Electronic Supplementary Information #1
Spectroscopic Studies

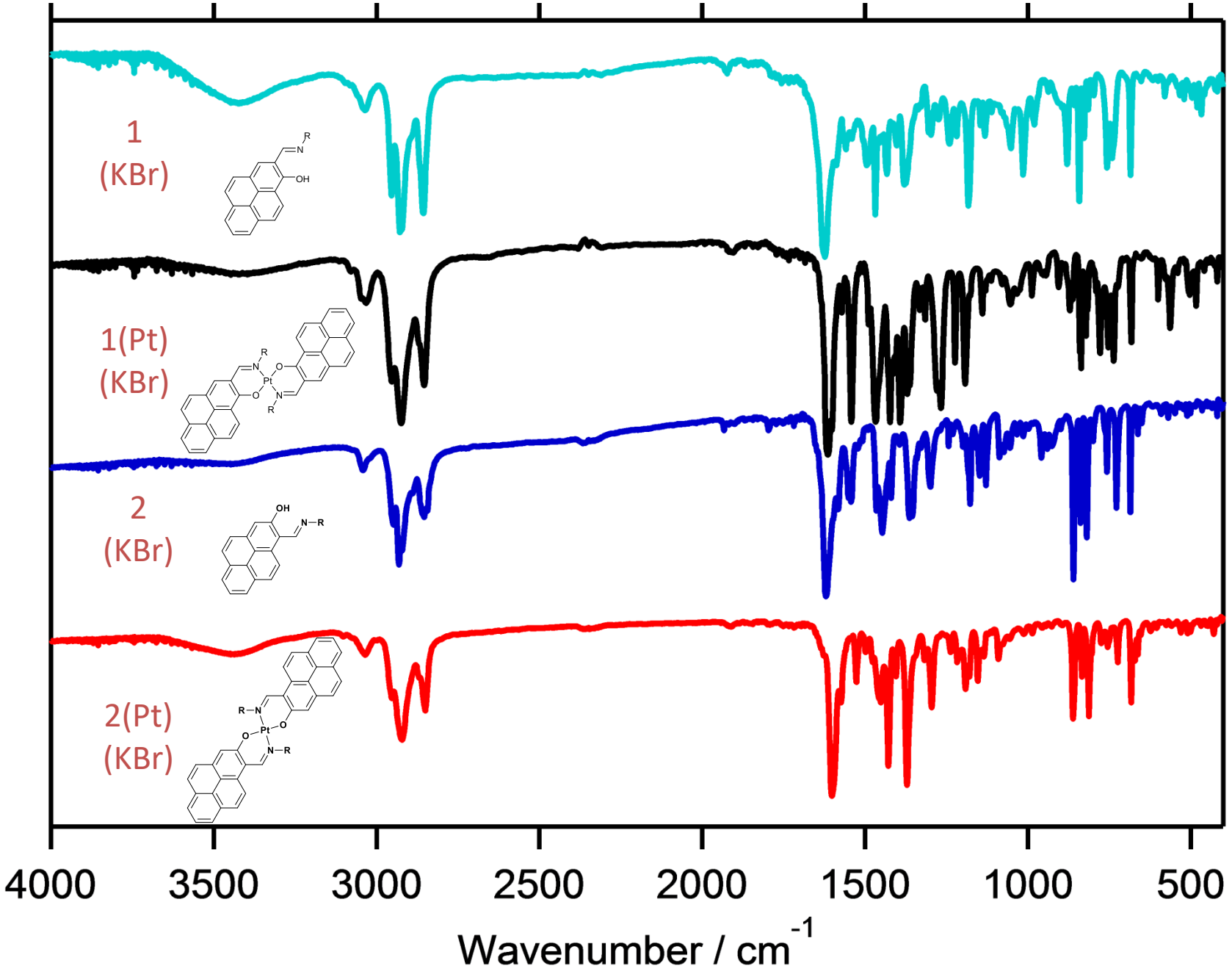
Title: Metal Complexes of π-Expanded Ligands (7): Syntheses, Structures and Properties of Pt(II) Complexes Containing Isomeric 1- and 2-alkyliminomethyl Pyrene Ligands.

Authors: Luong Xuan Dien[1,2]*, Nguyen Xuan Truong[1]

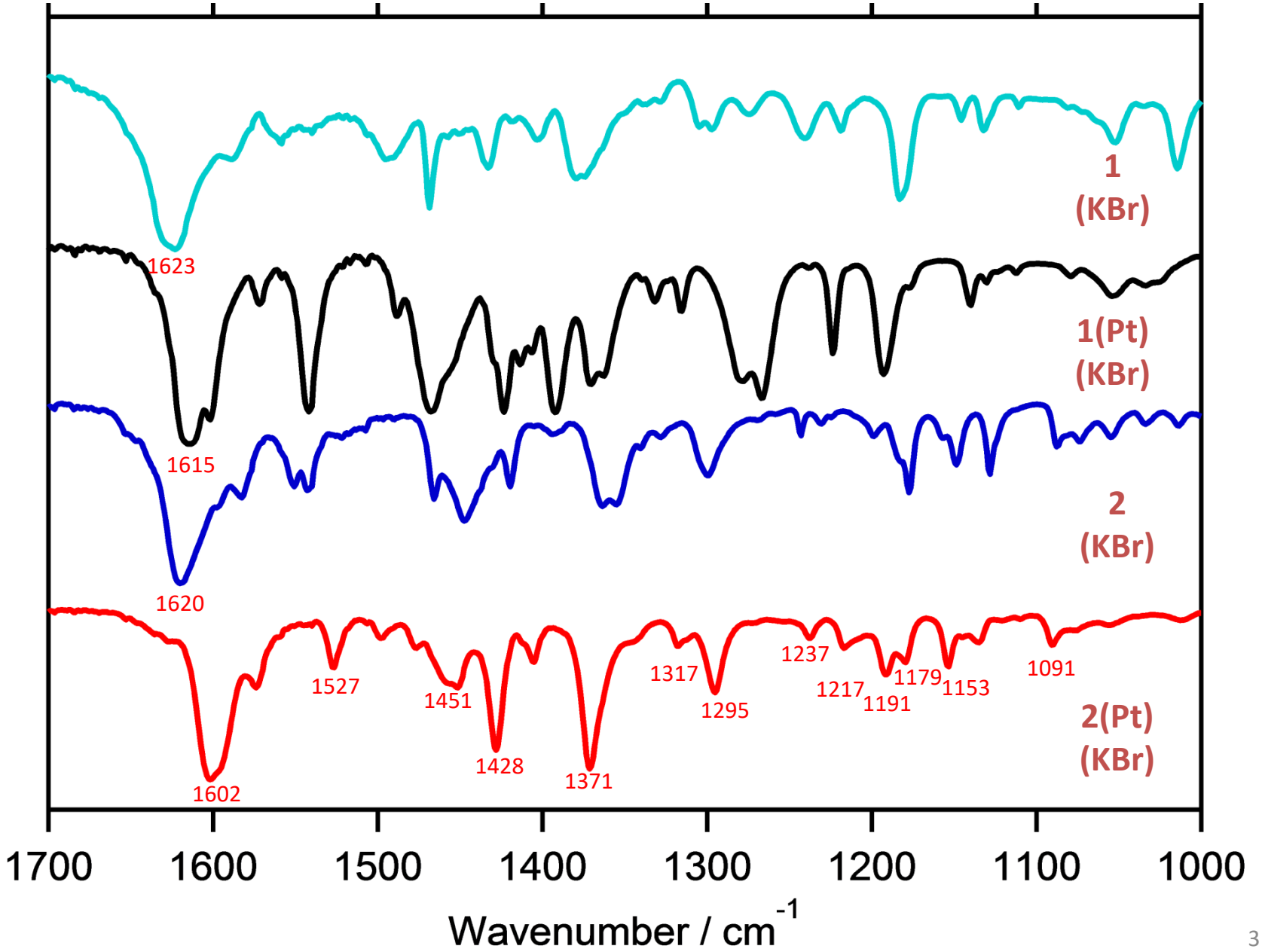
Organization: [1] *School of Chemical Engineering, Hanoi University of Science and Technology, 1 Dai Co Viet, Hanoi, Vietnam*

[2] *Department of Chemistry, Graduate School of Science and Engineering, Tokyo Metropolitan University, 1-1 Minami-Ohsawa, Hachi-Oji, Tokyo 192-0397, Japan*

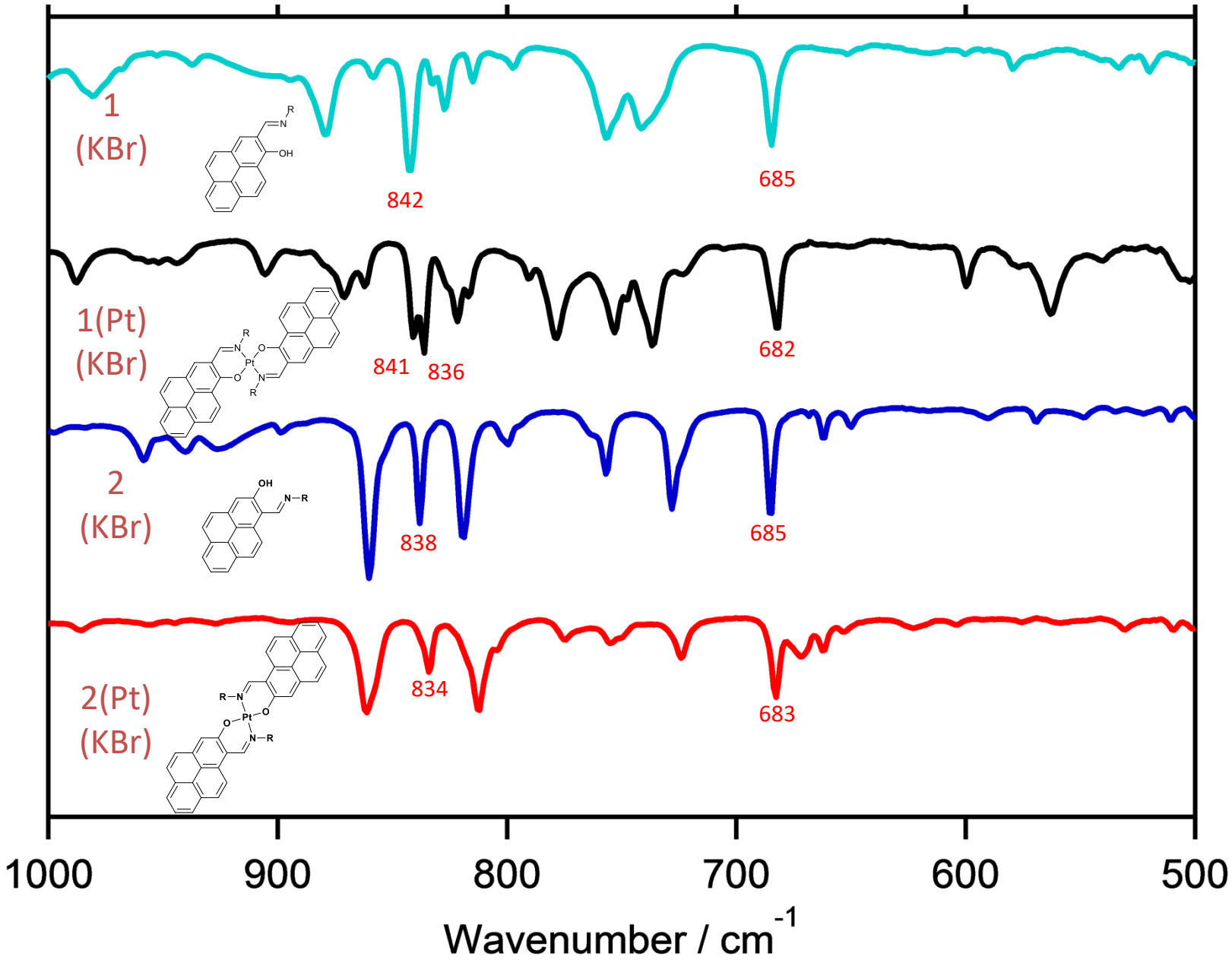
Comparison of IR Spectra of Ligands and Complexes



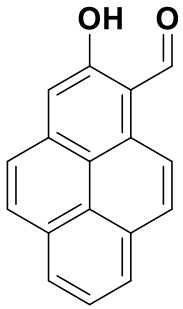
Expanded Plots of IR Spectra



Expanded Plots of IR Spectra



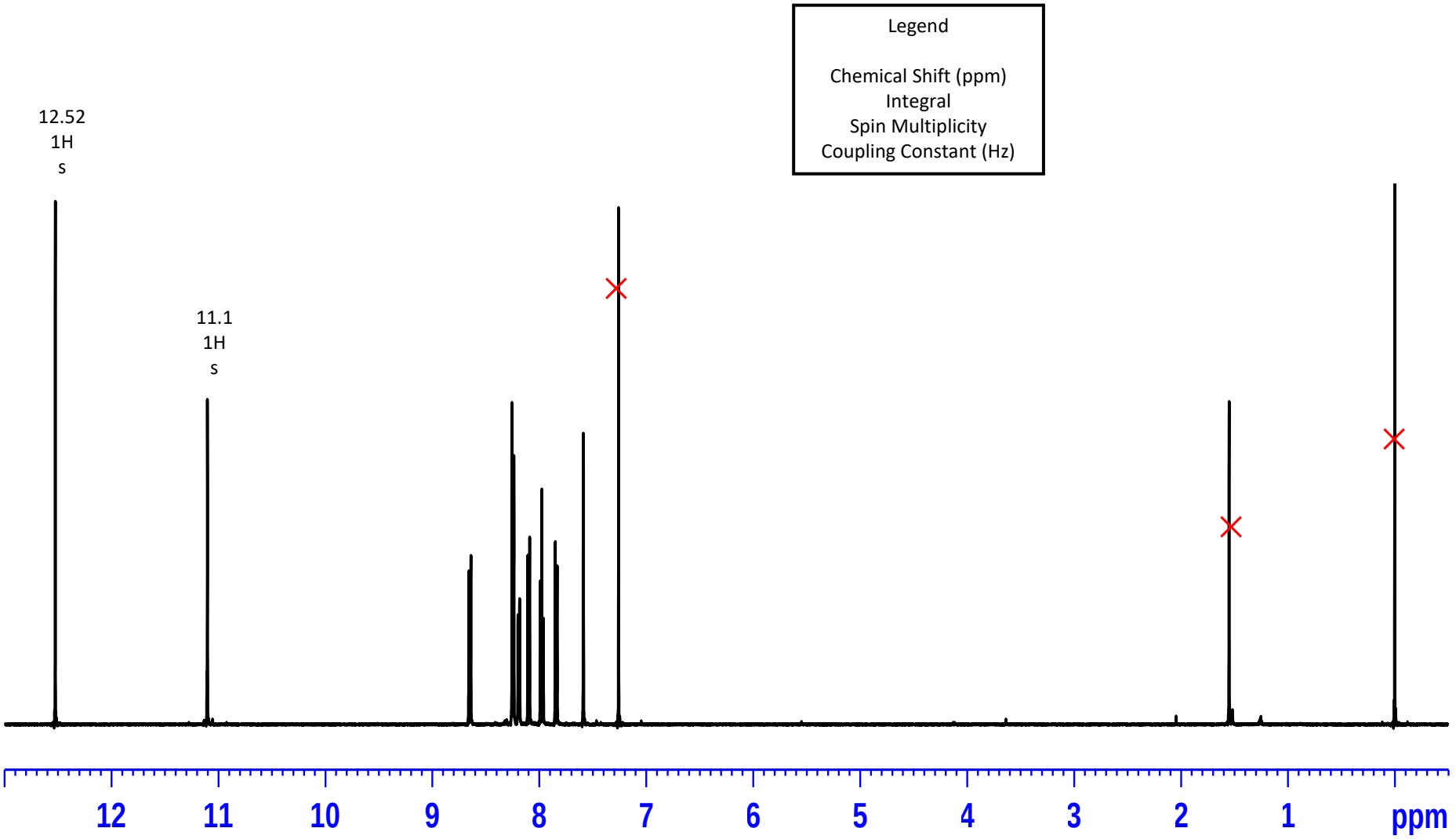
Compound 9



This important intermediate, 2-hydroxypyrene-1-carbaldehyde **9**, was prepared according to a different way compared to the literature: P. Demerseman, J. Einhorn, J. F. Gourvest and R. Royer, *J. Org. Chem.*, 1988, 53(17), 3936.

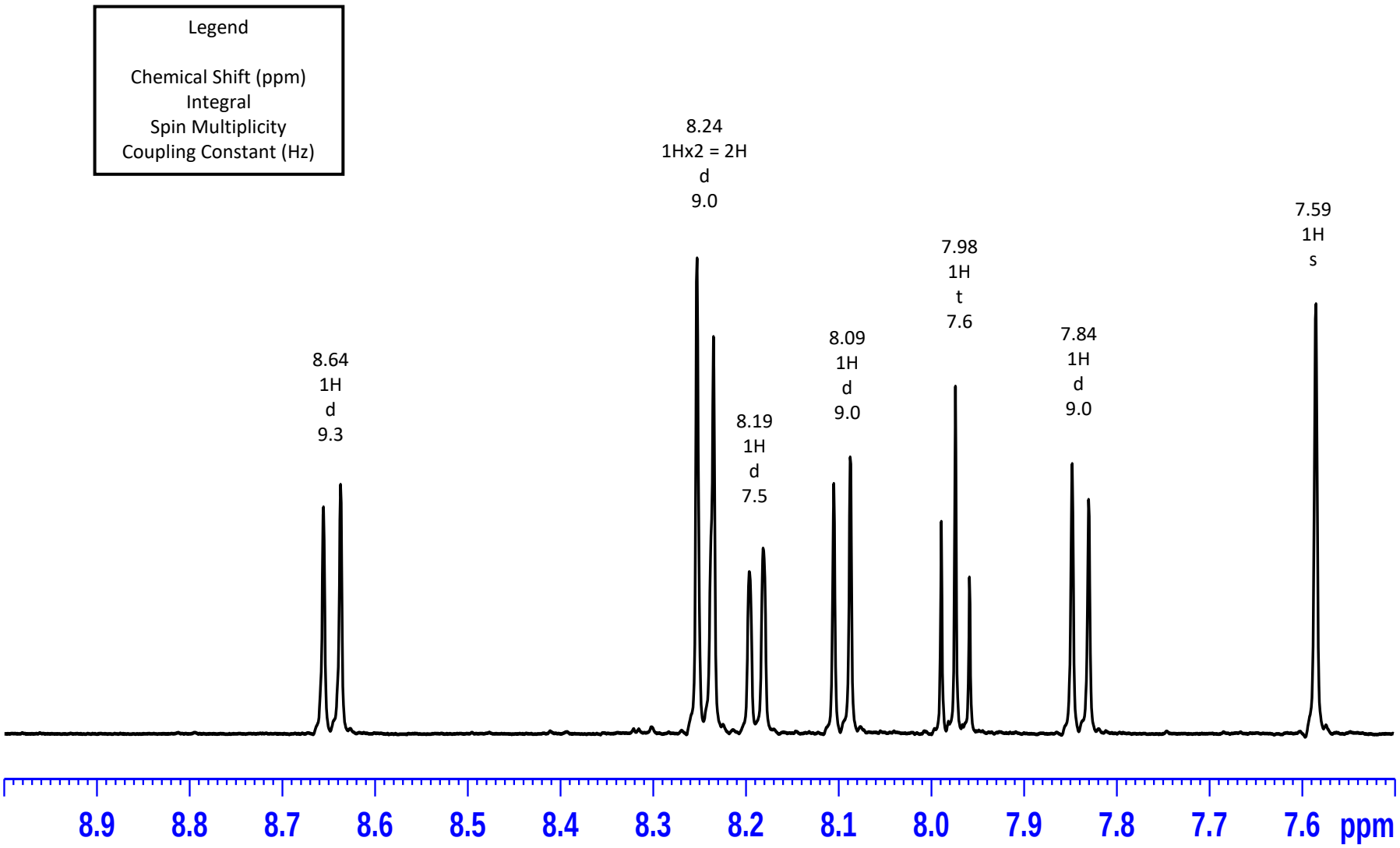
Yield:	95%
mp:	180 ºC (from ethyl acetate)
Chemical Formula:	$C_{17}H_{10}O_2$
Molecular Weight:	246.27

NMR Spectrum ($CDCl_3$)

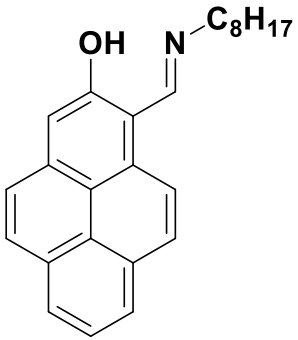


Chemical Shift / ppm

NMR Spectrum: Expanded Plot ($CDCl_3$)



Compound **2**



Yield:	99%
mp:	88 ^{o}C (from hexane)
Chemical Formula:	$C_{25}H_{27}NO$
Molecular Weight:	357.49

Elemental Analysis

	C	H	N
Calcd.	83.99	7.61	3.92
Found.	83.80	7.61	3.93
Δ	-0.19	0.00	+0.01

calcd. for $C_{25}H_{27}NO$

found

Request & Report Sheet of Elemental Analysis

Date(month/day): /

Department Name: Chemistry
Lab. Name: Inorganic Chemistry

Approval from Teaching Staff: 4T

Your Name: LUONG XUAN DIEN

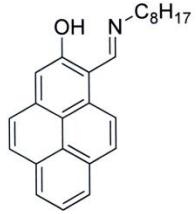
Your Position : □Staff ☑Student (grade: PhD) Your access extension#: 3567
Your E-mail: dienlx306@gmail.com

Sample Name(Symbolic): DL171

Molecular Formula: $C_{25}H_{27}NO$ Molecular Weight: 357.50

property
- mp : ℃
- bp : ℃
- Decompose point ℃
- State: □Liquid ☑solid
- □hygroscopic □poisonous □sublimate or volatile □photodegradability
- □handling in Ar atmosphere

Structural Formula:



Sample Wt. 6.26 mg

Comment & request for measuring:
(Ex.□Double time measuring, etc.)

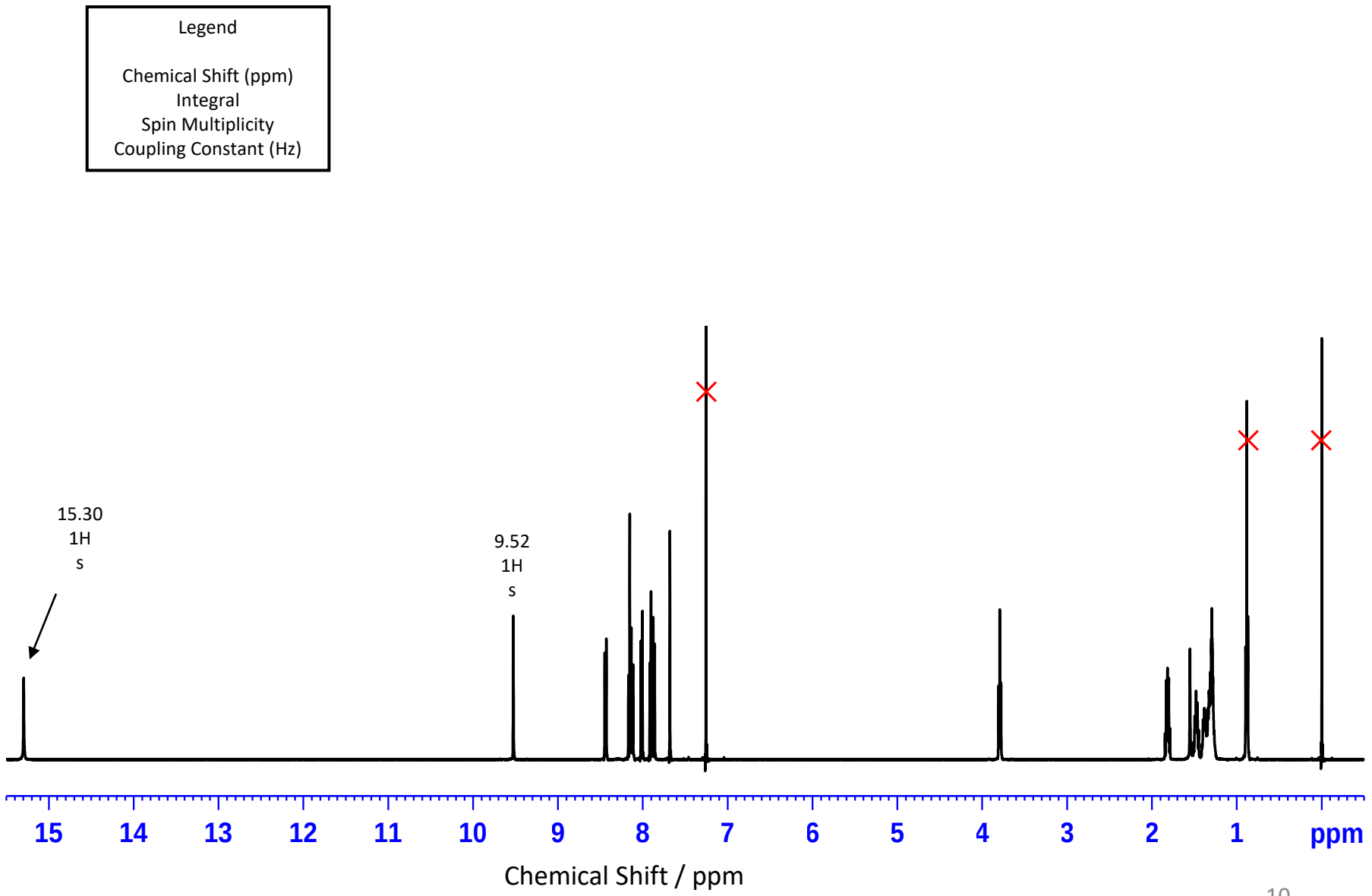
Theoretical cont. (Wt.%)	C: 83.99	H: 7.61	N: 3.92	O: 4.48	

Result of (Single time) Measurement

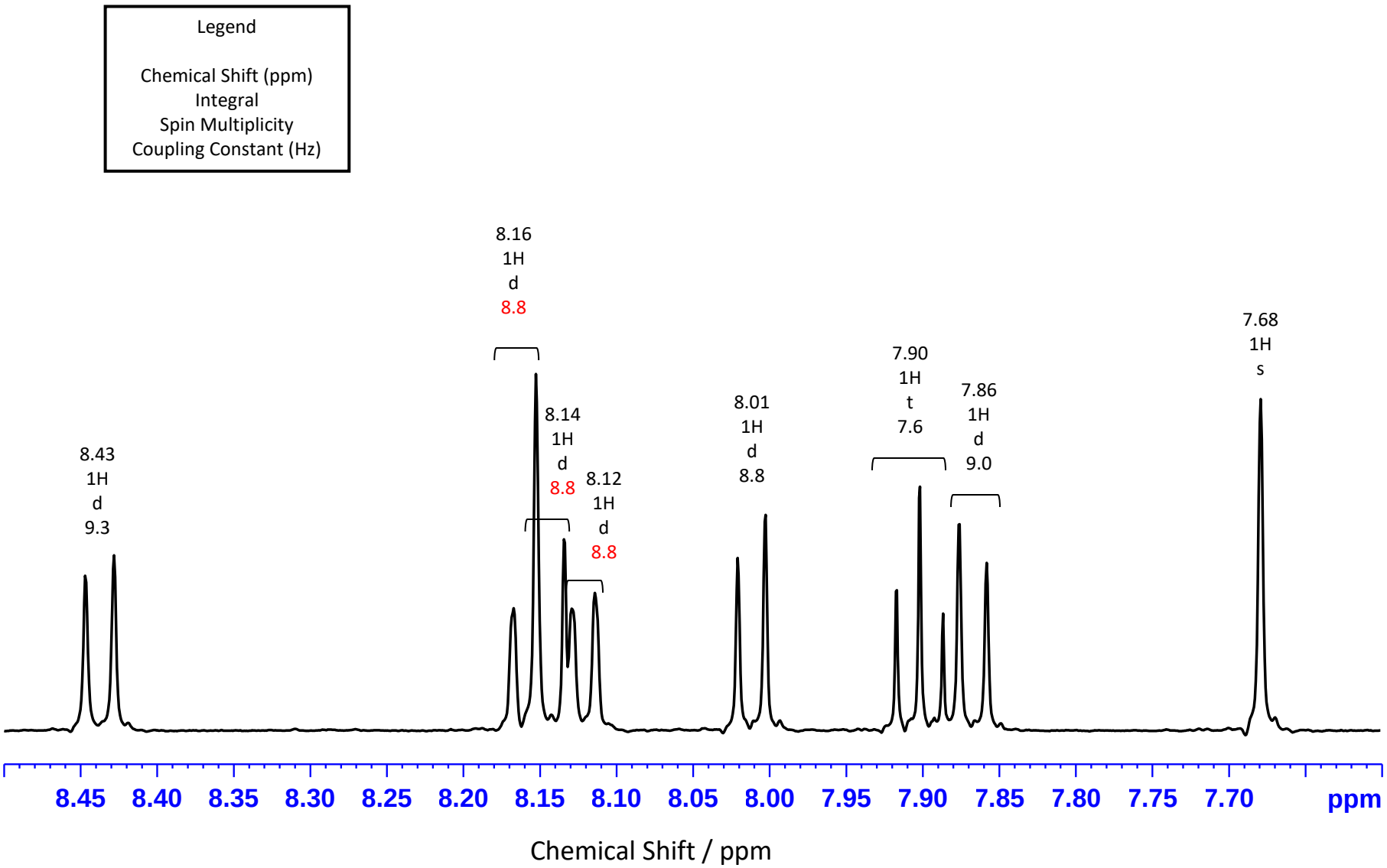
Measured cont. (Wt.%)	C: 83.80	H: 7.61	N: 3.93			Used Sample Wt. (mg)
K-factor	C: 22.797	H: 63.672	N: 7.888			1.398

Measuring Date (month/day): 4/16 (Counter#: 8204) Report No: 17

NMR Spectrum ($CDCl_3$)



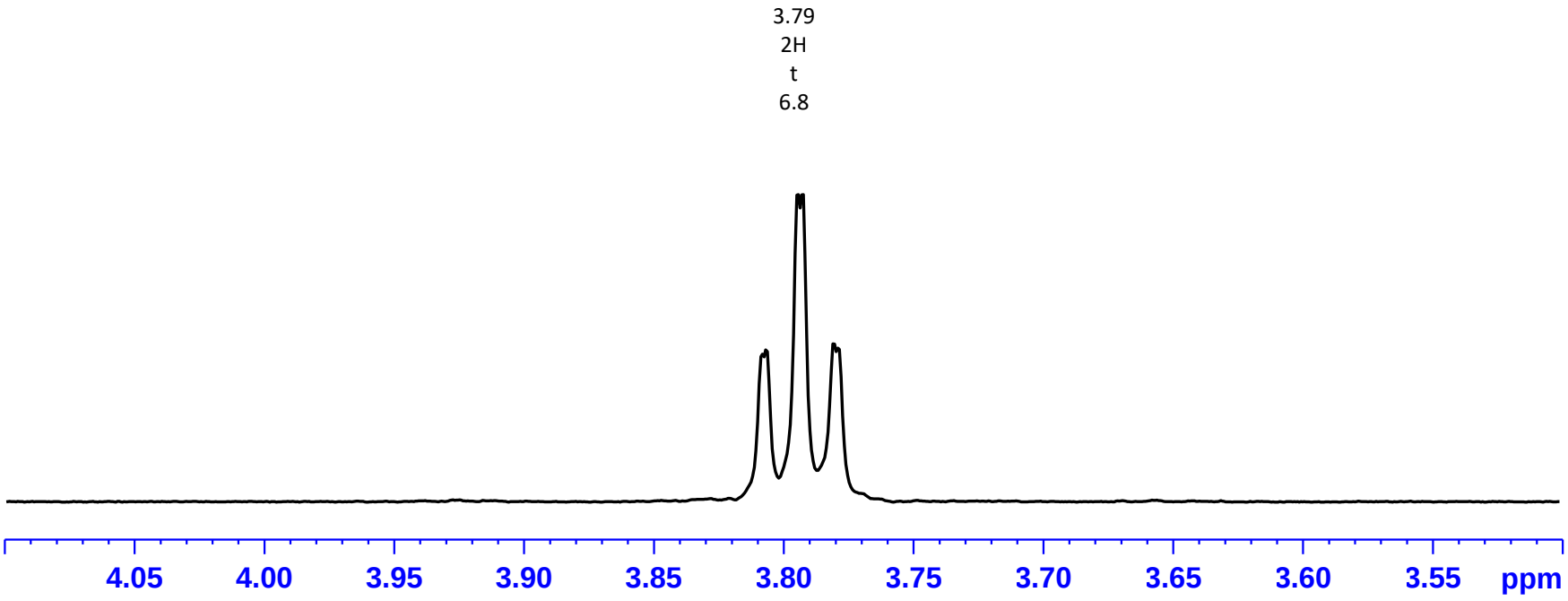
NMR Spectrum: Expanded Plot ($CDCl_3$)



NMR Spectrum: Expanded Plot ($CDCl_3$)

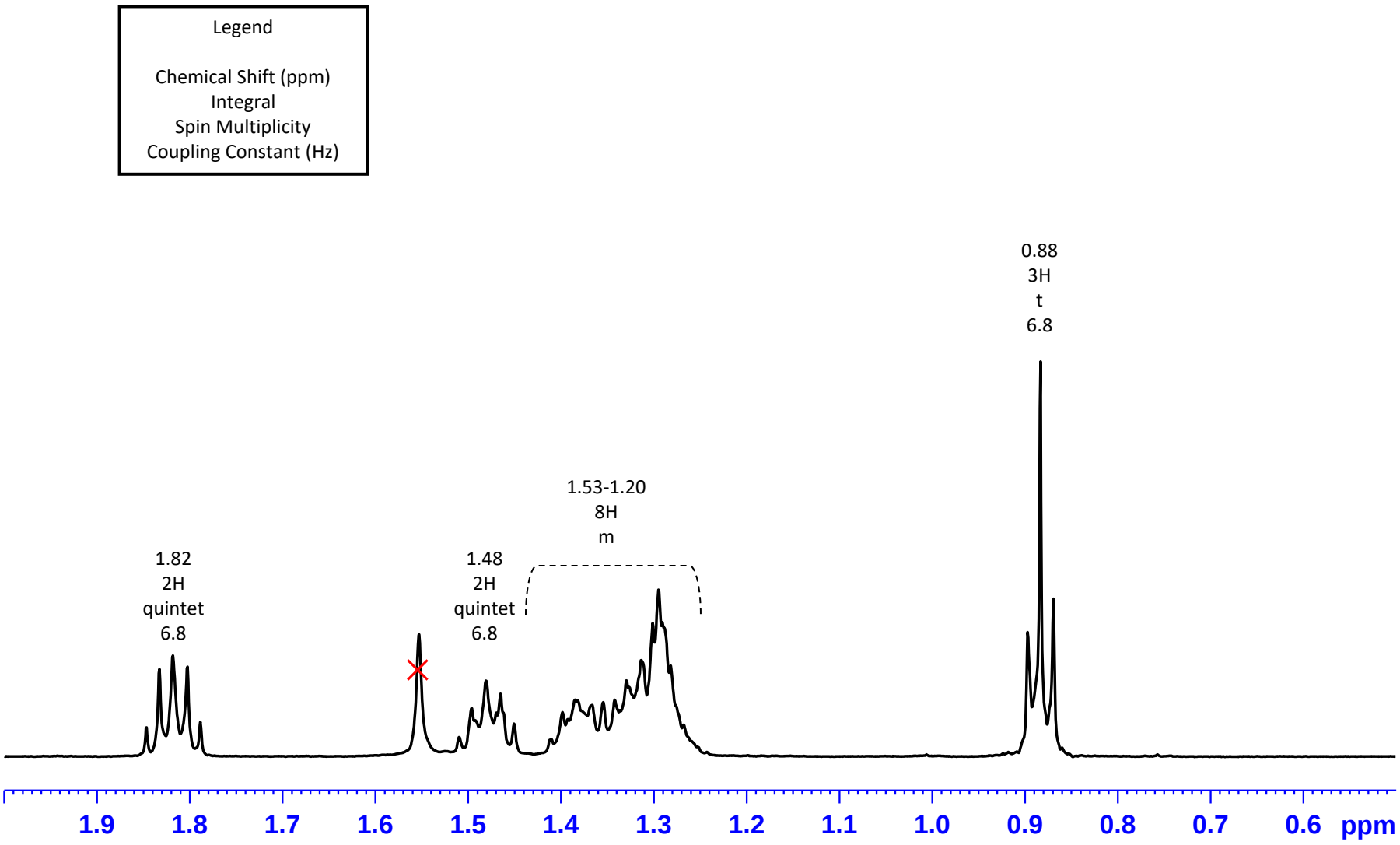
Legend

Chemical Shift (ppm)
Integral
Spin Multiplicity
Coupling Constant (Hz)

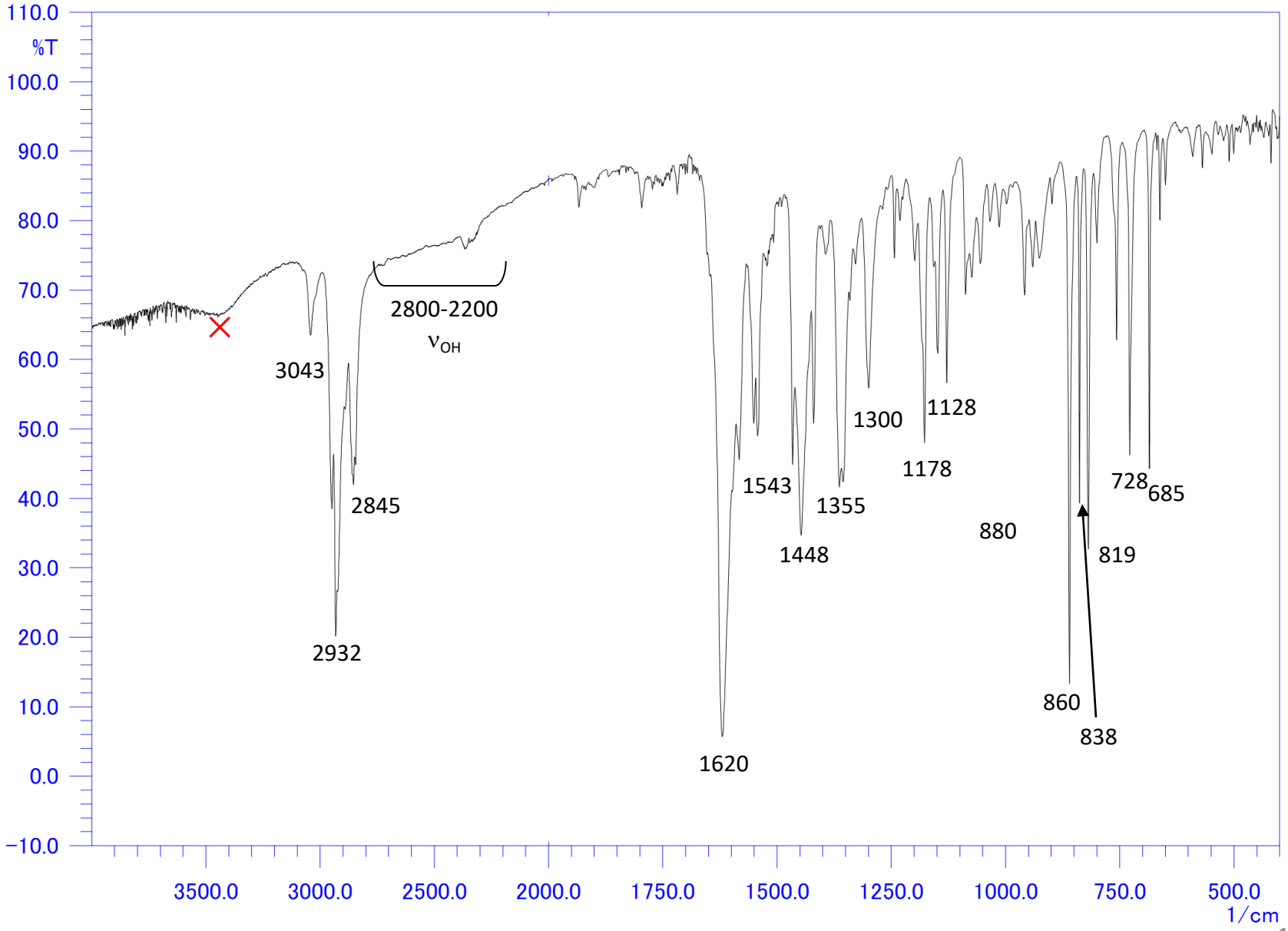


Chemical Shift / ppm

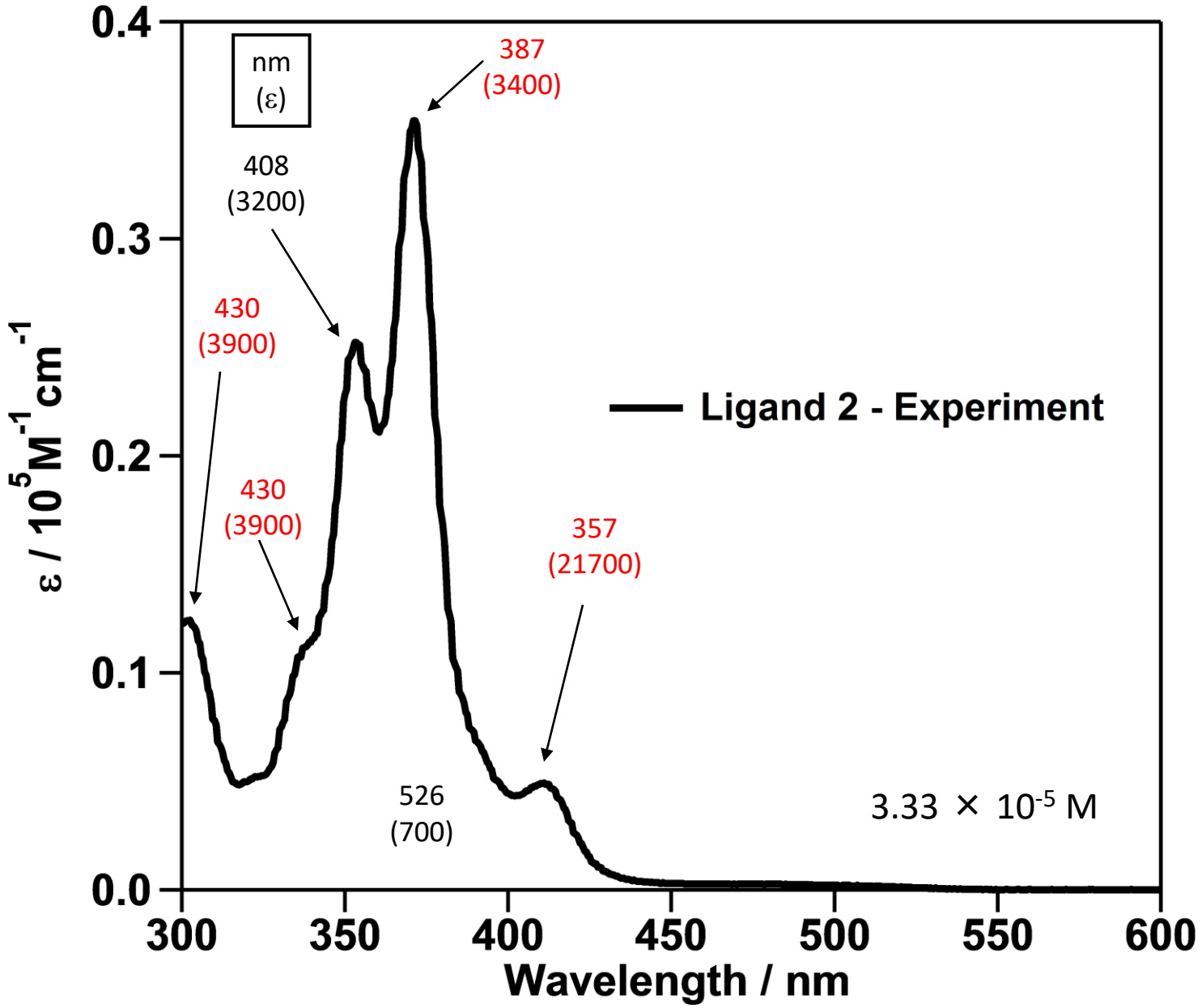
NMR Spectrum: Expanded Plot ($CDCl_3$)



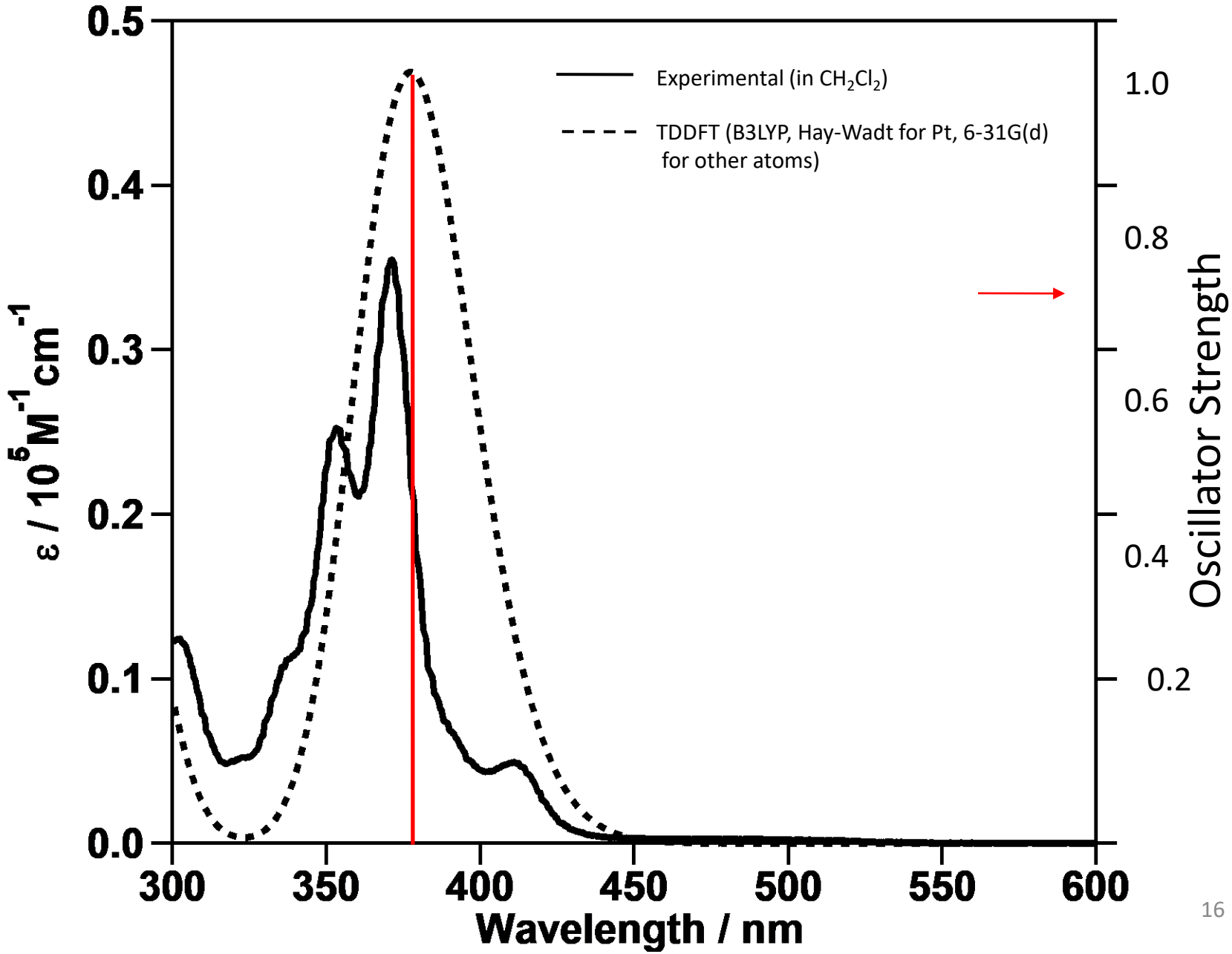
IR Spectrum (KBr Pellet)



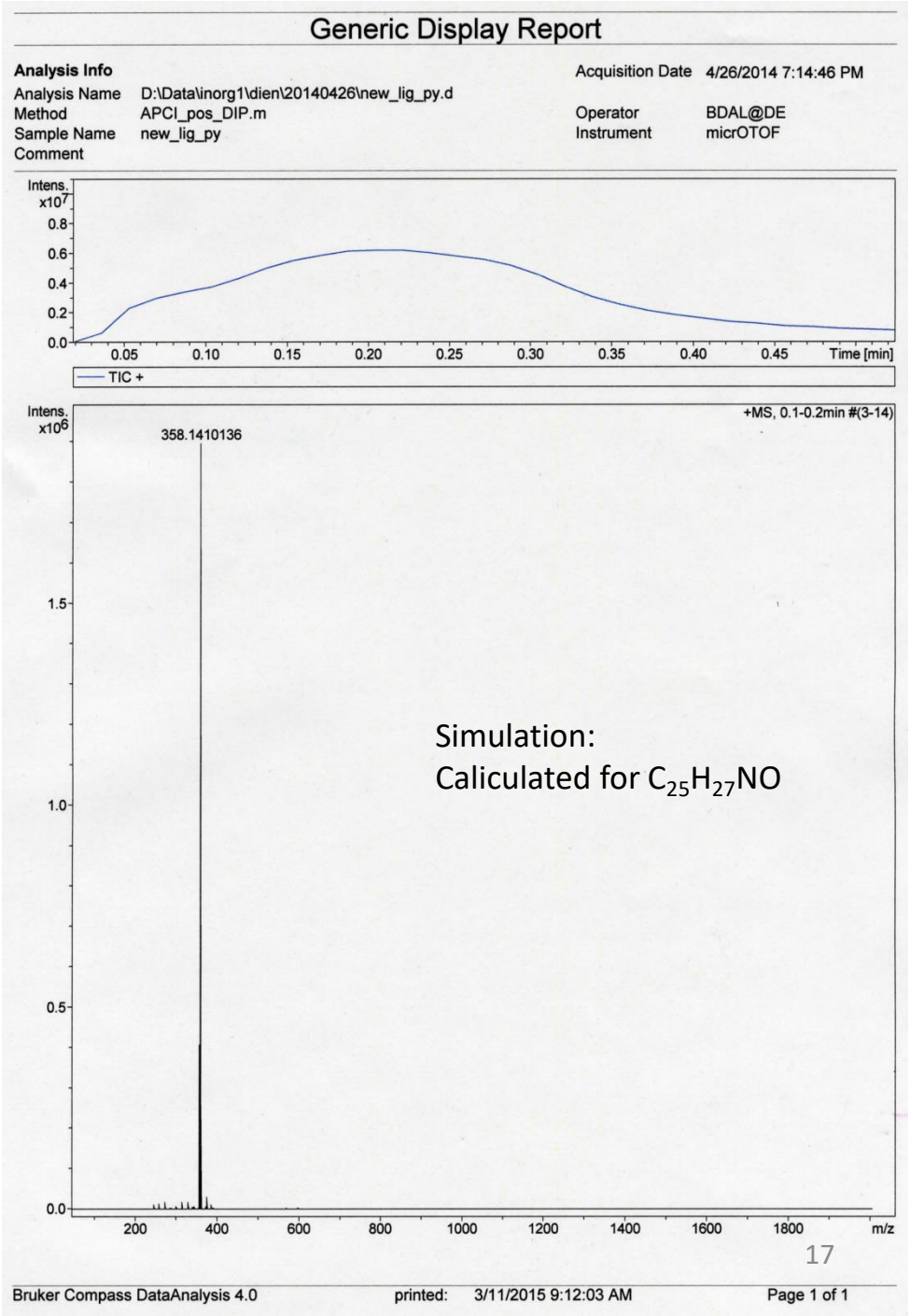
Absorption Spectrum (CH_2Cl_2)



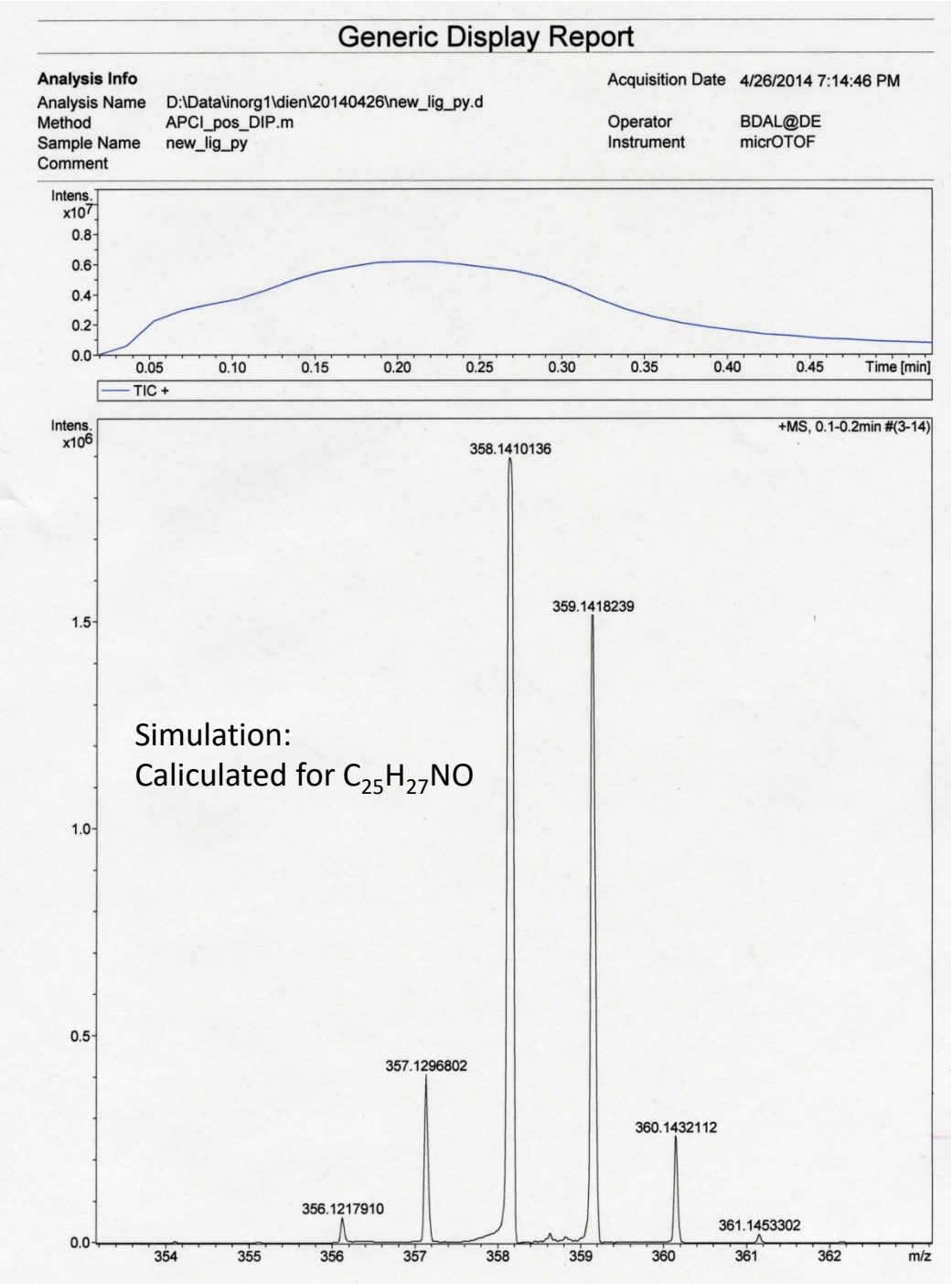
Obs. and Calcd. Absorption Spectra



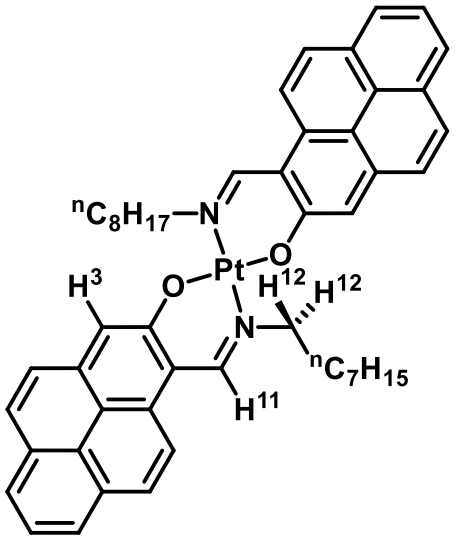
High Resolution Atmospheric Pressure Chemical Ionization Mass Spectrum



Expanded Plot of
High Resolution Atmospheric
Pressure Chemical Ionization
Mass Spectrum

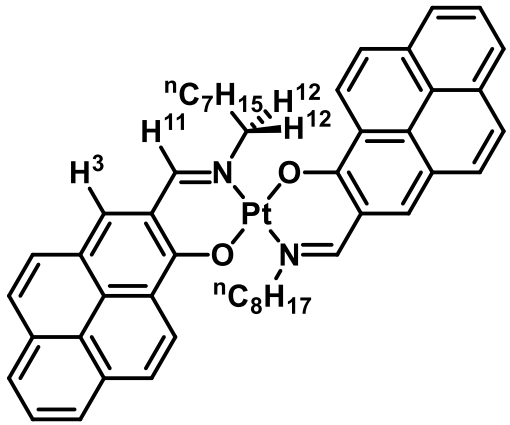


2(Pt)



Yield:	70 %
mp:	216 ºC (dec., from PhCl)
Chemical Formula:	$C_{50}H_{52}N_2O_2Pt$
Molecular Weight:	908.06

1(Pt)



Yield:	80 %
mp:	285 ºC (dec., from PhCl)
Chemical Formula:	$C_{50}H_{52}N_2O_2Pt$
Molecular Weight:	908.06

Elemental Analysis

	C	H	N
Calcd.	66.14	5.77	3.09
Found.	66.11	6.01	2.94
Δ	+0.03	-0.24	+0.15

calcd. for $C_{50}H_{52}N_2O_2Pt$

found

Date(month/day): 4 / 15

Department Name: Chemistry
Lab. Name: Inorganic Chemistry

Approval from Teaching Staff: LT

Your Name: LUONG XUAN DIEN

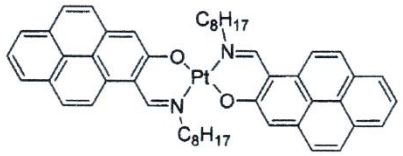
Your Position : □Staff ☑Student (grade: PhD) Your access extension#: 3567
Your E-mail: dienlx306@gmail.com

Sample Name(Symbolic): DL173

Molecular Formula: $C_{50}H_{52}N_2O_2Pt$ Molecular Weight: 908.06

property
- mp : ℃
- bp : ℃
- Decompose point ℃
- State: □Liquid ☑solid
- □hygroscopic □poisonous
- □sublimate or volatile
- □photodegradability
- □handling in Ar atmosphere

Structural Formula:



Sample Wt. 2.99 mg

Comment & request for measuring:
(Ex.□Double time measuring, etc.)

Theoretical cont. (Wt.%)	C: 66.14	H: 5.77	N: 3.09	O: 3.52	Pt: 21.48

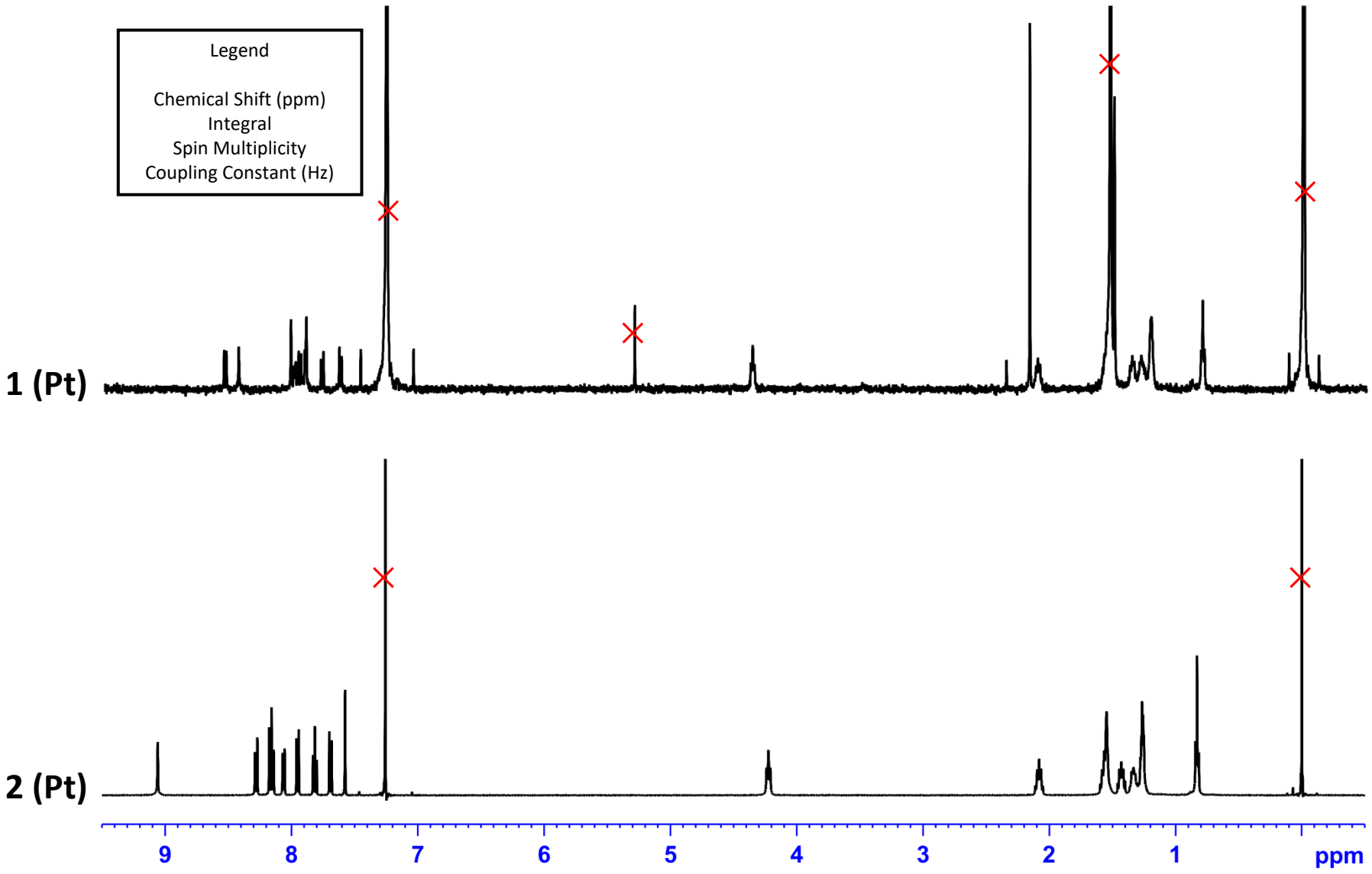
Result of (Single time) Measurement

Measured cont. (Wt.%)	C: 66.11	H: 6.01	N: 2.94			Used Sample Wt. (mg)
K-factor	C: 22.713	H: 42.583	N: 7.871			1.726

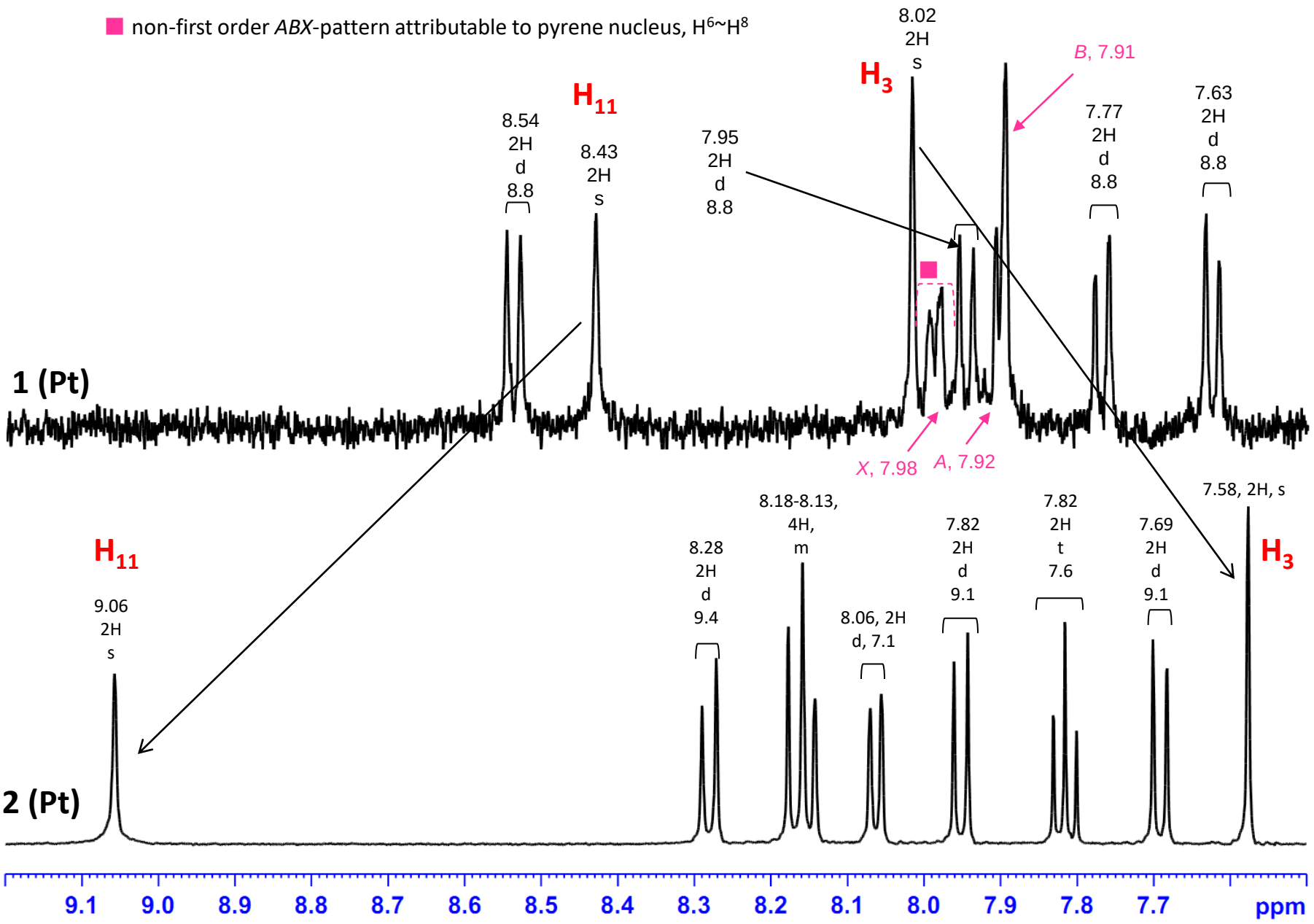
Measuring Date (month/day): 4/17 (Counter#: 8239) Report No: 18

Access: TMU Department of Chemistry Elemental Analysis Room (Building# 8 Room #384 ,Ext.#: 3463)

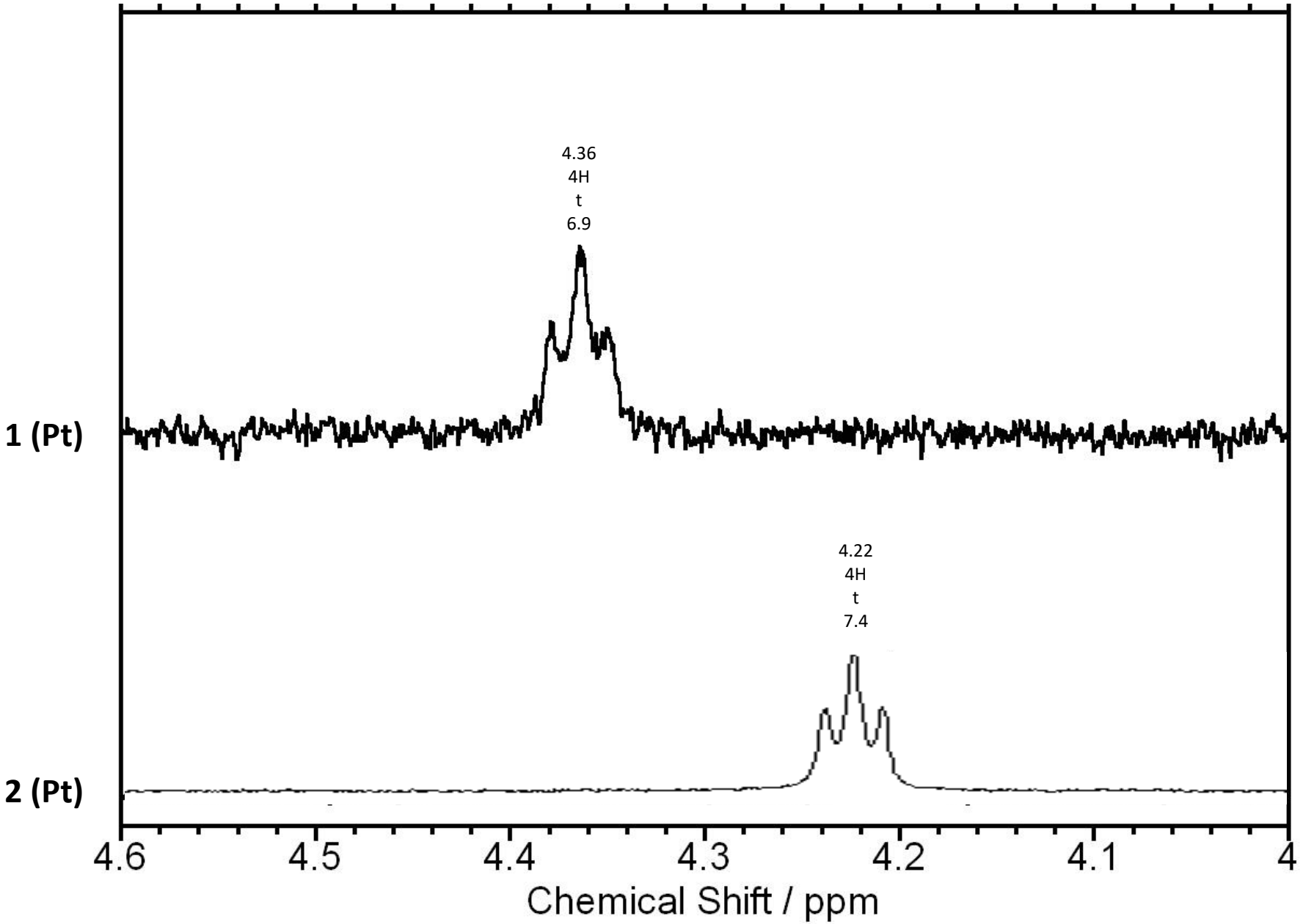
NMR Spectrum ($CDCl_3$)



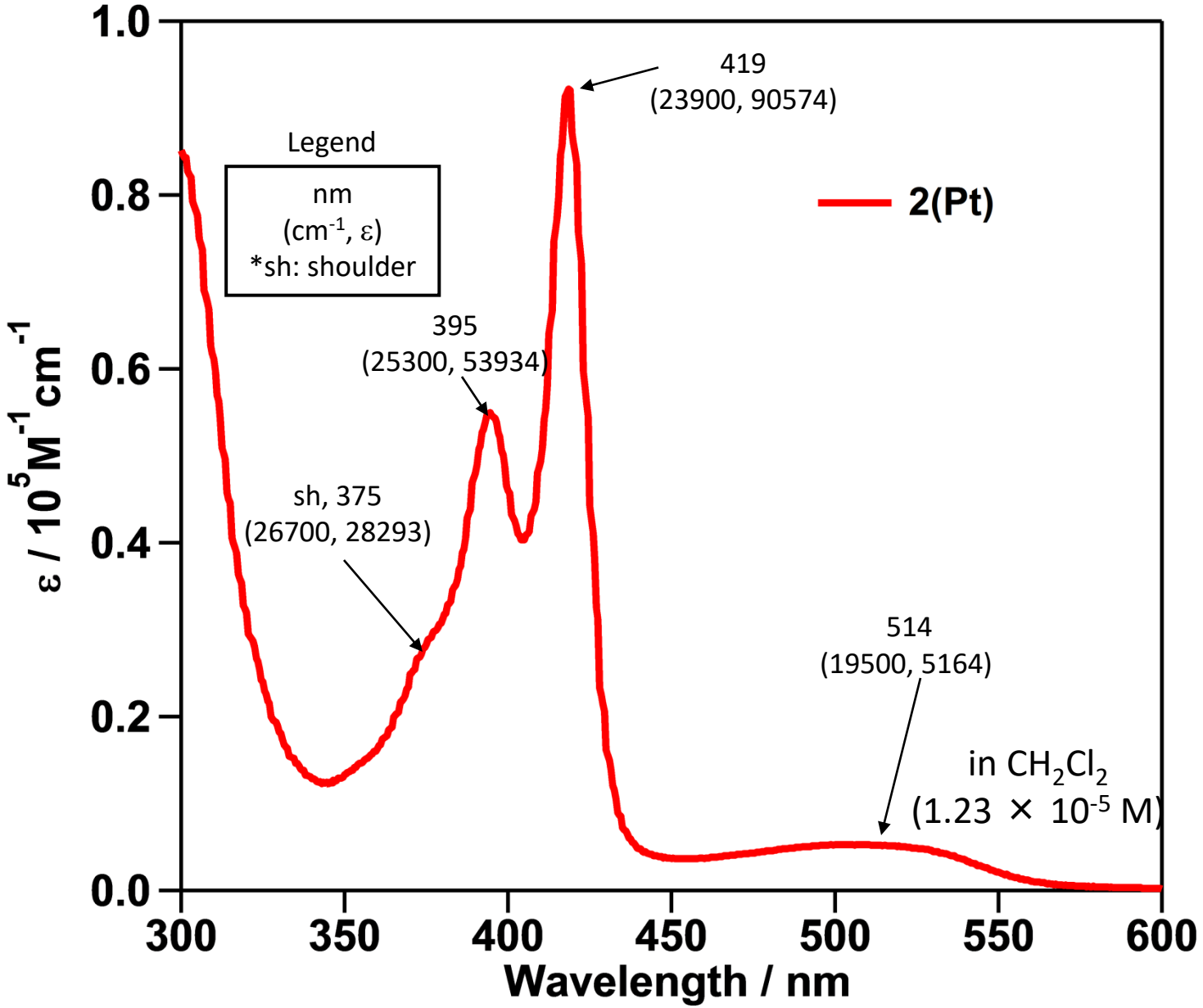
NMR Spectrum: Expanded Plot ($CDCl_3$)



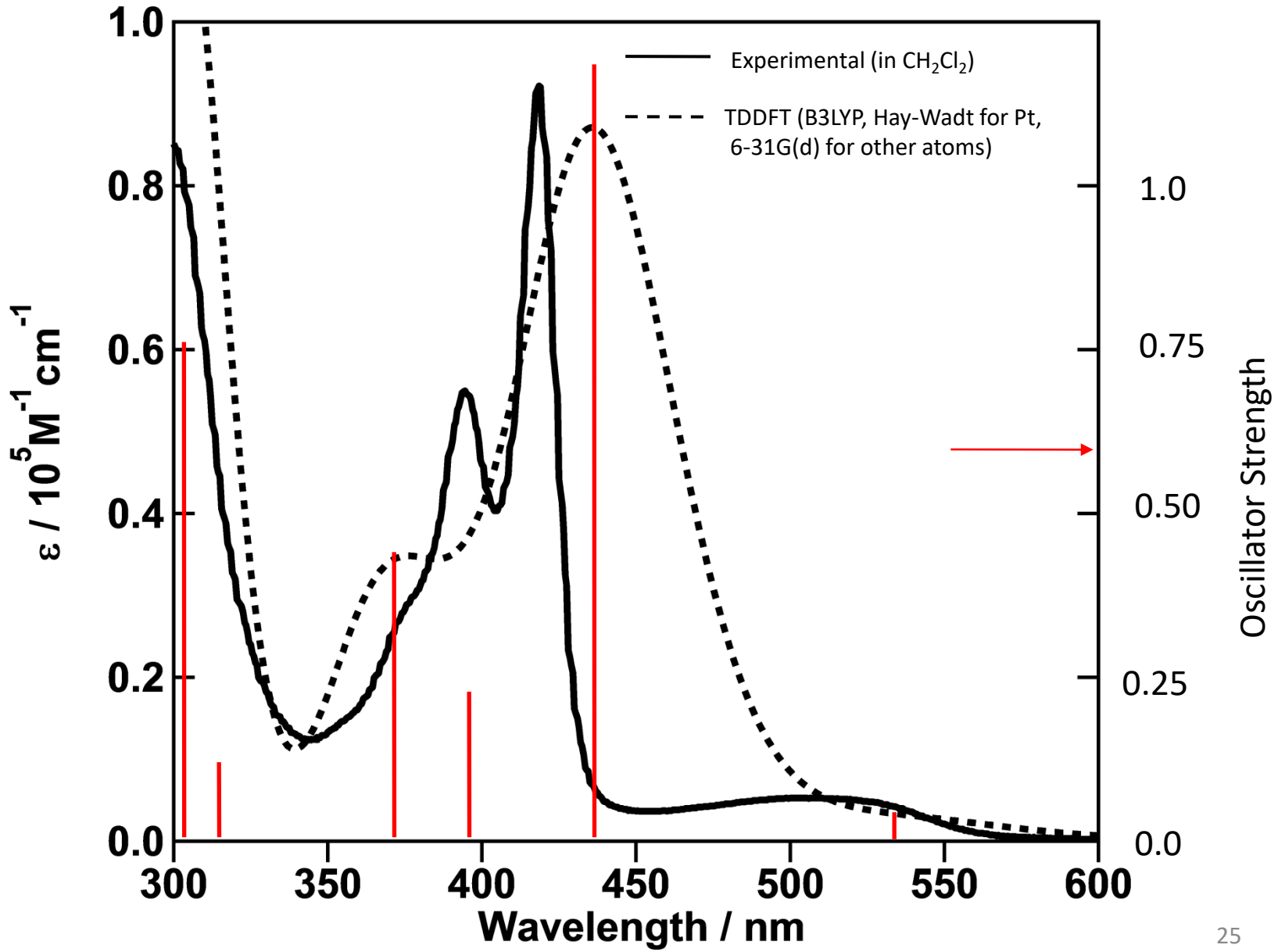
NMR Spectrum: Expanded Plot ($CDCl_3$)



Absorption Spectrum (CH_2Cl_2)



Obs. and Calcd. Absorption Spectra



Assignment of Absorption Spectrum of ***2(Pt)***

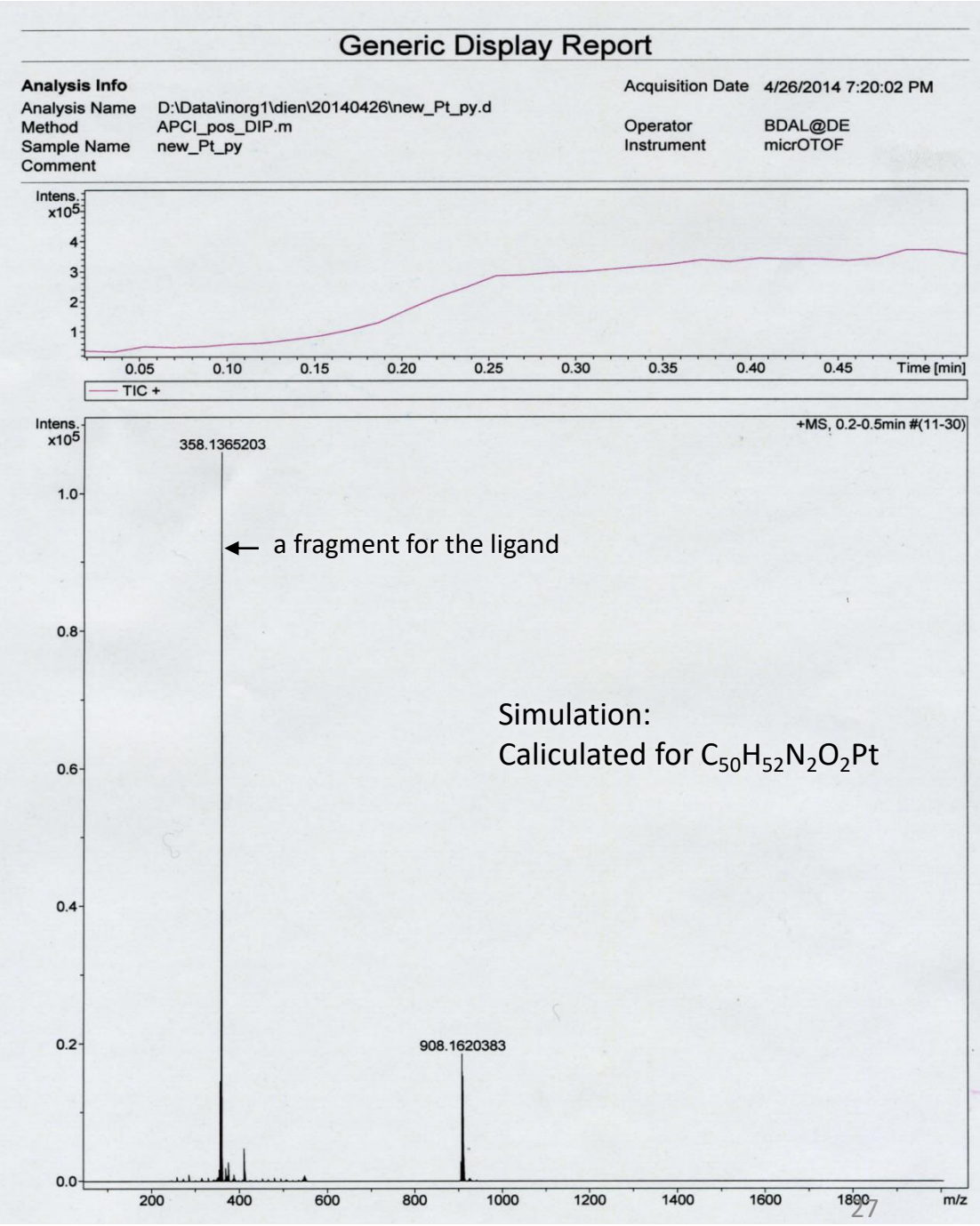
# of Transition	Observed Transition Energy / eV (nm)	Calculated Transition Energy / eV (nm)	Oscillator Strength *f*	Composition	CI
1	2.42 (514)	2.34 (529.8)	0.04	HOMO (ϕ_{144}) → LUMO(ϕ_{145})	0.97
2	2.96 (419)	2.54 (436.6)	1.17	HOMO-1 (ϕ_{143}) → LUMO(ϕ_{145})	0.96
3	3.14 (395)	3.17(391.3)	0.22	HOMO-2 (ϕ_{142}) → LUMO+1(ϕ_{146})	0.92
4	sh,† 3.31 (375)	3.39 (365.7)	0.36	HOMO-3 (ϕ_{141}) → LUMO+1(ϕ_{146})	0.84
5	-	3.94 (314.4)	0.11	HOMO-6(ϕ_{138}) → LUMO(ϕ_{145})	0.76
6	-	4.07(304.9)	0.75	HOMO(ϕ_{144}) → LUMO+4 (ϕ_{149})	0.46
		4.08(303.9)	0.40	HOMO -8(ϕ_{136}) → LUMO(ϕ_{145})	0.67

Program: Gaussian R-09W Ver.7 + Gauss View Ver.5
Method: B3LYP / TD-DFT
Basis Set: Hay-Wadt for Pt, 6-31G(d) for C, N, O, and H

50 excited states were calculated. Excited states having oscillator strength $f > 0.01$ are considered. The main configuration with configuration interaction (CI) coefficient >0.3 were considered.

† shoulder

High Resolution Atmospheric Pressure Chemical Ionization Mass Spectrum



Expanded Plot of
High Resolution Atmospheric
Pressure Chemical Ionization
Mass Spectrum