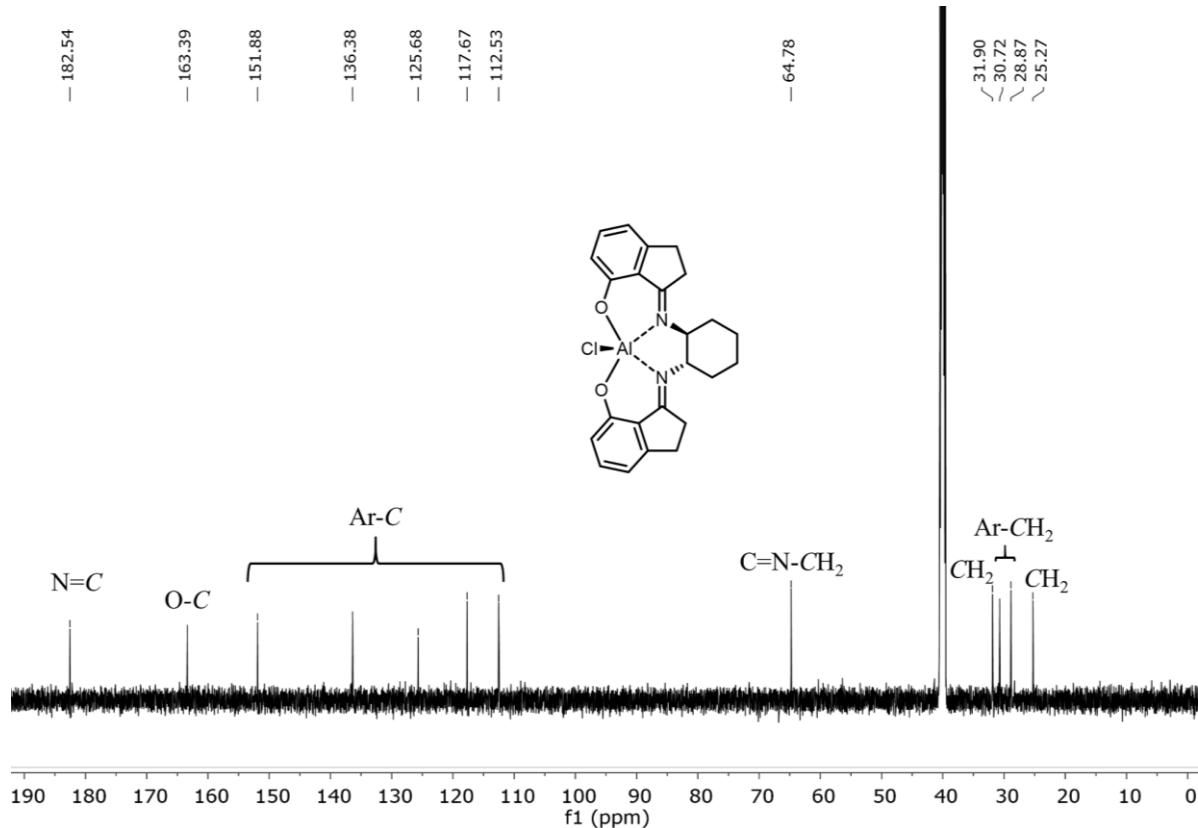


Figure S26 $^{13}\text{C}\{\text{H}\}$ NMR spectrum (150 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2f**.

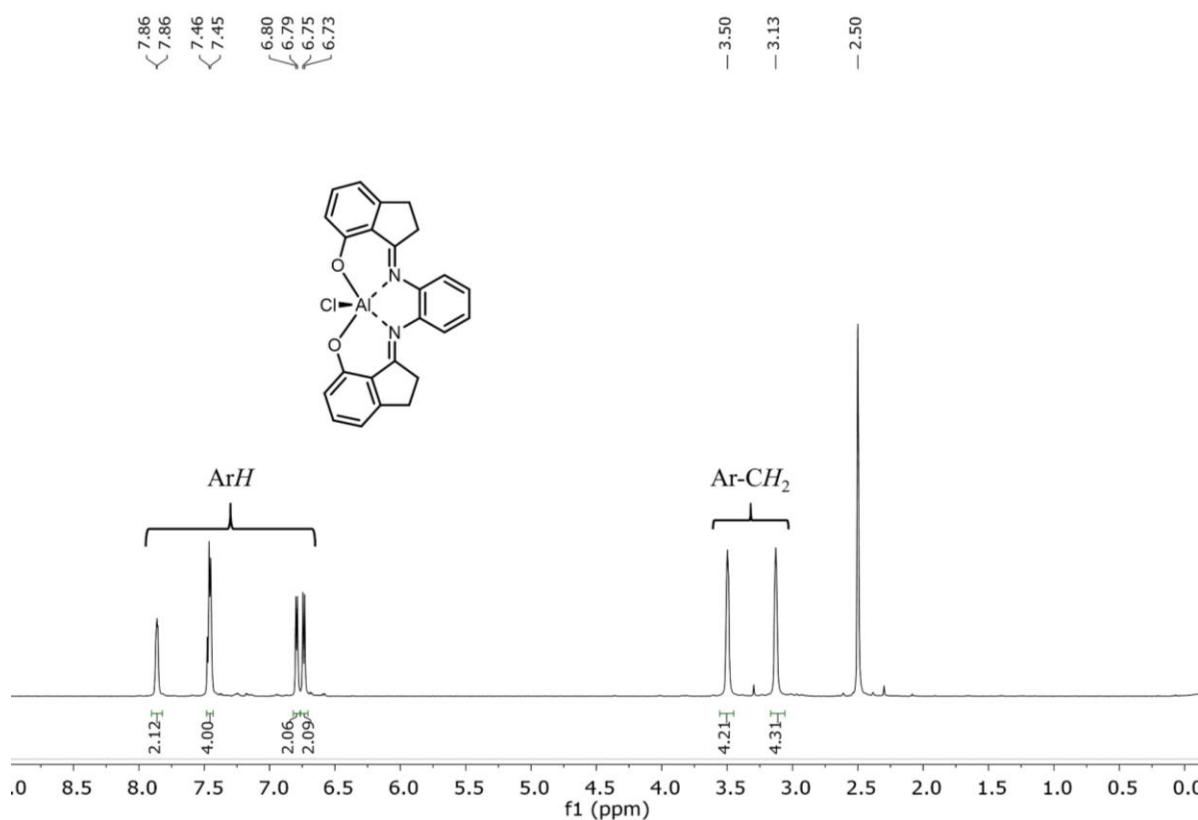


Figure S27 ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2g**.

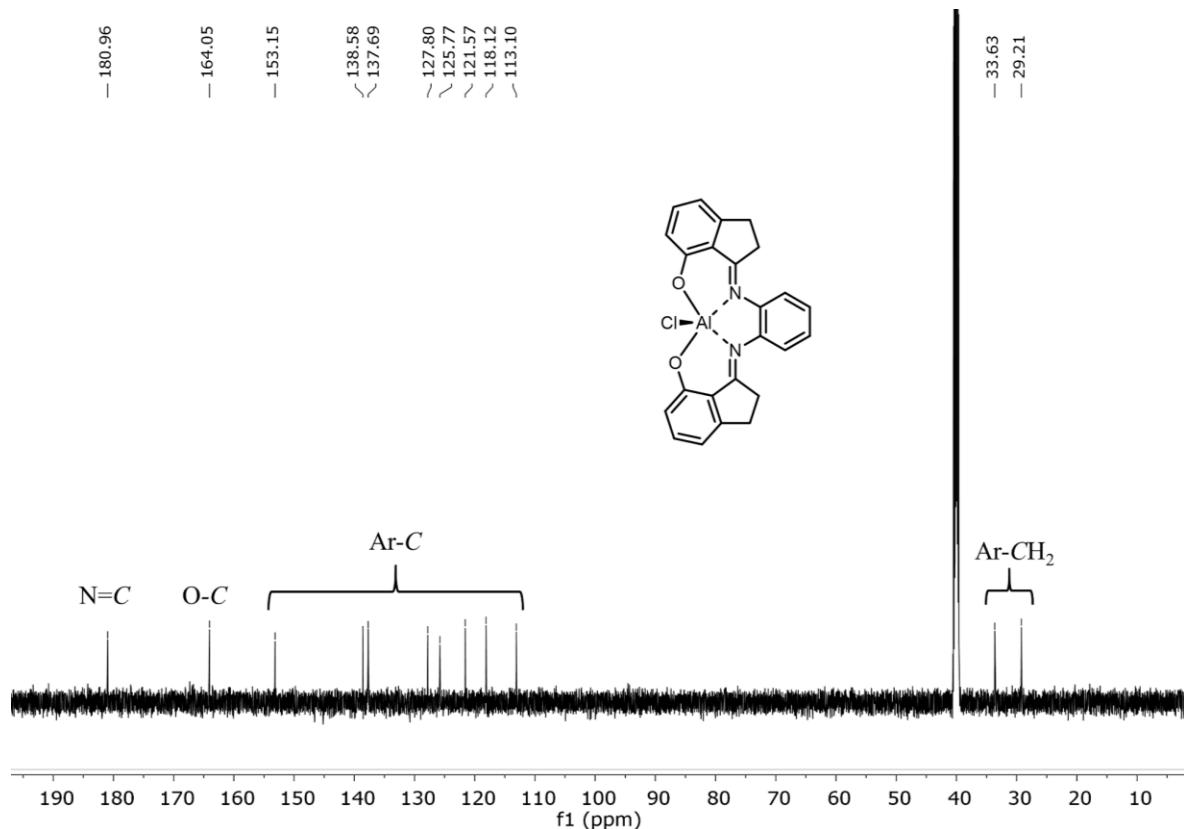


Figure S28 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (150 MHz, $\text{DMSO}-d_6$, 30 °C) of complex **2g**.

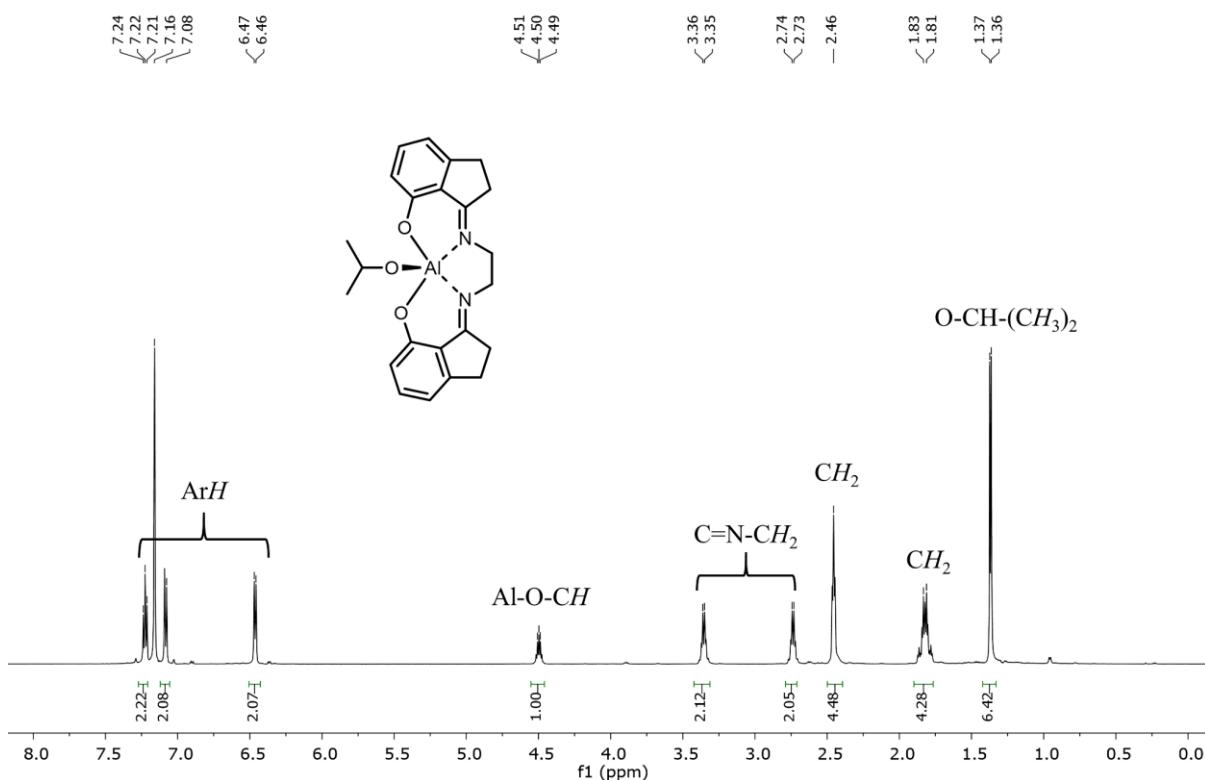


Figure S29 ^1H NMR spectrum (600 MHz, C_6D_6 , 30 °C) of complex **3a**.

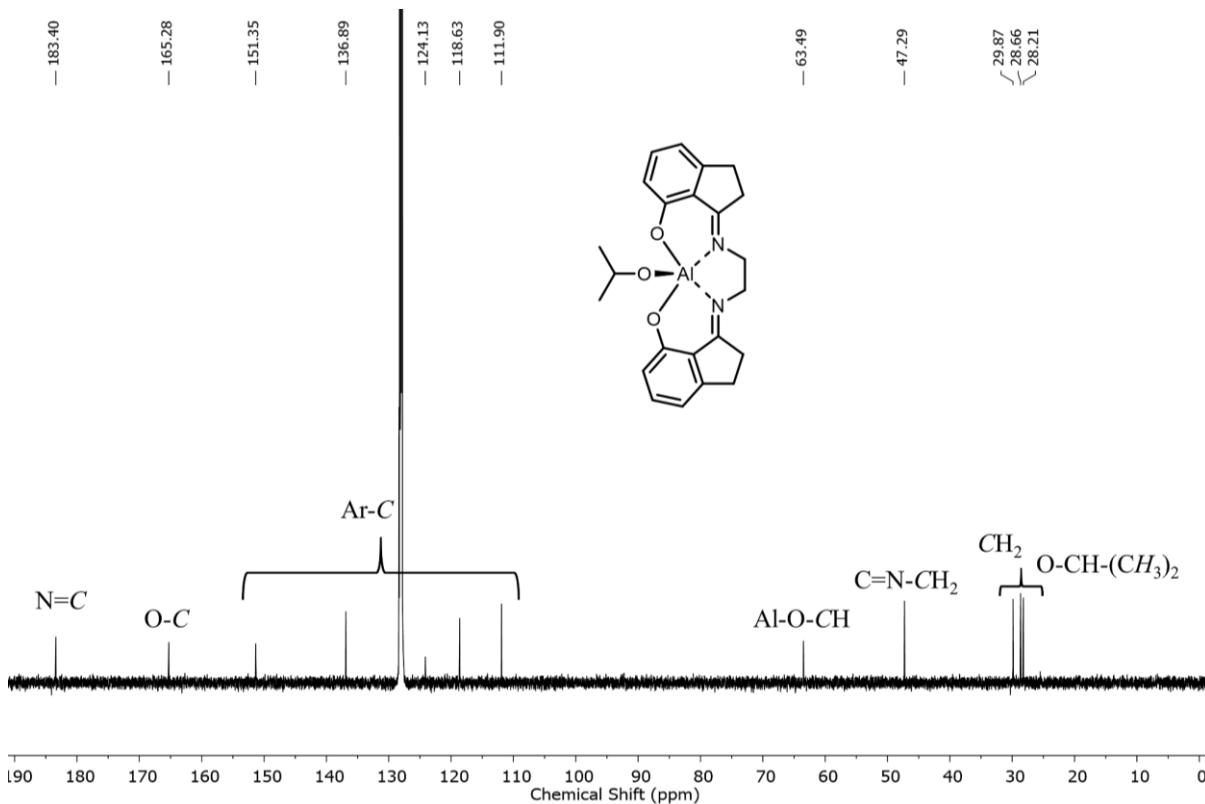


Figure S30 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (150 MHz, C_6D_6 , 30 °C) of complex **3a**.

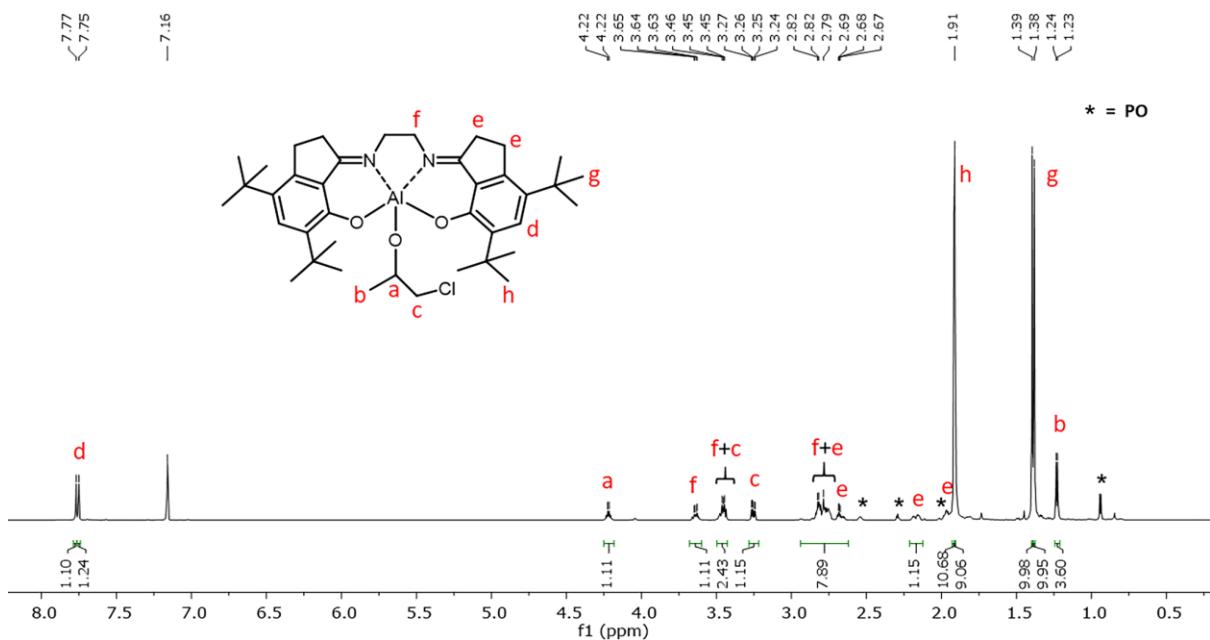


Figure S31 ^1H NMR spectrum (600 MHz, C_6D_6 , 30 °C) of complex **2c** with PO.

^1H NMR (600 MHz, C_6D_6 , 30 °C): δ 7.76 (d, $J = 11.3$ Hz, 2H, ArH), 4.22 (dq, $J = 5.7$ Hz, 1H, $\text{OCH}(\text{CH}_3)\text{CH}_2\text{Cl}$), 3.67 – 3.60 (m, 1H, C=N-CH₂), 3.50 – 3.40 (m, 2H, C=N-CH₂, $\text{OCH}(\text{CH}_3)\text{CH}_2\text{Cl}$), 3.25 (dd, $J = 10.1, 4.7$ Hz, 1H, $\text{OCH}(\text{CH}_3)\text{CH}_2\text{Cl}$), 2.92 – 2.61 (m, 8H, C=N-CH₂, Ar-CH₂), 2.17 (ddd, $J = 18.2, 7.6, 3.7$ Hz, 1H, Ar-CH₂), 1.91 (d, 19H, Ar-CH₂, Ar-C(CH₃)₃), 1.39 (d, $J = 8.5$ Hz, 18H, Ar-C(CH₃)₃), 1.23 (d, $J = 6.0$ Hz, 3H, $\text{OCH}(\text{CH}_3)\text{CH}_2\text{Cl}$).

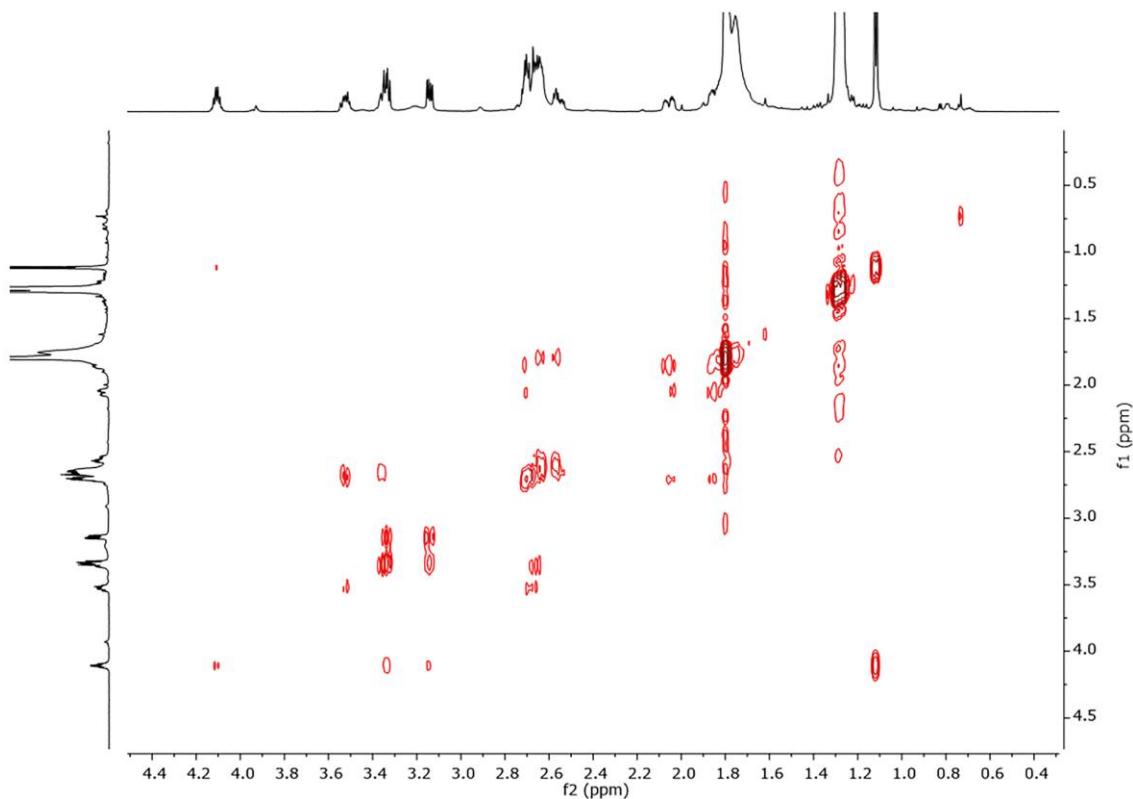


Figure S32 COSY NMR spectrum (600 MHz, C_6D_6 , 30 °C) of complex **2c** with PO.

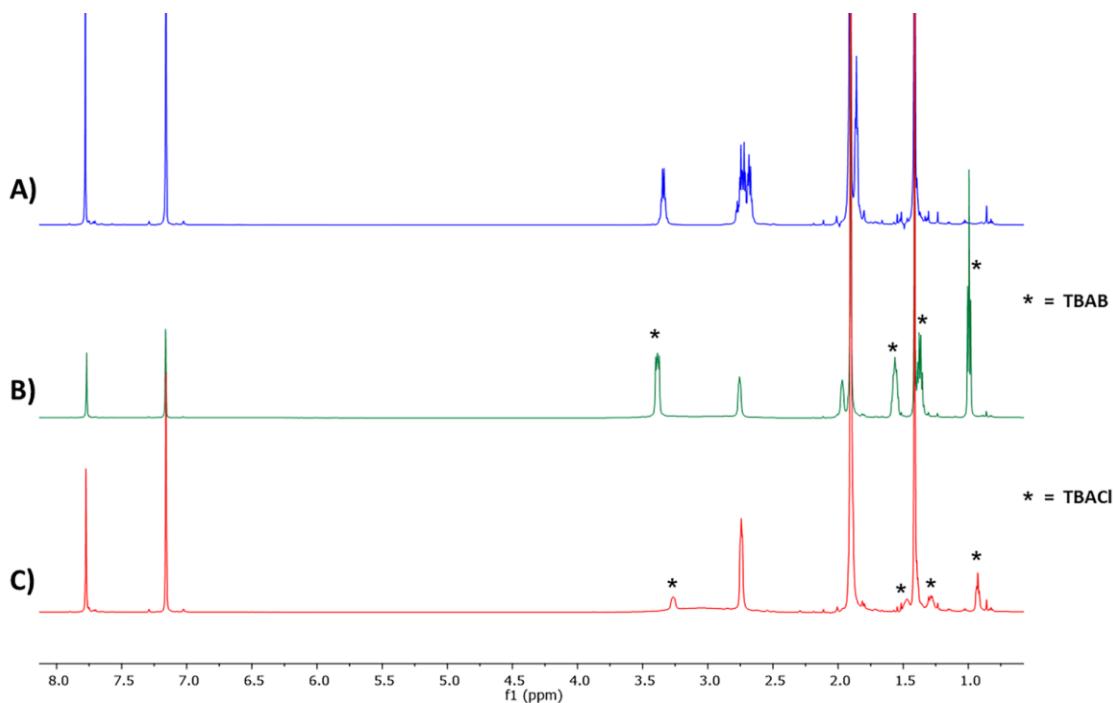


Figure S33 Series of ^1H NMR spectra (600 MHz, C_6D_6 , 30 °C) of (A) complex **2c**, (B) 1.0 equiv. of complex **2c** + 1.0 equiv. of TBAB for 5 min at room temperature, (C) 1.0 equiv. of complex **2c** + 1.0 equiv. of TBACl for 5 min at room temperature.

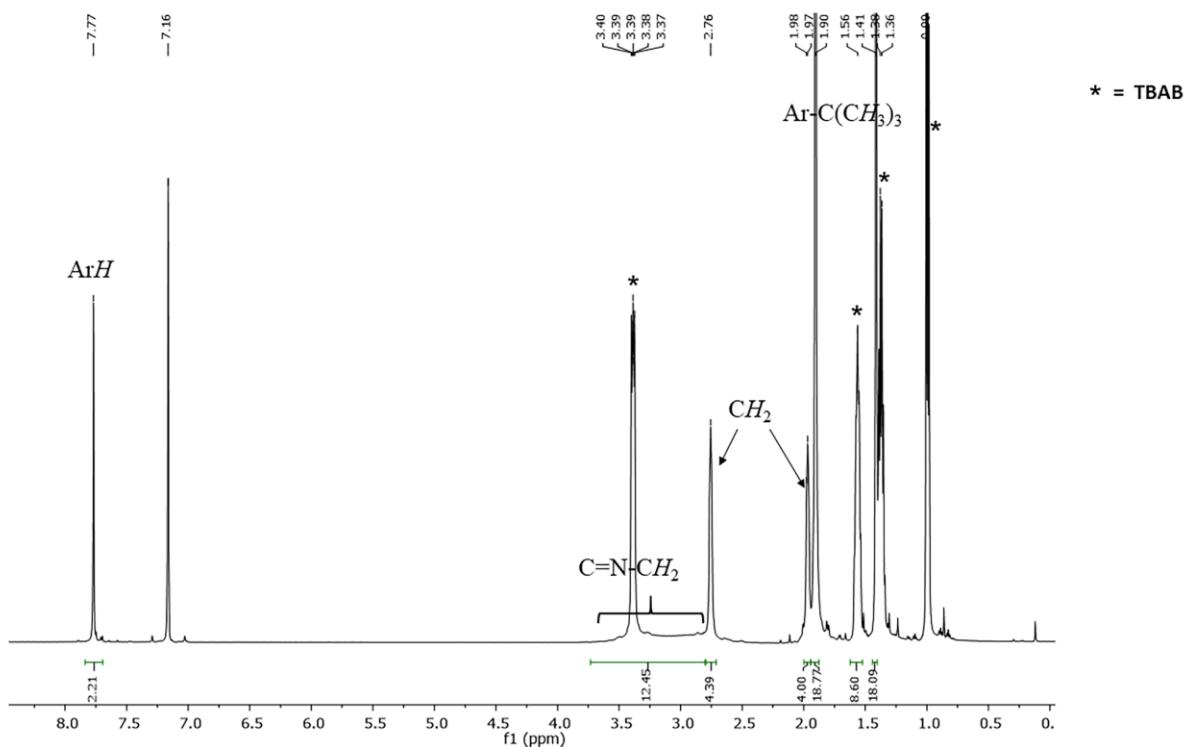


Figure S34 ^1H NMR spectrum (600 MHz, C_6D_6 , 30 °C) of 1.0 equiv. of complex **2c** and 1.0 equiv. of TBAB for 5 min at room temperature.

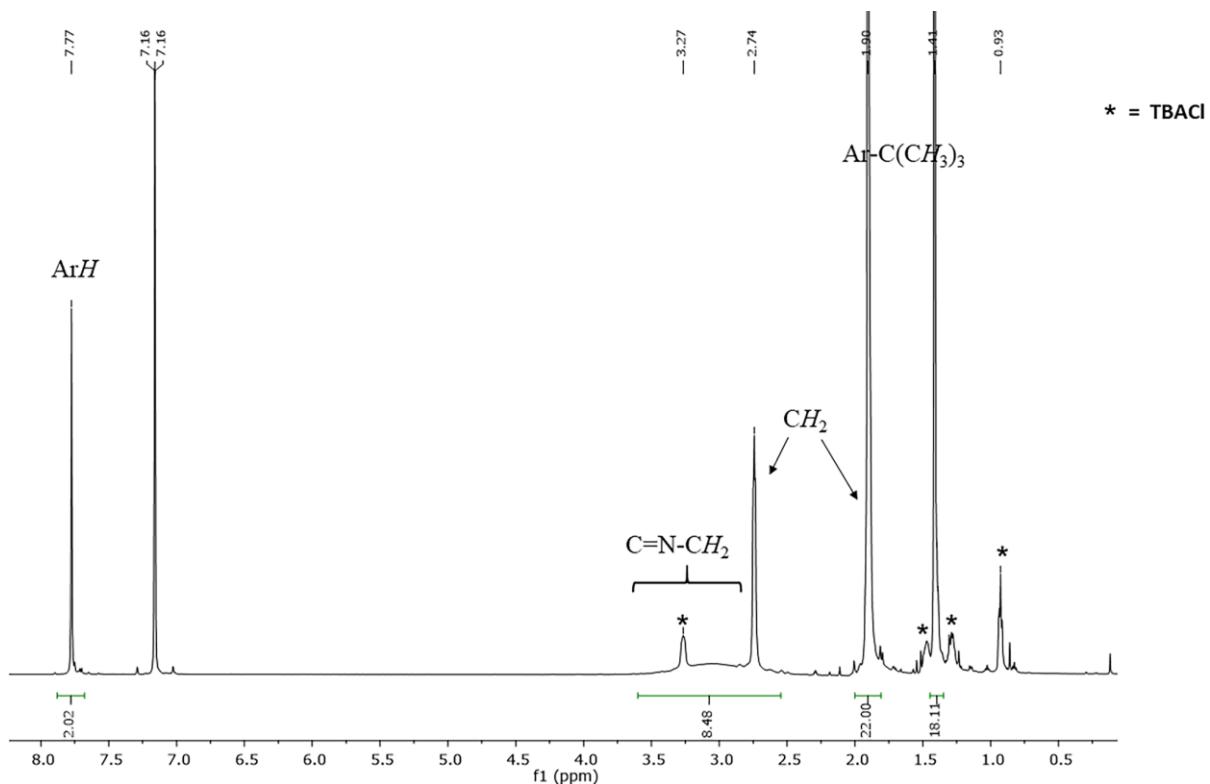


Figure S35 ^1H NMR spectrum (600 MHz, C_6D_6 , 30 °C) of 1.0 equiv of complex **2c** and 1.0 equiv of TBACl for 5 min at room temperature.

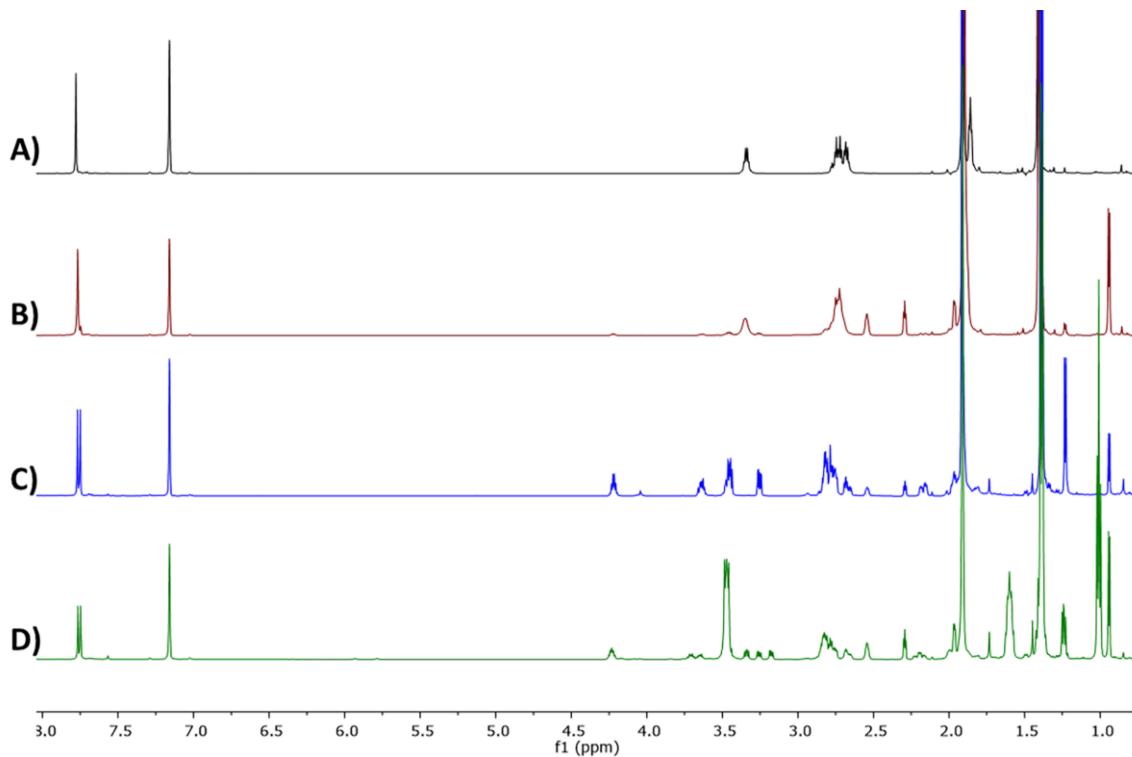


Figure S36 Series of ^1H NMR spectra (600 MHz, C_6D_6 , 30 °C) of (A) complex **2c**, (B) then the addition of 1.0 equiv. of PO for 5 min at room temperature, (C) then left for 4 h at room temperature, (D) 1.0 equiv. of PO was added to the mixture of complex **2c** and TBAB for 5 min.

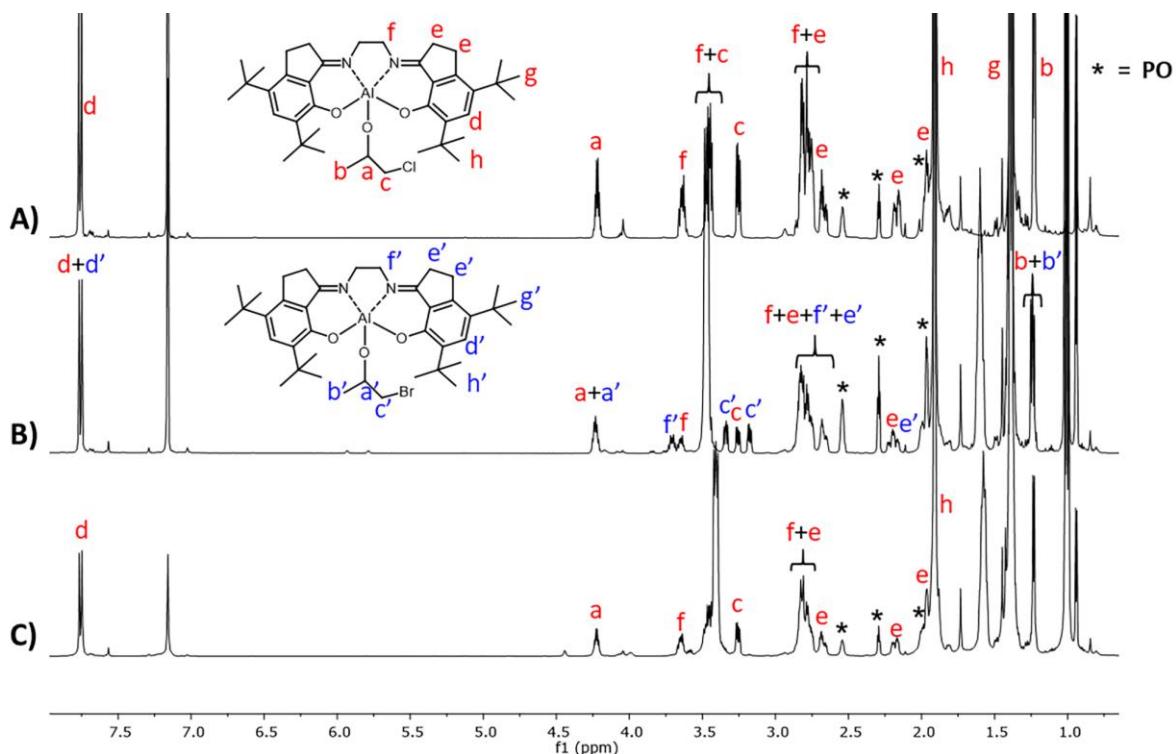


Figure S37 Series of ^1H NMR spectra (600 MHz, C_6D_6 , 30 °C) of (A) the mixture of complex **2c** and PO for 4 h at room temperature, (B) the mixture of complex **2c** and TBAB, then the addition of 1.0 equiv. of PO for 5 min, (C) then left overnight.

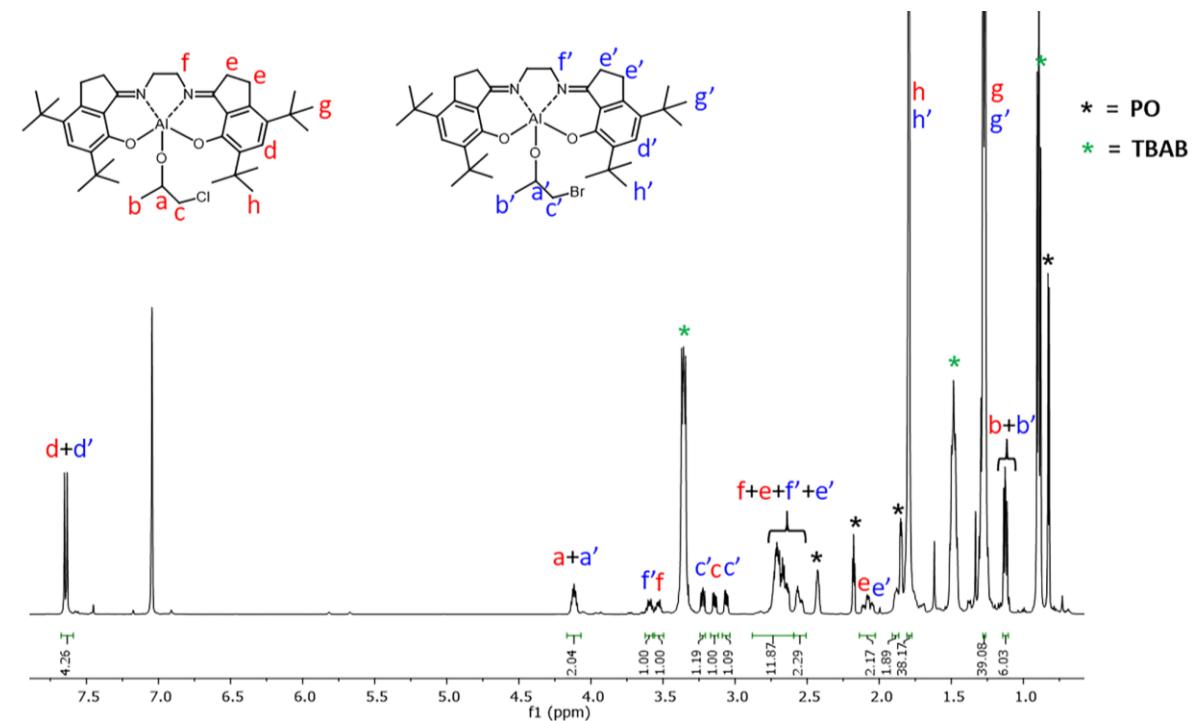


Figure S38 ^1H NMR spectrum (600 MHz, C_6D_6 , 30 °C) of the mixture of complex **2c** and TBAB, then the addition of 1.0 equiv of PO for 5 min.

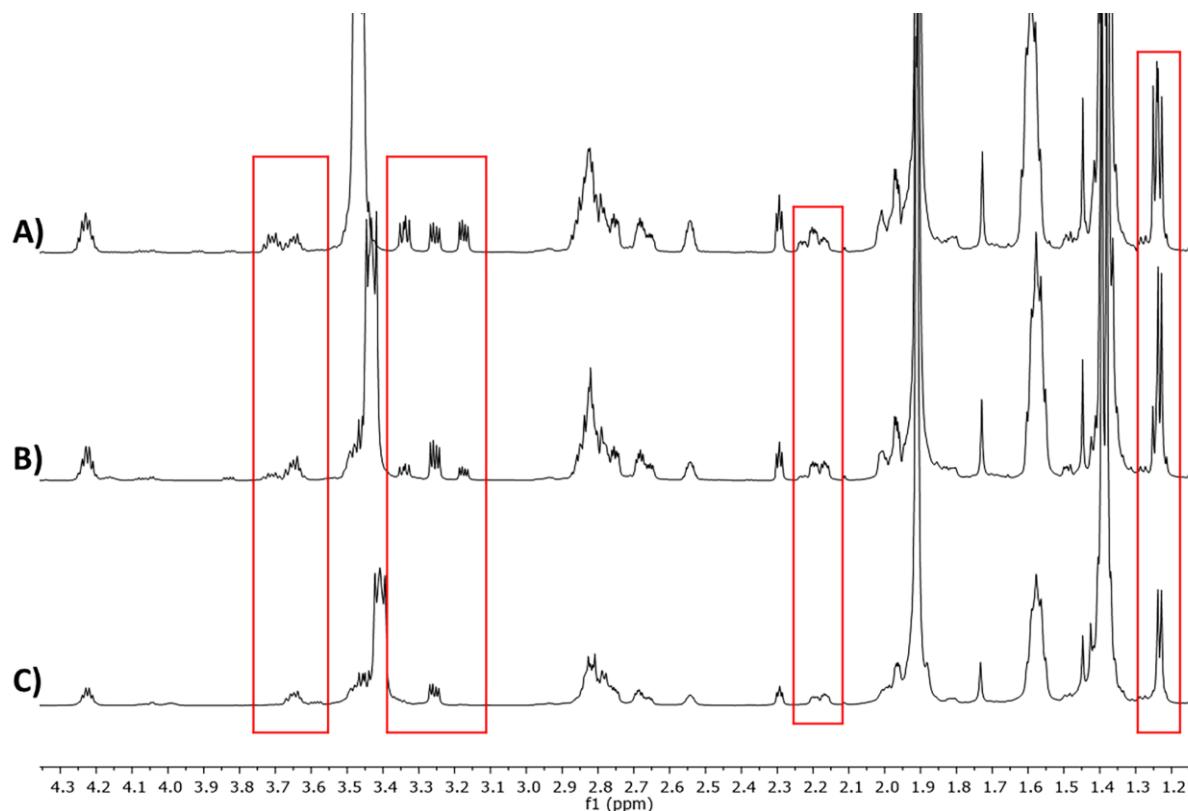


Figure S39 Series of ^1H NMR spectra (600 MHz, C_6D_6 , 30 °C) of (A) PO was added into the solution of complex **2c** first followed by TBAB at room temperature, (B) then left it for 8 h, (C) then left overnight.

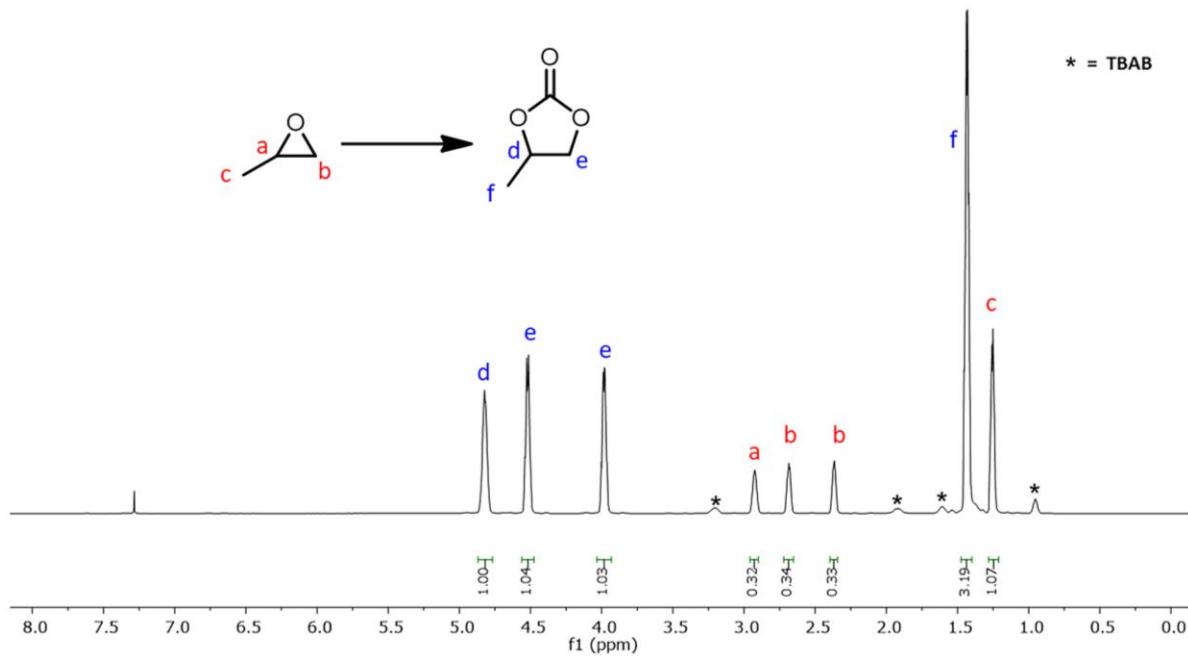


Figure S40 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the crude propylene carbonate from Table 1, entry 14

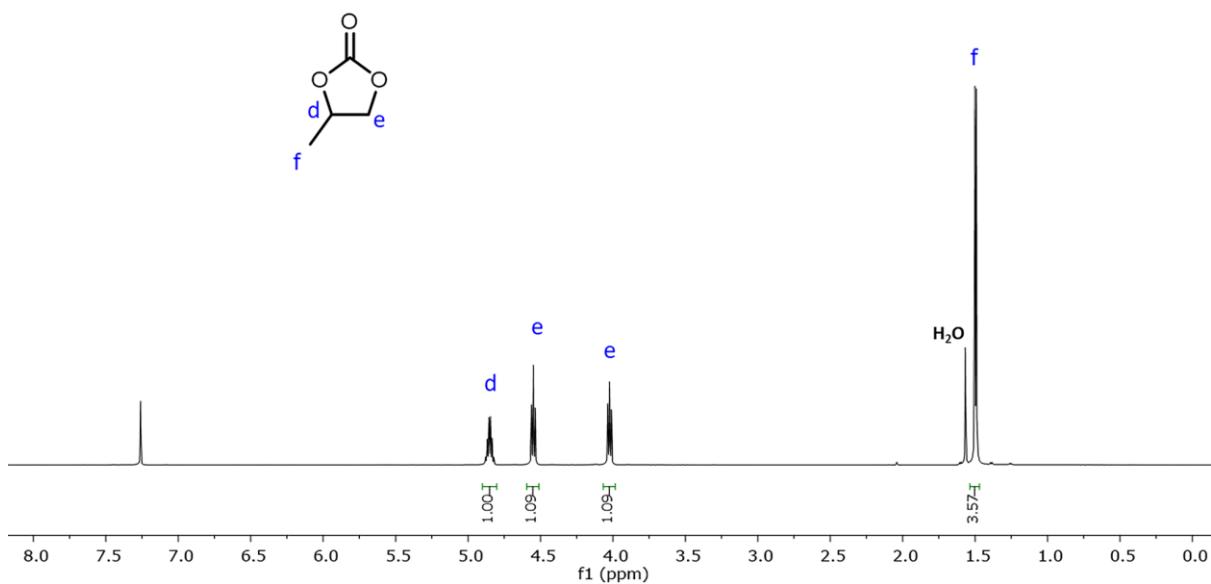


Figure S41 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the purified propylene carbonate.

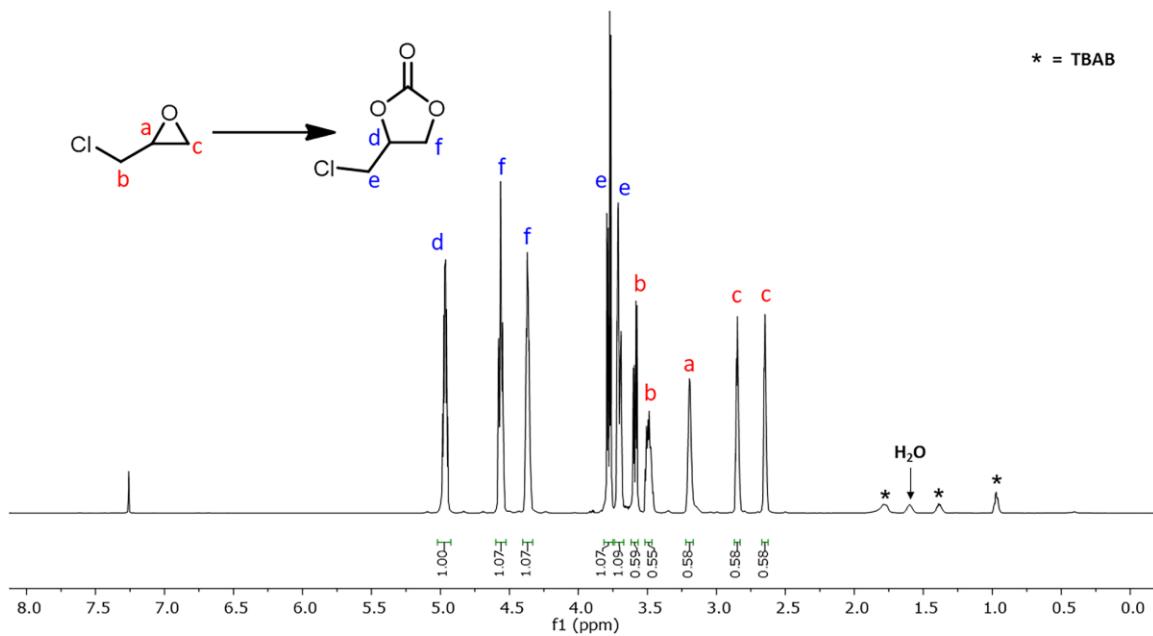


Figure S42 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the crude 3-chloropropylene carbonate (**5a**) from Fig. 6.

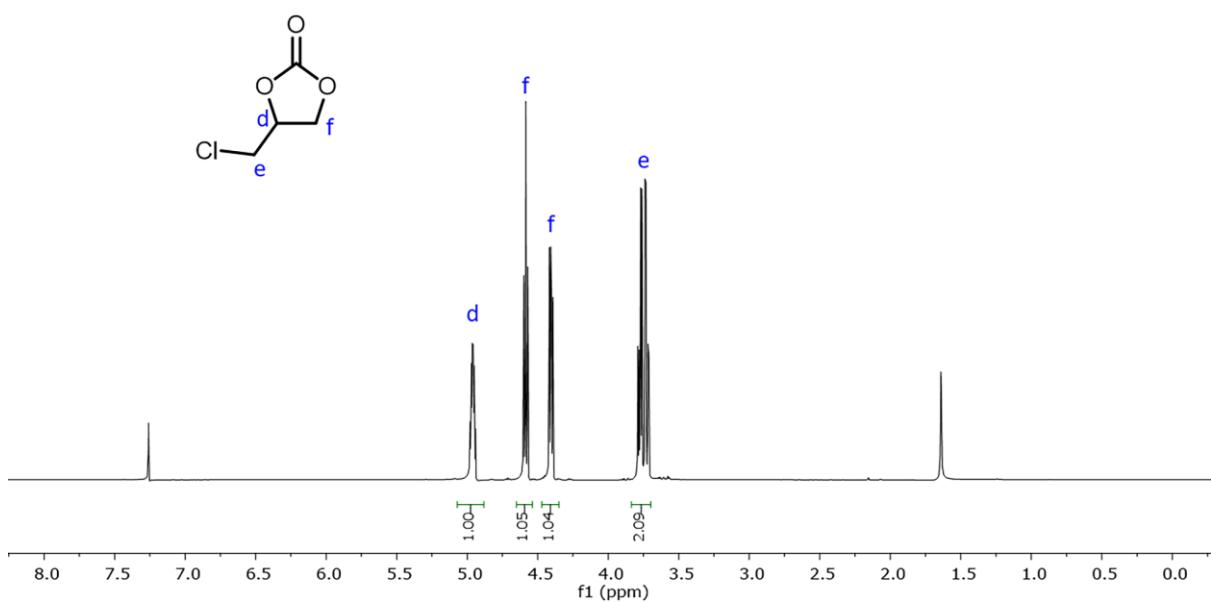


Figure S43 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the purified 3-chloropropylene carbonate (**5a**) from Fig. 6.

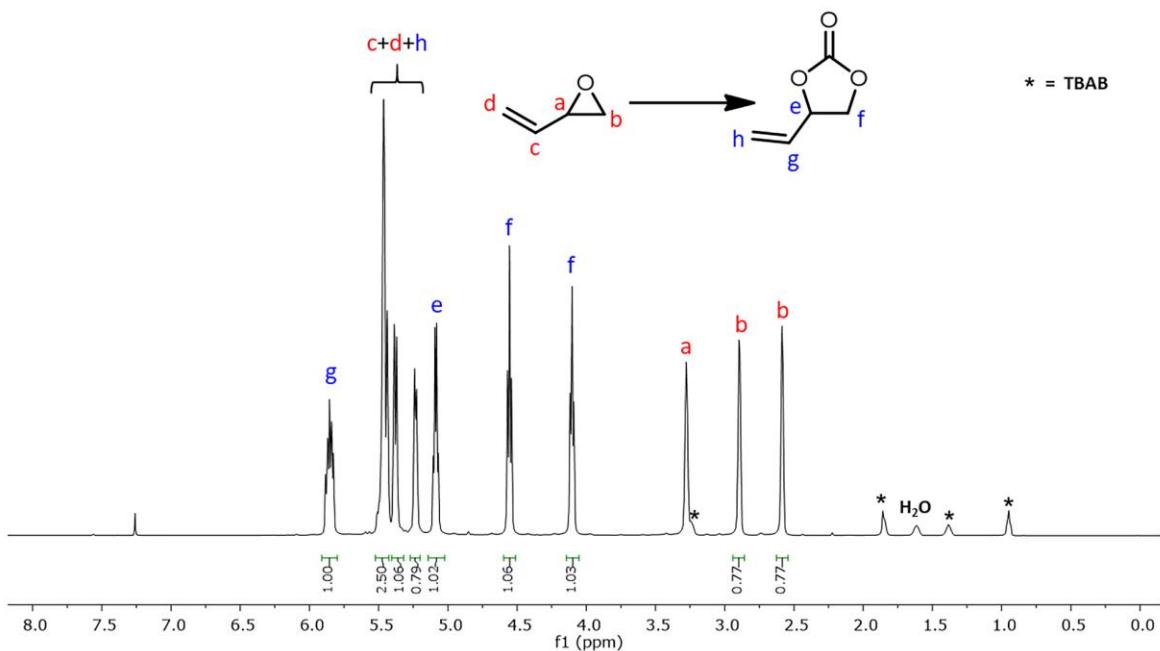


Figure S44 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the crude vinyl ethylene carbonate (**5b**) from Fig. 6.

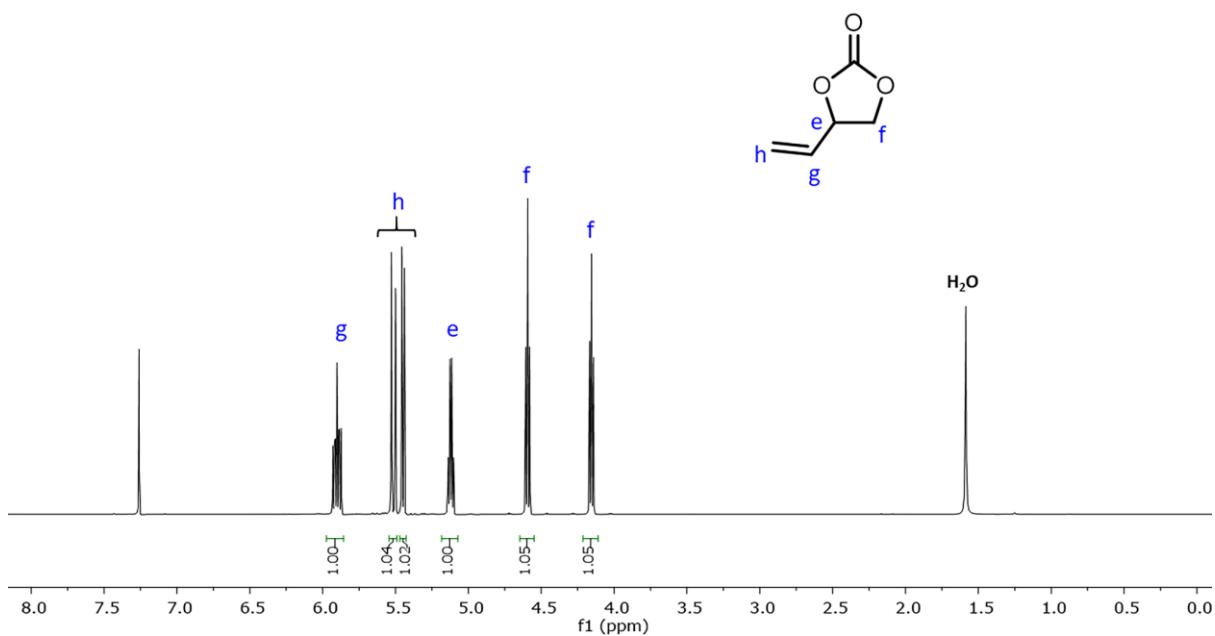


Figure S45 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the purified vinyl ethylene carbonate (**5b**) from Fig. 6.

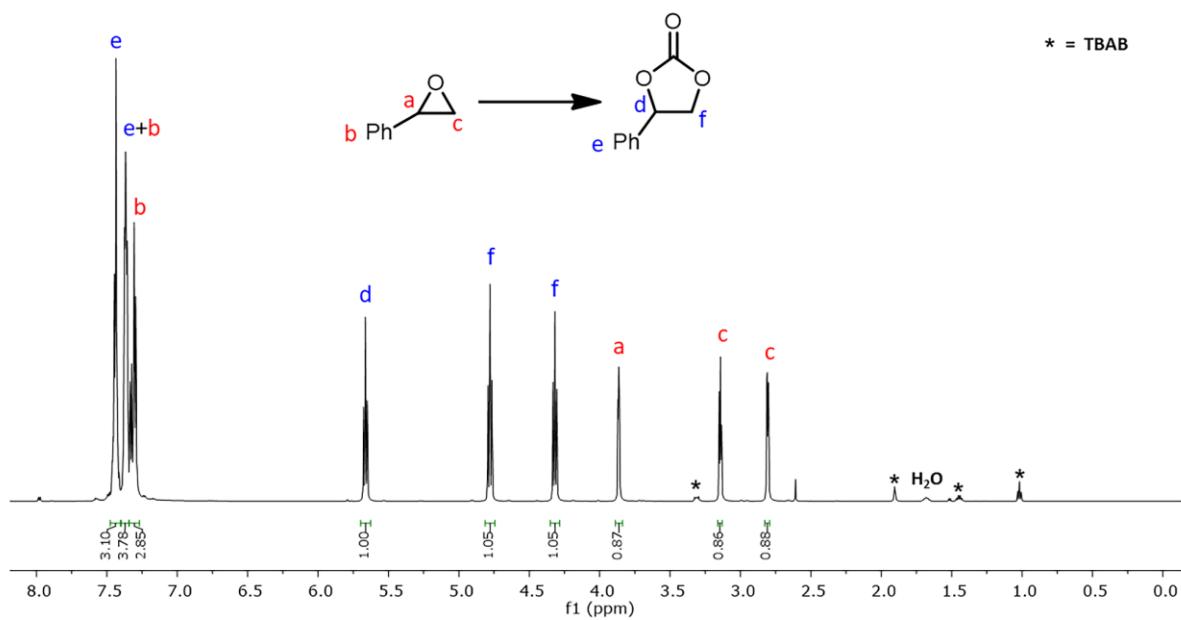


Figure S46 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the crude styrene carbonate (**5c**) from Fig. 6.

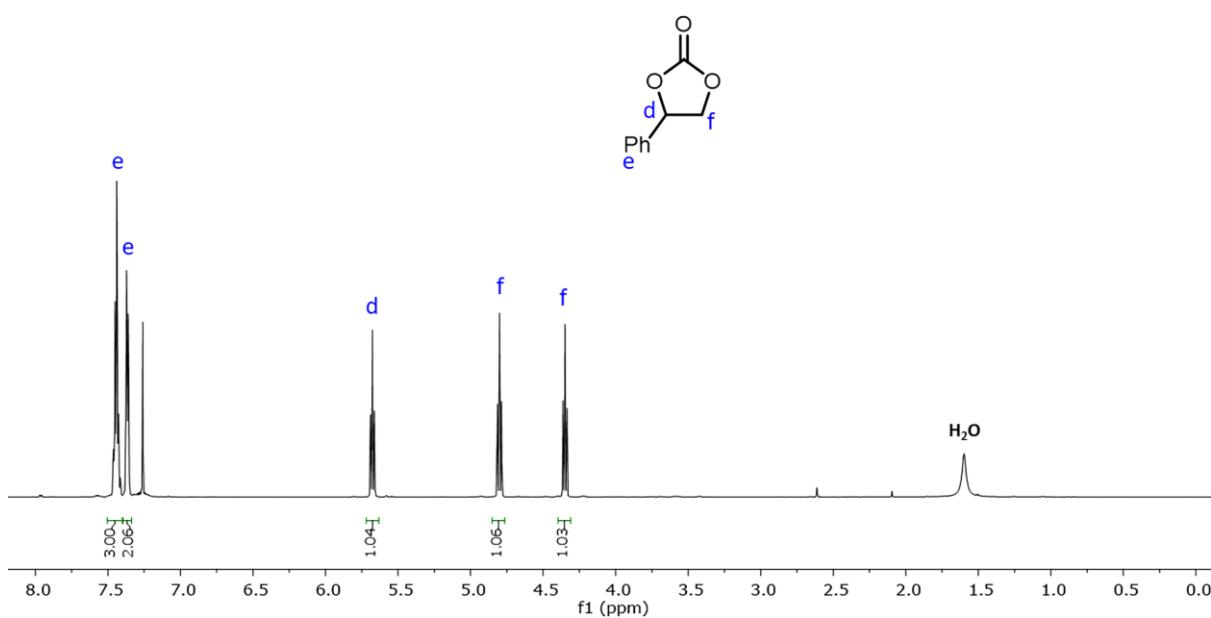


Figure S47 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the purified styrene carbonate (**5c**) from Fig. 6.

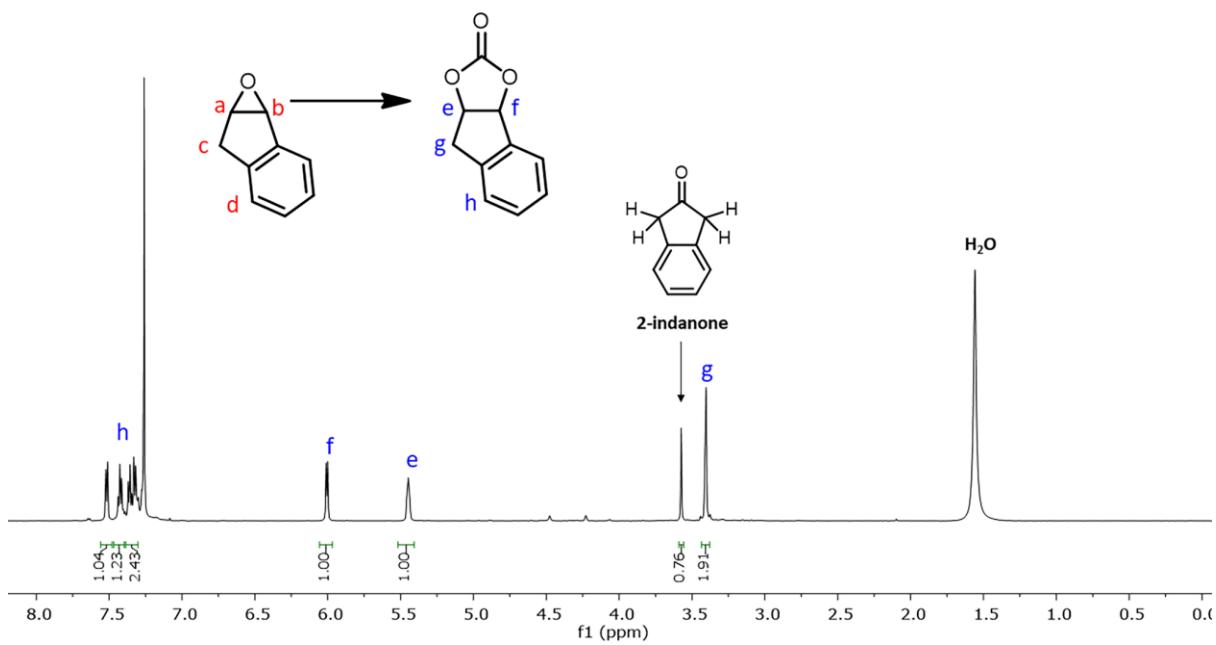


Figure S48 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the crude indene carbonate (**5d**) from Fig. 6.

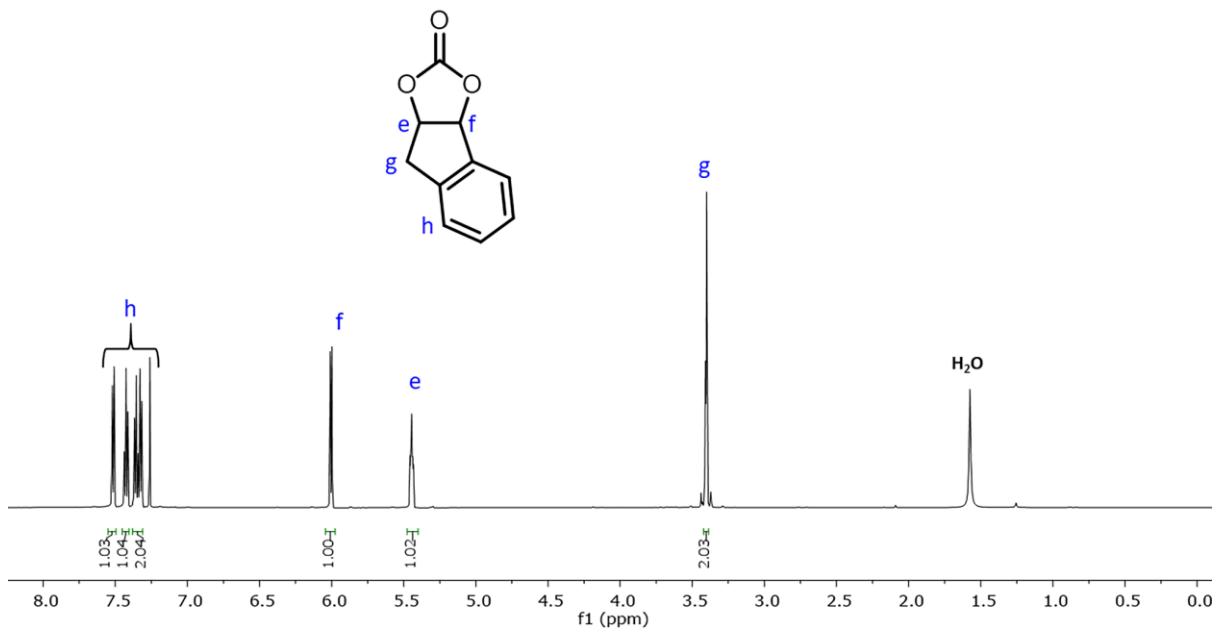


Figure S49 ¹H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the purified indene carbonate (**5d**) from Fig. 6.

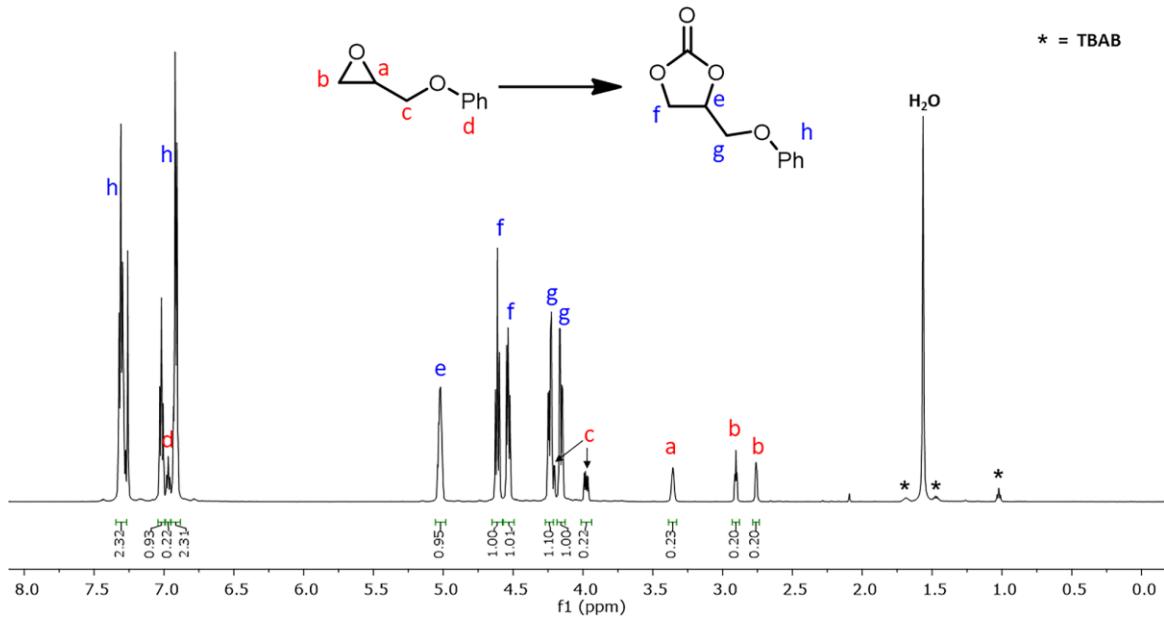


Figure S50 ¹H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the crude 3-phenoxypropylene carbonate (**5e**) from Fig. 6.

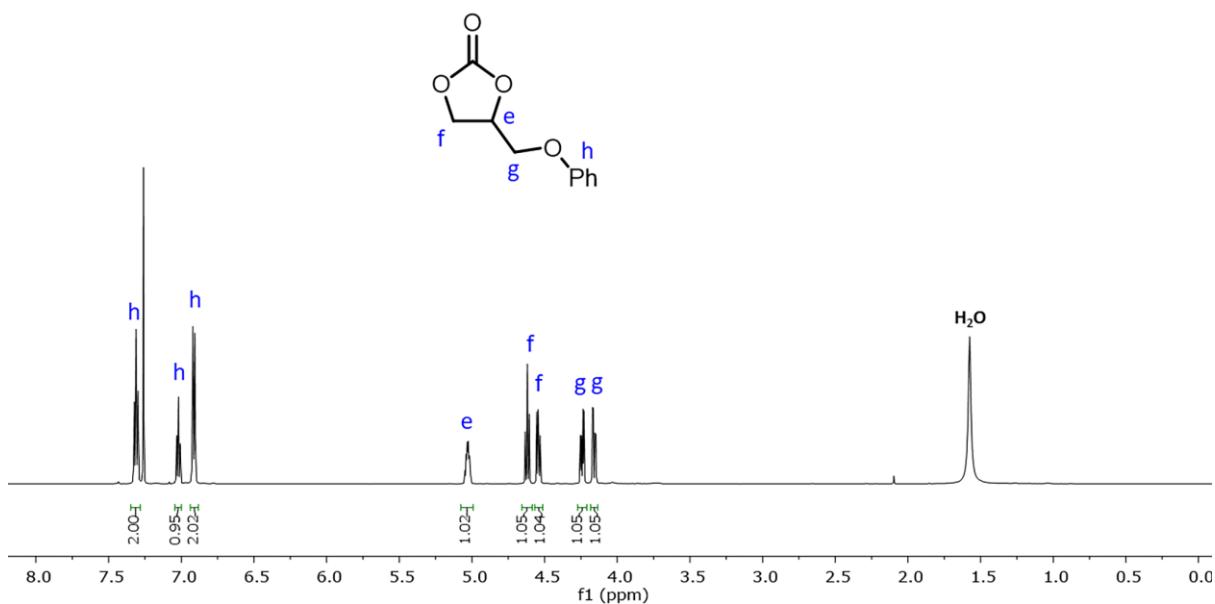


Figure S51 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the purified 3-phenoxypropylene carbonate (**5e**) from Fig. 6.

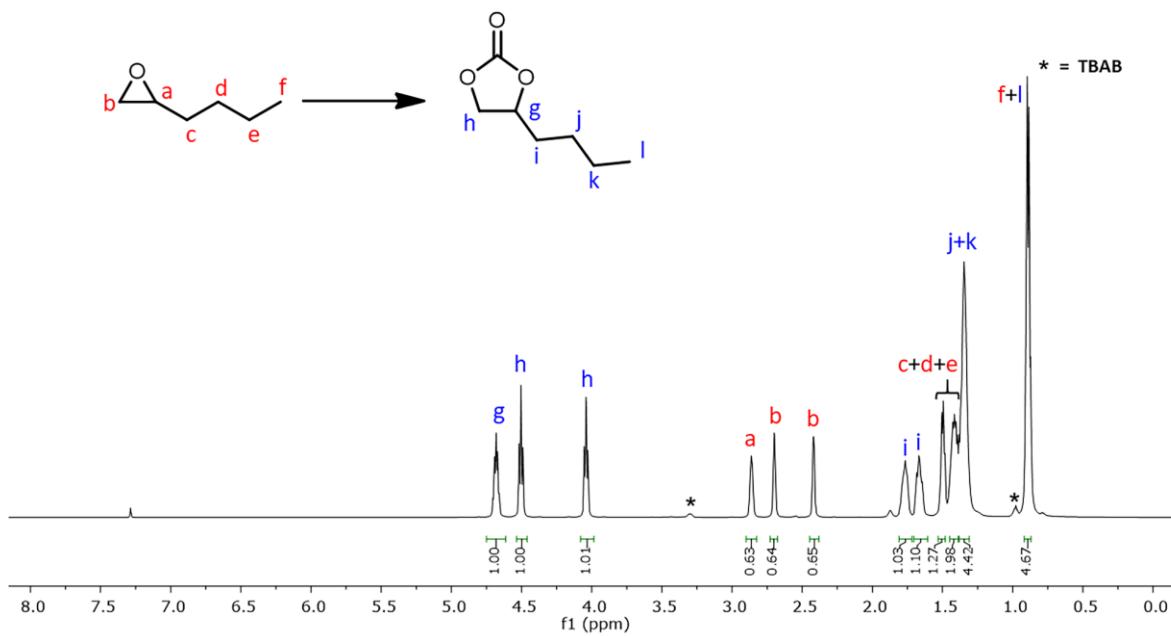


Figure S52 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the crude 1,2-hexylene carbonate (**5f**) from Fig. 6.

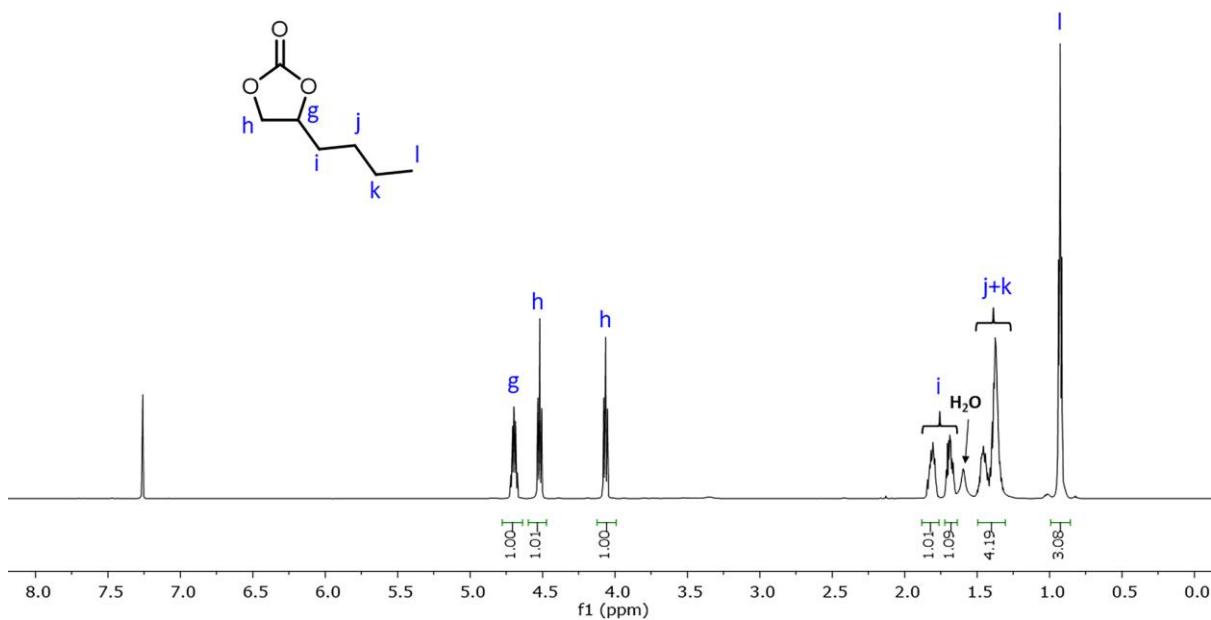


Figure S53 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the purified 1,2-hexylene carbonate (**5f**) from Fig. 6.

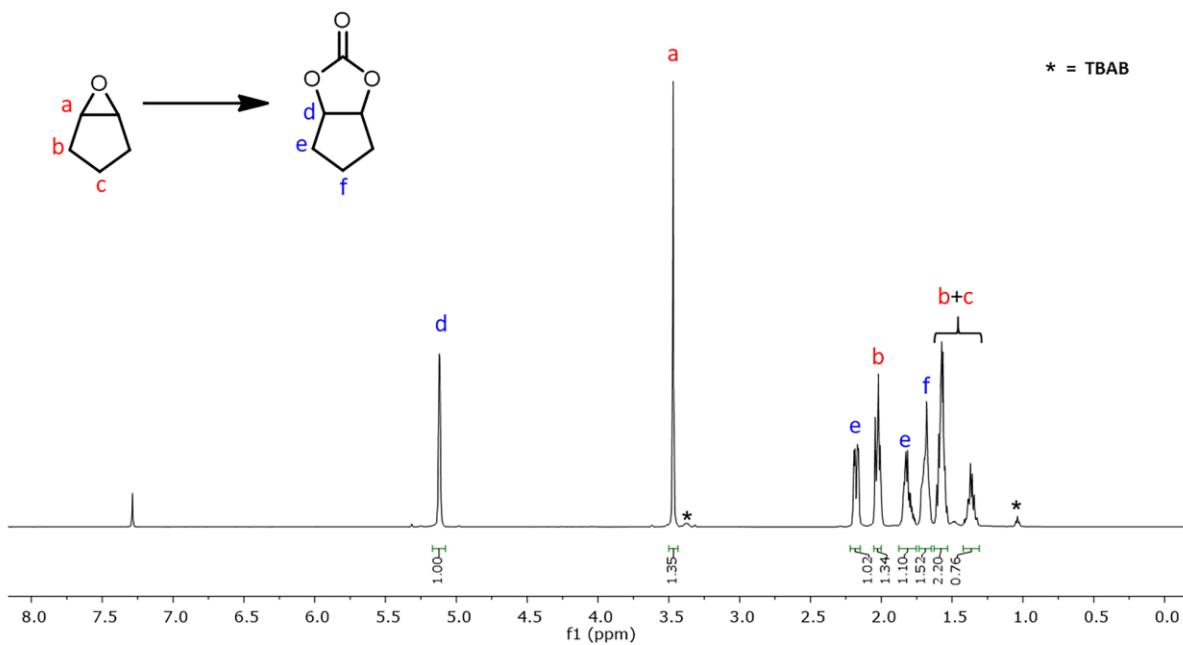


Figure S54 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the crude cyclopentene carbonate (**5g**) from Fig. 6.

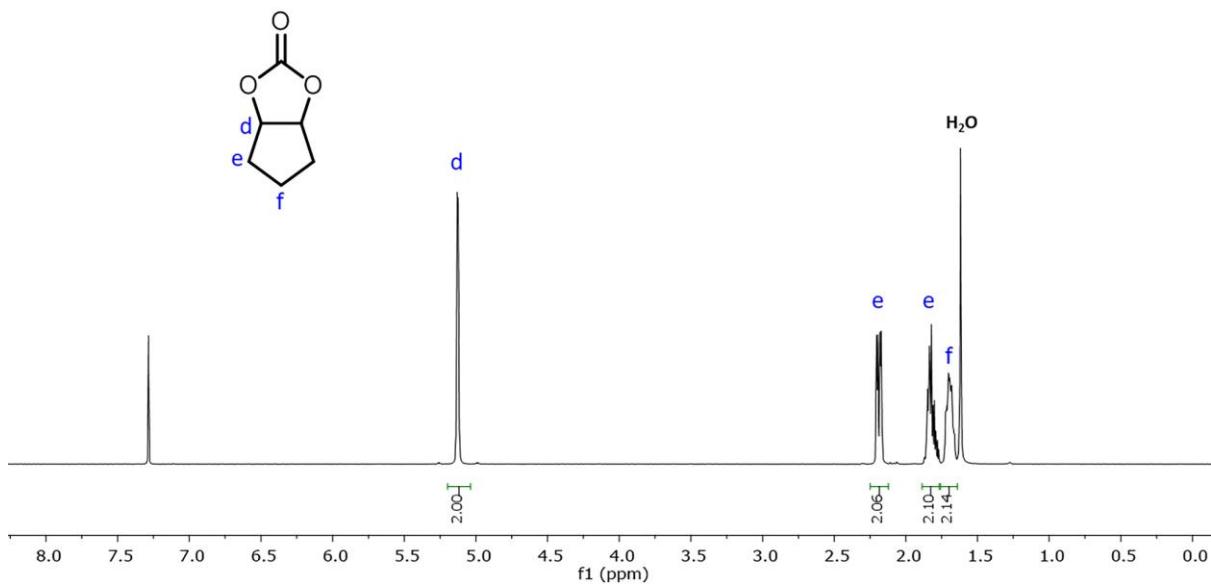


Figure S55 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the purified cyclopentene carbonate (**5g**) from Fig. 6.

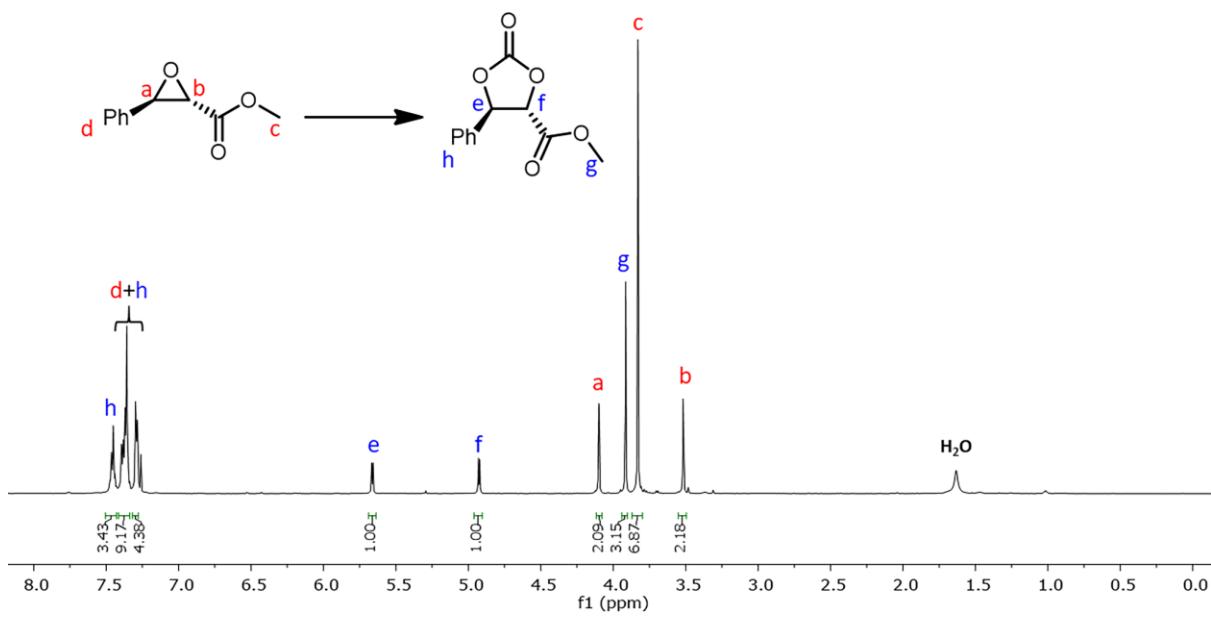


Figure S56 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the crude methyl 2-oxo-5-phenyl-1,3-dioxolane-4-carboxylate (**5h**) from Fig. 6.

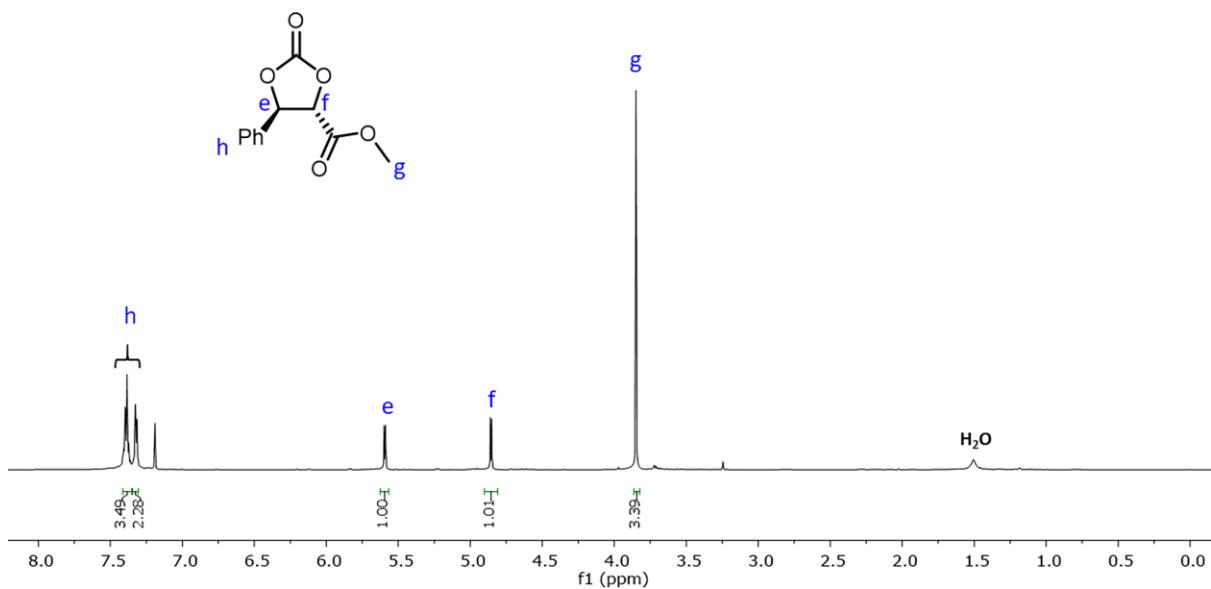


Figure S57 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the purified methyl 2-oxo-5-phenyl-1,3-dioxolane-4-carboxylate (**5h**) from Fig. 6.

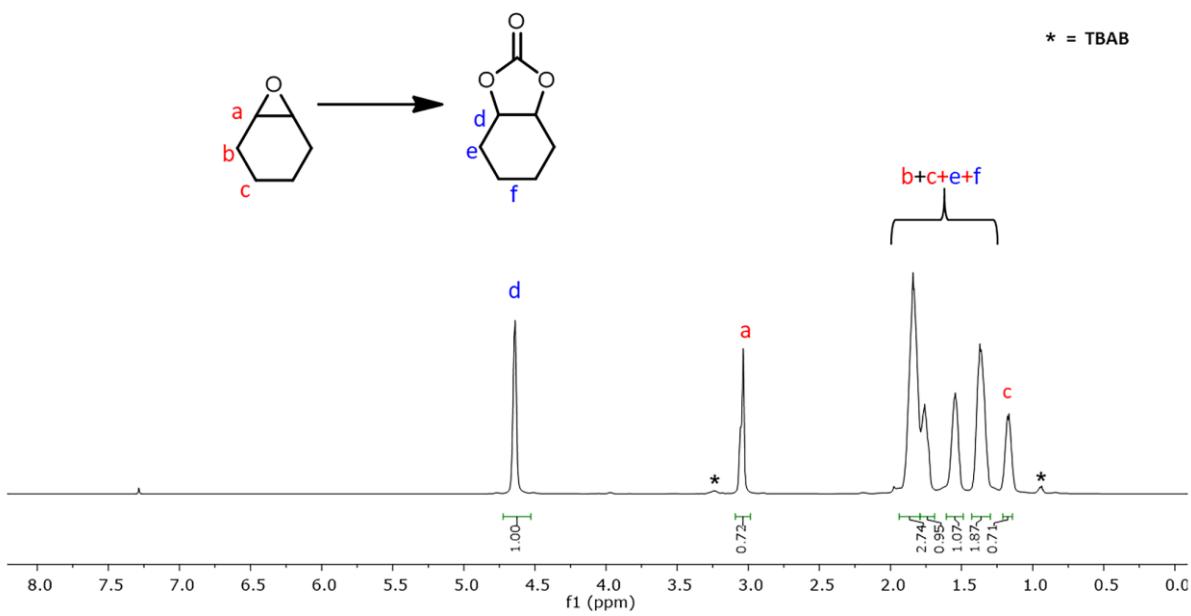


Figure S58 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the crude cyclohexene carbonate (**5i**) from Fig. 6.

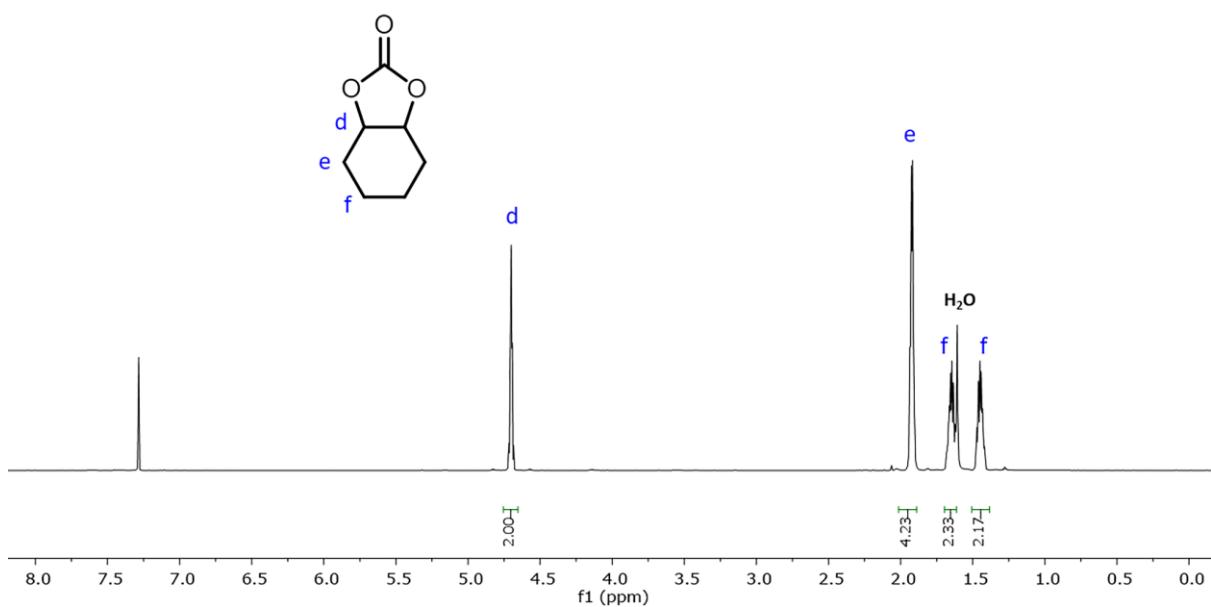


Figure S59 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the purified cyclohexene carbonate (**5i**) from Fig. 6.

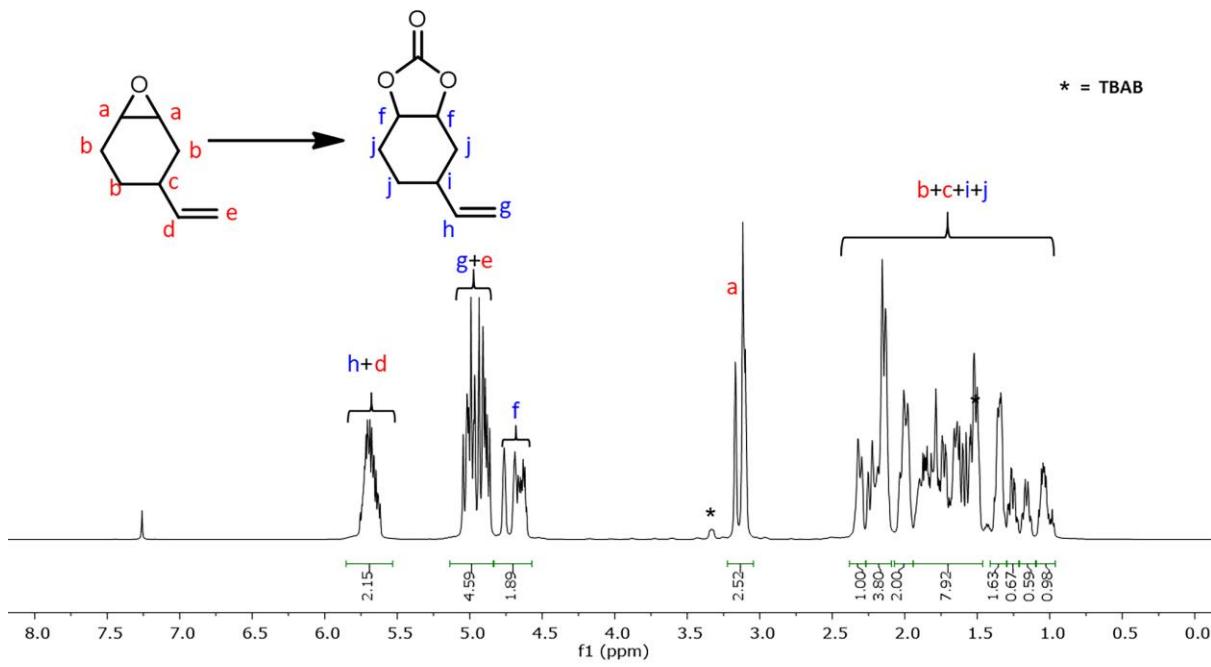


Figure S60 ^1H NMR spectrum (600 MHz, CDCl_3 , 30 °C) of the crude 4-vinylcyclohexene carbonate (**5j**) from Fig. 6.

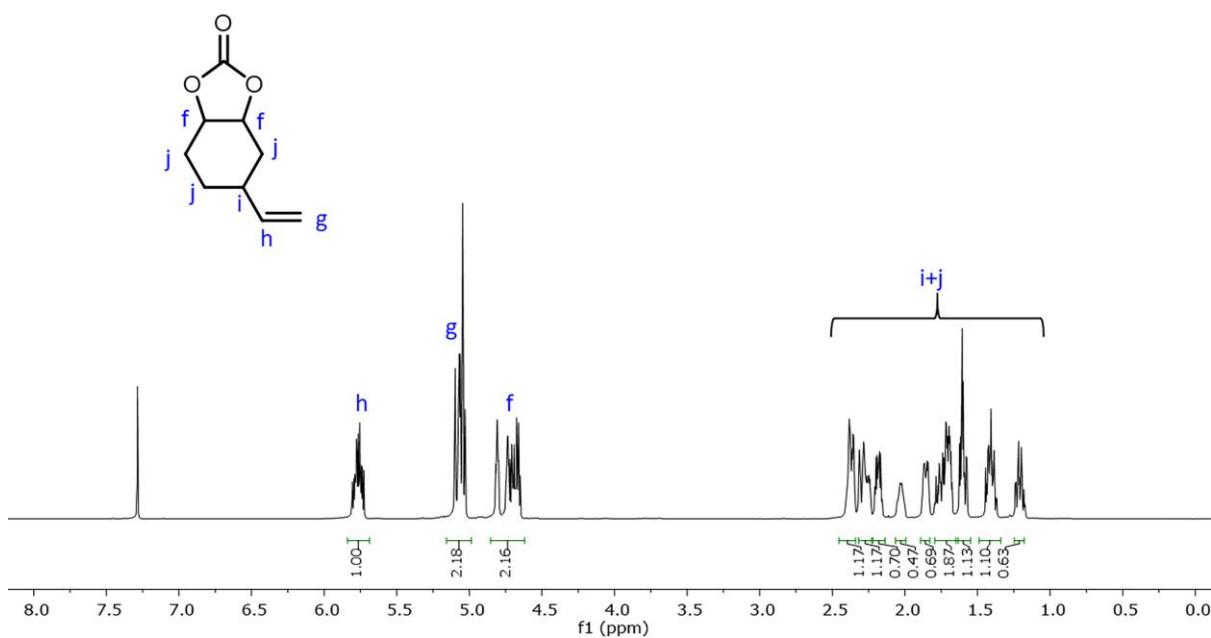


Figure S61 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the purified 4-vinylcyclohexene carbonate (**5j**) from Fig. 6.

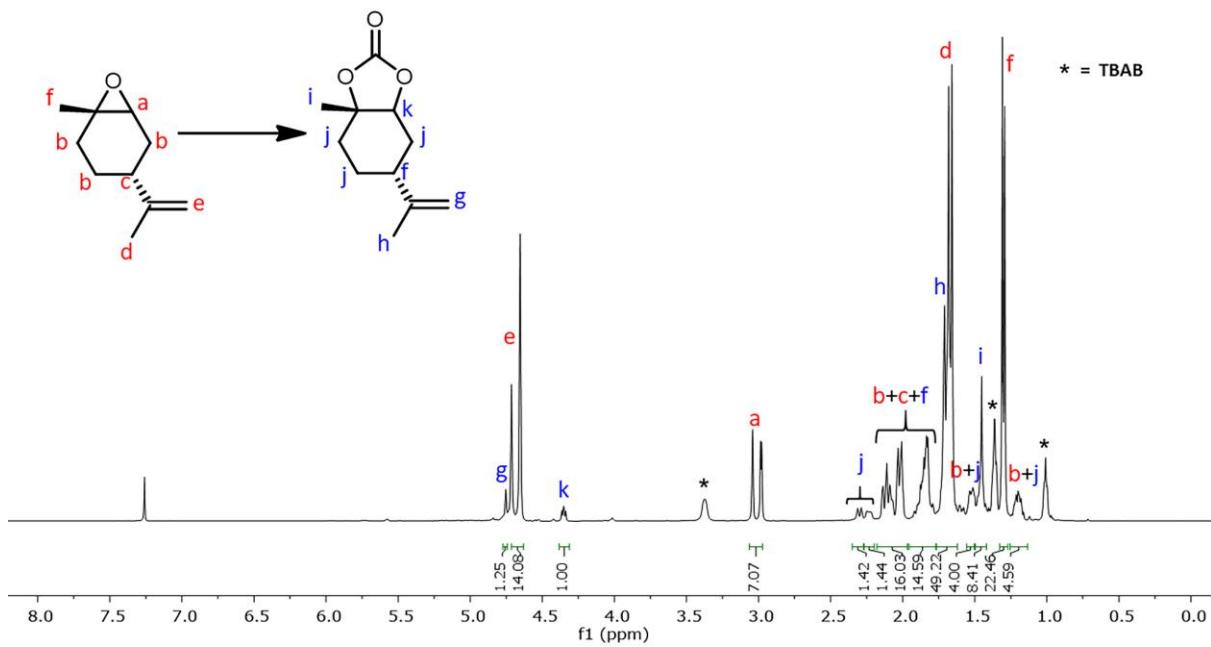


Figure S62 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the crude limonene carbonate (**5k**) from Fig. 6.

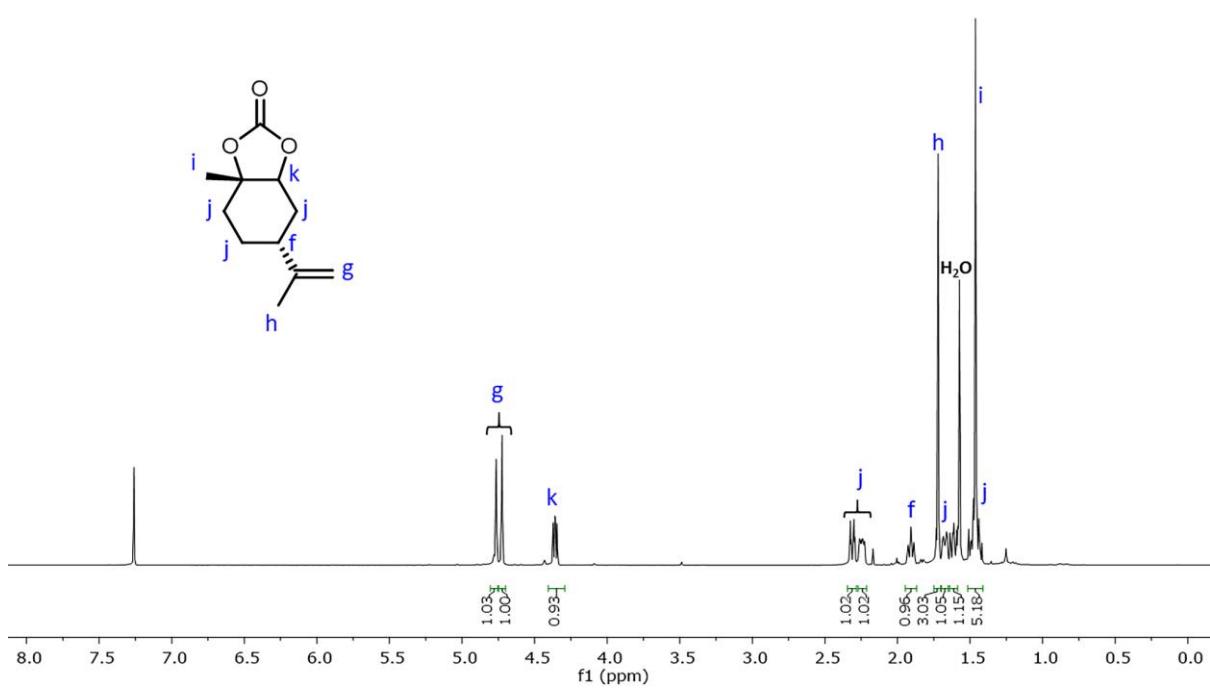


Figure S63 ¹H NMR spectrum (600 MHz, CDCl₃, 30 °C) of the purified limonene carbonate (**5k**) from Fig. 6.

Single-Crystal X-ray Crystallography

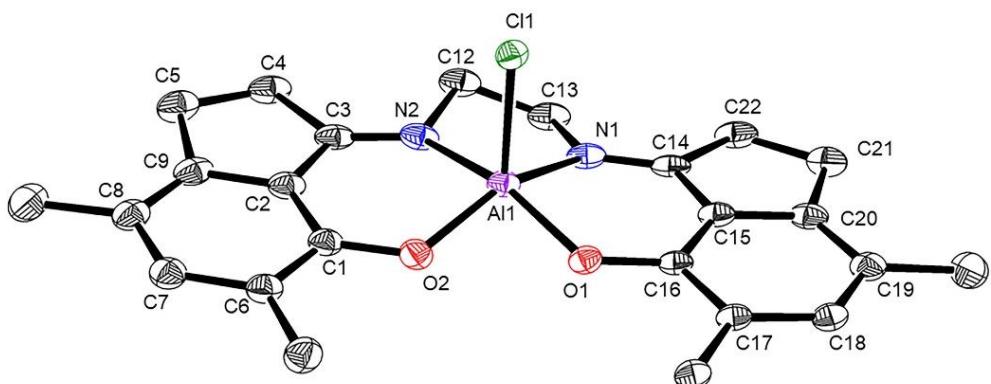


Table S1. Crystal data and structure refinement for complex **2b**

Complex	2b
CCDC	2072656
Chemical formula	4(C ₂₄ H ₂₆ AlClN ₂ O ₂)·C ₂ H ₈ Cl ₄
Formula weight	1921.47
Temperature (K)	120
Wavelength (Å)	0.71073
Space group	<i>P</i> 12/n 1
Crystal size (mm)	0.42 × 0.19 × 0.09
Crystal system	Monoclinic
a (Å)	17.714 (1)
b (Å)	10.239 (1)
c (Å)	25.344 (2)
V (Å ³)	4559.8 (6)
Z	2
Density (calcd.) (mg/m ³)	1.399
μ (mm ⁻¹)	0.35
Theta range for data collection (°)	2.4–26.4
<i>F</i> (000)	2016
Reflection collected	134693
Unique reflections	8984
Goodness-of-fit-on <i>F</i> ²	1.034
R1(<i>F</i>), <i>wR</i> (<i>F</i> ²)	0.0319, 0.094
Largest diff. peak and hole [e Å ⁻³]	0.29 and -0.90

Table S2 Selected bond distances and angles for complex **2b**

Bond distances (Å)		Bond angles (deg)	
Cl1—Al1	2.195 (1)	O1—Al1—Cl1	104.9 (1)
Al1—O1	1.803 (1)	O1—Al1—N1	92.2 (1)
Al1—O2	1.796 (1)	O1—Al1—N2	159.6 (1)
Al1—N1	2.001 (1)	O2—Al1—Cl1	107.9 (1)
Al1—N2	2.009 (1)	O2—Al1—O1	86.4 (1)
O1—C16	1.324 (2)	O2—Al1—N1	151.3 (1)
O2—C1	1.327 (2)	O2—Al1—N2	91.9 (1)
N1—C14	1.298 (2)	N1—Al1—Cl1	100.2 (1)
N1—C13	1.475 (2)	N1—Al1—N2	79.7 (1)
N2—C3	1.294 (2)	N2—Al1—Cl1	95.0 (1)
N2—C12	1.467 (2)	C16—O1—Al1	130.0 (1)
C16—C15	1.400 (2)	C1—O2—Al1	129.3 (1)
C16—C17	1.409 (2)	C14—N1—Al1	123.4 (1)
C14—C15	1.436 (2)	C14—N1—C13	118.5 (1)
C14—C22	1.511 (2)	C13—N1—Al1	117.9 (1)
C15—C20	1.398 (2)	C3—N2—Al1	123.4 (1)
C20—C19	1.384 (2)	C3—N2—C12	119.8 (1)
C20—C21	1.516 (2)	C12—N2—Al1	115.0 (1)
C17—C18	1.400 (2)	O1—C16—C15	121.0 (1)
C7—C6	1.394 (2)	O1—C16—C17	121.4 (1)
C7—C8	1.406 (2)	C15—C16—C17	117.6 (1)
C1—C6	1.408 (2)	N1—C14—C15	122.8 (1)
C1—C2	1.399 (2)	N1—C14—C22	128.5 (1)
C18—C19	1.410 (2)	C15—C14—C22	108.6 (1)
C3—C4	1.516 (2)	C16—C15—C14	125.7 (2)
C3—C2	1.432 (2)	C20—C15—C16	123.2 (2)
C12—C13	1.519 (3)	C20—C15—C14	111.0 (1)
C8—C9	1.380 (3)	O2—C1—C6	121.6 (1)
C9—C2	1.403 (2)	O2—C1—C2	121.1 (2)
C9—C5	1.510 (2)	C2—C1—C6	117.3 (1)
C4—C5	1.550 (3)	N2—C3—C4	128.4 (2)

C21—C22	1.546 (3)	N2—C3—C2	123.0 (1)
		C2—C3—C4	108.6 (2)
		N2—C12—C13	108.7 (1)
		N1—C13—C12	108.8 (1)
		C1—C2—C3	125.6 (2)
		C1—C2—C9	123.1 (2)
		C9—C2—C3	111.3 (1)

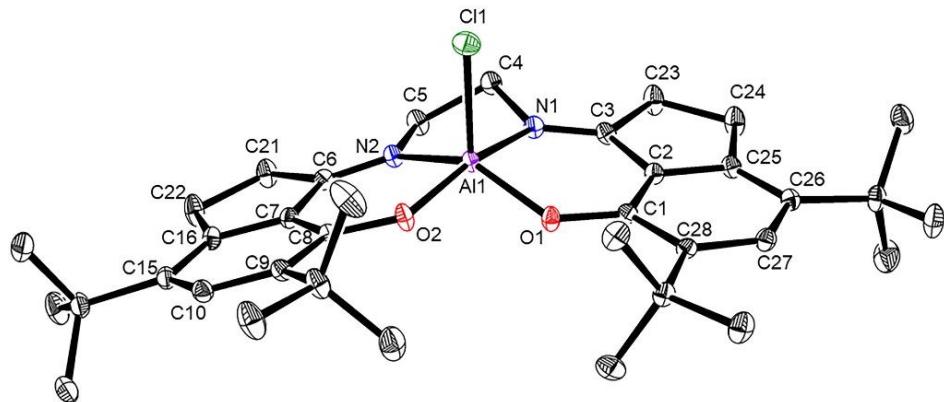


Table S3. Crystal data and structure refinement for complex **2c**

Complex	2c
CCDC	2072657
Chemical formula	C ₃₆ H ₅₀ AlClN ₂ O ₂ ·C ₆ H ₆
Formula weight	683.31
Temperature (K)	120
Wavelength (Å)	0.71073
Space group	P ₂ 12 ₁ 2 ₁
Crystal size (mm)	0.24 × 0.24 × 0.23
Crystal system	Orthorhombic
a (Å)	9.991 (1)
b (Å)	12.723 (1)
c (Å)	29.726 (2)
V (Å ³)	3778.4 (4)
Z	4
Density (calcd.) (mg/m ³)	1.201
μ (mm ⁻¹)	0.16
Theta range for data collection (°)	2.6–30.5
F (000)	1472
Reflection collected	133165
Unique reflections	11587
Goodness-of-fit-on F ²	1.057
R1(F), wR(F ²)	0.0314, 0.08
Largest diff. peak and hole [e Å ⁻³]	0.32 and -0.23

Table S4. Selected bond distances and angles for complex **2c**

Bond distances (\AA)		Bond angles (deg)	
Cl1—Al1	2.195 (1)	O1—Al1—Cl1	111.4 (1)
Al1—O1	1.792 (1)	O1—Al1—O2	88.5 (1)
Al1—O2	1.801 (1)	O1—Al1—N1	91.0 (1)
Al1—N1	1.993 (1)	O1—Al1—N2	143.7 (1)
Al1—N2	1.991 (1)	O2—Al1—Cl1	101.6 (1)
O1—C1	1.329 (2)	O2—Al1—N1	163.1 (1)
O2—C8	1.320 (2)	O2—Al1—N2	91.2 (1)
N1—C4	1.468 (2)	N1—Al1—Cl1	94.3 (1)
N1—C3	1.292 (2)	N2—Al1—Cl1	104.2 (1)
N2—C6	1.298 (2)	N2—Al1—N1	79.3 (1)
N2—C5	1.478 (2)	C1—O1—Al1	131.7 (1)
C1—C2	1.404 (2)	C8—O2—Al1	133.8 (1)
C1—C28	1.420 (2)	C4—N1—Al1	112.9 (1)
C2—C3	1.436 (2)	C3—N1—Al1	125.4 (1)
C2—C25	1.407 (2)	C3—N1—C4	121.0 (1)
C6—C7	1.436 (2)	C6—N2—Al1	125.1 (1)
C6—C21	1.508 (2)	C6—N2—C5	117.7 (1)
C8—C7	1.405 (2)	C5—N2—Al1	117.2 (1)
C8—C9	1.424 (2)	O1—C1—C2	120.4 (1)
C7—C16	1.411 (2)	C1—C2—C3	124.5 (1)
C4—C5	1.522 (2)	C1—C2—C25	124.5 (1)
C3—C23	1.507 (2)	C25—C2—C3	111.0 (1)
C9—C10	1.389 (2)	N2—C6—C7	124.6 (1)
C28—C27	1.400 (2)	O2—C8—C7	120.4 (1)
C10—C15	1.418 (2)	C8—C7—C6	123.9 (1)
C27—C26	1.410 (2)	C8—C7—C16	124.7 (1)
C25—C26	1.395 (2)	C16—C7—C6	111.3 (1)
C25—C24	1.520 (2)	N1—C4—C5	106.5 (1)
C23—C24	1.543 (2)	N1—C3—C2	123.3 (1)
C16—C15	1.392 (2)	N2—C5—C4	108.0 (1)
C16—C22	1.523 (2)	N2—C6—C21	126.5 (1)
C22—C21	1.542 (2)	C7—C6—C21	108.9 (1)
		N1—C3—C23	127.4 (1)
		C2—C3—C23	109.3 (1)
		O1—C1—C28	122.8 (1)
		C2—C1—C28	116.8 (1)
		O2—C8—C9	122.9 (1)
		C7—C8—C9	116.7 (1)

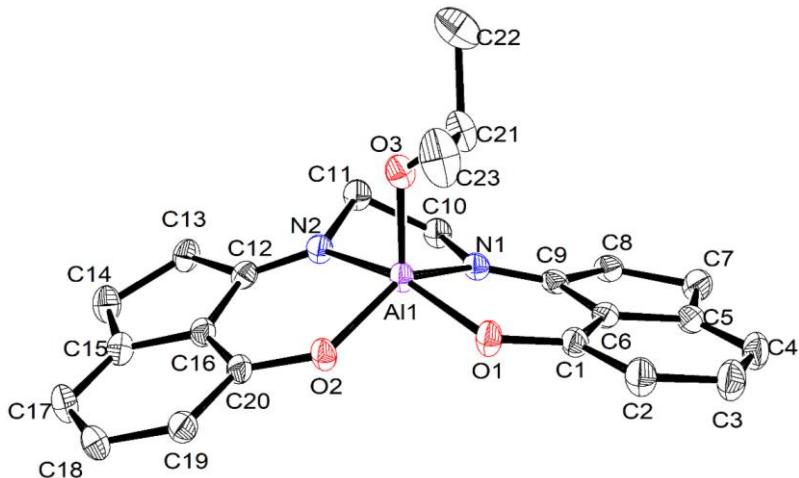


Table S5. Crystal data and structure refinement for complex **3a**

Complex	3a
CCDC	2085880
Chemical formula	C ₂₃ H ₂₅ AlN ₂ O ₃
Formula weight	404.43
Temperature (K)	100
Wavelength (Å)	0.71073
Space group	C 1 2/c 1
Crystal size (mm)	0.22 × 0.22 × 0.18
Crystal system	Monoclinic
a (Å)	22.813 (1)
b (Å)	15.194 (1)
c (Å)	13.992 (1)
V (Å ³)	4627.7 (3)
Z	8
Density (calcd.) (mg/m ³)	1.161
μ (mm ⁻¹)	0.11
Theta range for data collection (°)	2.4–26.4
F (000)	1712
Reflection collected	36235
Unique reflections	4739
Goodness-of-fit-on F ²	1.030
R1(F), wR(F ²)	0.0336, 0.0855
Largest diff. peak and hole [e Å ⁻³]	0.24 and -0.25

Table S6. Selected bond distances and angles for complex **3a**

Bond distances (Å)		Bond angles (deg)	
Al1—O2	1.817 (1)	O2—Al1—O1	86.4 (1)
Al1—O3	1.734 (1)	O2—Al1—N2	90.9 (1)
Al1—O1	1.831 (1)	O2—Al1—N1	140.3 (1)
Al1—N1	2.031 (1)	O3—Al1—O2	113.8 (1)
Al1—N2	2.017 (1)	O3—Al1—O1	105.4 (1)
O2—C20	1.326 (2)	O3—Al1—N2	94.6 (1)
O3—C21	1.411 (2)	O3—Al1—N1	105.1 (1)
O1—C1	1.319 (2)	O1—Al1—N2	159.2 (1)
N2—C12	1.288 (2)	O1—Al1—N1	91.3 (1)
N2—C11	1.466 (1)	N2—Al1—N1	77.7 (1)
N1—C9	1.293 (2)	C20—O2—Al1	131.9 (1)
N1—C10	1.477 (2)	C21—O3—Al1	128.1 (1)
C12—C16	1.437 (2)	C1—O1—Al1	130.8 (1)
C12—C13	1.514 (2)	C12—N2—Al1	127.3 (1)
C6—C9	1.436 (2)	C12—N2—C11	121.2 (1)
C6—C1	1.404 (2)	C11—N2—Al1	111.5 (1)
C6—C5	1.398 (2)	C9—N1—Al1	124.6 (1)
C9—C8	1.509 (2)	C9—N1—C10	117.9 (1)
C1—C2	1.403 (2)	C10—N1—Al1	117.3 (1)
C20—C16	1.402 (2)	N2—C12—C16	121.8 (1)
C20—C19	1.407 (2)	N2—C12—C13	129.5 (1)
C5—C7	1.513 (2)	C16—C12—C13	108.7 (1)
C5—C4	1.377 (2)	C1—C6—C9	125.7 (1)
C16—C15	1.397 (2)	C5—C6—C9	110.8 (1)
C8—C7	1.548 (2)	C5—C6—C1	123.4 (2)
C11—C10	1.522 (2)	N1—C9—C6	123.4 (2)
C15—C14	1.509 (2)	N1—C9—C8	127.7 (1)
C15—C17	1.386 (2)	C6—C9—C8	108.9 (1)
C19—C18	1.392 (2)	O1—C1—C6	121.2 (2)
C2—C3	1.389 (2)	O1—C1—C2	122.7 (1)
C18—C17	1.396 (2)	C2—C1—C6	116.2 (2)

C13—C14	1.548 (2)	O2—C20—C16	121.7 (1)
C21—C23	1.521 (2)	O2—C20—C19	122.0 (1)
C21—C22	1.515 (2)	C16—C20—C19	116.2 (1)
C3—C4	1.402 (2)	C20—C16—C12	125.6 (1)
		C15—C16—C12	110.9 (1)
		C15—C16—C20	123.6 (1)
		N2—C11—C10	106.3 (1)
		N1—C10—C11	106.8 (1)