

Supporting Information

Titanium Isopropoxide Complexes of a Series of Sterically Demanding Aryloxo Based $[\text{N}_2\text{O}_2]^{2-}$ Ligands as Precatalysts for Ethylene Polymerization

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Supplementary Material (ESI) for Dalton Transactions
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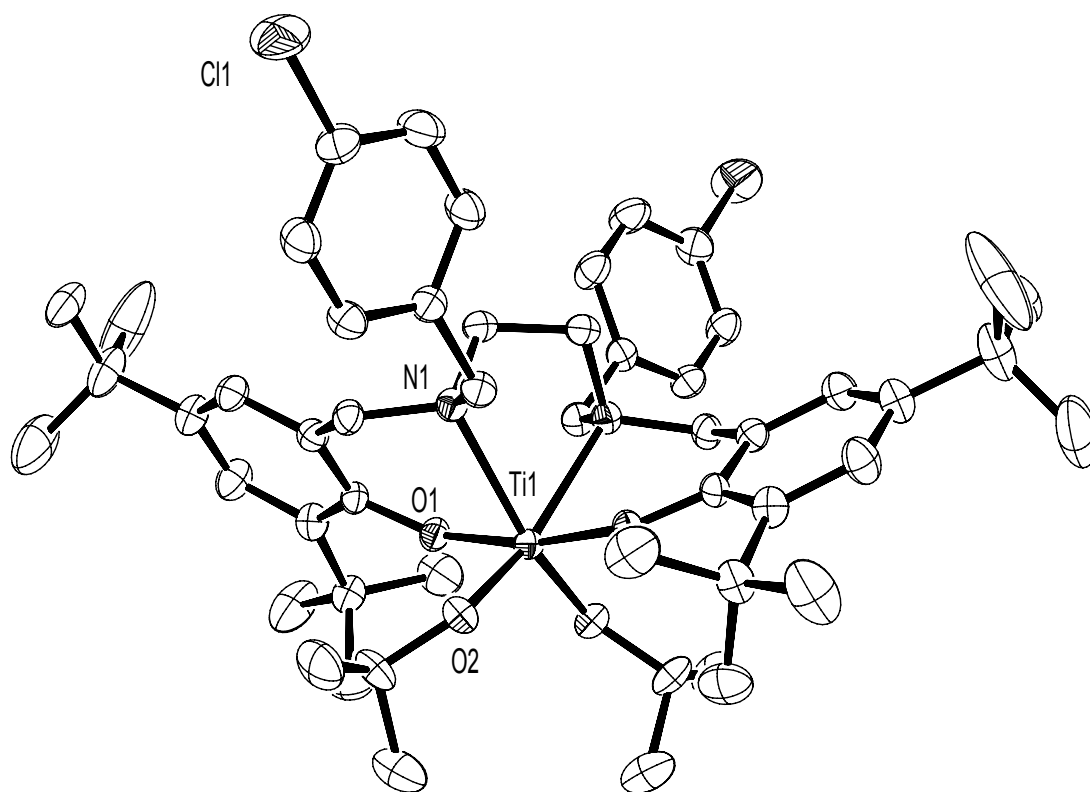


Figure S1. ORTEP view of the solid state structure of **5b**. The thermal ellipsoids are shown in 50 % probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°) are given: Ti1-O1 1.887(2), Ti1-O2 1.823(2), Ti1-N1 2.401(3), O1-Ti1-O2 91.37(10), O1-Ti1-N1 90.86(10), O2-Ti1-N1 89.36(10).

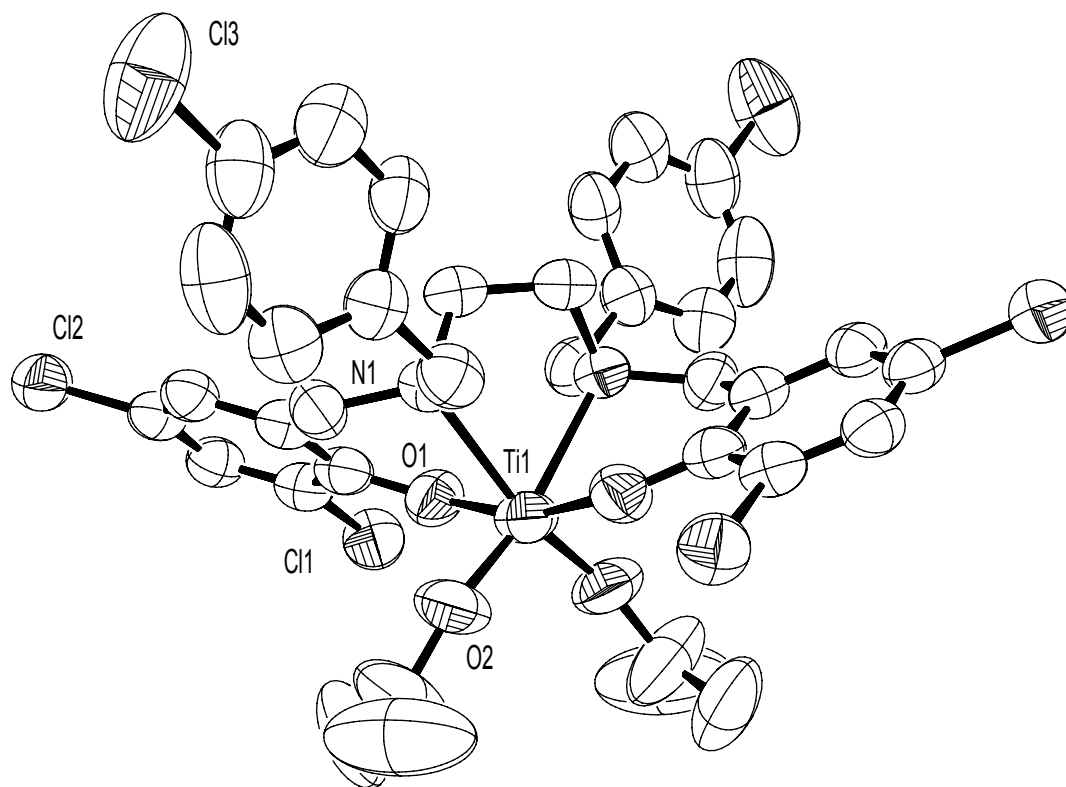


Figure S2. ORTEP view of the solid state structure of **6b**. The thermal ellipsoids are shown in 50 % probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°) are given: Ti1-O1 1.909(4), Ti1-O2 1.767(4), Ti1-N1 2.354(4), O1-Ti1-O2 96.81(19), O2-Ti1-N1 164.39(17), O1-Ti1-N1 85.56(16).

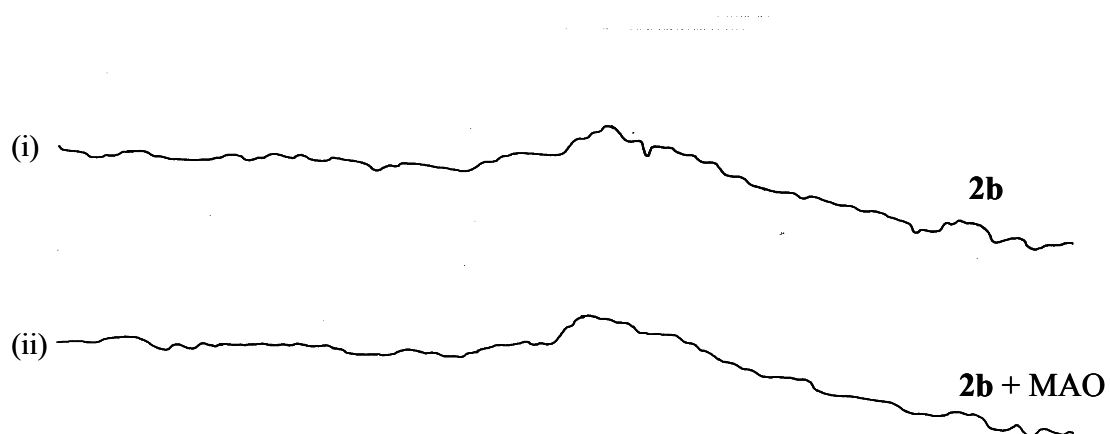
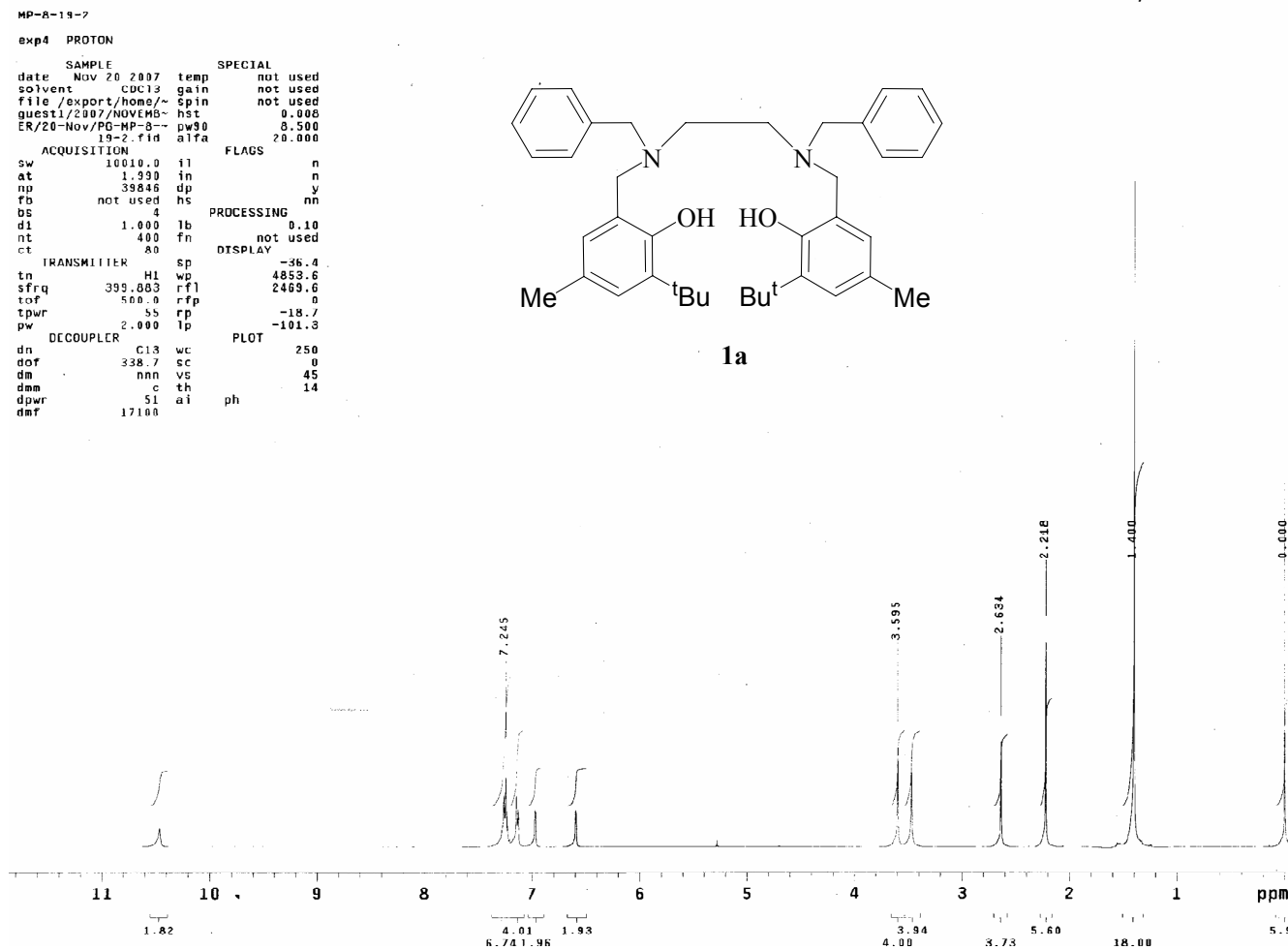


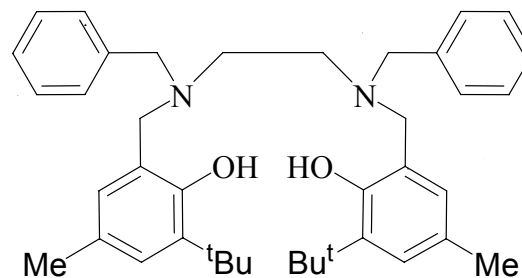
Figure S3. ESR spectrum (i) of the complex **2b** and (ii) of the complex **2b** when activated by MAO and both recorded at 77 K.



```

MP-12-186-13C
exp4 CARBON
SAMPLE
date Nov 5 2008 temp not used
solvent CDCl3 gain not used
file /export/home/~ spin not used
pgl/MANAS/2008/Nov~ hst 0.008
08/5-Nov/PG-MP-12~ pw90 14.000
186-13C.fid alfa 20.000
ACQUISITION
sw 25125.6 il n
at 1.199 tn n
np 60270 dp y
fb 13800 hs nn
bs 4
dl 1.000 lb PROCESSING 1.00
nt 20000 fn not used
ct 2084 DISPLAY
TRANSMITTER
tn C13 sp -146.4
sfrq 100.561 wp 20403.7
tof 1554.3 rfl 9268.3
tpwr 56 rfp 7768.5
pw 7.000 lp -309.3
DECOUPLER
dn H1 wc PLOT 250
dof 0 sc 0
dm yyy vs 34
dmm w th 7
dpwr 41 ai
dmf 11900 ph

```



1a

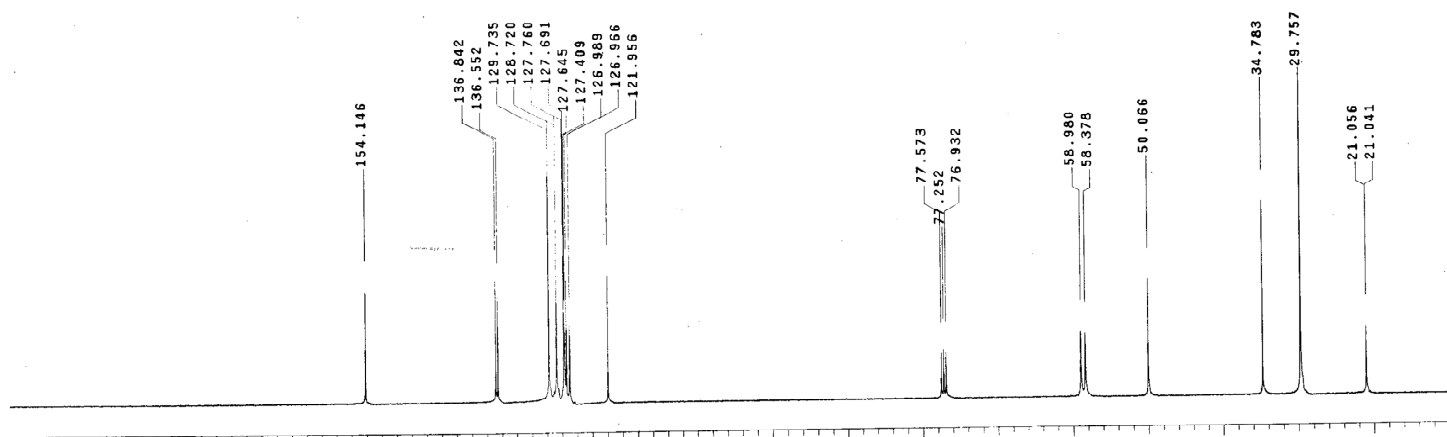
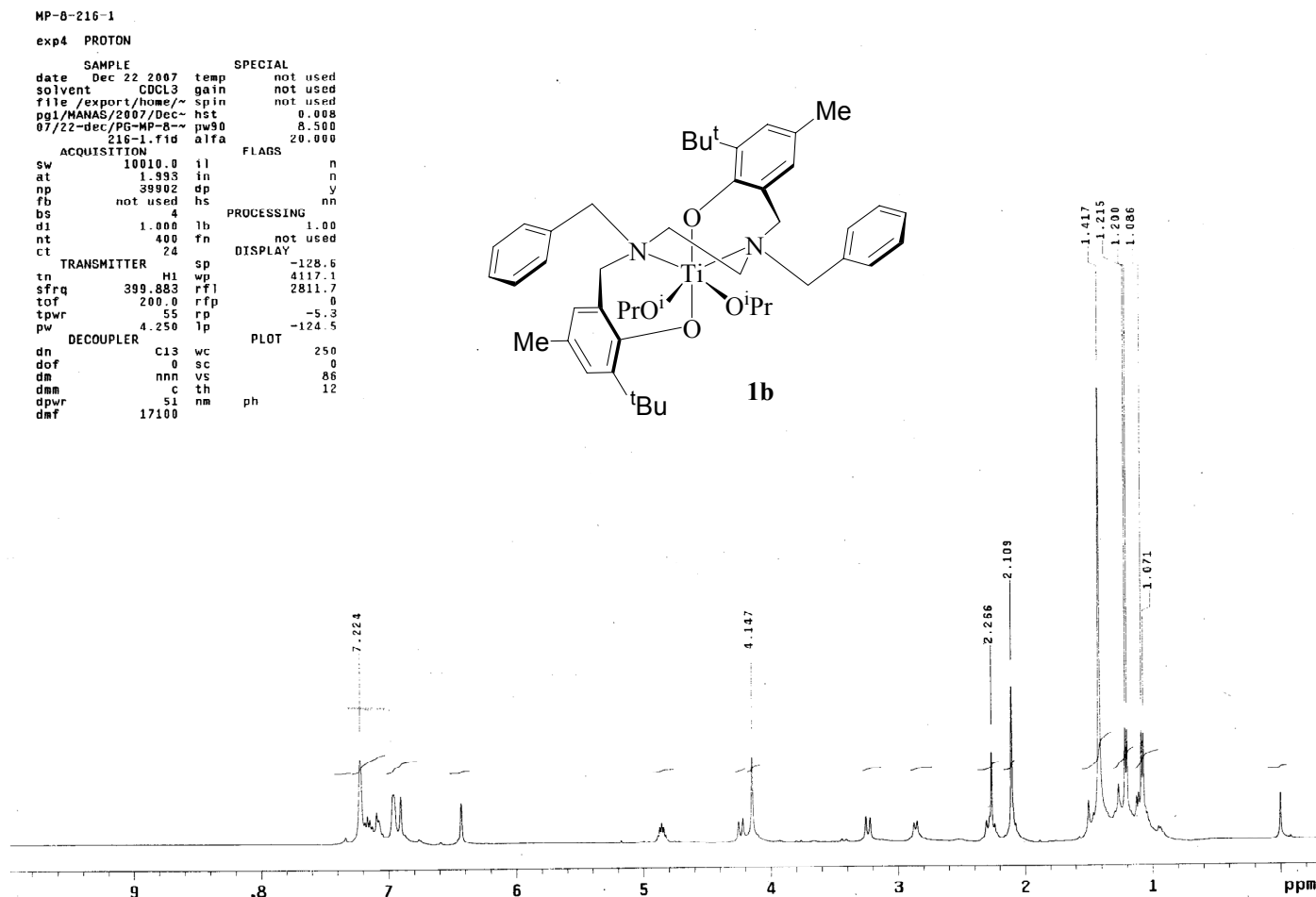


Figure S5. ^{13}C NMR spectrum of **1a** in CDCl_3 .



MP-8-216-13C
exp4 CARBON

SAMPLE		SPECTRAL	
date	Dec 23 2007	temp	not used
solvent	CDCl3	gain	not used
file	/export/home/~	spin	not used
pg1/MANAS/2007/Dec-		hst	0.008
07/23-dec/PG-MP-8-		pw90	14.000
216-13C.fid		alpha	20.000

ACQUISITION		FLAGS	
sw	25125.6	il	n
at	1.199	in	n
np	60270	dp	y
fb	13800	hs	nn
bs	4		
d1	1.000	l b	1.00
nt	20000	fn	not used
ct	7004		

TRANSMITTER		PROCESSING	
tn	G13	sp	-356.4
sfrq	100.561	wp	20416.0
tof	1554.3	rfl	9249.9
tpwr	56	rfp	7762.5
pw	7.000	rp	-31.1
		lp	-313.6

DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	83
dmm	w	th	10
dpwr	41	ai	ph
dmf	11900		

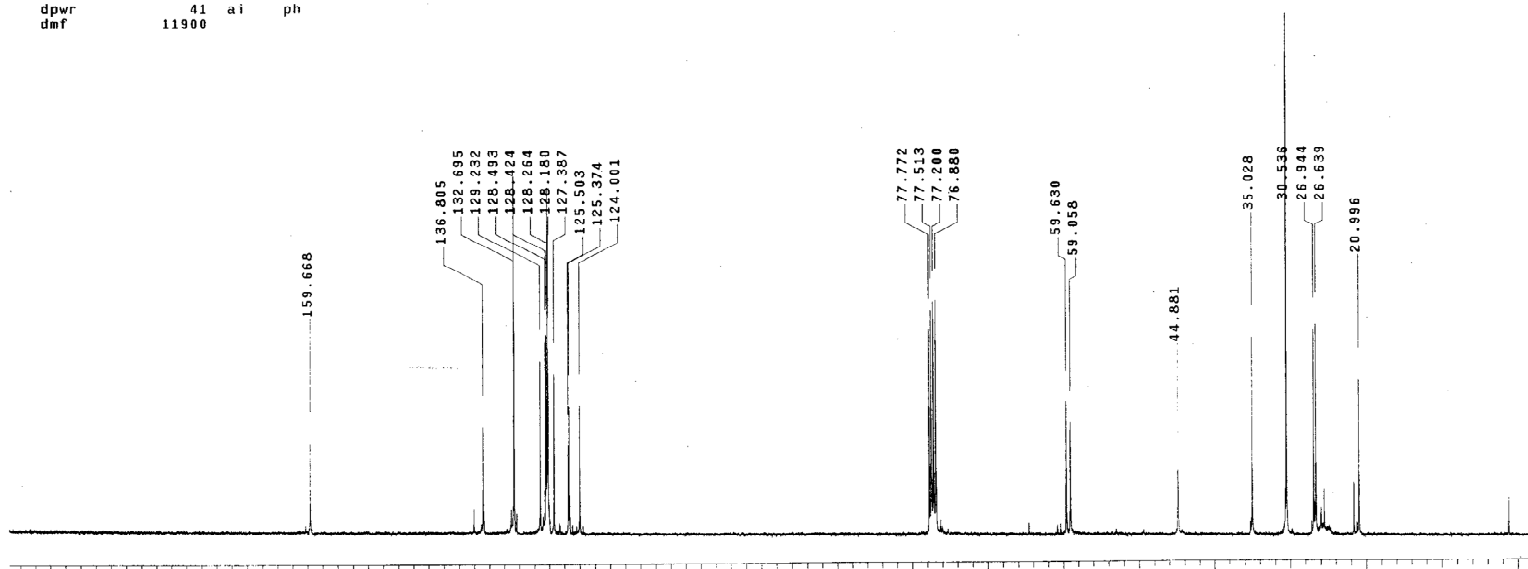
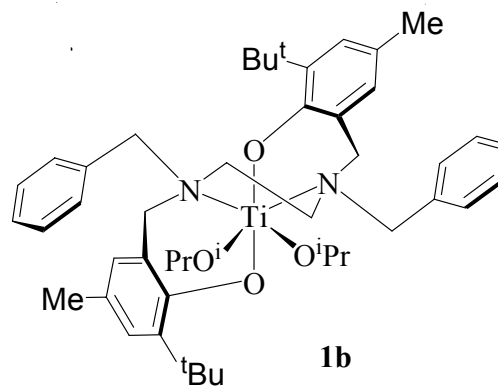


Figure S7. ^{13}C NMR spectrum of **1b** in CDCl_3 .

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ARR-2-108-1
exp4  PROTON

SAMPLE
date   Oct 25 2008
solvent CDCl3
file   /export/home/~
pg1/RAJSEKHAR/2008~
/Oct08/25-oct/PG-A~
RR-2-108-1.fid
ACQUISITION
sw      10010.0
at      1.993
np      39902
fb      not used
bs      4
d1      1.000
nt      400
ct      8
TRANSMITTER
tn      H1
sfrq    399.883
tof     200.0
tpwr    55
pw      4.250
DECOUPLER
dn      C13
dof     0
dm      nnn
dmm     c
dpwr    51
dmf     17100

SPECIAL
temp    not used
gain    not used
spin    not used
hst     0.008
pw90    8.500
alfa    20.000

FLAGS
il      n
in      n
dp      y
hs      nn

PROCESSING
lb      1.00
fn      not used

DISPLAY
sp      -71.5
wp      4968.2
rfl     2765.0
rfp     0
rp      51.6
lp      -151.8

PLOT
wc      250
sc      0
vs      87
th      6
ph


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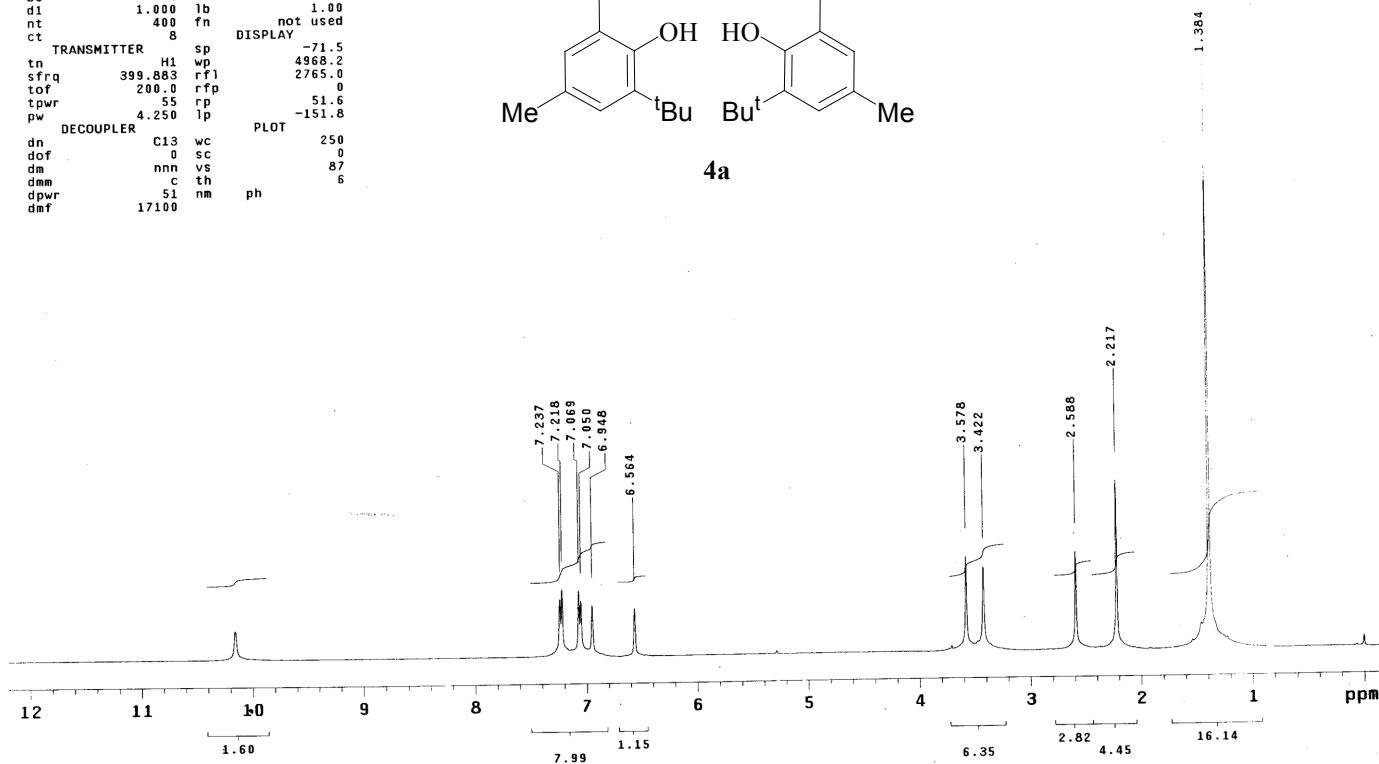
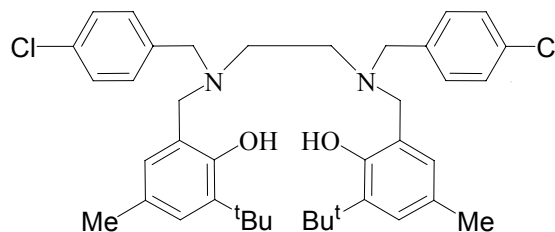


Figure S8. ^1H NMR spectrum of **4a** in CDCl_3 .

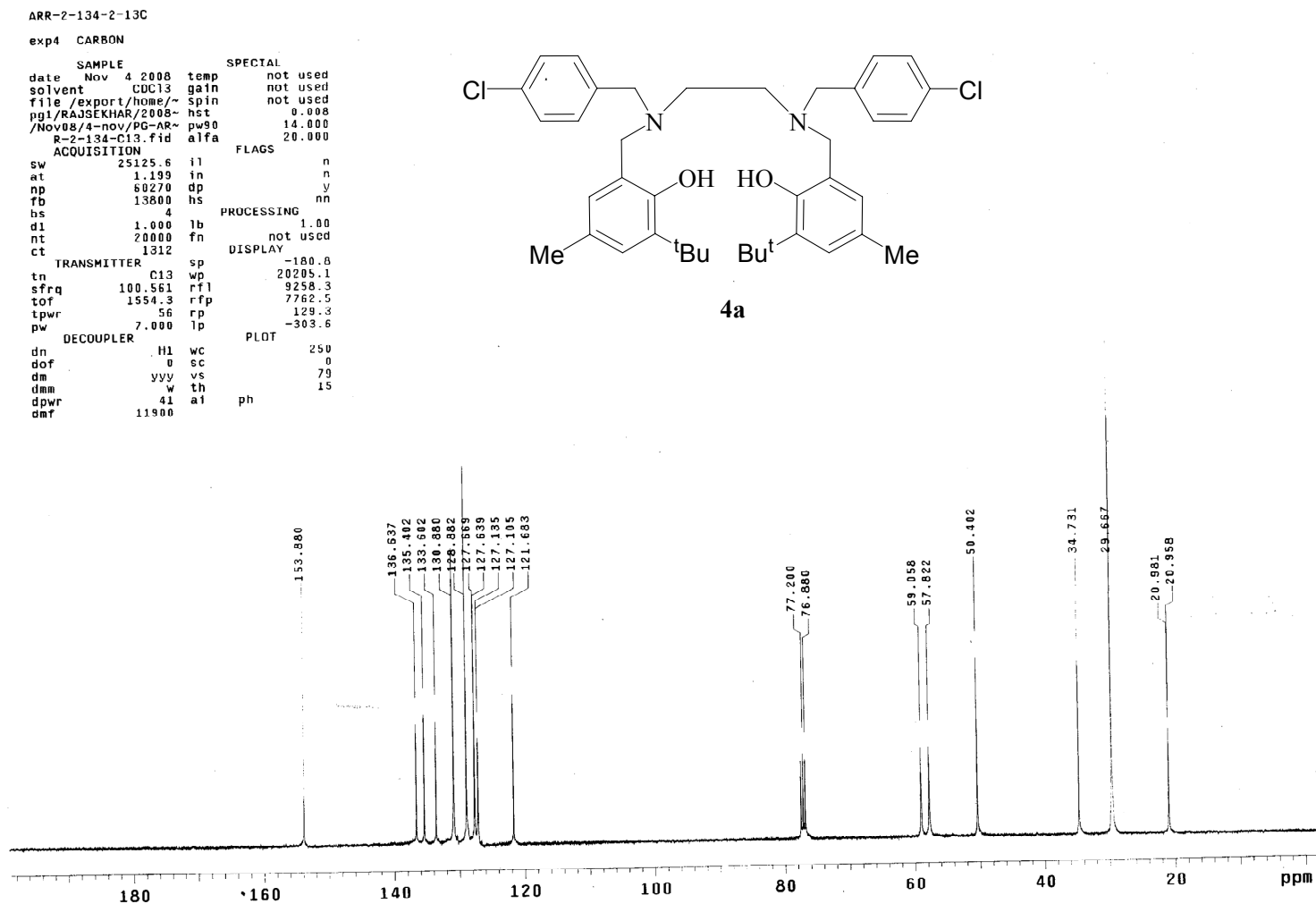


Figure S9. ¹³C NMR spectrum of **4a** in CDCl₃.

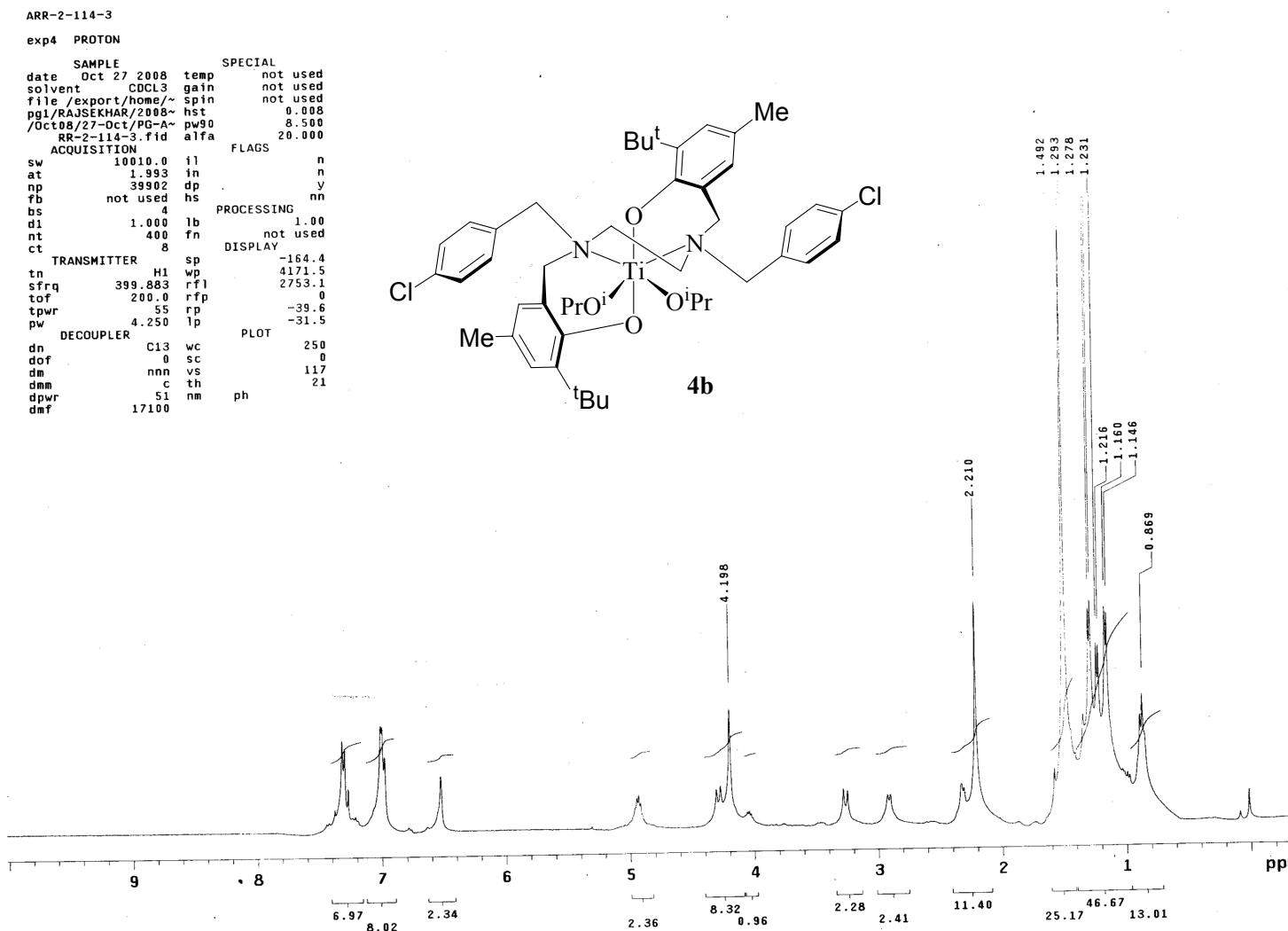
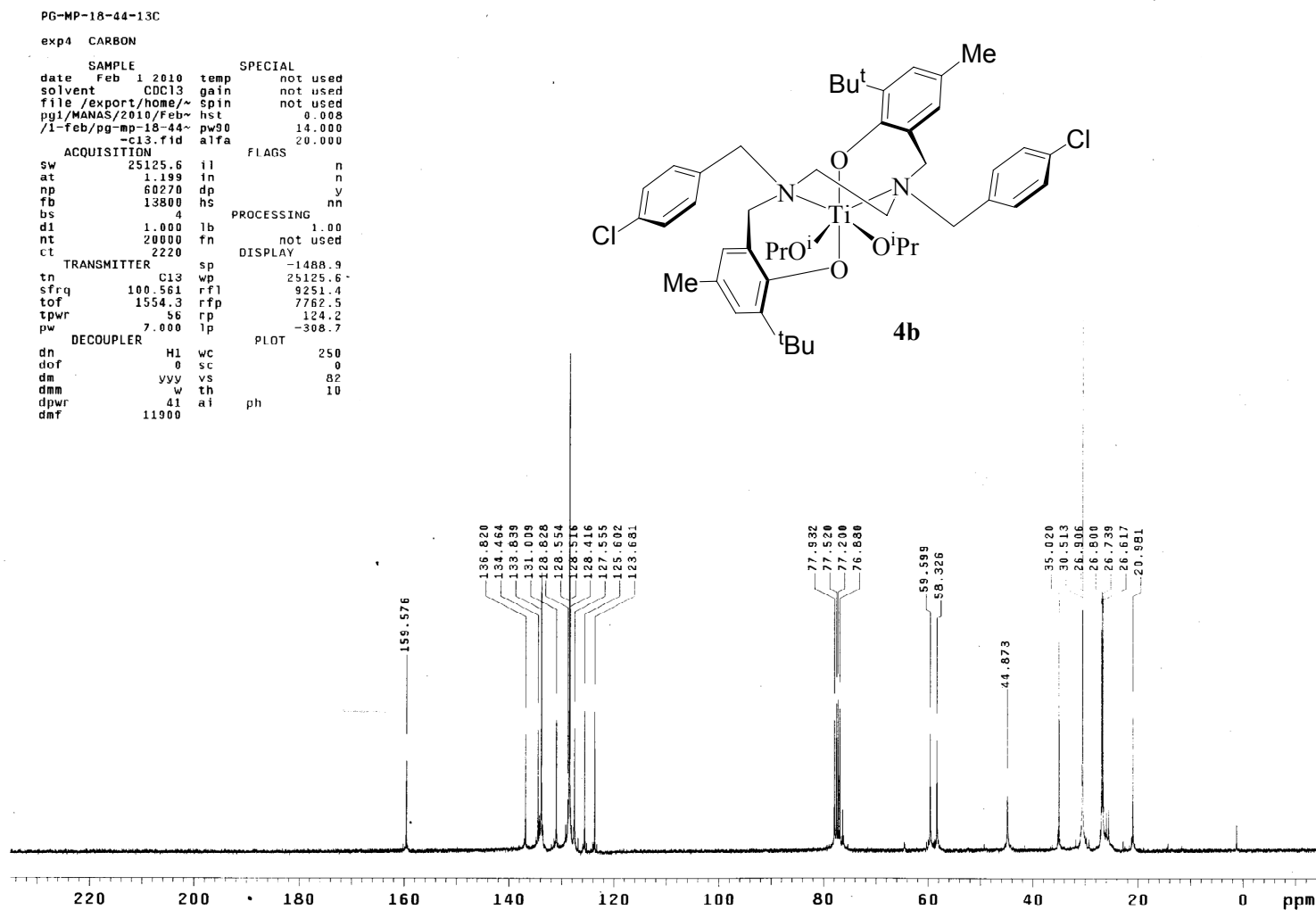
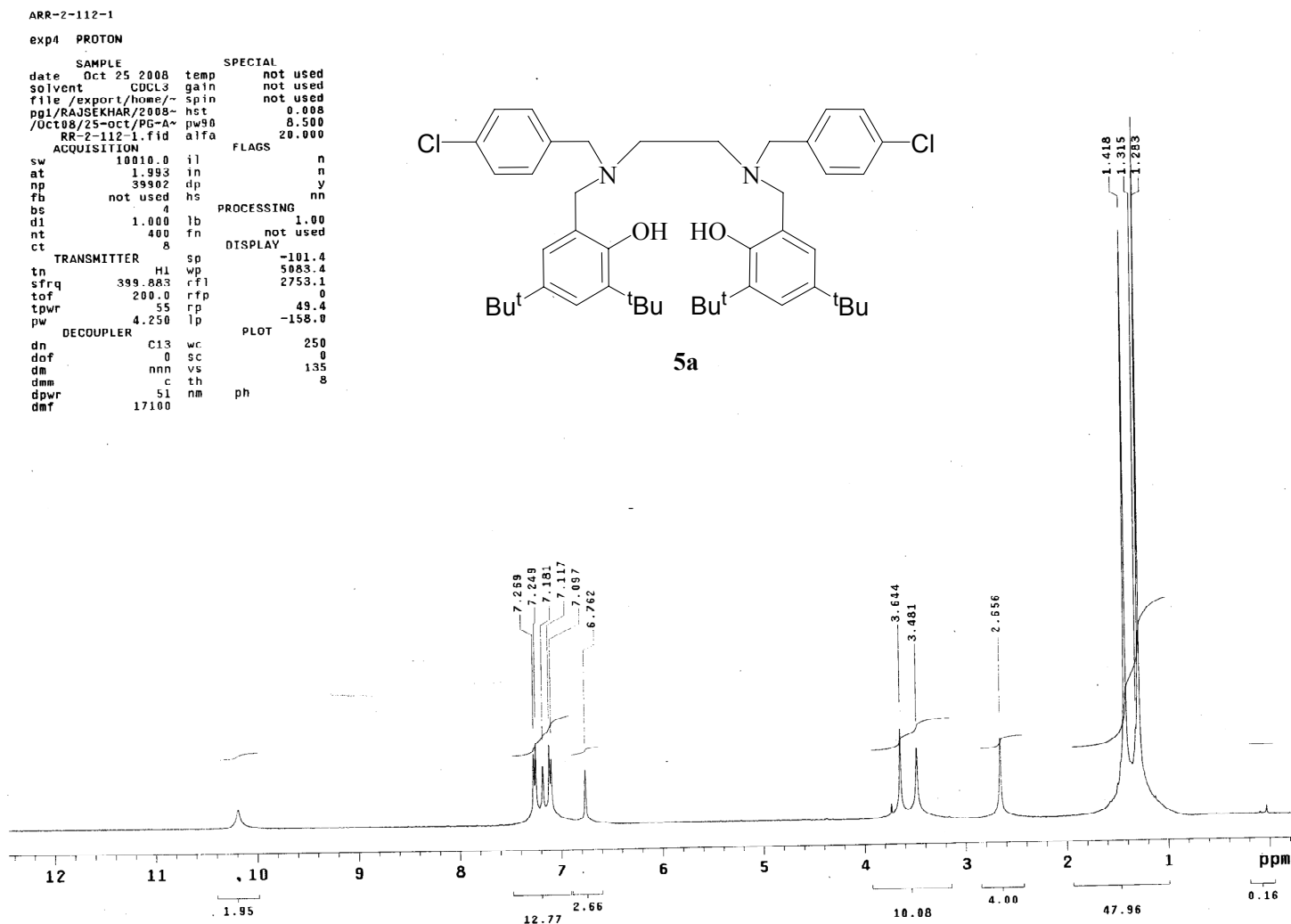


Figure S10. ¹H NMR spectrum of **4b** in CDCl₃.





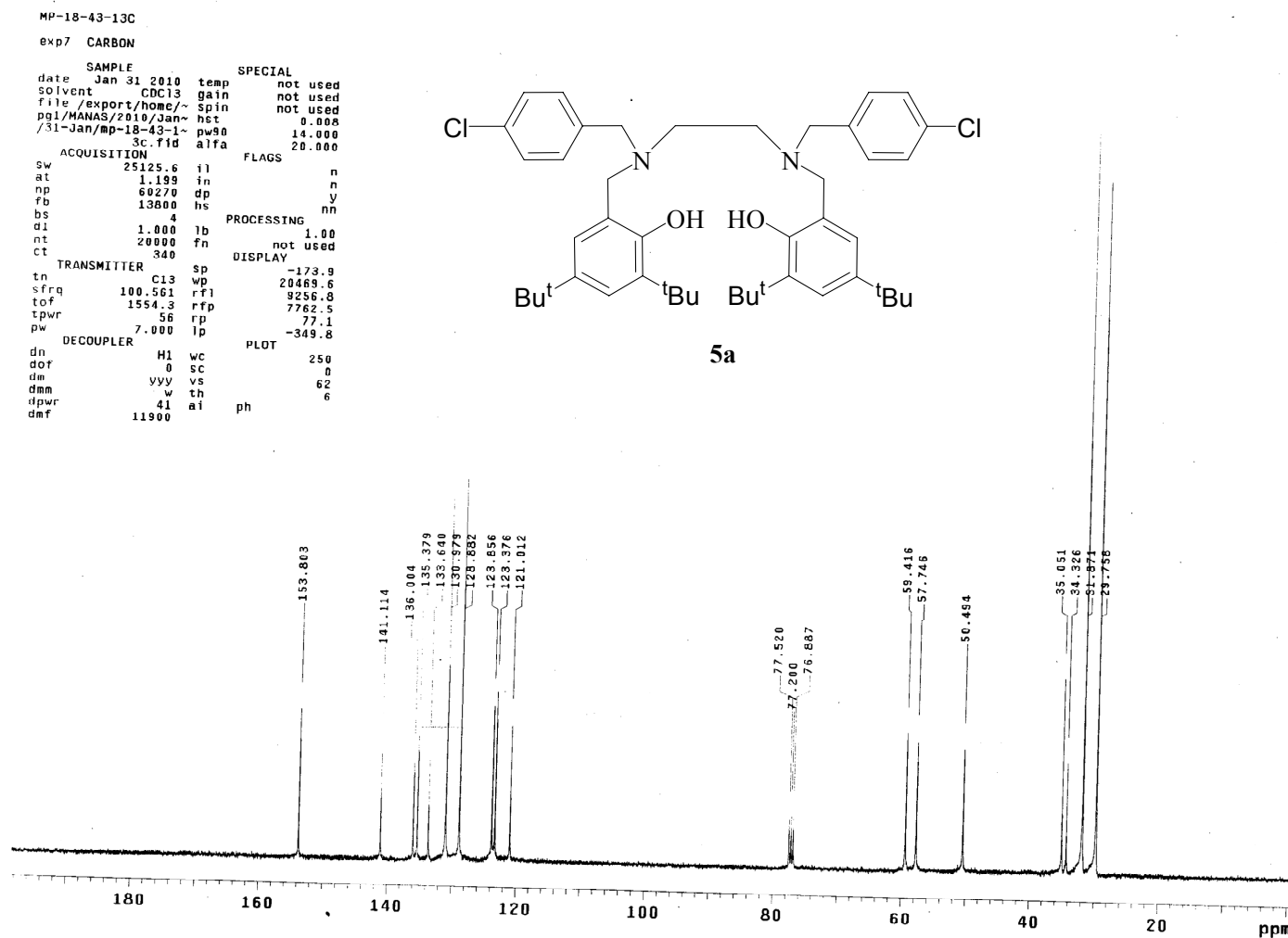
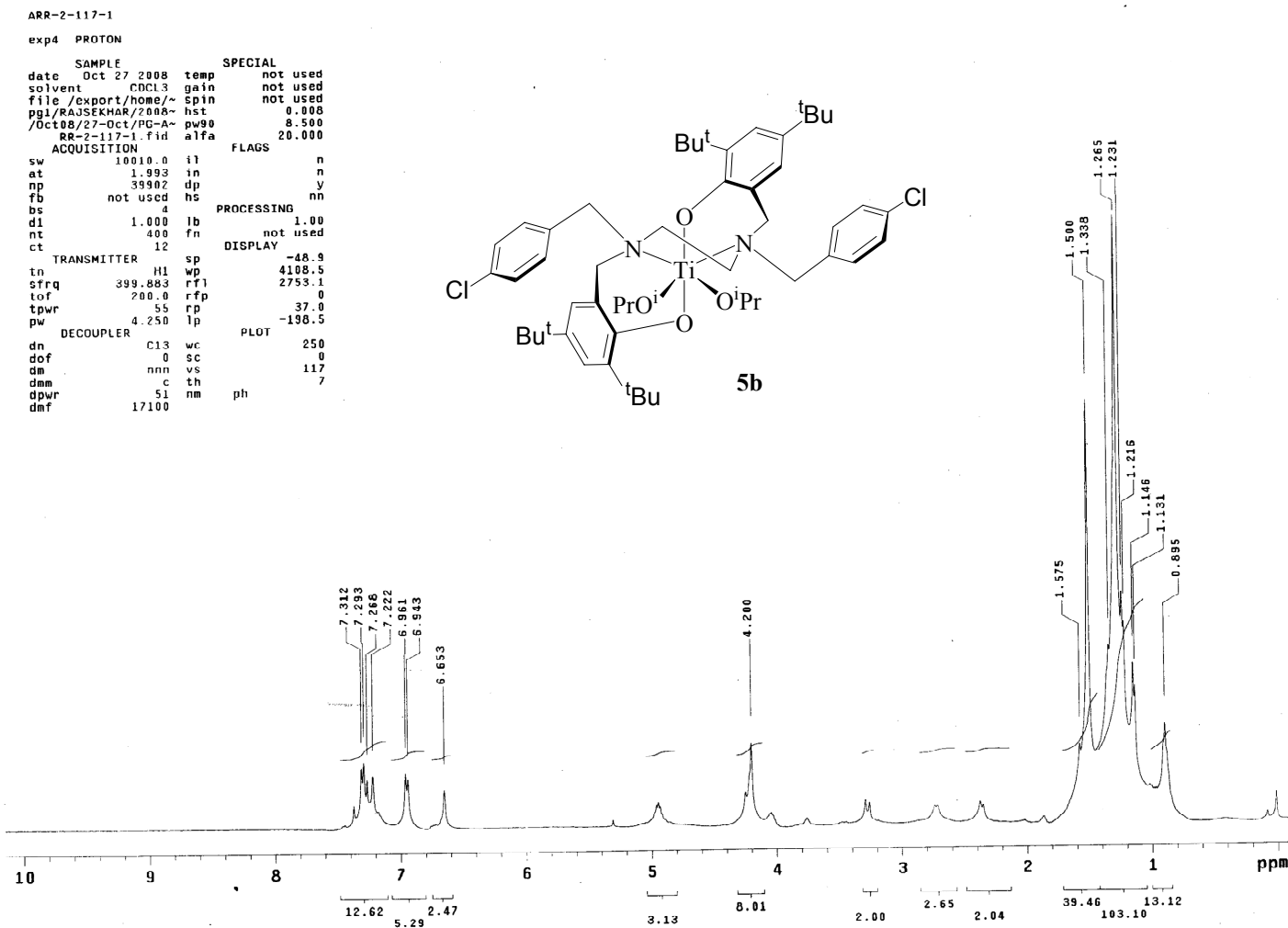


Figure S13. ^{13}C NMR spectrum of **5a** in CDCl_3 .



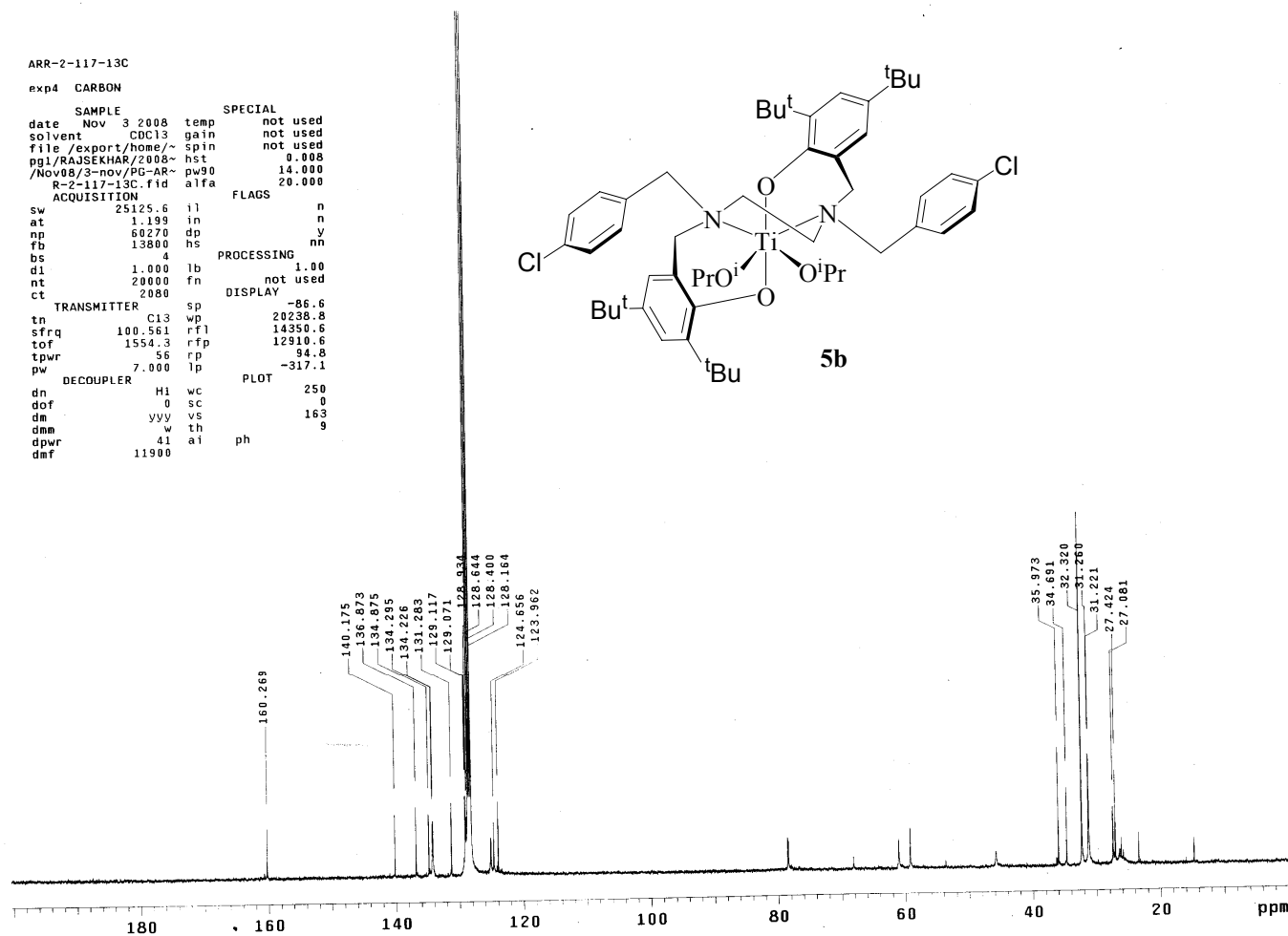
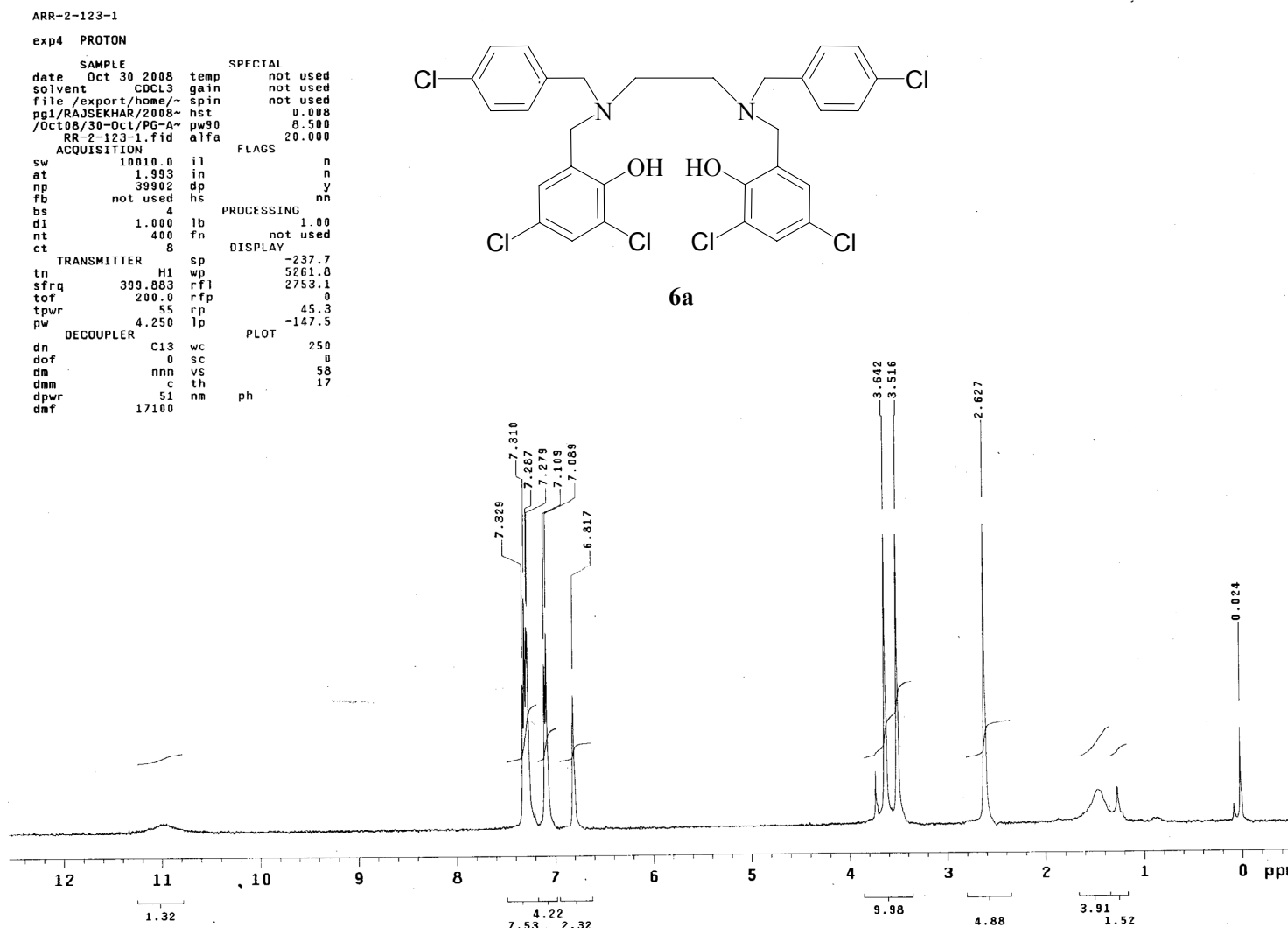


Figure S15. ^{13}C NMR spectrum of **5b** in C_6D_6 .



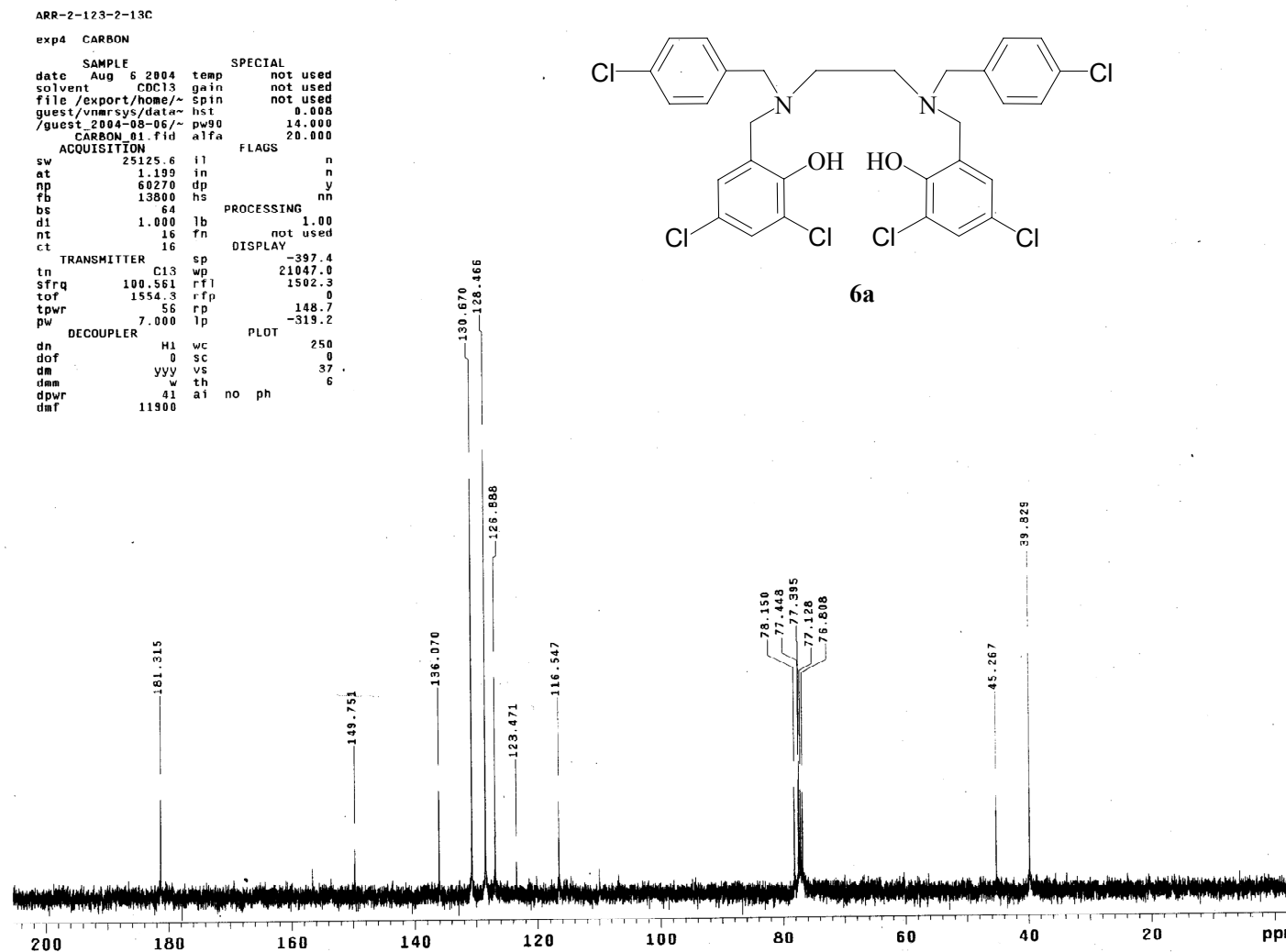


Figure S17. ^{13}C NMR spectrum of 6a in CDCl_3 .

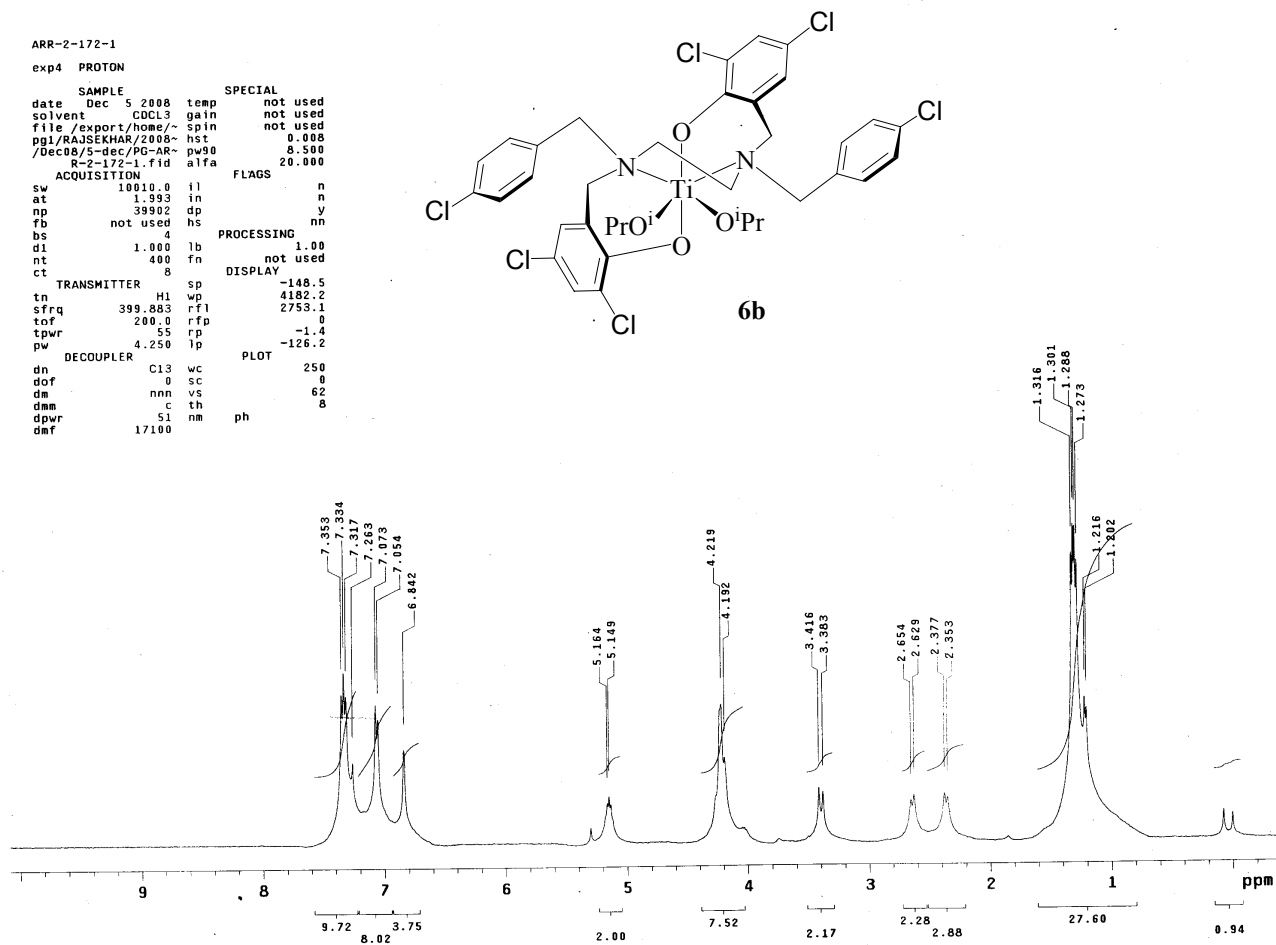


Figure S18. ^1H NMR spectrum of **6b** in CDCl_3 .

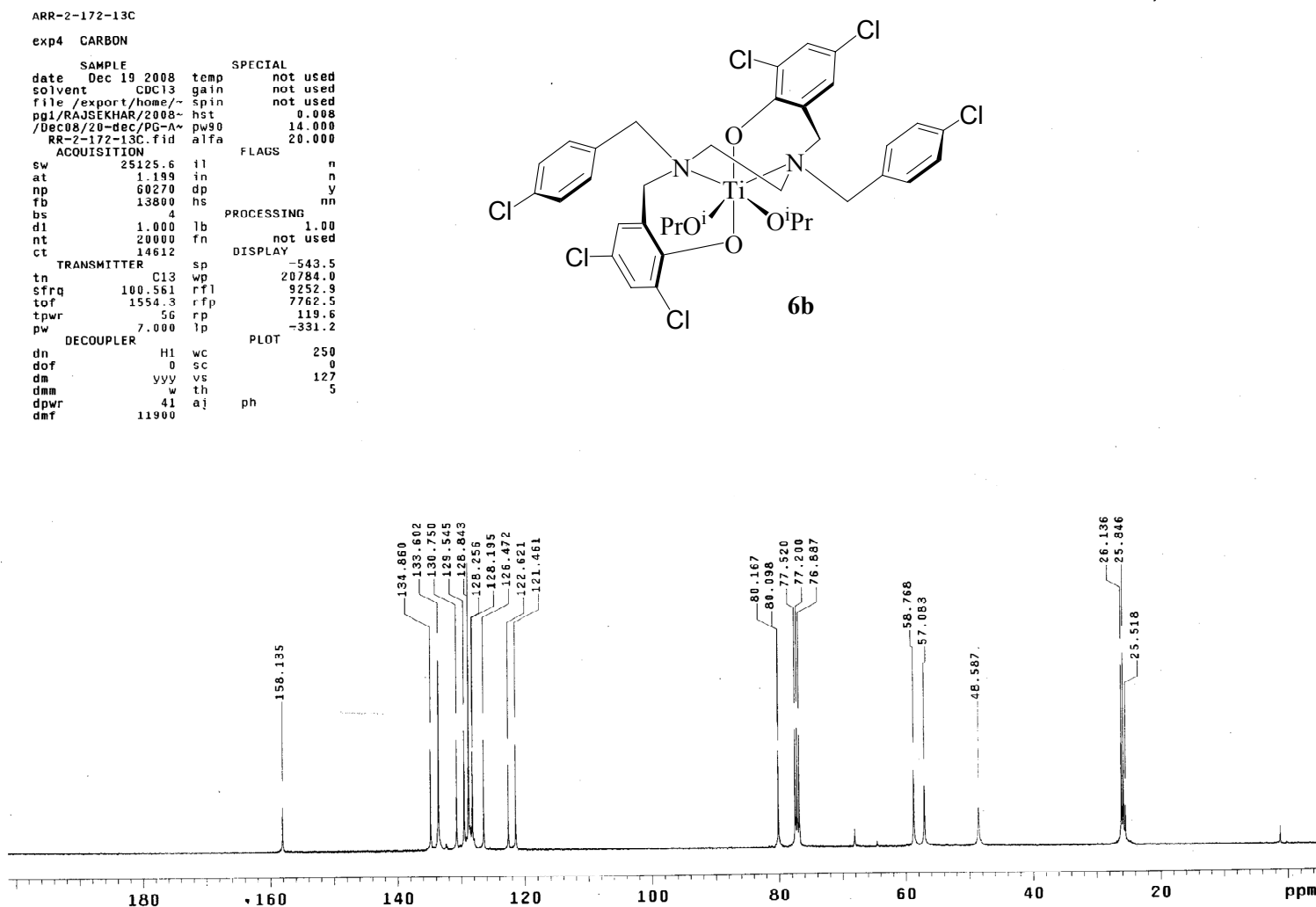


Figure S19. ¹³C NMR spectrum of **6b** in CDCl₃.