

Cyclometallated platinum(II) complexes of 1,3-di(2-pyridyl)benzenes: tuning excimer emission from red to near-infrared for NIR-OLEDs

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M. Cocchi and J. A. G. Williams

Supporting Information

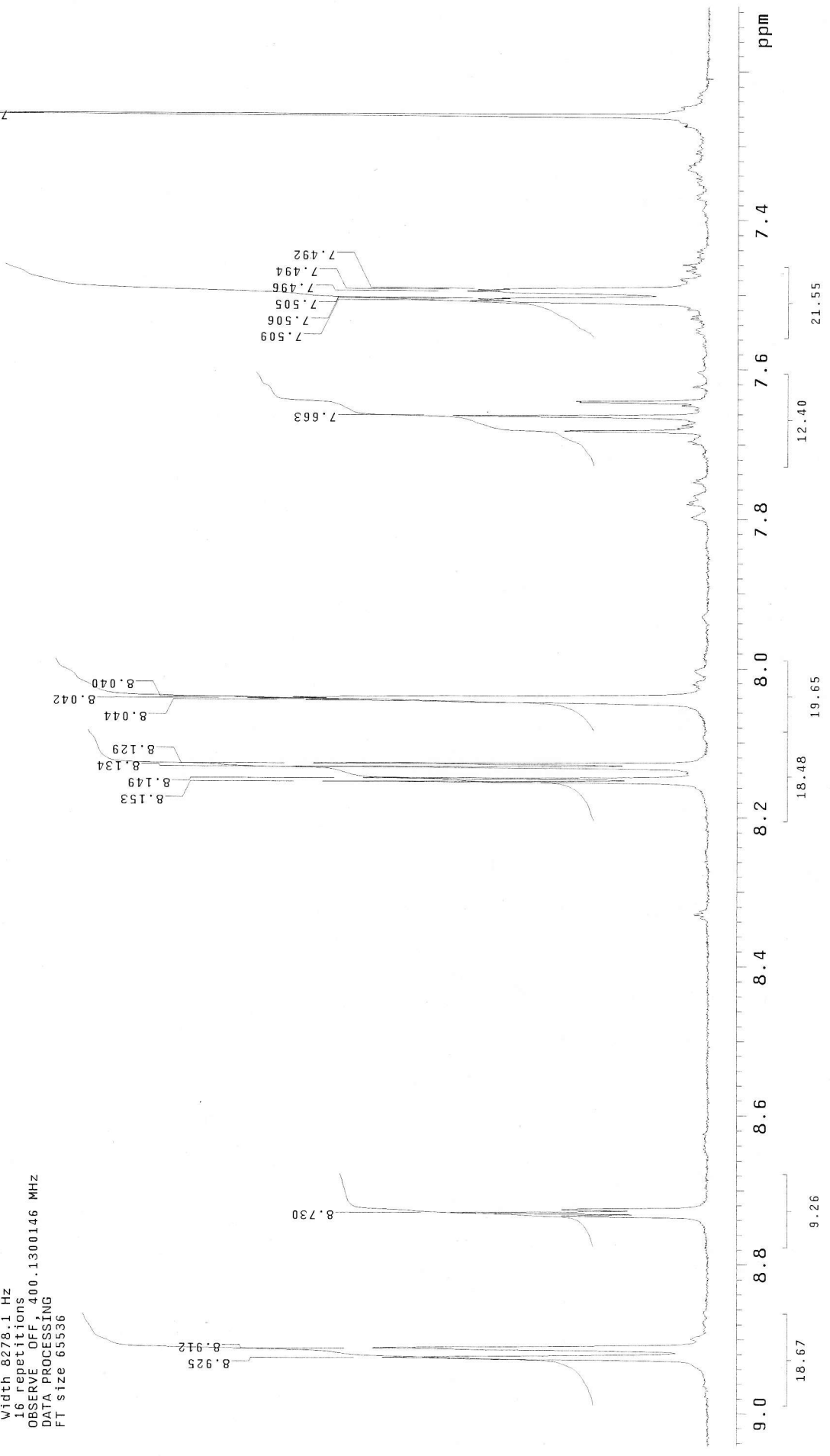
- Section 1.** ^1H and ^{19}F NMR spectra of ligands HL^{27-29} and complexes $\text{PtL}^{27-29}\text{Cl}$.
- Section 2.** Emission spectra of $\text{PtL}^{27-29}\text{Cl}$ in CH_2Cl_2 solution at varying concentrations.
- Section 3.** Plots of the decay rate constant k_{obs} versus concentration for $\text{PtL}^{27-29}\text{Cl}$ in CH_2Cl_2 at 298 ± 3 K.
- Section 4.** Emission spectra of $\text{PtL}^{27-29}\text{Cl}$ at 77 K in a frozen glass of diethyl ether / isopentane / ethanol (2:2:1 v/v), $\lambda_{\text{ex}} = 420$ nm.
- Section 5.** Emission spectra of $\text{PtL}^{27-29}\text{Cl}$ in the solid state obtained by evaporation from CH_2Cl_2 solution, $\lambda_{\text{ex}} = 374$ nm.

1. ^1H and ^{19}F NMR spectra

HL ^{27}H NMR in CDCl_3

Bruker data converted from file /data/tempdat/10114223/10
p1b23(A1203)

Pulse Sequence: zg30
Solvent: cdcl_3
Temp. 24.2 C / 297.3 K
File: ./10114223-10.cv
Experiment run on 03-10-08
Processed on "moodus"
Relax. delay 1.000 sec
1st pulse 90.0 degrees
2nd pulse 90.0 degrees
Acq. time 7.899 sec
Width 8278.1 Hz
16 repetitions
OBSERVE OFF, 400.1300146 MHz
DATA PROCESSING
FT size 65536



PLB23

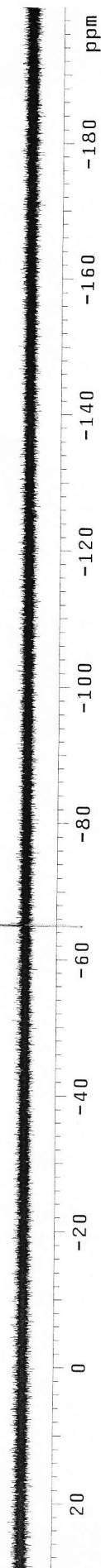
Automation directory: /export/home/vnmr1/automation/Ved1202_auto
File : /data/i50803/12180750-04

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
Sample #8
File: i50803/12180750-04
Experiment run on Mar 13 2008
INOVA-500 "black"

Relax. delay 1.500 sec
Pulse 30.0 degrees
Acq. time 1.050 sec
Width 108.1 kHz
16 repetitions
OBSERVE F19, 470.2520382 MHz
DECOUPLE H1, 499.7711057 MHz
power 42 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.2 Hz
FT size 262144
Total time 0 min, 40 sec

HL²⁷ ¹⁹F NMR in CDCl₃



PLB 25

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 24.0 C / 297.1 K

File: Mar14150309/PROTON_01

Experiment run on Mar 15 2008

Processed on "moodus"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.910 sec

Width 11261.3 Hz

32 repetitions

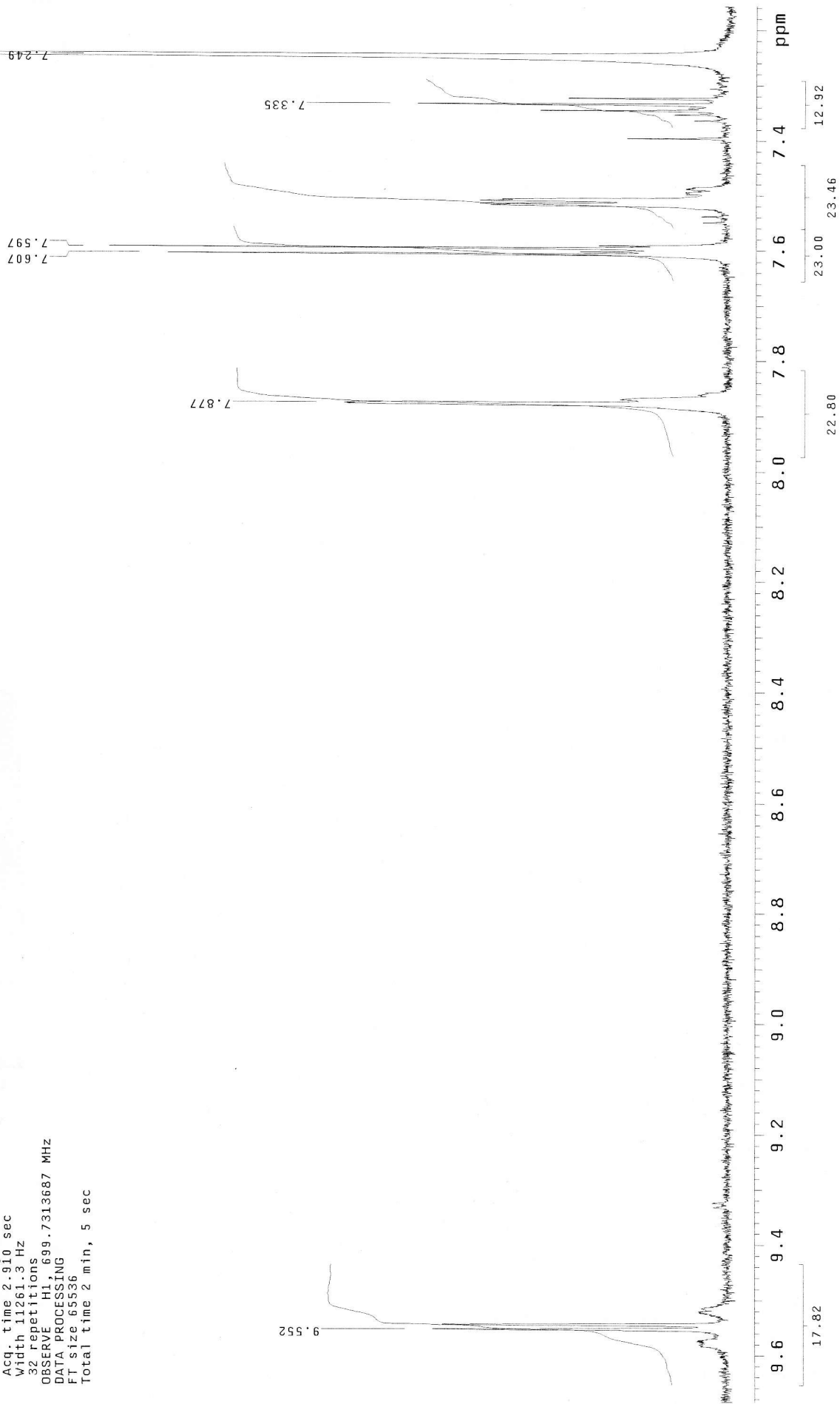
OBSERVE H1, 699.7313687 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 5 sec

PdL²⁷Cl¹H NMR in CDCl₃





VARIAN

PLB 25

Sample Name:

service

Data Collected on:

huple-vnmrs700

Archive directory:

/data/d70803

Sample directory:

Mar17115930

FidFile: FLUORINE_01

Pulse Sequence: FLUORINE (s2pul)

Solvent: cdcl3

Data collected on: Mar 17 2008

Temp. 24.0 C / 297.1 K

Sample #8, Operator: service

Relax. delay 1.000 sec

Pulse 35.0 degrees

Acq. time 0.839 sec

Width 156.2 kHz

16 repetitions

OBSERVE F19, 658.4053110 MHz

DATA PROCESSING

FT size 262144

Total time 0 min 30 sec

PtL²⁷Cl ¹⁹F NMR in CDCl₃

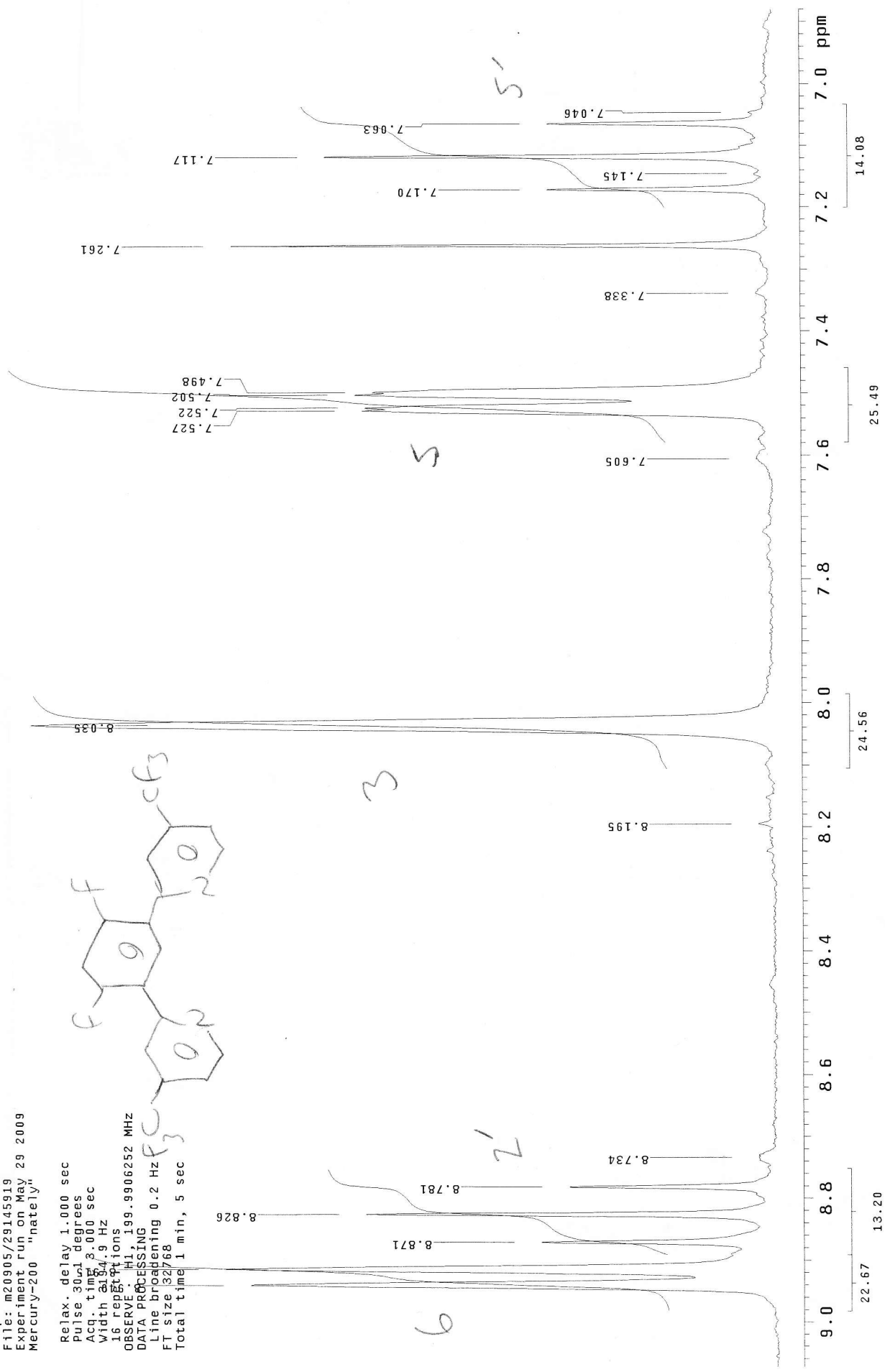
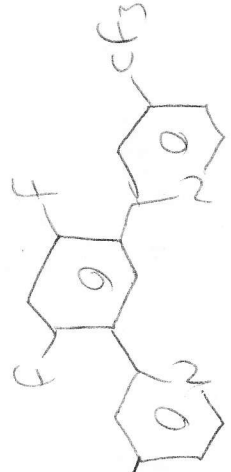
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

LM Expt 162 F3-4

HL²⁸ ¹H NMR in CDCl₃

Pulse Sequence: s2pul
Solvent: CDCl₃
Ambient temperature
Sample #31
File: m20905/29145919
Experiment run on May 29 2009
Mercury-200 "natel"

Relax. delay 1.000 sec
Pulse 30.01 degrees
Acq. time 3.000 sec
Width 3184.9 Hz
16 repetitions
OBSERVE: H1, 199.9906252 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 1 min, 5 sec

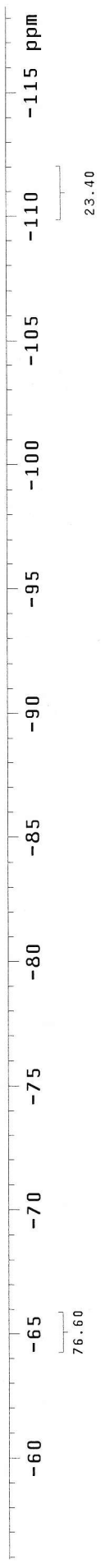


LM Expt 162 F spec

HL²⁸ ¹⁹F NMR in CDCl₃

Pulse Sequence: s2pul
Solvent: CDCl₃
Ambient temperature
Sample #31
File: m20905/29150146
Experiment run on May 29 2009
Mercury-200 "natel"

Relax. delay 3.000 sec
Pulse 30.0 degrees
Acq. time 1.000 sec
Width 59880.2 Hz
16 repetitions
OBSERVE F19, 188.1792744 MHz
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 min, 11 sec



LM CF3F2CX

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

File: Dec15174828/PROTON_01

Experiment run on Dec 16 2009

Processed on "dreedle"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.910 sec

Width 11261.3 Hz

4 repetitions

OBSERVE H1, 699.7313687 MHz

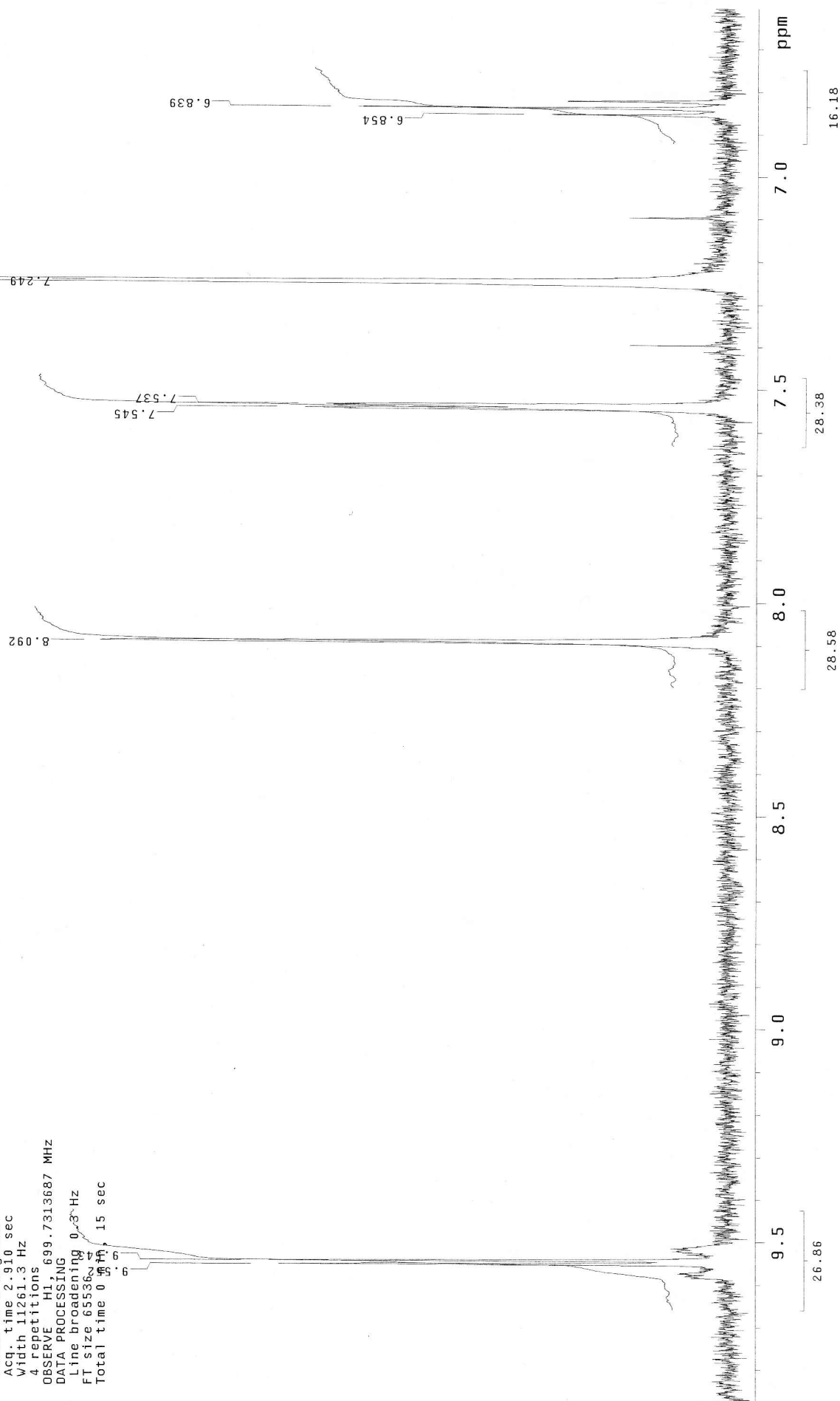
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 0.15 sec

PtL²⁸Cl¹H NMR in CDCl₃





VARIAN

LM CF3F2CX

PtL²⁸Cl¹⁹F NMR in CDCl₃

Sample Name:

service

Data Collected on:

huple-vnmrs700

Archive directory:

/data/d70912

Sample directory:

Dec15174828

FidFile: FLUORINE_01

Pulse Sequence: FLUORINE (s2pul)

Solvent: cdcl3

Data collected on: Dec 17 2009

Temp. 25.0 C / 298.1 K

Sample #25, Operator: service

Relax. delay 1.000 sec

Pulse 35.0 degrees

Acq. time 0.839 sec

Width 156.2 kHz

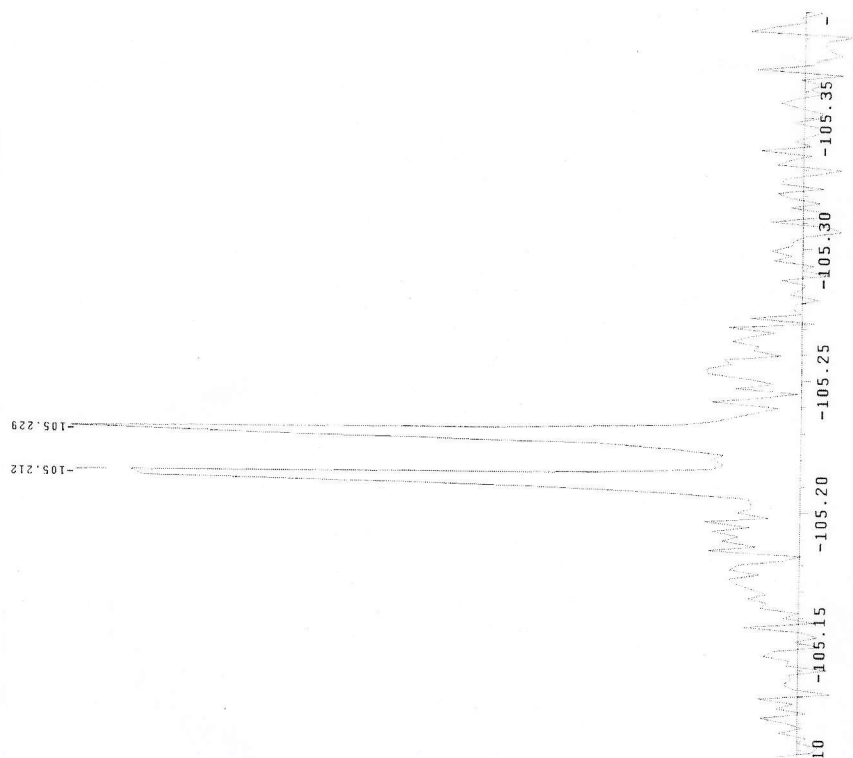
16 repetitions

OBSERVE F19, 658.4053110 MHz

DATA PROCESSING

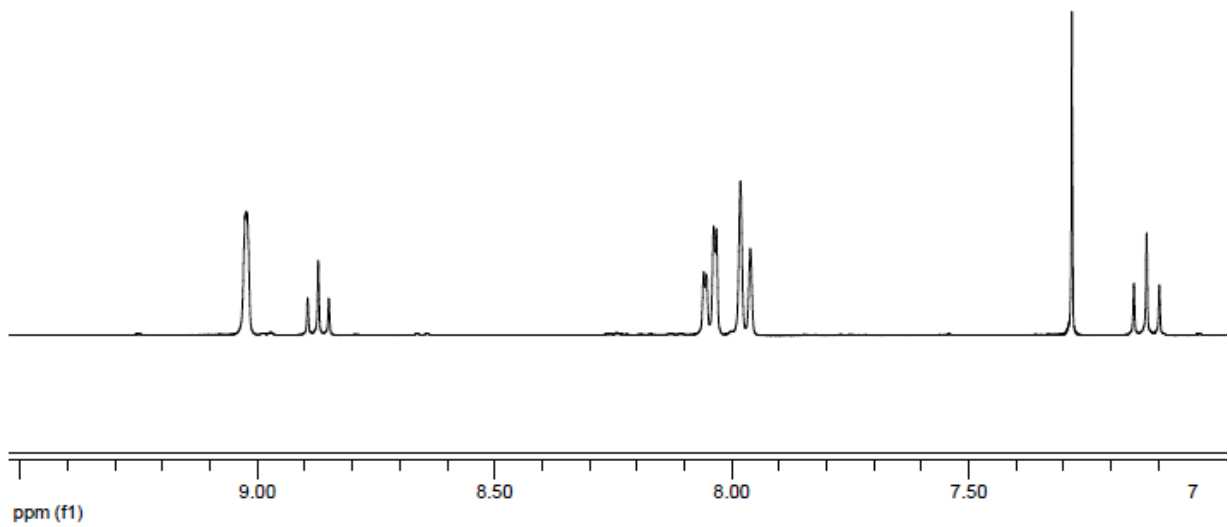
FT size 262144

Total time 0 min 30 sec

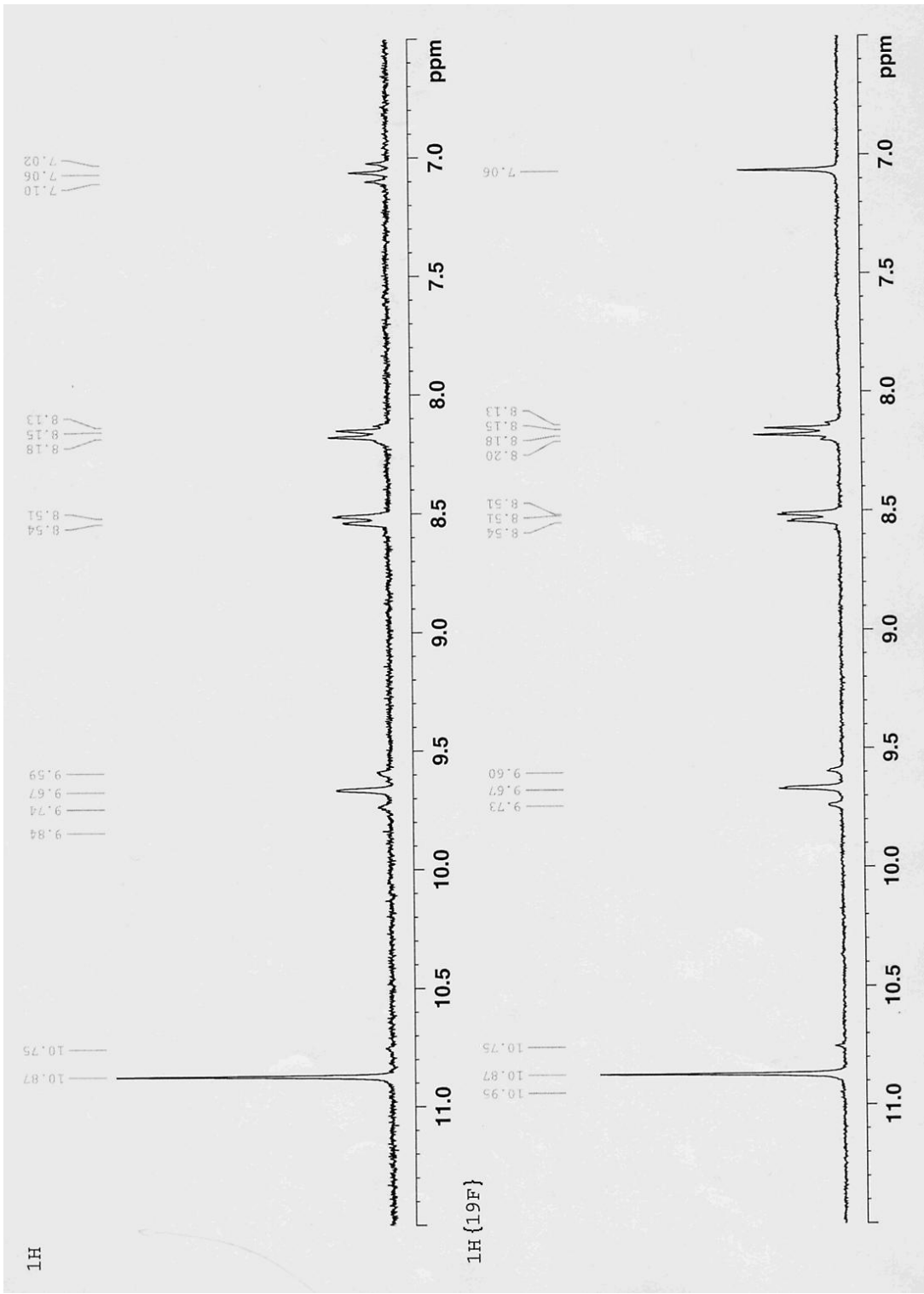


20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

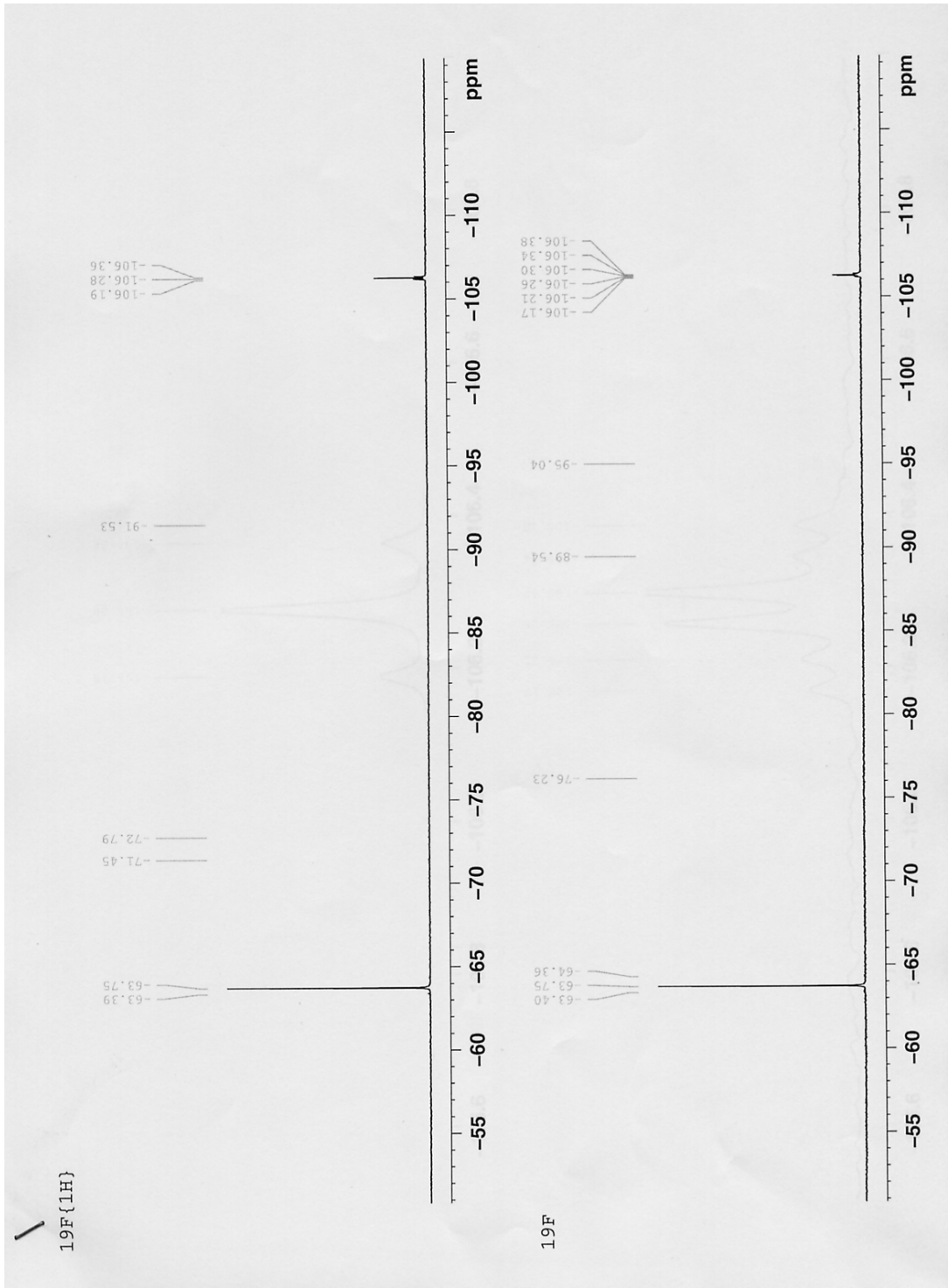
HL²⁹ ¹H NMR in CDCl₃ at 400 MHz

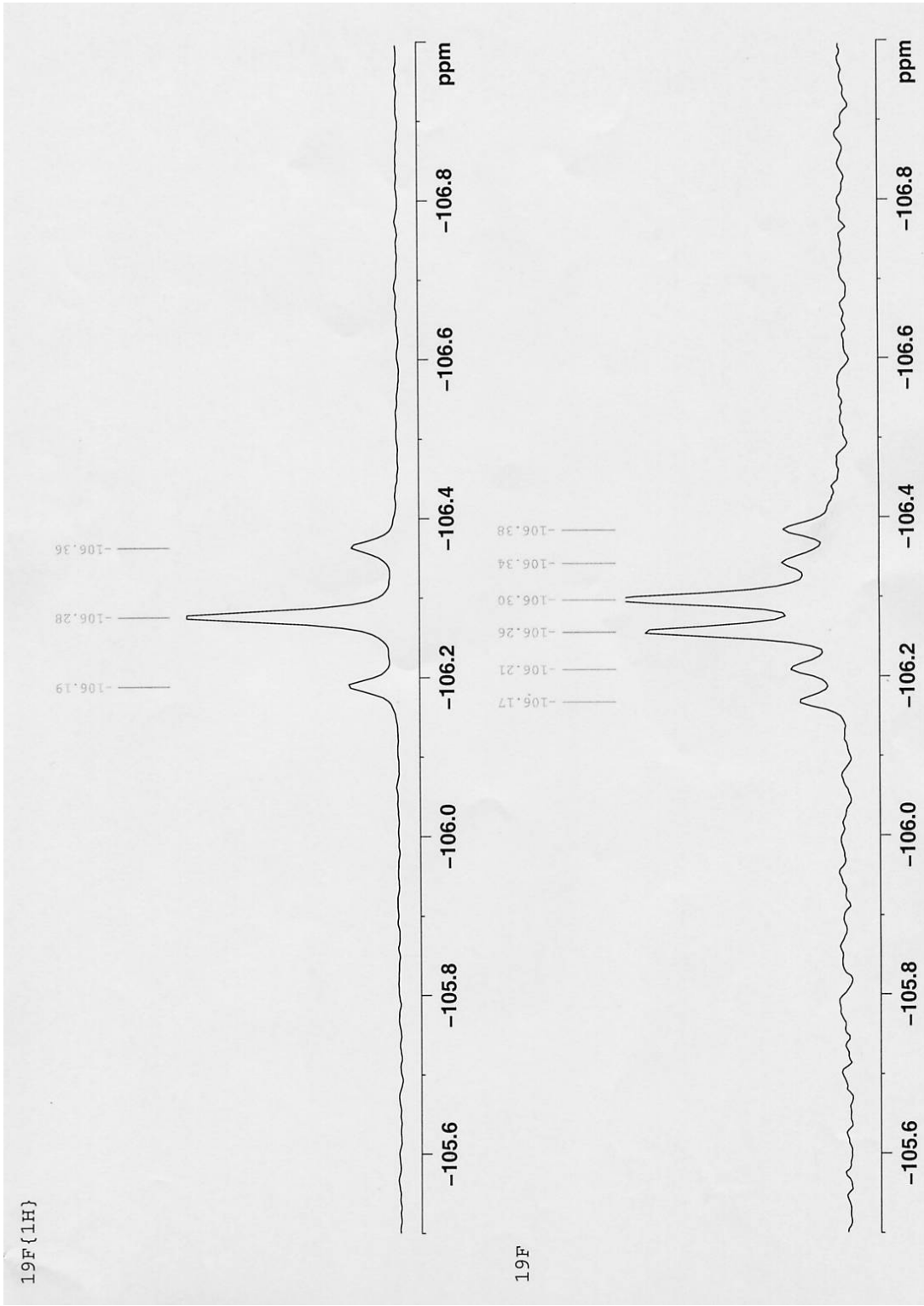


PtL²⁹Cl ¹H NMR in *d*₈-THF at 300 MHz coupled and decoupled to fluorine



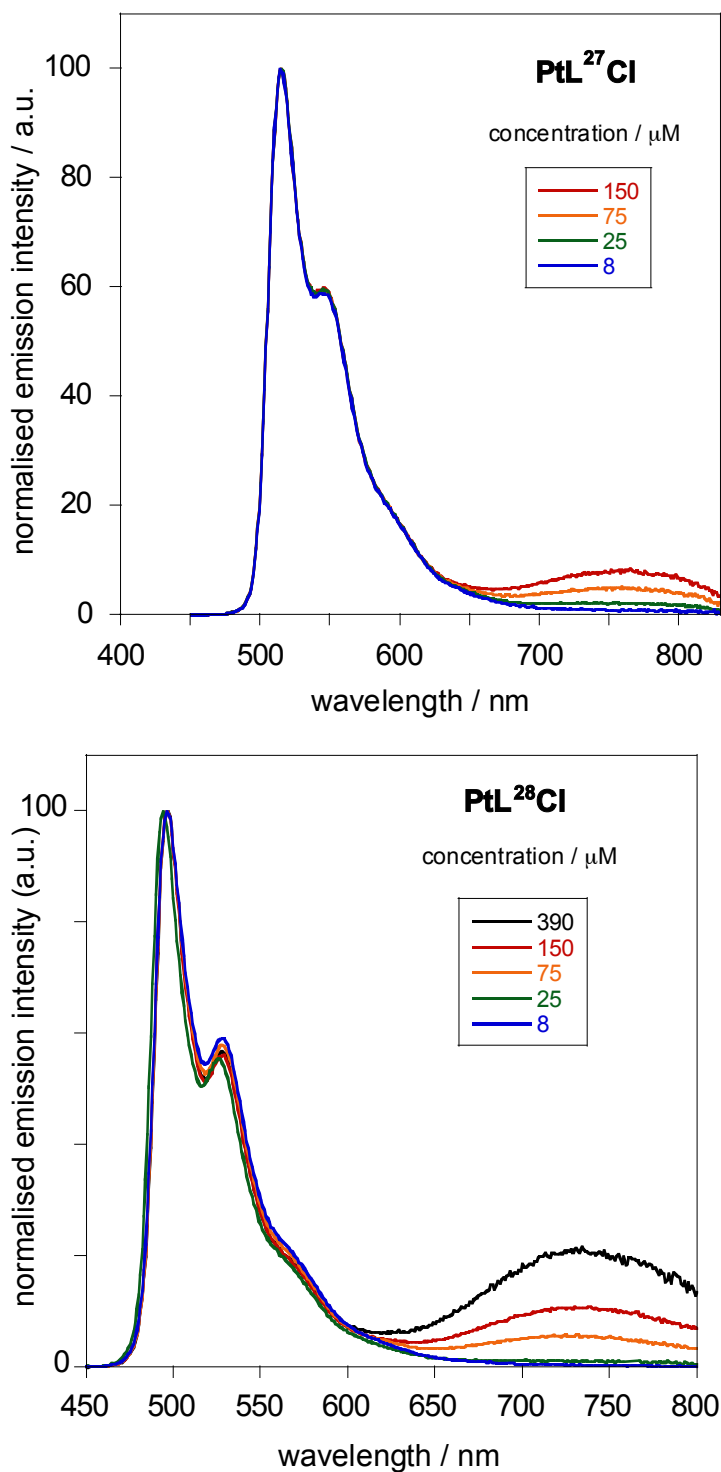
PtL²⁹Cl ¹⁹F NMR in *d*₈-THF at 282 MHz, coupled and decoupled to proton.

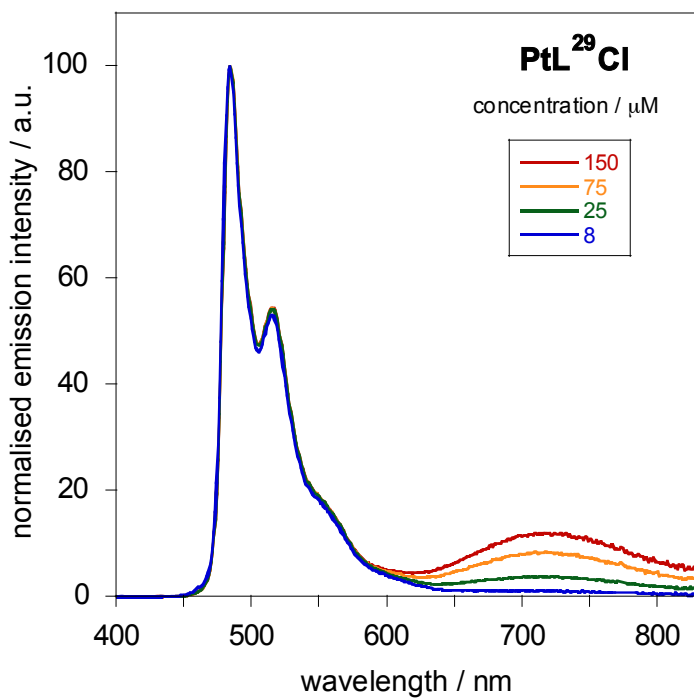




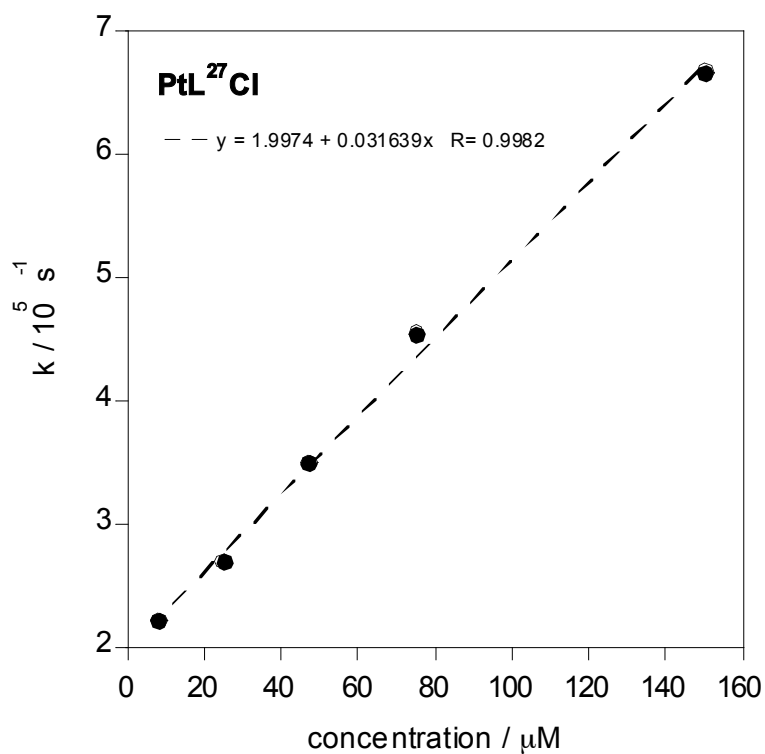


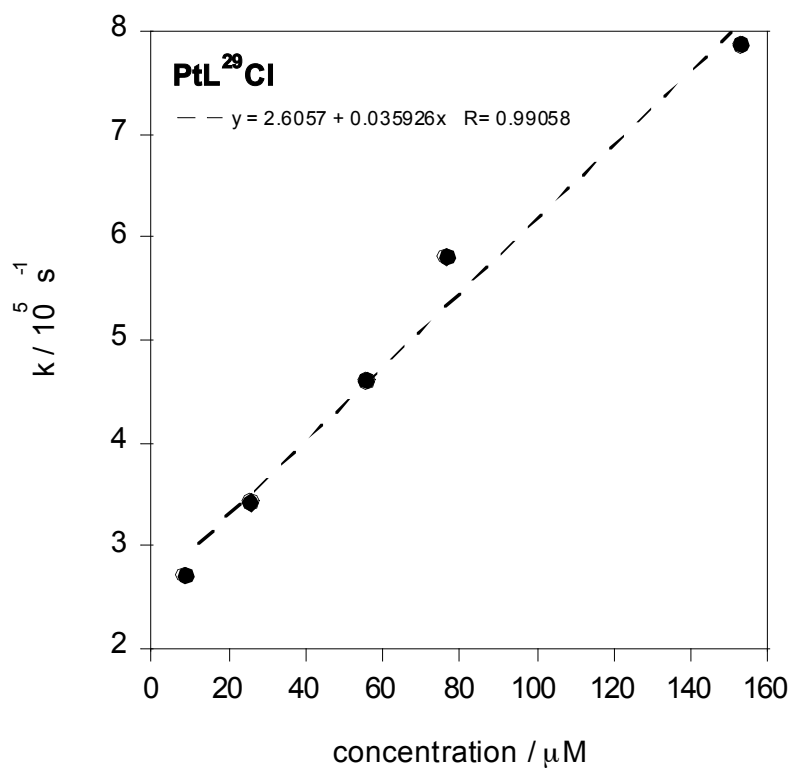
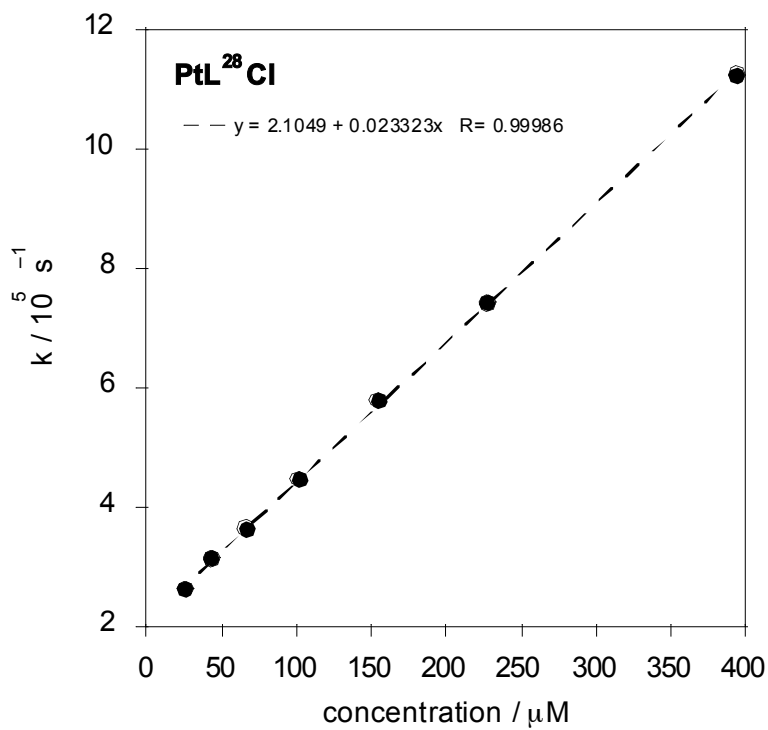
2. Emission spectra of PtL^{27}Cl – PtL^{29}Cl in CH_2Cl_2 solution at the varying concentrations indicated, showing the appearance of the excimer band as the concentration is raised; at $298 \pm 3 \text{ K}$, $\lambda_{\text{ex}} = 420 \text{ nm}$.



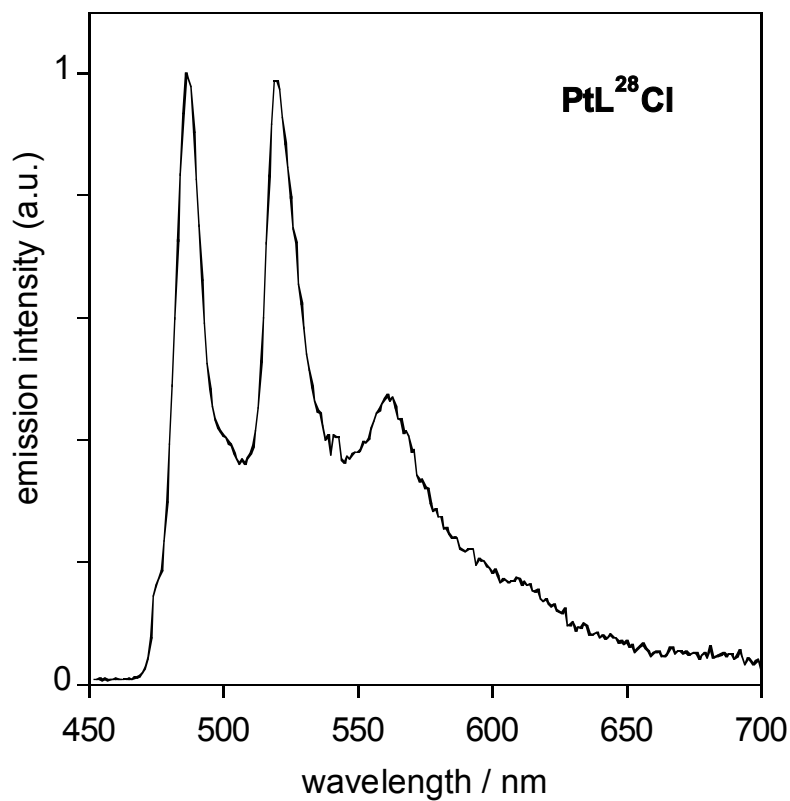
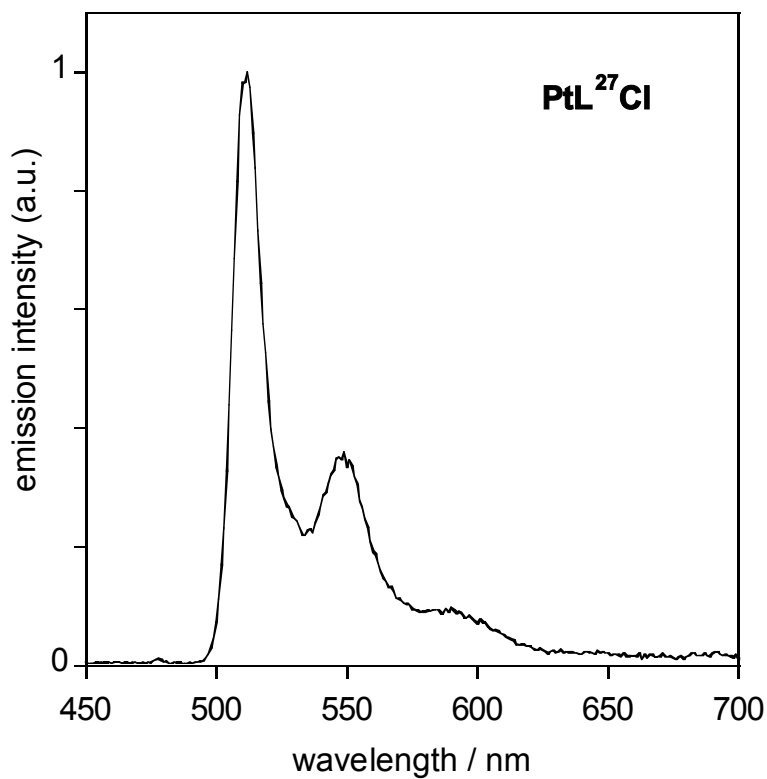


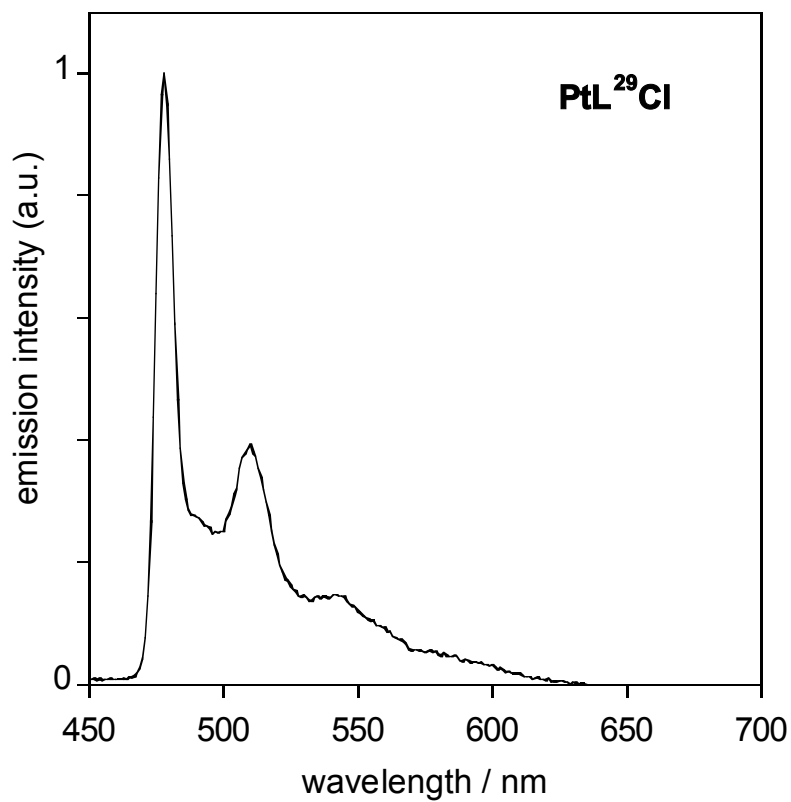
3. Plots of the decay rate constant k_{obs} versus concentration for PtL^{27}Cl – PtL^{29}Cl in CH_2Cl_2 at $298 \pm 3 \text{ K}$.





4. Emission spectra of PtL^{27}Cl – PtL^{29}Cl at 77 K in a frozen glass of diethyl ether / isopentane / ethanol (2:2:1 v/v), $\lambda_{\text{ex}} = 420 \text{ nm}$.





5. Emission spectra of PtL^{27}Cl – PtL^{29}Cl in the solid state obtained by evaporation from CH_2Cl_2 solution, $\lambda_{\text{ex}} = 374$ nm.

